



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1S5L
Title : Architecture of the photosynthetic oxygen evolving center
Authors : Ferreira, K.N.; Iverson, T.M.; Maghlaoui, K.; Barber, J.; Iwata, S.
Deposited on : 2004-01-21
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

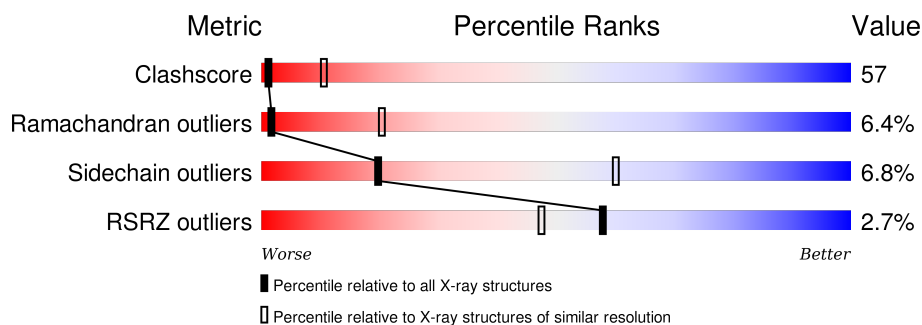
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>3%</div> <div>28%</div> <div>57%</div> <div>11%</div> <div>• •</div> </div>
1	a	344	<div> <div>%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
2	B	510	<div> <div>3%</div> <div>30%</div> <div>56%</div> <div>6%</div> <div>7%</div> </div>
2	b	510	<div> <div>2%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
3	C	473	<div> <div>2%</div> <div>22%</div> <div>57%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>
3	c	473	<div> <div>2%</div> <div>79%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>
4	D	352	<div> <div>2%</div> <div>30%</div> <div>59%</div> <div>7%</div> <div>•</div> </div>

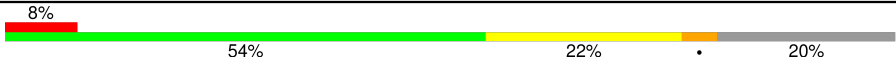

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Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	246	
13	o	246	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	X	50	
17	x	50	
18	N	37	
18	n	37	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	348	X	-	-	-
23	CLA	A	349	X	-	-	-
23	CLA	A	350	X	-	-	-
23	CLA	A	352	X	-	-	-
23	CLA	B	511	X	-	-	X
23	CLA	B	512	X	-	-	-
23	CLA	B	513	X	-	-	-
23	CLA	B	514	X	-	-	-
23	CLA	B	515	X	-	-	-
23	CLA	B	516	X	-	-	X
23	CLA	B	517	X	-	-	-
23	CLA	B	518	X	-	-	-
23	CLA	B	519	X	-	-	X
23	CLA	B	520	X	-	-	-
23	CLA	B	521	X	-	-	-
23	CLA	B	522	X	-	-	-
23	CLA	B	523	X	-	-	-
23	CLA	B	524	X	-	X	X
23	CLA	B	525	X	-	-	-
23	CLA	B	527	X	-	-	X
23	CLA	C	474	X	-	-	-
23	CLA	C	475	X	-	-	-
23	CLA	C	476	X	-	-	-
23	CLA	C	477	X	-	-	-
23	CLA	C	478	X	-	-	-
23	CLA	C	479	X	-	-	-
23	CLA	C	480	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	481	X	-	-	X
23	CLA	C	482	X	-	-	X
23	CLA	C	483	X	-	-	X
23	CLA	C	484	X	-	-	-
23	CLA	C	485	X	-	-	-
23	CLA	C	486	X	-	-	-
23	CLA	C	487	X	-	-	X
23	CLA	D	354	X	-	-	-
23	CLA	D	356	X	-	-	-
23	CLA	a	2348	X	-	-	-
23	CLA	a	2349	X	-	-	X
23	CLA	a	2351	X	-	-	-
23	CLA	b	2511	X	-	-	-
23	CLA	b	2512	X	-	-	-
23	CLA	b	2513	X	-	-	-
23	CLA	b	2514	X	-	-	-
23	CLA	b	2515	X	-	-	-
23	CLA	b	2516	X	-	-	X
23	CLA	b	2517	X	-	-	X
23	CLA	b	2518	X	-	-	-
23	CLA	b	2519	X	-	-	X
23	CLA	b	2520	X	-	-	-
23	CLA	b	2521	X	-	-	-
23	CLA	b	2522	X	-	-	X
23	CLA	b	2523	X	-	-	-
23	CLA	b	2524	X	-	-	X
23	CLA	b	2525	X	-	-	-
23	CLA	b	2526	X	-	-	X
23	CLA	c	2474	X	-	-	-
23	CLA	c	2475	X	-	-	-
23	CLA	c	2476	X	-	-	-
23	CLA	c	2477	X	-	-	X
23	CLA	c	2478	X	-	-	X
23	CLA	c	2479	X	-	-	X
23	CLA	c	2480	X	-	-	-
23	CLA	c	2481	X	-	-	-
23	CLA	c	2482	X	-	-	-
23	CLA	c	2483	X	-	-	-
23	CLA	c	2484	X	-	-	-
23	CLA	c	2485	X	-	-	X
23	CLA	c	2486	X	-	-	X
23	CLA	c	2487	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	2354	X	-	-	-
23	CLA	d	2355	X	-	-	X
23	CLA	d	2357	X	-	-	-
25	HEM	e	2084	-	-	-	X
26	PL9	A	353	-	-	-	X
26	PL9	D	357	-	-	-	X
26	PL9	a	2352	-	-	-	X
26	PL9	d	2358	-	-	-	X
27	LMT	d	2359	-	-	-	X
28	BCR	B	528	-	-	-	X
28	BCR	B	529	-	-	-	X
28	BCR	C	488	-	-	-	X
28	BCR	C	489	-	-	-	X
28	BCR	F	48	-	-	-	X
28	BCR	K	50	-	-	-	X
28	BCR	b	2527	-	-	-	X
28	BCR	b	2528	-	-	-	X
28	BCR	c	2488	-	-	-	X
28	BCR	c	2489	-	-	-	X
28	BCR	d	2360	-	-	-	X
28	BCR	k	2050	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45945 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2616	1714	430	457	15			

- Molecule 2 is a protein called photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			
2	b	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			
3	c	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INSERTION	UNP Q8DIF8
C	2	LYS	-	INSERTION	UNP Q8DIF8
C	3	THR	-	INSERTION	UNP Q8DIF8
C	4	LEU	-	INSERTION	UNP Q8DIF8
C	5	SER	-	INSERTION	UNP Q8DIF8
C	6	SER	-	INSERTION	UNP Q8DIF8
C	7	GLN	-	INSERTION	UNP Q8DIF8
C	8	LYS	-	INSERTION	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ARG	-	INSERTION	UNP Q8DIF8
C	10	TYR	-	INSERTION	UNP Q8DIF8
C	11	SER	-	INSERTION	UNP Q8DIF8
C	12	PRO	-	INSERTION	UNP Q8DIF8
C	13	VAL	-	INSERTION	UNP Q8DIF8
c	2001	MET	-	INSERTION	UNP Q8DIF8
c	2002	LYS	-	INSERTION	UNP Q8DIF8
c	2003	THR	-	INSERTION	UNP Q8DIF8
c	2004	LEU	-	INSERTION	UNP Q8DIF8
c	2005	SER	-	INSERTION	UNP Q8DIF8
c	2006	SER	-	INSERTION	UNP Q8DIF8
c	2007	GLN	-	INSERTION	UNP Q8DIF8
c	2008	LYS	-	INSERTION	UNP Q8DIF8
c	2009	ARG	-	INSERTION	UNP Q8DIF8
c	2010	TYR	-	INSERTION	UNP Q8DIF8
c	2011	SER	-	INSERTION	UNP Q8DIF8
c	2012	PRO	-	INSERTION	UNP Q8DIF8
c	2013	VAL	-	INSERTION	UNP Q8DIF8

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			
4	d	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			

- Molecule 5 is a protein called Cytochrome b559 alpha subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			624	411	99	114			
5	e	76	Total	C	N	O	0	0	0
			624	411	99	114			

- Molecule 6 is a protein called Cytochrome b559 beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

- Molecule 7 is a protein called photosystem II PsbH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			
7	h	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			

- Molecule 8 is a protein called Photosystem II reaction center I protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

- Molecule 9 is a protein called Photosystem II reaction center J protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center L protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			
12	m	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			
13	o	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			

- Molecule 14 is a protein called photosystem II PsbT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			
14	t	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	105	Total	C	N	O		0	0	0
			827	521	137	169				
15	u	105	Total	C	N	O		0	0	0
			827	521	137	169				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called photosystem II PsbX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O		0	0	0
			296	197	47	52				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	x	40	Total	C	N	O	0	0	0
			296	197	47	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	INSERTION	UNP Q9F1R6
X	2	ILE	-	INSERTION	UNP Q9F1R6
X	3	GLN	-	INSERTION	UNP Q9F1R6
X	4	SER	-	INSERTION	UNP Q9F1R6
X	5	ALA	-	INSERTION	UNP Q9F1R6
X	6	SER	-	INSERTION	UNP Q9F1R6
X	7	SER	-	INSERTION	UNP Q9F1R6
X	8	LEU	-	INSERTION	UNP Q9F1R6
X	9	LEU	-	INSERTION	UNP Q9F1R6
X	10	LEU	-	INSERTION	UNP Q9F1R6
x	2001	MET	-	INSERTION	UNP Q9F1R6
x	2002	ILE	-	INSERTION	UNP Q9F1R6
x	2003	GLN	-	INSERTION	UNP Q9F1R6
x	2004	SER	-	INSERTION	UNP Q9F1R6
x	2005	ALA	-	INSERTION	UNP Q9F1R6
x	2006	SER	-	INSERTION	UNP Q9F1R6
x	2007	SER	-	INSERTION	UNP Q9F1R6
x	2008	LEU	-	INSERTION	UNP Q9F1R6
x	2009	LEU	-	INSERTION	UNP Q9F1R6
x	2010	LEU	-	INSERTION	UNP Q9F1R6

- Molecule 18 is a protein called Photosystem II PsbN protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	N	37	Total	C	N	O	0	0	0
			186	111	37	38			
18	n	37	Total	C	N	O	0	0	0
			186	111	37	38			

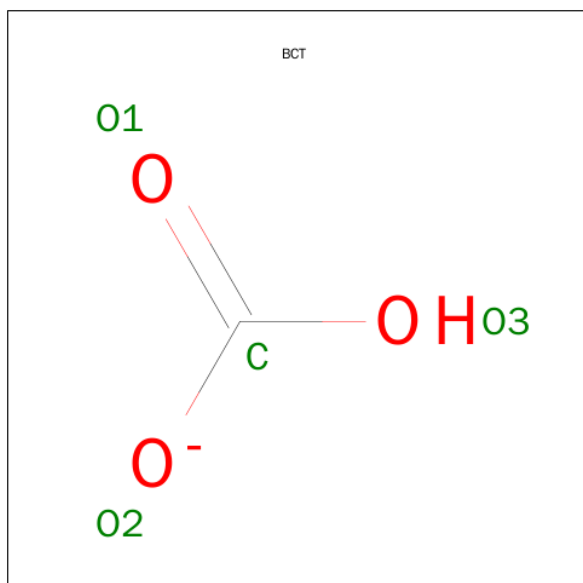
- Molecule 19 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			
19	z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			

- Molecule 20 is FE (III) ION (three-letter code: FE) (formula: Fe).

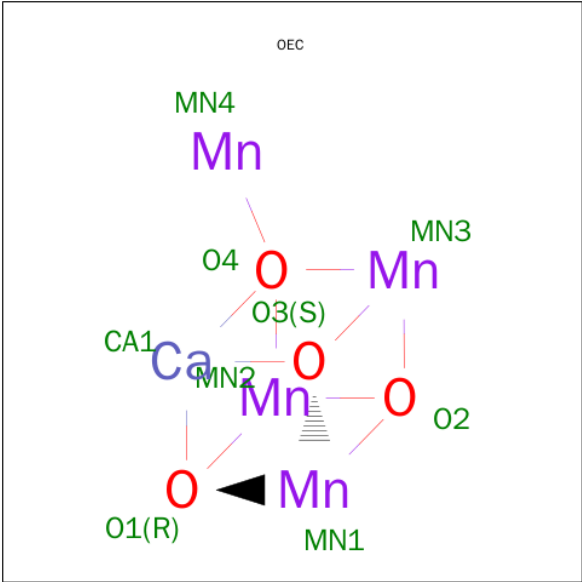
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3^-).



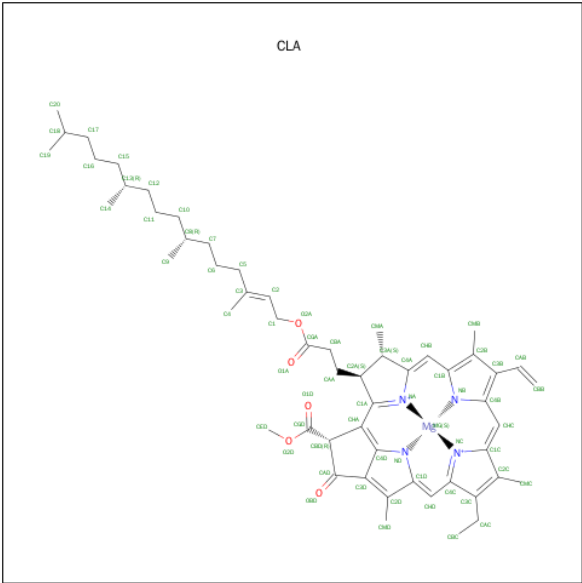
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	1	3		
21	D	1	Total	C	O	0	0
			4	1	3		
21	a	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	Ca	Mn	O	0	0
			9	1	4	4		
22	a	1	Total	Ca	Mn	O	0	0
			9	1	4	4		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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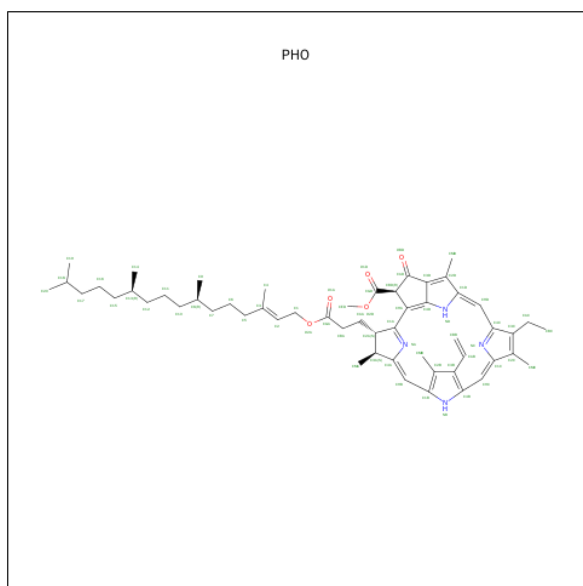
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

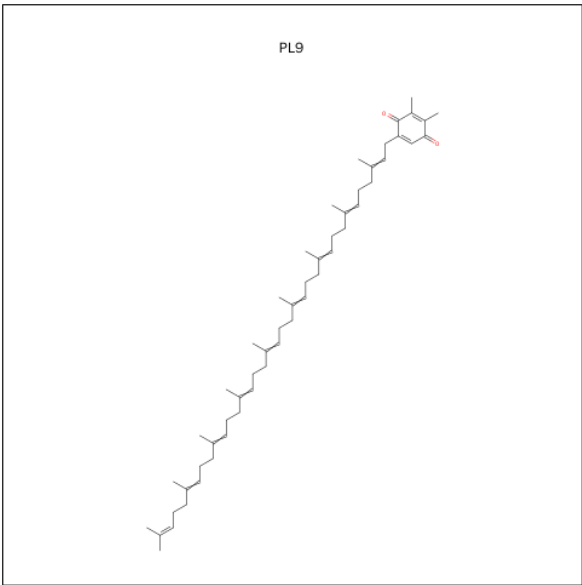
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

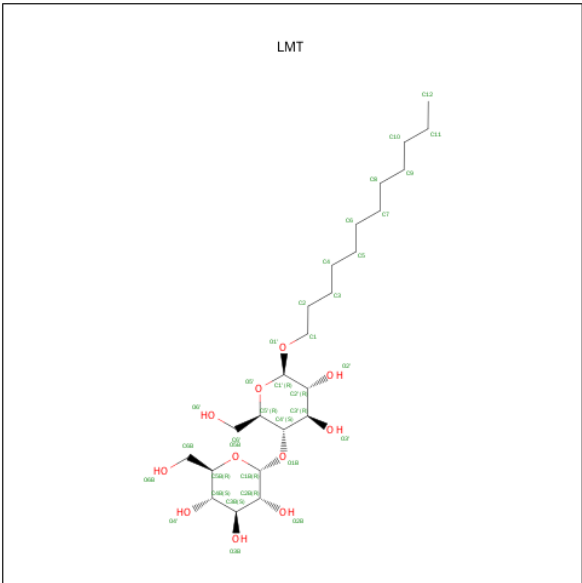
-
- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



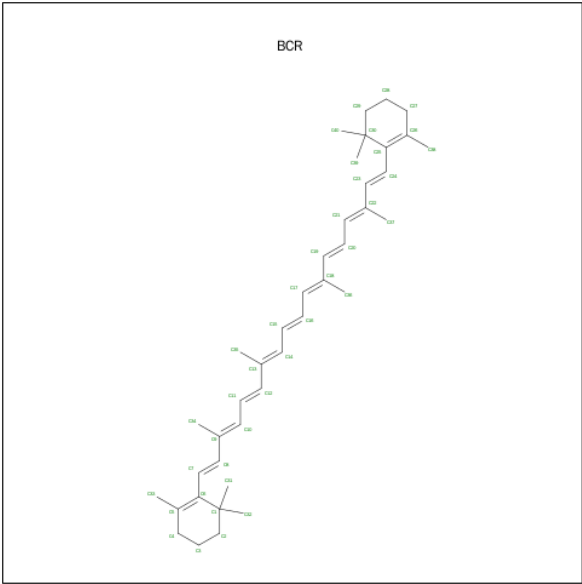
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	D	1	Total	C	O	0	0
			45	43	2		
26	A	1	Total	C	O	0	0
			45	43	2		
26	d	1	Total	C	O	0	0
			45	43	2		
26	a	1	Total	C	O	0	0
			45	43	2		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	1	Total	C	O	0	0
			35	24	11		
27	d	1	Total	C	O	0	0
			35	24	11		

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	1	Total	C	0	0
			40	40		
28	C	1	Total	C	0	0
			40	40		
28	K	1	Total	C	0	0
			40	40		
28	C	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		
28	J	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		
28	d	1	Total	C	0	0
			40	40		
28	c	1	Total	C	0	0
			40	40		
28	k	1	Total	C	0	0
			40	40		

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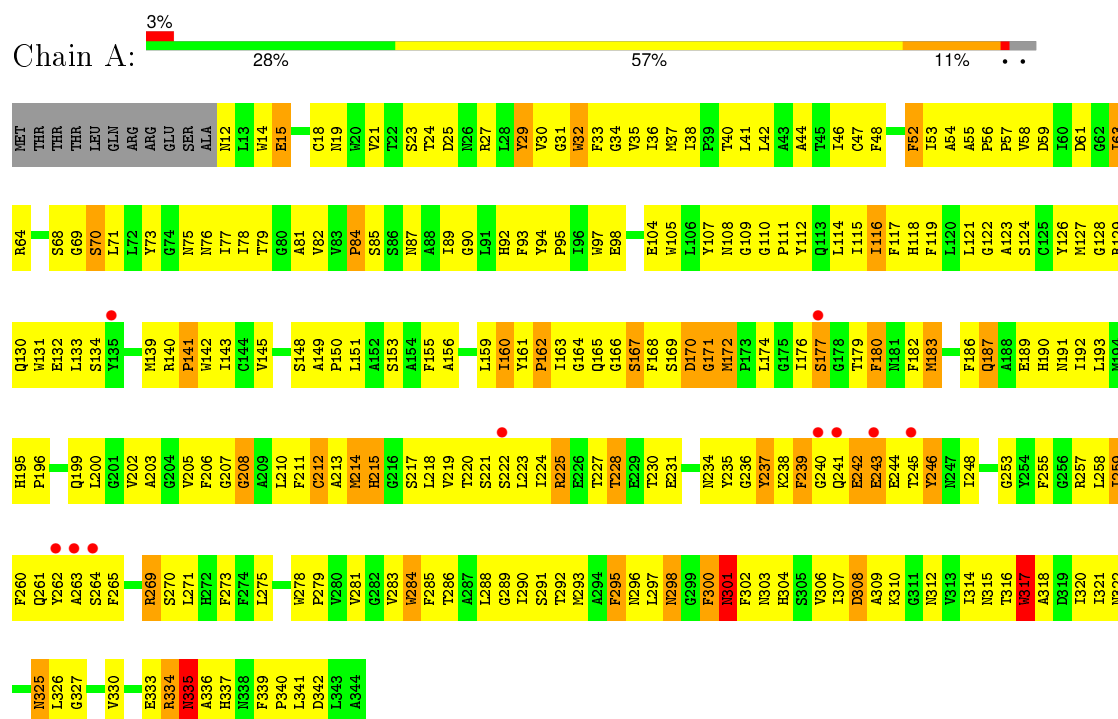
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	j	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0

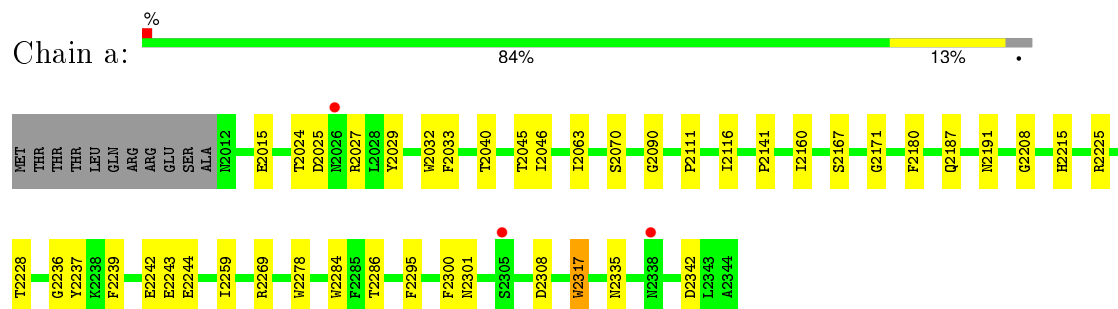
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem Q(B) protein

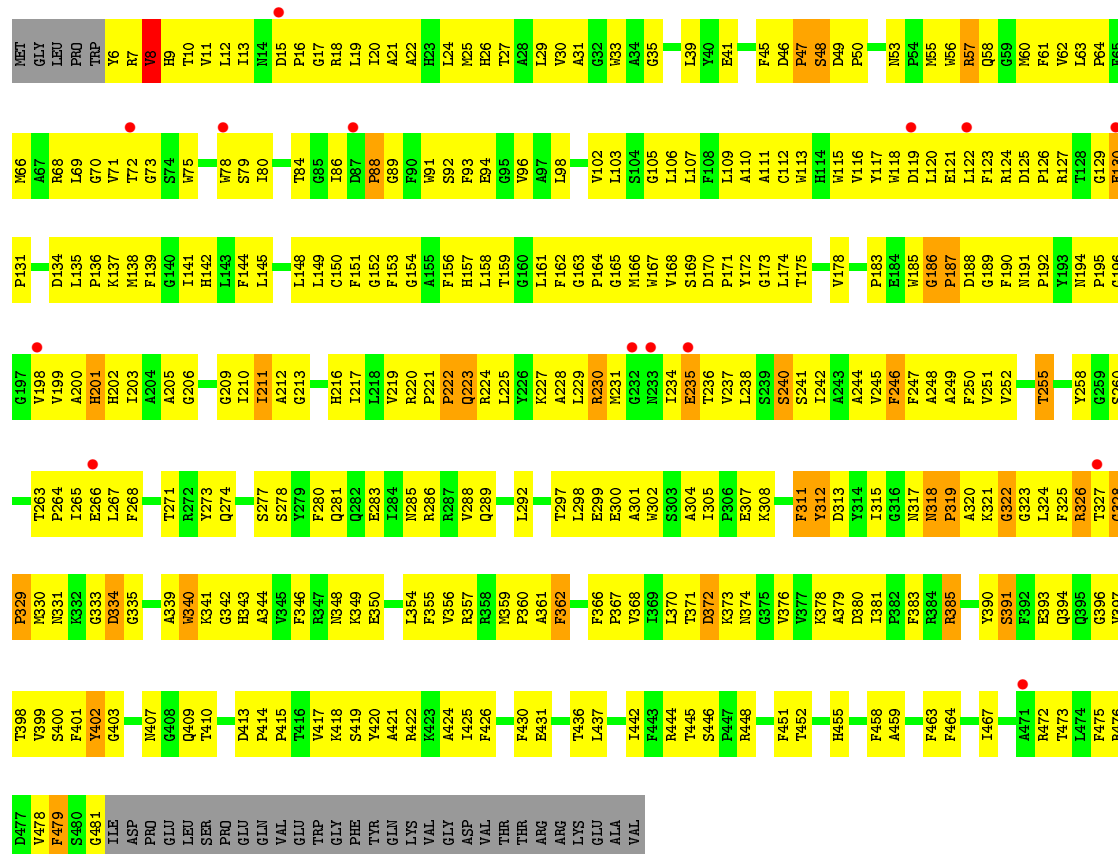


- Molecule 1: Photosystem Q(B) protein

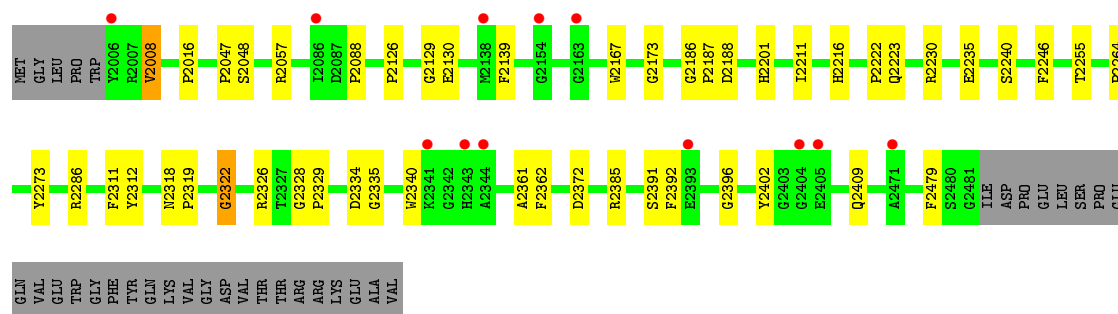
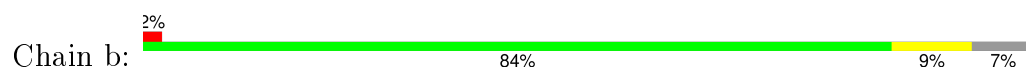


- Molecule 2: photosystem II core light harvesting protein

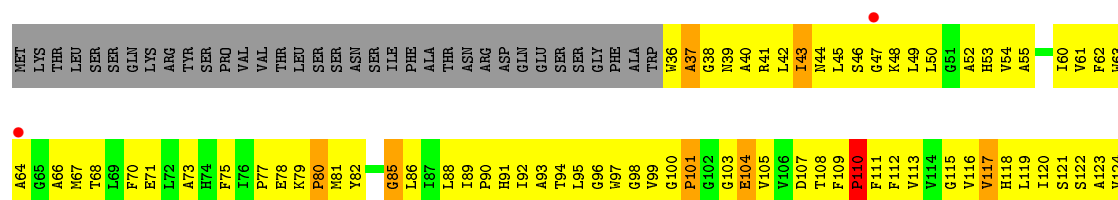


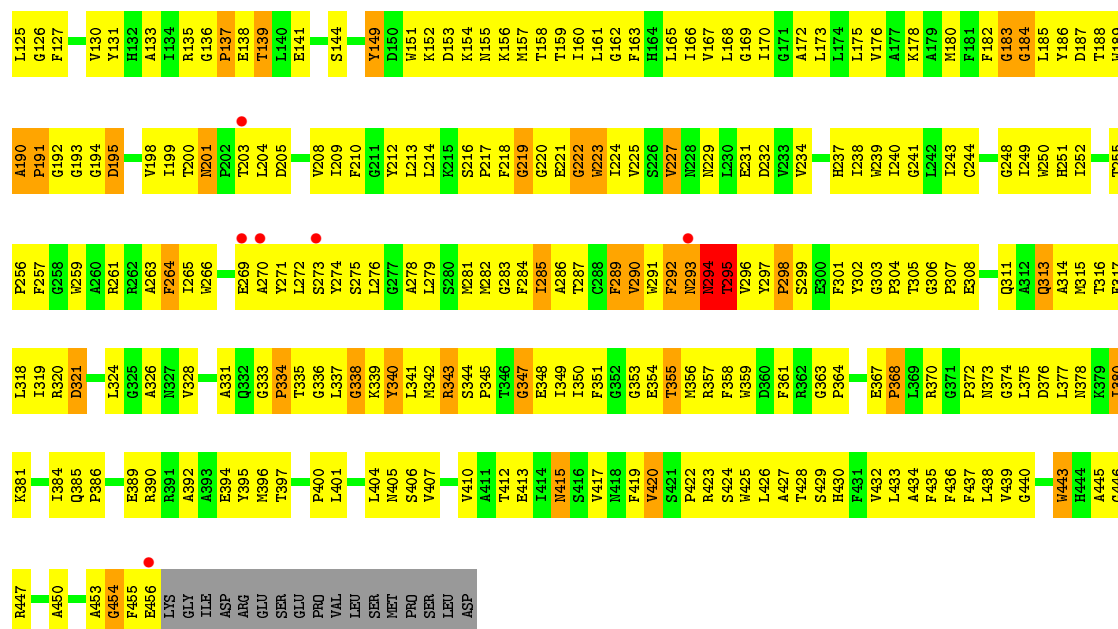


• Molecule 2: photosystem II core light harvesting protein

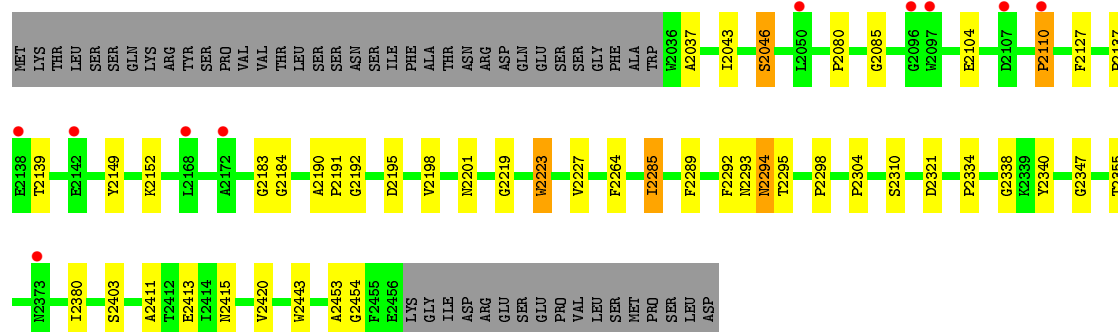
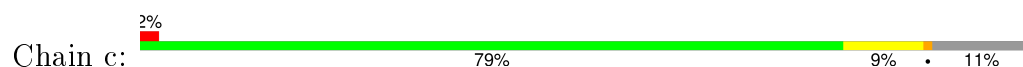


• Molecule 3: photosystem II CP43 protein

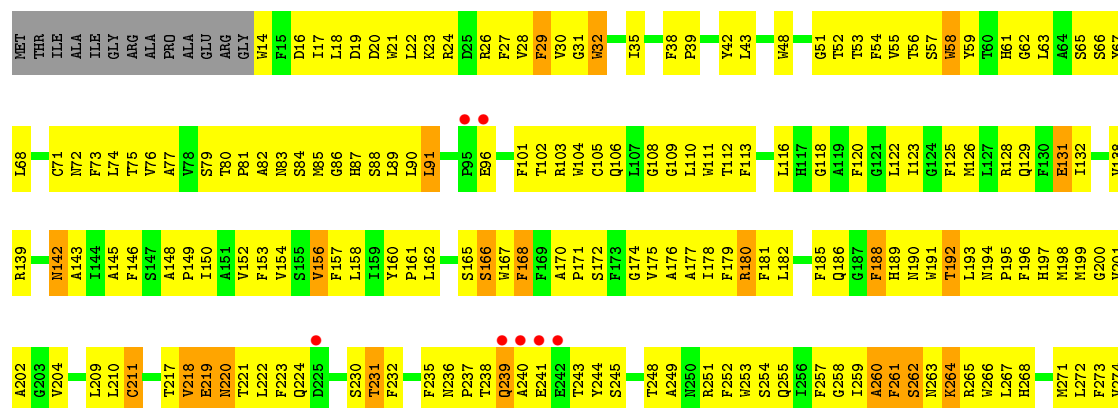


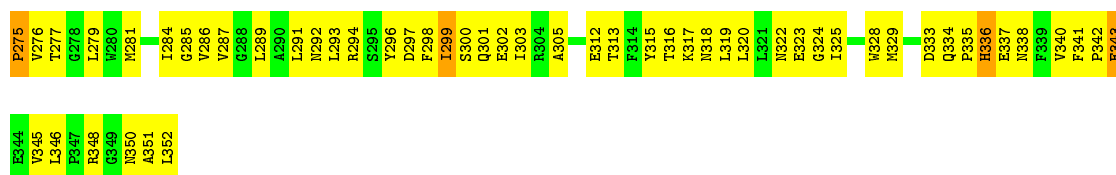


• Molecule 3: photosystem II CP43 protein

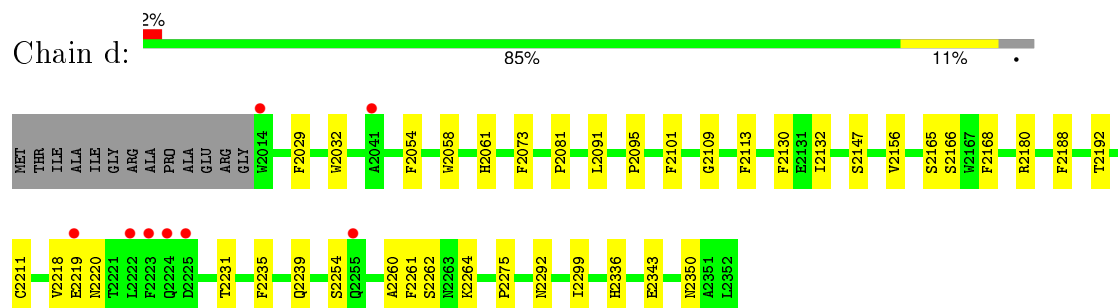


• Molecule 4: photosystem II reaction center D2 protein

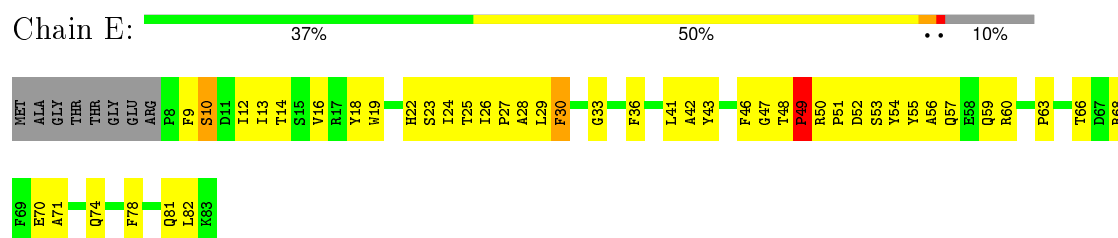




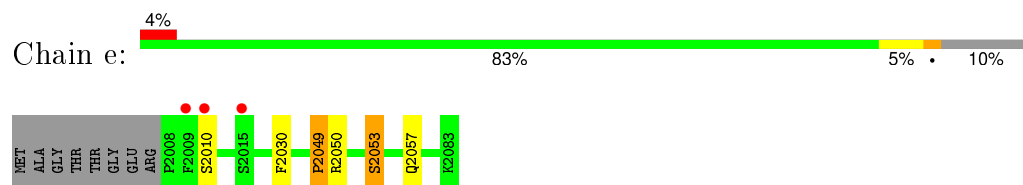
- Molecule 4: photosystem II reaction center D2 protein



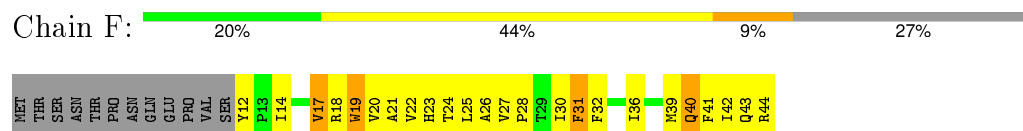
- Molecule 5: Cytochrome b559 alpha subunit



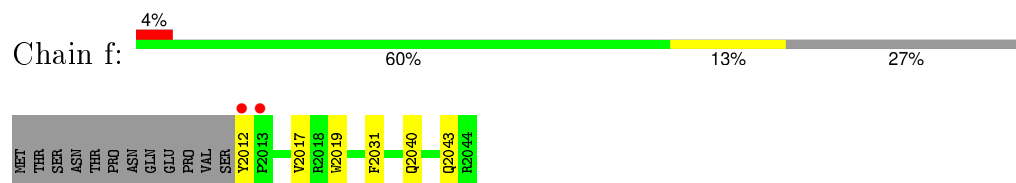
- Molecule 5: Cytochrome b559 alpha subunit



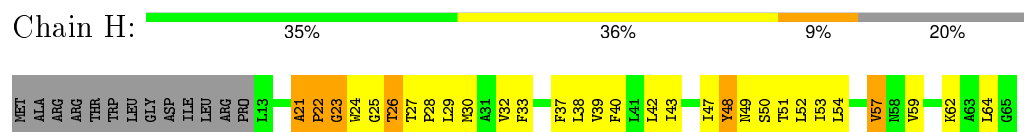
- Molecule 6: Cytochrome b559 beta subunit



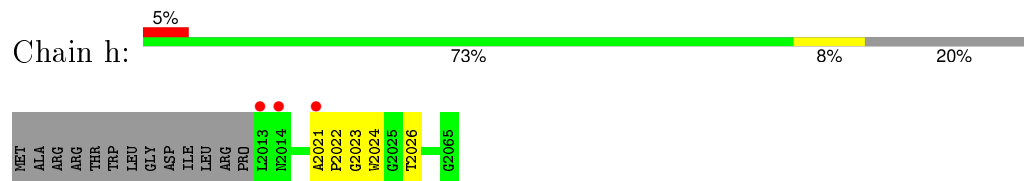
- Molecule 6: Cytochrome b559 beta subunit



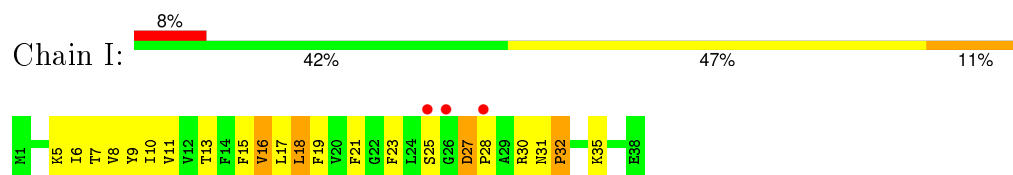
- Molecule 7: photosystem II PsbH protein



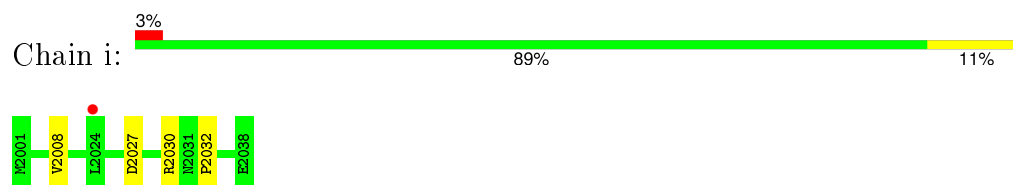
- Molecule 7: photosystem II PsbH protein



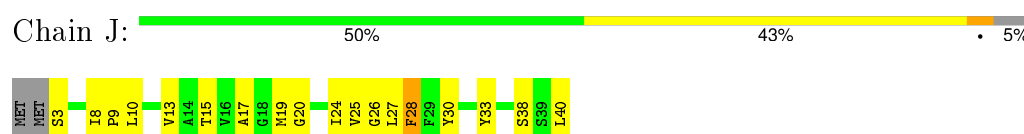
- Molecule 8: Photosystem II reaction center I protein



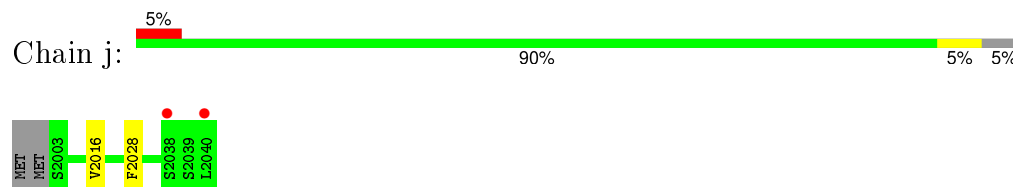
- Molecule 8: Photosystem II reaction center I protein



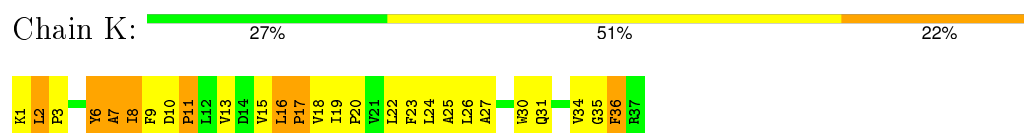
- Molecule 9: Photosystem II reaction center J protein




- Molecule 9: Photosystem II reaction center J protein



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

Chain k:  84% 16%




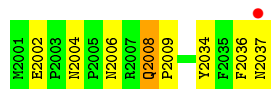
- Molecule 11: Photosystem II reaction center L protein

Chain L:  5% 30% 51% 14% 5%



- Molecule 11: Photosystem II reaction center L protein

Chain l:  3% 78% 19% .




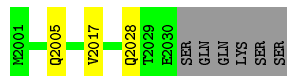
- Molecule 12: Photosystem II reaction center M protein

Chain M:  28% 50% 6% 17%



- Molecule 12: Photosystem II reaction center M protein

Chain m:  75% 8% 17%

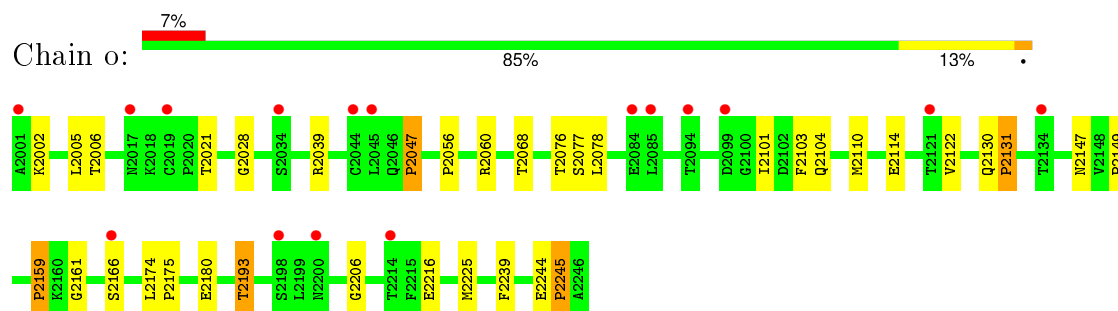


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

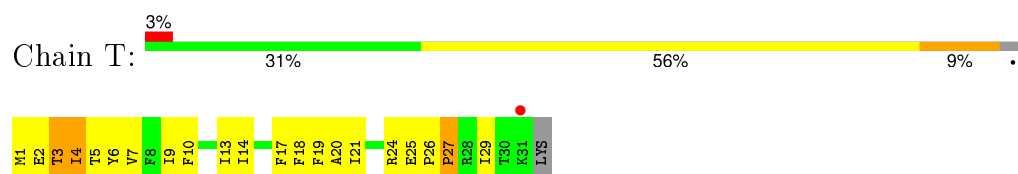
Chain O:  2% 30% 55% 13% .



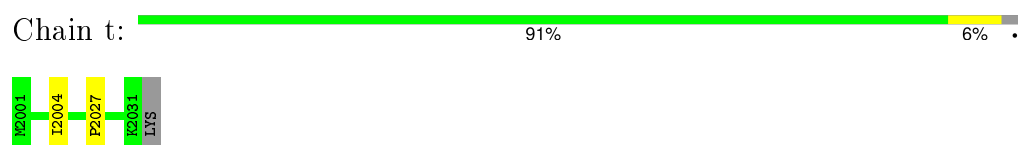
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



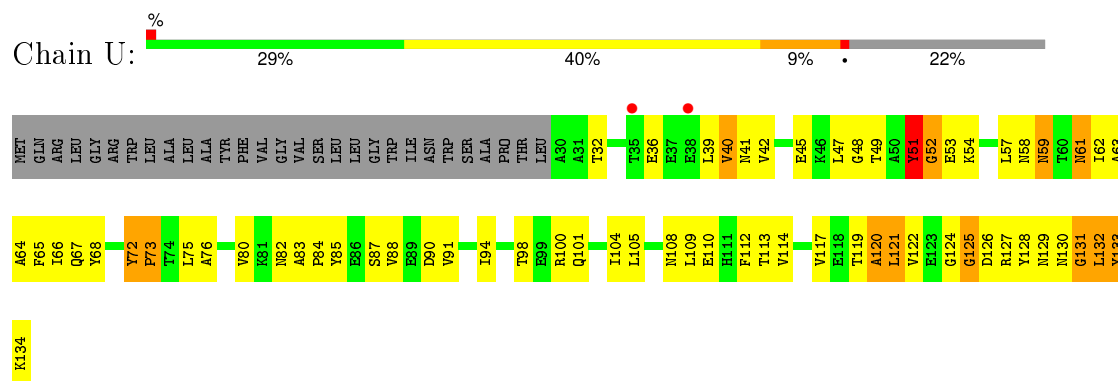
- Molecule 14: photosystem II PsbT protein



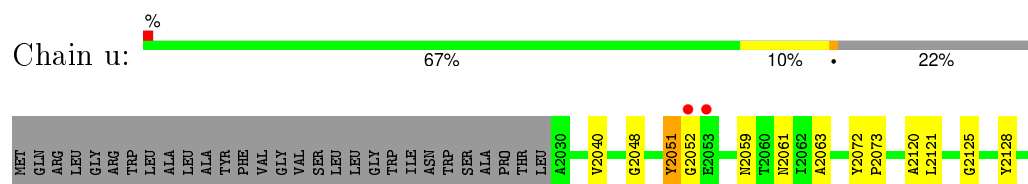
- Molecule 14: photosystem II PsbT protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

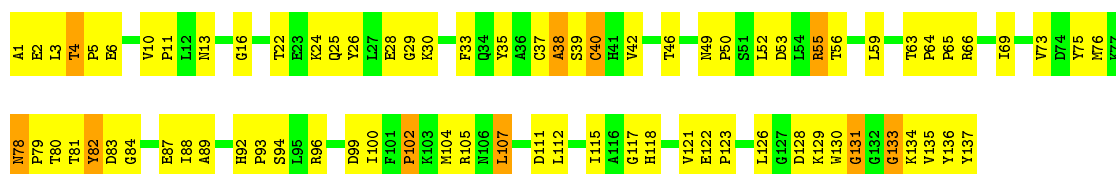


- Molecule 15: Photosystem II 12 kDa extrinsic protein

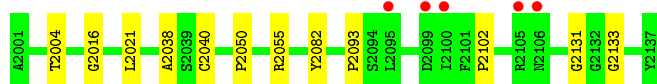
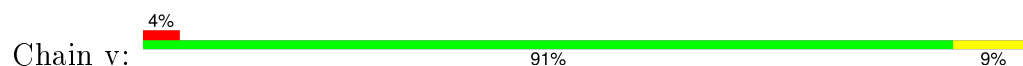


- Molecule 16: Cytochrome c-550

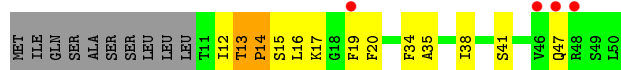




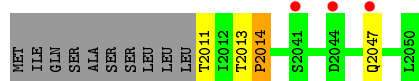
- Molecule 16: Cytochrome c-550



- Molecule 17: photosystem II PsbX protein



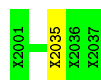
- Molecule 17: photosystem II PsbX protein



- Molecule 18: Photosystem II PsbN protein



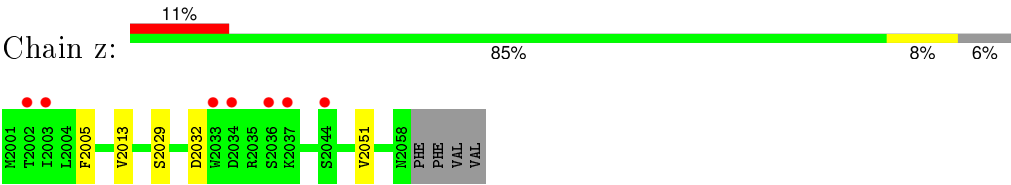
- Molecule 18: Photosystem II PsbN protein



- Molecule 19: Photosystem II reaction center Z protein



- Molecule 19: Photosystem II reaction center Z protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 228.85Å 309.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 74.07 – 3.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 84.1 (74.07-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.296 , 0.342 0.307 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 97.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 105247 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	45945	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, LMT, CLA, PL9, BCT, FE, OEC, HEM, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/2702	0.85	2/3685 (0.1%)
1	a	0.62	0/2701	0.83	2/3685 (0.1%)
2	B	0.57	0/3870	0.80	3/5271 (0.1%)
2	b	0.56	0/3870	0.80	4/5271 (0.1%)
3	C	0.60	0/3361	0.81	3/4579 (0.1%)
3	c	0.57	0/3361	0.80	3/4579 (0.1%)
4	D	0.62	0/2797	0.82	1/3813 (0.0%)
4	d	0.62	0/2797	0.83	2/3813 (0.1%)
5	E	0.59	0/643	0.89	1/876 (0.1%)
5	e	0.61	0/643	0.87	1/876 (0.1%)
6	F	0.74	0/278	0.84	0/379
6	f	0.68	0/278	0.84	0/379
7	H	0.58	0/419	0.81	0/570
7	h	0.60	0/419	0.81	0/570
8	I	0.63	0/319	0.73	0/429
8	i	0.61	0/319	0.73	0/429
9	J	0.60	0/278	0.80	0/376
9	j	0.62	0/278	0.84	0/376
10	K	0.66	0/303	0.92	0/416
10	k	0.63	0/303	0.86	0/416
11	L	0.74	1/311 (0.3%)	0.87	0/422
11	l	0.73	1/311 (0.3%)	0.91	0/422
12	M	0.63	0/237	0.77	0/324
12	m	0.70	0/237	0.80	0/324
13	O	0.67	0/1919	0.97	4/2601 (0.2%)
13	o	0.68	0/1919	0.96	3/2601 (0.1%)
14	T	0.71	0/274	0.78	0/370
14	t	0.74	0/274	0.80	0/370
15	U	0.68	0/838	0.91	1/1137 (0.1%)
15	u	0.62	0/838	0.87	0/1137
16	V	0.62	0/1085	0.78	0/1473
16	v	0.56	0/1085	0.77	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.57	0/299	0.72	0/403
17	x	0.61	0/299	0.75	0/403
19	Z	0.54	0/451	0.74	0/617
19	z	0.54	0/451	0.72	0/617
All	All	0.61	2/40767 (0.0%)	0.83	30/55482 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	b	0	1
11	l	0	1
13	O	0	1
15	U	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	2037	ASN	C-OXT	5.21	1.33	1.23
11	L	37	ASN	C-OXT	5.18	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2171	GLY	N-CA-C	-7.28	94.91	113.10
1	A	171	GLY	N-CA-C	-7.27	94.93	113.10
13	O	131	PRO	N-CA-C	6.48	128.95	112.10
1	a	2236	GLY	N-CA-C	6.41	129.12	113.10
4	D	231	THR	N-CA-C	-6.30	93.98	111.00
1	A	236	GLY	N-CA-C	6.29	128.83	113.10
4	d	2231	THR	N-CA-C	-6.18	94.30	111.00
13	o	2131	PRO	N-CA-C	6.08	127.89	112.10
2	B	129	GLY	N-CA-C	-5.90	98.35	113.10
2	b	2129	GLY	N-CA-C	-5.73	98.78	113.10
15	U	121	LEU	CA-CB-CG	-5.67	102.25	115.30
13	o	2193	THR	N-CA-C	5.46	125.75	111.00
13	o	2002	LYS	N-CA-C	5.42	125.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	2335	GLY	N-CA-C	-5.40	99.60	113.10
13	O	193	THR	N-CA-C	5.36	125.47	111.00
3	C	222	GLY	N-CA-C	-5.31	99.83	113.10
2	b	2329	PRO	N-CA-C	-5.25	98.46	112.10
2	B	329	PRO	N-CA-C	-5.23	98.49	112.10
3	c	2294	ASN	N-CA-C	-5.23	96.88	111.00
5	e	2053	SER	N-CA-C	5.22	125.10	111.00
2	B	335	GLY	N-CA-C	-5.19	100.13	113.10
13	O	23	ASP	N-CA-C	5.18	125.00	111.00
3	c	2223	TRP	CA-CB-CG	5.17	123.53	113.70
4	d	2054	PHE	N-CA-C	5.17	124.96	111.00
3	C	347	GLY	N-CA-C	5.12	125.91	113.10
3	C	294	ASN	N-CA-C	-5.11	97.19	111.00
13	O	2	LYS	N-CA-C	5.11	124.80	111.00
2	b	2322	GLY	N-CA-C	5.10	125.84	113.10
3	c	2347	GLY	N-CA-C	5.08	125.80	113.10
5	E	53	SER	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain
2	B	273	TYR	Sidechain
13	O	240	TYR	Sidechain
15	U	133	TYR	Sidechain
15	U	51	TYR	Sidechain
2	b	2273	TYR	Sidechain
11	l	2034	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	451	0
1	a	2616	0	2514	0	0
2	B	3739	0	3613	450	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3739	0	3613	0	0
3	C	3253	0	3192	532	0
3	c	3253	0	3192	0	0
4	D	2702	0	2605	412	0
4	d	2702	0	2605	0	0
5	E	624	0	613	95	0
5	e	624	0	613	0	0
6	F	269	0	277	43	0
6	f	269	0	277	0	0
7	H	409	0	424	52	0
7	h	409	0	424	0	0
8	I	312	0	329	25	0
8	i	312	0	326	0	0
9	J	272	0	279	43	0
9	j	272	0	279	0	0
10	K	293	0	308	57	0
10	k	293	0	305	0	0
11	L	304	0	316	49	0
11	l	304	0	313	0	0
12	M	234	0	255	32	0
12	m	234	0	252	0	0
13	O	1888	0	1867	274	6
13	o	1888	0	1864	0	0
14	T	265	0	275	41	0
14	t	265	0	272	0	0
15	U	827	0	819	121	0
15	u	827	0	819	0	0
16	V	1064	0	1075	124	0
16	v	1064	0	1070	0	0
17	X	296	0	328	14	0
17	x	296	0	328	0	0
18	N	186	0	40	10	0
18	n	186	0	40	0	6
19	Z	442	0	480	61	0
19	z	442	0	477	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	4	0	0	0	0
21	D	4	0	0	0	0
21	a	4	0	0	0	0
21	d	4	0	0	0	0
22	A	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	9	0	0	0	0
23	A	260	0	288	29	0
23	B	1040	0	1152	116	0
23	C	910	0	1008	104	0
23	D	130	0	144	18	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	910	0	1008	0	0
23	d	195	0	216	0	0
24	A	64	0	74	6	0
24	D	64	0	74	8	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	E	43	0	30	16	0
25	V	43	0	30	10	0
25	e	43	0	30	0	0
25	v	43	0	30	0	0
26	A	45	0	61	8	0
26	D	45	0	61	5	0
26	a	45	0	61	0	0
26	d	45	0	61	0	0
27	B	35	0	46	0	0
27	d	35	0	46	0	0
28	B	80	0	112	16	0
28	C	80	0	112	23	0
28	F	40	0	56	3	0
28	J	40	0	56	2	0
28	K	40	0	56	13	0
28	b	80	0	112	0	0
28	c	80	0	112	0	0
28	d	40	0	56	0	0
28	j	40	0	56	0	0
28	k	40	0	56	0	0
All	All	45945	0	45912	2600	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (2600) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:138:HEM:CMB	25:V:138:HEM:C2B	1.74	1.63
25:V:138:HEM:C2C	25:V:138:HEM:CMC	1.75	1.62
16:V:37:CYS:SG	25:V:138:HEM:HAB	1.57	1.44
5:E:12:ILE:CG2	5:E:18:TYR:HB2	1.44	1.43
5:E:12:ILE:HD12	25:E:84:HEM:O2D	1.31	1.25
6:F:40:GLN:NE2	9:J:27:LEU:HG	1.52	1.24
5:E:12:ILE:HG22	5:E:18:TYR:CB	1.71	1.21
13:O:40:ILE:HG12	13:O:84:GLU:OE1	1.07	1.19
2:B:75:TRP:H	2:B:94:GLU:HG3	1.07	1.18
3:C:158:THR:HG22	3:C:251:HIS:HB3	1.23	1.17
5:E:14:THR:HG22	9:J:8:ILE:HB	1.24	1.16
3:C:158:THR:CG2	3:C:251:HIS:HB3	1.75	1.16
6:F:39:MET:O	6:F:42:ILE:HG22	1.47	1.14
2:B:326:ARG:CD	2:B:327:THR:H	1.61	1.14
13:O:122:VAL:HA	13:O:146:PHE:CE2	1.85	1.12
3:C:308:GLU:HG2	3:C:361:PHE:CE1	1.85	1.10
5:E:60:ARG:HH22	16:V:129:LYS:HE3	1.05	1.10
3:C:455:PHE:HE1	4:D:224:GLN:HA	1.07	1.10
13:O:146:PHE:HB2	13:O:195:GLY:HA3	1.10	1.09
3:C:138:GLU:HG2	3:C:139:THR:H	1.09	1.09
4:D:298:PHE:HA	11:L:37:ASN:HD21	0.93	1.09
4:D:298:PHE:HA	11:L:37:ASN:ND2	1.67	1.09
5:E:14:THR:CG2	9:J:8:ILE:HB	1.83	1.08
1:A:186:PHE:HD2	1:A:192:ILE:HD11	1.05	1.08
3:C:344:SER:HB3	3:C:350:ILE:HD11	1.34	1.08
13:O:130:GLN:HB3	13:O:131:PRO:CD	1.83	1.08
5:E:12:ILE:HG22	5:E:18:TYR:HB2	1.10	1.07
3:C:223:TRP:CD1	3:C:224:ILE:HG13	1.90	1.07
16:V:37:CYS:SG	25:V:138:HEM:CAB	2.41	1.07
15:U:57:LEU:HD21	15:U:112:PHE:HD2	1.02	1.07
5:E:10:SER:HA	5:E:13:ILE:HD12	1.37	1.07
1:A:150:PRO:HB2	23:A:348:CLA:H62	1.38	1.06
15:U:59:ASN:N	15:U:59:ASN:HD22	1.33	1.06
5:E:14:THR:CG2	9:J:8:ILE:HD12	1.85	1.06
13:O:121:THR:HG21	13:O:148:VAL:HG22	1.37	1.06
13:O:40:ILE:CG1	13:O:84:GLU:OE1	2.04	1.05
2:B:326:ARG:HD2	2:B:327:THR:H	0.88	1.05
5:E:60:ARG:NH2	16:V:129:LYS:HE3	1.71	1.05
13:O:47:PRO:HG3	13:O:76:THR:HG21	1.36	1.04
3:C:223:TRP:HD1	3:C:224:ILE:HG13	1.19	1.04
2:B:57:ARG:HD3	2:B:331:ASN:HD21	1.17	1.04
15:U:57:LEU:HD21	15:U:112:PHE:CD2	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:THR:HG21	9:J:8:ILE:CD1	1.89	1.02
2:B:138:MET:HG2	23:B:522:CLA:HBC2	1.37	1.02
2:B:47:PRO:HB3	2:B:78:TRP:CD1	1.94	1.02
3:C:294:ASN:N	3:C:294:ASN:HD22	1.52	1.02
2:B:326:ARG:HD2	2:B:327:THR:N	1.74	1.01
5:E:14:THR:HG21	9:J:8:ILE:HD12	1.38	1.01
13:O:81:ILE:HG22	13:O:82:GLN:H	1.24	1.00
3:C:77:PRO:HA	3:C:104:GLU:OE2	1.59	1.00
1:A:186:PHE:CD2	1:A:192:ILE:HD11	1.95	1.00
3:C:62:PHE:CZ	10:K:19:ILE:HD11	1.95	1.00
15:U:132:LEU:H	15:U:132:LEU:HD23	1.20	1.00
4:D:336:HIS:CD2	4:D:336:HIS:H	1.78	1.00
6:F:40:GLN:OE1	9:J:28:PHE:HA	1.61	0.99
13:O:130:GLN:CB	13:O:131:PRO:HD2	1.91	0.99
3:C:104:GLU:HG2	3:C:105:VAL:HG23	1.40	0.99
5:E:12:ILE:CG2	5:E:18:TYR:CB	2.35	0.99
13:O:106:VAL:HG13	13:O:117:PRO:HG3	1.43	0.99
2:B:222:PRO:HB3	7:H:25:GLY:HA2	1.43	0.98
13:O:193:THR:HG22	13:O:194:LYS:H	1.27	0.98
13:O:39:ARG:HB3	13:O:245:PRO:HG3	1.42	0.98
3:C:343:ARG:HD2	3:C:343:ARG:C	1.84	0.98
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.46	0.97
3:C:158:THR:HG22	3:C:251:HIS:CB	1.95	0.97
3:C:455:PHE:CE1	4:D:224:GLN:HA	1.97	0.97
4:D:198:MET:HE1	11:L:30:LEU:HD11	1.46	0.97
3:C:320:ARG:NE	15:U:128:TYR:CE2	2.33	0.96
13:O:47:PRO:HA	13:O:237:GLY:HA3	1.47	0.95
19:Z:19:MET:O	19:Z:23:VAL:HG23	1.65	0.95
2:B:130:GLU:HG2	2:B:131:PRO:HD3	1.48	0.95
4:D:158:LEU:O	4:D:162:LEU:HG	1.66	0.95
23:C:478:CLA:H62	23:C:485:CLA:H12	1.48	0.95
2:B:326:ARG:HH11	2:B:327:THR:CB	1.80	0.95
4:D:88:SER:HB3	5:E:68:ARG:HH21	1.29	0.95
2:B:475:PHE:HB3	2:B:478:VAL:HB	1.46	0.95
15:U:59:ASN:N	15:U:59:ASN:ND2	2.05	0.95
13:O:130:GLN:HB3	13:O:131:PRO:HD2	0.96	0.94
3:C:42:LEU:HG	23:C:486:CLA:HED1	1.49	0.94
5:E:14:THR:HG21	9:J:8:ILE:CG1	1.95	0.94
23:B:521:CLA:HAB	23:B:527:CLA:HED1	1.47	0.94
13:O:81:ILE:HG22	13:O:82:GLN:N	1.80	0.94
2:B:6:TYR:OH	12:M:21:PHE:HZ	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:ALA:HB2	15:U:127:ARG:HD2	1.50	0.93
16:V:133:GLY:O	16:V:137:TYR:HB2	1.69	0.93
15:U:72:TYR:CD2	15:U:73:PRO:N	2.36	0.93
3:C:71:GLU:OE1	3:C:86:LEU:HB3	1.69	0.93
3:C:320:ARG:HE	15:U:128:TYR:HE2	1.08	0.93
1:A:225:ARG:HB3	2:B:481:GLY:C	1.88	0.93
15:U:59:ASN:HD22	15:U:59:ASN:H	0.99	0.93
13:O:44:CYS:HB3	13:O:240:TYR:HB3	1.51	0.93
3:C:271:TYR:HA	3:C:274:TYR:CD1	2.04	0.93
3:C:308:GLU:OE2	3:C:361:PHE:HZ	1.52	0.92
3:C:157:MET:HE2	3:C:160:ILE:HD12	1.50	0.92
4:D:319:LEU:HA	4:D:322:ASN:HD22	1.34	0.92
4:D:52:THR:HG22	4:D:67:TYR:HE1	1.35	0.91
3:C:344:SER:HB3	3:C:350:ILE:CD1	1.99	0.91
3:C:62:PHE:HZ	10:K:19:ILE:HD11	1.32	0.91
6:F:40:GLN:HE22	9:J:27:LEU:C	1.74	0.91
28:C:488:BCR:H312	19:Z:9:LEU:HD11	1.50	0.91
4:D:68:LEU:HA	6:F:39:MET:HE1	1.52	0.90
2:B:57:ARG:HD3	2:B:331:ASN:ND2	1.85	0.90
1:A:237:TYR:CZ	1:A:245:THR:HG23	2.06	0.90
1:A:317:TRP:HA	4:D:63:LEU:HD13	1.54	0.90
13:O:43:LEU:HD12	13:O:240:TYR:O	1.72	0.90
2:B:56:TRP:CZ3	2:B:266:GLU:HA	2.07	0.90
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.54	0.89
5:E:12:ILE:HG21	5:E:18:TYR:HB2	1.53	0.89
5:E:14:THR:HG22	9:J:8:ILE:CB	2.02	0.89
3:C:138:GLU:HG2	3:C:139:THR:N	1.87	0.89
1:A:300:PHE:HB3	1:A:302:PHE:HE1	1.36	0.89
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.51	0.89
2:B:318:ASN:HD22	2:B:319:PRO:N	1.70	0.89
16:V:4:THR:HG22	16:V:5:PRO:HD2	1.53	0.89
16:V:37:CYS:HG	25:V:138:HEM:CAB	1.84	0.89
13:O:104:GLN:OE1	13:O:104:GLN:N	2.05	0.89
16:V:46:THR:HG22	16:V:49:ASN:H	1.38	0.89
3:C:43:ILE:HG13	3:C:44:ASN:H	1.36	0.89
1:A:307:ILE:CG1	1:A:314:ILE:HD11	2.03	0.88
1:A:89:ILE:HG12	13:O:73:ARG:NH2	1.88	0.88
3:C:55:ALA:HB1	28:C:488:BCR:H373	1.55	0.88
1:A:239:PHE:HZ	4:D:223:PHE:HZ	1.22	0.88
2:B:56:TRP:HZ3	2:B:266:GLU:HA	1.38	0.88
19:Z:33:TRP:HE3	19:Z:37:LYS:HD3	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:GLY:HA2	2:B:325:PHE:CE1	2.08	0.88
1:A:334:ARG:HH11	4:D:320:LEU:HD11	1.38	0.88
1:A:286:THR:HG22	23:A:348:CLA:O1D	1.73	0.88
4:D:71:CYS:HB2	4:D:76:VAL:HG23	1.55	0.87
13:O:146:PHE:HB2	13:O:195:GLY:CA	2.01	0.87
3:C:307:PRO:HB3	3:C:358:PHE:CD2	2.09	0.87
3:C:116:VAL:HG13	28:C:488:BCR:H332	1.57	0.87
13:O:164:LEU:HD23	15:U:42:VAL:HG13	1.56	0.87
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.38	0.87
3:C:305:THR:HA	3:C:423:ARG:NH1	1.90	0.87
13:O:163:GLY:HA2	13:O:188:LYS:HG3	1.57	0.87
4:D:198:MET:CE	11:L:30:LEU:HD11	2.03	0.87
13:O:155:ASN:HD22	15:U:129:ASN:ND2	1.72	0.87
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.56	0.87
13:O:140:THR:HB	13:O:201:VAL:H	1.40	0.87
1:A:230:THR:HG22	1:A:231:GLU:H	1.39	0.87
13:O:146:PHE:CB	13:O:195:GLY:HA3	2.01	0.86
19:Z:51:VAL:HG12	19:Z:52:LEU:HD23	1.53	0.86
3:C:285:ILE:HA	23:C:487:CLA:HMB2	1.56	0.86
2:B:326:ARG:HD3	28:B:529:BCR:H402	1.56	0.86
11:L:7:ARG:C	11:L:9:PRO:HD3	1.96	0.86
2:B:9:HIS:HB2	23:B:523:CLA:HBA2	1.55	0.86
13:O:155:ASN:ND2	15:U:129:ASN:ND2	2.23	0.86
13:O:140:THR:HG21	13:O:201:VAL:O	1.74	0.86
5:E:60:ARG:HH22	16:V:129:LYS:CE	1.87	0.86
1:A:57:PRO:HG2	13:O:115:ARG:NH1	1.91	0.86
5:E:14:THR:CG2	9:J:8:ILE:CB	2.53	0.86
3:C:269:GLU:OE2	3:C:447:ARG:HG2	1.75	0.86
16:V:75:TYR:HE2	16:V:80:THR:H	1.22	0.86
1:A:214:MET:CE	1:A:214:MET:HA	2.05	0.86
2:B:120:LEU:HD23	2:B:130:GLU:HA	1.58	0.85
7:H:39:VAL:O	7:H:43:ILE:HG13	1.76	0.85
1:A:142:TRP:NE1	3:C:443:TRP:CH2	2.45	0.85
11:L:31:PHE:HB3	11:L:35:PHE:HE1	1.40	0.85
2:B:280:PHE:CE1	2:B:312:TYR:HB3	2.12	0.85
16:V:55:ARG:HH21	16:V:131:GLY:HA3	1.39	0.85
3:C:305:THR:H	3:C:308:GLU:HG3	1.41	0.85
1:A:223:LEU:HD22	1:A:245:THR:HG22	1.57	0.85
23:B:518:CLA:H141	23:B:524:CLA:HMA2	1.59	0.85
1:A:307:ILE:HG13	1:A:314:ILE:HD11	1.58	0.85
4:D:197:HIS:O	4:D:201:VAL:HG23	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:HD2	1:A:133:LEU:CD1	1.90	0.85
13:O:47:PRO:HG3	13:O:76:THR:CG2	2.06	0.85
2:B:122:LEU:HD12	23:B:525:CLA:HMA2	1.57	0.85
12:M:19:SER:O	12:M:23:ILE:HG12	1.77	0.84
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.12	0.84
3:C:282:MET:HA	3:C:285:ILE:HG13	1.57	0.84
3:C:257:PHE:O	3:C:261:ARG:HG3	1.77	0.84
4:D:90:LEU:HD11	4:D:96:GLU:OE1	1.78	0.84
13:O:126:VAL:O	13:O:144:GLY:HA3	1.78	0.84
13:O:43:LEU:CD1	13:O:241:ALA:HB2	2.08	0.84
2:B:318:ASN:HD22	2:B:318:ASN:C	1.79	0.84
2:B:357:ARG:HH22	4:D:337:GLU:HB3	1.41	0.83
2:B:339:ALA:HB3	2:B:430:PHE:HD1	1.43	0.83
2:B:322:GLY:HA2	2:B:325:PHE:CD1	2.13	0.83
1:A:334:ARG:NH1	4:D:320:LEU:HD11	1.93	0.83
5:E:14:THR:CG2	9:J:8:ILE:CG1	2.56	0.83
3:C:294:ASN:N	3:C:294:ASN:ND2	2.21	0.83
1:A:221:SER:HA	4:D:139:ARG:HB2	1.60	0.83
1:A:243:GLU:HA	4:D:240:ALA:HB1	1.58	0.83
23:B:512:CLA:H191	23:B:520:CLA:H151	1.61	0.83
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.43	0.83
3:C:279:LEU:HB3	23:C:481:CLA:HBC1	1.59	0.83
10:K:25:ALA:HB1	28:K:50:BCR:H19C	1.60	0.82
2:B:339:ALA:HB3	2:B:430:PHE:CD1	2.14	0.82
4:D:174:GLY:O	4:D:178:ILE:HG12	1.80	0.82
3:C:55:ALA:HB1	28:C:488:BCR:C37	2.09	0.82
23:A:350:CLA:HED1	4:D:175:VAL:HG13	1.61	0.82
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.14	0.82
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.14	0.82
2:B:212:ALA:HB2	23:B:511:CLA:HMC3	1.62	0.82
5:E:12:ILE:HD12	25:E:84:HEM:CGD	2.09	0.82
4:D:195:PRO:HA	4:D:198:MET:HE2	1.59	0.82
1:A:306:VAL:HG22	1:A:307:ILE:H	1.42	0.82
1:A:330:VAL:CG1	4:D:348:ARG:HG3	2.10	0.82
4:D:195:PRO:HA	4:D:198:MET:CE	2.09	0.82
3:C:203:THR:HG22	3:C:208:VAL:HG11	1.62	0.82
15:U:91:VAL:O	15:U:94:ILE:HG13	1.80	0.82
16:V:80:THR:HG23	16:V:84:GLY:HA2	1.62	0.81
4:D:71:CYS:HB2	4:D:76:VAL:CG2	2.09	0.81
3:C:292:PHE:N	3:C:292:PHE:HD2	1.78	0.81
1:A:156:ALA:HA	1:A:160:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:56:THR:HA	16:V:59:LEU:HD12	1.60	0.81
4:D:102:THR:HG22	4:D:106:GLN:HE21	1.43	0.81
1:A:301:ASN:HD21	3:C:407:VAL:CG2	1.93	0.81
2:B:413:ASP:HB3	2:B:415:PRO:HD2	1.60	0.81
13:O:95:PHE:CB	13:O:127:ALA:HB3	2.10	0.81
13:O:81:ILE:CG2	13:O:82:GLN:H	1.94	0.81
13:O:39:ARG:CB	13:O:245:PRO:HG3	2.10	0.81
1:A:326:LEU:HD13	3:C:412:THR:HG21	1.60	0.81
1:A:92:HIS:HD2	3:C:219:GLY:HA3	1.44	0.81
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.62	0.81
13:O:40:ILE:HG22	13:O:41:ALA:H	1.46	0.81
13:O:40:ILE:HG12	13:O:84:GLU:CD	2.02	0.81
3:C:295:THR:O	3:C:298:PRO:HD3	1.79	0.80
2:B:222:PRO:HB3	7:H:25:GLY:CA	2.11	0.80
2:B:248:ALA:HA	23:B:517:CLA:H42	1.62	0.80
9:J:40:LEU:HD23	16:V:30:LYS:HE2	1.61	0.80
2:B:170:ASP:OD1	2:B:175:THR:HG22	1.81	0.80
3:C:199:ILE:HD12	3:C:234:VAL:HG21	1.62	0.80
3:C:120:ILE:O	3:C:124:VAL:HG23	1.82	0.80
3:C:212:TYR:O	3:C:223:TRP:HB2	1.81	0.80
2:B:63:LEU:HB3	2:B:64:PRO:HD3	1.62	0.80
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.17	0.80
2:B:302:TRP:O	2:B:341:LYS:HE3	1.81	0.80
3:C:126:GLY:O	3:C:130:VAL:HG23	1.80	0.80
2:B:75:TRP:N	2:B:94:GLU:HG3	1.93	0.80
2:B:136:PRO:HD3	2:B:231:MET:HE1	1.64	0.80
3:C:308:GLU:HG2	3:C:361:PHE:HE1	1.42	0.80
19:Z:8:ALA:O	19:Z:11:ALA:HB3	1.82	0.80
4:D:138:VAL:HG12	4:D:139:ARG:N	1.97	0.80
2:B:478:VAL:HG11	4:D:139:ARG:HA	1.64	0.80
4:D:190:ASN:HB2	4:D:296:TYR:HD1	1.44	0.80
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.64	0.80
1:A:29:TYR:HD1	1:A:29:TYR:C	1.85	0.79
3:C:405:ASN:HB2	3:C:407:VAL:HG23	1.62	0.79
1:A:246:TYR:CE1	1:A:248:ILE:HG12	2.17	0.79
13:O:122:VAL:HA	13:O:146:PHE:HE2	1.47	0.79
16:V:4:THR:HG22	16:V:5:PRO:CD	2.12	0.79
11:L:12:LEU:HD11	11:L:16:SER:HB3	1.64	0.79
4:D:336:HIS:H	4:D:336:HIS:HD2	1.28	0.79
1:A:210:LEU:HD12	1:A:210:LEU:O	1.82	0.79
3:C:334:PRO:HA	13:O:153:THR:HB	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:56:ALA:HB2	5:E:82:LEU:HD23	1.62	0.79
23:B:512:CLA:H193	23:B:523:CLA:H102	1.62	0.79
3:C:292:PHE:CD2	3:C:292:PHE:N	2.50	0.79
15:U:132:LEU:N	15:U:132:LEU:HD23	1.96	0.79
5:E:14:THR:CG2	9:J:8:ILE:CD1	2.54	0.79
3:C:285:ILE:HA	23:C:487:CLA:CMB	2.11	0.79
16:V:79:PRO:HB2	16:V:88:ILE:CG1	2.13	0.79
3:C:264:PHE:HD2	3:C:264:PHE:N	1.81	0.79
1:A:14:TRP:CZ3	1:A:18:CYS:SG	2.76	0.79
1:A:239:PHE:HZ	4:D:223:PHE:CZ	2.01	0.79
13:O:95:PHE:HB3	13:O:127:ALA:HB3	1.65	0.79
1:A:296:ASN:CG	3:C:401:LEU:HD23	2.04	0.78
3:C:273:SER:HB3	3:C:445:ALA:HB2	1.66	0.78
13:O:140:THR:HB	13:O:201:VAL:HG23	1.64	0.78
2:B:264:PRO:HG3	2:B:267:LEU:HD12	1.64	0.78
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.18	0.78
13:O:75:THR:HG22	13:O:103:PHE:HD2	1.47	0.78
10:K:16:LEU:HB3	10:K:17:PRO:CD	2.13	0.78
8:I:27:ASP:HB2	8:I:28:PRO:CD	2.13	0.78
23:A:350:CLA:H121	26:A:353:PL9:H162	1.66	0.78
2:B:221:PRO:HG3	2:B:225:LEU:HD12	1.64	0.78
1:A:239:PHE:CE1	4:D:245:SER:HA	2.19	0.78
1:A:253:GLY:O	1:A:257:ARG:HG2	1.83	0.78
4:D:236:ASN:OD1	4:D:239:GLN:HB2	1.83	0.78
3:C:86:LEU:HD13	3:C:89:ILE:HD12	1.64	0.78
1:A:301:ASN:ND2	3:C:407:VAL:HG21	1.99	0.78
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.18	0.77
5:E:22:HIS:HA	5:E:25:THR:HB	1.64	0.77
3:C:347:GLY:HA3	13:O:17:ASN:OD1	1.85	0.77
4:D:298:PHE:CA	11:L:37:ASN:HD21	1.87	0.77
2:B:145:LEU:HD13	23:B:522:CLA:HMB1	1.65	0.77
4:D:176:ALA:HA	4:D:179:PHE:HD1	1.48	0.77
6:F:36:ILE:HA	6:F:39:MET:HG3	1.67	0.77
10:K:2:LEU:N	10:K:3:PRO:HD3	1.98	0.77
23:B:522:CLA:H171	23:B:525:CLA:CMD	2.14	0.77
5:E:12:ILE:HG22	5:E:18:TYR:CG	2.20	0.77
3:C:320:ARG:HH12	16:V:50:PRO:HD2	1.46	0.77
2:B:327:THR:HG22	2:B:329:PRO:HD3	1.67	0.77
2:B:478:VAL:CG1	4:D:139:ARG:HA	2.15	0.77
16:V:37:CYS:HG	25:V:138:HEM:HAB	1.37	0.77
16:V:79:PRO:HB2	16:V:88:ILE:HG12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD11	1:A:336:ALA:HB2	1.67	0.77
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.67	0.77
3:C:320:ARG:NH1	16:V:50:PRO:HD2	1.99	0.77
2:B:326:ARG:CD	2:B:327:THR:N	2.41	0.76
26:D:357:PL9:H38	14:T:18:PHE:HB2	1.66	0.76
1:A:306:VAL:HG22	1:A:307:ILE:N	1.99	0.76
2:B:326:ARG:NH1	2:B:327:THR:OG1	2.17	0.76
2:B:113:TRP:HB3	23:B:525:CLA:HED1	1.67	0.76
8:I:7:THR:O	8:I:11:VAL:HG23	1.85	0.76
2:B:142:HIS:CE1	23:B:524:CLA:H142	2.21	0.76
1:A:295:PHE:HB3	3:C:291:TRP:CZ3	2.20	0.76
1:A:301:ASN:HD21	3:C:407:VAL:HG21	1.48	0.76
4:D:323:GLU:HG2	13:O:168:TYR:OH	1.86	0.76
1:A:142:TRP:HE1	3:C:443:TRP:HH2	1.33	0.76
3:C:175:LEU:HD11	23:C:479:CLA:HED3	1.67	0.76
1:A:29:TYR:HD1	1:A:30:VAL:N	1.83	0.76
5:E:12:ILE:CD1	25:E:84:HEM:O1A	2.34	0.76
9:J:15:THR:HA	28:K:50:BCR:H372	1.67	0.76
1:A:87:ASN:HD21	3:C:357:ARG:HH11	1.32	0.76
2:B:326:ARG:HH11	2:B:327:THR:HB	1.48	0.75
23:B:522:CLA:H171	23:B:525:CLA:HMD3	1.68	0.75
1:A:148:SER:HB2	1:A:284:TRP:HH2	1.50	0.75
1:A:141:PRO:HG2	3:C:443:TRP:HZ3	1.52	0.75
2:B:118:TRP:CZ2	11:L:3:PRO:HB3	2.21	0.75
1:A:172:MET:HE2	23:A:349:CLA:HMC3	1.69	0.75
23:C:479:CLA:H92	23:C:479:CLA:HAB	1.69	0.75
4:D:31:GLY:HA3	4:D:131:GLU:OE1	1.86	0.75
2:B:305:ILE:O	2:B:305:ILE:HG13	1.86	0.75
3:C:264:PHE:CD2	3:C:264:PHE:N	2.54	0.75
1:A:57:PRO:HB3	1:A:68:SER:HB3	1.68	0.75
2:B:25:MET:HB3	28:B:529:BCR:H332	1.69	0.75
13:O:7:TYR:O	13:O:11:VAL:HG23	1.86	0.75
1:A:56:PRO:HA	1:A:73:TYR:CE1	2.22	0.75
1:A:159:LEU:HD21	23:C:487:CLA:HBD	1.69	0.75
4:D:336:HIS:CD2	4:D:336:HIS:N	2.52	0.75
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.68	0.74
3:C:98:GLY:O	3:C:99:VAL:HG23	1.86	0.74
2:B:187:PRO:O	2:B:190:PHE:N	2.20	0.74
3:C:89:ILE:HB	3:C:90:PRO:HD3	1.69	0.74
4:D:88:SER:CB	5:E:68:ARG:HH21	1.98	0.74
3:C:285:ILE:HG21	23:C:479:CLA:H51	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:GLY:HA2	13:O:7:TYR:CE1	2.22	0.74
11:L:4:ASN:N	11:L:5:PRO:HD3	2.03	0.74
4:D:19:ASP:OD1	4:D:23:LYS:HD2	1.87	0.74
3:C:293:ASN:C	3:C:294:ASN:HD22	1.89	0.74
2:B:172:TYR:CE2	2:B:283:GLU:HB2	2.23	0.74
3:C:308:GLU:HG2	3:C:361:PHE:CZ	2.22	0.74
3:C:363:GLY:O	3:C:367:GLU:HG2	1.87	0.74
2:B:112:CYS:O	2:B:116:VAL:HG23	1.87	0.74
4:D:68:LEU:CA	6:F:39:MET:HE1	2.18	0.74
5:E:9:PHE:O	5:E:10:SER:HB3	1.85	0.74
1:A:29:TYR:CD1	1:A:29:TYR:C	2.59	0.74
4:D:235:PHE:HA	4:D:239:GLN:OE1	1.86	0.74
5:E:43:TYR:CD2	5:E:50:ARG:HG2	2.22	0.74
3:C:229:ASN:HB3	3:C:232:ASP:OD1	1.88	0.74
3:C:350:ILE:HG12	3:C:359:TRP:HB2	1.70	0.74
2:B:63:LEU:HD11	2:B:93:PHE:CE1	2.22	0.74
4:D:71:CYS:HB3	4:D:75:THR:HB	1.68	0.74
4:D:51:GLY:HA2	4:D:55:VAL:HG23	1.69	0.74
5:E:19:TRP:HZ2	9:J:13:VAL:HG22	1.50	0.74
3:C:320:ARG:NE	15:U:128:TYR:HE2	1.79	0.74
4:D:152:VAL:O	4:D:156:VAL:HG23	1.88	0.74
1:A:78:ILE:HD11	11:L:34:TYR:CE1	2.23	0.74
3:C:227:VAL:HG23	3:C:294:ASN:HB3	1.68	0.74
3:C:61:VAL:HG22	23:C:480:CLA:HAC2	1.70	0.74
3:C:41:ARG:HB2	23:C:486:CLA:HED3	1.69	0.74
10:K:19:ILE:HA	10:K:22:LEU:HD12	1.70	0.74
3:C:101:PRO:N	3:C:195:ASP:HB3	2.03	0.73
13:O:43:LEU:HD13	13:O:241:ALA:HB2	1.69	0.73
10:K:2:LEU:H	10:K:3:PRO:HD3	1.51	0.73
2:B:27:THR:O	23:B:518:CLA:HBC1	1.88	0.73
3:C:138:GLU:CG	3:C:139:THR:H	1.96	0.73
4:D:267:LEU:O	4:D:271:MET:HG3	1.87	0.73
4:D:56:THR:HB	5:E:48:THR:HG23	1.71	0.73
1:A:317:TRP:HA	4:D:63:LEU:CD1	2.19	0.73
2:B:357:ARG:NH2	4:D:337:GLU:HB3	2.04	0.73
2:B:368:VAL:HA	2:B:425:ILE:HD11	1.69	0.73
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.69	0.73
14:T:18:PHE:HD2	14:T:19:PHE:CD1	2.07	0.73
3:C:248:GLY:O	3:C:252:ILE:HG13	1.89	0.73
3:C:123:ALA:HB1	19:Z:47:TRP:HH2	1.53	0.73
13:O:50:PHE:HZ	13:O:76:THR:HG23	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HH12	13:O:159:PRO:HA	1.53	0.72
1:A:76:ASN:HB3	14:T:2:GLU:OE2	1.90	0.72
4:D:238:THR:O	4:D:240:ALA:N	2.20	0.72
2:B:246:PHE:HE1	2:B:463:PHE:HB2	1.53	0.72
1:A:69:GLY:HA2	1:A:75:ASN:OD1	1.90	0.72
2:B:66:MET:O	2:B:71:VAL:HG23	1.89	0.72
19:Z:41:PHE:HD1	19:Z:41:PHE:H	1.35	0.72
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.71	0.72
1:A:182:PHE:O	1:A:186:PHE:HB2	1.88	0.72
3:C:271:TYR:HA	3:C:274:TYR:HD1	1.50	0.72
2:B:172:TYR:CZ	2:B:283:GLU:HB2	2.25	0.72
2:B:400:SER:OG	2:B:410:THR:HG23	1.88	0.72
4:D:194:ASN:O	4:D:198:MET:HG3	1.88	0.72
2:B:340:TRP:CZ3	2:B:342:GLY:HA3	2.24	0.72
4:D:235:PHE:CD1	4:D:236:ASN:N	2.57	0.72
13:O:162:ARG:O	13:O:162:ARG:HG2	1.90	0.72
3:C:42:LEU:CG	23:C:486:CLA:HED1	2.18	0.72
15:U:132:LEU:H	15:U:132:LEU:CD2	1.96	0.72
4:D:319:LEU:HA	4:D:322:ASN:ND2	2.04	0.72
3:C:42:LEU:HD13	23:C:486:CLA:HMA3	1.70	0.72
15:U:83:ALA:HA	15:U:85:TYR:CE2	2.25	0.72
8:I:15:PHE:HA	8:I:18:LEU:HG	1.72	0.72
13:O:201:VAL:HG13	13:O:211:ILE:HG23	1.71	0.72
5:E:14:THR:HG21	9:J:8:ILE:HG13	1.71	0.72
23:C:477:CLA:CMD	23:C:485:CLA:HAB	2.19	0.72
13:O:223:ASP:HB3	13:O:230:PRO:HG3	1.71	0.72
23:B:518:CLA:C14	23:B:524:CLA:HMA2	2.20	0.71
2:B:68:ARG:HH12	23:B:516:CLA:HED1	1.54	0.71
12:M:18:PRO:O	12:M:22:LEU:HG	1.89	0.71
3:C:343:ARG:HA	3:C:348:GLU:O	1.90	0.71
23:B:520:CLA:HBC3	23:B:523:CLA:H41	1.72	0.71
3:C:99:VAL:HG22	3:C:104:GLU:O	1.90	0.71
1:A:29:TYR:CD2	1:A:133:LEU:CD1	2.72	0.71
1:A:326:LEU:CD1	3:C:412:THR:HG21	2.20	0.71
2:B:248:ALA:O	2:B:252:VAL:HG23	1.89	0.71
13:O:40:ILE:HG22	13:O:41:ALA:N	2.04	0.71
1:A:239:PHE:CZ	4:D:223:PHE:HZ	2.08	0.71
3:C:437:PHE:HA	23:C:483:CLA:CMC	2.19	0.71
1:A:63:ILE:HD11	1:A:336:ALA:CB	2.20	0.71
2:B:17:GLY:O	2:B:20:ILE:HG22	1.89	0.71
3:C:385:GLN:OE1	3:C:386:PRO:HD2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:HB3	2:B:78:TRP:HD1	1.51	0.71
3:C:43:ILE:HG13	3:C:44:ASN:N	2.06	0.71
1:A:330:VAL:HG11	4:D:348:ARG:HG3	1.72	0.71
2:B:397:VAL:HG12	2:B:398:THR:N	2.05	0.71
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.72	0.71
4:D:244:TYR:OH	4:D:264:LYS:NZ	2.21	0.71
2:B:318:ASN:C	2:B:318:ASN:ND2	2.44	0.71
1:A:309:ALA:O	16:V:3:LEU:N	2.24	0.71
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.71	0.71
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.54	0.71
1:A:243:GLU:CA	4:D:240:ALA:HB1	2.21	0.71
1:A:29:TYR:HE1	1:A:31:GLY:CA	2.03	0.71
4:D:190:ASN:CB	4:D:296:TYR:HD1	2.04	0.71
4:D:262:SER:O	4:D:263:ASN:ND2	2.24	0.71
3:C:345:PRO:O	13:O:74:GLU:HB2	1.90	0.71
1:A:159:LEU:HG	1:A:163:ILE:HD11	1.73	0.71
2:B:339:ALA:HB2	2:B:431:GLU:H	1.56	0.71
15:U:73:PRO:HB2	16:V:83:ASP:OD2	1.91	0.71
2:B:57:ARG:NH1	2:B:317:ASN:OD1	2.23	0.71
2:B:321:LYS:CE	2:B:325:PHE:HZ	2.04	0.71
2:B:348:ASN:OD1	2:B:349:LYS:N	2.17	0.71
1:A:89:ILE:HG21	1:A:94:TYR:HB2	1.73	0.70
13:O:71:VAL:HG21	13:O:108:VAL:HG23	1.71	0.70
13:O:17:ASN:O	13:O:46:GLN:HG3	1.91	0.70
1:A:214:MET:HE2	1:A:214:MET:HA	1.71	0.70
4:D:221:THR:O	4:D:221:THR:HG22	1.90	0.70
1:A:307:ILE:O	1:A:309:ALA:N	2.23	0.70
3:C:350:ILE:HG21	3:C:359:TRP:HB3	1.73	0.70
1:A:214:MET:HE1	4:D:142:ASN:OD1	1.91	0.70
13:O:164:LEU:O	13:O:165:ALA:HB3	1.89	0.70
3:C:343:ARG:CD	3:C:343:ARG:C	2.59	0.70
4:D:16:ASP:O	4:D:19:ASP:HB3	1.90	0.70
13:O:211:ILE:HB	13:O:241:ALA:HB3	1.73	0.70
1:A:159:LEU:HD11	23:C:487:CLA:OBD	1.92	0.70
10:K:15:VAL:HG11	18:N:13:UNK:CB	2.21	0.70
5:E:52:ASP:O	16:V:1:ALA:HB3	1.90	0.70
13:O:155:ASN:ND2	15:U:129:ASN:HD22	1.88	0.70
3:C:450:ALA:HA	3:C:454:GLY:HA3	1.73	0.70
1:A:142:TRP:NE1	3:C:443:TRP:HH2	1.89	0.70
6:F:31:PHE:O	6:F:31:PHE:HD2	1.74	0.70
3:C:42:LEU:CD1	23:C:486:CLA:HMA3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:ND2	1:A:79:THR:HG21	2.05	0.70
12:M:15:VAL:HG12	12:M:16:LEU:HD23	1.73	0.70
7:H:59:VAL:O	7:H:59:VAL:HG12	1.91	0.70
4:D:68:LEU:HA	6:F:39:MET:CE	2.19	0.70
2:B:414:PRO:HG2	2:B:415:PRO:HD3	1.72	0.70
1:A:317:TRP:CA	4:D:63:LEU:HD13	2.22	0.70
4:D:90:LEU:CD1	4:D:96:GLU:HB3	2.21	0.70
4:D:118:GLY:HA3	24:D:355:PHO:H71	1.72	0.69
3:C:121:SER:O	3:C:125:LEU:HG	1.91	0.69
4:D:18:LEU:O	4:D:22:LEU:HB3	1.92	0.69
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.22	0.69
16:V:37:CYS:O	16:V:39:SER:N	2.26	0.69
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.74	0.69
3:C:123:ALA:CB	19:Z:47:TRP:HH2	2.04	0.69
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.26	0.69
2:B:397:VAL:HG12	2:B:398:THR:H	1.56	0.69
16:V:75:TYR:CD2	16:V:79:PRO:HA	2.26	0.69
2:B:41:GLU:OE1	2:B:63:LEU:HB2	1.91	0.69
3:C:305:THR:HA	3:C:423:ARG:HH11	1.56	0.69
13:O:118:LEU:CD1	13:O:233:VAL:HG11	2.23	0.69
2:B:324:LEU:CD1	11:L:34:TYR:HB3	2.22	0.69
10:K:30:TRP:CE3	10:K:31:GLN:NE2	2.60	0.69
1:A:235:TYR:HA	4:D:265:ARG:NH2	2.06	0.69
4:D:186:GLN:HB2	23:D:354:CLA:HBC1	1.73	0.69
4:D:87:HIS:NE2	4:D:166:SER:HA	2.08	0.69
4:D:90:LEU:HD11	4:D:96:GLU:CD	2.13	0.69
16:V:133:GLY:O	16:V:137:TYR:CB	2.41	0.69
1:A:320:ILE:HG22	1:A:320:ILE:O	1.93	0.69
1:A:219:VAL:HG11	4:D:268:HIS:CG	2.28	0.69
13:O:28:GLY:HA3	13:O:137:THR:HG22	1.73	0.69
1:A:161:TYR:HB3	1:A:162:PRO:CD	2.21	0.69
3:C:343:ARG:HD2	3:C:343:ARG:O	1.92	0.69
2:B:30:VAL:HG12	23:B:518:CLA:HHD	1.73	0.69
1:A:281:VAL:HG12	1:A:281:VAL:O	1.91	0.69
3:C:176:VAL:O	3:C:180:MET:HG2	1.93	0.69
13:O:75:THR:HG22	13:O:103:PHE:CD2	2.28	0.69
13:O:47:PRO:CG	13:O:76:THR:HG21	2.20	0.69
3:C:319:ILE:HD13	3:C:389:GLU:HG2	1.74	0.69
13:O:211:ILE:HG22	13:O:212:ALA:N	2.08	0.69
23:B:519:CLA:HMD1	23:B:524:CLA:HAB	1.75	0.69
2:B:57:ARG:HH11	2:B:57:ARG:CG	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:PHE:HB2	2:B:448:ARG:HE	1.56	0.69
13:O:140:THR:CB	13:O:201:VAL:H	2.06	0.68
15:U:62:ILE:HG23	15:U:76:ALA:HB1	1.74	0.68
3:C:158:THR:HG23	3:C:251:HIS:HB3	1.74	0.68
2:B:57:ARG:HH11	2:B:57:ARG:HG3	1.56	0.68
4:D:138:VAL:HG12	4:D:139:ARG:H	1.55	0.68
1:A:29:TYR:HD2	1:A:133:LEU:HD13	1.59	0.68
1:A:76:ASN:HD21	4:D:298:PHE:HE2	1.39	0.68
3:C:203:THR:CG2	3:C:208:VAL:HG11	2.23	0.68
1:A:301:ASN:OD1	3:C:407:VAL:HG21	1.94	0.68
13:O:22:LEU:O	13:O:203:LYS:HD3	1.94	0.68
3:C:116:VAL:HG21	28:C:489:BCR:H323	1.75	0.68
4:D:53:THR:HA	4:D:67:TYR:CD1	2.29	0.68
1:A:81:ALA:HB3	1:A:174:LEU:O	1.93	0.68
2:B:145:LEU:HD13	23:B:522:CLA:CMB	2.23	0.68
3:C:443:TRP:CE3	3:C:443:TRP:HA	2.28	0.68
4:D:261:PHE:HA	14:T:24:ARG:HH22	1.59	0.68
13:O:163:GLY:HA3	13:O:188:LYS:HE2	1.76	0.68
2:B:105:GLY:HA2	28:B:528:BCR:H383	1.75	0.68
26:D:357:PL9:H261	14:T:21:ILE:HD11	1.74	0.68
3:C:156:LYS:O	3:C:160:ILE:HG13	1.93	0.68
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.29	0.68
23:C:475:CLA:HBD	28:J:53:BCR:HC21	1.76	0.68
2:B:86:ILE:O	2:B:88:PRO:HD3	1.93	0.68
2:B:124:ARG:HG2	2:B:125:ASP:N	2.07	0.68
4:D:80:THR:HG21	4:D:167:TRP:O	1.94	0.68
2:B:6:TYR:HH	12:M:21:PHE:HZ	0.74	0.68
3:C:275:SER:HB3	23:C:485:CLA:HAA1	1.76	0.68
1:A:61:ASP:HA	1:A:87:ASN:HB2	1.75	0.68
9:J:9:PRO:O	9:J:10:LEU:HD23	1.94	0.68
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.74	0.68
2:B:383:PHE:O	13:O:166:SER:HA	1.93	0.68
10:K:34:VAL:HG12	10:K:34:VAL:O	1.93	0.68
28:C:488:BCR:H341	28:K:50:BCR:HC31	1.76	0.67
7:H:57:VAL:O	7:H:57:VAL:CG1	2.41	0.67
5:E:33:GLY:HA2	6:F:31:PHE:CE2	2.29	0.67
7:H:53:ILE:HG23	17:X:13:THR:OG1	1.94	0.67
2:B:113:TRP:O	2:B:117:TYR:HB2	1.94	0.67
3:C:308:GLU:OE2	3:C:361:PHE:CZ	2.43	0.67
3:C:149:TYR:CD2	3:C:156:LYS:HG3	2.29	0.67
4:D:86:GLY:C	4:D:87:HIS:HD2	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:THR:HG21	10:K:2:LEU:HG	1.76	0.67
2:B:86:ILE:HG22	2:B:86:ILE:O	1.94	0.67
2:B:326:ARG:NH1	2:B:327:THR:CB	2.56	0.67
24:A:351:PHO:NC	4:D:209:LEU:HD12	2.09	0.67
3:C:305:THR:CA	3:C:423:ARG:NH1	2.57	0.67
19:Z:48:ILE:O	19:Z:52:LEU:HG	1.95	0.67
16:V:76:MET:HE3	16:V:115:ILE:HG21	1.76	0.67
3:C:141:GLU:HB3	3:C:144:SER:OG	1.93	0.67
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.76	0.67
1:A:206:PHE:HE1	23:A:348:CLA:HMB1	1.57	0.67
3:C:282:MET:HA	3:C:285:ILE:CG1	2.24	0.67
2:B:266:GLU:HG2	2:B:266:GLU:O	1.93	0.67
3:C:141:GLU:HB2	3:C:144:SER:HB2	1.75	0.67
4:D:108:GLY:O	4:D:110:LEU:N	2.27	0.67
1:A:75:ASN:ND2	1:A:79:THR:CG2	2.57	0.67
2:B:135:LEU:HB2	2:B:231:MET:HE3	1.77	0.67
13:O:104:GLN:N	13:O:104:GLN:CD	2.46	0.67
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.09	0.67
13:O:168:TYR:CE1	13:O:172:ILE:HD11	2.29	0.67
13:O:125:LEU:HD12	13:O:145:GLU:O	1.93	0.67
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.24	0.67
5:E:26:ILE:CG1	5:E:27:PRO:HD3	2.25	0.67
2:B:162:PHE:HB3	23:B:515:CLA:HMD3	1.75	0.67
13:O:243:ILE:O	13:O:244:GLU:HB2	1.95	0.67
2:B:324:LEU:HD12	11:L:34:TYR:HB3	1.77	0.67
3:C:291:TRP:HB3	3:C:292:PHE:CD2	2.29	0.67
2:B:414:PRO:CD	2:B:415:PRO:HD3	2.24	0.67
3:C:419:PHE:O	3:C:420:VAL:HG23	1.95	0.67
25:E:84:HEM:HAC	6:F:26:ALA:HB1	1.75	0.67
6:F:40:GLN:HE21	9:J:27:LEU:HG	1.55	0.67
1:A:141:PRO:HG3	3:C:446:GLY:O	1.94	0.67
13:O:164:LEU:H	13:O:188:LYS:HE2	1.60	0.66
4:D:29:PHE:CD2	4:D:29:PHE:C	2.67	0.66
3:C:131:TYR:HE1	3:C:135:ARG:HD3	1.60	0.66
1:A:180:PHE:CE2	4:D:192:THR:HG22	2.31	0.66
1:A:290:ILE:HD11	23:A:348:CLA:CGD	2.25	0.66
14:T:3:THR:O	14:T:5:THR:N	2.28	0.66
23:A:348:CLA:H192	26:D:357:PL9:H252	1.77	0.66
2:B:380:ASP:OD1	2:B:390:TYR:HB2	1.95	0.66
13:O:140:THR:CG2	13:O:201:VAL:HB	2.24	0.66
1:A:255:PHE:HD2	1:A:264:SER:HA	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ALA:HA	23:C:483:CLA:O1A	1.95	0.66
13:O:164:LEU:CD2	15:U:42:VAL:HG13	2.25	0.66
1:A:222:SER:O	1:A:246:TYR:HB2	1.96	0.66
13:O:102:ASP:OD2	13:O:119:LEU:HD11	1.96	0.66
2:B:58:GLN:O	2:B:329:PRO:CB	2.43	0.66
3:C:450:ALA:HB1	3:C:455:PHE:O	1.96	0.66
16:V:78:ASN:HB2	16:V:96:ARG:HH11	1.60	0.66
15:U:39:LEU:O	15:U:41:ASN:N	2.28	0.66
5:E:12:ILE:HD13	25:E:84:HEM:O1A	1.95	0.66
2:B:58:GLN:O	2:B:329:PRO:HB2	1.94	0.66
3:C:269:GLU:CD	3:C:447:ARG:HG2	2.16	0.66
2:B:6:TYR:OH	23:B:520:CLA:HMD3	1.96	0.66
15:U:88:VAL:HG22	15:U:114:VAL:HG23	1.78	0.66
3:C:443:TRP:HE3	3:C:443:TRP:HA	1.61	0.66
19:Z:7:LEU:O	19:Z:11:ALA:HB2	1.95	0.66
5:E:19:TRP:CZ2	9:J:13:VAL:HG22	2.30	0.66
13:O:118:LEU:HD13	13:O:233:VAL:HG11	1.78	0.66
4:D:189:HIS:ND1	4:D:294:ARG:NE	2.43	0.66
3:C:208:VAL:HG13	3:C:209:ILE:N	2.10	0.65
2:B:92:SER:O	2:B:96:VAL:HG23	1.96	0.65
3:C:380:ILE:HG22	3:C:381:LYS:N	2.10	0.65
8:I:18:LEU:N	8:I:18:LEU:HD23	2.10	0.65
1:A:119:PHE:O	1:A:123:ALA:HB2	1.96	0.65
4:D:14:TRP:HA	4:D:17:ILE:HD12	1.78	0.65
13:O:224:ASP:C	13:O:225:MET:HG2	2.16	0.65
1:A:29:TYR:CE1	1:A:31:GLY:N	2.63	0.65
1:A:219:VAL:HG11	4:D:268:HIS:CD2	2.30	0.65
3:C:320:ARG:HH12	16:V:50:PRO:CD	2.10	0.65
13:O:158:ASP:HB2	13:O:159:PRO:HD2	1.78	0.65
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.27	0.65
3:C:108:THR:HG23	10:K:2:LEU:HD23	1.79	0.65
1:A:200:LEU:HD13	1:A:285:PHE:CD1	2.31	0.65
2:B:84:THR:O	2:B:84:THR:HG22	1.95	0.65
4:D:210:LEU:HD13	4:D:271:MET:HG2	1.79	0.65
7:H:27:THR:N	7:H:28:PRO:HD2	2.10	0.65
13:O:27:ARG:HG3	13:O:29:ALA:HB3	1.77	0.65
15:U:72:TYR:HD2	15:U:73:PRO:N	1.93	0.65
3:C:249:ILE:HA	3:C:252:ILE:HD12	1.78	0.65
1:A:29:TYR:HE1	1:A:31:GLY:N	1.95	0.65
13:O:128:SER:O	13:O:142:PHE:HA	1.96	0.65
3:C:285:ILE:HG23	23:C:487:CLA:HMB1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:PRO:CG	2:B:415:PRO:HD3	2.26	0.65
8:I:17:LEU:O	8:I:21:PHE:HB2	1.96	0.65
4:D:28:VAL:HB	6:F:17:VAL:HG13	1.79	0.65
2:B:280:PHE:CZ	2:B:312:TYR:HB3	2.32	0.65
3:C:61:VAL:HG22	23:C:480:CLA:CAC	2.25	0.65
10:K:25:ALA:HB1	28:K:50:BCR:C19	2.27	0.65
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.79	0.65
1:A:221:SER:HB3	4:D:138:VAL:HG12	1.78	0.65
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.11	0.65
13:O:152:ARG:NH1	13:O:156:PHE:CZ	2.65	0.65
1:A:97:TRP:HZ3	8:I:8:VAL:HG21	1.62	0.65
2:B:238:LEU:O	2:B:242:ILE:HG13	1.97	0.64
23:B:520:CLA:H161	12:M:17:VAL:HG11	1.79	0.64
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.78	0.64
7:H:49:ASN:OD1	7:H:49:ASN:O	2.15	0.64
3:C:293:ASN:OD1	3:C:297:TYR:O	2.15	0.64
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.78	0.64
1:A:183:MET:HE2	23:A:349:CLA:HMD3	1.79	0.64
2:B:154:GLY:HA2	2:B:158:LEU:HD12	1.79	0.64
4:D:52:THR:HG22	4:D:67:TYR:CE1	2.26	0.64
9:J:15:THR:HA	28:K:50:BCR:C37	2.27	0.64
15:U:132:LEU:N	15:U:132:LEU:CD2	2.57	0.64
6:F:40:GLN:NE2	9:J:27:LEU:CG	2.46	0.64
23:B:513:CLA:H91	23:B:516:CLA:HAA1	1.77	0.64
23:B:520:CLA:H161	12:M:17:VAL:CG1	2.27	0.64
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.29	0.64
1:A:285:PHE:O	1:A:288:LEU:HB2	1.97	0.64
13:O:20:PRO:HB2	13:O:240:TYR:CE1	2.33	0.64
10:K:9:PHE:O	10:K:13:VAL:HG23	1.96	0.64
1:A:221:SER:HB3	4:D:138:VAL:CG1	2.27	0.64
11:L:2:GLU:N	11:L:3:PRO:CD	2.61	0.64
13:O:66:VAL:HG13	13:O:67:PRO:HD2	1.80	0.64
6:F:25:LEU:O	6:F:28:PRO:HD2	1.98	0.64
4:D:57:SER:OG	4:D:65:SER:HB2	1.98	0.64
3:C:42:LEU:HG	23:C:486:CLA:CED	2.24	0.64
2:B:478:VAL:HG12	4:D:139:ARG:HG2	1.80	0.64
3:C:319:ILE:CD1	3:C:389:GLU:HG2	2.28	0.64
5:E:59:GLN:HE21	5:E:81:GLN:NE2	1.96	0.64
2:B:138:MET:CG	23:B:522:CLA:HBC2	2.20	0.64
2:B:130:GLU:HG2	2:B:131:PRO:CD	2.26	0.64
2:B:271:THR:OG1	2:B:274:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:39:LEU:C	15:U:41:ASN:H	2.01	0.64
1:A:310:LYS:HB3	1:A:312:ASN:ND2	2.13	0.64
10:K:2:LEU:N	10:K:3:PRO:CD	2.60	0.64
3:C:162:GLY:O	3:C:165:LEU:HB2	1.95	0.64
2:B:73:GLY:O	2:B:92:SER:HB2	1.98	0.64
1:A:159:LEU:HG	1:A:163:ILE:CD1	2.28	0.63
8:I:27:ASP:HB2	8:I:28:PRO:HD3	1.80	0.63
3:C:348:GLU:OE1	3:C:348:GLU:N	2.31	0.63
1:A:281:VAL:HA	1:A:284:TRP:CD1	2.33	0.63
3:C:305:THR:CA	3:C:423:ARG:HH12	2.11	0.63
4:D:263:ASN:O	4:D:265:ARG:N	2.31	0.63
13:O:238:VAL:HG12	13:O:239:PHE:N	2.12	0.63
2:B:221:PRO:HB3	2:B:225:LEU:HB2	1.78	0.63
13:O:39:ARG:CA	13:O:245:PRO:HG3	2.28	0.63
13:O:155:ASN:HD22	15:U:129:ASN:HD21	1.42	0.63
3:C:426:LEU:O	3:C:430:HIS:HB2	1.98	0.63
2:B:221:PRO:CG	2:B:225:LEU:HD12	2.29	0.63
2:B:326:ARG:NH1	2:B:327:THR:HB	2.13	0.63
3:C:78:GLU:H	3:C:104:GLU:CD	2.01	0.63
1:A:29:TYR:HD2	1:A:133:LEU:HD12	1.63	0.63
4:D:39:PRO:O	4:D:43:LEU:HG	1.99	0.63
1:A:206:PHE:HE1	23:A:348:CLA:CMB	2.11	0.63
3:C:160:ILE:O	3:C:163:PHE:HB2	1.98	0.63
1:A:63:ILE:HG23	3:C:335:THR:CG2	2.28	0.63
8:I:19:PHE:CZ	8:I:23:PHE:HE1	2.16	0.63
19:Z:46:LEU:O	19:Z:50:LEU:HG	1.99	0.63
3:C:321:ASP:OD1	3:C:321:ASP:N	2.31	0.63
16:V:75:TYR:HE2	16:V:80:THR:N	1.95	0.63
4:D:52:THR:HG23	4:D:76:VAL:HG12	1.81	0.63
4:D:222:LEU:HA	4:D:243:THR:O	1.98	0.63
4:D:253:TRP:HA	4:D:253:TRP:CE3	2.33	0.63
8:I:25:SER:HB2	8:I:28:PRO:HD2	1.80	0.63
2:B:327:THR:OG1	28:B:529:BCR:H401	1.99	0.63
15:U:113:THR:HG22	15:U:114:VAL:N	2.13	0.63
1:A:59:ASP:OD2	1:A:63:ILE:O	2.17	0.63
4:D:42:TYR:CZ	6:F:24:THR:HG23	2.33	0.63
4:D:298:PHE:CA	11:L:37:ASN:ND2	2.54	0.62
3:C:119:LEU:O	3:C:122:SER:OG	2.17	0.62
12:M:8:LEU:HD22	14:T:1:MET:CE	2.29	0.62
5:E:12:ILE:HD11	25:E:84:HEM:O1A	1.99	0.62
16:V:102:PRO:HA	16:V:105:ARG:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:489:BCR:H312	19:Z:55:GLY:HA2	1.81	0.62
3:C:120:ILE:HG21	28:C:489:BCR:H353	1.81	0.62
1:A:322:ASN:OD1	3:C:412:THR:HG23	1.99	0.62
3:C:370:ARG:HD3	3:C:375:LEU:CD2	2.29	0.62
1:A:261:GLN:HG3	1:A:262:TYR:N	2.13	0.62
1:A:161:TYR:CE1	1:A:186:PHE:HE1	2.17	0.62
23:A:350:CLA:HED1	4:D:175:VAL:CG1	2.29	0.62
2:B:106:LEU:HD22	23:B:522:CLA:H143	1.80	0.62
2:B:234:ILE:O	2:B:236:THR:N	2.32	0.62
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.67	0.62
4:D:56:THR:HG23	4:D:56:THR:O	1.98	0.62
2:B:225:LEU:HD13	2:B:231:MET:SD	2.38	0.62
23:B:520:CLA:HAA2	23:B:520:CLA:HBD	1.81	0.62
3:C:70:PHE:O	3:C:73:ALA:HB3	1.99	0.62
1:A:180:PHE:HE2	4:D:192:THR:O	1.82	0.62
1:A:239:PHE:HE1	4:D:245:SER:HA	1.61	0.62
10:K:15:VAL:HG21	18:N:9:UNK:O	1.99	0.62
1:A:309:ALA:HB1	16:V:1:ALA:O	2.00	0.62
19:Z:37:LYS:O	19:Z:41:PHE:CD1	2.52	0.62
13:O:162:ARG:O	13:O:162:ARG:CG	2.48	0.62
2:B:323:GLY:HA2	4:D:293:LEU:HG	1.81	0.62
3:C:320:ARG:NH1	16:V:49:ASN:HA	2.15	0.62
4:D:186:GLN:HA	4:D:186:GLN:NE2	2.14	0.62
10:K:10:ASP:HB3	10:K:11:PRO:HD3	1.81	0.62
13:O:168:TYR:CD1	13:O:172:ILE:HD11	2.35	0.62
3:C:216:SER:O	3:C:221:GLU:O	2.18	0.62
5:E:12:ILE:HD13	25:E:84:HEM:CGA	2.30	0.62
1:A:180:PHE:HD1	1:A:180:PHE:H	1.47	0.62
15:U:57:LEU:CD2	15:U:112:PHE:HD2	1.95	0.62
13:O:11:VAL:O	13:O:11:VAL:HG12	2.00	0.62
2:B:69:LEU:HD12	23:B:518:CLA:HBA2	1.82	0.62
2:B:29:LEU:HB3	28:B:528:BCR:H351	1.82	0.62
28:B:528:BCR:H331	28:B:528:BCR:HC8	1.82	0.62
16:V:129:LYS:CE	16:V:135:VAL:HG23	2.30	0.62
3:C:120:ILE:CG2	28:C:489:BCR:H353	2.30	0.62
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.81	0.62
5:E:56:ALA:O	5:E:57:GLN:C	2.37	0.62
4:D:180:ARG:C	4:D:180:ARG:HD3	2.21	0.62
23:B:524:CLA:H13	23:B:524:CLA:OBD	2.00	0.61
5:E:9:PHE:O	5:E:10:SER:CB	2.47	0.61
19:Z:44:SER:O	19:Z:48:ILE:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:CE2	1:A:245:THR:HA	2.35	0.61
7:H:53:ILE:HG23	17:X:13:THR:HG1	1.65	0.61
3:C:103:GLY:O	3:C:104:GLU:C	2.39	0.61
3:C:38:GLY:HA2	3:C:41:ARG:HE	1.64	0.61
3:C:405:ASN:HB2	3:C:407:VAL:CG2	2.30	0.61
13:O:53:LYS:HE2	13:O:234:LYS:HB2	1.82	0.61
4:D:91:LEU:HD23	4:D:91:LEU:N	2.14	0.61
3:C:225:VAL:HB	23:C:487:CLA:HMC3	1.81	0.61
28:C:489:BCR:H341	19:Z:51:VAL:HG13	1.82	0.61
1:A:89:ILE:HD12	1:A:108:ASN:HB3	1.83	0.61
13:O:50:PHE:HZ	13:O:76:THR:CG2	2.13	0.61
5:E:12:ILE:CG1	25:E:84:HEM:O2D	2.47	0.61
15:U:59:ASN:H	15:U:59:ASN:ND2	1.80	0.61
13:O:102:ASP:O	13:O:103:PHE:CD1	2.53	0.61
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.31	0.61
13:O:163:GLY:CA	13:O:188:LYS:HE2	2.30	0.61
4:D:108:GLY:C	4:D:110:LEU:H	2.02	0.61
14:T:4:ILE:HG13	14:T:5:THR:N	2.15	0.61
1:A:114:LEU:CD1	1:A:118:HIS:CE1	2.84	0.61
2:B:135:LEU:HD23	2:B:138:MET:SD	2.40	0.61
3:C:285:ILE:HG12	23:C:487:CLA:HMB2	1.82	0.61
28:C:489:BCR:C34	19:Z:51:VAL:HG13	2.31	0.61
13:O:94:THR:HA	13:O:127:ALA:O	2.01	0.61
13:O:40:ILE:CG2	13:O:41:ALA:H	2.14	0.61
3:C:282:MET:HA	3:C:285:ILE:HB	1.83	0.61
3:C:283:GLY:HA3	3:C:434:ALA:HB2	1.81	0.61
3:C:265:ILE:HG22	3:C:266:TRP:H	1.66	0.61
1:A:296:ASN:OD1	3:C:401:LEU:HD23	2.00	0.61
2:B:271:THR:HG22	2:B:448:ARG:NH1	2.15	0.61
1:A:301:ASN:CG	3:C:407:VAL:HG21	2.19	0.61
15:U:82:ASN:O	15:U:85:TYR:HE2	1.84	0.61
15:U:127:ARG:O	15:U:128:TYR:HD1	1.82	0.61
1:A:149:ALA:HA	1:A:284:TRP:CZ3	2.36	0.61
4:D:157:PHE:O	4:D:158:LEU:HD23	2.00	0.61
4:D:171:PRO:HG3	4:D:181:PHE:CE1	2.36	0.61
3:C:227:VAL:HG23	3:C:227:VAL:O	2.00	0.61
3:C:36:TRP:O	3:C:38:GLY:N	2.31	0.61
4:D:22:LEU:HD21	4:D:32:TRP:CE3	2.35	0.61
13:O:92:SER:HB2	13:O:129:THR:O	2.01	0.61
13:O:137:THR:O	13:O:140:THR:HG23	2.01	0.61
25:E:84:HEM:C4A	6:F:19:TRP:HH2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HA	3:C:42:LEU:HD12	1.82	0.61
1:A:224:ILE:HG21	1:A:227:THR:OG1	2.01	0.61
1:A:306:VAL:CG2	1:A:307:ILE:H	2.13	0.61
3:C:333:GLY:O	3:C:335:THR:N	2.34	0.61
4:D:18:LEU:HA	17:X:41:SER:OG	2.01	0.61
13:O:112:GLY:C	13:O:114:GLU:H	2.03	0.61
16:V:75:TYR:HE1	25:V:138:HEM:C2A	2.19	0.60
1:A:180:PHE:CD2	4:D:192:THR:HB	2.37	0.60
3:C:272:LEU:O	3:C:276:LEU:HB2	2.00	0.60
4:D:83:ASN:O	4:D:83:ASN:ND2	2.34	0.60
1:A:322:ASN:O	1:A:326:LEU:HB2	2.00	0.60
13:O:95:PHE:HB2	13:O:127:ALA:HB3	1.81	0.60
13:O:28:GLY:HA3	13:O:137:THR:CG2	2.30	0.60
1:A:187:GLN:HG3	1:A:193:LEU:HG	1.83	0.60
2:B:57:ARG:CG	2:B:57:ARG:NH1	2.64	0.60
2:B:98:LEU:O	2:B:102:VAL:HG23	2.01	0.60
3:C:433:LEU:O	3:C:437:PHE:HB2	2.02	0.60
23:C:486:CLA:H61	28:C:488:BCR:H393	1.83	0.60
2:B:321:LYS:HE3	2:B:325:PHE:HZ	1.66	0.60
1:A:279:PRO:HG2	4:D:211:CYS:HB3	1.81	0.60
2:B:7:ARG:HA	23:B:523:CLA:O1A	2.01	0.60
10:K:6:TYR:O	10:K:8:ILE:N	2.34	0.60
4:D:253:TRP:HE3	4:D:253:TRP:HA	1.67	0.60
4:D:77:ALA:CB	4:D:174:GLY:HA3	2.31	0.60
3:C:95:LEU:HD21	23:C:479:CLA:OBD	2.01	0.60
3:C:275:SER:CB	23:C:485:CLA:HAA1	2.30	0.60
1:A:223:LEU:HD22	1:A:245:THR:CG2	2.30	0.60
4:D:138:VAL:CG1	4:D:139:ARG:N	2.65	0.60
11:L:23:LEU:O	11:L:27:LEU:HB2	2.01	0.60
4:D:196:PHE:HD1	4:D:285:GLY:HA2	1.66	0.60
2:B:399:VAL:HG23	2:B:417:VAL:HG13	1.83	0.60
4:D:188:PHE:CD1	4:D:188:PHE:N	2.69	0.60
2:B:123:PHE:CG	2:B:123:PHE:O	2.54	0.60
2:B:229:LEU:O	2:B:230:ARG:C	2.40	0.60
2:B:142:HIS:ND1	23:B:524:CLA:H142	2.16	0.60
3:C:95:LEU:HA	3:C:185:LEU:HD12	1.84	0.60
3:C:78:GLU:HA	3:C:78:GLU:OE1	2.01	0.60
23:C:486:CLA:H42	10:K:30:TRP:NE1	2.17	0.60
7:H:30:MET:O	7:H:33:PHE:N	2.35	0.60
13:O:95:PHE:HB3	13:O:127:ALA:CB	2.31	0.60
1:A:261:GLN:HG3	1:A:262:TYR:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:474:CLA:H8	23:C:477:CLA:H143	1.84	0.60
13:O:88:ASN:ND2	13:O:92:SER:OG	2.34	0.60
1:A:321:ILE:O	1:A:325:ASN:ND2	2.34	0.60
2:B:191:ASN:HB2	2:B:192:PRO:HD2	1.83	0.60
4:D:145:ALA:HB2	4:D:272:LEU:HD11	1.83	0.60
1:A:104:GLU:OE2	13:O:73:ARG:HD3	2.02	0.60
2:B:372:ASP:OD2	2:B:376:VAL:HG23	2.02	0.60
16:V:38:ALA:O	16:V:42:VAL:HG23	2.01	0.60
3:C:297:TYR:CD2	3:C:302:TYR:HE1	2.19	0.60
2:B:321:LYS:CE	2:B:325:PHE:CZ	2.84	0.60
11:L:8:GLN:N	11:L:9:PRO:HD3	2.17	0.60
4:D:261:PHE:HD1	4:D:266:TRP:CD1	2.19	0.60
17:X:12:ILE:HG22	17:X:16:LEU:HD13	1.82	0.60
5:E:12:ILE:HG23	5:E:18:TYR:HB2	1.70	0.60
4:D:58:TRP:HA	4:D:62:GLY:H	1.67	0.60
11:L:1:MET:C	11:L:3:PRO:HD2	2.23	0.60
11:L:36:PHE:O	12:M:3:VAL:HG23	2.01	0.60
7:H:28:PRO:O	7:H:32:VAL:HG23	2.02	0.60
5:E:59:GLN:HE21	5:E:81:GLN:HE22	1.50	0.60
2:B:355:PHE:CE1	2:B:373:LYS:HB3	2.36	0.60
3:C:240:ILE:HG22	3:C:244:CYS:SG	2.42	0.59
16:V:118:HIS:CD2	16:V:122:GLU:OE1	2.55	0.59
3:C:62:PHE:CZ	10:K:19:ILE:CD1	2.81	0.59
5:E:26:ILE:HG12	5:E:27:PRO:HD3	1.84	0.59
1:A:57:PRO:HG2	13:O:115:ARG:HH11	1.67	0.59
1:A:281:VAL:CG1	1:A:281:VAL:O	2.50	0.59
2:B:235:GLU:HB3	2:B:473:THR:OG1	2.02	0.59
2:B:190:PHE:CE1	23:B:527:CLA:HED3	2.38	0.59
13:O:27:ARG:C	13:O:29:ALA:H	2.04	0.59
3:C:349:ILE:C	3:C:350:ILE:HG13	2.22	0.59
10:K:6:TYR:O	10:K:7:ALA:C	2.41	0.59
13:O:194:LYS:HG3	13:O:194:LYS:O	2.01	0.59
4:D:101:PHE:CE2	4:D:105:CYS:SG	2.95	0.59
3:C:169:GLY:O	3:C:173:LEU:HG	2.02	0.59
6:F:40:GLN:HE22	9:J:27:LEU:HG	1.58	0.59
1:A:281:VAL:HG22	1:A:284:TRP:HD1	1.67	0.59
23:C:486:CLA:H172	19:Z:23:VAL:HG21	1.84	0.59
2:B:171:PRO:CG	7:H:62:LYS:HA	2.33	0.59
3:C:299:SER:HB2	3:C:303:GLY:O	2.02	0.59
16:V:69:ILE:O	16:V:73:VAL:HG23	2.01	0.59
2:B:12:LEU:HD11	2:B:18:ARG:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.84	0.59
13:O:233:VAL:HG12	13:O:234:LYS:N	2.17	0.59
3:C:141:GLU:HB2	3:C:144:SER:CB	2.32	0.59
2:B:380:ASP:OD1	2:B:390:TYR:CB	2.50	0.59
16:V:117:GLY:O	16:V:121:VAL:HG23	2.03	0.59
4:D:66:SER:HA	4:D:76:VAL:HG13	1.85	0.59
3:C:223:TRP:CD1	3:C:224:ILE:N	2.71	0.59
16:V:55:ARG:HG3	16:V:56:THR:N	2.16	0.59
2:B:174:LEU:HG	2:B:174:LEU:O	2.01	0.59
2:B:302:TRP:O	2:B:305:ILE:HG12	2.02	0.59
19:Z:47:TRP:CD1	19:Z:47:TRP:C	2.76	0.59
2:B:321:LYS:HE2	2:B:325:PHE:CZ	2.37	0.59
13:O:164:LEU:O	13:O:165:ALA:CB	2.51	0.59
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.37	0.59
4:D:235:PHE:CG	4:D:236:ASN:N	2.70	0.59
3:C:374:GLY:HA2	13:O:7:TYR:HE1	1.65	0.59
7:H:53:ILE:HG22	17:X:15:SER:HB2	1.85	0.59
1:A:265:PHE:HB2	1:A:271:LEU:HD21	1.85	0.59
15:U:32:THR:O	15:U:36:GLU:HG3	2.03	0.59
2:B:225:LEU:O	2:B:231:MET:HG2	2.03	0.59
3:C:284:PHE:HD1	3:C:434:ALA:HB1	1.66	0.59
3:C:437:PHE:HA	23:C:483:CLA:HMC3	1.84	0.59
10:K:15:VAL:HG12	10:K:15:VAL:O	2.02	0.59
2:B:301:ALA:O	2:B:304:ALA:HB3	2.02	0.59
3:C:429:SER:O	3:C:432:VAL:HB	2.03	0.59
3:C:239:TRP:O	3:C:243:ILE:HG13	2.03	0.58
5:E:30:PHE:HD2	5:E:30:PHE:O	1.84	0.58
2:B:136:PRO:HD3	2:B:231:MET:CE	2.32	0.58
2:B:46:ASP:HB3	2:B:58:GLN:OE1	2.03	0.58
4:D:88:SER:OG	5:E:68:ARG:NE	2.36	0.58
2:B:340:TRP:CD1	2:B:340:TRP:N	2.71	0.58
2:B:171:PRO:HG3	7:H:62:LYS:HA	1.86	0.58
2:B:223:GLN:HG3	2:B:227:LYS:HE3	1.85	0.58
4:D:27:PHE:HB3	6:F:17:VAL:HG11	1.84	0.58
2:B:234:ILE:HG21	23:B:513:CLA:HAC1	1.85	0.58
3:C:62:PHE:CE1	3:C:119:LEU:HD11	2.39	0.58
1:A:307:ILE:HG13	1:A:314:ILE:CD1	2.30	0.58
13:O:156:PHE:O	13:O:188:LYS:NZ	2.36	0.58
1:A:29:TYR:CD2	1:A:133:LEU:HD12	2.37	0.58
13:O:221:SER:OG	13:O:231:HIS:N	2.36	0.58
8:I:19:PHE:CE1	8:I:23:PHE:HE1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.31	0.58
1:A:210:LEU:HD13	24:D:355:PHO:ND	2.18	0.58
3:C:77:PRO:O	3:C:78:GLU:HB2	2.03	0.58
3:C:266:TRP:HA	3:C:271:TYR:HE2	1.68	0.58
4:D:32:TRP:N	4:D:131:GLU:OE2	2.35	0.58
3:C:373:ASN:OD1	13:O:16:ALA:HA	2.03	0.58
16:V:63:THR:HB	16:V:83:ASP:O	2.03	0.58
3:C:293:ASN:OD1	3:C:423:ARG:NH2	2.37	0.58
3:C:71:GLU:HB3	3:C:89:ILE:HD11	1.85	0.58
4:D:29:PHE:HE2	4:D:31:GLY:CA	2.16	0.58
4:D:267:LEU:O	4:D:271:MET:HE2	2.03	0.58
1:A:98:GLU:HG3	1:A:98:GLU:O	2.02	0.58
13:O:215:PHE:O	13:O:216:GLU:HB2	2.02	0.58
28:B:529:BCR:H311	28:B:529:BCR:H342	1.86	0.58
3:C:271:TYR:HA	3:C:274:TYR:CE1	2.39	0.58
3:C:113:VAL:O	3:C:117:VAL:HG23	2.03	0.58
13:O:215:PHE:HB3	13:O:237:GLY:H	1.69	0.58
13:O:40:ILE:HG23	13:O:84:GLU:OE2	2.04	0.58
2:B:150:CYS:HB2	23:B:517:CLA:HMC3	1.84	0.58
4:D:35:ILE:O	4:D:39:PRO:HD2	2.03	0.58
3:C:63:TRP:CE2	3:C:67:MET:HG3	2.39	0.58
23:C:477:CLA:H142	23:C:477:CLA:H101	1.84	0.58
1:A:334:ARG:HH11	4:D:320:LEU:CD1	2.13	0.58
17:X:34:PHE:O	17:X:38:ILE:HG13	2.04	0.58
16:V:75:TYR:CE2	16:V:79:PRO:HA	2.39	0.58
13:O:39:ARG:HA	13:O:245:PRO:HG3	1.85	0.58
3:C:243:ILE:O	23:C:474:CLA:HMC1	2.03	0.58
14:T:3:THR:O	14:T:6:TYR:N	2.33	0.58
23:B:521:CLA:CAB	23:B:527:CLA:HED1	2.27	0.58
3:C:63:TRP:CZ2	3:C:67:MET:HG3	2.39	0.58
3:C:123:ALA:HB1	19:Z:47:TRP:CH2	2.37	0.58
1:A:14:TRP:HH2	8:I:25:SER:HB3	1.68	0.58
4:D:28:VAL:H	6:F:17:VAL:HG11	1.69	0.57
1:A:78:ILE:O	1:A:177:SER:HB2	2.03	0.57
23:B:520:CLA:HAA2	23:B:520:CLA:CBD	2.33	0.57
11:L:27:LEU:HD23	12:M:14:PHE:CE2	2.39	0.57
13:O:53:LYS:HG2	13:O:65:PHE:CD2	2.39	0.57
16:V:76:MET:O	16:V:94:SER:HA	2.04	0.57
3:C:188:THR:O	3:C:188:THR:HG22	2.03	0.57
1:A:228:THR:HG22	1:A:228:THR:O	2.04	0.57
3:C:344:SER:O	3:C:347:GLY:N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:215:PHE:HB3	13:O:237:GLY:N	2.19	0.57
16:V:38:ALA:O	16:V:42:VAL:CG2	2.52	0.57
23:B:518:CLA:H142	23:B:524:CLA:HBA1	1.86	0.57
3:C:286:ALA:O	3:C:289:PHE:HB3	2.03	0.57
3:C:305:THR:O	3:C:308:GLU:HB2	2.04	0.57
3:C:94:THR:C	3:C:96:GLY:H	2.07	0.57
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.39	0.57
10:K:11:PRO:HB3	18:N:9:UNK:CB	2.34	0.57
8:I:5:LYS:O	8:I:9:TYR:HD1	1.86	0.57
13:O:200:ASN:O	13:O:213:GLY:HA3	2.04	0.57
3:C:436:PHE:O	3:C:439:VAL:HB	2.04	0.57
6:F:14:ILE:HG13	6:F:14:ILE:O	2.03	0.57
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.19	0.57
1:A:89:ILE:HD13	1:A:94:TYR:CG	2.39	0.57
1:A:218:LEU:CD2	4:D:142:ASN:HD22	2.16	0.57
1:A:286:THR:CG2	23:A:348:CLA:O1D	2.50	0.57
1:A:141:PRO:HG3	3:C:446:GLY:C	2.24	0.57
10:K:24:LEU:O	10:K:27:ALA:HB3	2.04	0.57
3:C:318:LEU:HD22	3:C:328:VAL:HG21	1.87	0.57
2:B:368:VAL:HG21	2:B:422:ARG:HG2	1.86	0.57
12:M:8:LEU:HD22	14:T:1:MET:HE3	1.85	0.57
19:Z:12:LEU:HD12	19:Z:12:LEU:O	2.04	0.57
1:A:161:TYR:CE2	1:A:165:GLN:HG3	2.40	0.57
1:A:263:ALA:HB1	26:A:353:PL9:H151	1.86	0.57
1:A:69:GLY:O	1:A:81:ALA:HA	2.04	0.57
3:C:291:TRP:HB3	3:C:292:PHE:CE2	2.39	0.57
1:A:142:TRP:CD1	3:C:443:TRP:CH2	2.92	0.57
1:A:341:LEU:HD21	15:U:134:LYS:NZ	2.19	0.57
2:B:192:PRO:HG3	7:H:48:TYR:CE1	2.40	0.57
1:A:15:GLU:O	1:A:19:ASN:ND2	2.38	0.57
4:D:72:ASN:OD1	4:D:74:LEU:HB2	2.03	0.57
14:T:9:ILE:HG22	14:T:9:ILE:O	2.05	0.57
15:U:75:LEU:HD21	15:U:101:GLN:HE21	1.69	0.57
1:A:142:TRP:HB2	4:D:220:ASN:HB2	1.86	0.57
3:C:155:ASN:HB3	3:C:255:THR:OG1	2.05	0.57
4:D:261:PHE:CD1	4:D:266:TRP:CD1	2.93	0.57
14:T:24:ARG:HG2	14:T:25:GLU:N	2.19	0.57
4:D:68:LEU:N	6:F:39:MET:HE1	2.20	0.57
2:B:45:PHE:CE2	2:B:78:TRP:CZ2	2.92	0.57
23:B:524:CLA:O1A	23:B:524:CLA:H2	2.04	0.57
4:D:122:LEU:HD21	23:D:354:CLA:C9	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:PHE:C	2:B:479:PHE:HD2	2.07	0.57
1:A:143:ILE:HD13	4:D:253:TRP:CH2	2.40	0.57
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.03	0.57
1:A:316:THR:O	1:A:318:ALA:N	2.37	0.57
2:B:250:PHE:CD1	2:B:459:ALA:HB1	2.40	0.57
2:B:247:PHE:CE1	23:B:521:CLA:H72	2.40	0.57
4:D:168:PHE:HD2	4:D:168:PHE:C	2.08	0.57
2:B:479:PHE:C	2:B:479:PHE:CD2	2.78	0.57
2:B:414:PRO:N	2:B:415:PRO:CD	2.67	0.57
4:D:110:LEU:O	4:D:113:PHE:HB3	2.05	0.57
3:C:284:PHE:O	3:C:285:ILE:C	2.42	0.57
3:C:292:PHE:HE1	23:C:487:CLA:HBC3	1.69	0.57
3:C:42:LEU:CD2	23:C:486:CLA:HED1	2.35	0.57
16:V:22:THR:H	16:V:25:GLN:NE2	2.03	0.57
13:O:78:LEU:O	13:O:79:ASP:OD1	2.23	0.57
3:C:282:MET:CA	3:C:285:ILE:HG13	2.32	0.57
1:A:335:ASN:HD22	1:A:335:ASN:C	2.08	0.57
2:B:414:PRO:N	2:B:415:PRO:HD3	2.20	0.57
13:O:102:ASP:O	13:O:103:PHE:HD1	1.85	0.57
4:D:52:THR:O	4:D:67:TYR:HD1	1.88	0.57
4:D:86:GLY:C	4:D:87:HIS:CD2	2.78	0.57
13:O:39:ARG:HA	13:O:245:PRO:CB	2.35	0.57
3:C:155:ASN:OD1	3:C:156:LYS:HG2	2.04	0.57
4:D:29:PHE:C	4:D:29:PHE:HD2	2.08	0.57
2:B:10:THR:O	2:B:13:ILE:HG22	2.04	0.57
15:U:40:VAL:HG12	15:U:40:VAL:O	2.05	0.57
3:C:314:ALA:HB3	3:C:351:PHE:CD1	2.40	0.56
3:C:417:VAL:HG21	16:V:42:VAL:HG22	1.86	0.56
3:C:326:ALA:CB	15:U:127:ARG:HD2	2.31	0.56
2:B:414:PRO:O	2:B:418:LYS:HG3	2.04	0.56
1:A:29:TYR:CD1	1:A:30:VAL:N	2.69	0.56
3:C:412:THR:HG22	16:V:136:TYR:HE2	1.69	0.56
13:O:53:LYS:CE	13:O:234:LYS:HB2	2.35	0.56
3:C:141:GLU:CB	3:C:144:SER:OG	2.53	0.56
13:O:66:VAL:CG1	13:O:67:PRO:HD2	2.35	0.56
17:X:12:ILE:HA	17:X:16:LEU:HD12	1.87	0.56
1:A:114:LEU:HD11	1:A:118:HIS:CE1	2.39	0.56
1:A:214:MET:HE3	1:A:214:MET:HA	1.83	0.56
1:A:52:PHE:CE1	1:A:81:ALA:HB2	2.40	0.56
23:B:512:CLA:H203	23:B:523:CLA:H192	1.87	0.56
4:D:186:GLN:HE21	4:D:186:GLN:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:CD1	1:A:237:TYR:N	2.73	0.56
4:D:138:VAL:CG1	4:D:139:ARG:H	2.17	0.56
4:D:329:MET:O	4:D:329:MET:HG2	2.05	0.56
2:B:348:ASN:CG	2:B:349:LYS:H	2.07	0.56
3:C:324:LEU:HD21	15:U:72:TYR:OH	2.05	0.56
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.87	0.56
2:B:458:PHE:CE1	23:B:516:CLA:HBB1	2.41	0.56
3:C:88:LEU:O	3:C:91:HIS:HB2	2.05	0.56
23:C:476:CLA:H12	23:C:483:CLA:H2	1.86	0.56
11:L:7:ARG:O	11:L:9:PRO:HD3	2.05	0.56
4:D:261:PHE:HA	14:T:24:ARG:NH2	2.20	0.56
23:B:511:CLA:HMD1	7:H:26:THR:HB	1.86	0.56
3:C:229:ASN:OD1	3:C:231:GLU:HG3	2.05	0.56
7:H:53:ILE:HG23	7:H:53:ILE:O	2.04	0.56
13:O:149:PRO:HA	13:O:192:LEU:HD12	1.86	0.56
13:O:43:LEU:HD12	13:O:241:ALA:HB2	1.87	0.56
3:C:281:MET:O	3:C:284:PHE:HB2	2.05	0.56
4:D:231:THR:HG22	4:D:232:PHE:N	2.20	0.56
1:A:110:GLY:O	1:A:111:PRO:C	2.43	0.56
3:C:284:PHE:CD1	3:C:434:ALA:HB1	2.41	0.56
16:V:129:LYS:NZ	16:V:135:VAL:CG2	2.69	0.56
1:A:133:LEU:HD23	4:D:252:PHE:CD1	2.41	0.56
14:T:24:ARG:HG2	14:T:25:GLU:H	1.70	0.56
2:B:372:ASP:OD2	2:B:374:ASN:HB2	2.03	0.56
1:A:195:HIS:O	1:A:199:GLN:HG3	2.06	0.56
3:C:350:ILE:CG2	3:C:359:TRP:HB3	2.35	0.56
1:A:114:LEU:CD1	1:A:118:HIS:HE1	2.19	0.56
4:D:87:HIS:CD2	4:D:166:SER:HA	2.41	0.56
1:A:330:VAL:HG13	4:D:348:ARG:HG3	1.87	0.56
11:L:12:LEU:HD11	11:L:16:SER:CB	2.34	0.56
13:O:192:LEU:HD22	15:U:119:THR:HG23	1.88	0.56
2:B:394:GLN:NE2	15:U:52:GLY:HA3	2.21	0.56
3:C:279:LEU:HB3	23:C:481:CLA:CBC	2.35	0.56
2:B:371:THR:HG22	2:B:372:ASP:O	2.05	0.56
16:V:22:THR:H	16:V:25:GLN:HE21	1.52	0.56
1:A:93:PHE:CZ	23:A:352:CLA:HBA1	2.41	0.56
7:H:47:ILE:HG12	7:H:52:LEU:HD23	1.87	0.56
2:B:41:GLU:HG2	2:B:60:MET:SD	2.45	0.56
4:D:32:TRP:HA	4:D:32:TRP:CE3	2.41	0.56
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.36	0.56
1:A:281:VAL:HG22	1:A:284:TRP:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:VAL:HG11	3:C:121:SER:HB2	1.88	0.56
10:K:16:LEU:HB3	10:K:17:PRO:HD3	1.88	0.56
1:A:205:VAL:HG12	4:D:204:VAL:HG12	1.87	0.56
23:B:519:CLA:H142	23:D:356:CLA:H42	1.88	0.56
4:D:87:HIS:CD2	4:D:87:HIS:N	2.73	0.56
13:O:118:LEU:CD1	13:O:233:VAL:HG21	2.35	0.56
5:E:59:GLN:NE2	5:E:81:GLN:NE2	2.54	0.56
1:A:95:PRO:HD2	1:A:98:GLU:HB3	1.87	0.56
13:O:32:ILE:C	13:O:34:SER:H	2.10	0.56
1:A:316:THR:O	1:A:317:TRP:C	2.43	0.55
4:D:168:PHE:CD2	4:D:168:PHE:C	2.79	0.55
10:K:30:TRP:CZ3	10:K:31:GLN:NE2	2.74	0.55
4:D:257:PHE:CZ	26:D:357:PL9:H253	2.41	0.55
1:A:159:LEU:CG	1:A:163:ILE:HD11	2.36	0.55
3:C:101:PRO:CA	3:C:195:ASP:HB3	2.36	0.55
11:L:2:GLU:N	11:L:3:PRO:HD2	2.21	0.55
4:D:302:GLU:O	4:D:305:ALA:HB3	2.06	0.55
3:C:331:ALA:O	3:C:338:GLY:HA2	2.05	0.55
4:D:118:GLY:CA	24:D:355:PHO:H71	2.37	0.55
1:A:221:SER:CA	4:D:139:ARG:HB2	2.33	0.55
3:C:173:LEU:HA	3:C:176:VAL:HG23	1.88	0.55
1:A:142:TRP:HH2	1:A:273:PHE:HE1	1.54	0.55
3:C:342:MET:HE3	3:C:353:GLY:H	1.70	0.55
1:A:139:MET:HE2	4:D:248:THR:CG2	2.36	0.55
13:O:68:THR:HA	13:O:110:MET:HE1	1.87	0.55
4:D:59:TYR:HE1	5:E:49:PRO:HG2	1.72	0.55
2:B:326:ARG:HD3	28:B:529:BCR:C40	2.31	0.55
3:C:285:ILE:HG12	23:C:487:CLA:CMB	2.37	0.55
3:C:294:ASN:O	3:C:296:VAL:N	2.40	0.55
4:D:198:MET:HE1	11:L:30:LEU:CD1	2.30	0.55
2:B:418:LYS:HZ1	15:U:45:GLU:CD	2.10	0.55
16:V:55:ARG:O	16:V:59:LEU:HG	2.07	0.55
23:B:511:CLA:HBC3	7:H:33:PHE:CD2	2.42	0.55
1:A:12:ASN:O	1:A:15:GLU:HG3	2.06	0.55
2:B:12:LEU:HG	2:B:19:LEU:HB2	1.87	0.55
15:U:88:VAL:CG2	15:U:114:VAL:HG23	2.36	0.55
13:O:153:THR:HG22	13:O:154:ALA:N	2.22	0.55
1:A:325:ASN:N	1:A:325:ASN:HD22	2.05	0.55
1:A:297:LEU:HD22	3:C:428:THR:HG21	1.87	0.55
13:O:19:CYS:HB3	13:O:240:TYR:HB2	1.89	0.55
2:B:12:LEU:HD21	2:B:19:LEU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:TYR:N	2:B:6:TYR:CD2	2.75	0.55
7:H:21:ALA:HB3	7:H:22:PRO:CD	2.37	0.55
1:A:224:ILE:HG22	1:A:224:ILE:O	2.06	0.55
3:C:187:ASP:O	3:C:194:GLY:O	2.25	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.88	0.55
3:C:158:THR:O	3:C:161:LEU:HB3	2.07	0.55
2:B:47:PRO:HA	2:B:78:TRP:HE1	1.72	0.55
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.41	0.55
3:C:98:GLY:O	3:C:105:VAL:HG13	2.07	0.55
3:C:116:VAL:HG13	28:C:488:BCR:C33	2.33	0.55
23:C:478:CLA:C9	23:C:482:CLA:HAA1	2.36	0.55
3:C:447:ARG:O	3:C:447:ARG:HG3	2.06	0.55
1:A:301:ASN:HD21	3:C:407:VAL:HG23	1.71	0.55
13:O:32:ILE:C	13:O:34:SER:N	2.59	0.55
1:A:180:PHE:CD2	4:D:192:THR:CG2	2.90	0.55
15:U:57:LEU:HD11	15:U:112:PHE:HB3	1.89	0.55
23:C:478:CLA:H162	23:C:482:CLA:HMD2	1.89	0.55
1:A:224:ILE:HD11	1:A:243:GLU:HG3	1.89	0.55
4:D:29:PHE:HE2	4:D:31:GLY:HA3	1.72	0.55
2:B:356:VAL:HG23	2:B:370:LEU:HD23	1.89	0.55
2:B:327:THR:C	2:B:329:PRO:HD3	2.27	0.55
12:M:17:VAL:HG12	12:M:18:PRO:N	2.22	0.55
15:U:124:GLY:O	15:U:125:GLY:C	2.46	0.55
2:B:153:PHE:N	23:B:515:CLA:HMC3	2.22	0.55
16:V:66:ARG:HH11	16:V:66:ARG:HG3	1.72	0.55
2:B:231:MET:HE2	2:B:231:MET:O	2.07	0.54
1:A:291:SER:O	1:A:295:PHE:CE1	2.59	0.54
3:C:90:PRO:HB2	3:C:302:TYR:HE2	1.72	0.54
2:B:342:GLY:HA2	2:B:403:GLY:HA3	1.89	0.54
1:A:14:TRP:CH2	8:I:25:SER:HB3	2.42	0.54
13:O:211:ILE:CG2	13:O:212:ALA:N	2.70	0.54
4:D:71:CYS:HB3	4:D:75:THR:CB	2.38	0.54
10:K:19:ILE:HG13	10:K:20:PRO:HD3	1.89	0.54
2:B:302:TRP:CZ3	2:B:343:HIS:HB2	2.43	0.54
3:C:182:PHE:O	3:C:184:GLY:N	2.41	0.54
15:U:51:TYR:O	15:U:53:GLU:N	2.40	0.54
2:B:458:PHE:CD1	23:B:516:CLA:HMC3	2.42	0.54
2:B:6:TYR:OH	12:M:21:PHE:CZ	2.35	0.54
1:A:142:TRP:N	4:D:220:ASN:OD1	2.40	0.54
10:K:9:PHE:O	10:K:10:ASP:C	2.44	0.54
19:Z:17:PHE:O	19:Z:21:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LEU:O	3:C:54:VAL:HG23	2.07	0.54
1:A:334:ARG:O	1:A:335:ASN:ND2	2.40	0.54
2:B:212:ALA:CB	23:B:511:CLA:HMC3	2.36	0.54
13:O:22:LEU:O	13:O:203:LYS:CD	2.55	0.54
1:A:97:TRP:CE3	8:I:5:LYS:HA	2.43	0.54
16:V:92:HIS:ND1	16:V:93:PRO:HD2	2.22	0.54
2:B:159:THR:O	2:B:159:THR:HG22	2.07	0.54
4:D:30:VAL:HG22	4:D:38:PHE:HE1	1.71	0.54
13:O:140:THR:HG21	13:O:201:VAL:HB	1.88	0.54
13:O:243:ILE:HG22	13:O:244:GLU:N	2.22	0.54
1:A:278:TRP:HE1	23:A:350:CLA:H42	1.73	0.54
2:B:45:PHE:HE1	2:B:55:MET:HA	1.72	0.54
3:C:36:TRP:C	3:C:38:GLY:H	2.10	0.54
4:D:90:LEU:HD13	4:D:96:GLU:HB3	1.87	0.54
1:A:303:ASN:C	1:A:304:HIS:HD1	2.10	0.54
3:C:199:ILE:CD1	3:C:234:VAL:HG21	2.33	0.54
3:C:200:THR:C	3:C:201:ASN:HD22	2.10	0.54
2:B:372:ASP:CG	2:B:373:LYS:N	2.60	0.54
2:B:15:ASP:OD1	2:B:15:ASP:C	2.45	0.54
2:B:321:LYS:HE2	2:B:325:PHE:HZ	1.71	0.54
2:B:225:LEU:C	2:B:231:MET:HG2	2.28	0.54
1:A:180:PHE:HD2	4:D:192:THR:HB	1.72	0.54
3:C:88:LEU:O	3:C:91:HIS:N	2.40	0.54
1:A:302:PHE:N	1:A:302:PHE:CD1	2.75	0.54
1:A:133:LEU:HD21	4:D:252:PHE:HA	1.90	0.54
1:A:63:ILE:HG23	3:C:335:THR:HG21	1.89	0.54
4:D:29:PHE:HD2	4:D:29:PHE:O	1.91	0.54
2:B:371:THR:HG22	2:B:372:ASP:N	2.23	0.54
2:B:402:TYR:HD1	2:B:402:TYR:N	2.06	0.54
6:F:19:TRP:CH2	6:F:23:HIS:NE2	2.76	0.54
4:D:52:THR:O	4:D:76:VAL:HG11	2.08	0.54
2:B:110:ALA:O	2:B:113:TRP:N	2.37	0.54
4:D:87:HIS:CE1	4:D:162:LEU:HA	2.43	0.54
4:D:336:HIS:N	4:D:336:HIS:HD2	1.99	0.54
19:Z:37:LYS:O	19:Z:41:PHE:HD1	1.90	0.54
1:A:258:LEU:O	4:D:128:ARG:NH2	2.40	0.54
1:A:89:ILE:CG2	1:A:94:TYR:HB2	2.38	0.54
2:B:183:PRO:HD3	2:B:199:VAL:HG11	1.90	0.54
4:D:182:LEU:HA	23:D:354:CLA:HMD2	1.90	0.54
28:C:489:BCR:C31	19:Z:55:GLY:HA2	2.37	0.54
13:O:193:THR:HG22	13:O:194:LYS:N	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:HA	4:D:240:ALA:CB	2.34	0.54
4:D:221:THR:O	4:D:221:THR:CG2	2.56	0.54
4:D:281:MET:O	4:D:284:ILE:N	2.40	0.54
2:B:134:ASP:OD2	2:B:220:ARG:NH2	2.40	0.54
3:C:285:ILE:O	23:C:487:CLA:HBB1	2.07	0.54
4:D:83:ASN:HB3	4:D:336:HIS:ND1	2.23	0.54
1:A:320:ILE:O	1:A:320:ILE:CG2	2.55	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.76	0.54
7:H:57:VAL:HG12	7:H:57:VAL:O	2.07	0.54
2:B:153:PHE:O	2:B:158:LEU:HG	2.07	0.54
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.07	0.54
15:U:72:TYR:HD2	15:U:73:PRO:CD	2.20	0.54
1:A:114:LEU:HD12	1:A:118:HIS:CE1	2.43	0.54
23:A:349:CLA:H51	24:A:351:PHO:HMB3	1.89	0.54
4:D:156:VAL:CG1	4:D:171:PRO:HG2	2.38	0.54
3:C:151:TRP:C	3:C:153:ASP:H	2.10	0.54
2:B:209:GLY:HA3	23:B:518:CLA:H201	1.90	0.53
2:B:21:ALA:O	2:B:24:LEU:HB2	2.08	0.53
4:D:152:VAL:HG13	23:D:354:CLA:CED	2.38	0.53
3:C:324:LEU:HD12	15:U:128:TYR:CZ	2.43	0.53
15:U:73:PRO:HG2	16:V:83:ASP:CG	2.28	0.53
3:C:417:VAL:HG22	16:V:38:ALA:HB1	1.90	0.53
5:E:68:ARG:HH12	7:H:50:SER:HB3	1.72	0.53
4:D:96:GLU:CD	5:E:68:ARG:O	2.46	0.53
4:D:319:LEU:CA	4:D:322:ASN:HD22	2.14	0.53
13:O:152:ARG:HD2	13:O:156:PHE:CD2	2.43	0.53
16:V:22:THR:N	16:V:25:GLN:HE21	2.06	0.53
19:Z:36:SER:HA	19:Z:39:LEU:HD12	1.89	0.53
2:B:137:LYS:O	2:B:141:ILE:HG12	2.09	0.53
23:B:513:CLA:H18	23:B:524:CLA:CGA	2.38	0.53
23:B:518:CLA:C14	23:B:524:CLA:HBA1	2.38	0.53
2:B:6:TYR:CE1	2:B:8:VAL:HG21	2.42	0.53
4:D:179:PHE:HA	4:D:182:LEU:CD1	2.38	0.53
3:C:88:LEU:HD22	23:C:480:CLA:CGD	2.39	0.53
3:C:437:PHE:HA	23:C:483:CLA:HMC1	1.90	0.53
3:C:55:ALA:HB1	28:C:488:BCR:H371	1.90	0.53
4:D:195:PRO:O	4:D:198:MET:HB2	2.09	0.53
13:O:133:VAL:HG12	13:O:133:VAL:O	2.07	0.53
13:O:79:ASP:HA	13:O:101:ILE:HG21	1.91	0.53
1:A:213:ALA:O	1:A:217:SER:HB2	2.08	0.53
2:B:234:ILE:CG2	23:B:524:CLA:H193	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:ASN:CB	4:D:336:HIS:HD1	2.22	0.53
3:C:165:LEU:HD21	23:C:474:CLA:CBB	2.38	0.53
4:D:201:VAL:O	4:D:201:VAL:HG12	2.09	0.53
1:A:292:THR:HG23	3:C:428:THR:HG23	1.91	0.53
3:C:316:THR:HG21	3:C:396:MET:HE1	1.91	0.53
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.91	0.53
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.89	0.53
23:C:477:CLA:HMD1	23:C:485:CLA:HAB	1.91	0.53
2:B:174:LEU:HD22	2:B:308:LYS:HZ2	1.74	0.53
2:B:321:LYS:HE3	2:B:325:PHE:CZ	2.43	0.53
3:C:318:LEU:HD22	3:C:328:VAL:CG2	2.38	0.53
15:U:75:LEU:HD21	15:U:101:GLN:NE2	2.24	0.53
16:V:40:CYS:SG	25:V:138:HEM:CAC	2.97	0.53
2:B:313:ASP:O	2:B:313:ASP:OD1	2.26	0.53
3:C:176:VAL:HG13	3:C:234:VAL:HG13	1.91	0.53
5:E:26:ILE:HG13	5:E:27:PRO:HD3	1.89	0.53
15:U:72:TYR:CG	15:U:73:PRO:N	2.74	0.53
3:C:291:TRP:O	3:C:305:THR:HG23	2.08	0.53
16:V:122:GLU:HB3	16:V:123:PRO:CD	2.39	0.53
16:V:100:ILE:C	16:V:102:PRO:HD3	2.29	0.53
2:B:308:LYS:HE2	2:B:312:TYR:CE2	2.43	0.53
3:C:384:ILE:O	3:C:384:ILE:HG23	2.06	0.53
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.33	0.53
16:V:52:LEU:HD23	25:V:138:HEM:HAD2	1.90	0.53
2:B:62:VAL:HG11	23:B:518:CLA:HED3	1.91	0.53
14:T:10:PHE:CE2	14:T:14:ILE:HD11	2.43	0.53
2:B:479:PHE:O	4:D:139:ARG:NH2	2.29	0.53
2:B:263:THR:HG22	2:B:263:THR:O	2.09	0.53
1:A:306:VAL:CG2	1:A:307:ILE:N	2.69	0.53
1:A:29:TYR:HE1	1:A:31:GLY:HA3	1.73	0.53
1:A:31:GLY:O	1:A:34:GLY:N	2.38	0.53
2:B:340:TRP:CE3	2:B:342:GLY:HA3	2.44	0.53
2:B:381:ILE:O	2:B:381:ILE:HG22	2.09	0.53
1:A:307:ILE:C	1:A:309:ALA:N	2.62	0.53
16:V:78:ASN:ND2	16:V:87:GLU:OE2	2.42	0.53
13:O:110:MET:H	13:O:110:MET:HE2	1.73	0.53
2:B:236:THR:O	2:B:240:SER:HB3	2.09	0.53
2:B:458:PHE:CG	23:B:516:CLA:HMC3	2.44	0.53
3:C:112:PHE:O	3:C:116:VAL:HG23	2.09	0.53
1:A:23:SER:OG	1:A:24:THR:N	2.41	0.53
6:F:30:ILE:O	6:F:30:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:GLY:O	3:C:223:TRP:C	2.47	0.52
19:Z:37:LYS:HA	19:Z:40:ILE:HD12	1.91	0.52
2:B:344:ALA:HB2	2:B:401:PHE:HE1	1.74	0.52
2:B:421:ALA:O	2:B:424:ALA:HB3	2.08	0.52
10:K:16:LEU:HB3	10:K:17:PRO:HD2	1.90	0.52
1:A:63:ILE:CD1	1:A:336:ALA:HB2	2.38	0.52
5:E:48:THR:O	5:E:49:PRO:O	2.27	0.52
1:A:217:SER:OG	4:D:142:ASN:HA	2.09	0.52
3:C:292:PHE:CE1	23:C:487:CLA:HBC3	2.43	0.52
7:H:22:PRO:O	7:H:23:GLY:O	2.26	0.52
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.44	0.52
4:D:108:GLY:C	4:D:110:LEU:N	2.60	0.52
2:B:46:ASP:OD1	2:B:48:SER:OG	2.19	0.52
2:B:103:LEU:HD21	23:B:518:CLA:HMC3	1.91	0.52
1:A:218:LEU:HD23	4:D:142:ASN:HD22	1.74	0.52
14:T:18:PHE:HD2	14:T:19:PHE:HD1	1.56	0.52
1:A:223:LEU:O	1:A:225:ARG:HG3	2.09	0.52
2:B:328:GLY:HA3	23:B:514:CLA:O1A	2.10	0.52
1:A:189:GLU:CD	22:A:347:OEC:O1	2.37	0.52
23:D:356:CLA:H12	7:H:42:LEU:HD21	1.91	0.52
10:K:19:ILE:CG1	10:K:20:PRO:HD3	2.39	0.52
4:D:83:ASN:OD1	4:D:336:HIS:ND1	2.39	0.52
3:C:201:ASN:O	3:C:201:ASN:ND2	2.41	0.52
1:A:246:TYR:HE1	1:A:248:ILE:HG12	1.74	0.52
5:E:43:TYR:O	5:E:47:GLY:N	2.42	0.52
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.52
13:O:201:VAL:CG1	13:O:211:ILE:HG23	2.37	0.52
1:A:52:PHE:O	1:A:52:PHE:CD2	2.63	0.52
2:B:62:VAL:CG1	23:B:518:CLA:HED3	2.40	0.52
4:D:268:HIS:O	4:D:271:MET:HB2	2.10	0.52
7:H:51:THR:HG22	7:H:51:THR:O	2.10	0.52
2:B:110:ALA:O	2:B:111:ALA:C	2.46	0.52
4:D:87:HIS:HA	4:D:167:TRP:NE1	2.25	0.52
1:A:295:PHE:CD1	1:A:295:PHE:N	2.76	0.52
1:A:53:ILE:O	1:A:53:ILE:HG22	2.10	0.52
2:B:247:PHE:O	2:B:251:VAL:HG23	2.09	0.52
2:B:110:ALA:HA	23:B:522:CLA:H203	1.90	0.52
4:D:286:VAL:HG21	23:D:354:CLA:HED2	1.92	0.52
23:B:520:CLA:H201	12:M:18:PRO:HB3	1.92	0.52
3:C:278:ALA:O	3:C:282:MET:HG3	2.09	0.52
3:C:122:SER:O	28:C:488:BCR:H363	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:VAL:CG2	23:C:482:CLA:HMB2	2.39	0.52
1:A:303:ASN:O	1:A:304:HIS:ND1	2.40	0.52
19:Z:5:PHE:CZ	19:Z:54:VAL:HG13	2.45	0.52
8:I:31:ASN:O	8:I:31:ASN:CG	2.48	0.52
15:U:62:ILE:O	15:U:64:ALA:N	2.42	0.52
1:A:153:SER:OG	23:A:348:CLA:HED1	2.09	0.52
4:D:122:LEU:HD21	23:D:354:CLA:H92	1.92	0.52
14:T:18:PHE:CD2	14:T:19:PHE:CD1	2.95	0.52
13:O:122:VAL:HA	13:O:146:PHE:CD2	2.43	0.52
3:C:289:PHE:HD2	3:C:289:PHE:O	1.92	0.52
4:D:83:ASN:HB3	4:D:336:HIS:HD1	1.75	0.52
13:O:38:TYR:O	13:O:245:PRO:HB2	2.09	0.52
3:C:264:PHE:CZ	23:C:474:CLA:CGA	2.92	0.52
13:O:52:VAL:HG11	13:O:116:ILE:HD13	1.91	0.52
3:C:131:TYR:HE1	3:C:135:ARG:CD	2.23	0.52
3:C:316:THR:HG21	3:C:396:MET:CE	2.39	0.52
8:I:32:PRO:HG2	8:I:35:LYS:O	2.09	0.52
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.45	0.52
1:A:340:PRO:O	4:D:352:LEU:HD23	2.10	0.52
3:C:350:ILE:HG22	3:C:351:PHE:O	2.10	0.52
13:O:17:ASN:ND2	13:O:77:SER:OG	2.43	0.52
16:V:79:PRO:HG3	16:V:88:ILE:C	2.30	0.52
1:A:260:PHE:O	1:A:263:ALA:HB3	2.09	0.52
13:O:233:VAL:CG1	13:O:234:LYS:N	2.72	0.52
1:A:337:HIS:CE1	4:D:352:LEU:HD12	2.44	0.51
23:B:521:CLA:H112	23:D:356:CLA:H92	1.92	0.51
3:C:390:ARG:NH1	16:V:100:ILE:CG2	2.73	0.51
23:C:486:CLA:H42	10:K:30:TRP:HE1	1.74	0.51
2:B:451:PHE:CD1	2:B:451:PHE:C	2.84	0.51
7:H:21:ALA:CB	7:H:22:PRO:CD	2.87	0.51
3:C:340:TYR:CD1	3:C:340:TYR:N	2.77	0.51
2:B:393:GLU:N	2:B:393:GLU:OE1	2.43	0.51
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.68	0.51
3:C:138:GLU:O	3:C:139:THR:HB	2.09	0.51
4:D:318:ASN:O	4:D:322:ASN:ND2	2.44	0.51
7:H:37:PHE:O	7:H:40:PHE:HB3	2.11	0.51
13:O:93:LEU:O	13:O:128:SER:HA	2.11	0.51
12:M:5:GLN:O	12:M:5:GLN:HG3	2.10	0.51
3:C:354:GLU:C	3:C:356:MET:H	2.13	0.51
2:B:250:PHE:CE1	2:B:459:ALA:HB1	2.45	0.51
4:D:220:ASN:ND2	4:D:220:ASN:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:HG22	1:A:309:ALA:CB	2.40	0.51
11:L:27:LEU:HD23	12:M:14:PHE:HE2	1.75	0.51
2:B:246:PHE:C	2:B:246:PHE:CD2	2.83	0.51
2:B:168:VAL:HG12	2:B:169:SER:N	2.24	0.51
16:V:63:THR:CG2	16:V:83:ASP:O	2.59	0.51
1:A:70:SER:O	1:A:75:ASN:HB2	2.10	0.51
4:D:80:THR:HG22	4:D:81:PRO:HD2	1.92	0.51
4:D:90:LEU:HD11	4:D:96:GLU:HB3	1.90	0.51
13:O:164:LEU:HG	13:O:188:LYS:HB2	1.93	0.51
1:A:131:TRP:O	1:A:134:SER:HB2	2.10	0.51
2:B:164:PRO:HB3	23:B:515:CLA:HED2	1.93	0.51
3:C:68:THR:HB	3:C:115:GLY:HA2	1.93	0.51
13:O:1:ALA:O	13:O:2:LYS:HB2	2.10	0.51
3:C:343:ARG:HB3	13:O:78:LEU:CD1	2.40	0.51
1:A:162:PRO:HG3	1:A:171:GLY:HA2	1.93	0.51
23:B:519:CLA:HMD1	23:B:524:CLA:CAB	2.40	0.51
4:D:258:GLY:O	14:T:21:ILE:HG23	2.10	0.51
3:C:105:VAL:HG12	3:C:107:ASP:O	2.10	0.51
5:E:68:ARG:HH12	7:H:50:SER:CB	2.24	0.51
2:B:318:ASN:O	2:B:320:ALA:N	2.43	0.51
13:O:152:ARG:HD2	13:O:156:PHE:CE2	2.46	0.51
5:E:26:ILE:HA	5:E:29:LEU:HD12	1.93	0.51
4:D:58:TRP:HB3	4:D:63:LEU:O	2.10	0.51
6:F:36:ILE:CA	6:F:39:MET:HG3	2.40	0.51
23:B:521:CLA:H172	23:D:356:CLA:H72	1.92	0.51
2:B:308:LYS:HE2	2:B:312:TYR:CZ	2.46	0.51
19:Z:41:PHE:CD1	19:Z:41:PHE:N	2.73	0.51
13:O:188:LYS:HD2	13:O:225:MET:HG3	1.93	0.51
2:B:340:TRP:CZ3	2:B:342:GLY:CA	2.92	0.51
16:V:64:PRO:HD2	16:V:66:ARG:HH22	1.76	0.51
1:A:333:GLU:OE1	3:C:354:GLU:OE2	2.29	0.51
3:C:166:ILE:O	3:C:170:ILE:HG13	2.10	0.51
4:D:175:VAL:HG12	4:D:179:PHE:HE1	1.76	0.51
14:T:3:THR:O	14:T:4:ILE:C	2.48	0.51
2:B:452:THR:HG22	4:D:291:LEU:HD11	1.92	0.51
1:A:176:ILE:O	1:A:179:THR:HB	2.11	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
1:A:116:ILE:HG22	1:A:117:PHE:N	2.25	0.51
3:C:343:ARG:NH1	3:C:345:PRO:HD3	2.25	0.51
25:E:84:HEM:C4A	6:F:19:TRP:CH2	2.99	0.51
4:D:52:THR:O	4:D:67:TYR:CD1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:30:LYS:HG2	16:V:118:HIS:CD2	2.46	0.51
4:D:298:PHE:O	4:D:299:ILE:C	2.49	0.51
19:Z:23:VAL:O	19:Z:27:TYR:CD1	2.64	0.51
3:C:318:LEU:HD21	3:C:340:TYR:CB	2.40	0.51
4:D:261:PHE:CD2	14:T:24:ARG:NH2	2.79	0.51
13:O:27:ARG:O	13:O:29:ALA:N	2.44	0.51
4:D:71:CYS:HB2	4:D:76:VAL:HG22	1.89	0.51
2:B:62:VAL:HG13	23:B:518:CLA:O1D	2.11	0.51
4:D:199:MET:O	4:D:202:ALA:HB3	2.11	0.51
2:B:321:LYS:NZ	4:D:297:ASP:OD2	2.42	0.51
14:T:20:ALA:O	14:T:24:ARG:HB2	2.11	0.51
11:L:4:ASN:N	11:L:5:PRO:CD	2.72	0.51
2:B:402:TYR:N	2:B:402:TYR:CD1	2.78	0.51
4:D:82:ALA:H	4:D:85:MET:CE	2.24	0.51
16:V:33:PHE:CD2	16:V:37:CYS:SG	3.04	0.50
1:A:210:LEU:HD13	24:D:355:PHO:C1D	2.40	0.50
23:A:348:CLA:CAB	23:A:350:CLA:HMD2	2.41	0.50
3:C:37:ALA:HA	23:C:483:CLA:HBA1	1.92	0.50
16:V:133:GLY:O	16:V:137:TYR:CA	2.59	0.50
2:B:420:TYR:O	2:B:424:ALA:N	2.44	0.50
4:D:54:PHE:HB3	5:E:46:PHE:CD1	2.46	0.50
1:A:126:TYR:O	1:A:130:GLN:HG3	2.11	0.50
1:A:57:PRO:CB	1:A:68:SER:HB3	2.37	0.50
1:A:316:THR:HB	4:D:75:THR:CG2	2.40	0.50
1:A:317:TRP:N	4:D:63:LEU:HD13	2.26	0.50
3:C:123:ALA:CB	19:Z:47:TRP:CH2	2.91	0.50
2:B:340:TRP:CH2	2:B:342:GLY:HA3	2.45	0.50
3:C:301:PHE:N	3:C:301:PHE:CD2	2.79	0.50
1:A:316:THR:HB	4:D:75:THR:HG21	1.93	0.50
1:A:183:MET:CE	23:A:349:CLA:HMD3	2.41	0.50
3:C:305:THR:H	3:C:308:GLU:CG	2.19	0.50
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.46	0.50
13:O:54:GLU:OE1	13:O:231:HIS:CD2	2.64	0.50
3:C:420:VAL:HG12	3:C:425:TRP:CD1	2.46	0.50
16:V:64:PRO:O	16:V:66:ARG:NH1	2.44	0.50
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.94	0.50
13:O:41:ALA:N	13:O:83:GLY:O	2.43	0.50
1:A:177:SER:O	1:A:180:PHE:HB2	2.12	0.50
13:O:121:THR:HG21	13:O:148:VAL:CG2	2.26	0.50
1:A:237:TYR:CE2	1:A:245:THR:HG23	2.46	0.50
15:U:42:VAL:HG12	15:U:45:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:LYS:NZ	15:U:45:GLU:OE2	2.45	0.50
2:B:246:PHE:CE1	2:B:463:PHE:HB2	2.42	0.50
15:U:85:TYR:N	15:U:85:TYR:CD2	2.75	0.50
3:C:377:LEU:HD21	13:O:99:ASP:CG	2.32	0.50
3:C:350:ILE:HG22	3:C:351:PHE:N	2.27	0.50
1:A:148:SER:HB2	1:A:284:TRP:CH2	2.37	0.50
1:A:278:TRP:CB	1:A:279:PRO:HD3	2.35	0.50
1:A:334:ARG:NH1	13:O:159:PRO:HA	2.25	0.50
8:I:6:ILE:O	8:I:10:ILE:HG13	2.11	0.50
6:F:31:PHE:HD2	6:F:31:PHE:C	2.15	0.50
3:C:183:GLY:O	3:C:184:GLY:O	2.30	0.50
1:A:200:LEU:O	1:A:203:ALA:HB3	2.11	0.50
6:F:40:GLN:OE1	9:J:28:PHE:CD2	2.65	0.50
1:A:180:PHE:N	1:A:180:PHE:CD1	2.77	0.50
1:A:78:ILE:HD13	11:L:34:TYR:OH	2.10	0.50
15:U:105:LEU:O	15:U:109:LEU:N	2.41	0.50
15:U:108:ASN:O	15:U:109:LEU:C	2.50	0.50
15:U:54:LYS:HD2	15:U:113:THR:OG1	2.11	0.50
1:A:237:TYR:CD2	1:A:241:GLN:OE1	2.65	0.50
13:O:120:PHE:HE1	13:O:235:ILE:HG21	1.77	0.50
16:V:37:CYS:O	16:V:38:ALA:C	2.50	0.50
16:V:75:TYR:CE2	16:V:80:THR:N	2.70	0.50
2:B:136:PRO:CD	2:B:231:MET:HE1	2.40	0.50
2:B:240:SER:OG	2:B:241:SER:N	2.44	0.50
2:B:29:LEU:HD11	28:B:529:BCR:H331	1.94	0.50
4:D:200:GLY:O	4:D:204:VAL:HG23	2.11	0.50
3:C:287:THR:O	3:C:290:VAL:HB	2.11	0.50
3:C:302:TYR:O	3:C:422:PRO:HD2	2.12	0.50
23:C:487:CLA:HBC2	23:C:487:CLA:HHD	1.94	0.50
4:D:222:LEU:HD22	4:D:243:THR:HB	1.93	0.50
11:L:6:ASN:HD22	11:L:6:ASN:H	1.59	0.50
4:D:261:PHE:HD2	14:T:24:ARG:NH2	2.10	0.50
13:O:168:TYR:CZ	13:O:172:ILE:HD11	2.46	0.50
1:A:95:PRO:HG2	1:A:98:GLU:CB	2.41	0.50
1:A:24:THR:CB	4:D:251:ARG:NH2	2.74	0.50
19:Z:5:PHE:CE2	19:Z:54:VAL:HG13	2.47	0.50
6:F:40:GLN:OE1	9:J:28:PHE:HD2	1.95	0.50
1:A:320:ILE:HG21	4:D:333:ASP:OD2	2.12	0.50
2:B:206:GLY:O	2:B:210:ILE:HG13	2.11	0.50
13:O:54:GLU:CD	13:O:231:HIS:CE1	2.85	0.50
1:A:89:ILE:HD13	1:A:94:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:238:VAL:CG1	13:O:239:PHE:N	2.75	0.50
15:U:72:TYR:HD2	15:U:73:PRO:HG3	1.77	0.50
1:A:150:PRO:O	1:A:153:SER:HB3	2.12	0.50
13:O:39:ARG:HA	13:O:245:PRO:HB3	1.92	0.50
1:A:300:PHE:CB	1:A:302:PHE:HE1	2.16	0.50
15:U:84:PRO:C	15:U:85:TYR:CD2	2.85	0.50
4:D:24:ARG:HB3	4:D:26:ARG:HE	1.77	0.50
2:B:205:ALA:O	23:B:518:CLA:H191	2.12	0.49
23:C:487:CLA:H51	23:C:487:CLA:H102	1.94	0.49
3:C:98:GLY:O	3:C:99:VAL:CG2	2.58	0.49
4:D:198:MET:HE3	11:L:30:LEU:HD11	1.90	0.49
13:O:189:ARG:NE	15:U:39:LEU:HD23	2.27	0.49
1:A:183:MET:HB3	23:A:348:CLA:HBC2	1.94	0.49
2:B:244:ALA:O	2:B:247:PHE:HB3	2.11	0.49
23:A:348:CLA:HBB1	23:D:354:CLA:NC	2.27	0.49
3:C:91:HIS:O	3:C:94:THR:HB	2.11	0.49
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.94	0.49
23:C:486:CLA:H192	19:Z:19:MET:HG2	1.94	0.49
6:F:31:PHE:CD2	6:F:31:PHE:C	2.83	0.49
7:H:24:TRP:CE3	7:H:24:TRP:HA	2.46	0.49
3:C:349:ILE:O	3:C:350:ILE:HG13	2.13	0.49
3:C:345:PRO:HB3	13:O:73:ARG:CZ	2.41	0.49
16:V:33:PHE:HD2	16:V:37:CYS:SG	2.34	0.49
4:D:56:THR:CG2	4:D:56:THR:O	2.60	0.49
3:C:278:ALA:HB1	23:C:479:CLA:H142	1.94	0.49
3:C:88:LEU:O	3:C:89:ILE:C	2.50	0.49
1:A:308:ASP:O	1:A:309:ALA:C	2.50	0.49
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.42	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.49
2:B:194:ASN:C	2:B:196:GLY:N	2.66	0.49
16:V:63:THR:HB	16:V:83:ASP:C	2.32	0.49
1:A:215:HIS:HA	26:A:353:PL9:O1	2.12	0.49
3:C:291:TRP:HB3	3:C:292:PHE:HD2	1.74	0.49
3:C:149:TYR:CG	3:C:156:LYS:HG3	2.47	0.49
2:B:472:ARG:NE	2:B:479:PHE:HE1	2.11	0.49
3:C:337:LEU:HA	13:O:104:GLN:HE21	1.75	0.49
13:O:118:LEU:CD2	13:O:233:VAL:HG21	2.43	0.49
5:E:26:ILE:HG13	5:E:27:PRO:CD	2.42	0.49
2:B:297:THR:O	2:B:298:LEU:C	2.48	0.49
5:E:48:THR:HG22	5:E:48:THR:O	2.13	0.49
2:B:12:LEU:CD2	2:B:19:LEU:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:450:ALA:HA	3:C:454:GLY:CA	2.42	0.49
28:K:50:BCR:H333	19:Z:17:PHE:HA	1.94	0.49
2:B:260:SER:H	2:B:263:THR:HB	1.77	0.49
2:B:289:GLN:HA	2:B:289:GLN:OE1	2.12	0.49
1:A:75:ASN:HD22	1:A:79:THR:HG21	1.77	0.49
2:B:61:PHE:O	2:B:64:PRO:HD2	2.12	0.49
3:C:286:ALA:HA	3:C:289:PHE:HB3	1.95	0.49
3:C:285:ILE:CA	23:C:487:CLA:HMB2	2.35	0.49
3:C:138:GLU:CG	3:C:139:THR:N	2.61	0.49
13:O:50:PHE:O	13:O:68:THR:OG1	2.31	0.49
6:F:17:VAL:O	6:F:18:ARG:C	2.50	0.49
2:B:234:ILE:HG23	23:B:513:CLA:HMD2	1.95	0.49
2:B:326:ARG:HG2	12:M:4:ASN:HD22	1.78	0.49
3:C:297:TYR:O	3:C:298:PRO:C	2.51	0.49
3:C:52:ALA:HB1	23:C:486:CLA:HMB3	1.95	0.49
2:B:311:PHE:O	2:B:313:ASP:N	2.45	0.49
11:L:12:LEU:CD1	11:L:16:SER:HB3	2.39	0.49
3:C:66:ALA:HB1	10:K:17:PRO:HB3	1.95	0.49
13:O:65:PHE:CD1	13:O:65:PHE:N	2.81	0.49
15:U:75:LEU:CD2	15:U:101:GLN:HE21	2.25	0.49
2:B:451:PHE:CZ	2:B:455:HIS:ND1	2.80	0.49
1:A:166:GLY:O	1:A:167:SER:HB3	2.13	0.49
5:E:12:ILE:HD12	25:E:84:HEM:CBD	2.42	0.49
2:B:45:PHE:CE2	2:B:46:ASP:O	2.66	0.49
3:C:99:VAL:CG1	3:C:100:GLY:N	2.74	0.49
3:C:109:PHE:CZ	28:C:489:BCR:HC32	2.47	0.49
4:D:195:PRO:CA	4:D:198:MET:HE2	2.38	0.49
2:B:422:ARG:NH2	13:O:169:ASP:HB3	2.28	0.49
2:B:397:VAL:CG1	2:B:398:THR:N	2.76	0.49
2:B:156:PHE:HA	2:B:161:LEU:HB2	1.93	0.49
4:D:188:PHE:HD1	4:D:188:PHE:N	2.10	0.49
5:E:63:PRO:HB3	5:E:78:PHE:CD2	2.47	0.49
1:A:124:SER:O	1:A:127:MET:HB3	2.12	0.49
2:B:24:LEU:HD12	2:B:111:ALA:HA	1.93	0.49
2:B:6:TYR:CE1	2:B:8:VAL:CG2	2.96	0.49
2:B:78:TRP:HZ3	2:B:93:PHE:CE1	2.30	0.49
2:B:326:ARG:HG2	12:M:4:ASN:ND2	2.27	0.49
16:V:128:ASP:HB3	16:V:134:LYS:HG3	1.95	0.49
2:B:305:ILE:O	2:B:341:LYS:HD2	2.12	0.49
8:I:27:ASP:N	8:I:27:ASP:OD1	2.46	0.49
4:D:18:LEU:HD12	17:X:41:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:53:VAL:O	19:Z:57:LEU:HG	2.13	0.49
1:A:255:PHE:CE2	26:A:353:PL9:H152	2.48	0.49
3:C:296:VAL:O	3:C:298:PRO:HD2	2.13	0.49
3:C:71:GLU:C	3:C:73:ALA:H	2.15	0.49
1:A:243:GLU:N	4:D:240:ALA:HB1	2.28	0.49
1:A:301:ASN:O	1:A:301:ASN:CG	2.51	0.49
3:C:97:TRP:HA	3:C:97:TRP:CE3	2.48	0.49
11:L:10:VAL:O	12:M:28:GLN:NE2	2.46	0.49
15:U:47:LEU:C	15:U:49:THR:H	2.16	0.49
3:C:304:PRO:HB3	3:C:395:TYR:CG	2.48	0.49
4:D:20:ASP:O	4:D:21:TRP:C	2.50	0.49
12:M:9:ILE:O	12:M:13:LEU:HG	2.13	0.49
6:F:43:GLN:HG2	6:F:44:ARG:HG2	1.94	0.49
2:B:360:PRO:C	2:B:362:PHE:H	2.16	0.49
2:B:31:ALA:N	23:B:518:CLA:HBC3	2.28	0.48
2:B:62:VAL:O	2:B:63:LEU:C	2.51	0.48
4:D:158:LEU:O	4:D:161:PRO:HD2	2.13	0.48
7:H:23:GLY:C	7:H:25:GLY:N	2.66	0.48
13:O:38:TYR:O	13:O:245:PRO:CG	2.61	0.48
4:D:315:TYR:CE2	4:D:319:LEU:HD11	2.48	0.48
4:D:196:PHE:HD1	4:D:285:GLY:CA	2.25	0.48
9:J:24:ILE:O	9:J:27:LEU:HB3	2.12	0.48
23:B:512:CLA:O2A	23:B:512:CLA:H2A	2.13	0.48
3:C:282:MET:O	3:C:285:ILE:HB	2.13	0.48
23:C:486:CLA:CHB	28:C:488:BCR:H402	2.43	0.48
2:B:475:PHE:O	2:B:476:ARG:C	2.51	0.48
4:D:333:ASP:OD1	4:D:333:ASP:O	2.31	0.48
3:C:186:TYR:CD2	3:C:186:TYR:C	2.86	0.48
1:A:107:TYR:HD1	13:O:115:ARG:CZ	2.26	0.48
1:A:89:ILE:CG1	13:O:73:ARG:NH2	2.71	0.48
15:U:72:TYR:HD2	15:U:73:PRO:CG	2.26	0.48
6:F:22:VAL:O	6:F:26:ALA:HB3	2.13	0.48
6:F:39:MET:O	6:F:41:PHE:N	2.46	0.48
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.48	0.48
3:C:153:ASP:OD1	3:C:155:ASN:OD1	2.30	0.48
1:A:242:GLU:O	4:D:241:GLU:HA	2.12	0.48
3:C:208:VAL:CG1	3:C:209:ILE:N	2.77	0.48
4:D:236:ASN:HB2	4:D:237:PRO:HD2	1.96	0.48
1:A:200:LEU:HD13	1:A:285:PHE:HD1	1.75	0.48
2:B:84:THR:O	2:B:84:THR:CG2	2.61	0.48
4:D:112:THR:HG22	4:D:116:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:347:GLY:O	13:O:16:ALA:HB3	2.13	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CA	2.96	0.48
15:U:76:ALA:O	15:U:80:VAL:HG23	2.14	0.48
3:C:320:ARG:HH11	16:V:49:ASN:HA	1.78	0.48
1:A:211:PHE:CE2	1:A:278:TRP:CD1	3.02	0.48
4:D:154:VAL:HG13	4:D:158:LEU:HD12	1.94	0.48
3:C:71:GLU:C	3:C:73:ALA:N	2.67	0.48
10:K:19:ILE:HD12	28:K:50:BCR:H342	1.95	0.48
3:C:162:GLY:CA	3:C:248:GLY:HA2	2.43	0.48
4:D:343:GLU:OE2	16:V:134:LYS:NZ	2.40	0.48
16:V:133:GLY:O	16:V:137:TYR:N	2.47	0.48
1:A:307:ILE:C	1:A:309:ALA:H	2.16	0.48
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.43	0.48
3:C:316:THR:OG1	3:C:392:ALA:HB1	2.14	0.48
4:D:84:SER:HB2	5:E:66:THR:O	2.13	0.48
13:O:45:LEU:HD11	13:O:215:PHE:CE1	2.48	0.48
23:B:519:CLA:C14	23:D:356:CLA:H11	2.43	0.48
3:C:293:ASN:CG	3:C:423:ARG:NH2	2.67	0.48
2:B:57:ARG:HA	2:B:330:MET:HG3	1.96	0.48
3:C:109:PHE:O	3:C:111:PHE:N	2.47	0.48
3:C:40:ALA:O	3:C:43:ILE:HG23	2.12	0.48
16:V:33:PHE:CD2	16:V:37:CYS:HB2	2.48	0.48
1:A:259:ILE:HD13	26:A:353:PL9:H172	1.95	0.48
23:C:479:CLA:HAB	23:C:479:CLA:C9	2.41	0.48
1:A:224:ILE:CG2	1:A:227:THR:OG1	2.61	0.48
2:B:302:TRP:C	2:B:304:ALA:H	2.17	0.48
3:C:367:GLU:O	3:C:370:ARG:N	2.37	0.48
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.96	0.48
15:U:61:ASN:CB	15:U:126:ASP:O	2.62	0.48
1:A:129:ARG:NH2	4:D:255:GLN:O	2.46	0.48
16:V:13:ASN:C	16:V:13:ASN:OD1	2.51	0.48
15:U:65:PHE:HD1	15:U:76:ALA:HB1	1.78	0.48
16:V:46:THR:HG22	16:V:49:ASN:N	2.19	0.48
16:V:63:THR:O	16:V:80:THR:HG21	2.14	0.48
1:A:180:PHE:HE2	4:D:192:THR:C	2.17	0.48
1:A:284:TRP:HA	1:A:284:TRP:CE3	2.49	0.48
2:B:71:VAL:O	2:B:93:PHE:HE2	1.96	0.48
4:D:129:GLN:HE21	4:D:142:ASN:HB3	1.78	0.48
7:H:29:LEU:O	7:H:33:PHE:HD1	1.96	0.48
2:B:372:ASP:HB3	2:B:376:VAL:HB	1.95	0.48
2:B:360:PRO:O	2:B:362:PHE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:20:VAL:O	6:F:21:ALA:C	2.52	0.48
3:C:372:PRO:O	3:C:373:ASN:HB2	2.14	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CD	2.96	0.48
1:A:150:PRO:O	1:A:153:SER:N	2.47	0.48
1:A:278:TRP:HA	1:A:278:TRP:CE3	2.48	0.48
2:B:199:VAL:O	2:B:203:ILE:HG13	2.13	0.48
2:B:63:LEU:HB3	2:B:64:PRO:CD	2.38	0.48
3:C:289:PHE:CE2	3:C:294:ASN:OD1	2.67	0.48
3:C:294:ASN:O	3:C:295:THR:C	2.50	0.48
13:O:161:GLY:O	13:O:168:TYR:N	2.43	0.48
13:O:71:VAL:CG2	13:O:108:VAL:HG23	2.39	0.48
2:B:91:TRP:CB	23:B:515:CLA:H43	2.44	0.48
1:A:119:PHE:O	1:A:123:ALA:CB	2.62	0.48
13:O:32:ILE:O	13:O:35:SER:N	2.45	0.48
15:U:61:ASN:HB3	15:U:126:ASP:O	2.14	0.48
10:K:26:LEU:HD21	18:N:20:UNK:CB	2.43	0.48
13:O:137:THR:HG23	13:O:138:THR:N	2.29	0.48
13:O:45:LEU:HB3	13:O:79:ASP:HB2	1.96	0.48
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.48	0.48
3:C:282:MET:HA	3:C:285:ILE:CB	2.44	0.48
3:C:282:MET:HE2	23:C:479:CLA:H41	1.95	0.48
8:I:27:ASP:HB2	8:I:28:PRO:HD2	1.94	0.48
15:U:47:LEU:O	15:U:49:THR:N	2.46	0.48
8:I:31:ASN:O	8:I:31:ASN:OD1	2.31	0.48
2:B:235:GLU:HA	2:B:235:GLU:OE1	2.14	0.48
2:B:237:VAL:HG22	23:B:524:CLA:HBC2	1.96	0.48
4:D:152:VAL:CG1	23:D:354:CLA:H43	2.44	0.48
3:C:305:THR:N	3:C:308:GLU:HG3	2.21	0.48
3:C:64:ALA:HB3	3:C:118:HIS:HB3	1.95	0.48
2:B:57:ARG:NH2	2:B:334:ASP:OD2	2.45	0.48
1:A:238:LYS:O	1:A:240:GLY:N	2.47	0.48
1:A:242:GLU:O	1:A:244:GLU:N	2.47	0.48
1:A:307:ILE:HD13	5:E:54:TYR:HB2	1.95	0.48
2:B:385:ARG:HG3	13:O:165:ALA:HA	1.95	0.48
6:F:27:VAL:N	6:F:28:PRO:CD	2.77	0.48
16:V:25:GLN:O	16:V:26:TYR:C	2.52	0.48
15:U:66:ILE:O	15:U:66:ILE:HG22	2.13	0.48
1:A:104:GLU:HG2	1:A:105:TRP:N	2.29	0.47
13:O:46:GLN:O	13:O:238:VAL:O	2.31	0.47
16:V:79:PRO:HG3	16:V:89:ALA:N	2.29	0.47
1:A:284:TRP:HE3	1:A:284:TRP:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HG	2:B:19:LEU:CD1	2.43	0.47
10:K:35:GLY:O	10:K:36:PHE:HB2	2.13	0.47
4:D:90:LEU:HD11	4:D:96:GLU:CB	2.44	0.47
2:B:328:GLY:HA2	2:B:444:ARG:HD3	1.95	0.47
4:D:191:TRP:HE1	4:D:197:HIS:CD2	2.31	0.47
3:C:208:VAL:HG13	3:C:209:ILE:H	1.79	0.47
3:C:370:ARG:HD3	3:C:375:LEU:HD23	1.94	0.47
2:B:148:LEU:O	2:B:151:PHE:HB3	2.13	0.47
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.47
1:A:205:VAL:CG1	4:D:204:VAL:HG12	2.44	0.47
1:A:75:ASN:HD21	4:D:313:THR:HG21	1.79	0.47
2:B:247:PHE:HE1	23:B:521:CLA:H72	1.77	0.47
2:B:326:ARG:C	28:B:529:BCR:H292	2.34	0.47
4:D:178:ILE:O	4:D:182:LEU:HG	2.14	0.47
4:D:243:THR:HG22	4:D:243:THR:O	2.13	0.47
4:D:83:ASN:CB	4:D:336:HIS:ND1	2.77	0.47
13:O:164:LEU:N	13:O:188:LYS:HE2	2.29	0.47
3:C:339:LYS:HB2	3:C:340:TYR:CE1	2.49	0.47
2:B:394:GLN:CD	15:U:52:GLY:HA3	2.34	0.47
3:C:376:ASP:OD1	3:C:378:ASN:HB2	2.14	0.47
1:A:283:VAL:O	1:A:284:TRP:C	2.52	0.47
4:D:80:THR:CG2	4:D:168:PHE:HA	2.43	0.47
23:A:348:CLA:H191	14:T:17:PHE:CZ	2.49	0.47
13:O:193:THR:CG2	13:O:194:LYS:H	2.05	0.47
16:V:53:ASP:OD1	16:V:55:ARG:HB3	2.14	0.47
4:D:348:ARG:NH1	15:U:133:TYR:CE1	2.82	0.47
15:U:61:ASN:HB3	15:U:130:ASN:ND2	2.28	0.47
1:A:42:LEU:O	1:A:46:ILE:HG12	2.14	0.47
6:F:19:TRP:CZ3	6:F:23:HIS:CE1	3.03	0.47
19:Z:19:MET:HE1	19:Z:43:GLY:HA3	1.97	0.47
1:A:225:ARG:CB	2:B:481:GLY:C	2.72	0.47
4:D:337:GLU:O	4:D:338:ASN:HB2	2.14	0.47
1:A:301:ASN:HB2	1:A:303:ASN:HD21	1.79	0.47
3:C:199:ILE:HD12	3:C:234:VAL:CG2	2.39	0.47
17:X:12:ILE:O	17:X:12:ILE:HG13	2.15	0.47
2:B:198:VAL:O	2:B:201:HIS:HB3	2.14	0.47
1:A:161:TYR:CE1	1:A:186:PHE:CE1	3.00	0.47
1:A:202:VAL:HG21	23:A:350:CLA:OBD	2.15	0.47
1:A:180:PHE:CE2	4:D:192:THR:CG2	2.97	0.47
15:U:58:ASN:C	15:U:59:ASN:HD22	2.08	0.47
13:O:81:ILE:CG2	13:O:82:GLN:N	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:LEU:HD21	23:C:474:CLA:H171	1.97	0.47
3:C:249:ILE:O	3:C:252:ILE:HB	2.15	0.47
23:C:478:CLA:H91	23:C:482:CLA:HAA1	1.96	0.47
2:B:264:PRO:HG2	2:B:267:LEU:HB2	1.96	0.47
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.14	0.47
23:B:514:CLA:H202	11:L:27:LEU:HD11	1.96	0.47
13:O:27:ARG:C	13:O:29:ALA:N	2.68	0.47
3:C:392:ALA:O	3:C:396:MET:HB3	2.15	0.47
5:E:74:GLN:O	5:E:78:PHE:CD1	2.67	0.47
13:O:211:ILE:HG22	13:O:212:ALA:H	1.79	0.47
15:U:73:PRO:HG2	16:V:83:ASP:OD1	2.13	0.47
3:C:154:LYS:O	3:C:158:THR:OG1	2.15	0.47
1:A:315:ASN:HB2	4:D:63:LEU:HD23	1.95	0.47
1:A:44:ALA:CB	24:A:351:PHO:H91	2.44	0.47
2:B:464:PHE:HD2	23:B:523:CLA:HAC2	1.79	0.47
15:U:112:PHE:N	15:U:112:PHE:CD1	2.82	0.47
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.97	0.47
1:A:139:MET:HE2	4:D:248:THR:HG21	1.96	0.47
7:H:24:TRP:HA	7:H:24:TRP:HE3	1.78	0.47
5:E:25:THR:HG21	25:E:84:HEM:C4B	2.50	0.47
4:D:71:CYS:HB3	4:D:75:THR:CG2	2.45	0.47
23:B:519:CLA:CBB	4:D:123:ILE:HG12	2.44	0.47
1:A:52:PHE:CD1	1:A:81:ALA:HB2	2.50	0.47
2:B:124:ARG:CG	2:B:125:ASP:N	2.76	0.47
12:M:21:PHE:CD2	12:M:22:LEU:HD23	2.50	0.47
3:C:79:LYS:O	3:C:80:PRO:C	2.53	0.47
23:C:476:CLA:HED3	23:C:483:CLA:H71	1.96	0.47
10:K:31:GLN:HB3	10:K:36:PHE:HD2	1.80	0.47
13:O:39:ARG:HA	13:O:245:PRO:CG	2.44	0.47
1:A:143:ILE:HG21	4:D:253:TRP:HH2	1.80	0.47
2:B:252:VAL:O	2:B:255:THR:HB	2.15	0.47
13:O:118:LEU:HD13	13:O:233:VAL:HG21	1.96	0.47
7:H:54:LEU:HB2	7:H:57:VAL:HB	1.97	0.47
17:X:13:THR:O	17:X:15:SER:N	2.47	0.47
4:D:291:LEU:O	4:D:293:LEU:N	2.48	0.47
15:U:66:ILE:HG23	16:V:82:TYR:CE2	2.49	0.47
13:O:147:ASN:HA	13:O:147:ASN:HD22	1.43	0.47
1:A:210:LEU:HD12	1:A:210:LEU:C	2.36	0.47
2:B:187:PRO:HA	2:B:190:PHE:HB2	1.95	0.47
4:D:153:PHE:CZ	24:D:355:PHO:H92	2.50	0.47
3:C:227:VAL:HG23	3:C:294:ASN:CB	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	23:C:483:CLA:HBA2	1.96	0.47
2:B:11:VAL:HG13	11:L:6:ASN:CB	2.45	0.47
3:C:97:TRP:CZ3	3:C:178:LYS:HE3	2.50	0.47
5:E:23:SER:O	5:E:27:PRO:HG2	2.15	0.47
1:A:261:GLN:CG	1:A:262:TYR:H	2.28	0.47
3:C:343:ARG:HB3	13:O:78:LEU:HD12	1.97	0.47
3:C:320:ARG:HG2	15:U:128:TYR:HE2	1.80	0.47
15:U:72:TYR:CB	15:U:73:PRO:CD	2.91	0.47
9:J:27:LEU:O	9:J:30:TYR:N	2.48	0.47
5:E:14:THR:CB	9:J:8:ILE:HD12	2.43	0.47
1:A:186:PHE:CD2	1:A:192:ILE:CD1	2.85	0.47
2:B:250:PHE:HB3	23:B:521:CLA:H142	1.96	0.47
3:C:305:THR:O	3:C:306:GLY:C	2.52	0.47
23:C:476:CLA:HBD	23:C:486:CLA:CBB	2.45	0.47
19:Z:37:LYS:O	19:Z:41:PHE:CE1	2.68	0.47
13:O:158:ASP:CB	13:O:159:PRO:CD	2.92	0.47
2:B:153:PHE:O	2:B:157:HIS:HB3	2.14	0.47
1:A:271:LEU:O	1:A:275:LEU:HG	2.15	0.47
18:N:31:UNK:HA	19:Z:30:PRO:CG	2.45	0.47
4:D:52:THR:HG23	4:D:76:VAL:CG1	2.44	0.47
2:B:26:HIS:HB2	23:B:513:CLA:HMB2	1.96	0.47
1:A:291:SER:O	1:A:295:PHE:HE1	1.98	0.47
4:D:83:ASN:CG	4:D:336:HIS:HD1	2.16	0.47
13:O:152:ARG:HD2	13:O:156:PHE:CG	2.50	0.47
2:B:340:TRP:HH2	2:B:401:PHE:CD1	2.33	0.47
13:O:54:GLU:OE1	13:O:231:HIS:NE2	2.48	0.47
2:B:390:TYR:O	2:B:391:SER:O	2.33	0.47
7:H:27:THR:N	7:H:28:PRO:CD	2.78	0.47
2:B:224:ARG:O	2:B:228:ALA:HB3	2.15	0.47
13:O:210:GLU:HA	13:O:210:GLU:OE1	2.15	0.47
5:E:70:GLU:O	5:E:71:ALA:C	2.52	0.47
2:B:183:PRO:HB2	2:B:200:ALA:HB2	1.96	0.46
23:B:519:CLA:HBB2	4:D:123:ILE:HG12	1.97	0.46
2:B:45:PHE:CE2	2:B:78:TRP:HZ2	2.32	0.46
13:O:122:VAL:HG12	13:O:122:VAL:O	2.15	0.46
1:A:36:ILE:HD13	23:C:487:CLA:H141	1.97	0.46
16:V:126:LEU:O	16:V:129:LYS:HG3	2.15	0.46
7:H:21:ALA:HB3	7:H:22:PRO:HD2	1.97	0.46
3:C:337:LEU:HA	13:O:104:GLN:NE2	2.29	0.46
2:B:401:PHE:HZ	2:B:420:TYR:CD2	2.34	0.46
2:B:467:ILE:HD13	4:D:126:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:PHE:H	4:D:188:PHE:HD1	1.63	0.46
2:B:234:ILE:O	2:B:235:GLU:C	2.53	0.46
2:B:25:MET:HB3	28:B:529:BCR:C33	2.42	0.46
3:C:292:PHE:H	3:C:292:PHE:HD2	1.56	0.46
23:C:480:CLA:H42	23:C:481:CLA:HBD	1.98	0.46
1:A:230:THR:HG22	1:A:231:GLU:N	2.18	0.46
3:C:412:THR:O	3:C:412:THR:HG22	2.14	0.46
11:L:12:LEU:CD1	11:L:16:SER:CB	2.93	0.46
1:A:288:LEU:O	1:A:289:GLY:C	2.54	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.97	0.46
13:O:180:GLU:HG3	13:O:181:GLU:H	1.80	0.46
2:B:119:ASP:HB3	2:B:121:GLU:HG3	1.97	0.46
28:B:529:BCR:H393	28:B:529:BCR:H371	1.97	0.46
23:C:477:CLA:HMD3	23:C:485:CLA:HAB	1.96	0.46
1:A:31:GLY:O	1:A:33:PHE:N	2.48	0.46
13:O:114:GLU:OE2	13:O:231:HIS:NE2	2.47	0.46
13:O:32:ILE:O	13:O:34:SER:N	2.48	0.46
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.50	0.46
1:A:211:PHE:HE2	1:A:278:TRP:CD1	2.33	0.46
23:B:518:CLA:H61	23:B:518:CLA:H41	1.79	0.46
9:J:19:MET:SD	28:K:50:BCR:H361	2.55	0.46
4:D:325:ILE:O	4:D:329:MET:HB3	2.14	0.46
3:C:108:THR:CG2	10:K:2:LEU:HD23	2.44	0.46
4:D:72:ASN:OD1	4:D:74:LEU:CB	2.63	0.46
15:U:100:ARG:HG3	15:U:104:ILE:HD11	1.98	0.46
3:C:93:ALA:HB3	3:C:301:PHE:CE1	2.51	0.46
2:B:297:THR:O	2:B:300:GLU:N	2.49	0.46
13:O:137:THR:CG2	13:O:138:THR:N	2.77	0.46
16:V:33:PHE:CD2	16:V:37:CYS:CB	2.99	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD1	2.38	0.46
28:K:50:BCR:HC42	19:Z:17:PHE:CD1	2.49	0.46
1:A:33:PHE:CD1	1:A:128:GLY:C	2.89	0.46
3:C:200:THR:O	3:C:201:ASN:ND2	2.32	0.46
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.15	0.46
2:B:163:GLY:O	2:B:165:GLY:N	2.46	0.46
2:B:185:TRP:O	2:B:186:GLY:O	2.33	0.46
3:C:347:GLY:O	13:O:16:ALA:CB	2.64	0.46
13:O:46:GLN:HB3	13:O:46:GLN:HE21	1.50	0.46
1:A:75:ASN:ND2	1:A:79:THR:HG22	2.31	0.46
3:C:281:MET:O	3:C:285:ILE:HG13	2.16	0.46
3:C:71:GLU:O	3:C:75:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:ALA:O	10:K:1:LYS:HA	2.14	0.46
3:C:100:GLY:O	3:C:101:PRO:C	2.53	0.46
1:A:261:GLN:CG	1:A:262:TYR:N	2.78	0.46
2:B:53:ASN:ND2	2:B:58:GLN:OE1	2.49	0.46
3:C:293:ASN:HD22	3:C:293:ASN:N	2.12	0.46
10:K:10:ASP:N	10:K:11:PRO:CD	2.79	0.46
4:D:238:THR:C	4:D:240:ALA:N	2.68	0.46
2:B:307:GLU:O	2:B:308:LYS:C	2.48	0.46
1:A:312:ASN:HB3	5:E:55:TYR:CE1	2.51	0.46
3:C:335:THR:O	3:C:335:THR:HG22	2.16	0.46
4:D:267:LEU:C	4:D:271:MET:HE2	2.35	0.46
4:D:110:LEU:O	4:D:113:PHE:N	2.49	0.46
13:O:238:VAL:HG12	13:O:239:PHE:H	1.78	0.46
16:V:81:THR:O	16:V:83:ASP:N	2.49	0.46
13:O:40:ILE:CG2	13:O:41:ALA:N	2.72	0.46
2:B:234:ILE:HG13	23:B:524:CLA:H191	1.97	0.46
2:B:55:MET:HE1	2:B:80:ILE:HD13	1.97	0.46
4:D:87:HIS:HE1	4:D:162:LEU:HA	1.80	0.46
4:D:165:SER:O	4:D:166:SER:HB3	2.16	0.46
3:C:286:ALA:HA	3:C:289:PHE:CB	2.46	0.46
3:C:99:VAL:HG12	3:C:100:GLY:O	2.15	0.46
2:B:222:PRO:CB	7:H:25:GLY:HA2	2.30	0.46
4:D:329:MET:O	4:D:333:ASP:HB2	2.15	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.97	0.46
1:A:109:GLY:O	1:A:110:GLY:C	2.53	0.46
13:O:40:ILE:O	13:O:243:ILE:HG23	2.16	0.46
2:B:19:LEU:HD21	23:B:524:CLA:H192	1.97	0.46
1:A:218:LEU:CD2	4:D:142:ASN:ND2	2.79	0.46
14:T:7:VAL:O	14:T:10:PHE:HB3	2.16	0.46
3:C:95:LEU:HD11	23:C:480:CLA:HBA2	1.97	0.46
1:A:141:PRO:HG2	3:C:443:TRP:CZ3	2.41	0.46
19:Z:48:ILE:HG12	19:Z:48:ILE:O	2.15	0.46
13:O:152:ARG:NH1	13:O:156:PHE:CE2	2.84	0.46
3:C:406:SER:OG	23:C:475:CLA:O1A	2.34	0.46
16:V:78:ASN:HB2	16:V:96:ARG:NH1	2.28	0.46
11:L:28:ALA:O	11:L:29:LEU:C	2.53	0.46
13:O:28:GLY:HA2	13:O:204:VAL:HB	1.96	0.46
11:L:24:ILE:HD13	12:M:18:PRO:HB2	1.97	0.46
3:C:48:LYS:NZ	23:C:486:CLA:HBA1	2.31	0.46
4:D:148:ALA:HB1	4:D:279:LEU:HB2	1.98	0.46
5:E:43:TYR:CE2	5:E:50:ARG:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:39:LEU:C	15:U:41:ASN:N	2.68	0.46
2:B:346:PHE:O	2:B:354:LEU:HB2	2.16	0.46
13:O:136:ILE:HG22	13:O:204:VAL:HG21	1.98	0.45
1:A:159:LEU:CD2	1:A:163:ILE:HD11	2.46	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG23	2.31	0.45
3:C:210:PHE:O	3:C:213:LEU:HB2	2.16	0.45
2:B:479:PHE:C	2:B:481:GLY:N	2.69	0.45
2:B:280:PHE:O	2:B:281:GLN:C	2.55	0.45
13:O:53:LYS:HB3	13:O:64:GLU:O	2.16	0.45
7:H:53:ILE:HG22	17:X:15:SER:CB	2.45	0.45
18:N:22:UNK:C	18:N:24:UNK:N	2.75	0.45
1:A:112:TYR:CZ	1:A:116:ILE:HD11	2.51	0.45
3:C:341:LEU:HD22	3:C:349:ILE:HG22	1.97	0.45
1:A:169:SER:O	1:A:170:ASP:HB2	2.16	0.45
1:A:172:MET:HE2	23:A:349:CLA:CMC	2.44	0.45
2:B:249:ALA:CB	2:B:459:ALA:HB2	2.47	0.45
23:B:521:CLA:HAB	23:B:527:CLA:CED	2.31	0.45
2:B:19:LEU:HD21	23:B:524:CLA:C19	2.46	0.45
3:C:285:ILE:HD12	23:C:479:CLA:H71	1.98	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG21	2.32	0.45
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.99	0.45
1:A:320:ILE:HD13	4:D:333:ASP:HA	1.98	0.45
16:V:66:ARG:NH1	16:V:66:ARG:HG3	2.31	0.45
15:U:72:TYR:O	15:U:76:ALA:HB3	2.16	0.45
28:B:529:BCR:H361	28:B:529:BCR:H20C	1.66	0.45
4:D:65:SER:OG	4:D:77:ALA:O	2.31	0.45
14:T:17:PHE:O	14:T:18:PHE:C	2.55	0.45
1:A:155:PHE:O	1:A:159:LEU:N	2.41	0.45
11:L:37:ASN:OXT	11:L:37:ASN:ND2	2.50	0.45
19:Z:51:VAL:HG12	19:Z:52:LEU:CD2	2.36	0.45
3:C:151:TRP:C	3:C:153:ASP:N	2.70	0.45
2:B:171:PRO:HD3	7:H:64:LEU:HD11	1.98	0.45
1:A:117:PHE:O	1:A:121:LEU:HG	2.16	0.45
23:A:350:CLA:H121	26:A:353:PL9:C16	2.43	0.45
16:V:30:LYS:HG2	16:V:118:HIS:NE2	2.32	0.45
28:C:488:BCR:C21	10:K:23:PHE:HE2	2.29	0.45
3:C:169:GLY:O	3:C:173:LEU:CD1	2.65	0.45
1:A:14:TRP:CH2	1:A:18:CYS:SG	3.09	0.45
2:B:194:ASN:O	2:B:196:GLY:N	2.50	0.45
19:Z:2:THR:O	19:Z:6:GLN:HG3	2.17	0.45
3:C:313:GLN:O	3:C:317:PHE:HD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:110:MET:CE	13:O:110:MET:H	2.28	0.45
5:E:25:THR:HG21	25:E:84:HEM:C3B	2.51	0.45
1:A:52:PHE:O	1:A:52:PHE:HD2	1.98	0.45
4:D:279:LEU:N	4:D:279:LEU:HD23	2.32	0.45
1:A:303:ASN:HB2	3:C:415:ASN:OD1	2.16	0.45
1:A:63:ILE:HD11	1:A:336:ALA:HB1	1.99	0.45
3:C:178:LYS:O	3:C:178:LYS:CG	2.64	0.45
3:C:435:PHE:O	3:C:436:PHE:C	2.55	0.45
15:U:100:ARG:O	15:U:101:GLN:C	2.55	0.45
2:B:219:VAL:HG12	2:B:220:ARG:N	2.32	0.45
3:C:456:GLU:C	4:D:230:SER:CB	2.85	0.45
5:E:25:THR:HG23	25:E:84:HEM:HAB	1.98	0.45
2:B:113:TRP:HB3	23:B:525:CLA:CED	2.41	0.45
2:B:12:LEU:HG	2:B:19:LEU:HD13	1.97	0.45
14:T:18:PHE:HD2	14:T:19:PHE:CE1	2.35	0.45
10:K:9:PHE:HE2	19:Z:13:VAL:HG21	1.81	0.45
13:O:38:TYR:O	13:O:245:PRO:CB	2.65	0.45
23:C:477:CLA:HAA2	23:C:477:CLA:HBD	1.97	0.45
3:C:336:GLY:O	13:O:104:GLN:HG2	2.17	0.45
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.49	0.45
3:C:229:ASN:HD21	3:C:231:GLU:HB2	1.82	0.45
2:B:422:ARG:H	2:B:422:ARG:HG3	1.57	0.45
16:V:111:ASP:O	16:V:115:ILE:HG13	2.16	0.45
8:I:5:LYS:HG3	8:I:9:TYR:HE1	1.82	0.45
4:D:231:THR:HG22	4:D:232:PHE:H	1.81	0.45
14:T:29:ILE:O	14:T:29:ILE:HG22	2.16	0.45
3:C:297:TYR:CG	3:C:302:TYR:HE1	2.35	0.45
15:U:58:ASN:HB2	15:U:59:ASN:ND2	2.32	0.45
19:Z:19:MET:CE	19:Z:43:GLY:HA3	2.47	0.45
1:A:224:ILE:HD11	1:A:243:GLU:CG	2.47	0.45
1:A:300:PHE:CD2	3:C:404:LEU:HB2	2.52	0.45
4:D:312:GLU:HB2	13:O:159:PRO:HG3	1.97	0.45
2:B:152:GLY:C	23:B:515:CLA:HMC3	2.37	0.45
12:M:8:LEU:HD22	14:T:1:MET:HE1	1.98	0.45
1:A:289:GLY:O	1:A:293:MET:HG3	2.16	0.45
2:B:194:ASN:C	2:B:196:GLY:H	2.20	0.45
1:A:193:LEU:HB3	4:D:179:PHE:CD2	2.52	0.45
2:B:135:LEU:O	2:B:138:MET:N	2.50	0.45
4:D:129:GLN:NE2	4:D:142:ASN:HB3	2.32	0.45
3:C:63:TRP:CZ3	3:C:88:LEU:HD11	2.52	0.45
3:C:80:PRO:O	3:C:81:MET:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:113:THR:CG2	15:U:114:VAL:N	2.78	0.45
3:C:276:LEU:HD23	3:C:440:GLY:O	2.17	0.45
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.99	0.45
2:B:315:ILE:HD13	2:B:359:MET:CE	2.47	0.45
28:B:529:BCR:H403	12:M:6:LEU:HD12	1.99	0.45
3:C:294:ASN:C	3:C:296:VAL:N	2.70	0.45
2:B:271:THR:HG22	2:B:448:ARG:HH11	1.82	0.45
16:V:5:PRO:O	16:V:6:GLU:C	2.55	0.45
2:B:302:TRP:CE3	2:B:343:HIS:HB2	2.52	0.45
2:B:302:TRP:CH2	2:B:343:HIS:CG	3.05	0.45
13:O:163:GLY:HA3	13:O:188:LYS:CE	2.45	0.45
4:D:19:ASP:O	4:D:23:LYS:HG3	2.16	0.45
3:C:395:TYR:O	3:C:396:MET:C	2.55	0.45
2:B:451:PHE:CD1	2:B:451:PHE:O	2.69	0.45
14:T:26:PRO:HA	14:T:27:PRO:HD3	1.83	0.45
1:A:161:TYR:O	1:A:162:PRO:C	2.54	0.45
1:A:307:ILE:HG12	1:A:314:ILE:HD11	1.92	0.45
19:Z:33:TRP:CE3	19:Z:37:LYS:HD3	2.30	0.45
3:C:205:ASP:O	3:C:208:VAL:HG12	2.17	0.45
1:A:87:ASN:HD21	3:C:357:ARG:NH1	2.08	0.45
1:A:235:TYR:HA	4:D:265:ARG:HH22	1.77	0.45
2:B:156:PHE:HB2	23:B:515:CLA:HAC1	1.99	0.45
16:V:64:PRO:HB2	16:V:65:PRO:HD2	1.98	0.45
1:A:38:ILE:O	1:A:42:LEU:HG	2.17	0.45
13:O:140:THR:HG22	13:O:201:VAL:HB	1.98	0.44
5:E:25:THR:O	5:E:28:ALA:HB3	2.16	0.44
9:J:8:ILE:HA	9:J:9:PRO:HD3	1.82	0.44
1:A:192:ILE:O	1:A:193:LEU:C	2.55	0.44
2:B:234:ILE:O	2:B:237:VAL:N	2.43	0.44
1:A:295:PHE:HB3	3:C:291:TRP:CH2	2.53	0.44
3:C:105:VAL:CG1	3:C:107:ASP:O	2.65	0.44
3:C:339:LYS:NZ	15:U:125:GLY:HA3	2.32	0.44
5:E:56:ALA:CB	5:E:82:LEU:HD23	2.38	0.44
16:V:25:GLN:O	16:V:28:GLU:N	2.51	0.44
2:B:258:TYR:N	2:B:258:TYR:CD2	2.85	0.44
13:O:68:THR:HA	13:O:110:MET:CE	2.47	0.44
23:A:350:CLA:HMA1	24:D:355:PHO:C20	2.47	0.44
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.83	0.44
5:E:10:SER:HA	5:E:13:ILE:CD1	2.27	0.44
1:A:224:ILE:HG13	1:A:245:THR:O	2.18	0.44
8:I:7:THR:HA	8:I:10:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:LEU:CB	4:D:91:LEU:HD21	2.47	0.44
1:A:95:PRO:CG	1:A:98:GLU:HB2	2.48	0.44
3:C:435:PHE:O	3:C:438:LEU:N	2.48	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
13:O:211:ILE:CG2	13:O:212:ALA:H	2.29	0.44
4:D:68:LEU:HD23	5:E:48:THR:HB	1.99	0.44
2:B:190:PHE:CE1	23:B:527:CLA:CED	3.01	0.44
4:D:156:VAL:O	4:D:161:PRO:HD3	2.17	0.44
3:C:296:VAL:HG21	23:C:479:CLA:HMA2	1.99	0.44
4:D:300:SER:N	11:L:37:ASN:OD1	2.51	0.44
10:K:27:ALA:O	10:K:31:GLN:HG2	2.18	0.44
1:A:29:TYR:CE1	1:A:31:GLY:CA	2.93	0.44
13:O:153:THR:CG2	13:O:154:ALA:N	2.81	0.44
4:D:281:MET:HE1	4:D:284:ILE:HD12	1.99	0.44
3:C:376:ASP:OD1	3:C:378:ASN:N	2.50	0.44
2:B:31:ALA:HB2	23:B:518:CLA:CBC	2.47	0.44
3:C:220:GLY:H	23:C:487:CLA:HBC1	1.82	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
4:D:102:THR:HG23	5:E:46:PHE:C	2.38	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HA	1.98	0.44
13:O:218:GLU:HG3	13:O:233:VAL:O	2.17	0.44
13:O:55:GLU:HG2	13:O:64:GLU:HG3	2.00	0.44
4:D:91:LEU:CD2	4:D:91:LEU:N	2.73	0.44
3:C:311:GLN:NE2	3:C:355:THR:O	2.50	0.44
3:C:136:GLY:HA2	3:C:137:PRO:HD3	1.77	0.44
2:B:436:THR:O	2:B:437:LEU:HD23	2.17	0.44
1:A:104:GLU:O	1:A:105:TRP:C	2.56	0.44
16:V:79:PRO:HG3	16:V:89:ALA:HA	1.99	0.44
9:J:25:VAL:O	9:J:26:GLY:C	2.54	0.44
3:C:286:ALA:O	3:C:290:VAL:N	2.49	0.44
3:C:50:LEU:HD23	23:C:482:CLA:HMD3	2.00	0.44
4:D:88:SER:CB	5:E:68:ARG:NH2	2.74	0.44
1:A:238:LYS:O	1:A:239:PHE:C	2.55	0.44
2:B:478:VAL:O	2:B:481:GLY:N	2.47	0.44
4:D:296:TYR:O	4:D:296:TYR:CG	2.70	0.44
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.52	0.44
2:B:397:VAL:CG1	2:B:398:THR:H	2.28	0.44
13:O:55:GLU:HB3	13:O:61:GLN:NE2	2.32	0.44
2:B:370:LEU:HD12	2:B:379:ALA:HB3	1.99	0.44
16:V:92:HIS:CE1	16:V:93:PRO:HD2	2.52	0.44
14:T:13:ILE:HG22	14:T:13:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HD21	2:B:22:ALA:CB	2.48	0.44
4:D:158:LEU:C	4:D:161:PRO:HD2	2.37	0.44
11:L:24:ILE:HD11	12:M:18:PRO:HB2	2.00	0.44
3:C:287:THR:HG23	3:C:427:ALA:HA	1.99	0.44
3:C:85:GLY:C	3:C:86:LEU:HD23	2.37	0.44
3:C:270:ALA:O	3:C:274:TYR:CE1	2.71	0.44
1:A:230:THR:CG2	1:A:231:GLU:H	2.20	0.44
1:A:330:VAL:HG12	4:D:348:ARG:HA	2.00	0.44
15:U:133:TYR:O	15:U:134:LYS:OXT	2.36	0.44
1:A:97:TRP:CZ3	8:I:8:VAL:HG21	2.49	0.44
4:D:42:TYR:CZ	6:F:24:THR:CG2	3.00	0.44
19:Z:39:LEU:HG	19:Z:39:LEU:H	1.39	0.44
1:A:269:ARG:HD3	1:A:270:SER:N	2.32	0.44
1:A:107:TYR:HD1	13:O:115:ARG:NH1	2.16	0.44
15:U:62:ILE:CG2	15:U:76:ALA:HB1	2.47	0.44
1:A:149:ALA:CA	1:A:284:TRP:CZ3	3.00	0.44
1:A:213:ALA:O	1:A:217:SER:CB	2.65	0.44
4:D:57:SER:CB	4:D:79:SER:HB2	2.48	0.44
1:A:78:ILE:CD1	11:L:34:TYR:CE1	2.99	0.44
3:C:217:PRO:HA	3:C:222:GLY:HA2	2.00	0.44
23:C:476:CLA:H61	23:C:483:CLA:H72	1.99	0.44
10:K:6:TYR:CD1	10:K:6:TYR:N	2.86	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HB3	2.52	0.44
19:Z:5:PHE:HD2	19:Z:5:PHE:O	2.01	0.44
3:C:93:ALA:CB	3:C:301:PHE:CE1	3.01	0.44
2:B:350:GLU:N	2:B:350:GLU:OE1	2.50	0.44
4:D:28:VAL:HG12	4:D:28:VAL:O	2.17	0.44
1:A:315:ASN:O	4:D:63:LEU:HD22	2.16	0.44
3:C:201:ASN:CG	3:C:201:ASN:O	2.57	0.44
13:O:33:ASP:O	13:O:36:GLN:HB2	2.17	0.44
4:D:350:ASN:HD22	4:D:351:ALA:N	2.16	0.44
4:D:350:ASN:ND2	4:D:351:ALA:N	2.65	0.44
3:C:317:PHE:O	3:C:321:ASP:OD1	2.36	0.44
26:A:353:PL9:H23	26:A:353:PL9:H271	1.42	0.44
2:B:200:ALA:C	23:B:521:CLA:HBB1	2.38	0.44
23:B:519:CLA:H142	23:D:356:CLA:H11	1.99	0.44
4:D:161:PRO:HG3	4:D:170:ALA:CB	2.46	0.44
3:C:89:ILE:HB	3:C:90:PRO:CD	2.44	0.44
3:C:157:MET:HE2	3:C:160:ILE:CD1	2.34	0.44
3:C:274:TYR:HB3	23:C:485:CLA:C3B	2.48	0.44
5:E:68:ARG:NH1	7:H:50:SER:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:PHE:O	4:D:149:PRO:HD2	2.18	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
4:D:101:PHE:O	4:D:102:THR:C	2.56	0.44
1:A:54:ALA:O	1:A:55:ALA:C	2.55	0.44
4:D:110:LEU:O	4:D:111:TRP:C	2.55	0.44
3:C:299:SER:O	3:C:303:GLY:O	2.36	0.44
15:U:75:LEU:CD2	15:U:101:GLN:NE2	2.81	0.44
13:O:31:PRO:HB2	13:O:33:ASP:H	1.83	0.44
13:O:190:PHE:CE1	15:U:120:ALA:HA	2.53	0.44
6:F:40:GLN:NE2	9:J:27:LEU:O	2.48	0.43
1:A:187:GLN:HE21	1:A:187:GLN:HB3	1.50	0.43
1:A:41:LEU:HD13	24:A:351:PHO:C2	2.48	0.43
3:C:243:ILE:HG22	23:C:474:CLA:HMC1	2.00	0.43
2:B:264:PRO:HD2	2:B:268:PHE:HE1	1.83	0.43
1:A:341:LEU:HD21	15:U:134:LYS:HZ2	1.81	0.43
1:A:326:LEU:HD13	3:C:412:THR:CG2	2.39	0.43
5:E:33:GLY:O	5:E:36:PHE:N	2.48	0.43
15:U:47:LEU:HB3	15:U:51:TYR:HD1	1.83	0.43
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.18	0.43
2:B:360:PRO:C	2:B:362:PHE:N	2.71	0.43
3:C:350:ILE:CG2	3:C:351:PHE:N	2.81	0.43
2:B:234:ILE:HG21	23:B:524:CLA:H193	2.00	0.43
12:M:16:LEU:O	12:M:17:VAL:C	2.53	0.43
15:U:88:VAL:HG12	15:U:109:LEU:CD1	2.48	0.43
16:V:134:LYS:C	16:V:137:TYR:H	2.22	0.43
4:D:101:PHE:O	4:D:104:TRP:N	2.52	0.43
13:O:32:ILE:HA	13:O:133:VAL:HG11	2.00	0.43
3:C:189:TRP:O	3:C:190:ALA:O	2.36	0.43
13:O:182:LEU:O	13:O:183:ALA:C	2.55	0.43
13:O:243:ILE:CG2	13:O:244:GLU:N	2.81	0.43
2:B:18:ARG:NH1	2:B:115:TRP:O	2.50	0.43
4:D:178:ILE:O	4:D:181:PHE:HB3	2.19	0.43
1:A:160:ILE:H	1:A:160:ILE:HG13	1.66	0.43
3:C:48:LYS:HD3	3:C:133:ALA:O	2.18	0.43
5:E:55:TYR:O	16:V:1:ALA:HB2	2.17	0.43
2:B:418:LYS:O	2:B:419:SER:C	2.55	0.43
7:H:59:VAL:O	7:H:59:VAL:CG1	2.64	0.43
2:B:156:PHE:CD1	2:B:156:PHE:N	2.86	0.43
2:B:91:TRP:HB3	23:B:515:CLA:H43	2.00	0.43
3:C:187:ASP:OD1	3:C:189:TRP:N	2.51	0.43
16:V:35:TYR:O	16:V:35:TYR:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:HIS:C	5:E:24:ILE:N	2.70	0.43
5:E:24:ILE:O	5:E:24:ILE:HG22	2.18	0.43
12:M:20:VAL:O	12:M:21:PHE:C	2.55	0.43
1:A:159:LEU:O	1:A:160:ILE:C	2.56	0.43
10:K:9:PHE:N	10:K:9:PHE:CD1	2.86	0.43
2:B:302:TRP:C	2:B:304:ALA:N	2.71	0.43
7:H:57:VAL:O	7:H:57:VAL:HG13	2.17	0.43
5:E:30:PHE:C	5:E:30:PHE:CD2	2.91	0.43
3:C:191:PRO:O	3:C:193:GLY:N	2.48	0.43
3:C:394:GLU:O	3:C:397:THR:HB	2.18	0.43
13:O:57:LYS:O	13:O:57:LYS:HG3	2.18	0.43
1:A:339:PHE:CE1	3:C:314:ALA:HA	2.53	0.43
1:A:162:PRO:CG	1:A:171:GLY:HA2	2.48	0.43
4:D:181:PHE:O	4:D:182:LEU:C	2.57	0.43
23:D:356:CLA:H12	7:H:42:LEU:CD2	2.48	0.43
3:C:94:THR:C	3:C:96:GLY:N	2.71	0.43
3:C:223:TRP:HD1	3:C:224:ILE:N	2.14	0.43
4:D:218:VAL:O	4:D:220:ASN:N	2.52	0.43
19:Z:13:VAL:HG13	19:Z:17:PHE:CE1	2.54	0.43
3:C:155:ASN:O	3:C:159:THR:OG1	2.27	0.43
3:C:167:VAL:CG1	23:C:482:CLA:H11	2.48	0.43
2:B:479:PHE:C	2:B:481:GLY:H	2.21	0.43
4:D:189:HIS:CE1	4:D:294:ARG:HH21	2.36	0.43
19:Z:42:LEU:O	19:Z:46:LEU:HB2	2.18	0.43
13:O:34:SER:O	13:O:35:SER:C	2.57	0.43
13:O:34:SER:C	13:O:36:GLN:N	2.69	0.43
4:D:273:PHE:O	4:D:277:THR:HB	2.17	0.43
2:B:234:ILE:HG23	23:B:524:CLA:H193	2.01	0.43
2:B:63:LEU:HD12	2:B:63:LEU:HA	1.87	0.43
4:D:195:PRO:HA	4:D:198:MET:HE3	1.95	0.43
4:D:195:PRO:O	4:D:199:MET:HG3	2.19	0.43
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.18	0.43
2:B:311:PHE:C	2:B:313:ASP:N	2.71	0.43
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.84	0.43
6:F:32:PHE:CE1	28:F:48:BCR:H14C	2.54	0.43
2:B:354:LEU:CD2	2:B:378:LYS:HG3	2.48	0.43
23:A:350:CLA:HMD3	4:D:182:LEU:HD11	2.01	0.43
2:B:327:THR:O	2:B:329:PRO:HD3	2.18	0.43
1:A:295:PHE:O	3:C:291:TRP:CH2	2.72	0.43
10:K:31:GLN:HB3	10:K:36:PHE:CD2	2.54	0.43
2:B:252:VAL:HG22	23:B:517:CLA:O1A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:22:LEU:CD2	4:D:32:TRP:CE3	3.01	0.43
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.33	0.43
16:V:22:THR:N	16:V:25:GLN:NE2	2.65	0.43
2:B:297:THR:HB	2:B:299:GLU:OE1	2.18	0.43
1:A:290:ILE:HD11	23:A:348:CLA:OBD	2.19	0.43
23:A:350:CLA:HMA1	24:D:355:PHO:H201	2.00	0.43
14:T:10:PHE:HE2	14:T:14:ILE:HD11	1.83	0.43
19:Z:7:LEU:O	19:Z:11:ALA:CB	2.63	0.43
3:C:256:PRO:HA	23:C:474:CLA:HED3	2.01	0.43
13:O:58:ASN:O	13:O:59:LYS:HB2	2.19	0.43
2:B:265:ILE:C	2:B:267:LEU:H	2.22	0.43
11:L:6:ASN:N	11:L:6:ASN:HD22	2.15	0.43
13:O:126:VAL:O	13:O:126:VAL:HG12	2.18	0.43
1:A:301:ASN:HD22	1:A:301:ASN:N	2.16	0.43
1:A:234:ASN:C	4:D:265:ARG:HH12	2.22	0.43
10:K:34:VAL:CG1	10:K:34:VAL:O	2.64	0.43
14:T:1:MET:C	14:T:3:THR:N	2.68	0.43
3:C:377:LEU:HD21	13:O:99:ASP:OD2	2.18	0.43
3:C:355:THR:OG1	3:C:355:THR:O	2.37	0.43
2:B:135:LEU:N	2:B:136:PRO:HD2	2.33	0.43
2:B:237:VAL:CG2	23:B:524:CLA:HBC2	2.49	0.43
1:A:29:TYR:CE1	1:A:31:GLY:HA3	2.53	0.43
2:B:149:LEU:O	2:B:150:CYS:C	2.56	0.43
2:B:88:PRO:O	2:B:89:GLY:C	2.57	0.43
7:H:49:ASN:CG	7:H:49:ASN:O	2.57	0.43
1:A:196:PRO:HA	1:A:199:GLN:HB2	2.01	0.43
4:D:21:TRP:O	4:D:26:ARG:NH2	2.40	0.43
16:V:112:LEU:HA	16:V:112:LEU:HD23	1.80	0.43
1:A:104:GLU:O	1:A:107:TYR:N	2.41	0.43
1:A:89:ILE:HD13	1:A:94:TYR:CD1	2.54	0.43
5:E:48:THR:O	5:E:49:PRO:C	2.57	0.43
1:A:168:PHE:O	1:A:169:SER:C	2.57	0.43
2:B:6:TYR:HE1	2:B:8:VAL:HG21	1.83	0.43
4:D:204:VAL:HG21	23:D:354:CLA:HMA1	2.01	0.43
4:D:55:VAL:O	4:D:65:SER:HB3	2.18	0.43
16:V:100:ILE:O	16:V:102:PRO:HD3	2.19	0.43
23:C:484:CLA:C4B	28:C:489:BCR:H393	2.48	0.43
10:K:8:ILE:H	10:K:8:ILE:HG13	1.68	0.43
13:O:152:ARG:HD2	13:O:156:PHE:CZ	2.54	0.43
5:E:33:GLY:O	5:E:36:PHE:HB3	2.18	0.43
16:V:35:TYR:C	16:V:35:TYR:CD2	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:87:SER:HB3	15:U:90:ASP:OD1	2.19	0.43
4:D:328:TRP:CE2	4:D:346:LEU:HD13	2.54	0.43
16:V:79:PRO:CB	16:V:88:ILE:HG12	2.44	0.42
23:B:522:CLA:H171	23:B:525:CLA:HMD1	1.99	0.42
15:U:58:ASN:C	15:U:59:ASN:ND2	2.70	0.42
10:K:10:ASP:O	10:K:11:PRO:C	2.58	0.42
3:C:274:TYR:CE2	23:C:477:CLA:HED3	2.53	0.42
11:L:6:ASN:OD1	11:L:8:GLN:HG2	2.19	0.42
2:B:368:VAL:HG22	2:B:425:ILE:HD12	2.01	0.42
13:O:33:ASP:O	13:O:37:THR:N	2.50	0.42
18:N:31:UNK:HA	19:Z:30:PRO:HG2	2.01	0.42
16:V:104:MET:HE3	16:V:107:LEU:HD12	2.00	0.42
13:O:43:LEU:HD11	13:O:239:PHE:CD1	2.53	0.42
25:E:84:HEM:O1D	6:F:18:ARG:NE	2.48	0.42
1:A:150:PRO:O	1:A:151:LEU:C	2.55	0.42
13:O:122:VAL:O	13:O:125:LEU:HB2	2.19	0.42
2:B:331:ASN:C	2:B:333:GLY:H	2.21	0.42
3:C:116:VAL:HG11	28:C:489:BCR:H321	2.00	0.42
3:C:276:LEU:HD13	23:C:483:CLA:HBB1	2.01	0.42
10:K:30:TRP:HE3	10:K:31:GLN:HE21	1.65	0.42
4:D:221:THR:HG22	4:D:245:SER:H	1.84	0.42
13:O:54:GLU:OE1	13:O:114:GLU:OE1	2.37	0.42
2:B:323:GLY:N	4:D:294:ARG:O	2.49	0.42
4:D:350:ASN:O	4:D:351:ALA:HB3	2.19	0.42
9:J:3:SER:N	18:N:32:UNK:CB	2.82	0.42
5:E:14:THR:HG22	9:J:8:ILE:CD1	2.44	0.42
5:E:14:THR:HG22	9:J:8:ILE:HD12	1.88	0.42
2:B:327:THR:O	2:B:329:PRO:N	2.53	0.42
4:D:170:ALA:O	4:D:171:PRO:C	2.56	0.42
1:A:142:TRP:HH2	1:A:273:PHE:CE1	2.34	0.42
3:C:204:LEU:HD12	3:C:239:TRP:HE1	1.84	0.42
13:O:104:GLN:HB3	13:O:151:TYR:HE1	1.85	0.42
1:A:307:ILE:HG22	1:A:309:ALA:HB3	2.00	0.42
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.02	0.42
3:C:108:THR:HG21	10:K:2:LEU:CG	2.47	0.42
3:C:315:MET:O	3:C:319:ILE:HG13	2.18	0.42
5:E:30:PHE:HD2	5:E:30:PHE:C	2.23	0.42
15:U:51:TYR:HB3	15:U:52:GLY:H	1.34	0.42
15:U:130:ASN:O	15:U:131:GLY:C	2.57	0.42
4:D:316:THR:O	4:D:317:LYS:C	2.58	0.42
1:A:57:PRO:CA	1:A:68:SER:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:LEU:HD23	3:C:324:LEU:HA	1.77	0.42
16:V:37:CYS:HB2	16:V:38:ALA:H	1.71	0.42
23:B:524:CLA:O1D	23:B:524:CLA:H93	2.20	0.42
3:C:81:MET:HE2	3:C:90:PRO:HG3	2.02	0.42
3:C:139:THR:HG23	3:C:139:THR:O	2.19	0.42
3:C:443:TRP:CA	3:C:443:TRP:CE3	3.00	0.42
3:C:168:LEU:HD21	23:C:478:CLA:H72	2.02	0.42
3:C:213:LEU:HD11	23:C:474:CLA:H171	2.01	0.42
3:C:159:THR:HA	3:C:252:ILE:HA	2.01	0.42
1:A:64:ARG:O	13:O:152:ARG:NH2	2.50	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.01	0.42
4:D:126:MET:SD	4:D:143:ALA:O	2.77	0.42
13:O:229:GLU:HA	13:O:230:PRO:HD3	1.91	0.42
1:A:77:ILE:HD11	14:T:6:TYR:CD2	2.54	0.42
1:A:139:MET:CE	4:D:248:THR:CG2	2.97	0.42
4:D:273:PHE:O	4:D:277:THR:CB	2.67	0.42
17:X:17:LYS:O	17:X:20:PHE:N	2.52	0.42
8:I:13:THR:O	8:I:16:VAL:HB	2.19	0.42
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.49	0.42
2:B:245:VAL:HG22	23:B:513:CLA:H172	2.02	0.42
15:U:108:ASN:O	15:U:110:GLU:N	2.53	0.42
3:C:48:LYS:HZ2	23:C:486:CLA:HBA1	1.83	0.42
9:J:15:THR:CA	28:K:50:BCR:H372	2.45	0.42
4:D:249:ALA:O	4:D:252:PHE:HB3	2.20	0.42
1:A:55:ALA:HA	1:A:56:PRO:HD3	1.92	0.42
3:C:97:TRP:CE3	3:C:178:LYS:CE	3.02	0.42
6:F:32:PHE:CD1	28:F:48:BCR:H14C	2.54	0.42
1:A:297:LEU:CD2	3:C:428:THR:HG21	2.50	0.42
2:B:168:VAL:CG1	2:B:169:SER:N	2.83	0.42
4:D:20:ASP:O	4:D:24:ARG:N	2.52	0.42
2:B:49:ASP:HA	2:B:50:PRO:HD3	1.87	0.42
25:V:138:HEM:HMC1	25:V:138:HEM:HBC2	2.02	0.42
1:A:180:PHE:CE2	4:D:192:THR:O	2.68	0.42
1:A:76:ASN:CB	14:T:2:GLU:OE2	2.64	0.42
1:A:142:TRP:CH2	1:A:273:PHE:HE1	2.35	0.42
3:C:37:ALA:O	3:C:38:GLY:C	2.57	0.42
9:J:15:THR:HG23	28:K:50:BCR:H372	2.01	0.42
19:Z:47:TRP:HE1	19:Z:51:VAL:HG23	1.85	0.42
1:A:31:GLY:HA3	1:A:132:GLU:OE2	2.19	0.42
10:K:16:LEU:O	10:K:18:VAL:N	2.52	0.42
2:B:277:SER:O	2:B:278:SER:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLY:O	2:B:39:LEU:HG	2.19	0.42
2:B:106:LEU:HB3	23:B:522:CLA:H121	2.02	0.42
23:B:523:CLA:HAA2	23:B:523:CLA:HBD	2.01	0.42
1:A:160:ILE:O	1:A:164:GLY:N	2.46	0.42
16:V:29:GLY:HA3	16:V:118:HIS:HB2	2.02	0.42
3:C:38:GLY:HA3	23:C:486:CLA:C1D	2.50	0.42
4:D:146:PHE:O	4:D:150:ILE:HG13	2.20	0.42
2:B:340:TRP:CE3	2:B:342:GLY:CA	3.02	0.42
23:B:511:CLA:H102	7:H:37:PHE:CD1	2.55	0.42
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.02	0.42
7:H:51:THR:CG2	7:H:51:THR:O	2.68	0.42
4:D:116:LEU:O	4:D:120:PHE:HD1	2.03	0.42
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.42
1:A:339:PHE:HB3	3:C:313:GLN:OE1	2.19	0.42
16:V:81:THR:HB	16:V:83:ASP:OD1	2.19	0.42
9:J:30:TYR:O	9:J:33:TYR:HB2	2.20	0.42
4:D:186:GLN:NE2	4:D:192:THR:OG1	2.53	0.42
4:D:80:THR:CG2	4:D:81:PRO:HD2	2.49	0.42
3:C:60:ILE:O	23:C:480:CLA:HMD3	2.20	0.42
1:A:142:TRP:O	1:A:145:VAL:N	2.49	0.42
9:J:19:MET:HG2	28:K:50:BCR:H361	2.01	0.42
3:C:210:PHE:O	3:C:214:LEU:HG	2.20	0.42
1:A:63:ILE:HG23	3:C:335:THR:HG23	1.99	0.42
1:A:73:TYR:CD2	1:A:73:TYR:N	2.88	0.42
2:B:463:PHE:CZ	2:B:467:ILE:HD11	2.54	0.42
23:C:475:CLA:H51	28:J:53:BCR:H342	2.01	0.42
11:L:36:PHE:C	12:M:3:VAL:HG23	2.40	0.42
2:B:399:VAL:CG2	2:B:417:VAL:HG13	2.49	0.42
4:D:30:VAL:HG22	4:D:38:PHE:CE1	2.53	0.42
4:D:281:MET:O	4:D:284:ILE:HB	2.19	0.42
2:B:451:PHE:CZ	2:B:455:HIS:CE1	3.08	0.42
15:U:67:GLN:O	15:U:68:TYR:CD2	2.73	0.42
9:J:17:ALA:O	9:J:20:GLY:N	2.53	0.42
2:B:366:PHE:HA	2:B:367:PRO:HD3	1.71	0.42
23:B:512:CLA:OBD	23:B:520:CLA:HHC	2.20	0.42
23:B:516:CLA:H111	23:B:522:CLA:H42	2.00	0.42
14:T:18:PHE:CD2	14:T:19:PHE:CE1	3.08	0.42
3:C:307:PRO:O	3:C:308:GLU:C	2.57	0.42
3:C:289:PHE:CD1	23:C:487:CLA:HBB2	2.55	0.42
19:Z:9:LEU:HD12	19:Z:9:LEU:HA	1.83	0.42
3:C:259:TRP:HZ3	23:C:474:CLA:O2A	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:ARG:NH1	7:H:50:SER:HB3	2.34	0.42
2:B:56:TRP:HH2	2:B:312:TYR:HE2	1.67	0.42
2:B:325:PHE:O	2:B:328:GLY:N	2.52	0.42
1:A:21:VAL:HG13	1:A:30:VAL:O	2.19	0.42
3:C:173:LEU:HA	3:C:176:VAL:CG2	2.49	0.42
3:C:425:TRP:CE2	23:C:475:CLA:HBA2	2.54	0.42
13:O:198:SER:O	13:O:199:LEU:HD23	2.20	0.42
4:D:43:LEU:HD22	28:F:48:BCR:H323	2.02	0.42
2:B:223:GLN:HG2	2:B:227:LYS:HG3	2.01	0.42
1:A:327:GLY:HA3	4:D:324:GLY:O	2.20	0.42
1:A:315:ASN:C	4:D:63:LEU:HD22	2.39	0.42
4:D:67:TYR:C	6:F:39:MET:HE1	2.40	0.42
1:A:214:MET:HG2	26:A:353:PL9:HC8	2.02	0.42
2:B:19:LEU:HD23	23:B:524:CLA:H201	2.02	0.42
26:D:357:PL9:H38	14:T:18:PHE:CB	2.44	0.42
3:C:172:ALA:N	23:C:479:CLA:HAC1	2.35	0.42
4:D:90:LEU:HD11	4:D:96:GLU:CG	2.49	0.42
2:B:264:PRO:O	2:B:448:ARG:NH2	2.52	0.42
4:D:103:ARG:C	4:D:105:CYS:N	2.72	0.42
4:D:291:LEU:C	4:D:293:LEU:N	2.73	0.42
13:O:142:PHE:O	13:O:143:LYS:HG2	2.19	0.42
7:H:47:ILE:CG1	7:H:52:LEU:HD23	2.50	0.42
2:B:72:THR:HG22	2:B:79:SER:HB2	2.02	0.42
1:A:89:ILE:HG21	1:A:94:TYR:CB	2.46	0.41
13:O:101:ILE:HG22	13:O:102:ASP:N	2.35	0.41
13:O:75:THR:O	13:O:76:THR:C	2.57	0.41
4:D:48:TRP:CE3	24:D:355:PHO:H161	2.55	0.41
1:A:291:SER:O	1:A:295:PHE:CD1	2.73	0.41
1:A:141:PRO:O	3:C:443:TRP:CZ3	2.73	0.41
3:C:273:SER:CB	3:C:445:ALA:HB2	2.44	0.41
1:A:220:THR:O	1:A:223:LEU:HG	2.20	0.41
3:C:339:LYS:HE2	15:U:129:ASN:OD1	2.19	0.41
10:K:16:LEU:CB	10:K:17:PRO:CD	2.85	0.41
13:O:118:LEU:HD22	13:O:233:VAL:HG21	2.01	0.41
4:D:189:HIS:CE1	4:D:294:ARG:HE	2.38	0.41
4:D:301:GLN:O	4:D:302:GLU:C	2.58	0.41
4:D:334:GLN:N	4:D:335:PRO:HD3	2.35	0.41
2:B:145:LEU:CD1	23:B:522:CLA:HAB	2.49	0.41
23:B:516:CLA:HAA2	23:B:516:CLA:HBD	2.02	0.41
16:V:129:LYS:NZ	16:V:135:VAL:HG23	2.35	0.41
3:C:49:LEU:O	3:C:52:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:19:MET:CG	28:K:50:BCR:H361	2.50	0.41
19:Z:52:LEU:O	19:Z:56:VAL:HG23	2.21	0.41
23:C:474:CLA:HBB2	23:C:485:CLA:HED1	2.01	0.41
3:C:339:LYS:HB2	3:C:340:TYR:CD1	2.54	0.41
3:C:199:ILE:HG22	3:C:200:THR:N	2.35	0.41
13:O:197:ILE:HG12	13:O:198:SER:N	2.35	0.41
14:T:9:ILE:CG2	14:T:9:ILE:O	2.68	0.41
13:O:207:ARG:O	13:O:210:GLU:OE2	2.38	0.41
5:E:41:LEU:O	5:E:42:ALA:C	2.59	0.41
1:A:337:HIS:ND1	4:D:352:LEU:HD12	2.35	0.41
15:U:62:ILE:HG12	15:U:80:VAL:HG21	2.02	0.41
16:V:63:THR:HG21	16:V:83:ASP:O	2.19	0.41
2:B:235:GLU:O	2:B:238:LEU:HB3	2.21	0.41
2:B:46:ASP:HA	2:B:47:PRO:HD3	1.68	0.41
3:C:89:ILE:O	3:C:92:ILE:N	2.53	0.41
3:C:195:ASP:OD1	3:C:195:ASP:N	2.53	0.41
3:C:78:GLU:HG3	16:V:105:ARG:NH1	2.35	0.41
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.37	0.41
11:L:31:PHE:O	11:L:32:SER:C	2.57	0.41
1:A:143:ILE:HD12	4:D:252:PHE:CE2	2.56	0.41
3:C:412:THR:HG22	16:V:136:TYR:CE2	2.52	0.41
2:B:175:THR:HG23	2:B:175:THR:O	2.21	0.41
8:I:27:ASP:CB	8:I:28:PRO:CD	2.88	0.41
2:B:372:ASP:OD1	2:B:373:LYS:N	2.53	0.41
17:X:34:PHE:O	17:X:35:ALA:C	2.58	0.41
16:V:22:THR:OG1	16:V:25:GLN:HG3	2.20	0.41
11:L:14:ARG:HA	12:M:26:TYR:CE1	2.55	0.41
1:A:339:PHE:CB	3:C:313:GLN:OE1	2.68	0.41
3:C:320:ARG:NE	15:U:128:TYR:CZ	2.77	0.41
1:A:160:ILE:HG21	1:A:291:SER:OG	2.20	0.41
4:D:199:MET:O	4:D:202:ALA:N	2.51	0.41
23:C:474:CLA:H122	23:C:485:CLA:H13	2.03	0.41
3:C:218:PHE:O	3:C:219:GLY:C	2.58	0.41
15:U:84:PRO:C	15:U:85:TYR:HD2	2.22	0.41
4:D:259:ILE:O	4:D:260:ALA:HB2	2.20	0.41
3:C:321:ASP:CG	15:U:128:TYR:CD2	2.94	0.41
16:V:79:PRO:CB	16:V:88:ILE:CG1	2.93	0.41
1:A:210:LEU:O	1:A:214:MET:HB2	2.20	0.41
3:C:222:GLY:O	3:C:223:TRP:O	2.38	0.41
3:C:98:GLY:C	3:C:99:VAL:HG23	2.41	0.41
1:A:140:ARG:HB2	4:D:220:ASN:CG	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:6:TYR:H	10:K:6:TYR:HD1	1.67	0.41
19:Z:47:TRP:CD1	19:Z:51:VAL:HG23	2.55	0.41
2:B:265:ILE:O	2:B:267:LEU:N	2.54	0.41
1:A:307:ILE:O	1:A:308:ASP:C	2.58	0.41
4:D:29:PHE:CD2	4:D:29:PHE:O	2.72	0.41
2:B:467:ILE:HD13	4:D:126:MET:HE3	2.01	0.41
18:N:22:UNK:O	18:N:23:UNK:C	2.68	0.41
14:T:27:PRO:HG2	14:T:27:PRO:O	2.21	0.41
4:D:342:PRO:HG2	4:D:345:VAL:CG2	2.51	0.41
2:B:288:VAL:O	2:B:292:LEU:HB2	2.21	0.41
1:A:58:VAL:HG13	1:A:107:TYR:O	2.21	0.41
3:C:320:ARG:HG2	15:U:128:TYR:CE2	2.56	0.41
3:C:343:ARG:HD3	3:C:344:SER:C	2.40	0.41
13:O:76:THR:HB	13:O:77:SER:H	1.29	0.41
1:A:207:GLY:HA3	1:A:278:TRP:CD1	2.56	0.41
14:T:14:ILE:O	14:T:17:PHE:HB2	2.21	0.41
3:C:90:PRO:CB	3:C:302:TYR:HE2	2.33	0.41
7:H:22:PRO:HG2	7:H:23:GLY:H	1.85	0.41
2:B:308:LYS:HE2	2:B:312:TYR:OH	2.20	0.41
7:H:43:ILE:HG12	17:X:19:PHE:CZ	2.56	0.41
3:C:190:ALA:HA	3:C:191:PRO:HA	1.49	0.41
13:O:157:LEU:HD23	13:O:157:LEU:HA	1.79	0.41
1:A:149:ALA:HA	1:A:284:TRP:CE3	2.56	0.41
23:B:513:CLA:H18	23:B:524:CLA:O1A	2.20	0.41
1:A:159:LEU:HD21	1:A:163:ILE:HD11	2.03	0.41
3:C:281:MET:C	3:C:285:ILE:HG13	2.41	0.41
3:C:443:TRP:CD1	23:C:483:CLA:HMD3	2.56	0.41
3:C:54:VAL:O	3:C:54:VAL:HG12	2.21	0.41
4:D:322:ASN:O	4:D:325:ILE:N	2.53	0.41
4:D:217:THR:OG1	4:D:253:TRP:HZ2	2.03	0.41
2:B:339:ALA:HB1	2:B:340:TRP:HD1	1.86	0.41
13:O:71:VAL:HG21	13:O:108:VAL:CG2	2.46	0.41
1:A:95:PRO:HG2	1:A:98:GLU:HB2	2.02	0.41
3:C:395:TYR:N	3:C:395:TYR:CD2	2.87	0.41
19:Z:31:GLN:O	19:Z:32:ASP:C	2.59	0.41
3:C:45:LEU:O	3:C:47:GLY:N	2.54	0.41
3:C:82:TYR:C	3:C:82:TYR:CD1	2.94	0.41
13:O:15:LEU:O	13:O:16:ALA:C	2.59	0.41
4:D:58:TRP:HA	4:D:62:GLY:N	2.32	0.41
1:A:40:THR:CG2	1:A:118:HIS:O	2.69	0.41
2:B:12:LEU:HD11	2:B:19:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HB2	2:B:231:MET:CE	2.47	0.41
3:C:175:LEU:HD23	3:C:237:HIS:CD2	2.55	0.41
15:U:113:THR:HG22	15:U:114:VAL:H	1.82	0.41
15:U:57:LEU:HD23	15:U:57:LEU:HA	1.78	0.41
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.21	0.41
4:D:218:VAL:O	4:D:219:GLU:C	2.59	0.41
3:C:273:SER:HB2	23:C:477:CLA:HED1	2.02	0.41
3:C:275:SER:OG	23:C:485:CLA:HAA1	2.21	0.41
3:C:53:HIS:ND1	23:C:478:CLA:H141	2.35	0.41
2:B:385:ARG:HG3	13:O:165:ALA:C	2.41	0.41
1:A:341:LEU:HD21	15:U:134:LYS:HZ3	1.86	0.41
5:E:19:TRP:HZ2	9:J:13:VAL:CG2	2.27	0.41
2:B:315:ILE:HD13	2:B:359:MET:HE2	2.02	0.41
13:O:118:LEU:HD22	13:O:221:SER:HA	2.01	0.41
2:B:288:VAL:O	2:B:292:LEU:CB	2.68	0.41
1:A:208:GLY:O	1:A:212:CYS:HB2	2.20	0.41
15:U:65:PHE:CD1	15:U:76:ALA:CB	3.04	0.41
9:J:25:VAL:O	9:J:28:PHE:N	2.54	0.41
1:A:180:PHE:HD1	1:A:180:PHE:N	2.12	0.41
1:A:41:LEU:HD21	1:A:122:GLY:C	2.40	0.41
2:B:187:PRO:O	2:B:189:GLY:N	2.53	0.41
2:B:12:LEU:HG	2:B:19:LEU:CB	2.51	0.41
2:B:9:HIS:HE1	23:B:512:CLA:HED1	1.86	0.41
23:B:520:CLA:H51	28:B:529:BCR:H313	2.02	0.41
4:D:156:VAL:HG23	23:D:354:CLA:HED1	2.03	0.41
4:D:51:GLY:HA2	4:D:55:VAL:CG2	2.46	0.41
3:C:290:VAL:HG12	3:C:291:TRP:N	2.35	0.41
3:C:172:ALA:N	23:C:479:CLA:CAC	2.84	0.41
3:C:101:PRO:HA	3:C:195:ASP:HB3	2.02	0.41
3:C:62:PHE:CD2	10:K:20:PRO:HG3	2.56	0.41
28:C:488:BCR:C20	10:K:23:PHE:HE2	2.33	0.41
19:Z:47:TRP:NE1	19:Z:51:VAL:HG23	2.36	0.41
3:C:249:ILE:HG13	3:C:250:TRP:N	2.36	0.41
3:C:263:ALA:HB3	3:C:264:PHE:CD2	2.55	0.41
2:B:472:ARG:O	2:B:472:ARG:HG2	2.19	0.41
1:A:309:ALA:HB1	16:V:2:GLU:HA	2.03	0.41
23:B:514:CLA:H61	23:B:514:CLA:H41	1.93	0.41
2:B:33:TRP:HE1	23:B:514:CLA:HBC2	1.86	0.41
13:O:224:ASP:O	13:O:224:ASP:OD1	2.38	0.41
2:B:340:TRP:CZ3	2:B:407:ASN:HB3	2.55	0.41
7:H:29:LEU:HD12	7:H:29:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:100:ARG:O	15:U:104:ILE:HG13	2.21	0.41
1:A:24:THR:OG1	4:D:251:ARG:NH2	2.53	0.41
13:O:205:ASP:O	13:O:206:GLY:C	2.58	0.41
4:D:125:PHE:CD2	4:D:125:PHE:O	2.74	0.41
2:B:135:LEU:O	2:B:137:LYS:N	2.54	0.41
2:B:9:HIS:CE1	23:B:512:CLA:HED1	2.55	0.41
23:B:516:CLA:H41	23:B:516:CLA:H61	1.94	0.41
3:C:81:MET:HE1	3:C:90:PRO:N	2.35	0.41
1:A:225:ARG:HG3	1:A:225:ARG:H	1.19	0.41
2:B:265:ILE:HG21	2:B:312:TYR:CE1	2.55	0.41
4:D:32:TRP:HA	4:D:32:TRP:HE3	1.82	0.41
1:A:325:ASN:H	1:A:325:ASN:HD22	1.69	0.41
2:B:201:HIS:CD2	2:B:202:HIS:N	2.89	0.41
4:D:341:PHE:HA	4:D:342:PRO:HD2	1.73	0.41
2:B:166:MET:CE	2:B:195:PRO:HB3	2.51	0.41
13:O:238:VAL:CG1	13:O:239:PHE:H	2.33	0.40
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.65	0.40
2:B:12:LEU:HD23	2:B:19:LEU:HD12	2.02	0.40
2:B:249:ALA:HB3	2:B:459:ALA:HB2	2.02	0.40
2:B:47:PRO:HA	2:B:78:TRP:NE1	2.36	0.40
7:H:42:LEU:HA	7:H:42:LEU:HD23	1.72	0.40
3:C:291:TRP:HZ3	3:C:424:SER:HA	1.86	0.40
19:Z:13:VAL:HG13	19:Z:17:PHE:HE1	1.86	0.40
2:B:271:THR:CG2	2:B:448:ARG:NH1	2.82	0.40
2:B:321:LYS:CG	2:B:322:GLY:N	2.84	0.40
2:B:325:PHE:CZ	4:D:297:ASP:OD2	2.74	0.40
13:O:152:ARG:HD2	13:O:156:PHE:CD1	2.56	0.40
2:B:211:ILE:HG22	2:B:212:ALA:N	2.36	0.40
1:A:53:ILE:O	1:A:53:ILE:CG2	2.69	0.40
5:E:50:ARG:HB3	5:E:51:PRO:HD2	2.03	0.40
2:B:91:TRP:CD1	23:B:515:CLA:H51	2.55	0.40
14:T:3:THR:C	14:T:5:THR:N	2.74	0.40
15:U:61:ASN:HB3	15:U:130:ASN:HD22	1.85	0.40
18:N:8:UNK:O	18:N:12:UNK:N	2.54	0.40
1:A:32:TRP:HA	1:A:35:VAL:CG2	2.51	0.40
2:B:445:THR:HG22	2:B:446:SER:N	2.35	0.40
4:D:303:ILE:HD13	12:M:2:GLU:OE1	2.21	0.40
7:H:38:LEU:HD23	7:H:38:LEU:HA	1.87	0.40
15:U:65:PHE:HD1	15:U:76:ALA:CB	2.34	0.40
1:A:183:MET:HA	23:A:348:CLA:HMD2	2.03	0.40
1:A:174:LEU:HD13	24:A:351:PHO:H143	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD21	1:A:122:GLY:HA3	2.04	0.40
1:A:40:THR:HG22	1:A:41:LEU:N	2.36	0.40
2:B:109:LEU:O	2:B:113:TRP:HE3	2.03	0.40
2:B:327:THR:N	28:B:529:BCR:H292	2.36	0.40
2:B:124:ARG:HG3	23:B:525:CLA:H43	2.03	0.40
3:C:297:TYR:HB3	3:C:302:TYR:HD1	1.86	0.40
3:C:305:THR:CB	3:C:308:GLU:HG3	2.51	0.40
23:C:479:CLA:CMD	23:C:481:CLA:H111	2.52	0.40
3:C:42:LEU:O	3:C:43:ILE:C	2.59	0.40
2:B:267:LEU:HA	2:B:267:LEU:HD23	1.95	0.40
1:A:131:TRP:O	1:A:134:SER:N	2.54	0.40
4:D:287:VAL:O	4:D:287:VAL:HG12	2.20	0.40
1:A:110:GLY:O	1:A:112:TYR:N	2.54	0.40
13:O:137:THR:O	13:O:140:THR:CG2	2.67	0.40
4:D:68:LEU:HA	4:D:68:LEU:HD12	1.84	0.40
1:A:52:PHE:CD1	1:A:81:ALA:CB	3.04	0.40
2:B:122:LEU:HB3	2:B:123:PHE:H	1.63	0.40
3:C:308:GLU:CG	3:C:361:PHE:CZ	2.98	0.40
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.86	0.40
15:U:108:ASN:C	15:U:112:PHE:HE1	2.25	0.40
10:K:19:ILE:O	10:K:23:PHE:HD1	2.05	0.40
28:C:489:BCR:H342	19:Z:51:VAL:HG13	2.03	0.40
3:C:271:TYR:N	3:C:271:TYR:CD2	2.90	0.40
1:A:239:PHE:C	1:A:241:GLN:N	2.73	0.40
3:C:176:VAL:HG11	3:C:238:ILE:HG12	2.04	0.40
13:O:168:TYR:CE1	13:O:172:ILE:CD1	3.01	0.40
3:C:425:TRP:NE1	23:C:475:CLA:HBA2	2.36	0.40
13:O:201:VAL:HG11	13:O:204:VAL:CG2	2.51	0.40
16:V:75:TYR:HD2	16:V:79:PRO:HA	1.82	0.40
16:V:81:THR:O	16:V:84:GLY:N	2.54	0.40
16:V:63:THR:CB	16:V:83:ASP:O	2.67	0.40
5:E:12:ILE:HB	25:E:84:HEM:HAD2	2.02	0.40
4:D:66:SER:O	4:D:71:CYS:SG	2.74	0.40
1:A:255:PHE:CD2	1:A:264:SER:HA	2.47	0.40
1:A:44:ALA:HB1	24:A:351:PHO:H91	2.02	0.40
3:C:240:ILE:HG13	23:C:479:CLA:HBB1	2.03	0.40
2:B:333:GLY:HA2	2:B:442:ILE:O	2.22	0.40
3:C:112:PHE:HE2	10:K:6:TYR:CZ	2.39	0.40
1:A:301:ASN:OD1	3:C:407:VAL:HG11	2.20	0.40
11:L:36:PHE:CE2	12:M:8:LEU:N	2.90	0.40
13:O:27:ARG:HG3	13:O:29:ALA:CB	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:24:LYS:HE2	16:V:28:GLU:OE2	2.21	0.40
3:C:189:TRP:O	3:C:190:ALA:C	2.59	0.40
2:B:258:TYR:N	2:B:258:TYR:HD2	2.19	0.40
1:A:48:PHE:HB2	1:A:115:ILE:HD13	2.03	0.40
16:V:10:VAL:HA	16:V:11:PRO:HD3	1.98	0.40
13:O:72:THR:HG22	13:O:75:THR:OG1	2.21	0.40
3:C:343:ARG:CB	13:O:78:LEU:CD1	2.99	0.40
2:B:225:LEU:HD23	2:B:229:LEU:HD12	2.03	0.40
23:D:356:CLA:H151	23:D:356:CLA:H112	1.92	0.40
19:Z:9:LEU:C	19:Z:11:ALA:N	2.73	0.40
3:C:162:GLY:HA3	3:C:248:GLY:O	2.21	0.40
1:A:243:GLU:O	1:A:244:GLU:HB2	2.22	0.40
4:D:190:ASN:ND2	4:D:193:LEU:CD1	2.85	0.40
2:B:346:PHE:CE2	2:B:399:VAL:HG22	2.57	0.40
13:O:120:PHE:HA	13:O:219:GLN:HE22	1.86	0.40
1:A:46:ILE:O	1:A:47:CYS:C	2.59	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:246:ALA:C	18:n:2035:UNK:O[2_555]	1.76	0.44
13:O:246:ALA:N	18:n:2035:UNK:O[2_555]	1.97	0.23
13:O:246:ALA:O	18:n:2035:UNK:O[2_555]	2.07	0.13
13:O:246:ALA:O	18:n:2035:UNK:CB[2_555]	2.15	0.05
13:O:246:ALA:N	18:n:2035:UNK:C[2_555]	2.17	0.03
13:O:246:ALA:CA	18:n:2035:UNK:O[2_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	251 (76%)	58 (18%)	22 (7%)	1	19
1	a	331/344 (96%)	253 (76%)	56 (17%)	22 (7%)	1	19
2	B	474/510 (93%)	367 (77%)	84 (18%)	23 (5%)	3	27
2	b	474/510 (93%)	367 (77%)	83 (18%)	24 (5%)	2	26
3	C	419/473 (89%)	326 (78%)	60 (14%)	33 (8%)	1	14
3	c	419/473 (89%)	326 (78%)	62 (15%)	31 (7%)	1	16
4	D	337/352 (96%)	274 (81%)	49 (14%)	14 (4%)	3	32
4	d	337/352 (96%)	270 (80%)	51 (15%)	16 (5%)	3	29
5	E	74/84 (88%)	62 (84%)	10 (14%)	2 (3%)	6	44
5	e	74/84 (88%)	57 (77%)	14 (19%)	3 (4%)	3	33
6	F	31/45 (69%)	23 (74%)	5 (16%)	3 (10%)	1	10
6	f	31/45 (69%)	22 (71%)	6 (19%)	3 (10%)	1	10
7	H	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	2	22
7	h	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	2	22
8	I	36/38 (95%)	25 (69%)	10 (28%)	1 (3%)	6	43
8	i	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	2	24
9	J	36/40 (90%)	32 (89%)	3 (8%)	1 (3%)	6	43
9	j	36/40 (90%)	30 (83%)	4 (11%)	2 (6%)	2	24
10	K	35/37 (95%)	27 (77%)	2 (6%)	6 (17%)	0	3
10	k	35/37 (95%)	26 (74%)	3 (9%)	6 (17%)	0	3
11	L	35/37 (95%)	28 (80%)	3 (9%)	4 (11%)	0	7
11	l	35/37 (95%)	27 (77%)	5 (14%)	3 (9%)	1	12
12	M	28/36 (78%)	22 (79%)	5 (18%)	1 (4%)	4	37
12	m	28/36 (78%)	22 (79%)	4 (14%)	2 (7%)	1	17
13	O	244/246 (99%)	180 (74%)	44 (18%)	20 (8%)	1	13
13	o	244/246 (99%)	179 (73%)	45 (18%)	20 (8%)	1	13
14	T	29/32 (91%)	23 (79%)	3 (10%)	3 (10%)	1	9
14	t	29/32 (91%)	22 (76%)	5 (17%)	2 (7%)	1	18
15	U	103/134 (77%)	78 (76%)	14 (14%)	11 (11%)	0	8
15	u	103/134 (77%)	81 (79%)	11 (11%)	11 (11%)	0	8
16	V	135/137 (98%)	111 (82%)	16 (12%)	8 (6%)	2	22
16	v	135/137 (98%)	106 (78%)	22 (16%)	7 (5%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	38/50 (76%)	36 (95%)	1 (3%)	1 (3%)	7	45
17	x	38/50 (76%)	35 (92%)	2 (5%)	1 (3%)	7	45
19	Z	56/62 (90%)	39 (70%)	15 (27%)	2 (4%)	4	37
19	z	56/62 (90%)	40 (71%)	13 (23%)	3 (5%)	2	25
All	All	4984/5446 (92%)	3864 (78%)	801 (16%)	319 (6%)	2	20

All (319) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	GLY
1	A	228	THR
1	A	242	GLU
1	A	308	ASP
2	B	88	PRO
2	B	126	PRO
2	B	173	GLY
2	B	235	GLU
2	B	326	ARG
2	B	391	SER
3	C	37	ALA
3	C	104	GLU
3	C	137	PRO
3	C	184	GLY
3	C	190	ALA
3	C	192	GLY
3	C	227	VAL
3	C	285	ILE
4	D	218	VAL
4	D	264	LYS
5	E	49	PRO
6	F	17	VAL
7	H	21	ALA
10	K	7	ALA
10	K	8	ILE
11	L	8	GLN
11	L	9	PRO
13	O	76	THR
13	O	77	SER
13	O	101	ILE
13	O	130	GLN
13	O	245	PRO

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Mol	Chain	Res	Type
15	U	40	VAL
15	U	52	GLY
15	U	72	TYR
16	V	38	ALA
17	X	14	PRO
1	a	2090	GLY
1	a	2141	PRO
1	a	2228	THR
2	b	2088	PRO
2	b	2126	PRO
2	b	2173	GLY
2	b	2235	GLU
2	b	2326	ARG
2	b	2391	SER
3	c	2037	ALA
3	c	2104	GLU
3	c	2184	GLY
3	c	2190	ALA
3	c	2191	PRO
3	c	2192	GLY
3	c	2285	ILE
4	d	2218	VAL
4	d	2264	LYS
5	e	2049	PRO
6	f	2017	VAL
7	h	2021	ALA
10	k	2007	ALA
10	k	2008	ILE
11	l	2009	PRO
13	o	2076	THR
13	o	2077	SER
13	o	2130	GLN
13	o	2245	PRO
15	u	2040	VAL
15	u	2051	TYR
15	u	2052	GLY
15	u	2072	TYR
16	v	2038	ALA
17	x	2014	PRO
1	A	32	TRP
1	A	141	PRO
1	A	160	ILE

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	239	PHE
1	A	243	GLU
1	A	317	TRP
1	A	335	ASN
2	B	186	GLY
2	B	201	HIS
2	B	230	ARG
2	B	328	GLY
2	B	396	GLY
3	C	43	ILE
3	C	183	GLY
3	C	219	GLY
3	C	295	THR
3	C	453	ALA
4	D	109	GLY
4	D	156	VAL
4	D	219	GLU
4	D	292	ASN
5	E	10	SER
6	F	40	GLN
7	H	23	GLY
10	K	11	PRO
10	K	17	PRO
13	O	56	PRO
13	O	131	PRO
13	O	206	GLY
13	O	216	GLU
14	T	4	ILE
15	U	48	GLY
15	U	51	TYR
15	U	63	ALA
15	U	73	PRO
15	U	120	ALA
15	U	121	LEU
15	U	125	GLY
15	U	131	GLY
16	V	82	TYR
19	Z	32	ASP
1	a	2032	TRP
1	a	2160	ILE
1	a	2225	ARG

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Mol	Chain	Res	Type
1	a	2239	PHE
1	a	2242	GLU
1	a	2243	GLU
1	a	2308	ASP
2	b	2186	GLY
2	b	2201	HIS
2	b	2230	ARG
2	b	2328	GLY
2	b	2396	GLY
3	c	2137	PRO
3	c	2183	GLY
3	c	2219	GLY
3	c	2227	VAL
3	c	2295	THR
3	c	2453	ALA
4	d	2109	GLY
4	d	2219	GLU
4	d	2292	ASN
4	d	2299	ILE
5	e	2010	SER
6	f	2040	GLN
7	h	2023	GLY
10	k	2011	PRO
11	l	2008	GLN
13	o	2056	PRO
13	o	2078	LEU
13	o	2101	ILE
13	o	2161	GLY
13	o	2206	GLY
14	t	2004	ILE
15	u	2048	GLY
15	u	2063	ALA
15	u	2073	PRO
15	u	2120	ALA
15	u	2121	LEU
15	u	2131	GLY
16	v	2082	TYR
1	A	215	HIS
2	B	187	PRO
2	B	222	PRO
2	B	223	GLN
2	B	312	TYR

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Mol	Chain	Res	Type
2	B	319	PRO
2	B	361	ALA
3	C	80	PRO
3	C	110	PRO
3	C	191	PRO
3	C	223	TRP
3	C	334	PRO
3	C	355	THR
3	C	415	ASN
3	C	454	GLY
4	D	260	ALA
4	D	299	ILE
7	H	22	PRO
9	J	28	PHE
13	O	28	GLY
13	O	78	LEU
13	O	149	PRO
13	O	161	GLY
16	V	16	GLY
16	V	99	ASP
1	a	2191	ASN
1	a	2259	ILE
1	a	2317	TRP
2	b	2187	PRO
2	b	2222	PRO
2	b	2223	GLN
2	b	2319	PRO
2	b	2361	ALA
3	c	2110	PRO
3	c	2152	LYS
3	c	2223	TRP
3	c	2355	THR
3	c	2413	GLU
3	c	2415	ASN
4	d	2239	GLN
4	d	2260	ALA
4	d	2343	GLU
6	f	2019	TRP
7	h	2022	PRO
9	j	2028	PHE
10	k	2017	PRO
13	o	2131	PRO

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Mol	Chain	Res	Type
13	o	2149	PRO
13	o	2180	GLU
13	o	2216	GLU
15	u	2125	GLY
16	v	2016	GLY
19	z	2032	ASP
1	A	167	SER
1	A	191	ASN
1	A	208	GLY
1	A	259	ILE
1	A	300	PHE
1	A	301	ASN
1	A	334	ARG
3	C	46	SER
3	C	85	GLY
3	C	152	LYS
3	C	195	ASP
3	C	298	PRO
3	C	420	VAL
4	D	132	ILE
4	D	166	SER
4	D	239	GLN
4	D	343	GLU
13	O	114	GLU
14	T	27	PRO
16	V	133	GLY
19	Z	29	SER
1	a	2167	SER
1	a	2208	GLY
1	a	2215	HIS
1	a	2300	PHE
1	a	2301	ASN
2	b	2188	ASP
2	b	2312	TYR
3	c	2043	ILE
3	c	2334	PRO
3	c	2411	ALA
3	c	2420	VAL
4	d	2166	SER
13	o	2047	PRO
13	o	2114	GLU
14	t	2027	PRO

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Mol	Chain	Res	Type
16	v	2021	LEU
16	v	2102	PRO
16	v	2131	GLY
2	B	188	ASP
3	C	413	GLU
4	D	131	GLU
6	F	19	TRP
8	I	32	PRO
10	K	16	LEU
13	O	47	PRO
13	O	180	GLU
16	V	102	PRO
16	V	107	LEU
16	V	131	GLY
1	a	2116	ILE
1	a	2244	GLU
2	b	2047	PRO
3	c	2046	SER
3	c	2080	PRO
3	c	2454	GLY
4	d	2101	PHE
5	e	2057	GLN
10	k	2016	LEU
12	m	2005	GLN
13	o	2028	GLY
16	v	2133	GLY
19	z	2029	SER
1	A	116	ILE
2	B	47	PRO
3	C	380	ILE
11	L	2	GLU
14	T	3	THR
3	c	2085	GLY
3	c	2195	ASP
3	c	2298	PRO
3	c	2338	GLY
4	d	2113	PHE
4	d	2132	ILE
11	l	2002	GLU
12	m	2017	VAL
13	o	2175	PRO
1	A	63	ILE

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Mol	Chain	Res	Type
2	B	16	PRO
3	C	101	PRO
3	C	117	VAL
13	O	159	PRO
13	O	244	GLU
1	a	2046	ILE
1	a	2063	ILE
2	b	2264	PRO
13	o	2159	PRO
2	B	211	ILE
2	B	322	GLY
3	C	338	GLY
13	O	122	VAL
2	b	2016	PRO
2	b	2211	ILE
2	b	2322	GLY
13	o	2122	VAL
10	K	2	LEU
11	L	4	ASN
2	b	2008	VAL
9	j	2016	VAL
2	B	8	VAL
3	C	410	VAL
4	D	275	PRO
12	M	17	VAL
3	c	2380	ILE
4	d	2156	VAL
8	i	2008	VAL
8	i	2032	PRO
10	k	2002	LEU
13	o	2244	GLU
13	O	175	PRO
4	d	2095	PRO
4	d	2275	PRO
19	z	2013	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	244 (90%)	26 (10%)	10	43
1	a	270/280 (96%)	249 (92%)	21 (8%)	16	53
2	B	377/407 (93%)	355 (94%)	22 (6%)	25	65
2	b	377/407 (93%)	355 (94%)	22 (6%)	25	65
3	C	326/374 (87%)	306 (94%)	20 (6%)	23	64
3	c	326/374 (87%)	307 (94%)	19 (6%)	25	65
4	D	275/283 (97%)	257 (94%)	18 (6%)	21	62
4	d	275/283 (97%)	253 (92%)	22 (8%)	15	52
5	E	68/73 (93%)	65 (96%)	3 (4%)	35	73
5	e	68/73 (93%)	64 (94%)	4 (6%)	24	65
6	F	27/39 (69%)	25 (93%)	2 (7%)	17	56
6	f	27/39 (69%)	24 (89%)	3 (11%)	8	35
7	H	44/55 (80%)	41 (93%)	3 (7%)	20	60
7	h	44/55 (80%)	42 (96%)	2 (4%)	34	73
8	I	35/35 (100%)	31 (89%)	4 (11%)	7	33
8	i	35/35 (100%)	33 (94%)	2 (6%)	25	66
9	J	26/28 (93%)	25 (96%)	1 (4%)	40	76
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	61
10	k	30/30 (100%)	30 (100%)	0	100	100
11	L	35/35 (100%)	31 (89%)	4 (11%)	7	33
11	l	35/35 (100%)	31 (89%)	4 (11%)	7	33
12	M	27/33 (82%)	26 (96%)	1 (4%)	41	76
12	m	27/33 (82%)	26 (96%)	1 (4%)	41	76
13	O	208/208 (100%)	187 (90%)	21 (10%)	9	40
13	o	208/208 (100%)	190 (91%)	18 (9%)	13	48
14	T	28/29 (97%)	28 (100%)	0	100	100
14	t	28/29 (97%)	28 (100%)	0	100	100
15	U	89/112 (80%)	85 (96%)	4 (4%)	34	73
15	u	89/112 (80%)	84 (94%)	5 (6%)	26	66
16	V	117/117 (100%)	112 (96%)	5 (4%)	35	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/117 (100%)	112 (96%)	5 (4%)	35	74
17	X	33/42 (79%)	30 (91%)	3 (9%)	12	46
17	x	33/42 (79%)	29 (88%)	4 (12%)	6	30
19	Z	48/52 (92%)	42 (88%)	6 (12%)	6	29
19	z	48/52 (92%)	46 (96%)	2 (4%)	36	74
All	All	4126/4464 (92%)	3847 (93%)	279 (7%)	20	60

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	25	ASP
1	A	27	ARG
1	A	29	TYR
1	A	52	PHE
1	A	70	SER
1	A	84	PRO
1	A	162	PRO
1	A	170	ASP
1	A	172	MET
1	A	177	SER
1	A	180	PHE
1	A	183	MET
1	A	187	GLN
1	A	212	CYS
1	A	214	MET
1	A	237	TYR
1	A	269	ARG
1	A	284	TRP
1	A	295	PHE
1	A	298	ASN
1	A	301	ASN
1	A	317	TRP
1	A	325	ASN
1	A	335	ASN
1	A	342	ASP
2	B	8	VAL
2	B	48	SER
2	B	57	ARG
2	B	130	GLU

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Mol	Chain	Res	Type
2	B	139	PHE
2	B	167	TRP
2	B	216	HIS
2	B	240	SER
2	B	246	PHE
2	B	255	THR
2	B	285	ASN
2	B	286	ARG
2	B	311	PHE
2	B	318	ASN
2	B	334	ASP
2	B	340	TRP
2	B	362	PHE
2	B	372	ASP
2	B	385	ARG
2	B	402	TYR
2	B	409	GLN
2	B	479	PHE
3	C	110	PRO
3	C	127	PHE
3	C	139	THR
3	C	149	TYR
3	C	198	VAL
3	C	201	ASN
3	C	264	PHE
3	C	289	PHE
3	C	290	VAL
3	C	292	PHE
3	C	293	ASN
3	C	294	ASN
3	C	295	THR
3	C	313	GLN
3	C	321	ASP
3	C	340	TYR
3	C	343	ARG
3	C	368	PRO
3	C	400	PRO
3	C	443	TRP
4	D	29	PHE
4	D	32	TRP
4	D	58	TRP
4	D	61	HIS

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Mol	Chain	Res	Type
4	D	73	PHE
4	D	91	LEU
4	D	142	ASN
4	D	168	PHE
4	D	180	ARG
4	D	188	PHE
4	D	192	THR
4	D	211	CYS
4	D	220	ASN
4	D	254	SER
4	D	261	PHE
4	D	262	SER
4	D	336	HIS
4	D	340	VAL
5	E	16	VAL
5	E	30	PHE
5	E	49	PRO
6	F	12	TYR
6	F	31	PHE
7	H	26	THR
7	H	48	TYR
7	H	57	VAL
8	I	16	VAL
8	I	18	LEU
8	I	27	ASP
8	I	30	ARG
9	J	38	SER
10	K	6	TYR
10	K	36	PHE
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
11	L	36	PHE
12	M	28	GLN
13	O	3	GLN
13	O	21	THR
13	O	34	SER
13	O	39	ARG
13	O	46	GLN
13	O	47	PRO
13	O	65	PHE
13	O	68	THR

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Mol	Chain	Res	Type
13	O	104	GLN
13	O	110	MET
13	O	126	VAL
13	O	142	PHE
13	O	147	ASN
13	O	162	ARG
13	O	166	SER
13	O	174	LEU
13	O	190	PHE
13	O	193	THR
13	O	219	GLN
13	O	225	MET
13	O	245	PRO
15	U	51	TYR
15	U	59	ASN
15	U	61	ASN
15	U	132	LEU
16	V	4	THR
16	V	40	CYS
16	V	55	ARG
16	V	78	ASN
16	V	130	TRP
17	X	13	THR
17	X	14	PRO
17	X	47	GLN
19	Z	5	PHE
19	Z	32	ASP
19	Z	34	ASP
19	Z	41	PHE
19	Z	42	LEU
19	Z	51	VAL
1	a	2015	GLU
1	a	2024	THR
1	a	2025	ASP
1	a	2027	ARG
1	a	2029	TYR
1	a	2033	PHE
1	a	2040	THR
1	a	2045	THR
1	a	2070	SER
1	a	2111	PRO
1	a	2180	PHE

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Mol	Chain	Res	Type
1	a	2187	GLN
1	a	2237	TYR
1	a	2269	ARG
1	a	2278	TRP
1	a	2284	TRP
1	a	2286	THR
1	a	2295	PHE
1	a	2317	TRP
1	a	2335	ASN
1	a	2342	ASP
2	b	2008	VAL
2	b	2048	SER
2	b	2057	ARG
2	b	2130	GLU
2	b	2139	PHE
2	b	2167	TRP
2	b	2216	HIS
2	b	2240	SER
2	b	2246	PHE
2	b	2255	THR
2	b	2286	ARG
2	b	2311	PHE
2	b	2318	ASN
2	b	2334	ASP
2	b	2340	TRP
2	b	2362	PHE
2	b	2372	ASP
2	b	2385	ARG
2	b	2392	PHE
2	b	2402	TYR
2	b	2409	GLN
2	b	2479	PHE
3	c	2046	SER
3	c	2110	PRO
3	c	2127	PHE
3	c	2139	THR
3	c	2149	TYR
3	c	2198	VAL
3	c	2201	ASN
3	c	2264	PHE
3	c	2285	ILE
3	c	2289	PHE

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Mol	Chain	Res	Type
3	c	2292	PHE
3	c	2293	ASN
3	c	2294	ASN
3	c	2304	PRO
3	c	2310	SER
3	c	2321	ASP
3	c	2340	TYR
3	c	2403	SER
3	c	2443	TRP
4	d	2029	PHE
4	d	2032	TRP
4	d	2058	TRP
4	d	2061	HIS
4	d	2073	PHE
4	d	2081	PRO
4	d	2091	LEU
4	d	2130	PHE
4	d	2147	SER
4	d	2165	SER
4	d	2168	PHE
4	d	2180	ARG
4	d	2188	PHE
4	d	2192	THR
4	d	2211	CYS
4	d	2220	ASN
4	d	2235	PHE
4	d	2254	SER
4	d	2261	PHE
4	d	2262	SER
4	d	2336	HIS
4	d	2350	ASN
5	e	2030	PHE
5	e	2049	PRO
5	e	2050	ARG
5	e	2053	SER
6	f	2012	TYR
6	f	2031	PHE
6	f	2043	GLN
7	h	2024	TRP
7	h	2026	THR
8	i	2027	ASP
8	i	2030	ARG

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Mol	Chain	Res	Type
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
11	l	2036	PHE
12	m	2028	GLN
13	o	2005	LEU
13	o	2006	THR
13	o	2021	THR
13	o	2039	ARG
13	o	2047	PRO
13	o	2060	ARG
13	o	2068	THR
13	o	2103	PHE
13	o	2104	GLN
13	o	2110	MET
13	o	2147	ASN
13	o	2159	PRO
13	o	2166	SER
13	o	2174	LEU
13	o	2193	THR
13	o	2225	MET
13	o	2239	PHE
13	o	2245	PRO
15	u	2051	TYR
15	u	2059	ASN
15	u	2061	ASN
15	u	2128	TYR
15	u	2132	LEU
16	v	2004	THR
16	v	2040	CYS
16	v	2050	PRO
16	v	2055	ARG
16	v	2093	PRO
17	x	2011	THR
17	x	2013	THR
17	x	2014	PRO
17	x	2047	GLN
19	z	2005	PHE
19	z	2051	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	165	GLN
1	A	187	GLN
1	A	191	ASN
1	A	199	GLN
1	A	296	ASN
1	A	301	ASN
1	A	303	ASN
1	A	312	ASN
1	A	322	ASN
1	A	325	ASN
2	B	233	ASN
2	B	285	ASN
2	B	318	ASN
2	B	331	ASN
2	B	374	ASN
2	B	395	GLN
2	B	438	ASN
3	C	39	ASN
3	C	201	ASN
3	C	294	ASN
3	C	311	GLN
3	C	378	ASN
4	D	83	ASN
4	D	87	HIS
4	D	106	GLN
4	D	129	GLN
4	D	164	GLN
4	D	186	GLN
4	D	255	GLN
4	D	263	ASN
4	D	322	ASN
4	D	338	ASN
4	D	350	ASN
5	E	81	GLN
6	F	40	GLN
6	F	43	GLN
10	K	31	GLN
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
12	M	4	ASN

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Mol	Chain	Res	Type
12	M	28	GLN
13	O	36	GLN
13	O	46	GLN
13	O	61	GLN
13	O	124	ASN
13	O	132	ASN
13	O	147	ASN
13	O	155	ASN
13	O	200	ASN
13	O	219	GLN
15	U	59	ASN
15	U	61	ASN
15	U	82	ASN
15	U	130	ASN
16	V	25	GLN
19	Z	6	GLN
1	a	2019	ASN
1	a	2092	HIS
1	a	2165	GLN
1	a	2187	GLN
1	a	2199	GLN
1	a	2296	ASN
1	a	2301	ASN
1	a	2303	ASN
1	a	2322	ASN
1	a	2325	ASN
1	a	2335	ASN
2	b	2285	ASN
2	b	2318	ASN
2	b	2331	ASN
2	b	2343	HIS
2	b	2374	ASN
2	b	2395	GLN
2	b	2438	ASN
3	c	2039	ASN
3	c	2201	ASN
3	c	2294	ASN
3	c	2322	GLN
3	c	2405	ASN
4	d	2083	ASN
4	d	2087	HIS
4	d	2129	GLN

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Mol	Chain	Res	Type
4	d	2142	ASN
4	d	2164	GLN
4	d	2186	GLN
4	d	2190	ASN
4	d	2250	ASN
4	d	2255	GLN
4	d	2263	ASN
4	d	2322	ASN
4	d	2338	ASN
4	d	2350	ASN
6	f	2040	GLN
6	f	2043	GLN
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
12	m	2004	ASN
12	m	2028	GLN
13	o	2036	GLN
13	o	2046	GLN
13	o	2061	GLN
13	o	2124	ASN
13	o	2147	ASN
13	o	2155	ASN
13	o	2236	GLN
15	u	2059	ASN
15	u	2061	ASN
15	u	2108	ASN
15	u	2111	HIS
15	u	2130	ASN
16	v	2078	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 2 are monoatomic - leaving 106 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
21	BCT	A	346	22	0,3,3	0.00	-	0,3,3	0.00	-
22	OEC	A	347	1,3,21	0,13,13	0.00	-	0,27,27	0.00	-
23	CLA	A	348	1	55,73,73	1.08	6 (10%)	61,113,113	1.52	13 (21%)
23	CLA	A	349	-	55,73,73	1.03	5 (9%)	61,113,113	1.71	14 (22%)
23	CLA	A	350	-	55,73,73	0.97	1 (1%)	61,113,113	1.56	13 (21%)
24	PHO	A	351	-	67,69,69	1.11	5 (7%)	84,99,99	1.34	11 (13%)
23	CLA	A	352	1	55,73,73	1.03	4 (7%)	61,113,113	1.49	11 (18%)
26	PL9	A	353	-	45,45,55	2.59	19 (42%)	56,57,69	2.52	19 (33%)
23	CLA	B	511	2	55,73,73	1.22	9 (16%)	61,113,113	1.79	16 (26%)
23	CLA	B	512	2	55,73,73	1.04	3 (5%)	61,113,113	1.52	10 (16%)
23	CLA	B	513	2	55,73,73	1.12	4 (7%)	61,113,113	1.89	15 (24%)
23	CLA	B	514	-	55,73,73	1.29	8 (14%)	61,113,113	1.73	14 (22%)
23	CLA	B	515	2	55,73,73	1.13	5 (9%)	61,113,113	1.68	15 (24%)
23	CLA	B	516	2	55,73,73	1.40	8 (14%)	61,113,113	1.62	12 (19%)
23	CLA	B	517	2	55,73,73	1.07	5 (9%)	61,113,113	1.66	15 (24%)
23	CLA	B	518	2	55,73,73	1.07	3 (5%)	61,113,113	1.75	10 (16%)
23	CLA	B	519	2	55,73,73	1.38	9 (16%)	61,113,113	1.97	11 (18%)
23	CLA	B	520	2	55,73,73	1.28	7 (12%)	61,113,113	2.27	10 (16%)
23	CLA	B	521	2	55,73,73	1.06	4 (7%)	61,113,113	1.39	8 (13%)
23	CLA	B	522	2	55,73,73	0.95	3 (5%)	61,113,113	1.56	14 (22%)
23	CLA	B	523	2	55,73,73	1.14	6 (10%)	61,113,113	1.74	15 (24%)
23	CLA	B	524	-	55,73,73	1.03	3 (5%)	61,113,113	1.66	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	525	2	55,73,73	1.15	6 (10%)	61,113,113	1.63	11 (18%)
27	LMT	B	526	-	36,36,36	1.31	4 (11%)	47,47,47	1.80	9 (19%)
23	CLA	B	527	-	55,73,73	1.19	8 (14%)	61,113,113	1.64	12 (19%)
28	BCR	B	528	-	41,41,41	1.98	6 (14%)	56,56,56	2.25	18 (32%)
28	BCR	B	529	-	41,41,41	2.05	9 (21%)	56,56,56	2.30	23 (41%)
23	CLA	C	474	3	55,73,73	1.07	4 (7%)	61,113,113	1.67	14 (22%)
23	CLA	C	475	-	55,73,73	1.44	9 (16%)	61,113,113	1.68	13 (21%)
23	CLA	C	476	3	55,73,73	1.00	3 (5%)	61,113,113	1.50	9 (14%)
23	CLA	C	477	3	55,73,73	1.14	5 (9%)	61,113,113	2.15	14 (22%)
23	CLA	C	478	3	55,73,73	1.14	5 (9%)	61,113,113	1.57	9 (14%)
23	CLA	C	479	3	55,73,73	1.04	3 (5%)	61,113,113	1.82	15 (24%)
23	CLA	C	480	3	55,73,73	0.94	2 (3%)	61,113,113	1.56	13 (21%)
23	CLA	C	481	3	55,73,73	0.95	3 (5%)	61,113,113	1.91	11 (18%)
23	CLA	C	482	3	55,73,73	1.11	4 (7%)	61,113,113	1.57	10 (16%)
23	CLA	C	483	3	55,73,73	1.15	6 (10%)	61,113,113	1.83	12 (19%)
23	CLA	C	484	3	55,73,73	1.11	4 (7%)	61,113,113	1.49	10 (16%)
23	CLA	C	485	-	55,73,73	1.06	3 (5%)	61,113,113	1.71	14 (22%)
23	CLA	C	486	3	55,73,73	1.07	4 (7%)	61,113,113	1.59	12 (19%)
23	CLA	C	487	-	55,73,73	1.27	5 (9%)	61,113,113	1.61	13 (21%)
28	BCR	C	488	-	41,41,41	1.80	10 (24%)	56,56,56	2.01	18 (32%)
28	BCR	C	489	-	41,41,41	1.73	7 (17%)	56,56,56	1.99	17 (30%)
21	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	354	4	55,73,73	1.02	4 (7%)	61,113,113	1.47	10 (16%)
24	PHO	D	355	-	67,69,69	0.98	4 (5%)	84,99,99	1.54	15 (17%)
23	CLA	D	356	4	55,73,73	1.12	4 (7%)	61,113,113	1.45	9 (14%)
26	PL9	D	357	-	45,45,55	2.52	18 (40%)	56,57,69	1.95	13 (23%)
25	HEM	E	84	5,6	30,50,50	3.02	15 (50%)	24,82,82	3.86	15 (62%)
28	BCR	F	48	-	41,41,41	1.97	8 (19%)	56,56,56	2.53	23 (41%)
28	BCR	J	53	-	41,41,41	1.89	6 (14%)	56,56,56	2.15	20 (35%)
28	BCR	K	50	-	41,41,41	2.06	17 (41%)	56,56,56	1.94	15 (26%)
25	HEM	V	138	16	30,50,50	5.60	16 (53%)	24,82,82	3.74	16 (66%)
21	BCT	a	2346	22	0,3,3	0.00	-	0,3,3	0.00	-
22	OEC	a	2347	1,3,21	0,13,13	0.00	-	0,27,27	0.00	-
23	CLA	a	2348	1	55,73,73	1.05	5 (9%)	61,113,113	1.50	13 (21%)
23	CLA	a	2349	-	55,73,73	0.95	1 (1%)	61,113,113	1.52	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	a	2350	-	67,69,69	1.13	5 (7%)	84,99,99	1.31	10 (11%)
23	CLA	a	2351	1	55,73,73	1.12	4 (7%)	61,113,113	1.49	10 (16%)
26	PL9	a	2352	-	45,45,55	2.61	19 (42%)	56,57,69	2.53	18 (32%)
23	CLA	b	2511	2	55,73,73	1.21	6 (10%)	61,113,113	1.80	15 (24%)
23	CLA	b	2512	2	55,73,73	1.04	3 (5%)	61,113,113	1.58	11 (18%)
23	CLA	b	2513	2	55,73,73	1.13	4 (7%)	61,113,113	1.86	14 (22%)
23	CLA	b	2514	-	55,73,73	1.30	7 (12%)	61,113,113	1.75	14 (22%)
23	CLA	b	2515	2	55,73,73	1.13	5 (9%)	61,113,113	1.66	16 (26%)
23	CLA	b	2516	2	55,73,73	1.45	9 (16%)	61,113,113	1.63	13 (21%)
23	CLA	b	2517	2	55,73,73	1.03	5 (9%)	61,113,113	1.67	12 (19%)
23	CLA	b	2518	2	55,73,73	1.15	8 (14%)	61,113,113	1.71	10 (16%)
23	CLA	b	2519	2	55,73,73	1.33	6 (10%)	61,113,113	1.95	12 (19%)
23	CLA	b	2520	2	55,73,73	1.30	7 (12%)	61,113,113	2.29	10 (16%)
23	CLA	b	2521	2	55,73,73	1.15	5 (9%)	61,113,113	1.39	9 (14%)
23	CLA	b	2522	2	55,73,73	1.06	4 (7%)	61,113,113	1.53	13 (21%)
23	CLA	b	2523	2	55,73,73	1.19	7 (12%)	61,113,113	1.72	14 (22%)
23	CLA	b	2524	-	55,73,73	1.01	3 (5%)	61,113,113	1.65	12 (19%)
23	CLA	b	2525	2	55,73,73	1.14	5 (9%)	61,113,113	1.66	11 (18%)
23	CLA	b	2526	-	55,73,73	1.10	4 (7%)	61,113,113	1.68	12 (19%)
28	BCR	b	2527	-	41,41,41	1.88	7 (17%)	56,56,56	2.27	20 (35%)
28	BCR	b	2528	-	41,41,41	2.03	8 (19%)	56,56,56	2.22	21 (37%)
23	CLA	c	2474	3	55,73,73	1.08	4 (7%)	61,113,113	1.67	12 (19%)
23	CLA	c	2475	-	55,73,73	1.47	10 (18%)	61,113,113	1.64	12 (19%)
23	CLA	c	2476	3	55,73,73	1.04	5 (9%)	61,113,113	1.49	9 (14%)
23	CLA	c	2477	3	55,73,73	1.17	4 (7%)	61,113,113	2.14	16 (26%)
23	CLA	c	2478	3	55,73,73	1.12	6 (10%)	61,113,113	1.59	12 (19%)
23	CLA	c	2479	3	55,73,73	1.12	5 (9%)	61,113,113	1.84	16 (26%)
23	CLA	c	2480	3	55,73,73	0.96	4 (7%)	61,113,113	1.57	10 (16%)
23	CLA	c	2481	3	55,73,73	0.97	5 (9%)	61,113,113	1.90	12 (19%)
23	CLA	c	2482	3	55,73,73	1.14	4 (7%)	61,113,113	1.49	11 (18%)
23	CLA	c	2483	3	55,73,73	1.18	5 (9%)	61,113,113	1.82	12 (19%)
23	CLA	c	2484	3	55,73,73	1.13	4 (7%)	61,113,113	1.47	11 (18%)
23	CLA	c	2485	-	55,73,73	1.09	4 (7%)	61,113,113	1.72	15 (24%)
23	CLA	c	2486	3	55,73,73	1.07	4 (7%)	61,113,113	1.62	12 (19%)
23	CLA	c	2487	-	55,73,73	1.22	7 (12%)	61,113,113	1.64	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	c	2488	-	41,41,41	1.95	11 (26%)	56,56,56	1.99	18 (32%)
28	BCR	c	2489	-	41,41,41	1.91	8 (19%)	56,56,56	2.01	17 (30%)
21	BCT	d	2353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	2354	4	55,73,73	0.98	3 (5%)	61,113,113	1.51	9 (14%)
23	CLA	d	2355	-	55,73,73	1.05	3 (5%)	61,113,113	1.65	13 (21%)
24	PHO	d	2356	-	67,69,69	1.02	3 (4%)	84,99,99	1.51	15 (17%)
23	CLA	d	2357	4	55,73,73	1.12	5 (9%)	61,113,113	1.44	10 (16%)
26	PL9	d	2358	-	45,45,55	2.60	18 (40%)	56,57,69	1.94	14 (25%)
27	LMT	d	2359	-	36,36,36	1.31	4 (11%)	47,47,47	1.78	8 (17%)
28	BCR	d	2360	-	41,41,41	1.98	8 (19%)	56,56,56	2.48	22 (39%)
25	HEM	e	2084	5,6	30,50,50	3.06	16 (53%)	24,82,82	3.68	10 (41%)
28	BCR	j	2053	-	41,41,41	2.13	8 (19%)	56,56,56	2.15	19 (33%)
28	BCR	k	2050	-	41,41,41	2.11	18 (43%)	56,56,56	1.91	14 (25%)
25	HEM	v	2138	16	30,50,50	3.80	18 (60%)	24,82,82	4.29	16 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCT	A	346	22	-	0/0/0/0	0/0/0/0
22	OEC	A	347	1,3,21	-	0/0/54/54	0/3/5/5
23	CLA	A	348	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	349	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	350	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	351	-	-	0/53/103/103	0/1/6/6
23	CLA	A	352	1	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	A	353	-	-	0/41/61/73	0/1/1/1
23	CLA	B	511	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	512	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	513	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	514	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	515	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	516	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	517	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	518	2	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	519	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	520	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	521	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	522	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	523	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	524	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	525	2	3/3/20/25	0/37/135/135	0/0/9/9
27	LMT	B	526	-	-	0/21/61/61	0/2/2/2
23	CLA	B	527	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	B	528	-	-	0/29/63/63	0/2/2/2
28	BCR	B	529	-	-	0/29/63/63	0/2/2/2
23	CLA	C	474	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	475	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	476	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	477	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	478	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	479	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	480	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	481	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	482	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	483	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	484	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	485	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	486	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	487	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	C	488	-	-	0/29/63/63	0/2/2/2
28	BCR	C	489	-	-	0/29/63/63	0/2/2/2
21	BCT	D	353	20	-	0/0/0/0	0/0/0/0
23	CLA	D	354	4	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	355	-	-	0/53/103/103	0/1/6/6
23	CLA	D	356	4	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	D	357	-	-	0/41/61/73	0/1/1/1
25	HEM	E	84	5,6	-	0/10/54/54	0/0/8/8
28	BCR	F	48	-	-	0/29/63/63	0/2/2/2
28	BCR	J	53	-	-	0/29/63/63	0/2/2/2
28	BCR	K	50	-	-	0/29/63/63	0/2/2/2
25	HEM	V	138	16	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCT	a	2346	22	-	0/0/0/0	0/0/0/0
22	OEC	a	2347	1,3,21	-	0/0/54/54	0/3/5/5
23	CLA	a	2348	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	2349	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	2350	-	-	0/53/103/103	0/1/6/6
23	CLA	a	2351	1	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	a	2352	-	-	0/41/61/73	0/1/1/1
23	CLA	b	2511	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2512	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2513	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2514	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2515	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2516	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2517	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2518	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2519	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2520	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2521	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2522	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2523	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2524	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2525	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2526	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	b	2527	-	-	0/29/63/63	0/2/2/2
28	BCR	b	2528	-	-	0/29/63/63	0/2/2/2
23	CLA	c	2474	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2475	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2476	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2477	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2478	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2479	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2480	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2481	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2482	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2483	3	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	2484	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2485	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2486	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2487	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	c	2488	-	-	0/29/63/63	0/2/2/2
28	BCR	c	2489	-	-	0/29/63/63	0/2/2/2
21	BCT	d	2353	20	-	0/0/0/0	0/0/0/0
23	CLA	d	2354	4	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	2355	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	d	2356	-	-	0/53/103/103	0/1/6/6
23	CLA	d	2357	4	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	d	2358	-	-	0/41/61/73	0/1/1/1
27	LMT	d	2359	-	-	0/21/61/61	0/2/2/2
28	BCR	d	2360	-	-	0/29/63/63	0/2/2/2
25	HEM	e	2084	5,6	-	0/10/54/54	0/0/8/8
28	BCR	j	2053	-	-	0/29/63/63	0/2/2/2
28	BCR	k	2050	-	-	0/29/63/63	0/2/2/2
25	HEM	v	2138	16	-	0/10/54/54	0/0/8/8

All (650) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	v	2138	HEM	C3D-C4D	-7.90	1.41	1.51
25	v	2138	HEM	C3B-C4B	-7.44	1.45	1.51
25	e	2084	HEM	C2D-C3D	-6.18	1.36	1.54
26	d	2358	PL9	C53-C6	-5.28	1.39	1.50
26	D	357	PL9	C53-C6	-5.16	1.40	1.50
26	d	2358	PL9	C52-C5	-5.15	1.40	1.50
25	v	2138	HEM	CAD-C3D	-5.14	1.43	1.54
26	a	2352	PL9	C22-C23	-4.98	1.36	1.50
26	a	2352	PL9	C53-C6	-4.94	1.40	1.50
25	v	2138	HEM	C2C-C1C	-4.91	1.43	1.52
26	A	353	PL9	C22-C23	-4.85	1.36	1.50
26	A	353	PL9	C52-C5	-4.80	1.40	1.50
25	E	84	HEM	C2D-C3D	-4.74	1.40	1.54
26	A	353	PL9	C53-C6	-4.69	1.41	1.50
28	k	2050	BCR	C17-C18	-4.66	1.29	1.35
28	K	50	BCR	C17-C18	-4.64	1.29	1.35
25	V	138	HEM	C3C-CAC	-4.60	1.42	1.51
26	a	2352	PL9	C52-C5	-4.48	1.41	1.50
25	e	2084	HEM	C3D-C4D	-4.44	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	357	PL9	C52-C5	-4.44	1.41	1.50
25	E	84	HEM	C3B-C4B	-4.29	1.48	1.51
24	A	351	PHO	CHB-C1B	-4.25	1.30	1.38
24	a	2350	PHO	CHB-C1B	-4.05	1.31	1.38
23	B	520	CLA	CAA-CBA	-3.95	1.39	1.52
23	b	2520	CLA	CAA-CBA	-3.81	1.39	1.52
23	B	523	CLA	CAA-CBA	-3.77	1.40	1.52
23	b	2523	CLA	CAA-CBA	-3.76	1.40	1.52
23	b	2514	CLA	C1B-CHB	-3.70	1.29	1.39
23	A	348	CLA	C3B-C2B	-3.63	1.35	1.40
28	K	50	BCR	C23-C22	-3.62	1.37	1.45
28	k	2050	BCR	C19-C18	-3.56	1.38	1.45
28	k	2050	BCR	C23-C22	-3.56	1.38	1.45
27	B	526	LMT	C3B-C2B	-3.55	1.43	1.52
23	c	2477	CLA	CAA-CBA	-3.53	1.40	1.52
23	B	514	CLA	CAA-CBA	-3.52	1.40	1.52
23	B	514	CLA	C1B-CHB	-3.52	1.30	1.39
23	b	2514	CLA	CAA-CBA	-3.51	1.40	1.52
23	c	2479	CLA	CAA-CBA	-3.50	1.41	1.52
28	K	50	BCR	C19-C18	-3.45	1.38	1.45
25	E	84	HEM	C2C-C1C	-3.29	1.46	1.52
23	C	485	CLA	C1B-CHB	-3.23	1.30	1.39
23	C	477	CLA	CAA-CBA	-3.23	1.41	1.52
23	B	524	CLA	C1B-CHB	-3.22	1.31	1.39
23	B	519	CLA	C1B-CHB	-3.19	1.31	1.39
25	v	2138	HEM	C2D-C3D	-3.13	1.45	1.54
25	E	84	HEM	C3D-C4D	-3.13	1.47	1.51
27	d	2359	LMT	C3B-C2B	-3.12	1.44	1.52
23	B	515	CLA	C1B-CHB	-3.08	1.31	1.39
24	D	355	PHO	CHB-C1B	-3.07	1.33	1.38
26	a	2352	PL9	C17-C18	-3.04	1.42	1.50
23	b	2515	CLA	C1B-CHB	-3.02	1.31	1.39
23	b	2524	CLA	C1B-CHB	-3.00	1.31	1.39
23	B	511	CLA	CAA-CBA	-2.99	1.42	1.52
23	b	2519	CLA	C1B-CHB	-2.98	1.31	1.39
23	c	2485	CLA	C1B-CHB	-2.98	1.31	1.39
23	b	2518	CLA	CAA-CBA	-2.96	1.42	1.52
23	b	2511	CLA	C1B-CHB	-2.95	1.31	1.39
23	B	517	CLA	C1B-CHB	-2.94	1.31	1.39
23	a	2348	CLA	C1B-CHB	-2.90	1.31	1.39
23	C	479	CLA	CAA-CBA	-2.89	1.43	1.52
23	B	518	CLA	CAA-CBA	-2.89	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2515	CLA	CAA-CBA	-2.88	1.43	1.52
23	b	2519	CLA	CAA-CBA	-2.86	1.43	1.52
25	E	84	HEM	C2B-C1B	-2.85	1.42	1.51
26	A	353	PL9	C27-C28	-2.84	1.42	1.50
23	B	519	CLA	CAA-CBA	-2.83	1.43	1.52
23	A	348	CLA	C1B-CHB	-2.81	1.32	1.39
26	a	2352	PL9	C27-C28	-2.80	1.42	1.50
23	B	515	CLA	CAA-CBA	-2.79	1.43	1.52
28	K	50	BCR	C12-C13	-2.78	1.39	1.45
24	d	2356	PHO	CHB-C1B	-2.77	1.33	1.38
23	a	2349	CLA	CAA-CBA	-2.76	1.43	1.52
26	A	353	PL9	C17-C18	-2.75	1.42	1.50
23	C	480	CLA	CAA-CBA	-2.74	1.43	1.52
23	b	2511	CLA	CAA-CBA	-2.73	1.43	1.52
26	D	357	PL9	C32-C33	-2.73	1.42	1.50
28	K	50	BCR	C21-C22	-2.73	1.32	1.35
23	d	2355	CLA	C1B-CHB	-2.71	1.32	1.39
23	B	518	CLA	C1B-CHB	-2.71	1.32	1.39
23	B	511	CLA	C1B-CHB	-2.70	1.32	1.39
23	c	2481	CLA	CAA-CBA	-2.69	1.43	1.52
23	C	478	CLA	C1B-CHB	-2.68	1.32	1.39
23	c	2486	CLA	C1B-CHB	-2.64	1.32	1.39
23	c	2478	CLA	C1B-CHB	-2.63	1.32	1.39
23	b	2517	CLA	C1B-CHB	-2.61	1.32	1.39
23	c	2485	CLA	CAA-CBA	-2.61	1.43	1.52
23	C	475	CLA	C1B-CHB	-2.60	1.32	1.39
23	c	2483	CLA	CAA-CBA	-2.60	1.44	1.52
23	C	474	CLA	CAA-CBA	-2.59	1.44	1.52
28	k	2050	BCR	C12-C13	-2.58	1.40	1.45
23	C	483	CLA	CAA-CBA	-2.56	1.44	1.52
26	d	2358	PL9	C32-C33	-2.55	1.43	1.50
23	c	2480	CLA	CAA-CBA	-2.54	1.44	1.52
23	b	2521	CLA	CAA-CBA	-2.54	1.44	1.52
23	C	487	CLA	C1B-CHB	-2.53	1.32	1.39
23	B	516	CLA	CAA-CBA	-2.52	1.44	1.52
28	k	2050	BCR	C21-C22	-2.52	1.32	1.35
25	v	2138	HEM	C3C-CAC	-2.51	1.46	1.51
23	C	486	CLA	C1B-CHB	-2.50	1.32	1.39
23	B	525	CLA	C3B-C2B	-2.48	1.37	1.40
23	A	349	CLA	C1B-CHB	-2.48	1.33	1.39
23	b	2517	CLA	CAA-CBA	-2.47	1.44	1.52
23	b	2518	CLA	C1B-CHB	-2.45	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2479	CLA	C1B-CHB	-2.45	1.33	1.39
26	d	2358	PL9	C37-C38	-2.45	1.43	1.50
23	c	2474	CLA	CAA-CBA	-2.44	1.44	1.52
23	c	2485	CLA	CBA-CGA	-2.44	1.43	1.50
28	K	50	BCR	C20-C21	-2.44	1.36	1.43
23	b	2516	CLA	CAA-CBA	-2.44	1.44	1.52
23	B	521	CLA	CAA-CBA	-2.43	1.44	1.52
28	c	2488	BCR	C19-C18	-2.42	1.40	1.45
23	A	350	CLA	CAA-CBA	-2.42	1.44	1.52
28	k	2050	BCR	C20-C21	-2.41	1.36	1.43
25	v	2138	HEM	C2B-C1B	-2.41	1.44	1.51
23	C	479	CLA	C1B-CHB	-2.40	1.33	1.39
23	c	2475	CLA	C1B-CHB	-2.40	1.33	1.39
23	C	474	CLA	C1B-CHB	-2.39	1.33	1.39
28	K	50	BCR	C16-C15	-2.39	1.29	1.35
28	k	2050	BCR	C16-C17	-2.38	1.36	1.43
23	a	2351	CLA	C1B-CHB	-2.37	1.33	1.39
28	K	50	BCR	C16-C17	-2.37	1.36	1.43
28	k	2050	BCR	C16-C15	-2.37	1.29	1.35
23	A	348	CLA	CAA-CBA	-2.37	1.44	1.52
26	D	357	PL9	C37-C38	-2.36	1.43	1.50
23	B	517	CLA	CAA-CBA	-2.35	1.44	1.52
23	B	522	CLA	C1B-CHB	-2.33	1.33	1.39
23	A	352	CLA	C1B-CHB	-2.33	1.33	1.39
25	e	2084	HEM	C2B-C1B	-2.31	1.44	1.51
24	a	2350	PHO	C1D-C2D	-2.30	1.40	1.45
23	B	519	CLA	C3B-C2B	-2.30	1.37	1.40
26	D	357	PL9	C7-C8	-2.30	1.47	1.50
25	V	138	HEM	C2B-C1B	-2.30	1.44	1.51
23	c	2474	CLA	C1B-CHB	-2.29	1.33	1.39
23	b	2525	CLA	C3B-C2B	-2.29	1.37	1.40
28	K	50	BCR	C15-C14	-2.28	1.36	1.43
23	C	485	CLA	CAA-CBA	-2.28	1.45	1.52
23	C	475	CLA	CAA-CBA	-2.27	1.45	1.52
23	c	2475	CLA	CAA-CBA	-2.26	1.45	1.52
23	b	2515	CLA	C3A-C4A	-2.26	1.44	1.51
23	A	348	CLA	CBA-CGA	-2.25	1.43	1.50
24	A	351	PHO	C1D-C2D	-2.24	1.40	1.45
23	B	521	CLA	C1B-CHB	-2.24	1.33	1.39
23	c	2480	CLA	C1B-CHB	-2.24	1.33	1.39
23	C	481	CLA	CAA-CBA	-2.22	1.45	1.52
24	a	2350	PHO	CAA-CBA	-2.21	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2348	CLA	C3B-C2B	-2.20	1.37	1.40
23	b	2522	CLA	C1B-CHB	-2.20	1.33	1.39
23	B	515	CLA	C3A-C4A	-2.20	1.44	1.51
23	B	523	CLA	C1B-CHB	-2.20	1.33	1.39
26	d	2358	PL9	C22-C23	-2.20	1.44	1.50
23	b	2525	CLA	C1B-CHB	-2.19	1.33	1.39
28	C	488	BCR	C23-C22	-2.18	1.41	1.45
23	B	517	CLA	C3A-C4A	-2.18	1.44	1.51
23	A	349	CLA	CAA-CBA	-2.18	1.45	1.52
23	b	2518	CLA	C3D-CAD	-2.18	1.39	1.45
28	k	2050	BCR	C11-C10	-2.18	1.37	1.43
23	B	520	CLA	C1B-CHB	-2.17	1.33	1.39
26	d	2358	PL9	C7-C8	-2.17	1.47	1.50
28	C	488	BCR	C17-C18	-2.16	1.32	1.35
23	a	2348	CLA	CAA-CBA	-2.16	1.45	1.52
23	B	511	CLA	C3A-C4A	-2.15	1.44	1.51
23	B	514	CLA	C3A-C4A	-2.15	1.44	1.51
28	k	2050	BCR	C15-C14	-2.14	1.37	1.43
26	a	2352	PL9	C32-C33	-2.14	1.44	1.50
28	c	2488	BCR	C11-C10	-2.14	1.37	1.43
23	b	2518	CLA	C3B-C2B	-2.13	1.37	1.40
23	c	2487	CLA	C1B-CHB	-2.13	1.34	1.39
23	B	525	CLA	C3B-CAB	-2.11	1.43	1.47
23	b	2523	CLA	CBA-CGA	-2.11	1.44	1.50
28	B	529	BCR	C20-C21	-2.10	1.37	1.43
28	c	2488	BCR	C20-C21	-2.10	1.37	1.43
28	c	2488	BCR	C23-C22	-2.10	1.41	1.45
26	A	353	PL9	C21-C19	-2.09	1.46	1.51
26	a	2352	PL9	C37-C38	-2.09	1.44	1.50
26	A	353	PL9	C32-C33	-2.09	1.44	1.50
23	B	523	CLA	C2A-C1A	-2.09	1.48	1.52
23	D	356	CLA	CAA-CBA	-2.09	1.45	1.52
28	K	50	BCR	C14-C13	-2.07	1.33	1.35
23	c	2479	CLA	C3A-C4A	-2.07	1.45	1.51
23	C	477	CLA	C1B-CHB	-2.06	1.34	1.39
28	C	488	BCR	C11-C10	-2.05	1.37	1.43
28	k	2050	BCR	C14-C13	-2.05	1.33	1.35
26	D	357	PL9	C22-C23	-2.05	1.44	1.50
23	b	2514	CLA	C3A-C4A	-2.05	1.45	1.51
23	B	527	CLA	C1B-CHB	-2.04	1.34	1.39
23	b	2517	CLA	C3A-C4A	-2.04	1.45	1.51
28	C	488	BCR	C19-C18	-2.03	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	525	CLA	C1B-CHB	-2.03	1.34	1.39
23	b	2513	CLA	C1B-CHB	-2.02	1.34	1.39
23	b	2515	CLA	CBA-CGA	-2.02	1.44	1.50
23	b	2523	CLA	C1B-CHB	-2.02	1.34	1.39
23	c	2481	CLA	C1B-CHB	-2.01	1.34	1.39
23	d	2357	CLA	CAA-CBA	-2.01	1.46	1.52
24	D	355	PHO	C1D-C2D	-2.00	1.41	1.45
23	B	511	CLA	C1C-C2C	2.00	1.48	1.44
23	c	2486	CLA	C2-C3	2.00	1.36	1.33
23	A	352	CLA	C4C-C3C	2.01	1.48	1.45
23	D	354	CLA	C5-C3	2.01	1.55	1.51
23	B	527	CLA	OBD-CAD	2.01	1.25	1.22
23	C	474	CLA	CHC-C1C	2.02	1.41	1.35
23	c	2487	CLA	OBD-CAD	2.03	1.25	1.22
25	e	2084	HEM	C2A-C3A	2.03	1.43	1.37
23	a	2348	CLA	C4-C3	2.03	1.55	1.50
23	A	348	CLA	C4-C3	2.04	1.55	1.50
23	c	2481	CLA	CHC-C1C	2.04	1.41	1.35
23	c	2484	CLA	C1C-C2C	2.04	1.48	1.44
23	b	2512	CLA	CHC-C1C	2.04	1.41	1.35
23	B	517	CLA	CHC-C1C	2.05	1.41	1.35
24	D	355	PHO	C4-C3	2.05	1.55	1.50
23	c	2478	CLA	CHC-C1C	2.05	1.41	1.35
23	B	516	CLA	O2A-CGA	2.05	1.39	1.33
28	j	2053	BCR	C1-C6	2.05	1.56	1.53
23	c	2487	CLA	CMA-C3A	2.06	1.57	1.53
23	C	481	CLA	CHC-C1C	2.06	1.41	1.35
23	B	522	CLA	CHC-C1C	2.06	1.41	1.35
23	c	2481	CLA	C1C-C2C	2.06	1.48	1.44
23	C	477	CLA	C2-C3	2.06	1.37	1.33
26	a	2352	PL9	C2-C3	2.07	1.40	1.34
23	D	354	CLA	C1-C2	2.07	1.55	1.49
23	A	349	CLA	CHC-C1C	2.07	1.41	1.35
23	C	476	CLA	C4-C3	2.07	1.55	1.50
23	b	2514	CLA	CHC-C1C	2.07	1.41	1.35
23	B	514	CLA	O2A-CGA	2.07	1.39	1.33
23	c	2480	CLA	CHC-C1C	2.08	1.41	1.35
23	b	2526	CLA	C2-C3	2.08	1.37	1.33
23	C	483	CLA	CAA-C2A	2.08	1.58	1.54
23	B	519	CLA	CHC-C1C	2.08	1.41	1.35
23	c	2474	CLA	CHC-C1C	2.08	1.41	1.35
23	B	523	CLA	C5-C3	2.08	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	2357	CLA	CAA-C2A	2.09	1.58	1.54
26	a	2352	PL9	C40-C39	2.09	1.56	1.50
24	A	351	PHO	C3B-C4B	2.10	1.48	1.43
28	C	489	BCR	C33-C5	2.10	1.54	1.51
23	c	2475	CLA	OBD-CAD	2.10	1.25	1.22
23	B	511	CLA	C2-C3	2.10	1.37	1.33
23	C	482	CLA	C1-C2	2.10	1.55	1.49
23	c	2484	CLA	CHC-C1C	2.10	1.41	1.35
23	C	477	CLA	C1-C2	2.10	1.55	1.49
23	b	2516	CLA	CHC-C1C	2.10	1.41	1.35
23	B	513	CLA	CHC-C1C	2.11	1.41	1.35
23	b	2517	CLA	CHC-C1C	2.11	1.41	1.35
23	b	2524	CLA	CAA-C2A	2.12	1.58	1.54
23	B	511	CLA	C4-C3	2.12	1.55	1.50
28	F	48	BCR	C24-C23	2.12	1.39	1.33
23	d	2354	CLA	CHC-C1C	2.12	1.41	1.35
23	b	2518	CLA	O2A-CGA	2.13	1.39	1.33
25	v	2138	HEM	CBC-CAC	2.13	1.41	1.29
23	b	2518	CLA	C2-C3	2.13	1.37	1.33
28	b	2527	BCR	C38-C26	2.14	1.54	1.51
23	C	479	CLA	C2-C3	2.15	1.37	1.33
28	B	529	BCR	C5-C6	2.15	1.37	1.34
23	C	476	CLA	CHC-C1C	2.15	1.42	1.35
28	K	50	BCR	C5-C6	2.15	1.37	1.34
23	B	517	CLA	C4-C3	2.15	1.55	1.50
23	c	2477	CLA	CMB-C2B	2.16	1.56	1.51
23	c	2487	CLA	C5-C3	2.17	1.56	1.51
26	A	353	PL9	C2-C3	2.17	1.40	1.34
23	c	2478	CLA	O2A-CGA	2.17	1.39	1.33
23	B	527	CLA	CHC-C1C	2.17	1.42	1.35
23	C	483	CLA	CHC-C1C	2.18	1.42	1.35
23	c	2479	CLA	C4-C3	2.18	1.56	1.50
23	b	2521	CLA	CHC-C1C	2.18	1.42	1.35
23	D	356	CLA	CHC-C1C	2.18	1.42	1.35
23	B	522	CLA	C4-C3	2.19	1.56	1.50
23	c	2482	CLA	C4C-C3C	2.19	1.49	1.45
23	b	2522	CLA	CAA-C2A	2.19	1.58	1.54
23	c	2476	CLA	CMB-C2B	2.19	1.56	1.51
23	B	527	CLA	C1-C2	2.20	1.56	1.49
23	c	2476	CLA	C1C-C2C	2.20	1.49	1.44
28	J	53	BCR	C38-C26	2.20	1.54	1.51
25	e	2084	HEM	C3B-CAB	2.20	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	2357	CLA	CHC-C1C	2.21	1.42	1.35
24	D	355	PHO	C3B-C4B	2.21	1.48	1.43
23	C	486	CLA	C5-C3	2.21	1.56	1.51
28	d	2360	BCR	C24-C23	2.22	1.39	1.33
23	c	2477	CLA	CHC-C1C	2.22	1.42	1.35
23	D	354	CLA	CHC-C1C	2.22	1.42	1.35
23	B	515	CLA	CHC-C1C	2.22	1.42	1.35
23	A	349	CLA	CAA-C2A	2.23	1.58	1.54
23	C	475	CLA	CHC-C1C	2.23	1.42	1.35
23	c	2476	CLA	C4-C3	2.24	1.56	1.50
23	B	514	CLA	CHC-C1C	2.25	1.42	1.35
23	c	2479	CLA	C2-C3	2.26	1.37	1.33
23	b	2522	CLA	C5-C3	2.26	1.56	1.51
23	B	513	CLA	C4-C3	2.26	1.56	1.50
23	C	480	CLA	C4-C3	2.26	1.56	1.50
23	B	518	CLA	CHC-C1C	2.26	1.42	1.35
23	B	523	CLA	C4-C3	2.26	1.56	1.50
23	b	2521	CLA	CMB-C2B	2.26	1.56	1.51
24	d	2356	PHO	C4-C3	2.26	1.56	1.50
23	C	486	CLA	C4-C3	2.26	1.56	1.50
23	C	474	CLA	C4-C3	2.27	1.56	1.50
23	C	478	CLA	OBD-CAD	2.27	1.25	1.22
25	V	138	HEM	FE-NC	2.28	2.04	1.95
23	c	2482	CLA	C4-C3	2.28	1.56	1.50
23	b	2517	CLA	C4-C3	2.28	1.56	1.50
23	B	514	CLA	C2-C3	2.28	1.37	1.33
23	b	2516	CLA	O2A-CGA	2.28	1.40	1.33
23	d	2354	CLA	C5-C3	2.29	1.56	1.51
23	B	527	CLA	CMB-C2B	2.30	1.56	1.51
23	c	2475	CLA	CHC-C1C	2.30	1.42	1.35
23	B	512	CLA	CHC-C1C	2.30	1.42	1.35
23	c	2483	CLA	CHC-C1C	2.30	1.42	1.35
23	c	2478	CLA	OBD-CAD	2.31	1.25	1.22
28	c	2488	BCR	C33-C5	2.31	1.54	1.51
23	c	2476	CLA	CAA-C2A	2.31	1.58	1.54
24	A	351	PHO	C4-C3	2.31	1.56	1.50
23	b	2526	CLA	C4C-C3C	2.32	1.49	1.45
23	c	2480	CLA	C4-C3	2.32	1.56	1.50
23	b	2516	CLA	C6-C5	2.33	1.61	1.52
23	B	512	CLA	CAA-C2A	2.33	1.58	1.54
23	C	482	CLA	C4-C3	2.33	1.56	1.50
23	b	2523	CLA	C1C-C2C	2.34	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	478	CLA	CAA-C2A	2.34	1.58	1.54
23	b	2523	CLA	C5-C3	2.34	1.56	1.51
23	b	2516	CLA	C4-C3	2.34	1.56	1.50
23	B	519	CLA	C4-C3	2.35	1.56	1.50
23	C	484	CLA	OBD-CAD	2.35	1.25	1.22
28	B	529	BCR	C38-C26	2.35	1.54	1.51
23	b	2523	CLA	C4-C3	2.35	1.56	1.50
23	b	2526	CLA	CMB-C2B	2.35	1.56	1.51
23	C	483	CLA	C4-C3	2.35	1.56	1.50
28	j	2053	BCR	C33-C5	2.36	1.54	1.51
23	B	525	CLA	C4-C3	2.36	1.56	1.50
23	b	2521	CLA	C5-C3	2.36	1.56	1.51
23	B	511	CLA	C1-C2	2.37	1.56	1.49
23	B	521	CLA	CHC-C1C	2.37	1.42	1.35
23	B	527	CLA	C4C-C3C	2.38	1.49	1.45
23	c	2486	CLA	C4-C3	2.38	1.56	1.50
23	b	2518	CLA	CHC-C1C	2.38	1.42	1.35
23	b	2511	CLA	C1C-C2C	2.39	1.49	1.44
23	B	515	CLA	C4-C3	2.40	1.56	1.50
23	a	2351	CLA	CAA-C2A	2.40	1.58	1.54
23	b	2514	CLA	C2-C3	2.40	1.37	1.33
28	c	2489	BCR	C33-C5	2.41	1.55	1.51
23	B	514	CLA	C4-C3	2.41	1.56	1.50
23	B	523	CLA	CHC-C1C	2.41	1.42	1.35
23	B	520	CLA	C4-C3	2.41	1.56	1.50
27	B	526	LMT	O1'-C1'	2.42	1.44	1.40
23	b	2513	CLA	C2-C3	2.42	1.37	1.33
23	b	2520	CLA	C5-C3	2.43	1.56	1.51
23	c	2478	CLA	CAA-C2A	2.43	1.59	1.54
28	b	2528	BCR	C5-C6	2.44	1.38	1.34
25	E	84	HEM	C2A-C3A	2.45	1.44	1.37
24	a	2350	PHO	C4-C3	2.45	1.56	1.50
23	D	356	CLA	C1C-C2C	2.46	1.49	1.44
23	b	2526	CLA	C4-C3	2.46	1.56	1.50
23	C	478	CLA	O2A-CGA	2.46	1.40	1.33
28	k	2050	BCR	C5-C6	2.46	1.38	1.34
23	B	520	CLA	CHC-C1C	2.46	1.43	1.35
23	B	514	CLA	C5-C3	2.46	1.56	1.51
23	b	2513	CLA	C4-C3	2.47	1.56	1.50
25	e	2084	HEM	C3C-CAC	2.48	1.56	1.51
28	k	2050	BCR	C33-C5	2.48	1.55	1.51
28	F	48	BCR	C14-C13	2.48	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	511	CLA	O2A-CGA	2.48	1.40	1.33
23	b	2514	CLA	C4-C3	2.48	1.56	1.50
23	B	525	CLA	CAA-C2A	2.49	1.59	1.54
23	d	2355	CLA	CHC-C1C	2.49	1.43	1.35
23	C	484	CLA	CHC-C1C	2.49	1.43	1.35
23	C	478	CLA	C2-C3	2.49	1.37	1.33
27	B	526	LMT	C4'-C5'	2.49	1.59	1.52
26	D	357	PL9	C2-C3	2.50	1.41	1.34
28	c	2489	BCR	C21-C22	2.50	1.39	1.35
23	b	2519	CLA	C4-C3	2.50	1.56	1.50
23	b	2525	CLA	C4-C3	2.51	1.56	1.50
23	B	524	CLA	CAA-C2A	2.51	1.59	1.54
23	b	2511	CLA	C1-C2	2.51	1.57	1.49
23	C	487	CLA	C4-C3	2.51	1.56	1.50
28	j	2053	BCR	C38-C26	2.52	1.55	1.51
23	c	2485	CLA	C4-C3	2.52	1.56	1.50
23	c	2481	CLA	C4-C3	2.53	1.56	1.50
23	C	485	CLA	C4-C3	2.53	1.56	1.50
26	d	2358	PL9	C2-C3	2.54	1.41	1.34
26	D	357	PL9	C35-C34	2.54	1.56	1.50
23	c	2476	CLA	CHC-C1C	2.56	1.43	1.35
23	b	2512	CLA	CAA-C2A	2.56	1.59	1.54
23	A	349	CLA	O2A-CGA	2.56	1.41	1.33
23	a	2351	CLA	C4C-C3C	2.56	1.49	1.45
23	b	2520	CLA	CHC-C1C	2.56	1.43	1.35
28	b	2528	BCR	C38-C26	2.56	1.55	1.51
23	b	2523	CLA	CHC-C1C	2.57	1.43	1.35
23	d	2357	CLA	C5-C3	2.57	1.57	1.51
23	C	483	CLA	C2-C3	2.58	1.38	1.33
23	b	2518	CLA	C4-C3	2.58	1.57	1.50
26	A	353	PL9	C35-C34	2.58	1.57	1.50
23	b	2515	CLA	C4-C3	2.59	1.57	1.50
23	B	511	CLA	CHC-C1C	2.60	1.43	1.35
23	B	519	CLA	C5-C3	2.60	1.57	1.51
26	d	2358	PL9	C38-C39	2.60	1.40	1.32
26	A	353	PL9	C18-C19	2.61	1.38	1.33
23	b	2512	CLA	C4-C3	2.61	1.57	1.50
24	A	351	PHO	CHC-C1C	2.61	1.43	1.38
23	B	525	CLA	OBD-CAD	2.61	1.26	1.22
23	C	475	CLA	C1-C2	2.62	1.57	1.49
23	C	481	CLA	C4-C3	2.62	1.57	1.50
23	D	356	CLA	C4-C3	2.62	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2475	CLA	C1-C2	2.63	1.57	1.49
26	a	2352	PL9	C30-C29	2.63	1.57	1.50
25	e	2084	HEM	C4A-CHB	2.63	1.47	1.39
23	b	2511	CLA	O2A-CGA	2.63	1.41	1.33
28	B	528	BCR	C33-C5	2.63	1.55	1.51
23	b	2525	CLA	OBD-CAD	2.64	1.26	1.22
23	b	2522	CLA	C4-C3	2.64	1.57	1.50
23	B	516	CLA	C6-C5	2.64	1.62	1.52
26	D	357	PL9	C38-C39	2.65	1.40	1.32
23	b	2524	CLA	O2A-CGA	2.65	1.41	1.33
28	K	50	BCR	C33-C5	2.65	1.55	1.51
23	a	2351	CLA	C4-C3	2.65	1.57	1.50
23	B	516	CLA	C4-C3	2.65	1.57	1.50
23	C	487	CLA	OBD-CAD	2.65	1.26	1.22
24	d	2356	PHO	CHC-C1C	2.65	1.44	1.38
23	B	519	CLA	C1-C2	2.66	1.57	1.49
23	b	2511	CLA	CHC-C1C	2.66	1.43	1.35
27	d	2359	LMT	C4'-C5'	2.67	1.60	1.52
24	a	2350	PHO	C3B-C4B	2.68	1.49	1.43
23	b	2520	CLA	C1-C2	2.68	1.57	1.49
26	A	353	PL9	C30-C29	2.68	1.57	1.50
23	B	520	CLA	C1-C2	2.70	1.57	1.49
23	b	2520	CLA	O2A-CGA	2.70	1.41	1.33
26	d	2358	PL9	C35-C34	2.70	1.57	1.50
23	C	484	CLA	CAA-C2A	2.70	1.59	1.54
23	B	527	CLA	C4-C3	2.71	1.57	1.50
23	c	2482	CLA	C5-C3	2.71	1.57	1.51
26	a	2352	PL9	C35-C34	2.73	1.57	1.50
28	b	2528	BCR	C24-C23	2.73	1.41	1.33
23	B	513	CLA	C2-C3	2.74	1.38	1.33
23	A	352	CLA	C4-C3	2.75	1.57	1.50
23	A	348	CLA	CHC-C1C	2.75	1.43	1.35
23	c	2487	CLA	C4-C3	2.75	1.57	1.50
27	B	526	LMT	C2-C1	2.75	1.63	1.50
23	b	2519	CLA	C1-C2	2.75	1.58	1.49
23	A	352	CLA	CAA-C2A	2.76	1.59	1.54
23	b	2514	CLA	C5-C3	2.77	1.57	1.51
23	c	2484	CLA	CAA-C2A	2.77	1.59	1.54
23	d	2355	CLA	O2A-CGA	2.77	1.41	1.33
23	D	354	CLA	CAA-C2A	2.77	1.59	1.54
27	d	2359	LMT	C2-C1	2.78	1.63	1.50
23	c	2483	CLA	C4-C3	2.78	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	50	BCR	C1-C6	2.80	1.57	1.53
23	b	2525	CLA	CAA-C2A	2.80	1.59	1.54
23	B	524	CLA	O2A-CGA	2.80	1.41	1.33
23	b	2520	CLA	C4-C3	2.80	1.57	1.50
23	C	482	CLA	C5-C3	2.81	1.57	1.51
28	b	2527	BCR	C1-C6	2.81	1.57	1.53
28	d	2360	BCR	C14-C13	2.81	1.39	1.35
23	c	2478	CLA	C2-C3	2.84	1.38	1.33
23	C	476	CLA	CAA-C2A	2.84	1.59	1.54
23	a	2348	CLA	CHC-C1C	2.86	1.44	1.35
23	B	516	CLA	CAA-C2A	2.86	1.59	1.54
28	K	50	BCR	C2-C1	2.86	1.61	1.54
26	d	2358	PL9	C30-C29	2.87	1.57	1.50
23	c	2483	CLA	C5-C3	2.87	1.57	1.51
23	C	475	CLA	C4-C3	2.87	1.57	1.50
25	e	2084	HEM	CHD-C4C	2.87	1.43	1.36
23	c	2486	CLA	CAA-C2A	2.87	1.59	1.54
23	B	527	CLA	C2-C3	2.88	1.38	1.33
25	V	138	HEM	CHC-C4B	2.88	1.46	1.38
23	d	2357	CLA	C4-C3	2.89	1.57	1.50
23	C	484	CLA	C4-C3	2.90	1.57	1.50
23	d	2354	CLA	CAA-C2A	2.91	1.59	1.54
28	k	2050	BCR	C30-C25	2.91	1.57	1.53
23	c	2474	CLA	C4-C3	2.92	1.57	1.50
23	c	2484	CLA	C4-C3	2.94	1.57	1.50
28	C	489	BCR	C1-C6	2.95	1.58	1.53
23	b	2519	CLA	C2-C3	2.96	1.38	1.33
26	A	353	PL9	C8-C9	2.96	1.38	1.33
25	V	138	HEM	CBC-CAC	2.96	1.46	1.29
23	B	512	CLA	C4-C3	2.96	1.57	1.50
23	B	520	CLA	O2A-CGA	2.98	1.42	1.33
23	B	516	CLA	C1-C2	2.98	1.58	1.49
23	B	521	CLA	C4-C3	2.98	1.57	1.50
23	c	2483	CLA	C2-C3	2.99	1.38	1.33
23	b	2516	CLA	C1-C2	3.00	1.58	1.49
25	v	2138	HEM	C3B-CAB	3.01	1.57	1.51
23	B	519	CLA	C2-C3	3.02	1.38	1.33
23	C	475	CLA	O2A-CGA	3.03	1.42	1.33
25	e	2084	HEM	CMA-C3A	3.03	1.57	1.51
23	C	486	CLA	CAA-C2A	3.05	1.60	1.54
25	E	84	HEM	CMD-C2D	3.06	1.60	1.53
26	a	2352	PL9	C8-C9	3.06	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	353	PL9	C31-C29	3.08	1.58	1.51
23	c	2475	CLA	C4-C3	3.08	1.58	1.50
23	C	483	CLA	C5-C3	3.10	1.58	1.51
23	B	516	CLA	C5-C3	3.11	1.58	1.51
23	C	477	CLA	O2A-CGA	3.12	1.42	1.33
25	E	84	HEM	CMC-C2C	3.13	1.60	1.53
27	d	2359	LMT	O1'-C1'	3.13	1.45	1.40
23	b	2516	CLA	C5-C3	3.13	1.58	1.51
23	c	2475	CLA	C5-C3	3.14	1.58	1.51
23	B	520	CLA	C2-C3	3.17	1.39	1.33
26	D	357	PL9	C8-C9	3.18	1.39	1.33
28	k	2050	BCR	C2-C1	3.19	1.61	1.54
26	a	2352	PL9	C31-C29	3.20	1.58	1.51
23	c	2482	CLA	CAA-C2A	3.22	1.60	1.54
28	C	488	BCR	C26-C25	3.22	1.39	1.34
23	C	475	CLA	C5-C3	3.24	1.58	1.51
26	d	2358	PL9	C8-C9	3.25	1.39	1.33
25	e	2084	HEM	CHC-C1C	3.25	1.44	1.36
26	D	357	PL9	C13-C14	3.25	1.39	1.33
28	C	488	BCR	C5-C6	3.26	1.39	1.34
28	C	489	BCR	C5-C6	3.26	1.39	1.34
26	D	357	PL9	C30-C29	3.27	1.58	1.50
23	c	2475	CLA	O2A-CGA	3.27	1.43	1.33
25	v	2138	HEM	CMA-C3A	3.28	1.58	1.51
28	K	50	BCR	C26-C25	3.28	1.39	1.34
23	b	2521	CLA	C4-C3	3.29	1.58	1.50
23	c	2477	CLA	O2A-CGA	3.29	1.43	1.33
28	c	2488	BCR	C5-C6	3.30	1.39	1.34
23	c	2487	CLA	CAA-C2A	3.31	1.60	1.54
25	v	2138	HEM	C4C-NC	3.31	1.40	1.36
28	K	50	BCR	C29-C30	3.32	1.62	1.54
26	a	2352	PL9	C38-C39	3.32	1.42	1.32
28	J	53	BCR	C2-C1	3.35	1.62	1.54
28	B	529	BCR	C24-C23	3.35	1.42	1.33
25	e	2084	HEM	CMD-C2D	3.35	1.60	1.53
28	K	50	BCR	C30-C25	3.36	1.58	1.53
25	v	2138	HEM	C1A-CHA	3.37	1.49	1.39
23	C	482	CLA	CAA-C2A	3.37	1.60	1.54
28	C	489	BCR	C2-C1	3.38	1.62	1.54
23	c	2475	CLA	CAA-C2A	3.38	1.60	1.54
28	B	529	BCR	C1-C6	3.39	1.58	1.53
25	v	2138	HEM	CBB-CAB	3.39	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	529	BCR	C29-C30	3.41	1.62	1.54
23	b	2520	CLA	C2-C3	3.41	1.39	1.33
28	k	2050	BCR	C26-C25	3.43	1.39	1.34
28	C	489	BCR	C26-C25	3.43	1.39	1.34
28	F	48	BCR	C29-C30	3.44	1.62	1.54
28	c	2489	BCR	C2-C1	3.45	1.62	1.54
25	v	2138	HEM	CHD-C4C	3.46	1.44	1.36
23	C	487	CLA	CAA-C2A	3.46	1.61	1.54
28	k	2050	BCR	C29-C30	3.46	1.62	1.54
28	F	48	BCR	C2-C1	3.49	1.62	1.54
28	b	2528	BCR	C1-C6	3.55	1.58	1.53
28	c	2489	BCR	C5-C6	3.56	1.40	1.34
28	C	488	BCR	C2-C1	3.58	1.62	1.54
28	B	528	BCR	C2-C1	3.60	1.62	1.54
26	A	353	PL9	C38-C39	3.62	1.43	1.32
28	C	488	BCR	C1-C6	3.63	1.58	1.53
23	b	2516	CLA	CAA-C2A	3.64	1.61	1.54
28	b	2528	BCR	C29-C30	3.64	1.62	1.54
26	a	2352	PL9	C23-C24	3.65	1.40	1.33
26	D	357	PL9	C33-C34	3.66	1.40	1.33
26	a	2352	PL9	C33-C34	3.67	1.40	1.33
23	b	2519	CLA	O2A-CGA	3.67	1.44	1.33
28	c	2488	BCR	C26-C25	3.68	1.40	1.34
28	c	2488	BCR	C2-C1	3.68	1.63	1.54
28	j	2053	BCR	C29-C30	3.69	1.63	1.54
26	d	2358	PL9	C28-C29	3.70	1.40	1.33
28	J	53	BCR	C29-C30	3.70	1.63	1.54
23	B	519	CLA	O2A-CGA	3.70	1.44	1.33
23	c	2487	CLA	C4C-C3C	3.70	1.51	1.45
23	C	475	CLA	CAA-C2A	3.71	1.61	1.54
28	B	528	BCR	C29-C30	3.72	1.63	1.54
28	C	489	BCR	C29-C30	3.72	1.63	1.54
25	e	2084	HEM	CBC-CAC	3.74	1.50	1.29
28	j	2053	BCR	C2-C1	3.76	1.63	1.54
28	d	2360	BCR	C2-C1	3.78	1.63	1.54
26	d	2358	PL9	C13-C14	3.78	1.40	1.33
28	F	48	BCR	C5-C6	3.78	1.40	1.34
25	E	84	HEM	CBC-CAC	3.79	1.51	1.29
28	b	2527	BCR	C29-C30	3.79	1.63	1.54
28	c	2489	BCR	C26-C25	3.80	1.40	1.34
26	A	353	PL9	C23-C24	3.81	1.40	1.33
28	b	2527	BCR	C2-C1	3.84	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	k	2050	BCR	C1-C6	3.87	1.59	1.53
26	D	357	PL9	C28-C29	3.90	1.40	1.33
23	B	516	CLA	C2-C3	3.91	1.40	1.33
28	C	488	BCR	C29-C30	3.92	1.63	1.54
23	C	487	CLA	C4C-C3C	3.93	1.52	1.45
25	V	138	HEM	CBB-CAB	3.94	1.52	1.29
28	d	2360	BCR	C1-C6	4.00	1.59	1.53
28	C	488	BCR	C30-C25	4.00	1.59	1.53
28	c	2489	BCR	C29-C30	4.03	1.63	1.54
26	A	353	PL9	C13-C14	4.03	1.40	1.33
25	E	84	HEM	CMB-C2B	4.04	1.62	1.53
28	d	2360	BCR	C29-C30	4.07	1.63	1.54
26	d	2358	PL9	C33-C34	4.07	1.41	1.33
23	b	2513	CLA	CAA-C2A	4.08	1.62	1.54
28	c	2488	BCR	C29-C30	4.08	1.64	1.54
26	a	2352	PL9	C13-C14	4.10	1.41	1.33
28	J	53	BCR	C26-C25	4.14	1.40	1.34
25	E	84	HEM	CBB-CAB	4.17	1.53	1.29
28	B	529	BCR	C2-C1	4.17	1.64	1.54
26	D	357	PL9	C23-C24	4.21	1.41	1.33
28	F	48	BCR	C1-C6	4.22	1.59	1.53
25	e	2084	HEM	CBB-CAB	4.25	1.53	1.29
23	C	475	CLA	C2-C3	4.27	1.41	1.33
25	e	2084	HEM	CMB-C2B	4.28	1.63	1.53
28	c	2488	BCR	C30-C25	4.29	1.59	1.53
28	F	48	BCR	C26-C25	4.30	1.41	1.34
23	c	2475	CLA	C2-C3	4.36	1.41	1.33
28	b	2528	BCR	C2-C1	4.41	1.64	1.54
26	A	353	PL9	C28-C29	4.44	1.41	1.33
28	d	2360	BCR	C26-C25	4.44	1.41	1.34
23	b	2516	CLA	C2-C3	4.49	1.41	1.33
26	d	2358	PL9	C31-C29	4.52	1.61	1.51
23	B	513	CLA	CAA-C2A	4.53	1.63	1.54
28	c	2489	BCR	C1-C6	4.57	1.60	1.53
26	D	357	PL9	C18-C19	4.58	1.42	1.33
28	d	2360	BCR	C5-C6	4.63	1.41	1.34
25	v	2138	HEM	CMD-C2D	4.66	1.64	1.53
28	J	53	BCR	C5-C6	4.70	1.41	1.34
28	b	2527	BCR	C26-C25	4.72	1.41	1.34
25	E	84	HEM	CHD-C4C	4.73	1.47	1.36
28	b	2527	BCR	C30-C25	4.76	1.60	1.53
26	a	2352	PL9	C28-C29	4.77	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	2488	BCR	C1-C6	4.89	1.60	1.53
26	d	2358	PL9	C18-C19	4.90	1.42	1.33
26	A	353	PL9	C33-C34	4.90	1.42	1.33
25	E	84	HEM	CMA-C3A	4.91	1.61	1.51
28	B	528	BCR	C5-C6	4.91	1.42	1.34
28	b	2528	BCR	C26-C25	4.94	1.42	1.34
26	d	2358	PL9	C23-C24	5.00	1.42	1.33
25	v	2138	HEM	CMB-C2B	5.08	1.64	1.53
28	B	528	BCR	C26-C25	5.16	1.42	1.34
28	j	2053	BCR	C5-C6	5.27	1.42	1.34
26	D	357	PL9	C31-C29	5.28	1.63	1.51
28	b	2527	BCR	C5-C6	5.34	1.42	1.34
28	j	2053	BCR	C26-C25	5.37	1.42	1.34
28	c	2489	BCR	C30-C25	5.44	1.61	1.53
28	C	489	BCR	C30-C25	5.47	1.61	1.53
25	v	2138	HEM	CMC-C2C	5.48	1.65	1.53
28	B	529	BCR	C26-C25	5.61	1.43	1.34
25	E	84	HEM	C1C-NC	5.64	1.43	1.36
25	V	138	HEM	C2A-C3A	5.73	1.54	1.37
28	d	2360	BCR	C30-C25	5.74	1.61	1.53
28	b	2528	BCR	C30-C25	5.78	1.62	1.53
28	B	528	BCR	C30-C25	5.89	1.62	1.53
28	B	529	BCR	C30-C25	5.94	1.62	1.53
26	D	357	PL9	C7-C3	6.18	1.56	1.51
25	E	84	HEM	C4C-NC	6.23	1.43	1.36
26	d	2358	PL9	C7-C3	6.25	1.56	1.51
28	J	53	BCR	C30-C25	6.28	1.62	1.53
25	e	2084	HEM	C4C-NC	6.41	1.43	1.36
25	V	138	HEM	CHD-C4C	6.69	1.52	1.36
25	V	138	HEM	CMD-C2D	6.70	1.68	1.53
25	e	2084	HEM	C1C-NC	6.73	1.44	1.36
28	F	48	BCR	C30-C25	6.79	1.63	1.53
25	V	138	HEM	C1A-CHA	6.89	1.58	1.39
25	V	138	HEM	CMA-C3A	7.15	1.66	1.51
26	A	353	PL9	C7-C3	7.21	1.57	1.51
28	j	2053	BCR	C30-C25	7.38	1.64	1.53
26	a	2352	PL9	C7-C3	7.79	1.57	1.51
25	v	2138	HEM	C1C-NC	9.15	1.47	1.36
25	V	138	HEM	CMB-C2B	9.34	1.74	1.53
25	V	138	HEM	CMC-C2C	9.77	1.75	1.53
25	V	138	HEM	C3B-C4B	10.22	1.61	1.51
25	V	138	HEM	C4C-NC	10.77	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	138	HEM	C1C-NC	14.93	1.54	1.36

All (1333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	E	84	HEM	C3B-CAB-CBB	-11.71	106.50	124.46
25	e	2084	HEM	C3B-CAB-CBB	-11.63	106.62	124.46
25	v	2138	HEM	C3B-CAB-CBB	-11.62	106.63	124.46
25	V	138	HEM	C3B-CAB-CBB	-10.38	108.53	124.46
25	v	2138	HEM	CAA-C2A-C1A	-7.18	119.21	127.01
23	B	520	CLA	CAA-C2A-C1A	-7.12	87.37	112.47
23	b	2520	CLA	CAA-C2A-C1A	-7.10	87.43	112.47
26	A	353	PL9	C21-C22-C23	-6.89	93.65	111.69
25	e	2084	HEM	C3C-CAC-CBC	-6.64	114.28	124.46
26	a	2352	PL9	C21-C22-C23	-6.63	94.33	111.69
25	E	84	HEM	C3C-CAC-CBC	-6.44	114.57	124.46
23	b	2520	CLA	CAA-CBA-CGA	-6.33	94.80	113.32
23	B	520	CLA	CAA-CBA-CGA	-6.27	94.95	113.32
25	V	138	HEM	CBD-CAD-C3D	-5.92	96.33	113.55
23	c	2477	CLA	CAA-C2A-C1A	-5.90	91.66	112.47
23	C	477	CLA	CAA-C2A-C1A	-5.82	91.96	112.47
26	A	353	PL9	C35-C34-C36	-5.74	106.63	115.41
28	B	529	BCR	C20-C21-C22	-5.72	118.94	127.20
23	B	519	CLA	CAA-C2A-C1A	-5.49	93.09	112.47
23	b	2519	CLA	CAA-C2A-C1A	-5.48	93.15	112.47
26	a	2352	PL9	C35-C34-C36	-5.47	107.05	115.41
28	b	2528	BCR	C20-C21-C22	-5.30	119.53	127.20
26	a	2352	PL9	C26-C24-C23	-5.21	111.17	121.05
23	C	481	CLA	CAA-CBA-CGA	-5.17	98.19	113.32
26	D	357	PL9	C35-C34-C36	-5.11	107.61	115.41
23	c	2481	CLA	CAA-CBA-CGA	-5.10	98.38	113.32
26	d	2358	PL9	C35-C34-C36	-4.94	107.87	115.41
24	d	2356	PHO	CBD-CHA-C4D	-4.72	103.17	108.46
25	e	2084	HEM	CBA-CAA-C2A	-4.70	104.11	112.53
26	A	353	PL9	C26-C24-C23	-4.69	112.15	121.05
25	E	84	HEM	CBA-CAA-C2A	-4.59	104.30	112.53
25	v	2138	HEM	C3C-CAC-CBC	-4.58	117.43	124.46
23	C	477	CLA	CAA-CBA-CGA	-4.55	100.00	113.32
24	D	355	PHO	CBD-CHA-C4D	-4.55	103.36	108.46
23	c	2479	CLA	CAA-CBA-CGA	-4.49	100.16	113.32
28	F	48	BCR	C8-C9-C10	-4.49	111.76	118.98
28	b	2527	BCR	C33-C5-C4	-4.48	104.94	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2483	CLA	CAA-C2A-C1A	-4.47	96.70	112.47
23	c	2477	CLA	CAA-CBA-CGA	-4.44	100.31	113.32
23	C	483	CLA	CAA-C2A-C1A	-4.35	97.11	112.47
25	v	2138	HEM	CBD-CAD-C3D	-4.31	101.00	113.55
28	d	2360	BCR	C8-C9-C10	-4.29	112.07	118.98
27	d	2359	LMT	C1B-O1B-C4'	-4.26	106.88	118.01
23	C	479	CLA	CAA-CBA-CGA	-4.18	101.07	113.32
25	v	2138	HEM	C2C-C1C-CHC	-4.17	117.34	123.68
28	B	528	BCR	C33-C5-C4	-4.16	105.53	113.43
23	c	2477	CLA	C7-C6-C5	-4.16	100.77	113.06
23	C	477	CLA	C7-C6-C5	-4.11	100.93	113.06
23	B	525	CLA	C3B-CAB-CBB	-4.04	118.05	126.32
27	B	526	LMT	C1B-O1B-C4'	-4.04	107.46	118.01
23	B	519	CLA	CAA-CBA-CGA	-3.98	101.67	113.32
23	b	2525	CLA	C3B-CAB-CBB	-3.96	118.21	126.32
23	c	2481	CLA	CAA-C2A-C1A	-3.94	98.59	112.47
23	b	2524	CLA	C5-C3-C2	-3.93	113.61	121.05
28	d	2360	BCR	C33-C5-C4	-3.87	106.09	113.43
23	b	2526	CLA	CAA-CBA-CGA	-3.86	102.03	113.32
23	C	485	CLA	OBD-CAD-CBD	-3.85	120.13	125.94
28	b	2527	BCR	C38-C26-C27	-3.83	106.17	113.43
23	B	511	CLA	CAA-C2A-C1A	-3.82	99.00	112.47
24	A	351	PHO	CBD-CHA-C4D	-3.81	104.19	108.46
28	J	53	BCR	C33-C5-C4	-3.81	106.20	113.43
24	a	2350	PHO	CBD-CHA-C4D	-3.80	104.20	108.46
23	b	2511	CLA	CAA-C2A-C1A	-3.79	99.12	112.47
23	B	511	CLA	CAA-CBA-CGA	-3.76	102.31	113.32
23	B	524	CLA	C5-C3-C2	-3.74	113.97	121.05
28	F	48	BCR	C33-C5-C4	-3.73	106.35	113.43
23	b	2519	CLA	CAA-CBA-CGA	-3.73	102.39	113.32
23	B	527	CLA	CAA-CBA-CGA	-3.73	102.40	113.32
23	C	481	CLA	CAA-C2A-C1A	-3.73	99.33	112.47
23	B	524	CLA	OBD-CAD-CBD	-3.72	120.33	125.94
23	B	518	CLA	CAA-C2A-C1A	-3.71	99.37	112.47
25	V	138	HEM	C4B-CHC-C1C	-3.71	119.62	125.82
28	j	2053	BCR	C33-C5-C4	-3.70	106.41	113.43
28	B	529	BCR	C30-C25-C26	-3.69	117.24	122.66
28	B	528	BCR	C38-C26-C27	-3.69	106.44	113.43
23	c	2487	CLA	CMB-C2B-C1B	-3.68	122.28	128.36
28	F	48	BCR	C38-C26-C27	-3.67	106.46	113.43
23	b	2514	CLA	CAA-C2A-C3A	-3.66	102.69	113.22
23	B	523	CLA	CAA-CBA-CGA	-3.65	102.63	113.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2523	CLA	CAA-CBA-CGA	-3.63	102.68	113.32
26	A	353	PL9	C27-C26-C24	-3.63	100.89	112.71
23	B	514	CLA	CAA-C2A-C1A	-3.62	99.71	112.47
28	B	529	BCR	C38-C26-C27	-3.61	106.59	113.43
23	b	2518	CLA	CAA-C2A-C1A	-3.61	99.76	112.47
23	c	2485	CLA	OBD-CAD-CBD	-3.59	120.51	125.94
23	b	2511	CLA	CAA-CBA-CGA	-3.59	102.81	113.32
23	C	479	CLA	CAA-C2A-C1A	-3.59	99.82	112.47
23	B	523	CLA	CAA-C2A-C1A	-3.58	99.85	112.47
28	b	2528	BCR	C30-C25-C26	-3.57	117.41	122.66
28	C	488	BCR	C38-C26-C27	-3.57	106.66	113.43
23	B	514	CLA	CAA-C2A-C3A	-3.56	102.98	113.22
23	b	2524	CLA	OBD-CAD-CBD	-3.55	120.58	125.94
23	c	2479	CLA	CAA-C2A-C1A	-3.54	99.97	112.47
23	b	2514	CLA	CAA-C2A-C1A	-3.54	99.98	112.47
26	a	2352	PL9	C27-C26-C24	-3.54	101.19	112.71
28	C	489	BCR	C33-C5-C4	-3.54	106.72	113.43
23	b	2526	CLA	C7-C6-C5	-3.53	102.64	113.06
23	b	2523	CLA	CAA-C2A-C1A	-3.51	100.09	112.47
23	C	487	CLA	CMB-C2B-C1B	-3.50	122.58	128.36
23	B	527	CLA	C7-C6-C5	-3.48	102.78	113.06
28	d	2360	BCR	C38-C26-C27	-3.48	106.84	113.43
28	B	529	BCR	C1-C6-C5	-3.43	117.62	122.66
23	C	479	CLA	OBD-CAD-CBD	-3.41	120.79	125.94
28	b	2528	BCR	C1-C6-C5	-3.41	117.65	122.66
23	b	2517	CLA	OBD-CAD-CBD	-3.40	120.81	125.94
23	B	513	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
23	C	474	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
27	B	526	LMT	C1-O1'-C1'	-3.39	108.02	113.94
28	c	2488	BCR	C38-C26-C27	-3.38	107.02	113.43
23	A	348	CLA	OBD-CAD-CBD	-3.37	120.86	125.94
23	B	513	CLA	C7-C6-C5	-3.37	103.12	113.06
23	c	2476	CLA	C7-C6-C5	-3.36	103.12	113.06
28	c	2489	BCR	C33-C5-C4	-3.35	107.08	113.43
28	b	2528	BCR	C38-C26-C27	-3.35	107.08	113.43
25	V	138	HEM	C3B-C4B-NB	-3.33	105.26	111.63
23	c	2479	CLA	OBD-CAD-CBD	-3.33	120.92	125.94
28	c	2488	BCR	C8-C9-C10	-3.32	113.63	118.98
23	B	515	CLA	CAA-C2A-C3A	-3.31	103.70	113.22
28	C	488	BCR	C33-C5-C4	-3.30	107.17	113.43
23	B	515	CLA	CAA-CBA-CGA	-3.28	103.70	113.32
28	J	53	BCR	C38-C26-C27	-3.28	107.20	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	355	PHO	C7-C6-C5	-3.28	103.37	113.06
23	A	349	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
28	j	2053	BCR	C8-C9-C10	-3.26	113.74	118.98
28	j	2053	BCR	C38-C26-C27	-3.25	107.27	113.43
23	B	512	CLA	OBD-CAD-CBD	-3.23	121.06	125.94
27	d	2359	LMT	C1-O1'-C1'	-3.22	108.31	113.94
23	b	2511	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
23	d	2355	CLA	C5-C3-C2	-3.21	114.97	121.05
23	b	2515	CLA	CAA-C2A-C3A	-3.20	104.00	113.22
28	j	2053	BCR	C23-C22-C21	-3.20	113.83	118.98
23	b	2513	CLA	C7-C6-C5	-3.20	103.62	113.06
28	C	488	BCR	C8-C9-C10	-3.19	113.84	118.98
25	v	2138	HEM	C4B-CHC-C1C	-3.18	120.50	125.82
23	b	2516	CLA	OBD-CAD-CBD	-3.17	121.15	125.94
23	b	2519	CLA	OBD-CAD-CBD	-3.17	121.16	125.94
23	B	517	CLA	OBD-CAD-CBD	-3.16	121.17	125.94
23	C	479	CLA	C7-C6-C5	-3.15	103.77	113.06
23	b	2515	CLA	CAA-CBA-CGA	-3.13	104.14	113.32
23	a	2349	CLA	C7-C6-C5	-3.13	103.81	113.06
25	E	84	HEM	CMA-C3A-C4A	-3.13	123.19	128.36
23	C	481	CLA	OBD-CAD-CBD	-3.13	121.22	125.94
26	D	357	PL9	C3-C2-C1	-3.13	121.06	122.97
28	c	2489	BCR	C38-C26-C27	-3.13	107.50	113.43
28	C	489	BCR	C38-C26-C27	-3.12	107.51	113.43
23	b	2525	CLA	C7-C6-C5	-3.12	103.86	113.06
23	D	354	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
23	A	349	CLA	C5-C3-C2	-3.11	115.15	121.05
23	B	520	CLA	OBD-CAD-CBD	-3.10	121.25	125.94
23	b	2513	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
23	B	516	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
23	A	350	CLA	C7-C6-C5	-3.09	103.94	113.06
23	a	2349	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
23	B	519	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
24	a	2350	PHO	C7-C6-C5	-3.07	104.00	113.06
23	c	2479	CLA	C7-C6-C5	-3.06	104.01	113.06
24	d	2356	PHO	C7-C6-C5	-3.06	104.02	113.06
23	a	2351	CLA	CAA-C2A-C3A	-3.06	104.42	113.22
23	C	486	CLA	OBD-CAD-CBD	-3.06	121.32	125.94
23	A	350	CLA	OBD-CAD-CBD	-3.05	121.33	125.94
28	c	2488	BCR	C33-C5-C4	-3.04	107.66	113.43
23	d	2355	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
23	B	524	CLA	C7-C6-C5	-3.04	104.09	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2486	CLA	O1D-CGD-CBD	-3.04	120.27	124.62
23	b	2521	CLA	OBD-CAD-CBD	-3.03	121.36	125.94
28	k	2050	BCR	C38-C26-C27	-3.03	107.69	113.43
28	J	53	BCR	C23-C22-C21	-3.03	114.11	118.98
23	B	518	CLA	CAA-C2A-C3A	-3.03	104.52	113.22
23	C	486	CLA	C7-C6-C5	-3.02	104.13	113.06
23	b	2512	CLA	CMB-C2B-C1B	-3.02	123.37	128.36
23	C	476	CLA	C7-C6-C5	-3.01	104.18	113.06
23	c	2481	CLA	C7-C6-C5	-3.00	104.19	113.06
28	B	529	BCR	C37-C22-C21	-3.00	118.47	122.90
23	b	2517	CLA	CAA-C2A-C3A	-3.00	104.59	113.22
28	d	2360	BCR	C30-C25-C26	-2.99	118.26	122.66
23	d	2354	CLA	OBD-CAD-CBD	-2.99	121.42	125.94
28	K	50	BCR	C38-C26-C27	-2.99	107.77	113.43
23	B	522	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
28	b	2528	BCR	C33-C5-C4	-2.98	107.77	113.43
28	F	48	BCR	C30-C25-C26	-2.97	118.29	122.66
23	C	478	CLA	CMB-C2B-C1B	-2.97	123.45	128.36
24	d	2356	PHO	CAA-C2A-C3A	-2.97	104.69	113.22
26	A	353	PL9	C27-C28-C29	-2.96	121.32	127.76
24	D	355	PHO	CAA-C2A-C3A	-2.96	104.71	113.22
23	b	2514	CLA	OBD-CAD-CBD	-2.96	121.47	125.94
28	J	53	BCR	C8-C9-C10	-2.95	114.22	118.98
24	A	351	PHO	C7-C6-C5	-2.95	104.34	113.06
26	a	2352	PL9	C32-C33-C34	-2.95	121.35	127.76
23	A	349	CLA	CAA-C2A-C1A	-2.94	102.09	112.47
23	c	2486	CLA	OBD-CAD-CBD	-2.94	121.51	125.94
26	d	2358	PL9	C31-C29-C28	-2.94	115.48	121.05
23	a	2348	CLA	CAA-C2A-C3A	-2.93	104.78	113.22
23	A	352	CLA	CAA-C2A-C3A	-2.93	104.78	113.22
23	c	2486	CLA	C7-C6-C5	-2.93	104.40	113.06
24	A	351	PHO	CAB-C3B-C2B	-2.93	118.58	128.41
26	D	357	PL9	C31-C29-C28	-2.93	115.49	121.05
23	B	521	CLA	OBD-CAD-CBD	-2.93	121.52	125.94
26	A	353	PL9	C3-C2-C1	-2.93	121.19	122.97
23	B	517	CLA	CAA-C2A-C3A	-2.93	104.80	113.22
23	c	2478	CLA	CMB-C2B-C1B	-2.92	123.53	128.36
23	B	512	CLA	C7-C6-C5	-2.92	104.45	113.06
23	C	481	CLA	C7-C6-C5	-2.91	104.46	113.06
23	c	2481	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
28	K	50	BCR	C33-C5-C4	-2.90	107.93	113.43
23	C	480	CLA	OBD-CAD-CBD	-2.89	121.57	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	475	CLA	O1A-CGA-CBA	-2.89	112.16	123.72
23	B	518	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
23	c	2474	CLA	C7-C6-C5	-2.89	104.54	113.06
23	c	2475	CLA	O1A-CGA-CBA	-2.88	112.19	123.72
23	D	356	CLA	O1D-CGD-CBD	-2.88	120.50	124.62
28	c	2489	BCR	C8-C9-C10	-2.88	114.35	118.98
28	b	2528	BCR	C37-C22-C21	-2.87	118.66	122.90
23	c	2474	CLA	CAA-C2A-C1A	-2.86	102.37	112.47
23	C	485	CLA	C7-C6-C5	-2.86	104.60	113.06
23	d	2355	CLA	CAA-C2A-C1A	-2.86	102.38	112.47
23	B	513	CLA	CAA-C2A-C3A	-2.85	105.01	113.22
23	c	2487	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
26	d	2358	PL9	C3-C2-C1	-2.85	121.23	122.97
26	d	2358	PL9	C20-C19-C21	-2.85	111.06	115.41
23	B	522	CLA	CMB-C2B-C1B	-2.85	123.65	128.36
28	B	528	BCR	C30-C25-C26	-2.85	118.48	122.66
28	B	529	BCR	C33-C5-C4	-2.84	108.04	113.43
23	c	2474	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
23	b	2512	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
23	b	2512	CLA	C7-C6-C5	-2.84	104.67	113.06
24	a	2350	PHO	CAB-C3B-C2B	-2.84	118.90	128.41
23	B	514	CLA	OBD-CAD-CBD	-2.83	121.66	125.94
23	B	525	CLA	C7-C6-C5	-2.83	104.70	113.06
28	b	2527	BCR	C30-C25-C26	-2.83	118.50	122.66
24	D	355	PHO	C2A-C1A-NA	-2.83	108.46	112.08
28	B	528	BCR	C1-C6-C5	-2.82	118.51	122.66
26	a	2352	PL9	C15-C14-C16	-2.82	111.10	115.41
28	b	2527	BCR	C1-C6-C5	-2.82	118.52	122.66
23	b	2522	CLA	CMB-C2B-C1B	-2.82	123.70	128.36
23	b	2520	CLA	OBD-CAD-CBD	-2.82	121.69	125.94
23	b	2524	CLA	C7-C6-C5	-2.81	104.75	113.06
28	K	50	BCR	C23-C22-C21	-2.81	114.45	118.98
26	a	2352	PL9	C27-C28-C29	-2.81	121.66	127.76
23	b	2519	CLA	CAA-C2A-C3A	-2.81	105.15	113.22
28	k	2050	BCR	C33-C5-C4	-2.80	108.13	113.43
24	d	2356	PHO	C12-C11-C10	-2.79	99.13	112.99
28	F	48	BCR	C1-C6-C5	-2.79	118.56	122.66
23	B	527	CLA	OBD-CAD-CBD	-2.78	121.74	125.94
23	b	2518	CLA	CAA-C2A-C3A	-2.78	105.21	113.22
25	V	138	HEM	C2C-C1C-CHC	-2.77	119.47	123.68
23	b	2520	CLA	O1D-CGD-CBD	-2.77	120.66	124.62
23	A	348	CLA	CAA-C2A-C3A	-2.76	105.27	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	CAA-C2A-C3A	-2.76	105.28	113.22
23	b	2517	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
23	a	2349	CLA	CAA-C2A-C1A	-2.76	102.75	112.47
23	b	2518	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
28	k	2050	BCR	C23-C22-C21	-2.75	114.55	118.98
23	C	474	CLA	CAA-C2A-C1A	-2.75	102.78	112.47
24	D	355	PHO	C12-C11-C10	-2.75	99.37	112.99
23	B	515	CLA	C7-C6-C5	-2.74	104.95	113.06
23	b	2525	CLA	OBD-CAD-CBD	-2.74	121.80	125.94
23	B	519	CLA	CAA-C2A-C3A	-2.74	105.33	113.22
23	B	512	CLA	CMB-C2B-C1B	-2.74	123.83	128.36
23	B	523	CLA	OBD-CAD-CBD	-2.74	121.81	125.94
23	c	2482	CLA	OBD-CAD-CBD	-2.74	121.81	125.94
23	a	2351	CLA	OBD-CAD-CBD	-2.73	121.83	125.94
26	D	357	PL9	C20-C19-C21	-2.72	111.25	115.41
28	k	2050	BCR	C8-C9-C10	-2.72	114.60	118.98
23	c	2485	CLA	C7-C6-C5	-2.72	105.04	113.06
23	b	2511	CLA	CAA-C2A-C3A	-2.71	105.41	113.22
23	A	348	CLA	C7-C6-C5	-2.71	105.05	113.06
25	E	84	HEM	C4B-CHC-C1C	-2.70	121.31	125.82
28	B	528	BCR	C8-C9-C10	-2.70	114.63	118.98
23	c	2480	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
23	b	2514	CLA	CAA-CBA-CGA	-2.70	105.41	113.32
23	c	2485	CLA	CAA-C2A-C3A	-2.69	105.47	113.22
23	C	483	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
23	b	2526	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
23	C	482	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
23	A	352	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
28	K	50	BCR	C8-C9-C10	-2.67	114.68	118.98
23	C	483	CLA	CAA-CBA-CGA	-2.67	105.50	113.32
23	C	484	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
24	d	2356	PHO	C2A-C1A-NA	-2.67	108.66	112.08
23	c	2484	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
23	c	2477	CLA	OBD-CAD-CBD	-2.66	121.92	125.94
23	C	475	CLA	CAA-C2A-C3A	-2.66	105.57	113.22
23	A	352	CLA	C7-C6-C5	-2.65	105.22	113.06
26	d	2358	PL9	C22-C21-C19	-2.65	104.07	112.71
23	C	486	CLA	O1D-CGD-CBD	-2.65	120.82	124.62
23	C	486	CLA	CAA-C2A-C3A	-2.64	105.62	113.22
26	A	353	PL9	C32-C33-C34	-2.64	122.02	127.76
28	C	488	BCR	C19-C18-C17	-2.64	114.73	118.98
23	C	485	CLA	CAA-C2A-C3A	-2.63	105.65	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	2359	LMT	C3'-C4'-C5'	-2.63	104.89	110.84
23	C	482	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
27	B	526	LMT	C3'-C4'-C5'	-2.63	104.90	110.84
23	A	350	CLA	CAA-C2A-C1A	-2.62	103.25	112.47
24	a	2350	PHO	C2A-C1A-NA	-2.61	108.73	112.08
23	d	2357	CLA	OBD-CAD-CBD	-2.61	122.00	125.94
28	C	489	BCR	C8-C9-C10	-2.61	114.78	118.98
23	d	2355	CLA	CMB-C2B-C1B	-2.61	124.05	128.36
23	a	2348	CLA	OBD-CAD-CBD	-2.61	122.01	125.94
23	c	2483	CLA	CAA-CBA-CGA	-2.59	105.73	113.32
23	b	2523	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
28	b	2527	BCR	C23-C22-C21	-2.58	114.82	118.98
23	B	515	CLA	OBD-CAD-CBD	-2.58	122.05	125.94
23	C	485	CLA	O1D-CGD-CBD	-2.58	120.93	124.62
23	b	2523	CLA	CMB-C2B-C1B	-2.57	124.11	128.36
23	B	511	CLA	OBD-CAD-CBD	-2.57	122.06	125.94
23	b	2517	CLA	CMB-C2B-C1B	-2.57	124.12	128.36
23	b	2513	CLA	CAA-C2A-C1A	-2.57	103.42	112.47
23	B	514	CLA	CAA-CBA-CGA	-2.56	105.83	113.32
23	c	2475	CLA	CAA-C2A-C3A	-2.56	105.87	113.22
23	C	480	CLA	CAA-C2A-C1A	-2.55	103.47	112.47
23	a	2351	CLA	C7-C6-C5	-2.55	105.53	113.06
23	B	524	CLA	CMB-C2B-C1B	-2.55	124.14	128.36
23	c	2483	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
28	d	2360	BCR	C1-C6-C5	-2.53	118.94	122.66
23	C	477	CLA	OBD-CAD-CBD	-2.53	122.11	125.94
24	D	355	PHO	CAB-C3B-C2B	-2.52	119.96	128.41
25	E	84	HEM	C2C-C1C-CHC	-2.52	119.85	123.68
23	B	514	CLA	CMB-C2B-C1B	-2.52	124.20	128.36
23	A	349	CLA	CAA-C2A-C3A	-2.51	105.99	113.22
23	D	356	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
23	C	487	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
24	d	2356	PHO	CAB-C3B-C2B	-2.51	120.00	128.41
23	b	2515	CLA	C7-C6-C5	-2.50	105.67	113.06
23	d	2354	CLA	O1D-CGD-CBD	-2.50	121.04	124.62
25	e	2084	HEM	CAA-C2A-C1A	-2.50	124.30	127.01
23	B	523	CLA	CMB-C2B-C1B	-2.50	124.23	128.36
28	B	528	BCR	C23-C22-C21	-2.50	114.96	118.98
23	B	513	CLA	CAA-C2A-C1A	-2.50	103.67	112.47
23	C	478	CLA	CAA-C2A-C3A	-2.49	106.05	113.22
23	b	2514	CLA	CMB-C2B-C1B	-2.49	124.24	128.36
23	C	474	CLA	C7-C6-C5	-2.49	105.71	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	348	CLA	O1D-CGD-CBD	-2.49	121.06	124.62
28	c	2488	BCR	C19-C18-C17	-2.49	114.98	118.98
23	a	2348	CLA	O1D-CGD-CBD	-2.48	121.06	124.62
28	c	2489	BCR	C1-C6-C5	-2.48	119.02	122.66
28	J	53	BCR	C30-C25-C26	-2.48	119.02	122.66
28	C	489	BCR	C30-C25-C26	-2.47	119.03	122.66
23	A	349	CLA	CMB-C2B-C1B	-2.47	124.27	128.36
28	C	489	BCR	C1-C6-C5	-2.47	119.03	122.66
26	D	357	PL9	C22-C21-C19	-2.47	104.66	112.71
23	B	511	CLA	CAA-C2A-C3A	-2.47	106.12	113.22
23	b	2522	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
23	c	2480	CLA	CAA-C2A-C1A	-2.45	103.83	112.47
23	c	2485	CLA	C12-C11-C10	-2.44	100.86	112.99
23	B	525	CLA	OBD-CAD-CBD	-2.44	122.25	125.94
23	B	521	CLA	CMB-C2B-C1B	-2.44	124.33	128.36
23	C	477	CLA	CMB-C2B-C1B	-2.44	124.33	128.36
23	c	2474	CLA	O1D-CGD-CBD	-2.43	121.14	124.62
23	c	2478	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
23	a	2348	CLA	C7-C6-C5	-2.43	105.89	113.06
25	v	2138	HEM	CMA-C3A-C4A	-2.43	124.35	128.36
23	C	480	CLA	C7-C6-C5	-2.42	105.90	113.06
23	b	2524	CLA	CMB-C2B-C1B	-2.42	124.35	128.36
28	b	2527	BCR	C8-C9-C10	-2.42	115.08	118.98
24	A	351	PHO	C2A-C1A-NA	-2.42	108.98	112.08
23	B	517	CLA	CMB-C2B-C1B	-2.42	124.36	128.36
23	c	2485	CLA	O1D-CGD-CBD	-2.42	121.16	124.62
23	B	520	CLA	O1D-CGD-CBD	-2.42	121.16	124.62
23	c	2480	CLA	C7-C6-C5	-2.41	105.93	113.06
23	c	2479	CLA	O1D-CGD-CBD	-2.41	121.16	124.62
23	c	2478	CLA	O1D-CGD-CBD	-2.41	121.17	124.62
26	D	357	PL9	C25-C24-C26	-2.41	111.73	115.41
23	c	2475	CLA	OBD-CAD-CBD	-2.41	122.31	125.94
23	C	485	CLA	C12-C11-C10	-2.40	101.07	112.99
26	d	2358	PL9	C25-C24-C26	-2.40	111.74	115.41
26	A	353	PL9	C15-C14-C16	-2.40	111.74	115.41
24	A	351	PHO	CAA-C2A-C3A	-2.40	106.31	113.22
23	c	2486	CLA	CAA-C2A-C3A	-2.40	106.33	113.22
23	c	2478	CLA	CAA-C2A-C3A	-2.39	106.34	113.22
25	V	138	HEM	CAA-CBA-CGA	-2.39	108.36	112.75
28	c	2488	BCR	C15-C16-C17	-2.39	118.11	123.39
23	B	511	CLA	CMB-C2B-C1B	-2.37	124.44	128.36
23	B	517	CLA	CAA-C2A-C1A	-2.37	104.12	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2526	CLA	CMB-C2B-C1B	-2.37	124.45	128.36
23	c	2483	CLA	C7-C6-C5	-2.37	106.08	113.06
23	B	518	CLA	O1D-CGD-CBD	-2.35	121.25	124.62
23	d	2357	CLA	O1D-CGD-CBD	-2.34	121.26	124.62
23	b	2516	CLA	O1A-CGA-CBA	-2.34	114.36	123.72
23	b	2516	CLA	CAA-C2A-C1A	-2.34	104.23	112.47
23	b	2521	CLA	CMB-C2B-C1B	-2.33	124.52	128.36
26	d	2358	PL9	C15-C14-C16	-2.32	111.86	115.41
23	b	2515	CLA	CAA-C2A-C1A	-2.32	104.29	112.47
23	c	2481	CLA	O1D-CGD-CBD	-2.32	121.30	124.62
28	C	488	BCR	C15-C16-C17	-2.32	118.27	123.39
23	B	527	CLA	CMB-C2B-C1B	-2.32	124.53	128.36
25	v	2138	HEM	CAA-CBA-CGA	-2.31	108.50	112.75
23	B	516	CLA	O1A-CGA-CBA	-2.31	114.47	123.72
23	d	2355	CLA	CAA-C2A-C3A	-2.31	106.57	113.22
23	b	2515	CLA	CMB-C2B-C1B	-2.31	124.54	128.36
28	j	2053	BCR	C30-C25-C26	-2.31	119.27	122.66
28	d	2360	BCR	C15-C16-C17	-2.31	118.29	123.39
23	b	2524	CLA	O1D-CGD-CBD	-2.31	121.32	124.62
26	a	2352	PL9	C3-C2-C1	-2.30	121.57	122.97
23	C	474	CLA	O1D-CGD-CBD	-2.30	121.33	124.62
23	B	517	CLA	O1D-CGD-CBD	-2.29	121.35	124.62
25	V	138	HEM	CAA-C2A-C1A	-2.29	124.53	127.01
23	B	525	CLA	O1D-CGD-CBD	-2.29	121.35	124.62
23	C	478	CLA	OBD-CAD-CBD	-2.28	122.49	125.94
28	c	2489	BCR	C30-C25-C26	-2.28	119.31	122.66
23	C	479	CLA	CAA-C2A-C3A	-2.28	106.66	113.22
27	d	2359	LMT	C3-C2-C1	-2.28	103.29	113.47
23	B	516	CLA	O2A-CGA-O1A	-2.27	117.63	123.49
28	b	2528	BCR	C35-C13-C14	-2.27	119.55	122.90
23	b	2515	CLA	OBD-CAD-CBD	-2.26	122.52	125.94
28	j	2053	BCR	C1-C6-C5	-2.26	119.34	122.66
28	B	528	BCR	C12-C13-C14	-2.26	115.34	118.98
23	b	2521	CLA	CAA-CBA-CGA	-2.24	106.75	113.32
23	B	523	CLA	C7-C6-C5	-2.24	106.43	113.06
28	B	529	BCR	C35-C13-C14	-2.24	119.59	122.90
23	C	475	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
23	B	516	CLA	CAA-C2A-C1A	-2.24	104.58	112.47
26	D	357	PL9	C15-C14-C16	-2.23	112.00	115.41
28	F	48	BCR	C15-C16-C17	-2.23	118.46	123.39
23	C	482	CLA	CMB-C2B-C1B	-2.23	124.68	128.36
28	J	53	BCR	C1-C6-C5	-2.23	119.39	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2487	CLA	C7-C6-C5	-2.22	106.49	113.06
23	b	2523	CLA	C7-C6-C5	-2.22	106.49	113.06
23	C	475	CLA	CMB-C2B-C1B	-2.22	124.69	128.36
23	c	2477	CLA	O1D-CGD-CBD	-2.22	121.44	124.62
23	b	2517	CLA	CAA-C2A-C1A	-2.22	104.65	112.47
23	A	350	CLA	O1D-CGD-CBD	-2.22	121.44	124.62
23	C	484	CLA	CAA-C2A-C3A	-2.22	106.84	113.22
23	B	523	CLA	C2C-C1C-NC	-2.21	108.60	110.24
23	B	521	CLA	CAA-CBA-CGA	-2.21	106.85	113.32
23	B	523	CLA	O1D-CGD-CBD	-2.21	121.46	124.62
24	A	351	PHO	O1D-CGD-CBD	-2.21	121.46	124.62
23	B	513	CLA	O1D-CGD-CBD	-2.20	121.46	124.62
27	B	526	LMT	C3-C2-C1	-2.20	103.63	113.47
23	c	2482	CLA	CMB-C2B-C1B	-2.20	124.72	128.36
23	A	350	CLA	CMB-C2B-C1B	-2.20	124.72	128.36
28	b	2528	BCR	C20-C19-C18	-2.20	119.85	126.32
23	c	2477	CLA	CMB-C2B-C1B	-2.19	124.74	128.36
23	A	350	CLA	CMA-C3A-C2A	-2.19	104.66	114.35
23	B	515	CLA	CMB-C2B-C1B	-2.19	124.74	128.36
23	c	2474	CLA	CMB-C2B-C1B	-2.19	124.75	128.36
23	b	2515	CLA	O1D-CGD-CBD	-2.19	121.49	124.62
23	C	483	CLA	C7-C6-C5	-2.18	106.62	113.06
28	c	2488	BCR	C30-C25-C26	-2.18	119.46	122.66
23	B	515	CLA	CAA-C2A-C1A	-2.18	104.79	112.47
23	b	2516	CLA	O2A-CGA-O1A	-2.18	117.88	123.49
23	b	2511	CLA	CMB-C2B-C1B	-2.18	124.77	128.36
23	c	2480	CLA	O1D-CGD-CBD	-2.17	121.50	124.62
23	C	480	CLA	CMB-C2B-C1B	-2.17	124.77	128.36
23	c	2476	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
23	c	2481	CLA	CMB-C2B-C1B	-2.15	124.80	128.36
23	B	524	CLA	O1D-CGD-CBD	-2.15	121.54	124.62
23	c	2485	CLA	CMB-C2B-C1B	-2.15	124.81	128.36
23	b	2511	CLA	C2C-C1C-NC	-2.15	108.64	110.24
23	b	2518	CLA	CMB-C2B-C1B	-2.15	124.81	128.36
23	c	2484	CLA	CMB-C2B-C1B	-2.14	124.82	128.36
23	C	485	CLA	C5-C3-C2	-2.14	116.99	121.05
23	d	2355	CLA	C2C-C1C-NC	-2.13	108.65	110.24
23	B	515	CLA	O1D-CGD-CBD	-2.13	121.56	124.62
24	a	2350	PHO	CAA-C2A-C3A	-2.13	107.09	113.22
23	C	481	CLA	CMB-C2B-C1B	-2.13	124.85	128.36
23	a	2349	CLA	CMA-C3A-C2A	-2.12	104.95	114.35
23	d	2357	CLA	C7-C6-C5	-2.11	106.84	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2485	CLA	C5-C3-C2	-2.10	117.06	121.05
28	c	2488	BCR	C23-C22-C21	-2.10	115.60	118.98
28	B	529	BCR	C20-C19-C18	-2.10	120.14	126.32
23	C	484	CLA	C7-C6-C5	-2.10	106.87	113.06
23	C	475	CLA	C3B-CAB-CBB	-2.10	122.03	126.32
23	C	480	CLA	O1D-CGD-CBD	-2.10	121.62	124.62
23	b	2523	CLA	C2C-C1C-NC	-2.09	108.68	110.24
28	C	488	BCR	C30-C25-C26	-2.09	119.59	122.66
23	B	517	CLA	C7-C6-C5	-2.09	106.88	113.06
26	A	353	PL9	C7-C3-C2	-2.09	121.68	123.42
23	A	349	CLA	O1D-CGD-CBD	-2.09	121.62	124.62
23	a	2349	CLA	O1D-CGD-CBD	-2.09	121.63	124.62
23	c	2475	CLA	C3B-CAB-CBB	-2.09	122.05	126.32
26	a	2352	PL9	C21-C19-C18	-2.09	117.09	121.05
23	D	356	CLA	C7-C6-C5	-2.09	106.90	113.06
28	d	2360	BCR	C40-C30-C29	-2.08	101.33	108.79
23	B	511	CLA	O1D-CGD-CBD	-2.08	121.64	124.62
26	A	353	PL9	C21-C19-C18	-2.07	117.12	121.05
23	a	2349	CLA	CAA-C2A-C3A	-2.06	107.28	113.22
23	b	2525	CLA	O1D-CGD-CBD	-2.06	121.67	124.62
25	E	84	HEM	CAA-C2A-C1A	-2.06	124.78	127.01
23	c	2484	CLA	C7-C6-C5	-2.06	106.99	113.06
23	A	350	CLA	CAA-C2A-C3A	-2.06	107.31	113.22
23	C	474	CLA	CAA-C2A-C3A	-2.05	107.31	113.22
23	b	2513	CLA	CMB-C2B-C1B	-2.05	124.97	128.36
28	K	50	BCR	C1-C6-C5	-2.05	119.65	122.66
23	C	479	CLA	O1D-CGD-CBD	-2.05	121.69	124.62
23	B	511	CLA	C2C-C1C-NC	-2.05	108.72	110.24
23	D	354	CLA	CMB-C2B-C1B	-2.05	124.98	128.36
23	c	2478	CLA	C7-C6-C5	-2.04	107.03	113.06
23	b	2519	CLA	CMB-C2B-C1B	-2.04	124.99	128.36
23	B	513	CLA	CMB-C2B-C1B	-2.04	124.99	128.36
23	b	2522	CLA	C7-C6-C5	-2.04	107.05	113.06
23	b	2511	CLA	O1D-CGD-CBD	-2.04	121.70	124.62
23	B	522	CLA	C7-C6-C5	-2.03	107.07	113.06
23	b	2516	CLA	CMB-C2B-C1B	-2.03	125.01	128.36
23	a	2348	CLA	C12-C11-C10	-2.02	102.95	112.99
23	A	348	CLA	C12-C11-C10	-2.02	102.96	112.99
26	d	2358	PL9	C7-C3-C2	-2.02	121.74	123.42
24	D	355	PHO	O1D-CGD-CBD	-2.02	121.73	124.62
23	C	485	CLA	CMB-C2B-C1B	-2.01	125.03	128.36
23	A	349	CLA	C2C-C1C-NC	-2.01	108.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	522	CLA	CAA-C2A-C3A	-2.01	107.44	113.22
23	C	474	CLA	CMB-C2B-C1B	-2.01	125.04	128.36
23	c	2479	CLA	CAA-C2A-C3A	-2.01	107.45	113.22
28	b	2527	BCR	C12-C13-C14	-2.01	115.75	118.98
23	c	2484	CLA	CAA-C2A-C3A	-2.00	107.45	113.22
23	b	2511	CLA	C7-C6-C5	-2.00	107.15	113.06
28	F	48	BCR	C40-C30-C29	-2.00	101.62	108.79
23	c	2485	CLA	C1C-NC-C4C	2.00	108.70	106.27
28	C	488	BCR	C1-C6-C7	2.00	121.42	115.82
28	b	2527	BCR	C15-C14-C13	2.00	130.09	127.20
23	c	2482	CLA	C16-C15-C13	2.00	122.14	115.49
23	b	2515	CLA	CMB-C2B-C3B	2.00	129.01	125.09
28	j	2053	BCR	C36-C18-C19	2.01	121.43	118.10
23	c	2475	CLA	C6-C7-C8	2.01	122.14	115.49
27	B	526	LMT	C1'-O5'-C5'	2.01	117.64	113.75
28	B	529	BCR	C10-C11-C12	2.01	129.25	123.13
28	C	488	BCR	C37-C22-C23	2.01	121.44	118.10
23	b	2524	CLA	CMB-C2B-C3B	2.01	129.02	125.09
23	B	517	CLA	C1C-NC-C4C	2.01	108.71	106.27
27	B	526	LMT	O6B-C6B-C5B	2.02	118.00	111.33
23	B	514	CLA	C1C-NC-C4C	2.02	108.72	106.27
23	b	2514	CLA	C2A-C1A-CHA	2.02	127.61	123.89
23	c	2475	CLA	CBA-CAA-C2A	2.02	119.44	113.73
23	b	2521	CLA	O2D-CGD-CBD	2.02	114.07	111.30
23	b	2512	CLA	C6-C7-C8	2.02	122.20	115.49
28	C	488	BCR	C28-C27-C26	2.02	117.08	113.87
28	J	53	BCR	C35-C13-C12	2.03	121.47	118.10
24	d	2356	PHO	C2A-C3A-C4A	2.03	105.75	101.10
23	c	2478	CLA	CAA-CBA-CGA	2.03	119.26	113.32
23	B	517	CLA	C6-C5-C3	2.03	116.94	112.48
23	a	2351	CLA	C2A-C1A-CHA	2.03	127.62	123.89
23	C	475	CLA	CAA-CBA-CGA	2.04	119.28	113.32
23	c	2475	CLA	C2A-C1A-CHA	2.04	127.64	123.89
23	a	2349	CLA	CED-O2D-CGD	2.04	120.77	115.99
28	K	50	BCR	C16-C17-C18	2.04	130.14	127.20
23	C	474	CLA	C6-C5-C3	2.04	116.96	112.48
23	A	348	CLA	C1C-NC-C4C	2.05	108.75	106.27
23	C	487	CLA	CBA-CAA-C2A	2.05	119.51	113.73
23	B	514	CLA	C2A-C1A-CHA	2.05	127.66	123.89
28	c	2489	BCR	C28-C27-C26	2.05	117.12	113.87
28	B	528	BCR	C15-C14-C13	2.05	130.16	127.20
23	A	352	CLA	O2A-CGA-CBA	2.05	118.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2515	CLA	C1C-NC-C4C	2.06	108.77	106.27
23	b	2519	CLA	C1C-NC-C4C	2.06	108.77	106.27
23	a	2351	CLA	CAA-CBA-CGA	2.07	119.37	113.32
23	C	483	CLA	C6-C7-C8	2.07	122.35	115.49
23	A	348	CLA	CBA-CAA-C2A	2.07	119.57	113.73
28	b	2528	BCR	C16-C17-C18	2.07	130.19	127.20
23	b	2523	CLA	O2D-CGD-CBD	2.07	114.14	111.30
23	D	354	CLA	C1C-NC-C4C	2.07	108.79	106.27
23	c	2482	CLA	O2A-CGA-CBA	2.08	118.23	111.90
28	B	528	BCR	C37-C22-C23	2.08	121.56	118.10
28	k	2050	BCR	C16-C17-C18	2.08	130.20	127.20
23	c	2483	CLA	C6-C7-C8	2.08	122.39	115.49
23	C	480	CLA	C1C-NC-C4C	2.08	108.80	106.27
28	C	489	BCR	C11-C10-C9	2.08	130.21	127.20
24	d	2356	PHO	CMD-C2D-C1D	2.09	128.45	125.06
23	d	2357	CLA	CBA-CAA-C2A	2.09	119.64	113.73
28	J	53	BCR	C11-C10-C9	2.09	130.22	127.20
23	C	487	CLA	CHD-C4C-C3C	2.09	128.18	124.94
28	c	2488	BCR	C28-C27-C26	2.09	117.19	113.87
25	E	84	HEM	C3B-C4B-CHC	2.10	126.12	123.16
23	C	475	CLA	C2A-C1A-CHA	2.10	127.75	123.89
23	b	2522	CLA	O2D-CGD-CBD	2.10	114.18	111.30
23	B	511	CLA	CHB-C4A-NA	2.11	127.42	124.51
28	c	2489	BCR	C34-C9-C8	2.11	121.61	118.10
23	b	2514	CLA	C1C-NC-C4C	2.11	108.83	106.27
28	b	2527	BCR	C35-C13-C12	2.11	121.61	118.10
23	a	2348	CLA	CBA-CAA-C2A	2.11	119.69	113.73
23	c	2487	CLA	CHD-C4C-C3C	2.12	128.22	124.94
23	A	352	CLA	C2A-C1A-CHA	2.12	127.78	123.89
28	b	2527	BCR	C34-C9-C8	2.12	121.62	118.10
28	c	2489	BCR	C32-C1-C6	2.12	113.63	110.30
28	J	53	BCR	C28-C27-C26	2.12	117.23	113.87
23	c	2479	CLA	CHB-C4A-NA	2.12	127.45	124.51
23	B	523	CLA	O2D-CGD-CBD	2.12	114.21	111.30
23	A	352	CLA	C6-C5-C3	2.13	117.15	112.48
23	A	349	CLA	C1C-NC-C4C	2.13	108.85	106.27
23	B	515	CLA	C6-C5-C3	2.13	117.15	112.48
23	A	350	CLA	C6-C5-C3	2.13	117.16	112.48
27	d	2359	LMT	O6B-C6B-C5B	2.13	118.37	111.33
23	B	519	CLA	CHB-C4A-NA	2.13	127.46	124.51
28	B	529	BCR	C3-C4-C5	2.13	117.25	113.87
28	B	529	BCR	C16-C17-C18	2.13	130.28	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	489	BCR	C28-C27-C26	2.13	117.25	113.87
28	B	529	BCR	C23-C24-C25	2.14	133.73	127.32
23	B	522	CLA	C16-C15-C13	2.14	122.58	115.49
23	C	476	CLA	C6-C7-C8	2.14	122.58	115.49
28	d	2360	BCR	C36-C18-C19	2.14	121.66	118.10
23	B	524	CLA	C1C-NC-C4C	2.14	108.87	106.27
28	B	529	BCR	C7-C8-C9	2.15	129.49	126.22
23	B	511	CLA	CMB-C2B-C3B	2.15	129.30	125.09
28	C	488	BCR	C11-C10-C9	2.15	130.31	127.20
23	b	2515	CLA	C6-C5-C3	2.16	117.22	112.48
28	J	53	BCR	C37-C22-C23	2.16	121.69	118.10
28	J	53	BCR	C20-C21-C22	2.16	130.32	127.20
28	C	489	BCR	C8-C7-C6	2.16	133.80	127.32
23	a	2351	CLA	O2A-CGA-CBA	2.16	118.49	111.90
23	C	475	CLA	O2D-CGD-CBD	2.16	114.27	111.30
23	c	2477	CLA	C1C-NC-C4C	2.16	108.90	106.27
28	F	48	BCR	C40-C30-C25	2.17	113.70	110.30
23	B	515	CLA	O2A-CGA-CBA	2.17	118.52	111.90
28	C	489	BCR	C34-C9-C8	2.17	121.71	118.10
23	A	348	CLA	C16-C15-C13	2.18	122.70	115.49
28	K	50	BCR	C34-C9-C8	2.18	121.72	118.10
28	d	2360	BCR	C8-C7-C6	2.18	133.86	127.32
28	c	2488	BCR	C36-C18-C19	2.18	121.72	118.10
28	b	2528	BCR	C3-C4-C5	2.18	117.33	113.87
23	a	2349	CLA	C6-C5-C3	2.18	117.27	112.48
23	B	514	CLA	CMB-C2B-C3B	2.18	129.36	125.09
23	C	474	CLA	C6-C7-C8	2.18	122.73	115.49
23	d	2355	CLA	C4-C3-C5	2.19	118.75	115.41
23	c	2487	CLA	C2A-C1A-CHA	2.19	127.91	123.89
23	c	2482	CLA	CAA-CBA-CGA	2.19	119.73	113.32
28	J	53	BCR	C30-C25-C24	2.19	121.95	115.82
28	F	48	BCR	C36-C18-C19	2.19	121.74	118.10
23	B	516	CLA	C1C-NC-C4C	2.19	108.93	106.27
28	b	2528	BCR	C23-C24-C25	2.19	133.91	127.32
23	b	2521	CLA	CBA-CAA-C2A	2.19	119.92	113.73
23	a	2348	CLA	C1C-NC-C4C	2.20	108.95	106.27
23	C	487	CLA	C2A-C1A-CHA	2.20	127.94	123.89
28	j	2053	BCR	C30-C25-C24	2.21	122.00	115.82
23	b	2516	CLA	CED-O2D-CGD	2.21	121.17	115.99
23	a	2348	CLA	C16-C15-C13	2.21	122.83	115.49
23	C	482	CLA	CAA-CBA-CGA	2.21	119.80	113.32
28	B	528	BCR	C7-C8-C9	2.22	129.60	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	2354	CLA	C6-C5-C3	2.22	117.36	112.48
23	B	527	CLA	C6-C7-C8	2.23	122.87	115.49
23	c	2477	CLA	C16-C15-C13	2.23	122.88	115.49
23	d	2357	CLA	CED-O2D-CGD	2.23	121.22	115.99
23	B	524	CLA	CMB-C2B-C3B	2.23	129.46	125.09
23	B	521	CLA	CBA-CAA-C2A	2.24	120.05	113.73
28	j	2053	BCR	C15-C14-C13	2.24	130.43	127.20
23	a	2348	CLA	O2A-CGA-CBA	2.24	118.72	111.90
28	J	53	BCR	C16-C17-C18	2.24	130.43	127.20
23	b	2514	CLA	CMB-C2B-C3B	2.24	129.47	125.09
28	b	2528	BCR	C7-C8-C9	2.24	129.63	126.22
23	B	522	CLA	O2D-CGD-CBD	2.25	114.38	111.30
28	c	2489	BCR	C11-C10-C9	2.25	130.45	127.20
23	A	352	CLA	CAA-CBA-CGA	2.25	119.91	113.32
28	F	48	BCR	C8-C7-C6	2.25	134.08	127.32
28	B	529	BCR	C30-C25-C24	2.26	122.14	115.82
28	B	529	BCR	C34-C9-C8	2.26	121.85	118.10
23	b	2522	CLA	C16-C15-C13	2.26	122.97	115.49
23	D	354	CLA	C6-C5-C3	2.26	117.44	112.48
23	A	348	CLA	O2A-CGA-CBA	2.26	118.80	111.90
23	b	2518	CLA	O2D-CGD-CBD	2.27	114.41	111.30
23	c	2479	CLA	C2A-C1A-CHA	2.27	128.06	123.89
23	B	512	CLA	CMB-C2B-C3B	2.28	129.54	125.09
23	B	512	CLA	CED-O2D-CGD	2.28	121.33	115.99
28	b	2527	BCR	C16-C17-C18	2.28	130.49	127.20
23	d	2357	CLA	O2A-CGA-CBA	2.28	118.85	111.90
23	c	2476	CLA	CBA-CAA-C2A	2.28	120.18	113.73
23	c	2475	CLA	C6-C5-C3	2.28	117.50	112.48
23	B	522	CLA	CMB-C2B-C3B	2.29	129.57	125.09
28	j	2053	BCR	C35-C13-C12	2.29	121.91	118.10
28	c	2488	BCR	C34-C9-C8	2.29	121.91	118.10
23	D	356	CLA	O2A-CGA-CBA	2.29	118.88	111.90
23	b	2526	CLA	C6-C7-C8	2.30	123.12	115.49
24	D	355	PHO	CMD-C2D-C1D	2.30	128.80	125.06
23	c	2485	CLA	C6-C5-C3	2.31	117.55	112.48
23	C	479	CLA	C2A-C1A-CHA	2.31	128.13	123.89
28	b	2527	BCR	C37-C22-C23	2.32	121.95	118.10
23	B	512	CLA	O2A-CGA-CBA	2.32	118.97	111.90
23	C	475	CLA	C6-C5-C3	2.32	117.58	112.48
23	C	480	CLA	C6-C5-C3	2.33	117.60	112.48
23	b	2522	CLA	CMB-C2B-C3B	2.34	129.66	125.09
28	k	2050	BCR	C23-C24-C25	2.34	134.33	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	2528	BCR	C34-C9-C8	2.35	122.00	118.10
23	C	477	CLA	C16-C15-C13	2.35	123.27	115.49
28	B	528	BCR	C16-C17-C18	2.35	130.59	127.20
23	D	354	CLA	CED-O2D-CGD	2.35	121.50	115.99
23	B	523	CLA	C6-C5-C3	2.36	117.65	112.48
23	b	2524	CLA	C4-C3-C5	2.36	119.01	115.41
23	B	512	CLA	O2D-CGD-CBD	2.36	114.53	111.30
23	c	2474	CLA	C6-C5-C3	2.36	117.67	112.48
23	a	2348	CLA	CED-O2D-CGD	2.37	121.54	115.99
23	B	522	CLA	CBA-CAA-C2A	2.37	120.41	113.73
26	a	2352	PL9	C36-C37-C38	2.38	117.91	111.69
23	b	2511	CLA	O2A-CGA-CBA	2.38	119.15	111.90
23	B	527	CLA	O2D-CGD-CBD	2.38	114.56	111.30
28	B	529	BCR	C24-C23-C22	2.38	129.84	126.22
23	b	2522	CLA	C2A-C1A-CHA	2.38	128.27	123.89
23	b	2512	CLA	O2A-CGA-CBA	2.39	119.18	111.90
28	C	488	BCR	C34-C9-C8	2.39	122.08	118.10
23	C	487	CLA	CMB-C2B-C3B	2.39	129.77	125.09
28	K	50	BCR	C23-C24-C25	2.39	134.51	127.32
28	c	2488	BCR	C32-C1-C6	2.40	114.06	110.30
25	v	2138	HEM	CMA-C3A-C2A	2.41	130.28	125.24
23	B	516	CLA	C6-C7-C8	2.41	123.48	115.49
23	c	2476	CLA	C6-C5-C3	2.41	117.78	112.48
26	A	353	PL9	C36-C37-C38	2.41	118.01	111.69
23	B	511	CLA	C2A-C1A-CHA	2.42	128.34	123.89
27	d	2359	LMT	O1'-C1'-C2'	2.42	111.09	108.04
23	b	2522	CLA	CBA-CAA-C2A	2.42	120.55	113.73
28	C	488	BCR	C36-C18-C19	2.42	122.12	118.10
23	C	476	CLA	CED-O2D-CGD	2.42	121.67	115.99
23	b	2516	CLA	C6-C7-C8	2.42	123.52	115.49
23	c	2484	CLA	O2D-CGD-CBD	2.42	114.62	111.30
28	b	2528	BCR	C35-C13-C12	2.42	122.13	118.10
23	c	2487	CLA	CMB-C2B-C3B	2.43	129.83	125.09
26	D	357	PL9	C8-C7-C3	2.43	119.20	111.60
28	C	489	BCR	C21-C20-C19	2.43	130.54	123.13
26	d	2358	PL9	C7-C8-C9	2.44	130.82	126.70
28	F	48	BCR	C20-C21-C22	2.44	130.72	127.20
28	j	2053	BCR	C16-C17-C18	2.44	130.72	127.20
28	j	2053	BCR	C37-C22-C23	2.44	122.16	118.10
23	C	476	CLA	CBA-CAA-C2A	2.44	120.62	113.73
28	K	50	BCR	C37-C22-C23	2.44	122.16	118.10
28	b	2528	BCR	C30-C25-C24	2.45	122.68	115.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	522	CLA	C2A-C1A-CHA	2.45	128.40	123.89
26	D	357	PL9	C7-C8-C9	2.46	130.86	126.70
23	B	521	CLA	O2A-CGA-CBA	2.46	119.39	111.90
23	b	2523	CLA	C16-C15-C13	2.46	123.65	115.49
23	B	517	CLA	CBA-CAA-C2A	2.47	120.69	113.73
28	k	2050	BCR	C37-C22-C23	2.48	122.22	118.10
23	b	2511	CLA	C2A-C1A-CHA	2.48	128.45	123.89
23	b	2512	CLA	CMB-C2B-C3B	2.48	129.94	125.09
23	B	523	CLA	C16-C15-C13	2.49	123.73	115.49
28	c	2488	BCR	C11-C10-C9	2.49	130.79	127.20
23	B	524	CLA	C4-C3-C5	2.49	119.21	115.41
23	C	477	CLA	C6-C7-C8	2.50	123.77	115.49
23	b	2523	CLA	C6-C5-C3	2.50	117.96	112.48
28	b	2527	BCR	C7-C8-C9	2.50	130.02	126.22
23	B	517	CLA	C2A-C1A-CHA	2.50	128.49	123.89
23	C	484	CLA	C6-C5-C3	2.50	117.98	112.48
23	c	2486	CLA	C2A-C1A-CHA	2.51	128.50	123.89
26	a	2352	PL9	C30-C29-C31	2.51	119.24	115.41
23	D	356	CLA	C6-C5-C3	2.51	118.00	112.48
28	B	529	BCR	C35-C13-C12	2.52	122.28	118.10
23	c	2477	CLA	C6-C7-C8	2.52	123.85	115.49
23	C	481	CLA	O2D-CGD-CBD	2.52	114.76	111.30
23	A	352	CLA	CED-O2D-CGD	2.53	121.91	115.99
28	c	2489	BCR	C21-C20-C19	2.53	130.84	123.13
23	C	485	CLA	O2A-CGA-CBA	2.53	119.61	111.90
23	b	2517	CLA	C2A-C1A-CHA	2.53	128.54	123.89
23	C	479	CLA	C6-C7-C8	2.53	123.88	115.49
24	a	2350	PHO	O2A-CGA-CBA	2.54	119.63	111.90
23	c	2476	CLA	CED-O2D-CGD	2.54	121.95	115.99
23	c	2474	CLA	CED-O2D-CGD	2.54	121.95	115.99
24	A	351	PHO	O2A-CGA-CBA	2.55	119.66	111.90
23	b	2521	CLA	O2A-CGA-CBA	2.55	119.66	111.90
28	k	2050	BCR	C36-C18-C19	2.55	122.34	118.10
23	C	487	CLA	C6-C5-C3	2.56	118.10	112.48
23	c	2484	CLA	C6-C5-C3	2.56	118.10	112.48
23	D	356	CLA	CED-O2D-CGD	2.56	122.00	115.99
23	d	2355	CLA	CED-O2D-CGD	2.56	122.00	115.99
23	C	487	CLA	O2D-CGD-CBD	2.56	114.82	111.30
28	b	2528	BCR	C1-C6-C7	2.57	123.00	115.82
23	c	2486	CLA	CBA-CAA-C2A	2.58	121.00	113.73
23	d	2354	CLA	CED-O2D-CGD	2.58	122.03	115.99
23	c	2487	CLA	O2A-CGA-CBA	2.58	119.76	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	486	CLA	CBA-CAA-C2A	2.58	121.02	113.73
26	d	2358	PL9	C8-C7-C3	2.58	119.67	111.60
28	K	50	BCR	C36-C18-C19	2.58	122.40	118.10
23	B	515	CLA	C1D-CHD-C4C	2.59	126.52	122.60
23	B	515	CLA	C2A-C1A-CHA	2.59	128.65	123.89
23	C	481	CLA	CED-O2D-CGD	2.59	122.07	115.99
23	B	511	CLA	O2A-CGA-CBA	2.60	119.81	111.90
28	d	2360	BCR	C24-C23-C22	2.60	130.18	126.22
28	j	2053	BCR	C8-C7-C6	2.60	135.12	127.32
23	C	479	CLA	O2A-CGA-CBA	2.60	119.82	111.90
28	b	2527	BCR	C8-C7-C6	2.60	135.14	127.32
23	b	2515	CLA	C2A-C1A-CHA	2.61	128.70	123.89
28	d	2360	BCR	C20-C21-C22	2.61	130.97	127.20
28	k	2050	BCR	C34-C9-C8	2.62	122.45	118.10
25	v	2138	HEM	C2C-C1C-NC	2.62	114.62	110.21
23	c	2487	CLA	C6-C5-C3	2.62	118.24	112.48
23	C	485	CLA	C6-C5-C3	2.63	118.25	112.48
23	c	2479	CLA	C6-C7-C8	2.63	124.21	115.49
23	A	349	CLA	CED-O2D-CGD	2.65	122.20	115.99
23	d	2355	CLA	C1D-CHD-C4C	2.66	126.63	122.60
28	B	529	BCR	C1-C6-C7	2.66	123.27	115.82
23	B	517	CLA	CED-O2D-CGD	2.66	122.23	115.99
23	b	2520	CLA	C1D-CHD-C4C	2.66	126.63	122.60
23	C	486	CLA	CED-O2D-CGD	2.67	122.24	115.99
23	C	487	CLA	O2A-CGA-CBA	2.67	120.02	111.90
23	b	2520	CLA	CED-O2D-CGD	2.67	122.25	115.99
23	D	354	CLA	CBA-CAA-C2A	2.67	121.28	113.73
23	B	514	CLA	CED-O2D-CGD	2.68	122.26	115.99
23	B	522	CLA	O2A-CGA-CBA	2.68	120.05	111.90
23	b	2517	CLA	CBA-CAA-C2A	2.68	121.28	113.73
28	d	2360	BCR	C30-C25-C24	2.68	123.31	115.82
23	b	2522	CLA	O2A-CGA-CBA	2.68	120.07	111.90
23	C	486	CLA	C2A-C1A-CHA	2.69	128.83	123.89
23	c	2476	CLA	O2A-CGA-CBA	2.69	120.10	111.90
28	F	48	BCR	C24-C23-C22	2.69	130.32	126.22
23	c	2484	CLA	CBA-CAA-C2A	2.69	121.33	113.73
24	D	355	PHO	CBA-CAA-C2A	2.69	121.33	113.73
24	d	2356	PHO	O2D-CGD-CBD	2.69	114.99	111.30
23	c	2479	CLA	O2A-CGA-CBA	2.70	120.12	111.90
28	J	53	BCR	C8-C7-C6	2.70	135.44	127.32
23	b	2512	CLA	O2D-CGD-CBD	2.70	115.01	111.30
23	C	484	CLA	CBA-CAA-C2A	2.71	121.37	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	484	CLA	O2D-CGD-CBD	2.71	115.01	111.30
23	c	2486	CLA	CED-O2D-CGD	2.71	122.36	115.99
23	C	476	CLA	C6-C5-C3	2.72	118.44	112.48
28	B	528	BCR	C8-C7-C6	2.72	135.50	127.32
27	B	526	LMT	O1'-C1'-C2'	2.72	111.48	108.04
23	b	2522	CLA	C6-C5-C3	2.73	118.48	112.48
26	A	353	PL9	C30-C29-C31	2.73	119.58	115.41
23	C	474	CLA	CED-O2D-CGD	2.74	122.41	115.99
23	b	2512	CLA	CED-O2D-CGD	2.74	122.41	115.99
24	d	2356	PHO	CBA-CAA-C2A	2.74	121.47	113.73
28	c	2489	BCR	C30-C25-C24	2.75	123.52	115.82
23	B	514	CLA	O2D-CGD-CBD	2.75	115.07	111.30
23	c	2482	CLA	C6-C5-C3	2.75	118.52	112.48
23	C	482	CLA	CED-O2D-CGD	2.75	122.44	115.99
23	A	348	CLA	C1D-CHD-C4C	2.75	126.77	122.60
23	b	2515	CLA	C1D-CHD-C4C	2.75	126.77	122.60
23	B	518	CLA	C1D-CHD-C4C	2.76	126.77	122.60
23	C	480	CLA	CED-O2D-CGD	2.76	122.46	115.99
23	d	2357	CLA	C6-C5-C3	2.77	118.56	112.48
23	b	2516	CLA	O2D-CGD-CBD	2.77	115.10	111.30
23	b	2520	CLA	O2A-CGA-CBA	2.78	120.36	111.90
23	d	2355	CLA	O2D-CGD-CBD	2.78	115.11	111.30
23	C	476	CLA	O2A-CGA-CBA	2.78	120.36	111.90
23	A	349	CLA	C1D-CHD-C4C	2.78	126.80	122.60
23	c	2485	CLA	O2A-CGA-CBA	2.78	120.36	111.90
23	b	2525	CLA	CBA-CAA-C2A	2.78	121.58	113.73
23	B	520	CLA	C1D-CHD-C4C	2.78	126.81	122.60
23	B	527	CLA	C2A-C1A-CHA	2.79	129.01	123.89
23	b	2517	CLA	C1D-CHD-C4C	2.79	126.82	122.60
23	D	354	CLA	O2D-CGD-CBD	2.79	115.13	111.30
23	c	2483	CLA	CED-O2D-CGD	2.79	122.54	115.99
23	c	2487	CLA	O2D-CGD-CBD	2.80	115.13	111.30
28	B	528	BCR	C23-C24-C25	2.80	135.72	127.32
23	a	2351	CLA	CED-O2D-CGD	2.80	122.55	115.99
28	C	489	BCR	C30-C25-C24	2.80	123.66	115.82
23	C	484	CLA	O2A-CGA-CBA	2.81	120.45	111.90
23	B	525	CLA	CBA-CAA-C2A	2.81	121.65	113.73
23	b	2518	CLA	C1D-CHD-C4C	2.81	126.85	122.60
23	C	483	CLA	CED-O2D-CGD	2.81	122.58	115.99
23	c	2482	CLA	CED-O2D-CGD	2.82	122.59	115.99
23	B	518	CLA	CED-O2D-CGD	2.83	122.62	115.99
23	A	348	CLA	CED-O2D-CGD	2.83	122.62	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	527	CLA	CED-O2D-CGD	2.83	122.62	115.99
23	c	2481	CLA	O2D-CGD-CBD	2.83	115.18	111.30
23	b	2524	CLA	CED-O2D-CGD	2.83	122.63	115.99
28	d	2360	BCR	C34-C9-C8	2.84	122.81	118.10
23	b	2513	CLA	C2A-C1A-CHA	2.84	129.11	123.89
23	c	2484	CLA	O2A-CGA-CBA	2.84	120.55	111.90
23	B	522	CLA	C6-C5-C3	2.84	118.73	112.48
23	C	479	CLA	O2D-CGD-CBD	2.85	115.20	111.30
23	c	2479	CLA	O2D-CGD-CBD	2.85	115.20	111.30
23	B	516	CLA	C5-C3-C2	2.85	126.46	121.05
28	F	48	BCR	C30-C25-C24	2.85	123.81	115.82
23	b	2524	CLA	C1D-CHD-C4C	2.86	126.93	122.60
23	B	520	CLA	CED-O2D-CGD	2.86	122.70	115.99
28	b	2527	BCR	C23-C24-C25	2.86	135.92	127.32
23	b	2525	CLA	C6-C5-C3	2.87	118.78	112.48
24	d	2356	PHO	CED-O2D-CGD	2.87	122.72	115.99
23	B	520	CLA	O2A-CGA-CBA	2.87	120.65	111.90
23	A	350	CLA	C1D-CHD-C4C	2.87	126.95	122.60
23	b	2526	CLA	O2D-CGD-CBD	2.87	115.24	111.30
23	B	519	CLA	CED-O2D-CGD	2.88	122.73	115.99
23	b	2521	CLA	C1D-CHD-C4C	2.88	126.95	122.60
23	b	2526	CLA	C2A-C1A-CHA	2.88	129.19	123.89
23	b	2526	CLA	CED-O2D-CGD	2.88	122.75	115.99
25	V	138	HEM	CAD-C3D-C4D	2.89	122.67	112.47
23	c	2480	CLA	C1D-CHD-C4C	2.90	126.99	122.60
23	B	524	CLA	CED-O2D-CGD	2.90	122.79	115.99
23	B	524	CLA	C1D-CHD-C4C	2.91	127.00	122.60
23	a	2349	CLA	C1D-CHD-C4C	2.91	127.01	122.60
23	C	486	CLA	C1D-CHD-C4C	2.92	127.02	122.60
23	C	478	CLA	CED-O2D-CGD	2.92	122.84	115.99
26	A	353	PL9	C31-C32-C33	2.92	119.34	111.69
23	b	2523	CLA	O2A-CGA-CBA	2.92	120.81	111.90
23	b	2514	CLA	CED-O2D-CGD	2.92	122.85	115.99
24	A	351	PHO	CED-O2D-CGD	2.92	122.85	115.99
23	c	2480	CLA	CED-O2D-CGD	2.93	122.86	115.99
23	c	2481	CLA	CED-O2D-CGD	2.93	122.87	115.99
28	F	48	BCR	C34-C9-C8	2.94	122.98	118.10
23	b	2518	CLA	CED-O2D-CGD	2.94	122.89	115.99
23	c	2481	CLA	C1D-CHD-C4C	2.95	127.06	122.60
23	c	2486	CLA	C1D-CHD-C4C	2.95	127.06	122.60
23	B	514	CLA	C1D-CHD-C4C	2.95	127.07	122.60
23	B	522	CLA	CED-O2D-CGD	2.95	122.92	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	518	CLA	O2D-CGD-CBD	2.96	115.36	111.30
23	A	350	CLA	O2A-CGA-CBA	2.96	120.93	111.90
28	J	53	BCR	C7-C8-C9	2.97	130.74	126.22
23	a	2351	CLA	C1D-CHD-C4C	2.97	127.10	122.60
24	a	2350	PHO	CED-O2D-CGD	2.97	122.96	115.99
23	b	2516	CLA	C5-C3-C2	2.97	126.69	121.05
23	C	484	CLA	CED-O2D-CGD	2.97	122.96	115.99
23	B	524	CLA	O2A-CGA-CBA	2.98	120.97	111.90
23	B	525	CLA	C6-C5-C3	2.98	119.02	112.48
28	c	2488	BCR	C23-C24-C25	2.98	136.27	127.32
23	B	511	CLA	O2D-CGD-CBD	2.98	115.39	111.30
23	C	486	CLA	O2D-CGD-CBD	2.99	115.39	111.30
26	a	2352	PL9	C31-C32-C33	2.99	119.51	111.69
28	C	489	BCR	C7-C8-C9	2.99	130.77	126.22
23	B	513	CLA	C2A-C1A-CHA	2.99	129.39	123.89
23	c	2474	CLA	C1D-CHD-C4C	2.99	127.13	122.60
23	C	480	CLA	C1D-CHD-C4C	2.99	127.13	122.60
23	C	478	CLA	O2D-CGD-CBD	2.99	115.40	111.30
23	b	2515	CLA	O2D-CGD-CBD	3.00	115.41	111.30
23	B	523	CLA	O2A-CGA-CBA	3.00	121.03	111.90
23	B	527	CLA	C1D-CHD-C4C	3.00	127.14	122.60
23	c	2481	CLA	O2A-CGA-CBA	3.00	121.05	111.90
23	c	2482	CLA	O2D-CGD-CBD	3.00	115.42	111.30
23	b	2514	CLA	O2D-CGD-CBD	3.01	115.42	111.30
23	B	513	CLA	C1D-CHD-C4C	3.01	127.16	122.60
23	a	2349	CLA	O2A-CGA-CBA	3.01	121.08	111.90
23	b	2514	CLA	C1D-CHD-C4C	3.01	127.16	122.60
23	C	479	CLA	C1D-CHD-C4C	3.01	127.16	122.60
23	a	2349	CLA	O2D-CGD-CBD	3.02	115.44	111.30
23	C	475	CLA	C1D-CHD-C4C	3.02	127.17	122.60
23	C	487	CLA	CED-O2D-CGD	3.02	123.08	115.99
23	b	2517	CLA	CED-O2D-CGD	3.02	123.08	115.99
23	B	516	CLA	C1D-CHD-C4C	3.02	127.18	122.60
23	b	2511	CLA	O2D-CGD-CBD	3.03	115.45	111.30
25	V	138	HEM	C3C-CAC-CBC	3.03	129.10	124.46
23	b	2523	CLA	C1D-CHD-C4C	3.03	127.19	122.60
23	c	2475	CLA	C1D-CHD-C4C	3.03	127.19	122.60
23	C	479	CLA	CED-O2D-CGD	3.03	123.11	115.99
23	c	2477	CLA	C1D-CHD-C4C	3.03	127.19	122.60
25	E	84	HEM	CMA-C3A-C2A	3.04	131.59	125.24
23	b	2511	CLA	C1D-CHD-C4C	3.04	127.20	122.60
24	D	355	PHO	CED-O2D-CGD	3.04	123.11	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	511	CLA	C1D-CHD-C4C	3.04	127.20	122.60
23	B	525	CLA	O2D-CGD-CBD	3.04	115.47	111.30
23	b	2522	CLA	CED-O2D-CGD	3.04	123.13	115.99
23	B	513	CLA	CED-O2D-CGD	3.05	123.15	115.99
23	C	480	CLA	O2D-CGD-CBD	3.05	115.49	111.30
23	B	521	CLA	C1D-CHD-C4C	3.05	127.22	122.60
23	c	2479	CLA	C1D-CHD-C4C	3.06	127.23	122.60
23	A	349	CLA	O2D-CGD-CBD	3.06	115.50	111.30
23	C	481	CLA	C1D-CHD-C4C	3.06	127.23	122.60
23	C	474	CLA	C1D-CHD-C4C	3.06	127.23	122.60
23	b	2524	CLA	O2A-CGA-CBA	3.07	121.24	111.90
23	c	2485	CLA	CBA-CAA-C2A	3.07	122.39	113.73
23	C	481	CLA	O2A-CGA-CBA	3.07	121.25	111.90
23	b	2513	CLA	CED-O2D-CGD	3.07	123.20	115.99
23	a	2351	CLA	O2D-CGD-CBD	3.08	115.52	111.30
23	b	2512	CLA	C1D-CHD-C4C	3.08	127.26	122.60
28	C	488	BCR	C23-C24-C25	3.08	136.57	127.32
23	c	2479	CLA	C6-C5-C3	3.09	119.26	112.48
23	B	525	CLA	O2A-CGA-CBA	3.09	121.31	111.90
23	b	2513	CLA	C1D-CHD-C4C	3.09	127.27	122.60
23	b	2525	CLA	O2A-CGA-CBA	3.09	121.31	111.90
23	A	352	CLA	O2D-CGD-CBD	3.09	115.54	111.30
23	d	2354	CLA	CBA-CAA-C2A	3.09	122.46	113.73
28	j	2053	BCR	C29-C30-C25	3.10	115.27	110.36
23	B	516	CLA	O2D-CGD-CBD	3.11	115.56	111.30
28	c	2488	BCR	C2-C1-C6	3.11	115.29	110.36
23	C	485	CLA	C1D-CHD-C4C	3.11	127.31	122.60
24	A	351	PHO	CBD-CHA-C1A	3.11	133.69	126.36
23	b	2519	CLA	C1D-CHD-C4C	3.12	127.32	122.60
24	a	2350	PHO	CBD-CHA-C1A	3.12	133.70	126.36
23	b	2511	CLA	CED-O2D-CGD	3.12	123.30	115.99
23	C	476	CLA	C1D-CHD-C4C	3.12	127.32	122.60
23	c	2478	CLA	CED-O2D-CGD	3.12	123.31	115.99
23	D	354	CLA	C1D-CHD-C4C	3.12	127.33	122.60
23	d	2357	CLA	C1D-CHD-C4C	3.12	127.33	122.60
23	b	2525	CLA	C1D-CHD-C4C	3.13	127.33	122.60
23	B	511	CLA	CED-O2D-CGD	3.13	123.33	115.99
23	c	2484	CLA	CED-O2D-CGD	3.13	123.33	115.99
23	c	2483	CLA	O2D-CGD-CBD	3.13	115.60	111.30
23	B	513	CLA	O2A-CGA-CBA	3.13	121.45	111.90
23	c	2482	CLA	CBA-CAA-C2A	3.14	122.58	113.73
23	B	512	CLA	C1D-CHD-C4C	3.14	127.35	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2519	CLA	CED-O2D-CGD	3.14	123.35	115.99
23	B	523	CLA	C1D-CHD-C4C	3.14	127.35	122.60
28	j	2053	BCR	C2-C1-C6	3.14	115.33	110.36
23	C	474	CLA	O2A-CGA-CBA	3.14	121.47	111.90
23	b	2519	CLA	O2A-CGA-CBA	3.14	121.48	111.90
23	c	2478	CLA	C1D-CHD-C4C	3.15	127.36	122.60
23	C	475	CLA	CED-O2D-CGD	3.15	123.38	115.99
24	d	2356	PHO	O2A-CGA-CBA	3.15	121.50	111.90
23	c	2480	CLA	O2A-CGA-CBA	3.15	121.51	111.90
25	V	138	HEM	C1D-CHD-C4C	3.16	131.10	125.82
28	c	2489	BCR	C23-C24-C25	3.16	136.80	127.32
23	c	2474	CLA	O2A-CGA-CBA	3.16	121.52	111.90
28	C	488	BCR	C2-C1-C6	3.16	115.37	110.36
23	a	2348	CLA	C1D-CHD-C4C	3.16	127.39	122.60
23	c	2476	CLA	C1D-CHD-C4C	3.17	127.39	122.60
23	c	2484	CLA	C1D-CHD-C4C	3.17	127.39	122.60
23	c	2483	CLA	C1D-CHD-C4C	3.17	127.39	122.60
23	c	2480	CLA	O2D-CGD-CBD	3.17	115.65	111.30
24	D	355	PHO	O2A-CGA-CBA	3.17	121.57	111.90
23	C	482	CLA	C6-C5-C3	3.17	119.45	112.48
24	D	355	PHO	C6-C5-C3	3.18	119.45	112.48
23	c	2477	CLA	O2D-CGD-CBD	3.18	115.66	111.30
28	k	2050	BCR	C7-C8-C9	3.18	131.06	126.22
23	b	2526	CLA	C1D-CHD-C4C	3.18	127.41	122.60
23	B	519	CLA	C1D-CHD-C4C	3.18	127.41	122.60
28	K	50	BCR	C7-C8-C9	3.19	131.08	126.22
23	c	2487	CLA	CED-O2D-CGD	3.19	123.48	115.99
23	C	482	CLA	CBA-CAA-C2A	3.20	122.75	113.73
23	c	2479	CLA	CED-O2D-CGD	3.20	123.48	115.99
23	D	356	CLA	C1D-CHD-C4C	3.20	127.44	122.60
23	b	2522	CLA	C1D-CHD-C4C	3.20	127.44	122.60
23	C	486	CLA	O2A-CGA-CBA	3.20	121.64	111.90
23	b	2521	CLA	CED-O2D-CGD	3.20	123.49	115.99
27	d	2359	LMT	O1B-C1B-C2B	3.20	115.89	108.10
23	b	2517	CLA	O2A-CGA-CBA	3.20	121.66	111.90
27	B	526	LMT	O1B-C1B-C2B	3.21	115.91	108.10
23	A	352	CLA	C1D-CHD-C4C	3.21	127.46	122.60
23	B	525	CLA	C1D-CHD-C4C	3.21	127.46	122.60
23	C	480	CLA	O2A-CGA-CBA	3.21	121.69	111.90
28	c	2489	BCR	C7-C8-C9	3.21	131.12	126.22
23	b	2516	CLA	CBA-CAA-C2A	3.22	122.83	113.73
23	C	483	CLA	O2D-CGD-CBD	3.23	115.72	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2485	CLA	CED-O2D-CGD	3.23	123.56	115.99
23	B	519	CLA	O2A-CGA-CBA	3.23	121.75	111.90
23	B	517	CLA	C1D-CHD-C4C	3.24	127.50	122.60
23	B	522	CLA	C1D-CHD-C4C	3.25	127.51	122.60
23	b	2519	CLA	O2D-CGD-CBD	3.25	115.76	111.30
23	c	2485	CLA	C1D-CHD-C4C	3.26	127.53	122.60
23	B	512	CLA	C6-C5-C3	3.26	119.63	112.48
28	J	53	BCR	C2-C1-C6	3.26	115.53	110.36
23	b	2515	CLA	CED-O2D-CGD	3.26	123.64	115.99
23	C	477	CLA	O2D-CGD-CBD	3.26	115.78	111.30
23	C	485	CLA	CBA-CAA-C2A	3.27	122.95	113.73
23	C	485	CLA	CED-O2D-CGD	3.27	123.67	115.99
23	C	483	CLA	C1D-CHD-C4C	3.27	127.55	122.60
23	C	479	CLA	C6-C5-C3	3.28	119.68	112.48
28	F	48	BCR	C23-C24-C25	3.28	137.17	127.32
23	b	2513	CLA	O2A-CGA-CBA	3.28	121.90	111.90
28	d	2360	BCR	C16-C15-C14	3.28	130.66	123.39
23	B	524	CLA	O2D-CGD-CBD	3.29	115.81	111.30
28	C	489	BCR	C23-C24-C25	3.29	137.19	127.32
23	c	2486	CLA	O2A-CGA-CBA	3.29	121.92	111.90
23	b	2524	CLA	O2D-CGD-CBD	3.29	115.82	111.30
24	A	351	PHO	O2D-CGD-CBD	3.30	115.82	111.30
23	c	2477	CLA	CED-O2D-CGD	3.30	123.73	115.99
23	b	2516	CLA	C1D-CHD-C4C	3.30	127.60	122.60
23	C	477	CLA	CED-O2D-CGD	3.31	123.75	115.99
23	b	2525	CLA	O2D-CGD-CBD	3.31	115.84	111.30
23	b	2512	CLA	C6-C5-C3	3.31	119.75	112.48
23	c	2482	CLA	C1D-CHD-C4C	3.32	127.62	122.60
23	B	517	CLA	O2A-CGA-CBA	3.32	122.02	111.90
23	B	516	CLA	CBA-CAA-C2A	3.32	123.11	113.73
24	a	2350	PHO	O2D-CGD-CBD	3.33	115.86	111.30
24	a	2350	PHO	C4A-NA-C1A	3.34	111.19	108.21
28	C	488	BCR	C29-C30-C25	3.34	115.66	110.36
23	d	2354	CLA	C1D-CHD-C4C	3.35	127.66	122.60
28	B	529	BCR	C29-C30-C25	3.35	115.67	110.36
24	D	355	PHO	CBD-CHA-C1A	3.35	134.26	126.36
23	c	2487	CLA	C1D-CHD-C4C	3.35	127.68	122.60
23	B	515	CLA	O2D-CGD-CBD	3.36	115.90	111.30
23	B	521	CLA	CED-O2D-CGD	3.36	123.86	115.99
28	j	2053	BCR	C7-C8-C9	3.36	131.34	126.22
23	C	483	CLA	C6-C5-C3	3.36	119.86	112.48
23	c	2478	CLA	O2D-CGD-CBD	3.36	115.91	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	523	CLA	CED-O2D-CGD	3.36	123.88	115.99
28	F	48	BCR	C16-C15-C14	3.38	130.86	123.39
28	F	48	BCR	C29-C30-C25	3.40	115.75	110.36
23	D	354	CLA	O2A-CGA-CBA	3.40	122.27	111.90
23	C	487	CLA	C1D-CHD-C4C	3.40	127.75	122.60
23	c	2475	CLA	CED-O2D-CGD	3.41	123.99	115.99
23	C	482	CLA	C1D-CHD-C4C	3.41	127.76	122.60
23	C	478	CLA	C1D-CHD-C4C	3.43	127.78	122.60
23	B	515	CLA	CED-O2D-CGD	3.43	124.02	115.99
23	d	2354	CLA	O2A-CGA-CBA	3.43	122.34	111.90
23	c	2478	CLA	C2A-C1A-CHA	3.43	130.21	123.89
28	k	2050	BCR	C29-C30-C25	3.45	115.82	110.36
28	c	2489	BCR	C29-C30-C25	3.45	115.82	110.36
24	d	2356	PHO	C6-C5-C3	3.45	120.05	112.48
23	b	2523	CLA	CED-O2D-CGD	3.45	124.08	115.99
24	d	2356	PHO	CBD-CHA-C1A	3.45	134.49	126.36
23	c	2476	CLA	O2D-CGD-CBD	3.45	116.04	111.30
25	e	2084	HEM	C2D-C3D-C4D	3.46	107.36	101.50
23	C	483	CLA	O2A-CGA-CBA	3.46	122.45	111.90
23	D	356	CLA	O2D-CGD-CBD	3.47	116.06	111.30
28	d	2360	BCR	C23-C24-C25	3.47	137.74	127.32
23	C	476	CLA	O2D-CGD-CBD	3.47	116.06	111.30
25	V	138	HEM	CMB-C2B-C3B	3.47	125.20	116.53
23	C	477	CLA	O2A-CGA-CBA	3.47	122.49	111.90
23	c	2487	CLA	CAC-C3C-C4C	3.48	129.88	124.83
26	d	2358	PL9	C32-C31-C29	3.48	124.06	112.71
23	B	519	CLA	O2D-CGD-CBD	3.49	116.08	111.30
23	d	2354	CLA	O2D-CGD-CBD	3.49	116.08	111.30
23	C	477	CLA	C1D-CHD-C4C	3.49	127.88	122.60
23	c	2477	CLA	O2A-CGA-CBA	3.49	122.54	111.90
23	C	478	CLA	C2A-C1A-CHA	3.49	130.32	123.89
26	A	353	PL9	C25-C24-C23	3.50	130.37	123.50
23	c	2483	CLA	C6-C5-C3	3.51	120.18	112.48
23	C	478	CLA	O2A-CGA-CBA	3.51	122.59	111.90
23	C	484	CLA	C1D-CHD-C4C	3.51	127.91	122.60
28	d	2360	BCR	C2-C1-C6	3.51	115.92	110.36
25	E	84	HEM	C2D-C3D-C4D	3.51	107.45	101.50
28	j	2053	BCR	C24-C23-C22	3.52	131.57	126.22
25	e	2084	HEM	CMD-C2D-C3D	3.52	129.90	114.35
23	c	2478	CLA	O2A-CGA-CBA	3.52	122.62	111.90
23	A	350	CLA	O2D-CGD-CBD	3.52	116.13	111.30
26	D	357	PL9	C32-C31-C29	3.52	124.19	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	513	CLA	C6-C5-C3	3.53	120.23	112.48
28	d	2360	BCR	C29-C30-C25	3.53	115.95	110.36
25	V	138	HEM	C3B-C4B-CHC	3.54	128.14	123.16
28	K	50	BCR	C29-C30-C25	3.54	115.97	110.36
28	b	2528	BCR	C29-C30-C25	3.54	115.97	110.36
23	B	525	CLA	CED-O2D-CGD	3.54	124.30	115.99
28	B	528	BCR	C24-C23-C22	3.55	131.62	126.22
28	c	2489	BCR	C2-C1-C6	3.56	115.99	110.36
28	J	53	BCR	C24-C23-C22	3.56	131.64	126.22
23	b	2513	CLA	C6-C5-C3	3.56	120.30	112.48
24	D	355	PHO	O2D-CGD-CBD	3.57	116.20	111.30
28	b	2528	BCR	C33-C5-C6	3.58	128.12	124.61
23	c	2483	CLA	O2A-CGA-CBA	3.58	122.80	111.90
23	d	2355	CLA	O2A-CGA-CBA	3.58	122.81	111.90
25	E	84	HEM	CMD-C2D-C3D	3.58	130.19	114.35
28	B	529	BCR	C33-C5-C6	3.58	128.12	124.61
28	F	48	BCR	C2-C1-C6	3.58	116.04	110.36
28	b	2527	BCR	C24-C23-C22	3.60	131.70	126.22
23	b	2513	CLA	O2D-CGD-CBD	3.61	116.25	111.30
23	b	2525	CLA	CED-O2D-CGD	3.61	124.45	115.99
23	C	486	CLA	C6-C5-C3	3.62	120.42	112.48
23	B	513	CLA	O2D-CGD-CBD	3.62	116.27	111.30
23	A	348	CLA	O2D-CGD-CBD	3.64	116.29	111.30
23	B	527	CLA	CBA-CAA-C2A	3.64	124.00	113.73
24	A	351	PHO	C4A-NA-C1A	3.64	111.46	108.21
23	b	2526	CLA	CBA-CAA-C2A	3.67	124.08	113.73
28	B	528	BCR	C29-C30-C25	3.67	116.18	110.36
23	c	2486	CLA	C6-C5-C3	3.68	120.55	112.48
28	C	489	BCR	C29-C30-C25	3.68	116.19	110.36
23	b	2514	CLA	O2A-CGA-CBA	3.69	123.14	111.90
23	C	477	CLA	C6-C5-C3	3.69	120.58	112.48
23	b	2517	CLA	O2D-CGD-CBD	3.70	116.37	111.30
23	B	517	CLA	O2D-CGD-CBD	3.71	116.38	111.30
23	C	487	CLA	CAC-C3C-C4C	3.73	130.24	124.83
28	J	53	BCR	C29-C30-C25	3.73	116.27	110.36
28	c	2488	BCR	C29-C30-C25	3.73	116.27	110.36
26	A	353	PL9	C32-C31-C29	3.73	124.87	112.71
23	B	520	CLA	O2D-CGD-CBD	3.73	116.42	111.30
28	C	489	BCR	C2-C1-C6	3.73	116.27	110.36
25	v	2138	HEM	C2D-C3D-C4D	3.73	107.83	101.50
23	b	2515	CLA	CBA-CAA-C2A	3.74	124.27	113.73
23	A	349	CLA	O2A-CGA-CBA	3.74	123.29	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	2527	BCR	C29-C30-C25	3.74	116.28	110.36
26	a	2352	PL9	C32-C31-C29	3.75	124.94	112.71
28	b	2527	BCR	C2-C1-C6	3.77	116.33	110.36
23	C	482	CLA	O2D-CGD-CBD	3.78	116.48	111.30
23	C	474	CLA	O2D-CGD-CBD	3.78	116.48	111.30
23	C	485	CLA	O2D-CGD-CBD	3.78	116.49	111.30
23	a	2349	CLA	CBA-CAA-C2A	3.83	124.55	113.73
23	C	480	CLA	CBA-CAA-C2A	3.84	124.56	113.73
23	B	515	CLA	CBA-CAA-C2A	3.84	124.58	113.73
23	c	2486	CLA	O2D-CGD-CBD	3.85	116.58	111.30
28	c	2488	BCR	C16-C17-C18	3.85	132.75	127.20
23	d	2357	CLA	O2D-CGD-CBD	3.86	116.59	111.30
23	B	514	CLA	O2A-CGA-CBA	3.86	123.67	111.90
23	c	2485	CLA	O2D-CGD-CBD	3.89	116.63	111.30
23	c	2487	CLA	C4A-NA-C1A	3.90	111.41	106.36
23	a	2348	CLA	O2D-CGD-CBD	3.91	116.67	111.30
23	c	2480	CLA	CBA-CAA-C2A	3.92	124.79	113.73
23	c	2477	CLA	C6-C5-C3	3.92	121.09	112.48
23	b	2514	CLA	CBA-CAA-C2A	3.93	124.83	113.73
23	c	2474	CLA	CBA-CAA-C2A	3.94	124.84	113.73
23	A	350	CLA	CBA-CAA-C2A	3.97	124.93	113.73
23	C	474	CLA	CBA-CAA-C2A	3.97	124.94	113.73
23	B	518	CLA	O2A-CGA-CBA	4.00	124.08	111.90
28	k	2050	BCR	C2-C1-C6	4.00	116.70	110.36
23	d	2355	CLA	CBA-CAA-C2A	4.01	125.04	113.73
28	B	528	BCR	C2-C1-C6	4.02	116.73	110.36
23	A	349	CLA	CBA-CAA-C2A	4.02	125.09	113.73
28	C	488	BCR	C16-C17-C18	4.04	133.03	127.20
26	A	353	PL9	C7-C8-C9	4.04	133.55	126.70
23	b	2518	CLA	O2A-CGA-CBA	4.04	124.22	111.90
28	K	50	BCR	C2-C1-C6	4.04	116.77	110.36
28	d	2360	BCR	C7-C8-C9	4.05	132.39	126.22
23	c	2474	CLA	O2D-CGD-CBD	4.08	116.89	111.30
23	b	2513	CLA	CBA-CAA-C2A	4.08	125.25	113.73
25	v	2138	HEM	CAD-C3D-C4D	4.09	126.89	112.47
23	B	514	CLA	CBA-CAA-C2A	4.09	125.28	113.73
23	a	2349	CLA	C4A-NA-C1A	4.11	111.68	106.36
26	a	2352	PL9	C25-C24-C23	4.12	131.59	123.50
26	a	2352	PL9	C7-C8-C9	4.12	133.68	126.70
23	B	513	CLA	CAA-CBA-CGA	4.14	125.44	113.32
25	e	2084	HEM	CAD-C3D-C4D	4.15	127.09	112.47
23	C	487	CLA	C4A-NA-C1A	4.15	111.72	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	2358	PL9	C30-C29-C31	4.16	121.75	115.41
28	b	2528	BCR	C2-C1-C6	4.16	116.94	110.36
23	C	477	CLA	C4A-NA-C1A	4.18	111.76	106.36
23	c	2479	CLA	CBA-CAA-C2A	4.18	125.53	113.73
28	b	2528	BCR	C21-C20-C19	4.18	135.88	123.13
25	E	84	HEM	CAD-C3D-C2D	4.18	125.24	113.22
25	v	2138	HEM	CAD-C3D-C2D	4.20	125.28	113.22
25	E	84	HEM	CAD-C3D-C4D	4.21	127.30	112.47
23	B	521	CLA	C4A-NA-C1A	4.21	111.81	106.36
25	V	138	HEM	CMD-C2D-C3D	4.22	133.03	114.35
23	b	2513	CLA	CAA-CBA-CGA	4.22	125.68	113.32
23	c	2477	CLA	C4A-NA-C1A	4.23	111.83	106.36
23	A	350	CLA	C4A-NA-C1A	4.23	111.83	106.36
26	d	2358	PL9	C36-C34-C33	4.23	129.07	121.05
28	B	529	BCR	C21-C20-C19	4.24	136.04	123.13
23	C	479	CLA	CBA-CAA-C2A	4.24	125.69	113.73
23	b	2521	CLA	C4A-NA-C1A	4.24	111.85	106.36
26	D	357	PL9	C36-C34-C33	4.28	129.17	121.05
24	d	2356	PHO	C4A-NA-C1A	4.28	112.03	108.21
25	e	2084	HEM	CAD-C3D-C2D	4.29	125.55	113.22
23	a	2348	CLA	C4A-NA-C1A	4.30	111.92	106.36
23	D	354	CLA	C4A-NA-C1A	4.30	111.92	106.36
28	F	48	BCR	C7-C8-C9	4.31	132.79	126.22
23	b	2520	CLA	O2D-CGD-CBD	4.31	117.22	111.30
23	d	2354	CLA	C4A-NA-C1A	4.32	111.94	106.36
23	C	485	CLA	C4A-NA-C1A	4.33	111.95	106.36
24	D	355	PHO	C4A-NA-C1A	4.33	112.08	108.21
26	D	357	PL9	C30-C29-C31	4.34	122.03	115.41
28	B	529	BCR	C2-C1-C6	4.36	117.27	110.36
23	c	2475	CLA	C4A-NA-C1A	4.37	112.01	106.36
23	B	515	CLA	C4A-NA-C1A	4.38	112.03	106.36
23	B	513	CLA	CBA-CAA-C2A	4.38	126.10	113.73
23	B	527	CLA	C4A-NA-C1A	4.41	112.06	106.36
23	A	348	CLA	C4A-NA-C1A	4.42	112.08	106.36
25	V	138	HEM	CAD-C3D-C2D	4.44	125.99	113.22
23	c	2485	CLA	C4A-NA-C1A	4.48	112.15	106.36
23	b	2526	CLA	C4A-NA-C1A	4.49	112.16	106.36
23	b	2515	CLA	C4A-NA-C1A	4.52	112.20	106.36
23	B	527	CLA	C6-C5-C3	4.53	122.42	112.48
23	b	2526	CLA	C6-C5-C3	4.56	122.50	112.48
23	C	486	CLA	C4A-NA-C1A	4.59	112.29	106.36
23	b	2514	CLA	C4A-NA-C1A	4.60	112.31	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	514	CLA	C4A-NA-C1A	4.61	112.32	106.36
23	c	2482	CLA	C4A-NA-C1A	4.61	112.33	106.36
25	V	138	HEM	CMC-C2C-C3C	4.63	128.08	116.53
23	C	475	CLA	C4A-NA-C1A	4.63	112.35	106.36
28	d	2360	BCR	C11-C10-C9	4.65	133.92	127.20
23	c	2476	CLA	C4A-NA-C1A	4.66	112.38	106.36
25	e	2084	HEM	CMC-C2C-C3C	4.67	128.18	116.53
23	c	2474	CLA	C4A-NA-C1A	4.67	112.40	106.36
23	b	2511	CLA	CBA-CAA-C2A	4.68	126.95	113.73
23	b	2516	CLA	C4A-NA-C1A	4.69	112.42	106.36
23	B	516	CLA	C4A-NA-C1A	4.69	112.43	106.36
23	C	484	CLA	C4A-NA-C1A	4.69	112.43	106.36
23	B	511	CLA	CBA-CAA-C2A	4.69	126.98	113.73
23	d	2355	CLA	C4A-NA-C1A	4.69	112.43	106.36
23	C	480	CLA	C4A-NA-C1A	4.70	112.43	106.36
23	c	2486	CLA	C4A-NA-C1A	4.71	112.45	106.36
23	B	520	CLA	C4A-NA-C1A	4.72	112.46	106.36
23	b	2517	CLA	C4A-NA-C1A	4.73	112.48	106.36
23	c	2480	CLA	C4A-NA-C1A	4.76	112.51	106.36
23	c	2481	CLA	C4A-NA-C1A	4.76	112.52	106.36
23	b	2519	CLA	C4A-NA-C1A	4.77	112.53	106.36
23	C	481	CLA	C4A-NA-C1A	4.78	112.54	106.36
23	c	2484	CLA	C4A-NA-C1A	4.80	112.56	106.36
23	B	525	CLA	C4A-NA-C1A	4.80	112.57	106.36
28	F	48	BCR	C11-C10-C9	4.80	134.14	127.20
23	b	2524	CLA	C4A-NA-C1A	4.81	112.57	106.36
25	v	2138	HEM	CMB-C2B-C3B	4.82	128.55	116.53
23	B	518	CLA	C4A-NA-C1A	4.82	112.59	106.36
23	b	2518	CLA	C4A-NA-C1A	4.82	112.59	106.36
23	C	482	CLA	C4A-NA-C1A	4.83	112.61	106.36
23	b	2518	CLA	CBA-CAA-C2A	4.84	127.38	113.73
23	C	478	CLA	C4A-NA-C1A	4.84	112.61	106.36
23	B	523	CLA	CBA-CAA-C2A	4.84	127.39	113.73
23	b	2523	CLA	CBA-CAA-C2A	4.85	127.41	113.73
23	C	474	CLA	C4A-NA-C1A	4.85	112.63	106.36
25	e	2084	HEM	CMB-C2B-C3B	4.85	128.64	116.53
23	b	2520	CLA	C4A-NA-C1A	4.86	112.64	106.36
23	a	2351	CLA	C4A-NA-C1A	4.86	112.64	106.36
23	B	522	CLA	C4A-NA-C1A	4.88	112.67	106.36
23	c	2478	CLA	C4A-NA-C1A	4.88	112.67	106.36
23	c	2483	CLA	C4A-NA-C1A	4.89	112.69	106.36
23	C	476	CLA	C4A-NA-C1A	4.90	112.69	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	524	CLA	C4A-NA-C1A	4.90	112.70	106.36
28	C	489	BCR	C38-C26-C25	4.90	129.42	124.61
23	b	2522	CLA	C4A-NA-C1A	4.90	112.70	106.36
23	b	2525	CLA	C4A-NA-C1A	4.92	112.72	106.36
23	A	349	CLA	C4A-NA-C1A	4.92	112.72	106.36
28	c	2489	BCR	C38-C26-C25	4.93	129.44	124.61
23	A	352	CLA	C4A-NA-C1A	4.94	112.75	106.36
23	C	483	CLA	C4A-NA-C1A	4.95	112.76	106.36
23	B	518	CLA	CBA-CAA-C2A	4.95	127.70	113.73
23	B	517	CLA	C4A-NA-C1A	4.96	112.77	106.36
23	B	512	CLA	C4A-NA-C1A	4.98	112.80	106.36
25	E	84	HEM	CMB-C2B-C3B	4.99	129.00	116.53
23	B	523	CLA	C4A-NA-C1A	5.02	112.85	106.36
25	E	84	HEM	CMC-C2C-C3C	5.05	129.13	116.53
23	b	2523	CLA	C4A-NA-C1A	5.07	112.92	106.36
28	k	2050	BCR	C33-C5-C6	5.07	129.59	124.61
23	b	2512	CLA	C4A-NA-C1A	5.10	112.95	106.36
23	C	479	CLA	C4A-NA-C1A	5.12	112.98	106.36
23	D	356	CLA	C4A-NA-C1A	5.13	112.99	106.36
23	d	2357	CLA	C4A-NA-C1A	5.13	113.00	106.36
23	b	2511	CLA	C4A-NA-C1A	5.17	113.05	106.36
23	B	519	CLA	C4A-NA-C1A	5.18	113.06	106.36
23	b	2516	CLA	O2A-CGA-CBA	5.21	127.76	111.90
28	c	2488	BCR	C33-C5-C6	5.21	129.72	124.61
23	B	511	CLA	C4A-NA-C1A	5.24	113.13	106.36
28	K	50	BCR	C33-C5-C6	5.24	129.75	124.61
28	c	2488	BCR	C38-C26-C25	5.24	129.75	124.61
23	B	516	CLA	O2A-CGA-CBA	5.25	127.90	111.90
23	c	2479	CLA	C4A-NA-C1A	5.28	113.19	106.36
26	a	2352	PL9	C36-C34-C33	5.29	131.08	121.05
28	C	488	BCR	C33-C5-C6	5.34	129.85	124.61
23	c	2475	CLA	O2A-CGA-CBA	5.37	128.27	111.90
23	B	513	CLA	C4A-NA-C1A	5.40	113.34	106.36
26	A	353	PL9	C36-C34-C33	5.41	131.30	121.05
23	C	475	CLA	O2A-CGA-CBA	5.42	128.40	111.90
28	C	488	BCR	C38-C26-C25	5.43	129.93	124.61
23	b	2513	CLA	C4A-NA-C1A	5.45	113.41	106.36
28	k	2050	BCR	C38-C26-C25	5.50	130.00	124.61
25	v	2138	HEM	CMD-C2D-C3D	5.55	138.92	114.35
28	d	2360	BCR	C38-C26-C25	5.60	130.10	124.61
28	d	2360	BCR	C16-C17-C18	5.60	135.29	127.20
28	F	48	BCR	C16-C17-C18	5.77	135.53	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	V	138	HEM	C2D-C3D-C4D	5.78	111.30	101.50
28	K	50	BCR	C38-C26-C25	5.81	130.31	124.61
28	F	48	BCR	C38-C26-C25	5.97	130.47	124.61
26	a	2352	PL9	C37-C36-C34	5.98	132.20	112.71
28	C	489	BCR	C33-C5-C6	5.99	130.49	124.61
28	j	2053	BCR	C38-C26-C25	6.04	130.53	124.61
26	A	353	PL9	C37-C36-C34	6.09	132.56	112.71
26	A	353	PL9	C22-C23-C24	6.12	141.08	127.76
28	c	2489	BCR	C33-C5-C6	6.13	130.63	124.61
28	b	2528	BCR	C38-C26-C25	6.20	130.70	124.61
28	J	53	BCR	C38-C26-C25	6.23	130.72	124.61
28	J	53	BCR	C33-C5-C6	6.23	130.72	124.61
28	B	528	BCR	C38-C26-C25	6.25	130.75	124.61
23	c	2483	CLA	CBA-CAA-C2A	6.29	131.48	113.73
28	b	2527	BCR	C38-C26-C25	6.43	130.92	124.61
28	j	2053	BCR	C33-C5-C6	6.43	130.92	124.61
28	F	48	BCR	C33-C5-C6	6.49	130.97	124.61
26	d	2358	PL9	C37-C36-C34	6.50	133.88	112.71
26	D	357	PL9	C37-C36-C34	6.53	133.97	112.71
23	C	483	CLA	CBA-CAA-C2A	6.55	132.20	113.73
23	B	519	CLA	CBA-CAA-C2A	6.59	132.33	113.73
26	a	2352	PL9	C22-C23-C24	6.76	142.47	127.76
28	d	2360	BCR	C33-C5-C6	6.78	131.26	124.61
23	b	2519	CLA	CBA-CAA-C2A	6.80	132.92	113.73
28	B	529	BCR	C38-C26-C25	6.92	131.40	124.61
23	c	2481	CLA	CBA-CAA-C2A	7.13	133.84	113.73
23	C	481	CLA	CBA-CAA-C2A	7.36	134.49	113.73
25	v	2138	HEM	CMC-C2C-C3C	7.52	135.30	116.53
28	B	528	BCR	C33-C5-C6	7.55	132.01	124.61
28	b	2527	BCR	C33-C5-C6	7.55	132.01	124.61
27	B	526	LMT	O1'-C1-C2	7.69	140.49	109.88
27	d	2359	LMT	O1'-C1-C2	7.71	140.53	109.88
23	c	2477	CLA	CBA-CAA-C2A	8.25	137.00	113.73
23	C	477	CLA	CBA-CAA-C2A	8.35	137.30	113.73
23	b	2520	CLA	CBA-CAA-C2A	10.33	142.88	113.73
23	B	520	CLA	CBA-CAA-C2A	10.35	142.93	113.73

All (216) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	520	CLA	NC
23	B	520	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	520	CLA	NA
23	c	2478	CLA	NC
23	c	2478	CLA	ND
23	c	2478	CLA	NA
23	C	477	CLA	NC
23	C	477	CLA	ND
23	C	477	CLA	NA
23	a	2348	CLA	NC
23	a	2348	CLA	ND
23	a	2348	CLA	NA
23	b	2518	CLA	NC
23	b	2518	CLA	ND
23	b	2518	CLA	NA
23	c	2487	CLA	NC
23	c	2487	CLA	ND
23	c	2487	CLA	NA
23	C	486	CLA	NC
23	C	486	CLA	ND
23	C	486	CLA	NA
23	c	2482	CLA	NC
23	c	2482	CLA	ND
23	c	2482	CLA	NA
23	b	2523	CLA	NC
23	b	2523	CLA	ND
23	b	2523	CLA	NA
23	C	478	CLA	NC
23	C	478	CLA	ND
23	C	478	CLA	NA
23	B	514	CLA	NC
23	B	514	CLA	ND
23	B	514	CLA	NA
23	c	2477	CLA	NC
23	c	2477	CLA	ND
23	c	2477	CLA	NA
23	c	2484	CLA	NC
23	c	2484	CLA	ND
23	c	2484	CLA	NA
23	B	517	CLA	NC
23	B	517	CLA	ND
23	B	517	CLA	NA
23	D	356	CLA	NC
23	D	356	CLA	ND

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Mol	Chain	Res	Type	Atom
23	D	356	CLA	NA
23	c	2486	CLA	NC
23	c	2486	CLA	ND
23	c	2486	CLA	NA
23	b	2512	CLA	NC
23	b	2512	CLA	ND
23	b	2512	CLA	NA
23	b	2526	CLA	NC
23	b	2526	CLA	ND
23	b	2526	CLA	NA
23	c	2483	CLA	NC
23	c	2483	CLA	ND
23	c	2483	CLA	NA
23	B	523	CLA	NC
23	B	523	CLA	ND
23	B	523	CLA	NA
23	A	350	CLA	NC
23	A	350	CLA	ND
23	A	350	CLA	NA
23	c	2481	CLA	NC
23	c	2481	CLA	ND
23	c	2481	CLA	NA
23	B	525	CLA	NC
23	B	525	CLA	ND
23	B	525	CLA	NA
23	B	519	CLA	NC
23	B	519	CLA	ND
23	B	519	CLA	NA
23	b	2514	CLA	NC
23	b	2514	CLA	ND
23	b	2514	CLA	NA
23	b	2522	CLA	NC
23	b	2522	CLA	ND
23	b	2522	CLA	NA
23	C	485	CLA	NC
23	C	485	CLA	ND
23	C	485	CLA	NA
23	d	2357	CLA	NC
23	d	2357	CLA	ND
23	d	2357	CLA	NA
23	A	349	CLA	NC
23	A	349	CLA	ND

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Mol	Chain	Res	Type	Atom
23	A	349	CLA	NA
23	B	511	CLA	NC
23	B	511	CLA	ND
23	B	511	CLA	NA
23	B	513	CLA	NC
23	B	513	CLA	ND
23	B	513	CLA	NA
23	D	354	CLA	NC
23	D	354	CLA	ND
23	D	354	CLA	NA
23	B	521	CLA	NC
23	B	521	CLA	ND
23	B	521	CLA	NA
23	C	481	CLA	NC
23	C	481	CLA	ND
23	C	481	CLA	NA
23	c	2480	CLA	NC
23	c	2480	CLA	ND
23	c	2480	CLA	NA
23	C	474	CLA	NC
23	C	474	CLA	ND
23	C	474	CLA	NA
23	c	2479	CLA	NC
23	c	2479	CLA	ND
23	c	2479	CLA	NA
23	C	487	CLA	NC
23	C	487	CLA	ND
23	C	487	CLA	NA
23	c	2476	CLA	NC
23	c	2476	CLA	ND
23	c	2476	CLA	NA
23	b	2521	CLA	NC
23	b	2521	CLA	ND
23	b	2521	CLA	NA
23	b	2519	CLA	NC
23	b	2519	CLA	ND
23	b	2519	CLA	NA
23	d	2354	CLA	NC
23	d	2354	CLA	ND
23	d	2354	CLA	NA
23	b	2520	CLA	NC
23	b	2520	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	2520	CLA	NA
23	B	515	CLA	NC
23	B	515	CLA	ND
23	B	515	CLA	NA
23	d	2355	CLA	NC
23	d	2355	CLA	ND
23	d	2355	CLA	NA
23	b	2511	CLA	NC
23	b	2511	CLA	ND
23	b	2511	CLA	NA
23	C	482	CLA	NC
23	C	482	CLA	ND
23	C	482	CLA	NA
23	C	479	CLA	NC
23	C	479	CLA	ND
23	C	479	CLA	NA
23	B	524	CLA	NC
23	B	524	CLA	ND
23	B	524	CLA	NA
23	C	476	CLA	NC
23	C	476	CLA	ND
23	C	476	CLA	NA
23	B	516	CLA	NC
23	B	516	CLA	ND
23	B	516	CLA	NA
23	c	2474	CLA	NC
23	c	2474	CLA	ND
23	c	2474	CLA	NA
23	b	2515	CLA	NC
23	b	2515	CLA	ND
23	b	2515	CLA	NA
23	C	475	CLA	NC
23	C	475	CLA	ND
23	C	475	CLA	NA
23	b	2517	CLA	NC
23	b	2517	CLA	ND
23	b	2517	CLA	NA
23	a	2349	CLA	NC
23	a	2349	CLA	ND
23	a	2349	CLA	NA
23	C	480	CLA	NC
23	C	480	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	480	CLA	NA
23	B	522	CLA	NC
23	B	522	CLA	ND
23	B	522	CLA	NA
23	B	512	CLA	NC
23	B	512	CLA	ND
23	B	512	CLA	NA
23	C	484	CLA	NC
23	C	484	CLA	ND
23	C	484	CLA	NA
23	b	2524	CLA	NC
23	b	2524	CLA	ND
23	b	2524	CLA	NA
23	b	2513	CLA	NC
23	b	2513	CLA	ND
23	b	2513	CLA	NA
23	A	352	CLA	NC
23	A	352	CLA	ND
23	A	352	CLA	NA
23	B	518	CLA	NC
23	B	518	CLA	ND
23	B	518	CLA	NA
23	a	2351	CLA	NC
23	a	2351	CLA	ND
23	a	2351	CLA	NA
23	A	348	CLA	NC
23	A	348	CLA	ND
23	A	348	CLA	NA
23	C	483	CLA	NC
23	C	483	CLA	ND
23	C	483	CLA	NA
23	c	2485	CLA	NC
23	c	2485	CLA	ND
23	c	2485	CLA	NA
23	c	2475	CLA	NC
23	c	2475	CLA	ND
23	c	2475	CLA	NA
23	B	527	CLA	NC
23	B	527	CLA	ND
23	B	527	CLA	NA
23	b	2525	CLA	NC
23	b	2525	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	2525	CLA	NA
23	b	2516	CLA	NC
23	b	2516	CLA	ND
23	b	2516	CLA	NA

There are no torsion outliers.

There are no ring outliers.

50 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	347	OEC	1	0
23	A	348	CLA	14	0
23	A	349	CLA	5	0
23	A	350	CLA	10	0
24	A	351	PHO	6	0
23	A	352	CLA	1	0
26	A	353	PL9	8	0
23	B	511	CLA	5	0
23	B	512	CLA	7	0
23	B	513	CLA	7	0
23	B	514	CLA	4	0
23	B	515	CLA	8	0
23	B	516	CLA	8	0
23	B	517	CLA	3	0
23	B	518	CLA	16	0
23	B	519	CLA	7	0
23	B	520	CLA	10	0
23	B	521	CLA	9	0
23	B	522	CLA	12	0
23	B	523	CLA	7	0
23	B	524	CLA	22	0
23	B	525	CLA	7	0
23	B	527	CLA	5	0
28	B	528	BCR	3	0
28	B	529	BCR	13	0
23	C	474	CLA	11	0
23	C	475	CLA	5	0
23	C	476	CLA	4	0
23	C	477	CLA	8	0
23	C	478	CLA	6	0
23	C	479	CLA	13	0
23	C	480	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	481	CLA	4	0
23	C	482	CLA	6	0
23	C	483	CLA	11	0
23	C	484	CLA	1	0
23	C	485	CLA	10	0
23	C	486	CLA	18	0
23	C	487	CLA	17	0
28	C	488	BCR	12	0
28	C	489	BCR	11	0
23	D	354	CLA	10	0
24	D	355	PHO	8	0
23	D	356	CLA	8	0
26	D	357	PL9	5	0
25	E	84	HEM	16	0
28	F	48	BCR	3	0
28	J	53	BCR	2	0
28	K	50	BCR	13	0
25	V	138	HEM	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/344 (96%)	0.14	10 (3%) 54 43	33, 60, 91, 104	0
1	a	333/344 (96%)	-0.14	3 (0%) 85 78	39, 63, 92, 105	0
2	B	476/510 (93%)	-0.04	14 (2%) 55 45	39, 65, 89, 105	0
2	b	476/510 (93%)	-0.02	12 (2%) 61 50	39, 65, 89, 106	0
3	C	421/473 (89%)	-0.12	8 (1%) 70 60	34, 69, 89, 103	0
3	c	421/473 (89%)	-0.07	10 (2%) 62 52	36, 71, 90, 107	0
4	D	339/352 (96%)	-0.09	7 (2%) 67 58	22, 60, 92, 106	0
4	d	339/352 (96%)	-0.16	8 (2%) 62 52	31, 62, 92, 106	0
5	E	76/84 (90%)	-0.18	0 100 100	55, 76, 94, 107	0
5	e	76/84 (90%)	-0.13	3 (3%) 43 35	60, 79, 96, 107	0
6	F	33/45 (73%)	-0.42	0 100 100	49, 68, 92, 107	0
6	f	33/45 (73%)	-0.20	2 (6%) 25 19	49, 70, 92, 101	0
7	H	53/66 (80%)	-0.33	0 100 100	46, 73, 104, 106	0
7	h	53/66 (80%)	-0.29	3 (5%) 27 21	56, 74, 106, 109	0
8	I	38/38 (100%)	0.19	3 (7%) 15 13	60, 76, 100, 102	0
8	i	38/38 (100%)	-0.53	1 (2%) 59 49	59, 76, 100, 104	0
9	J	38/40 (95%)	-0.30	0 100 100	60, 79, 99, 103	0
9	j	38/40 (95%)	0.11	2 (5%) 30 23	61, 82, 98, 107	0
10	K	37/37 (100%)	-0.60	0 100 100	61, 71, 95, 95	0
10	k	37/37 (100%)	-0.25	0 100 100	65, 73, 96, 97	0
11	L	37/37 (100%)	-0.06	2 (5%) 29 23	39, 58, 101, 104	0
11	l	37/37 (100%)	0.14	1 (2%) 58 47	34, 61, 99, 101	0
12	M	30/36 (83%)	0.00	0 100 100	45, 56, 79, 88	0
12	m	30/36 (83%)	0.06	0 100 100	44, 56, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	246/246 (100%)	0.01	5 (2%) 68 59	41, 75, 100, 110	0
13	o	246/246 (100%)	0.21	16 (6%) 22 17	46, 75, 99, 107	0
14	T	31/32 (96%)	0.20	1 (3%) 51 42	27, 54, 86, 89	0
14	t	31/32 (96%)	-0.42	0 100 100	32, 53, 90, 93	0
15	U	105/134 (78%)	0.04	2 (1%) 70 60	41, 67, 91, 104	0
15	u	105/134 (78%)	-0.14	2 (1%) 70 60	46, 68, 92, 103	0
16	V	137/137 (100%)	-0.30	0 100 100	42, 66, 80, 88	0
16	v	137/137 (100%)	0.00	5 (3%) 46 37	46, 70, 85, 90	0
17	X	40/50 (80%)	-0.09	4 (10%) 9 9	67, 74, 102, 109	0
17	x	40/50 (80%)	0.21	3 (7%) 17 14	67, 77, 104, 108	0
18	N	0/37	-	-	-	-
18	n	0/37	-	-	-	-
19	Z	58/62 (93%)	-0.32	1 (1%) 73 64	62, 80, 93, 102	0
19	z	58/62 (93%)	0.31	7 (12%) 6 6	70, 81, 94, 106	0
All	All	5056/5520 (91%)	-0.06	135 (2%) 58 47	22, 68, 95, 110	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	2026	ASN	6.9
8	I	25	SER	6.6
1	A	264	SER	5.6
16	v	2100	ILE	5.4
4	D	242	GLU	5.0
8	I	28	PRO	4.4
2	B	233	ASN	4.3
13	O	62	GLU	4.2
5	e	2009	PHE	4.0
6	f	2013	PRO	4.0
1	A	263	ALA	3.9
17	X	47	GLN	3.9
15	u	2053	GLU	3.7
1	A	241	GLN	3.6
3	C	203	THR	3.5
4	d	2222	LEU	3.5
2	B	235	GLU	3.4
2	b	2341	LYS	3.4
2	b	2138	MET	3.3

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Mol	Chain	Res	Type	RSRZ
4	d	2255	GLN	3.3
2	B	232	GLY	3.3
13	O	99	ASP	3.3
15	u	2052	GLY	3.3
3	C	47	GLY	3.3
7	h	2014	ASN	3.3
19	z	2036	SER	3.2
4	D	96	GLU	3.2
2	b	2006	TYR	3.1
4	D	95	PRO	3.1
1	A	243	GLU	3.1
13	o	2134	THR	3.1
15	U	35	THR	3.1
5	e	2010	SER	3.1
6	f	2012	TYR	3.0
19	z	2003	ILE	3.0
13	o	2214	THR	3.0
3	c	2050	LEU	3.0
13	o	2044	CYS	2.9
13	o	2019	CYS	2.9
16	v	2105	ARG	2.9
4	d	2225	ASP	2.8
2	b	2343	HIS	2.8
4	D	241	GLU	2.8
3	C	269	GLU	2.8
2	B	266	GLU	2.7
16	v	2099	ASP	2.7
16	v	2106	ASN	2.7
1	a	2338	ASN	2.7
13	o	2001	ALA	2.7
3	c	2110	PRO	2.6
2	b	2163	GLY	2.6
13	o	2094	THR	2.6
13	o	2198	SER	2.6
17	x	2044	ASP	2.6
4	d	2223	PHE	2.6
9	j	2038	SER	2.6
2	b	2405	GLU	2.6
19	Z	30	PRO	2.6
19	z	2044	SER	2.5
3	c	2096	GLY	2.5
13	o	2200	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
19	z	2037	LYS	2.5
2	B	87	ASP	2.5
7	h	2021	ALA	2.5
2	B	198	VAL	2.5
19	z	2034	ASP	2.5
1	a	2305	SER	2.5
13	o	2017	ASN	2.5
15	U	38	GLU	2.5
19	z	2033	TRP	2.5
17	x	2041	SER	2.5
3	c	2373	ASN	2.4
4	D	239	GLN	2.4
4	d	2041	ALA	2.4
1	A	245	THR	2.4
14	T	31	LYS	2.4
3	C	273	SER	2.4
4	d	2014	TRP	2.4
3	C	293	ASN	2.4
2	b	2154	GLY	2.4
4	d	2224	GLN	2.4
13	O	246	ALA	2.4
13	o	2121	THR	2.4
19	z	2002	THR	2.4
2	b	2086	ILE	2.4
1	A	240	GLY	2.4
16	v	2095	LEU	2.4
2	B	78	TRP	2.4
4	D	225	ASP	2.4
3	c	2172	ALA	2.4
2	B	130	GLU	2.3
1	A	135	TYR	2.3
2	b	2344	ALA	2.3
13	o	2084	GLU	2.3
13	o	2099	ASP	2.3
3	C	456	GLU	2.3
2	b	2471	ALA	2.3
9	j	2040	LEU	2.3
13	o	2166	SER	2.3
11	l	2037	ASN	2.3
2	B	327	THR	2.3
3	c	2097	TRP	2.3
17	X	46	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	2404	GLY	2.3
5	e	2015	SER	2.3
1	A	222	SER	2.2
17	X	19	PHE	2.2
3	c	2168	LEU	2.2
17	x	2047	GLN	2.2
2	B	72	THR	2.2
2	B	122	LEU	2.2
4	D	240	ALA	2.2
2	B	471	ALA	2.2
8	I	26	GLY	2.2
2	B	119	ASP	2.2
11	L	11	GLU	2.2
4	d	2219	GLU	2.1
2	b	2393	GLU	2.1
8	i	2024	LEU	2.1
3	c	2138	GLU	2.1
13	o	2085	LEU	2.1
13	O	93	LEU	2.1
11	L	4	ASN	2.1
13	O	88	ASN	2.1
3	C	270	ALA	2.1
1	A	177	SER	2.0
2	B	15	ASP	2.0
3	c	2107	ASP	2.0
1	A	262	TYR	2.0
13	o	2045	LEU	2.0
3	c	2142	GLU	2.0
17	X	48	ARG	2.0
3	C	64	ALA	2.0
13	o	2034	SER	2.0
7	h	2013	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CLA	C	487	65/65	0.57	0.78	8.16	87,101,114,118	0
28	BCR	K	50	40/40	0.67	0.61	7.85	79,85,96,101	0
28	BCR	C	489	40/40	0.73	0.49	6.64	85,90,100,100	0
28	BCR	b	2527	40/40	0.74	0.44	5.49	64,78,84,86	0
28	BCR	k	2050	40/40	0.64	0.72	4.99	80,85,97,101	0
28	BCR	c	2488	40/40	0.76	0.71	4.88	76,84,93,96	0
28	BCR	B	528	40/40	0.73	0.41	4.47	63,79,85,87	0
26	PL9	D	357	45/55	0.75	0.42	4.32	71,80,86,88	0
28	BCR	F	48	40/40	0.76	0.37	3.80	66,80,91,92	0
23	CLA	c	2487	65/65	0.52	0.63	3.60	88,101,114,118	0
28	BCR	d	2360	40/40	0.75	0.39	3.35	67,79,91,93	0
28	BCR	C	488	40/40	0.83	0.42	3.28	75,83,92,95	0
23	CLA	b	2526	65/65	0.82	0.45	2.87	82,89,106,110	0
28	BCR	B	529	40/40	0.39	0.69	2.53	76,93,105,106	0
23	CLA	b	2517	65/65	0.89	0.47	2.48	64,71,80,89	0
23	CLA	C	481	65/65	0.87	0.36	2.47	54,60,84,88	0
27	LMT	d	2359	35/35	0.77	0.38	2.42	73,82,91,92	0
23	CLA	d	2355	65/65	0.90	0.40	2.35	19,32,75,86	0
23	CLA	B	516	65/65	0.84	0.37	2.34	44,55,92,93	0
23	CLA	c	2486	65/65	0.76	0.50	2.33	79,84,92,94	0
23	CLA	a	2349	65/65	0.87	0.33	2.06	36,54,93,95	0
23	CLA	b	2516	65/65	0.91	0.28	2.05	42,54,93,94	0
28	BCR	b	2528	40/40	0.62	0.57	2.03	77,92,105,106	0
26	PL9	d	2358	45/55	0.73	0.40	1.95	70,80,87,89	0
23	CLA	b	2521	65/65	0.85	0.39	1.85	67,71,80,82	0
28	BCR	c	2489	40/40	0.70	0.51	1.85	85,90,100,100	0
23	CLA	C	480	65/65	0.84	0.48	1.83	64,79,82,87	0
26	PL9	a	2352	45/55	0.68	0.45	1.81	77,85,90,91	0
23	CLA	B	527	65/65	0.79	0.43	1.80	84,89,106,109	0
23	CLA	C	475	65/65	0.86	0.38	1.79	66,80,97,103	0
23	CLA	c	2477	65/65	0.82	0.44	1.78	73,79,98,101	0
23	CLA	C	485	65/65	0.81	0.39	1.78	64,75,91,95	0
23	CLA	b	2519	65/65	0.90	0.43	1.76	60,66,90,91	0
23	CLA	B	518	65/65	0.91	0.39	1.75	51,61,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	c	2485	65/65	0.86	0.46	1.69	61,75,90,94	0
23	CLA	a	2348	65/65	0.93	0.32	1.62	44,50,65,69	0
23	CLA	A	352	65/65	0.79	0.36	1.59	48,65,101,102	0
25	HEM	V	138	43/43	0.95	0.27	1.58	44,49,56,57	0
23	CLA	B	511	65/65	0.88	0.41	1.48	58,81,92,97	0
27	LMT	B	526	35/35	0.83	0.39	1.43	72,82,90,91	0
23	CLA	B	524	65/65	0.88	0.54	1.36	56,68,75,88	0
25	HEM	e	2084	43/43	0.89	0.47	1.32	75,79,100,108	0
23	CLA	B	519	65/65	0.82	0.46	1.30	58,67,90,91	0
23	CLA	d	2354	65/65	0.94	0.29	1.29	40,47,75,80	0
23	CLA	c	2483	65/65	0.85	0.31	1.26	68,74,100,106	0
24	PHO	D	355	64/64	0.87	0.32	1.23	62,69,103,111	0
23	CLA	c	2475	65/65	0.85	0.33	1.23	66,80,97,102	0
23	CLA	C	482	65/65	0.79	0.42	1.22	71,80,97,98	0
23	CLA	C	476	65/65	0.85	0.33	1.18	49,62,75,78	0
23	CLA	a	2351	65/65	0.84	0.27	1.16	50,66,101,102	0
23	CLA	c	2478	65/65	0.91	0.50	1.11	55,66,87,92	0
23	CLA	C	483	65/65	0.70	0.42	1.11	67,73,101,106	0
23	CLA	b	2513	65/65	0.88	0.29	1.10	45,57,102,106	0
24	PHO	a	2350	64/64	0.82	0.35	1.07	56,66,81,82	0
26	PL9	A	353	45/55	0.62	0.57	1.04	77,86,91,92	0
23	CLA	b	2511	65/65	0.82	0.39	1.02	58,81,92,97	0
23	CLA	C	486	65/65	0.88	0.31	0.99	78,84,91,95	0
23	CLA	D	354	65/65	0.92	0.33	0.97	42,46,76,81	0
23	CLA	D	356	65/65	0.87	0.28	0.89	69,77,90,95	0
23	CLA	d	2357	65/65	0.80	0.37	0.88	68,77,91,95	0
23	CLA	b	2518	65/65	0.89	0.37	0.87	53,60,86,88	0
23	CLA	b	2514	65/65	0.87	0.38	0.85	59,67,79,82	0
24	PHO	d	2356	64/64	0.86	0.32	0.80	62,70,103,111	0
23	CLA	B	514	65/65	0.80	0.38	0.78	60,67,79,82	0
23	CLA	c	2479	65/65	0.89	0.44	0.76	57,76,80,84	0
23	CLA	C	479	65/65	0.91	0.33	0.75	57,76,80,83	0
23	CLA	B	517	65/65	0.89	0.40	0.75	65,71,79,89	0
23	CLA	b	2525	65/65	0.83	0.30	0.71	73,80,89,91	0
23	CLA	c	2480	65/65	0.87	0.39	0.70	65,80,82,87	0
23	CLA	b	2522	65/65	0.88	0.44	0.67	69,75,87,88	0
23	CLA	c	2476	65/65	0.85	0.28	0.64	50,64,75,78	0
23	CLA	B	513	65/65	0.93	0.37	0.63	46,57,102,106	0
23	CLA	c	2481	65/65	0.87	0.33	0.59	55,60,85,89	0
23	CLA	C	484	65/65	0.78	0.39	0.58	76,87,101,102	0
23	CLA	B	512	65/65	0.93	0.26	0.55	37,50,63,67	0
23	CLA	C	478	65/65	0.91	0.40	0.53	55,65,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	b	2524	65/65	0.88	0.44	0.52	56,68,76,89	0
25	HEM	E	84	43/43	0.95	0.31	0.47	64,79,100,108	0
23	CLA	c	2474	65/65	0.87	0.30	0.46	70,76,88,89	0
23	CLA	B	521	65/65	0.85	0.33	0.44	67,72,80,81	0
23	CLA	A	349	65/65	0.93	0.35	0.43	19,31,76,86	0
23	CLA	A	348	65/65	0.93	0.34	0.38	44,50,65,70	0
23	CLA	b	2512	65/65	0.91	0.26	0.24	34,50,63,66	0
23	CLA	C	477	65/65	0.84	0.31	0.08	71,79,97,100	0
25	HEM	v	2138	43/43	0.94	0.25	0.06	40,50,55,57	0
23	CLA	A	350	65/65	0.87	0.37	0.05	36,52,92,95	0
23	CLA	b	2520	65/65	0.85	0.31	0.05	61,68,78,79	0
23	CLA	B	523	65/65	0.88	0.29	-0.05	60,64,94,109	0
23	CLA	B	515	65/65	0.87	0.28	-0.05	45,66,84,87	0
23	CLA	B	522	65/65	0.90	0.27	-0.06	71,75,87,88	0
23	CLA	B	520	65/65	0.85	0.28	-0.06	63,68,79,79	0
24	PHO	A	351	64/64	0.91	0.26	-0.10	55,65,80,82	0
23	CLA	b	2523	65/65	0.88	0.27	-0.12	59,64,94,108	0
23	CLA	C	474	65/65	0.86	0.24	-0.14	69,76,87,89	0
23	CLA	B	525	65/65	0.87	0.27	-0.20	72,80,89,92	0
23	CLA	c	2482	65/65	0.86	0.40	-0.24	72,81,97,98	0
23	CLA	c	2484	65/65	0.81	0.32	-0.27	77,87,101,102	0
21	BCT	D	353	4/4	0.96	0.20	-0.34	66,66,69,69	0
23	CLA	b	2515	65/65	0.90	0.24	-0.54	43,66,84,87	0
21	BCT	a	2346	4/4	0.93	0.22	-0.92	71,72,73,76	0
21	BCT	A	346	4/4	0.97	0.18	-1.65	70,70,71,74	0
21	BCT	d	2353	4/4	0.97	0.13	-1.66	66,68,69,69	0
22	OEC	A	347	9/9	0.93	0.21	-1.92	66,69,73,74	0
20	FE	A	345	1/1	0.97	0.11	-2.05	58,58,58,58	0
22	OEC	a	2347	9/9	0.94	0.17	-2.15	68,70,74,75	0
20	FE	a	2345	1/1	0.91	0.10	-2.18	67,67,67,67	0
28	BCR	J	53	40/40	0.70	0.51	-	70,88,100,100	0
28	BCR	j	2053	40/40	0.73	0.51	-	71,87,100,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.