



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 10:34 PM EST

PDB ID : 5KAI
Title : NH3-bound RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 2.8 Å resolution
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Deposited on : 2016-06-01
Resolution : 2.80 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)

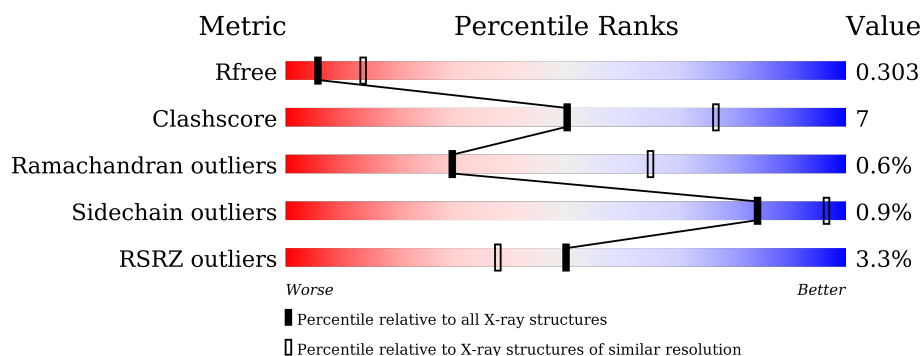
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 75%; height: 10px; background-color: green;"></div> <div style="width: 21%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 75% 21% .. </div> </div>
1	a	344	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 97%; height: 10px; background-color: green;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 97% . </div> </div>
2	B	510	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 2% <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 79% 20% . </div> </div>
2	b	510	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 5% <div style="width: 98%; height: 10px; background-color: green;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 98% . </div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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	LMG	A	603	-	-	-	X
23	LMG	B	621	-	-	-	X
23	LMG	C	501	-	-	-	X
23	LMG	C	521	-	-	-	X
23	LMG	D	409	-	-	-	X
23	LMG	b	626	-	-	-	X
23	LMG	b	627	-	-	-	X
23	LMG	c	519	-	-	-	X
23	LMG	c	520	-	-	-	X
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	707	X	-	-	-
25	CLA	a	708	X	-	-	-
25	CLA	a	711	X	-	-	-
25	CLA	a	719	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	619	X	-	-	-
25	CLA	b	620	X	-	-	-
25	CLA	b	621	X	-	-	-
25	CLA	b	622	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	X
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
27	BCR	D	405	-	-	-	X
27	BCR	t	103	-	-	-	X
28	PL9	A	611	-	-	-	X
28	PL9	a	713	-	-	-	X
29	SQD	B	623	-	-	-	X
29	SQD	B	626	-	-	-	X
29	SQD	I	102	-	-	-	X
29	SQD	b	601	-	-	-	X
30	UNL	b	604	-	-	-	X
30	UNL	b	605	-	-	-	X
30	UNL	b	606	-	-	-	X
30	UNL	t	101	-	-	-	X
30	UNL	t	102	-	-	-	X
30	UNL	z	101	-	-	-	X
32	LHG	D	407	-	-	-	X
32	LHG	E	101	-	-	-	X
32	LHG	e	101	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50284 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	1	0
			3968	2605	661	689	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			661	432	107	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	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 protein L.

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 protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			774	491	129	154				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

- 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 reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	38	Total	C	N	O		0	0	0
			279	187	45	47				

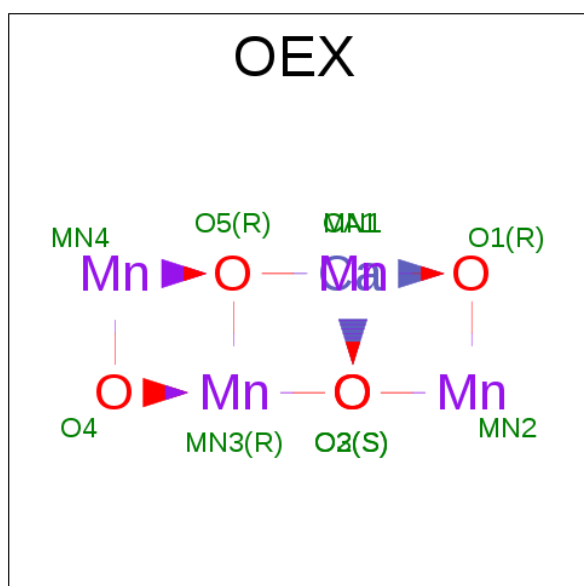
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			478	328	72	76	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O		0	0	0
			270	183	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

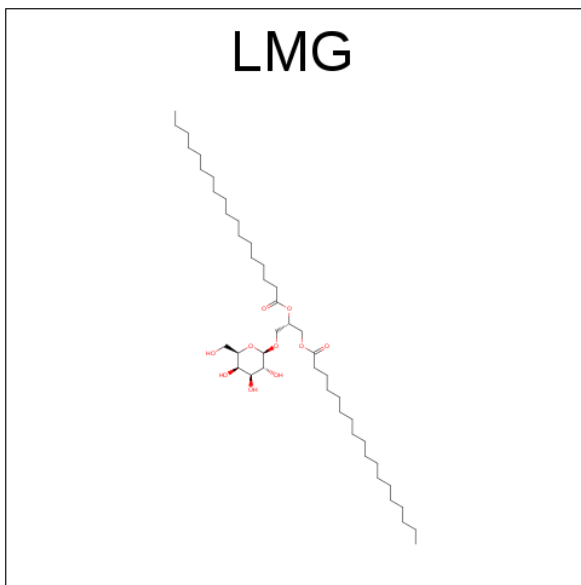
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Fe	0	0
			1	1		

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	M	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		

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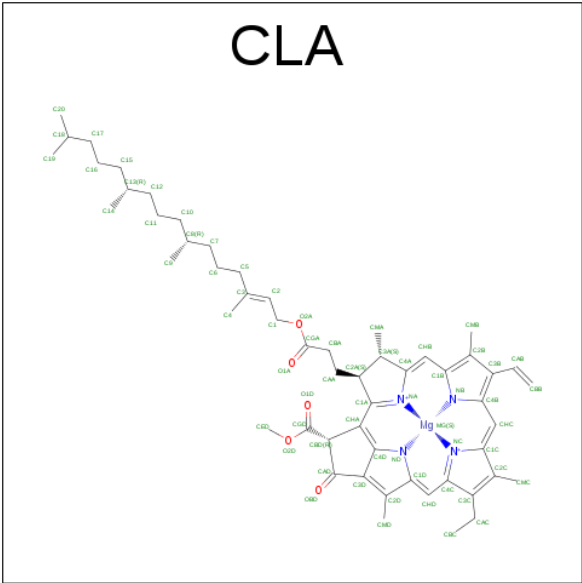
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	b	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C		0	0
			9	9			
23	c	1	Total	C	O	0	0
			51	41	10		
23	c	1	Total	C	O	0	0
			51	41	10		
23	d	1	Total	C	O	0	0
			40	35	5		
23	f	1	Total	C	O	0	0
			51	41	10		

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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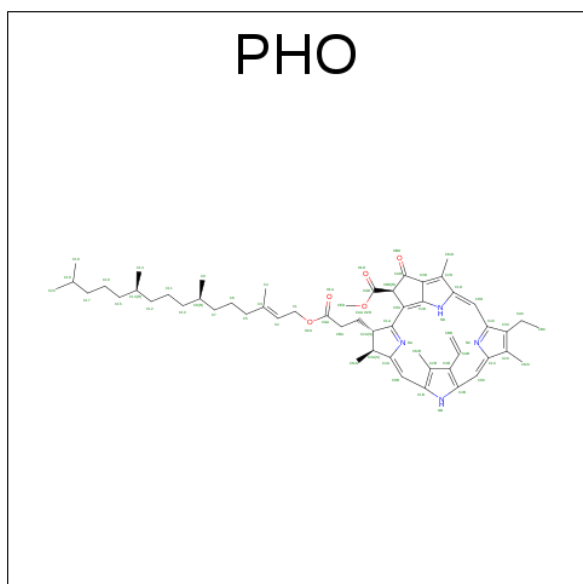
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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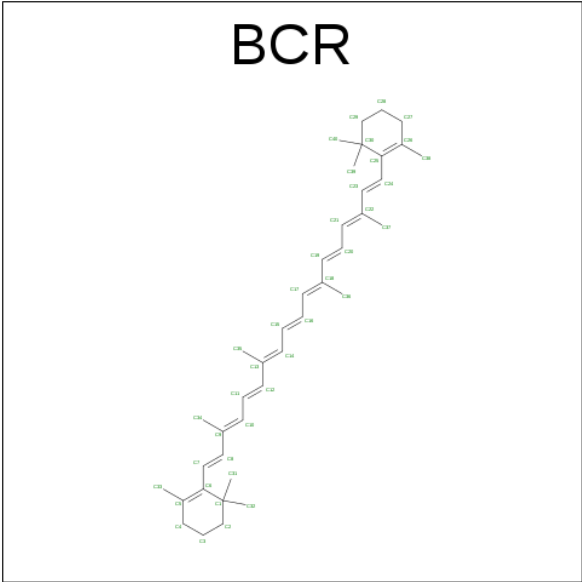
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



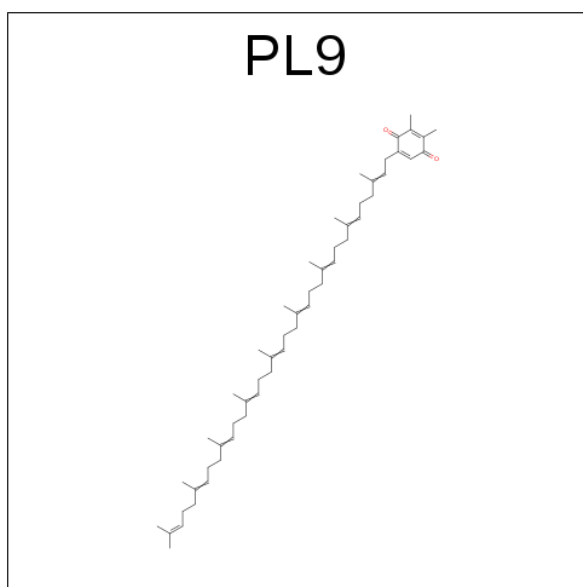
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- Molecule 28 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: $C_{53}H_{80}O_2$).



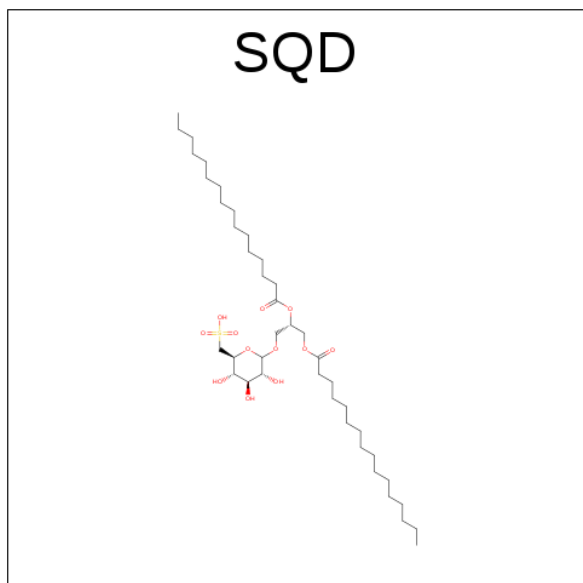
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).

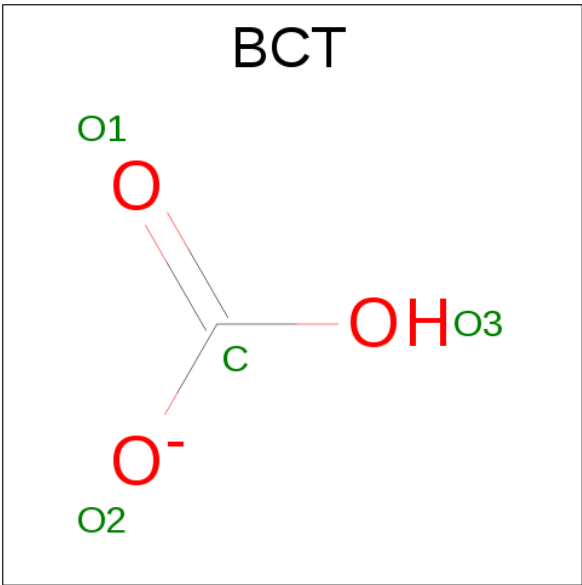


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			40	35	5			
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	I	1	Total	C	O		0	0
			40	35	5			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O	S	0	0
			54	41	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

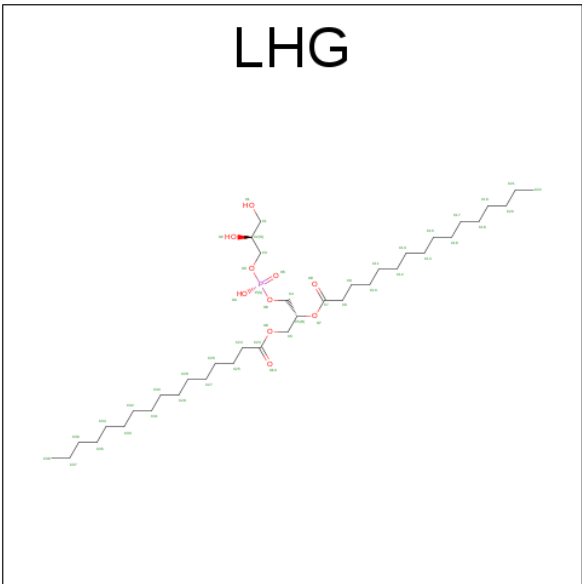
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	j	1	Total C 9 9	0	0
30	i	1	Total C 22 22	0	0
30	d	1	Total C 22 22	0	0
30	H	1	Total C 8 8	0	0
30	B	3	Total C 29 29	0	0
30	I	1	Total C 9 9	0	0
30	a	3	Total C 24 24	0	0
30	z	1	Total C 11 11	0	0
30	A	1	Total C 7 7	0	0
30	t	2	Total C 15 15	0	0
30	m	2	Total C 17 17	0	0
30	b	4	Total C 48 48	0	0
30	M	2	Total C 22 22	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



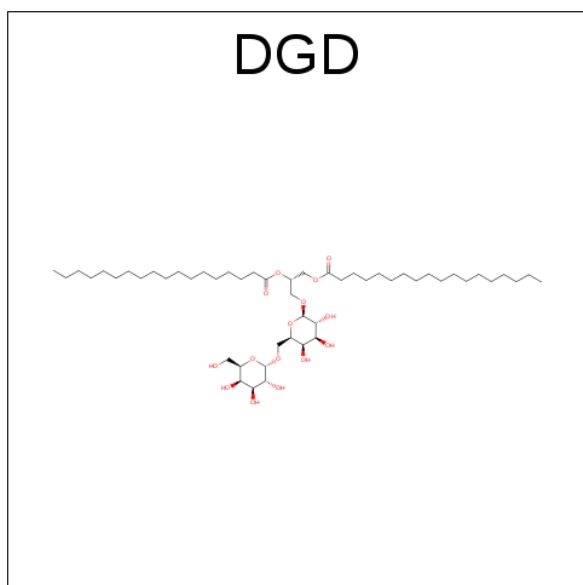
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			39	28	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



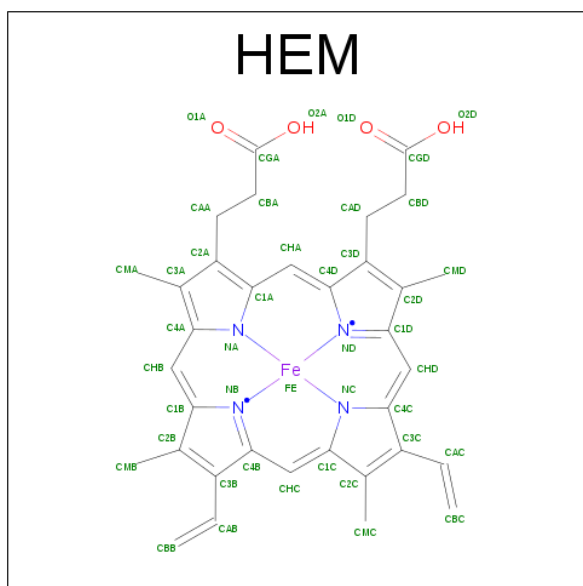
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	h	1	Total C O 62 47 15	0	0

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

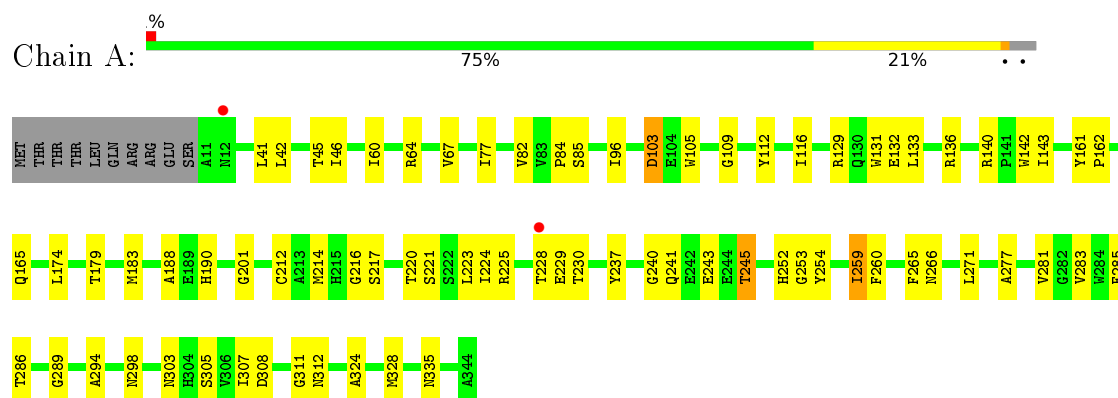
- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	14	Total O 14 14	0	0
35	B	5	Total O 5 5	0	0
35	C	2	Total O 2 2	0	0
35	D	5	Total O 5 5	0	0
35	H	1	Total O 1 1	0	0
35	K	1	Total O 1 1	0	0
35	L	1	Total O 1 1	0	0
35	M	1	Total O 1 1	0	0
35	O	9	Total O 9 9	0	0
35	U	1	Total O 1 1	0	0
35	V	6	Total O 6 6	0	0
35	a	13	Total O 13 13	0	0
35	b	12	Total O 12 12	0	0
35	c	8	Total O 8 8	0	0
35	d	11	Total O 11 11	0	0
35	e	1	Total O 1 1	0	0
35	h	1	Total O 1 1	0	0
35	l	1	Total O 1 1	0	0
35	o	5	Total O 5 5	0	0
35	u	5	Total O 5 5	0	0
35	v	3	Total O 3 3	0	0
35	z	1	Total O 1 1	0	0

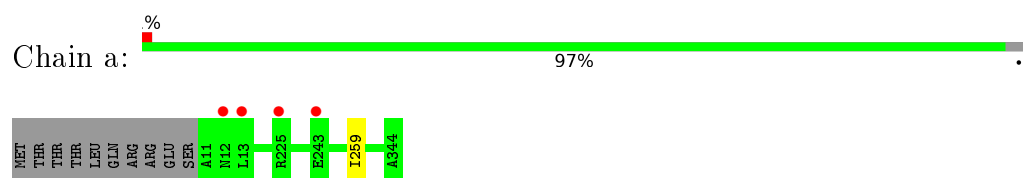
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

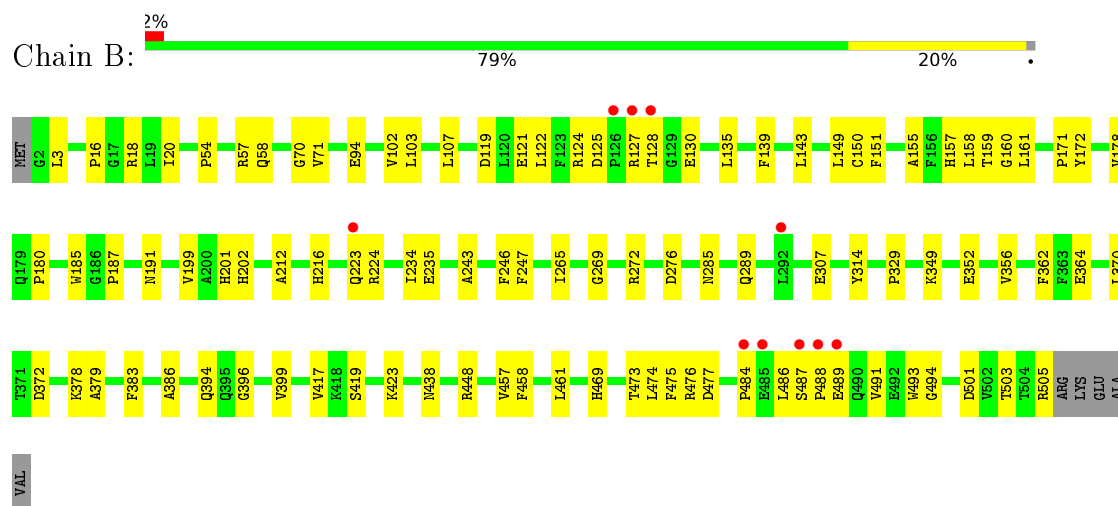
• Molecule 1: Photosystem II protein D1 1



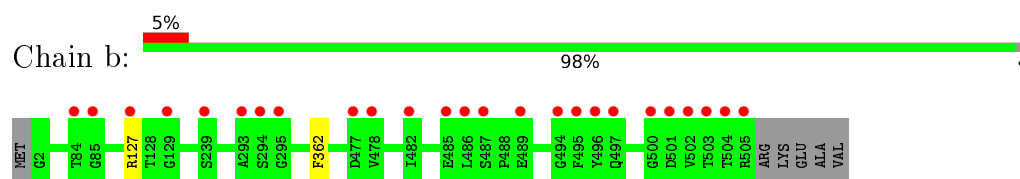
• Molecule 1: Photosystem II protein D1 1



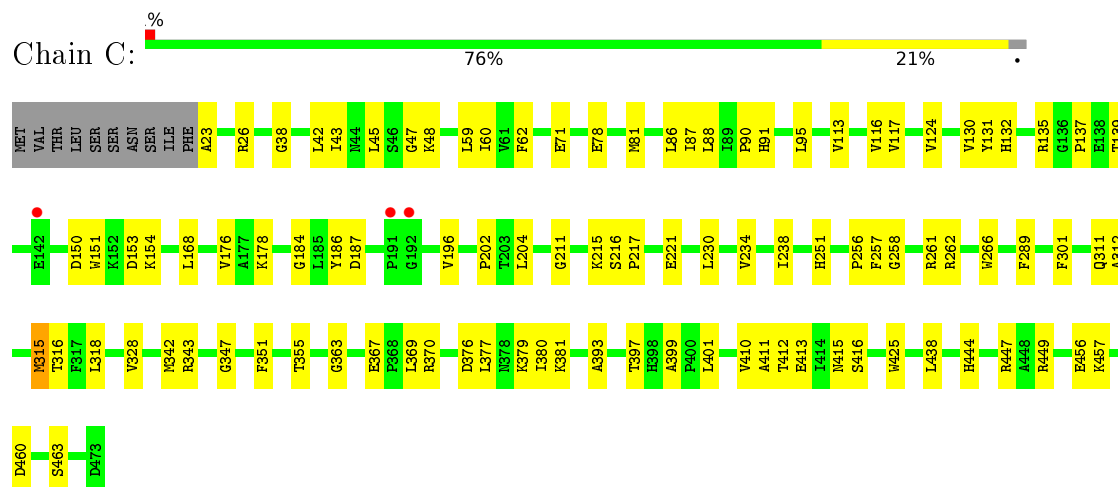
• Molecule 2: Photosystem II CP47 reaction center protein



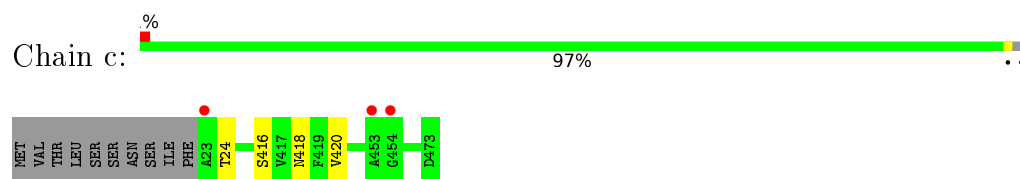
• Molecule 2: Photosystem II CP47 reaction center protein



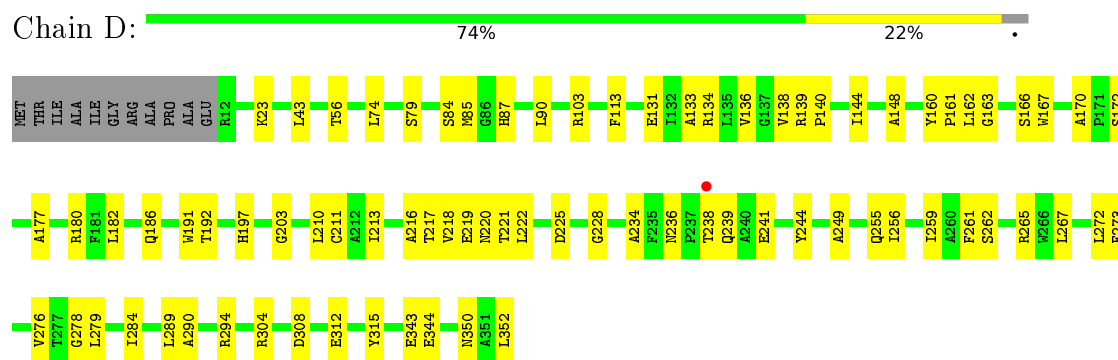
- Molecule 3: Photosystem II CP43 reaction center protein



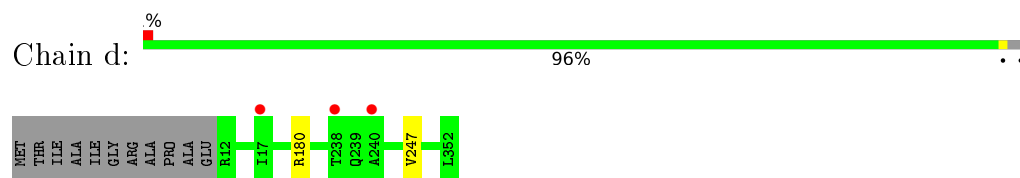
- Molecule 3: Photosystem II CP43 reaction center protein



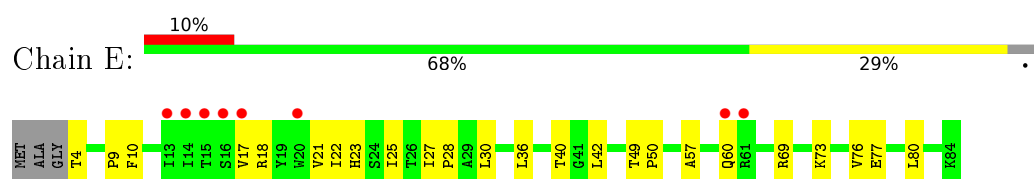
- Molecule 4: Photosystem II D2 protein



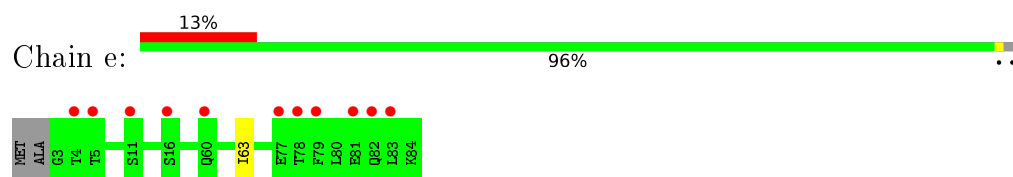
- Molecule 4: Photosystem II D2 protein



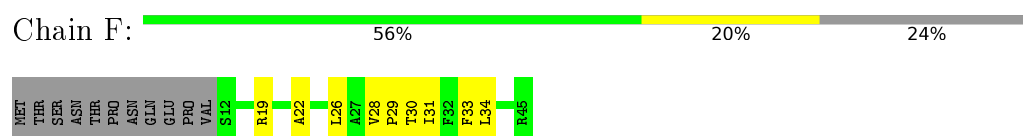
- Molecule 5: Cytochrome b559 subunit alpha



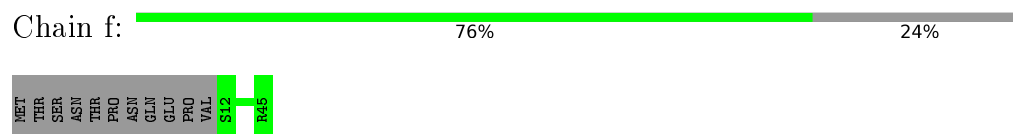
- Molecule 5: Cytochrome b559 subunit alpha



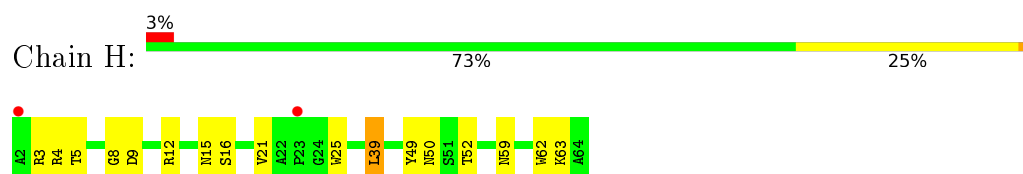
- Molecule 6: Cytochrome b559 subunit beta



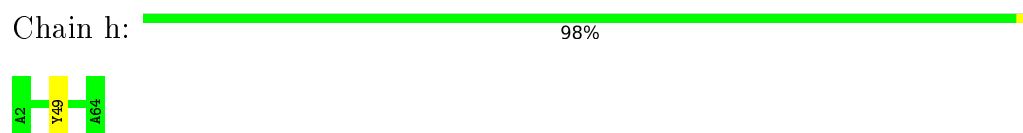
- Molecule 6: Cytochrome b559 subunit beta



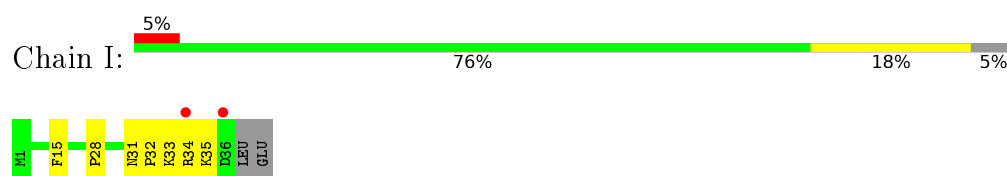
- Molecule 7: Photosystem II reaction center protein H



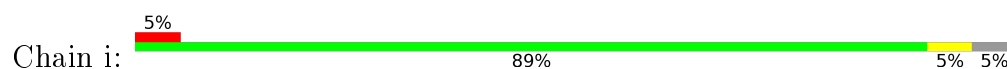
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

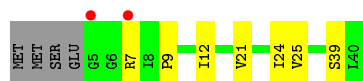


- Molecule 8: Photosystem II reaction center protein I

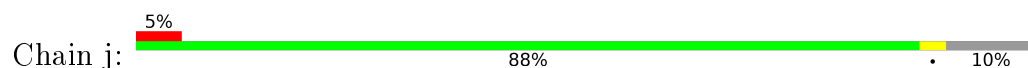




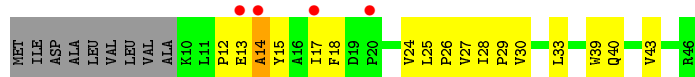
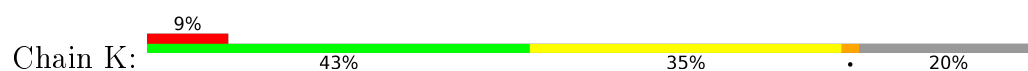
- Molecule 9: Photosystem II reaction center protein J



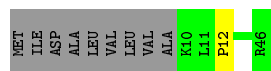
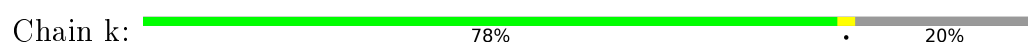
- Molecule 9: Photosystem II reaction center protein J



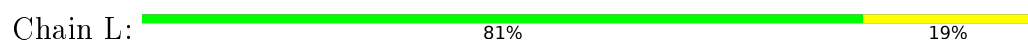
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

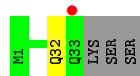
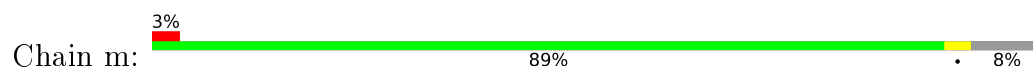


- Molecule 12: Photosystem II reaction center protein M

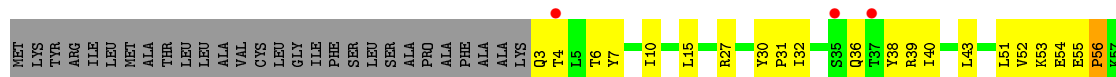




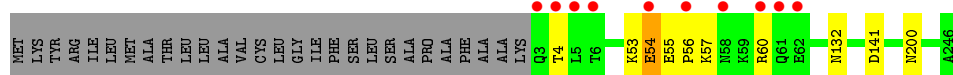
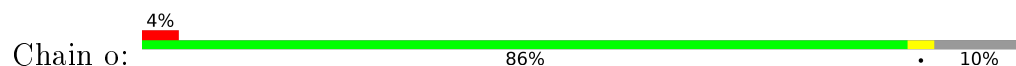
- Molecule 12: Photosystem II reaction center protein M



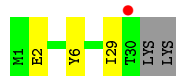
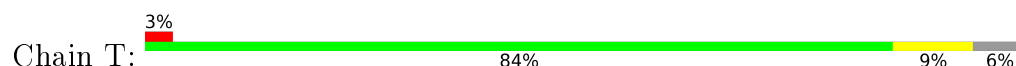
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



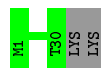
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

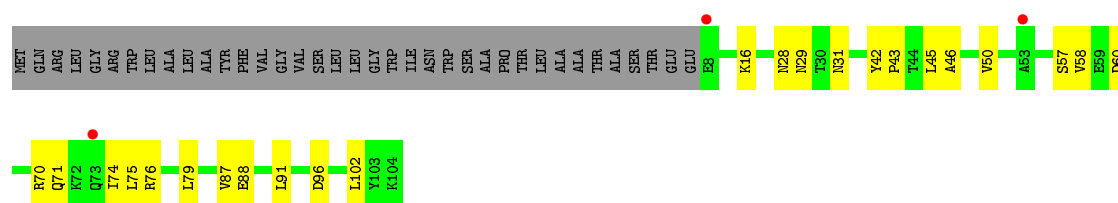


- Molecule 14: Photosystem II reaction center protein T



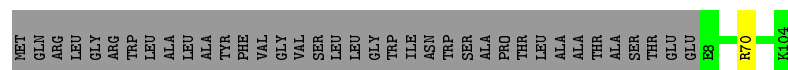
- Molecule 15: Photosystem II 12 kDa extrinsic protein





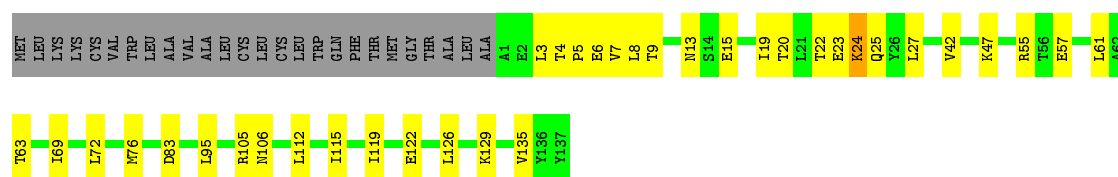
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 72% 28%



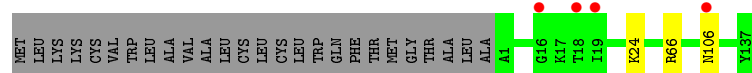
- Molecule 16: Cytochrome c-550

Chain V: 62% 21% 16%



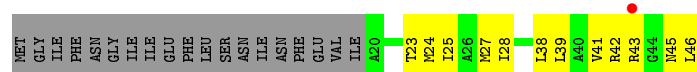
- Molecule 16: Cytochrome c-550

Chain v: 2% 82% 16%



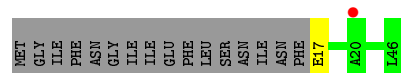
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 2% 33% 26% 41%



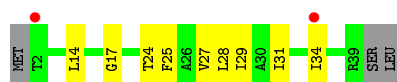
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 2% 63% 35%

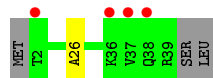
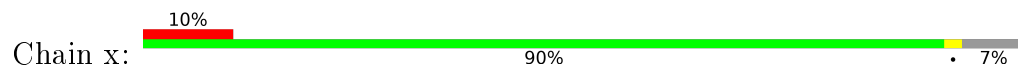


- Molecule 18: Photosystem II reaction center X protein

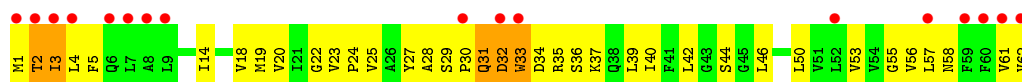
Chain X: 5% 71% 22% 7%



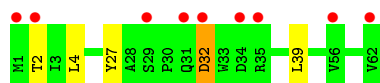
- Molecule 18: Photosystem II reaction center X protein



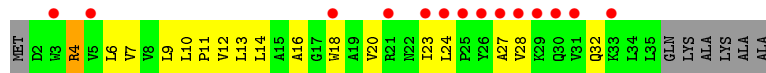
- Molecule 19: Photosystem II reaction center protein Z



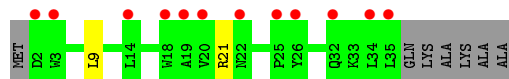
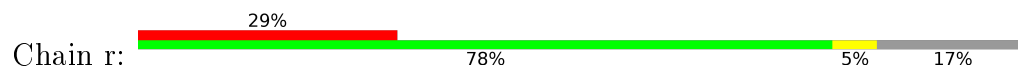
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.91Å 224.27Å 331.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 43.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.57-2.80) 87.7 (43.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_2411)	Depositor
R, R_{free}	0.250 , 0.300 0.253 , 0.303	Depositor DCC
R_{free} test set	1792 reflections (0.96%)	DCC
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50284	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, PHO, DGD, CL, CLA, PL9, LMG, FE2, BCT, HEM, FME, UNL, BCR, SQD

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	0.26	0/2707	0.42	0/3692
1	a	0.25	0/2707	0.40	0/3692
2	B	0.26	0/4109	0.41	0/5600
2	b	0.25	0/4111	0.41	0/5603
3	C	0.25	0/3599	0.40	0/4900
3	c	0.26	0/3599	0.43	0/4900
4	D	0.25	0/2811	0.40	0/3830
4	d	0.25	0/2811	0.40	0/3830
5	E	0.26	0/680	0.42	0/928
5	e	0.32	1/684 (0.1%)	0.40	0/933
6	F	0.25	0/284	0.40	0/387
6	f	0.24	0/284	0.36	0/387
7	H	0.27	0/511	0.44	0/697
7	h	0.24	0/511	0.41	0/697
8	I	0.26	0/293	0.40	0/396
8	i	0.56	1/293 (0.3%)	0.54	0/396
9	J	0.24	0/263	0.38	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.30	0/303	0.50	0/416
10	k	0.43	0/303	0.45	0/416
11	L	0.27	0/311	0.43	0/422
11	l	0.24	0/311	0.38	0/422
12	M	0.24	0/253	0.35	0/346
12	m	0.24	0/253	0.33	0/346
13	O	0.26	0/1905	0.46	0/2583
13	o	0.27	0/1905	0.52	1/2583 (0.0%)
14	T	0.27	0/257	0.36	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.24	0/785	0.43	0/1064
15	u	0.26	0/785	0.48	0/1064
16	V	0.23	0/1085	0.43	0/1473
16	v	0.23	0/1085	0.44	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.23	0/201	0.41	0/268
17	y	0.35	0/225	0.45	0/301
18	X	0.25	0/284	0.42	0/384
18	x	0.24	0/282	0.39	0/381
19	Z	0.30	0/490	0.51	0/669
19	z	0.35	0/489	0.52	0/669
20	R	0.27	0/279	0.52	0/383
20	r	0.25	0/276	0.51	0/379
All	All	0.26	2/42844 (0.0%)	0.42	1/58320 (0.0%)

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
13	o	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	CB-CG	-6.06	1.36	1.52
5	e	63	ILE	C-N	5.53	1.44	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	54	GLU	C-N-CA	5.75	136.08	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	4	THR	Peptide

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	2622	0	2519	70	0
1	a	2622	0	2519	0	0
2	B	3969	0	3828	92	0
2	b	3968	0	3829	0	0
3	C	3486	0	3407	82	0
3	c	3486	0	3407	0	0
4	D	2716	0	2621	68	0
4	d	2716	0	2621	0	0
5	E	661	0	648	27	0
5	e	665	0	651	0	0
6	F	275	0	282	9	0
6	f	275	0	282	0	0
7	H	498	0	518	18	0
7	h	498	0	518	0	0
8	I	296	0	311	7	0
8	i	296	0	311	0	0
9	J	257	0	268	4	0
9	j	257	0	268	0	0
10	K	293	0	305	12	0
10	k	293	0	305	0	0
11	L	304	0	316	7	0
11	l	304	0	316	0	0
12	M	260	0	275	6	0
12	m	260	0	275	0	0
13	O	1874	0	1846	63	0
13	o	1874	0	1846	0	0
14	T	258	0	261	3	0
14	t	258	0	261	0	0
15	U	774	0	773	18	0
15	u	774	0	773	0	0
16	V	1064	0	1073	32	0
16	v	1064	0	1073	0	0
17	Y	200	0	226	8	0
17	y	224	0	252	0	0
18	X	281	0	312	10	0
18	x	279	0	307	0	0
19	Z	479	0	516	38	0
19	z	478	0	516	0	0
20	R	273	0	305	24	0
20	r	270	0	296	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	51	0	72	2	0
23	B	51	0	72	1	0
23	C	153	0	216	1	0
23	D	51	0	72	3	0
23	M	51	0	72	3	0
23	a	102	0	144	0	0
23	b	111	0	158	0	0
23	c	102	0	144	0	0
23	d	40	0	61	0	0
23	f	51	0	72	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	184	0	192	4	0
25	B	1040	0	1152	59	0
25	C	845	0	936	48	0
25	D	195	0	216	12	0
25	a	260	0	288	0	0
25	b	1022	0	1115	0	0
25	c	838	0	919	0	0
25	d	130	0	144	0	0
26	A	64	0	74	2	0
26	D	64	0	74	3	0
26	a	128	0	148	0	0
27	A	40	0	56	4	0
27	B	120	0	168	4	0
27	C	80	0	112	5	0
27	D	40	0	56	4	0
27	H	40	0	56	3	0
27	K	40	0	56	3	0
27	Y	40	0	56	0	0
27	a	40	0	56	0	0
27	b	160	0	224	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	k	80	0	112	0	0
27	t	40	0	56	0	0
28	A	55	0	80	5	0
28	D	55	0	80	2	0
28	a	55	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	55	0	80	0	0
29	A	92	0	138	3	0
29	B	101	0	135	6	0
29	D	43	0	53	4	0
29	I	40	0	67	3	0
29	a	54	0	78	0	0
29	b	54	0	77	0	0
29	f	41	0	49	0	0
30	A	7	0	0	0	0
30	B	29	0	0	0	0
30	H	8	0	0	0	0
30	I	9	0	0	0	0
30	M	22	0	0	0	0
30	a	24	0	0	0	0
30	b	48	0	0	0	0
30	d	22	0	0	0	0
30	i	22	0	0	0	0
30	j	9	0	0	0	0
30	m	17	0	0	0	0
30	t	15	0	0	0	0
30	z	11	0	0	0	0
31	A	4	0	1	0	0
31	a	4	0	1	0	0
32	B	49	0	74	2	0
32	D	98	0	148	10	0
32	E	49	0	74	4	0
32	L	49	0	74	4	0
32	a	39	0	51	0	0
32	b	49	0	74	0	0
32	d	98	0	148	0	0
32	e	42	0	57	0	0
33	C	186	0	246	7	0
33	H	62	0	82	0	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	E	43	0	30	5	0
34	V	43	0	30	3	0
34	e	43	0	30	0	0
34	v	43	0	30	0	0
35	A	14	0	0	0	0
35	B	5	0	0	0	0
35	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	5	0	0	1	0
35	H	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	O	9	0	0	2	0
35	U	1	0	0	0	0
35	V	6	0	0	1	0
35	a	13	0	0	0	0
35	b	12	0	0	0	0
35	c	8	0	0	0	0
35	d	11	0	0	0	0
35	e	1	0	0	0	0
35	h	1	0	0	0	0
35	l	1	0	0	0	0
35	o	5	0	0	0	0
35	u	5	0	0	0	0
35	v	3	0	0	0	0
35	z	1	0	0	0	0
All	All	50284	0	51204	625	0

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 7.

All (625) 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)
7:H:4:ARG:NH2	7:H:9:ASP:OD2	1.66	1.23
13:O:54:GLU:HA	13:O:55:GLU:HB2	4.70	1.02
1:A:225:ARG:HD3	2:B:484:PRO:HD3	1.58	0.83
13:O:55:GLU:OE1	13:O:56:PRO:HD3	7.09	0.81
2:B:269:GLY:O	2:B:448:ARG:NH2	2.13	0.80
19:Z:36:SER:HA	19:Z:39:LEU:HD21	5.88	0.80
2:B:125:ASP:OD2	2:B:127:ARG:NH1	7.74	0.80
2:B:157:HIS:HE1	25:B:607:CLA:NA	1.81	0.78
19:Z:2:THR:N	19:Z:3:ILE:O	2.17	0.78
6:F:31:ILE:HA	6:F:34:LEU:HD23	1.65	0.77
2:B:18:ARG:NH2	29:B:626:SQD:O8	2.14	0.77
13:O:40:ILE:HD13	13:O:243:ILE:HD13	1.67	0.77
1:A:237:TYR:HB2	1:A:245:THR:HG21	1.66	0.76
34:E:102:HEM:HBC2	34:E:102:HEM:HHD	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:O	7:H:12:ARG:NH2	3.64	0.74
3:C:42:LEU:HD23	3:C:45:LEU:HD12	2.84	0.73
34:E:102:HEM:HHC	34:E:102:HEM:HBB2	4.74	0.73
2:B:155:ALA:O	2:B:159:THR:OG1	2.36	0.73
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.69	0.72
2:B:307:GLU:OE1	13:O:58:ASN:ND2	52.90	0.72
29:B:626:SQD:O10	11:L:14:ARG:NH2	29.72	0.72
5:E:27:ILE:HG23	5:E:28:PRO:HD3	1.71	0.72
25:C:504:CLA:H172	25:C:511:CLA:HBB2	1.73	0.71
4:D:236:ASN:H	4:D:239:GLN:HE22	4.19	0.70
1:A:240:GLY:HA3	14:T:29:ILE:HG23	2.95	0.70
2:B:349:LYS:HG2	2:B:396:GLY:HA3	1.73	0.70
2:B:187:PRO:HG3	25:B:602:CLA:HMD3	1.74	0.69
29:D:410:SQD:H252	18:X:31:ILE:HD13	1.72	0.69
13:O:83:GLY:HA2	13:O:98:GLU:HG3	5.15	0.69
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.93	0.69
3:C:26:ARG:NH2	17:Y:46:LEU:OXT	4.74	0.69
25:B:617:CLA:HMD1	7:H:5:THR:HG21	1.76	0.68
4:D:279:LEU:HD22	26:D:401:PHO:HBC3	1.76	0.68
4:D:192:THR:HG23	25:D:403:CLA:HBC2	1.76	0.68
2:B:157:HIS:HE1	25:B:612:CLA:NA	34.10	0.68
10:K:13:GLU:OE2	10:K:14:ALA:N	2.27	0.68
2:B:172:TYR:OH	7:H:63:LYS:NZ	4.13	0.67
25:C:509:CLA:H92	32:D:408:LHG:H371	1.75	0.67
7:H:5:THR:HG23	7:H:8:GLY:H	1.60	0.67
3:C:135:ARG:NH1	19:Z:27:TYR:CD2	7.21	0.67
3:C:116:VAL:HG21	27:C:515:BCR:H312	1.77	0.67
2:B:474:LEU:O	4:D:134:ARG:NH1	2.58	0.67
3:C:38:GLY:HA3	25:C:511:CLA:HMD3	15.96	0.67
12:M:24:ILE:HG23	12:M:27:VAL:HG21	6.97	0.66
3:C:425:TRP:CD1	25:C:505:CLA:H3A	2.31	0.66
19:Z:31:GLN:HG3	19:Z:32:ASP:HB2	6.39	0.66
1:A:142:TRP:CZ2	3:C:447:ARG:HG3	3.23	0.65
5:E:57:ALA:HB3	5:E:60:GLN:HB2	1.77	0.65
1:A:225:ARG:NH2	2:B:477:ASP:O	4.26	0.65
5:E:10:PHE:N	32:E:101:LHG:O4	2.29	0.65
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.93	0.65
32:D:408:LHG:H172	32:D:408:LHG:H352	1.79	0.64
32:D:408:LHG:H141	32:D:408:LHG:H372	1.79	0.64
3:C:60:ILE:HG23	25:C:510:CLA:HMC2	18.40	0.64
20:R:14:LEU:HD23	20:R:14:LEU:H	4.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:23:VAL:HG23	19:Z:27:TYR:CE1	7.48	0.63
16:V:24:LYS:H	16:V:24:LYS:HD2	2.40	0.63
1:A:217:SER:O	1:A:221:SER:OG	2.96	0.63
1:A:241:GLN:NE2	1:A:245:THR:HG23	2.12	0.63
13:O:53:LYS:NZ	13:O:55:GLU:OE2	7.73	0.63
3:C:410:VAL:HG13	3:C:412:THR:H	5.48	0.63
19:Z:19:MET:O	19:Z:23:VAL:HG12	4.94	0.63
2:B:150:CYS:HB2	25:B:609:CLA:HMC3	23.22	0.63
4:D:192:THR:HG23	25:D:402:CLA:HBC2	11.23	0.62
19:Z:24:PRO:HA	19:Z:27:TYR:HB2	2.70	0.62
3:C:38:GLY:HA3	25:C:512:CLA:HMD3	1.81	0.62
2:B:18:ARG:CZ	11:L:4:ASN:HD22	2.12	0.62
33:C:518:DGD:HO3D	33:C:519:DGD:HO5E	1.45	0.62
29:A:612:SQD:H251	32:D:408:LHG:H121	1.81	0.61
20:R:6:LEU:HD13	20:R:10:LEU:HD21	1.82	0.61
2:B:216:HIS:HE1	25:B:610:CLA:NA	1.97	0.61
16:V:55:ARG:NH1	16:V:57:GLU:OE1	5.99	0.61
3:C:137:PRO:HB2	3:C:139:THR:O	2.84	0.61
15:U:76:ARG:HA	15:U:79:LEU:HD23	2.05	0.61
29:B:626:SQD:O7	11:L:7:ARG:NH2	2.32	0.61
19:Z:32:ASP:O	19:Z:34:ASP:N	2.32	0.61
19:Z:19:MET:O	19:Z:22:GLY:N	3.39	0.61
13:O:87:VAL:HG22	13:O:93:LEU:HD22	2.32	0.61
20:R:16:ALA:O	20:R:20:VAL:HG23	2.01	0.61
19:Z:23:VAL:HG13	19:Z:24:PRO:HD3	4.52	0.61
3:C:154:LYS:HE3	3:C:261:ARG:HD2	1.83	0.60
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.83	0.60
13:O:54:GLU:CA	13:O:55:GLU:HB2	4.96	0.60
19:Z:3:ILE:O	19:Z:5:PHE:N	2.33	0.60
3:C:135:ARG:NH1	19:Z:27:TYR:CE2	7.94	0.60
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	3.42	0.60
5:E:77:GLU:HA	5:E:80:LEU:HD23	1.83	0.60
17:Y:42:ARG:NH1	19:Z:31:GLN:OE1	9.16	0.60
19:Z:39:LEU:H	19:Z:39:LEU:HD23	3.81	0.60
2:B:216:HIS:HE1	25:B:610:CLA:C1A	2.14	0.60
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	1.84	0.60
13:O:99:ASP:OD1	13:O:100:GLY:N	2.81	0.60
4:D:56:THR:HB	5:E:49:THR:HG23	2.02	0.60
8:I:28:PRO:O	8:I:31:ASN:ND2	2.84	0.60
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.35	0.59
13:O:84:GLU:OE2	13:O:86:LYS:NZ	4.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:105:ARG:NH2	35:V:301:HOH:O	2.35	0.59
4:D:163:GLY:HA3	4:D:290:ALA:HB1	1.84	0.59
16:V:5:PRO:HA	16:V:8:LEU:HD12	1.84	0.59
3:C:43:ILE:O	3:C:151:TRP:NE1	2.50	0.59
17:Y:39:LEU:HD21	19:Z:25:VAL:HG13	4.29	0.59
2:B:216:HIS:HE1	25:B:615:CLA:C1A	32.96	0.59
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.67	0.59
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.23	0.59
1:A:308:ASP:OD1	1:A:312:ASN:N	2.58	0.59
19:Z:25:VAL:O	19:Z:29:SER:OG	4.15	0.59
16:V:15:GLU:OE1	16:V:15:GLU:N	5.04	0.58
1:A:265:PHE:HB2	1:A:271:LEU:HD12	3.75	0.58
13:O:153:THR:HG22	13:O:154:ALA:H	1.68	0.58
1:A:143:ILE:HD11	4:D:217:THR:HA	2.50	0.58
25:B:617:CLA:H171	7:H:3:ARG:NH1	2.19	0.58
15:U:29:ASN:HD21	15:U:87:VAL:HA	1.67	0.58
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.08	0.58
1:A:243:GLU:OE1	1:A:243:GLU:N	2.83	0.58
13:O:158:ASP:OD1	13:O:162:ARG:N	2.34	0.58
2:B:103:LEU:HD21	25:B:611:CLA:HMC3	28.22	0.57
7:H:12:ARG:O	7:H:16:SER:OG	4.03	0.57
13:O:64:GLU:OE1	13:O:64:GLU:N	2.37	0.57
2:B:469:HIS:CE1	25:B:612:CLA:NA	2.72	0.57
3:C:311:GLN:NE2	3:C:355:THR:OG1	2.36	0.57
25:B:616:CLA:H2	25:B:617:CLA:HBB2	1.87	0.57
3:C:135:ARG:HH21	3:C:135:ARG:HG3	4.42	0.57
25:C:514:CLA:HMB1	25:C:514:CLA:HBB1	1.86	0.57
1:A:84:PRO:HA	1:A:112:TYR:CG	2.39	0.56
3:C:113:VAL:HA	3:C:116:VAL:HG22	1.87	0.56
1:A:253:GLY:HA2	2:B:493:TRP:CH2	2.40	0.56
2:B:185:TRP:HD1	23:B:621:LMG:HC2	1.69	0.56
25:D:403:CLA:HBB1	25:D:403:CLA:HMB1	3.03	0.56
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.77	0.56
25:C:512:CLA:HMB1	25:C:512:CLA:HBB1	1.93	0.56
19:Z:32:ASP:HB3	19:Z:35:ARG:HB3	8.48	0.56
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.88	0.56
17:Y:45:ASN:HB3	19:Z:28:ALA:HB1	1.87	0.56
3:C:87:ILE:HG13	3:C:88:LEU:HG	2.38	0.56
25:C:505:CLA:H51	33:C:519:DGD:HB62	1.86	0.56
13:O:27:ARG:NH2	13:O:202:ALA:O	6.63	0.56
1:A:303:ASN:O	3:C:415:ASN:ND2	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:HB2	25:B:610:CLA:HMC3	1.88	0.56
5:E:18:ARG:HH21	34:E:102:HEM:CGA	3.54	0.56
3:C:370:ARG:HD3	13:O:7:TYR:CE2	2.41	0.56
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.07	0.56
2:B:487:SER:O	2:B:489:GLU:N	2.35	0.56
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.87	0.56
25:D:404:CLA:H61	18:X:14:LEU:HD12	1.86	0.56
4:D:186:GLN:HB2	25:D:402:CLA:HBC1	11.94	0.55
25:B:617:CLA:HMB1	25:B:617:CLA:HBB1	1.88	0.55
5:E:76:VAL:O	5:E:80:LEU:HD22	2.05	0.55
25:B:607:CLA:H71	25:B:607:CLA:H12	6.84	0.55
27:B:618:BCR:H383	29:B:626:SQD:H91	1.88	0.55
2:B:102:VAL:HG23	25:B:612:CLA:H102	29.45	0.55
2:B:216:HIS:HE1	25:B:615:CLA:NA	32.23	0.55
25:B:602:CLA:HAC1	27:H:102:BCR:H383	1.88	0.55
25:B:612:CLA:HMB1	25:B:612:CLA:HBB1	1.88	0.55
3:C:204:LEU:HD22	3:C:238:ILE:HD11	5.31	0.55
1:A:131:TRP:CH2	25:C:506:CLA:HAA2	2.42	0.55
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.88	0.55
4:D:221:THR:HG21	4:D:249:ALA:HB2	1.89	0.55
34:E:102:HEM:HMB2	34:E:102:HEM:HBB2	1.88	0.55
6:F:26:LEU:O	6:F:30:THR:OG1	2.12	0.55
11:L:24:ILE:HD12	12:M:18:PRO:HG2	2.81	0.55
3:C:438:LEU:HD11	25:C:505:CLA:HBB1	20.99	0.55
2:B:457:VAL:HG13	4:D:284:ILE:HD12	4.70	0.55
13:O:40:ILE:HD13	13:O:243:ILE:HG22	5.28	0.55
1:A:64:ARG:O	13:O:152:ARG:NH1	2.64	0.55
13:O:201:VAL:HG12	13:O:239:PHE:HZ	5.06	0.55
25:B:617:CLA:OBD	7:H:5:THR:OG1	2.15	0.54
19:Z:2:THR:H	19:Z:3:ILE:C	2.09	0.54
19:Z:2:THR:HB	19:Z:3:ILE:HB	1.87	0.54
2:B:265:ILE:HA	2:B:448:ARG:HH22	1.72	0.54
25:C:509:CLA:H202	10:K:33:LEU:HD22	1.90	0.54
16:V:4:THR:HG23	16:V:6:GLU:H	1.72	0.54
2:B:150:CYS:HB2	25:B:604:CLA:HMC3	1.88	0.54
2:B:149:LEU:HD23	25:B:609:CLA:HBC1	21.16	0.54
10:K:25:LEU:HD22	27:K:101:BCR:H332	10.48	0.54
13:O:91:GLY:HA3	13:O:132:ASN:HA	2.06	0.54
16:V:4:THR:HG22	16:V:7:VAL:HG13	1.89	0.54
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.89	0.54
1:A:136:ARG:O	8:I:32:PRO:HG3	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.90	0.54
3:C:202:PRO:HB3	3:C:234:VAL:HG12	2.62	0.54
13:O:53:LYS:HE2	13:O:231:HIS:HA	5.50	0.54
16:V:24:LYS:N	16:V:24:LYS:HD2	2.21	0.54
4:D:304:ARG:NH1	35:D:502:HOH:O	18.13	0.54
25:B:614:CLA:H142	7:H:39:LEU:HD11	31.91	0.54
19:Z:19:MET:O	19:Z:23:VAL:N	2.94	0.54
1:A:183:MET:HA	25:A:606:CLA:HMD2	1.89	0.54
25:C:513:CLA:HMB1	25:C:513:CLA:HBB1	2.24	0.54
19:Z:23:VAL:CG2	19:Z:27:TYR:CE1	6.62	0.54
2:B:103:LEU:HB2	25:B:607:CLA:H62	1.90	0.54
1:A:214:MET:HB3	28:A:611:PL9:H103	1.90	0.53
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.90	0.53
4:D:304:ARG:NH2	4:D:308:ASP:OD2	2.41	0.53
13:O:124:ASN:HB2	13:O:147:ASN:HD22	2.69	0.53
18:X:31:ILE:HA	18:X:34:ILE:HG22	1.90	0.53
2:B:187:PRO:HB3	25:B:607:CLA:HMD3	30.64	0.53
2:B:476:ARG:HG3	2:B:477:ASP:N	3.98	0.53
34:V:201:HEM:HBB2	34:V:201:HEM:HMB2	1.89	0.53
1:A:241:GLN:HE22	1:A:245:THR:HG23	1.71	0.53
2:B:383:PHE:N	4:D:344:GLU:O	2.42	0.53
6:F:30:THR:HG22	6:F:34:LEU:HD21	1.90	0.53
15:U:31:ASN:ND2	15:U:96:ASP:O	3.09	0.53
20:R:24:LEU:HD12	20:R:27:ALA:HB3	1.90	0.53
16:V:122:GLU:HG3	16:V:126:LEU:HD12	2.88	0.53
3:C:377:LEU:HG	3:C:381:LYS:HE3	1.90	0.53
1:A:223:LEU:HD23	4:D:139:ARG:HH11	5.59	0.53
9:J:21:VAL:O	9:J:25:VAL:HG12	2.37	0.53
2:B:314:TYR:OH	13:O:176:GLN:NE2	2.42	0.52
29:A:612:SQD:H311	25:C:509:CLA:H71	1.90	0.52
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	40.92	0.52
2:B:372:ASP:HB3	2:B:378:LYS:HD2	2.41	0.52
2:B:364:GLU:OE1	4:D:294:ARG:NH2	2.95	0.52
1:A:41:LEU:O	1:A:45:THR:HG23	5.13	0.52
19:Z:50:LEU:HA	19:Z:53:VAL:HG12	1.90	0.52
1:A:237:TYR:CB	1:A:245:THR:HG21	2.39	0.52
3:C:413:GLU:OE2	16:V:47:LYS:NZ	3.50	0.52
5:E:25:ILE:HG21	20:R:18:TRP:CD1	5.47	0.52
13:O:10:ILE:HG23	13:O:15:LEU:HB2	2.96	0.52
25:C:512:CLA:H171	19:Z:20:VAL:HG22	1.92	0.52
2:B:370:LEU:HB2	2:B:379:ALA:HB3	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:21:VAL:HA	9:J:24:ILE:HG22	5.47	0.52
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.35	0.52
20:R:11:PRO:HA	20:R:14:LEU:HD21	5.65	0.52
4:D:312:GLU:HB2	13:O:159:PRO:HG3	1.92	0.52
20:R:23:ILE:O	20:R:27:ALA:N	2.86	0.52
1:A:224:ILE:O	4:D:265:ARG:NH2	2.42	0.52
3:C:312:ALA:O	3:C:316:THR:OG1	2.24	0.51
13:O:52:VAL:HG23	13:O:68:THR:HG21	2.55	0.51
25:D:403:CLA:H2	18:X:17:GLY:HA3	28.28	0.51
19:Z:23:VAL:O	19:Z:27:TYR:HD1	4.55	0.51
5:E:30:LEU:CD2	20:R:12:VAL:HG22	2.40	0.51
4:D:85:MET:HE2	4:D:90:LEU:HD21	2.21	0.51
5:E:42:LEU:HD12	20:R:4:ARG:HB2	4.31	0.51
15:U:88:GLU:HG3	15:U:91:LEU:HD23	5.05	0.51
25:C:506:CLA:H43	27:C:516:BCR:HC7	1.91	0.51
3:C:178:LYS:NZ	3:C:184:GLY:O	2.53	0.51
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.93	0.51
2:B:469:HIS:HE1	25:B:617:CLA:NA	26.40	0.51
25:C:509:CLA:H193	33:C:518:DGD:HAW2	1.93	0.51
16:V:4:THR:O	16:V:7:VAL:HG22	2.11	0.51
3:C:135:ARG:NH2	19:Z:27:TYR:O	5.38	0.51
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.02	0.51
27:D:405:BCR:H383	23:D:409:LMG:H161	1.92	0.51
6:F:30:THR:O	6:F:33:PHE:N	2.44	0.51
15:U:29:ASN:ND2	15:U:88:GLU:H	2.09	0.51
16:V:122:GLU:HG3	16:V:126:LEU:CD1	3.39	0.51
10:K:27:VAL:O	10:K:30:VAL:HG12	2.11	0.50
4:D:236:ASN:HB3	4:D:239:GLN:NE2	5.71	0.50
3:C:131:TYR:HA	19:Z:27:TYR:HE2	2.82	0.50
2:B:128:THR:OG1	2:B:130:GLU:OE1	6.01	0.50
3:C:87:ILE:O	3:C:91:HIS:ND1	2.64	0.50
15:U:71:GLN:O	15:U:75:LEU:HD12	2.11	0.50
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.92	0.50
28:A:611:PL9:H221	26:D:401:PHO:HMA2	1.93	0.50
2:B:201:HIS:HB2	25:B:608:CLA:C1B	26.99	0.50
1:A:142:TRP:HZ2	3:C:447:ARG:HG3	2.60	0.50
4:D:262:SER:OG	32:D:407:LHG:O4	2.96	0.50
13:O:58:ASN:O	13:O:60:ARG:N	2.44	0.50
13:O:38:TYR:OH	35:O:301:HOH:O	2.19	0.50
25:A:607:CLA:HMD3	4:D:182:LEU:HD11	1.93	0.50
13:O:210:GLU:OE1	13:O:240:TYR:OH	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:55:GLU:HB3	13:O:56:PRO:CD	4.17	0.50
1:A:201:GLY:HA3	1:A:286:THR:HB	1.93	0.49
10:K:14:ALA:HB1	19:Z:5:PHE:CE2	2.81	0.49
2:B:185:TRP:HB3	25:B:602:CLA:HMA3	1.93	0.49
3:C:176:VAL:HG23	3:C:234:VAL:HG13	4.03	0.49
29:A:614:SQD:H101	2:B:94:GLU:HG2	56.42	0.49
2:B:155:ALA:O	2:B:161:LEU:HD12	5.96	0.49
3:C:444:HIS:CE1	25:C:509:CLA:NA	2.80	0.49
7:H:50:ASN:OD1	7:H:52:THR:OG1	2.25	0.49
25:B:612:CLA:H142	32:L:101:LHG:H361	1.93	0.49
16:V:13:ASN:CG	16:V:15:GLU:OE1	5.08	0.49
28:A:611:PL9:H403	6:F:22:ALA:HB2	1.94	0.49
3:C:38:GLY:HA3	25:C:511:CLA:CMD	15.26	0.49
25:D:402:CLA:HED1	28:D:406:PL9:H371	1.95	0.49
4:D:222:LEU:HA	4:D:244:TYR:HA	2.36	0.49
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.95	0.49
1:A:64:ARG:NH1	13:O:105:PRO:O	2.44	0.49
5:E:23:HIS:O	5:E:27:ILE:HG22	2.11	0.49
18:X:25:PHE:O	18:X:28:LEU:N	3.40	0.49
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.95	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.94	0.49
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.48	0.49
8:I:31:ASN:O	8:I:35:LYS:NZ	5.59	0.49
19:Z:23:VAL:HG23	19:Z:27:TYR:HE1	7.83	0.49
16:V:23:GLU:HG2	16:V:24:LYS:NZ	2.27	0.49
4:D:259:ILE:HD13	32:D:407:LHG:H262	2.21	0.49
5:E:25:ILE:HD11	20:R:18:TRP:CD1	2.48	0.48
15:U:76:ARG:HA	15:U:79:LEU:CD2	2.86	0.48
2:B:356:VAL:HG22	2:B:370:LEU:HD22	3.98	0.48
2:B:121:GLU:O	7:H:12:ARG:NH2	2.46	0.48
13:O:30:TYR:CD2	13:O:243:ILE:HD11	6.17	0.48
25:B:614:CLA:H192	32:B:625:LHG:H223	1.95	0.48
3:C:47:GLY:HA3	3:C:137:PRO:O	2.29	0.48
4:D:236:ASN:N	4:D:239:GLN:HE22	4.91	0.48
3:C:216:SER:HB3	3:C:221:GLU:HG3	4.13	0.48
16:V:19:ILE:HG21	16:V:69:ILE:HG13	1.95	0.48
2:B:139:PHE:CZ	2:B:143:LEU:HD12	2.48	0.48
2:B:352:GLU:OE2	2:B:378:LYS:NZ	2.35	0.48
3:C:425:TRP:CD1	25:C:504:CLA:H3A	20.47	0.48
10:K:12:PRO:CB	10:K:15:TYR:HD2	3.68	0.48
16:V:13:ASN:OD1	16:V:15:GLU:OE1	5.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:72:LEU:O	16:V:76:MET:HG3	2.78	0.48
25:C:509:CLA:HMB3	25:C:510:CLA:HAA1	7.58	0.48
4:D:166:SER:OG	4:D:167:TRP:N	3.49	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.48
5:E:40:THR:HB	20:R:4:ARG:HG2	1.95	0.48
19:Z:14:ILE:O	19:Z:18:VAL:HG13	5.72	0.48
25:B:612:CLA:H93	25:B:612:CLA:H112	4.12	0.48
5:E:9:PRO:HB3	32:E:101:LHG:HC31	1.95	0.48
11:L:22:LEU:O	11:L:26:VAL:HG13	2.14	0.48
2:B:307:GLU:CD	13:O:58:ASN:HD21	53.20	0.48
16:V:57:GLU:O	16:V:61:LEU:HD12	3.67	0.48
1:A:132:GLU:O	1:A:136:ARG:HG2	2.24	0.47
1:A:277:ALA:O	1:A:281:VAL:HG12	5.04	0.47
2:B:501:ASP:OD1	2:B:503:THR:OG1	2.32	0.47
25:C:508:CLA:HBC3	25:C:510:CLA:H92	14.25	0.47
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.11	0.47
3:C:217:PRO:HB2	33:C:517:DGD:HA32	1.96	0.47
3:C:399:ALA:O	3:C:401:LEU:N	2.56	0.47
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.96	0.47
3:C:23:ALA:O	3:C:26:ARG:N	6.66	0.47
15:U:46:ALA:O	15:U:50:VAL:HG22	4.45	0.47
16:V:23:GLU:O	16:V:27:LEU:HG	2.56	0.47
13:O:96:VAL:HG13	13:O:126:VAL:HG22	1.95	0.47
1:A:42:LEU:HD13	27:A:610:BCR:H353	1.96	0.47
3:C:176:VAL:HG11	3:C:238:ILE:HG22	5.89	0.47
3:C:376:ASP:HB3	3:C:379:LYS:HB2	1.95	0.47
1:A:140:ARG:NE	4:D:219:GLU:O	2.46	0.47
1:A:283:VAL:HA	1:A:286:THR:HG22	1.96	0.47
25:B:605:CLA:H121	25:B:616:CLA:H42	1.96	0.47
15:U:70:ARG:O	15:U:74:ILE:HG13	2.15	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.52	0.47
3:C:59:LEU:HD13	25:C:511:CLA:HMD2	1.96	0.47
3:C:460:ASP:OD1	3:C:463:SER:OG	6.65	0.47
5:E:27:ILE:CG2	5:E:28:PRO:HD3	2.43	0.47
20:R:24:LEU:HD22	20:R:24:LEU:H	4.69	0.47
13:O:40:ILE:CD1	13:O:243:ILE:HD13	2.42	0.47
19:Z:58:ASN:O	19:Z:62:VAL:HG23	2.53	0.47
25:C:507:CLA:H162	25:C:507:CLA:H141	1.64	0.46
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.98	0.46
1:A:254:TYR:HE1	4:D:133:ALA:HB2	1.81	0.46
1:A:67:VAL:HG22	4:D:312:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:31:PRO:O	35:O:301:HOH:O	2.20	0.46
1:A:230:THR:O	2:B:3:LEU:HD23	2.52	0.46
1:A:190:HIS:O	1:A:298:ASN:HB3	2.25	0.46
3:C:318:LEU:HD21	3:C:328:VAL:HG21	1.97	0.46
7:H:5:THR:CG2	7:H:8:GLY:H	2.26	0.46
3:C:113:VAL:O	3:C:117:VAL:HG23	3.94	0.46
3:C:130:VAL:HG21	25:C:511:CLA:H161	18.58	0.46
2:B:191:ASN:ND2	7:H:59:ASN:O	2.47	0.46
15:U:28:ASN:HB3	15:U:87:VAL:HG22	2.04	0.46
25:B:609:CLA:HAB	25:B:611:CLA:H151	23.86	0.46
8:I:31:ASN:OD1	8:I:33:LYS:HB2	3.75	0.46
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.96	0.46
18:X:24:THR:O	18:X:28:LEU:HD12	3.21	0.46
25:B:607:CLA:H141	25:B:607:CLA:H161	4.69	0.46
3:C:444:HIS:CE1	25:C:508:CLA:NA	15.04	0.46
13:O:6:THR:OG1	13:O:7:TYR:N	2.51	0.46
25:B:606:CLA:H92	25:B:606:CLA:H62	1.76	0.46
25:B:613:CLA:HBB1	25:B:613:CLA:HMB1	1.97	0.46
27:B:620:BCR:H20C	27:B:620:BCR:H361	1.81	0.46
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.97	0.46
19:Z:56:VAL:HG23	19:Z:57:LEU:HD12	1.97	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.97	0.46
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.97	0.46
27:A:610:BCR:H371	27:A:610:BCR:H24C	1.79	0.46
25:B:605:CLA:H161	25:B:605:CLA:H141	1.62	0.46
8:I:33:LYS:HB3	8:I:34:ARG:H	2.47	0.46
2:B:119:ASP:OD1	2:B:124:ARG:NH2	2.49	0.45
2:B:487:SER:C	2:B:489:GLU:H	2.19	0.45
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.98	0.45
3:C:393:ALA:O	3:C:397:THR:HG23	2.75	0.45
13:O:53:LYS:NZ	13:O:231:HIS:HA	7.14	0.45
23:A:603:LMG:H342	23:A:603:LMG:H312	1.69	0.45
25:B:615:CLA:H61	25:B:615:CLA:H41	1.67	0.45
3:C:410:VAL:HG22	3:C:411:ALA:H	4.39	0.45
3:C:81:MET:HB3	3:C:86:LEU:HD12	2.43	0.45
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.98	0.45
25:C:503:CLA:H62	25:C:503:CLA:H101	3.55	0.45
27:C:516:BCR:H15C	27:C:516:BCR:H351	1.84	0.45
4:D:261:PHE:CG	4:D:267:LEU:HD12	2.52	0.45
1:A:60:ILE:HD12	1:A:84:PRO:HD2	3.45	0.45
3:C:116:VAL:HG23	3:C:117:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:95:PHE:O	13:O:126:VAL:HA	2.34	0.45
2:B:329:PRO:HD3	23:M:101:LMG:HC61	1.99	0.45
3:C:256:PRO:HA	25:C:507:CLA:HED2	1.98	0.45
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.03	0.45
27:H:102:BCR:H24C	27:H:102:BCR:H371	1.74	0.45
1:A:174:LEU:HD22	26:A:608:PHO:H151	1.98	0.45
13:O:53:LYS:HZ1	13:O:231:HIS:HA	7.62	0.45
3:C:370:ARG:HD3	13:O:7:TYR:CD2	2.52	0.45
13:O:40:ILE:HG13	13:O:95:PHE:CD1	3.28	0.45
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.87	0.45
13:O:53:LYS:CE	13:O:231:HIS:HA	6.46	0.45
3:C:363:GLY:O	3:C:367:GLU:HG2	2.18	0.45
25:C:509:CLA:H192	25:C:512:CLA:HAC1	13.05	0.45
10:K:17:ILE:HG23	10:K:18:PHE:CD1	6.19	0.45
1:A:131:TRP:HZ2	3:C:449:ARG:HD2	1.81	0.45
25:B:607:CLA:H72	25:B:607:CLA:C4D	11.64	0.45
32:E:101:LHG:H302	32:E:101:LHG:H271	4.43	0.45
2:B:235:GLU:HB3	2:B:473:THR:HG22	1.99	0.45
4:D:136:VAL:HG23	4:D:138:VAL:HG13	6.01	0.45
16:V:4:THR:HG23	16:V:6:GLU:N	2.32	0.45
3:C:90:PRO:HB3	3:C:301:PHE:HB3	2.20	0.44
1:A:217:SER:HA	4:D:272:LEU:HD12	2.10	0.44
20:R:24:LEU:O	20:R:28:VAL:HG12	2.17	0.44
15:U:29:ASN:HD21	15:U:88:GLU:H	1.65	0.44
18:X:24:THR:O	18:X:27:VAL:HG22	5.82	0.44
29:B:626:SQD:H202	29:B:626:SQD:H171	1.74	0.44
5:E:17:VAL:O	5:E:21:VAL:HG23	2.16	0.44
16:V:13:ASN:N	16:V:13:ASN:OD1	2.78	0.44
17:Y:23:THR:O	17:Y:27:MET:HG3	2.24	0.44
1:A:253:GLY:HA3	2:B:491:VAL:CG1	2.47	0.44
2:B:122:LEU:O	7:H:15:ASN:ND2	2.50	0.44
12:M:8:LEU:HG	12:M:9:ILE:HD12	6.45	0.44
13:O:30:TYR:CE2	13:O:243:ILE:HD11	6.20	0.44
3:C:78:GLU:HG2	16:V:106:ASN:HD21	1.83	0.44
18:X:25:PHE:O	18:X:27:VAL:N	3.27	0.44
25:A:607:CLA:H193	23:D:409:LMG:H401	1.99	0.44
2:B:285:ASN:O	2:B:289:GLN:HG2	2.18	0.44
3:C:257:PHE:O	3:C:261:ARG:HG3	2.19	0.44
33:C:518:DGD:HA62	4:D:74:LEU:HD21	11.73	0.44
25:B:602:CLA:H91	25:B:602:CLA:H111	1.74	0.44
25:B:610:CLA:H91	25:B:610:CLA:H112	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:343:ARG:NH1	3:C:347:GLY:O	2.51	0.44
3:C:369:LEU:HD22	3:C:380:ILE:HD13	5.27	0.44
8:I:15:PHE:CZ	29:I:102:SQD:H381	2.53	0.44
20:R:28:VAL:O	20:R:32:GLN:HG2	4.16	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
1:A:165:GLN:NE2	1:A:294:ALA:O	3.09	0.44
3:C:256:PRO:HA	25:C:506:CLA:HED2	17.32	0.44
3:C:42:LEU:HD22	3:C:48:LYS:HB3	2.40	0.44
25:C:510:CLA:HBB1	25:C:510:CLA:HMB1	2.44	0.44
11:L:10:VAL:O	12:M:28:GLN:NE2	2.47	0.44
12:M:17:VAL:HG21	23:M:101:LMG:H401	1.99	0.44
20:R:10:LEU:HA	20:R:13:LEU:HD23	5.14	0.44
15:U:16:LYS:HE3	15:U:88:GLU:HB2	2.00	0.44
1:A:85:SER:HA	1:A:109:GLY:HA3	2.21	0.44
2:B:223:GLN:HE21	2:B:224:ARG:HG2	6.37	0.44
25:C:512:CLA:H142	25:C:512:CLA:H111	4.69	0.44
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.69	0.44
4:D:225:ASP:HB2	4:D:234:ALA:HB1	2.00	0.44
25:D:403:CLA:H143	25:D:403:CLA:H162	3.30	0.44
27:K:101:BCR:H361	27:K:101:BCR:H20C	1.83	0.44
13:O:53:LYS:HD3	13:O:232:GLU:H	5.06	0.44
1:A:216:GLY:O	1:A:220:THR:OG1	2.67	0.44
3:C:315:MET:HB2	3:C:351:PHE:CZ	2.53	0.44
19:Z:42:LEU:O	19:Z:46:LEU:N	2.47	0.44
1:A:46:ILE:HD12	27:A:610:BCR:H15C	2.00	0.43
4:D:236:ASN:CG	4:D:238:THR:HG22	2.38	0.43
4:D:241:GLU:N	4:D:241:GLU:OE2	4.15	0.43
28:D:406:PL9:H351	28:D:406:PL9:H371	1.63	0.43
27:H:102:BCR:H15C	27:H:102:BCR:H351	1.87	0.43
4:D:140:PRO:O	4:D:144:ILE:HG12	2.18	0.43
13:O:36:GLN:HB3	13:O:38:TYR:CE2	3.91	0.43
25:C:509:CLA:H171	25:C:509:CLA:H13	1.84	0.43
16:V:13:ASN:OD1	16:V:15:GLU:CD	5.43	0.43
18:X:25:PHE:O	18:X:29:ILE:HD12	3.05	0.43
28:A:611:PL9:H121	28:A:611:PL9:HC8	1.53	0.43
25:D:402:CLA:H141	25:D:402:CLA:H162	1.69	0.43
6:F:31:ILE:HD13	6:F:34:LEU:HD23	2.00	0.43
5:E:27:ILE:HG13	6:F:31:ILE:HG21	2.00	0.43
13:O:39:ARG:NH2	13:O:82:GLN:OE1	6.44	0.43
20:R:10:LEU:O	20:R:14:LEU:N	2.29	0.43
2:B:201:HIS:HE2	25:B:604:CLA:C2B	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:ALA:HB3	15:U:102:LEU:HD22	2.13	0.43
25:C:504:CLA:H193	25:C:504:CLA:H161	1.85	0.43
27:D:405:BCR:H351	27:D:405:BCR:H15C	1.88	0.43
16:V:3:LEU:HG	16:V:8:LEU:HD21	1.99	0.43
3:C:186:TYR:HA	3:C:196:VAL:HA	2.24	0.43
8:I:33:LYS:NZ	8:I:33:LYS:HB3	2.33	0.43
2:B:469:HIS:HE1	25:B:612:CLA:NA	2.16	0.43
25:B:604:CLA:H192	25:B:604:CLA:H162	1.81	0.43
27:B:618:BCR:H341	27:B:618:BCR:H11C	1.87	0.43
25:C:514:CLA:H92	25:C:514:CLA:H62	1.79	0.43
33:C:517:DGD:HAH1	33:C:517:DGD:HAT2	1.73	0.43
2:B:419:SER:O	2:B:423:LYS:HG2	2.19	0.43
32:D:408:LHG:H122	32:D:408:LHG:H372	2.00	0.43
4:D:43:LEU:HD23	4:D:113:PHE:HZ	1.84	0.43
4:D:84:SER:O	5:E:69:ARG:HB2	2.18	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.05	0.43
15:U:58:VAL:HG12	15:U:79:LEU:HD13	2.00	0.43
1:A:228:THR:CG2	1:A:229:GLU:H	2.32	0.43
25:C:509:CLA:H142	25:C:509:CLA:H112	2.33	0.43
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.52	0.43
27:C:516:BCR:H371	27:C:516:BCR:H24C	1.84	0.43
13:O:140:THR:O	13:O:201:VAL:HG22	4.46	0.43
17:Y:24:MET:O	17:Y:28:ILE:HG12	4.25	0.43
1:A:307:ILE:HD11	1:A:311:GLY:O	5.82	0.42
3:C:168:LEU:HD11	25:C:509:CLA:H61	24.99	0.42
4:D:216:ALA:O	4:D:220:ASN:ND2	2.49	0.42
2:B:135:LEU:HD11	2:B:234:ILE:HA	2.81	0.42
2:B:265:ILE:HA	2:B:448:ARG:NH2	2.34	0.42
4:D:350:ASN:O	4:D:352:LEU:N	2.45	0.42
23:D:409:LMG:H192	23:D:409:LMG:H161	1.54	0.42
13:O:59:LYS:HB3	13:O:60:ARG:HH11	1.84	0.42
20:R:10:LEU:HB3	20:R:11:PRO:HD3	3.36	0.42
16:V:22:THR:H	16:V:25:GLN:NE2	4.61	0.42
1:A:305:SER:HA	9:J:39:SER:HB3	2.17	0.42
3:C:154:LYS:HD3	3:C:266:TRP:CE2	2.54	0.42
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.02	0.42
28:A:611:PL9:H512	29:D:410:SQD:H331	2.01	0.42
13:O:207:ARG:HB3	13:O:207:ARG:HE	1.67	0.42
20:R:9:LEU:HA	20:R:9:LEU:HD22	4.55	0.42
17:Y:38:LEU:O	17:Y:41:VAL:HG22	2.59	0.42
19:Z:40:ILE:O	19:Z:44:SER:OG	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ALA:O	1:A:328:MET:HG3	2.28	0.42
3:C:211:GLY:O	3:C:215:LYS:HG3	2.37	0.42
23:C:520:LMG:HC71	23:C:520:LMG:O2	4.27	0.42
3:C:95:LEU:HD21	25:C:502:CLA:OBD	2.19	0.42
2:B:475:PHE:CD1	4:D:140:PRO:HG3	2.59	0.42
26:D:401:PHO:HBB1	26:D:401:PHO:HMB1	2.01	0.42
3:C:258:GLY:O	3:C:262:ARG:HG2	3.85	0.42
25:C:512:CLA:H152	25:C:512:CLA:H112	1.73	0.42
4:D:23:LYS:NZ	4:D:131:GLU:OE1	2.52	0.42
13:O:53:LYS:HE2	13:O:231:HIS:CA	6.17	0.42
15:U:57:SER:OG	15:U:60:ASP:OD2	2.32	0.42
25:B:616:CLA:H162	25:B:616:CLA:H202	4.17	0.42
27:B:619:BCR:H361	27:B:619:BCR:H20C	1.83	0.42
3:C:187:ASP:HB2	3:C:230:LEU:HD12	2.60	0.42
16:V:63:THR:HB	16:V:83:ASP:HA	2.00	0.42
1:A:223:LEU:HD23	4:D:139:ARG:NH1	6.23	0.42
23:A:603:LMG:H372	23:A:603:LMG:H341	1.91	0.42
32:B:625:LHG:H152	32:L:101:LHG:H281	2.01	0.42
29:D:410:SQD:H272	29:D:410:SQD:H242	1.88	0.42
1:A:335:ASN:HD21	13:O:157:LEU:H	2.01	0.42
2:B:486:LEU:HD23	2:B:487:SER:N	2.34	0.42
25:B:607:CLA:H193	25:B:607:CLA:H161	1.83	0.42
25:B:615:CLA:H111	25:B:615:CLA:H143	1.88	0.42
25:C:502:CLA:H161	25:C:502:CLA:H202	1.85	0.42
11:L:7:ARG:HG2	11:L:7:ARG:H	1.67	0.42
20:R:20:VAL:O	20:R:24:LEU:HD22	4.34	0.42
29:B:623:SQD:H242	29:B:623:SQD:H82	2.01	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG11	2.10	0.42
4:D:218:VAL:O	4:D:222:LEU:HG	2.53	0.42
26:A:608:PHO:HMB3	25:D:402:CLA:H72	2.02	0.42
1:A:285:PHE:O	1:A:289:GLY:N	2.63	0.41
2:B:151:PHE:HA	2:B:202:HIS:O	2.50	0.41
2:B:494:GLY:HA3	5:E:4:THR:O	2.20	0.41
3:C:425:TRP:NE1	25:C:505:CLA:H3A	2.33	0.41
33:C:517:DGD:HO3D	33:C:518:DGD:HO5E	31.85	0.41
23:M:101:LMG:H421	23:M:101:LMG:H392	1.94	0.41
15:U:45:LEU:HD11	15:U:71:GLN:HB2	4.91	0.41
3:C:342:MET:HE3	3:C:342:MET:HB2	2.83	0.41
1:A:112:TYR:O	1:A:116:ILE:HG23	2.20	0.41
1:A:133:LEU:HD23	4:D:256:ILE:HG12	2.02	0.41
1:A:228:THR:CG2	1:A:229:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:HB2	25:B:615:CLA:HMC3	34.96	0.41
25:C:505:CLA:H41	25:C:505:CLA:H62	1.91	0.41
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.55	0.41
32:D:408:LHG:H321	32:D:408:LHG:H291	1.89	0.41
10:K:24:VAL:HB	17:Y:25:ILE:HD13	4.42	0.41
13:O:52:VAL:CG2	13:O:68:THR:HG21	3.02	0.41
19:Z:55:GLY:O	19:Z:58:ASN:HB3	2.66	0.41
1:A:179:THR:O	1:A:183:MET:HG3	2.20	0.41
1:A:228:THR:HG22	1:A:229:GLU:N	2.35	0.41
2:B:201:HIS:HB2	25:B:608:CLA:NB	27.66	0.41
25:B:610:CLA:H41	25:B:610:CLA:H62	4.34	0.41
32:D:407:LHG:H112	32:D:407:LHG:HC82	2.26	0.41
29:D:410:SQD:H271	29:D:410:SQD:H301	1.89	0.41
15:U:88:GLU:CG	15:U:91:LEU:HD23	5.56	0.41
16:V:9:THR:HG22	16:V:20:THR:HG23	2.01	0.41
18:X:27:VAL:O	18:X:31:ILE:HG13	2.20	0.41
2:B:16:PRO:O	2:B:20:ILE:HG12	3.99	0.41
25:B:603:CLA:H111	25:B:603:CLA:H152	1.83	0.41
25:B:604:CLA:H62	25:B:604:CLA:H41	1.82	0.41
13:O:78:LEU:HD13	13:O:122:VAL:HG22	2.02	0.41
25:C:503:CLA:H161	25:C:503:CLA:H193	4.45	0.41
13:O:32:ILE:HG22	13:O:135:SER:HA	6.05	0.41
1:A:259:ILE:HB	1:A:260:PHE:H	1.74	0.41
25:B:611:CLA:H202	25:B:611:CLA:H161	1.85	0.41
25:B:613:CLA:H122	25:B:613:CLA:H8	1.88	0.41
2:B:71:VAL:HG23	25:B:612:CLA:HMA2	36.04	0.41
3:C:251:HIS:HE1	25:C:507:CLA:NA	2.16	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	3.93	0.41
27:K:101:BCR:H11C	27:K:101:BCR:H341	1.95	0.41
10:K:26:PRO:O	10:K:29:PRO:HD2	2.33	0.41
13:O:115:ARG:O	13:O:117:PRO:HD3	2.33	0.41
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.41
4:D:203:GLY:HA3	4:D:278:GLY:HA3	2.16	0.41
27:D:405:BCR:H341	27:D:405:BCR:H11C	1.92	0.41
5:E:36:LEU:HD13	20:R:7:VAL:HG12	2.25	0.41
34:E:102:HEM:CGD	6:F:19:ARG:HH21	2.34	0.41
3:C:62:PHE:CZ	10:K:28:ILE:HD11	2.55	0.41
13:O:224:ASP:HB3	13:O:227:ALA:HB3	2.33	0.41
16:V:115:ILE:O	16:V:119:ILE:HG13	2.24	0.41
1:A:220:THR:HA	1:A:223:LEU:HD21	3.05	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:610:BCR:H15C	27:A:610:BCR:H351	1.87	0.41
2:B:477:ASP:OD1	2:B:477:ASP:N	2.52	0.41
3:C:215:LYS:HE2	3:C:215:LYS:HB3	1.92	0.41
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.55	0.41
15:U:42:TYR:HA	15:U:43:PRO:HA	1.83	0.41
1:A:252:HIS:CE1	1:A:266:ASN:HB3	2.55	0.41
25:B:605:CLA:H142	25:B:616:CLA:H62	2.02	0.41
3:C:124:VAL:O	25:C:513:CLA:HAC1	16.46	0.41
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.84	0.41
20:R:10:LEU:HD22	20:R:10:LEU:H	1.86	0.41
16:V:42:VAL:HG12	16:V:47:LYS:HE2	3.69	0.41
2:B:458:PHE:HB3	25:B:610:CLA:HBC2	29.46	0.41
2:B:247:PHE:HB2	25:B:614:CLA:HBC1	22.44	0.41
4:D:273:PHE:CE2	32:L:101:LHG:H112	2.56	0.41
32:D:407:LHG:O1	32:L:101:LHG:O4	2.29	0.41
1:A:103:ASP:OD1	1:A:103:ASP:N	2.54	0.40
2:B:265:ILE:HD11	7:H:62:TRP:CH2	7.09	0.40
25:A:609:CLA:HBC1	29:I:102:SQD:H182	2.02	0.40
10:K:40:GLN:HA	10:K:43:VAL:HG22	2.04	0.40
20:R:6:LEU:CD1	20:R:10:LEU:HD21	2.48	0.40
25:B:615:CLA:H141	25:B:615:CLA:H161	1.83	0.40
3:C:132:HIS:CE1	25:C:513:CLA:NA	12.06	0.40
4:D:79:SER:HA	4:D:172:SER:HB3	2.02	0.40
29:I:102:SQD:H212	29:I:102:SQD:H182	1.81	0.40
25:C:511:CLA:H2	10:K:39:TRP:NE1	17.78	0.40
19:Z:33:TRP:CG	19:Z:33:TRP:O	2.73	0.40
1:A:129:ARG:NH2	4:D:255:GLN:O	2.54	0.40
3:C:457:LYS:HE3	4:D:228:GLY:O	4.08	0.40
13:O:58:ASN:C	13:O:60:ARG:H	2.24	0.40
19:Z:14:ILE:HA	19:Z:14:ILE:HD13	1.94	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.10	0.40
2:B:58:GLN:C	2:B:329:PRO:HB3	2.42	0.40
25:D:402:CLA:H112	25:D:402:CLA:H91	1.91	0.40
27:D:405:BCR:H20C	27:D:405:BCR:H361	1.85	0.40
13:O:3:GLN:O	13:O:4:THR:HG23	2.60	0.40
32:E:101:LHG:H261	32:E:101:LHG:H291	1.71	0.40
5:E:22:ILE:HA	20:R:18:TRP:HE1	1.87	0.40

There are no symmetry-related clashes.

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	332/344 (96%)	324 (98%)	7 (2%)	1 (0%)	46	79
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	46	79
2	B	502/510 (98%)	482 (96%)	19 (4%)	1 (0%)	52	84
2	b	503/510 (99%)	484 (96%)	19 (4%)	0	100	100
3	C	449/461 (97%)	431 (96%)	17 (4%)	1 (0%)	52	84
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	39	74
4	D	339/352 (96%)	325 (96%)	14 (4%)	0	100	100
4	d	339/352 (96%)	323 (95%)	16 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
7	h	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	29 (85%)	5 (15%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	6	19
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	6	19
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	6	19
11	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	5	17
12	m	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	5	17
13	O	242/272 (89%)	230 (95%)	10 (4%)	2 (1%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	223 (92%)	15 (6%)	4 (2%)	11	36
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	88 (93%)	7 (7%)	0	100	100
16	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	36/41 (88%)	32 (89%)	3 (8%)	1 (3%)	6	21
19	Z	60/62 (97%)	51 (85%)	1 (2%)	8 (13%)	0	1
19	z	60/62 (97%)	53 (88%)	4 (7%)	3 (5%)	3	8
20	R	32/41 (78%)	29 (91%)	3 (9%)	0	100	100
20	r	32/41 (78%)	30 (94%)	1 (3%)	1 (3%)	5	17
All	All	5237/5694 (92%)	4987 (95%)	220 (4%)	30 (1%)	30	65

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	30	PRO
19	Z	31	GLN
19	Z	33	TRP
19	Z	61	VAL
3	c	24	THR
10	k	12	PRO
13	o	53	LYS
13	o	55	GLU
19	z	32	ASP
3	C	416	SER
10	K	14	ALA
12	M	32	GLN
19	Z	3	ILE
19	Z	32	ASP
3	c	416	SER
18	x	26	ALA
13	O	132	ASN

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Mol	Chain	Res	Type
19	Z	2	THR
13	o	54	GLU
1	a	259	ILE
19	z	2	THR
19	z	4	LEU
20	r	21	ARG
13	O	56	PRO
19	Z	4	LEU
12	m	32	GLN
2	B	488	PRO
9	j	6	GLY
1	A	259	ILE
13	o	56	PRO

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%)	268 (99%)	2 (1%)	88	97
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	402/407 (99%)	397 (99%)	5 (1%)	78	95
2	b	402/407 (99%)	400 (100%)	2 (0%)	92	98
3	C	352/362 (97%)	350 (99%)	2 (1%)	90	98
3	c	352/362 (97%)	350 (99%)	2 (1%)	90	98
4	D	276/283 (98%)	274 (99%)	2 (1%)	88	97
4	d	276/283 (98%)	274 (99%)	2 (1%)	88	97
5	E	72/73 (99%)	72 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	53/53 (100%)	51 (96%)	2 (4%)	40	74
7	h	53/53 (100%)	52 (98%)	1 (2%)	65	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	47	81
9	J	24/28 (86%)	23 (96%)	1 (4%)	36	71
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	207/228 (91%)	206 (100%)	1 (0%)	92	98
13	o	207/228 (91%)	202 (98%)	5 (2%)	57	87
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	78	95
16	V	117/138 (85%)	116 (99%)	1 (1%)	84	96
16	v	117/138 (85%)	114 (97%)	3 (3%)	54	86
17	Y	20/37 (54%)	19 (95%)	1 (5%)	30	64
17	y	23/37 (62%)	22 (96%)	1 (4%)	35	70
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	30/34 (88%)	30 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	91
19	z	52/52 (100%)	49 (94%)	3 (6%)	25	57
20	R	29/33 (88%)	28 (97%)	1 (3%)	44	78
20	r	28/33 (85%)	27 (96%)	1 (4%)	42	76
All	All	4339/4650 (93%)	4298 (99%)	41 (1%)	84	96

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	A	245	THR

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Mol	Chain	Res	Type
2	B	107	LEU
2	B	362	PHE
2	B	394	GLN
2	B	438	ASN
2	B	505	ARG
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	315	TYR
7	H	39	LEU
7	H	49	TYR
9	J	7	ARG
13	O	118	LEU
16	V	24	LYS
17	Y	43	ARG
19	Z	1	MET
20	R	4	ARG
2	b	127	ARG
2	b	362	PHE
3	c	418	ASN
3	c	420	VAL
4	d	180	ARG
4	d	247	VAL
7	h	49	TYR
8	i	35	LYS
13	o	57	LYS
13	o	60	ARG
13	o	132	ASN
13	o	141	ASP
13	o	200	ASN
15	u	70	ARG
16	v	24	LYS
16	v	66	ARG
16	v	106	ASN
17	y	17	GLU
19	z	27	TYR
19	z	32	ASP
19	z	39	LEU
20	r	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	252	HIS
1	A	312	ASN
2	B	216	HIS
2	B	409	GLN
3	C	201	ASN
3	C	311	GLN
4	D	98	GLN
5	E	74	GLN
11	L	6	ASN
13	O	82	GLN
13	O	130	GLN
13	O	200	ASN
15	U	29	ASN
16	V	106	ASN
20	R	32	GLN
1	a	261	GLN
1	a	335	ASN
2	b	216	HIS
2	b	223	GLN
2	b	409	GLN
3	c	311	GLN
4	d	239	GLN
5	e	74	GLN
13	o	46	GLN
13	o	61	GLN
13	o	147	ASN
13	o	236	GLN
16	v	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.88	0	5,9,11	1.21	0
12	FME	M	1	12	8,9,10	0.83	0	5,9,11	0.89	0
14	FME	T	1	14	8,9,10	0.88	0	5,9,11	0.97	0
8	FME	i	1	8	8,9,10	0.87	0	5,9,11	0.93	0
12	FME	m	1	12	8,9,10	0.87	0	5,9,11	0.92	0
14	FME	t	1	14	8,9,10	0.87	0	5,9,11	0.89	0

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
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 23 are unknown and 6 are monoatomic - leaving 151 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	OEX	A	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
23	LMG	A	603	-	51,51,55	0.93	2 (3%)	59,59,63	1.40	8 (13%)
25	CLA	A	606	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	A	607	35	57,73,73	1.15	5 (8%)	61,113,113	1.09	5 (8%)
26	PHO	A	608	-	67,69,69	1.23	7 (10%)	86,99,99	1.08	8 (9%)
25	CLA	A	609	-	46,62,73	1.26	4 (8%)	47,99,113	1.20	5 (10%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	A	611	-	54,55,55	0.85	2 (3%)	68,69,69	1.44	14 (20%)
29	SQD	A	612	-	51,52,54	0.96	5 (9%)	60,63,65	2.04	10 (16%)
29	SQD	A	614	-	39,39,54	0.87	2 (5%)	41,41,65	1.20	3 (7%)
31	BCT	A	615	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	B	602	35	57,73,73	1.14	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	B	603	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	B	604	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	B	605	-	57,73,73	1.14	4 (7%)	61,113,113	1.22	7 (11%)
25	CLA	B	606	-	57,73,73	1.14	4 (7%)	61,113,113	1.07	6 (9%)
25	CLA	B	607	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	B	608	35	57,73,73	1.13	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	B	609	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	B	610	-	57,73,73	1.15	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	B	611	35	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	B	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	B	613	-	57,73,73	1.13	5 (8%)	61,113,113	1.18	6 (9%)
25	CLA	B	614	-	57,73,73	1.14	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	B	615	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	B	616	-	57,73,73	1.14	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	B	617	-	57,73,73	1.12	5 (8%)	61,113,113	1.20	7 (11%)
27	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	8 (14%)
27	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	B	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	5 (8%)
23	LMG	B	621	-	51,51,55	0.73	1 (1%)	59,59,63	1.37	9 (15%)
29	SQD	B	623	-	46,47,54	1.01	3 (6%)	55,58,65	2.07	13 (23%)
32	LHG	B	625	-	48,48,48	0.62	0	49,54,54	1.28	6 (12%)
29	SQD	B	626	-	53,54,54	0.94	5 (9%)	62,65,65	2.16	9 (14%)
23	LMG	C	501	-	51,51,55	0.72	0	59,59,63	1.31	6 (10%)
25	CLA	C	502	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C	503	-	57,73,73	1.14	5 (8%)	61,113,113	1.13	7 (11%)
25	CLA	C	504	-	57,73,73	1.13	5 (8%)	61,113,113	1.15	7 (11%)
25	CLA	C	505	35	57,73,73	1.13	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	C	506	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	C	507	-	57,73,73	1.14	4 (7%)	61,113,113	1.08	7 (11%)
25	CLA	C	508	35	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	C	509	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	C	510	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	C	511	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	7 (11%)
25	CLA	C	512	3	57,73,73	1.12	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	C	513	-	57,73,73	1.12	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	C	514	-	57,73,73	1.12	5 (8%)	61,113,113	1.19	7 (11%)
27	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	8 (14%)
27	BCR	C	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	5 (8%)
33	DGD	C	517	-	63,63,67	0.83	1 (1%)	77,77,81	1.42	9 (11%)
33	DGD	C	518	-	63,63,67	0.90	4 (6%)	77,77,81	1.45	11 (14%)
33	DGD	C	519	-	63,63,67	0.86	1 (1%)	77,77,81	1.42	10 (12%)
23	LMG	C	520	-	51,51,55	0.73	0	59,59,63	1.31	6 (10%)
23	LMG	C	521	-	51,51,55	0.78	1 (1%)	59,59,63	1.36	5 (8%)
26	PHO	D	401	-	67,69,69	1.23	8 (11%)	86,99,99	1.07	7 (8%)
25	CLA	D	402	35	57,73,73	1.13	5 (8%)	61,113,113	1.13	4 (6%)
25	CLA	D	403	-	57,73,73	1.15	5 (8%)	61,113,113	1.07	5 (8%)
25	CLA	D	404	-	57,73,73	1.15	4 (7%)	61,113,113	1.13	7 (11%)
27	BCR	D	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	7 (12%)
28	PL9	D	406	-	54,55,55	0.85	2 (3%)	68,69,69	1.46	15 (22%)
32	LHG	D	407	-	48,48,48	0.60	1 (2%)	49,54,54	1.26	6 (12%)
32	LHG	D	408	-	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
23	LMG	D	409	-	51,51,55	0.72	0	59,59,63	1.30	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	D	410	-	42,43,54	1.06	5 (11%)	51,54,65	2.04	9 (17%)
32	LHG	E	101	-	48,48,48	0.67	1 (2%)	49,54,54	1.22	6 (12%)
34	HEM	E	102	5,6	24,50,50	2.03	5 (20%)	16,82,82	1.38	2 (12%)
27	BCR	H	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	7 (12%)
33	DGD	H	103	-	63,63,67	0.85	1 (1%)	77,77,81	1.35	7 (9%)
29	SQD	I	102	-	39,39,54	0.84	2 (5%)	41,41,65	1.23	2 (4%)
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	5 (8%)
32	LHG	L	101	-	48,48,48	0.61	1 (2%)	49,54,54	1.26	6 (12%)
23	LMG	M	101	-	51,51,55	0.73	0	59,59,63	1.32	6 (10%)
34	HEM	V	201	16	24,50,50	2.05	5 (20%)	16,82,82	1.33	2 (12%)
27	BCR	Y	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.18	4 (7%)
23	LMG	a	701	-	51,51,55	0.79	0	59,59,63	1.32	7 (11%)
21	OEX	a	702	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
31	BCT	a	706	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	a	707	-	57,73,73	1.14	4 (7%)	61,113,113	1.13	4 (6%)
25	CLA	a	708	35	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
26	PHO	a	709	-	67,69,69	1.24	7 (10%)	86,99,99	1.06	8 (9%)
26	PHO	a	710	-	67,69,69	1.23	7 (10%)	86,99,99	1.08	7 (8%)
25	CLA	a	711	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
27	BCR	a	712	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
28	PL9	a	713	-	54,55,55	0.83	2 (3%)	68,69,69	1.42	12 (17%)
29	SQD	a	714	-	53,54,54	0.94	4 (7%)	62,65,65	1.95	11 (17%)
23	LMG	a	715	-	51,51,55	0.74	0	59,59,63	1.32	6 (10%)
25	CLA	a	719	35	57,73,73	1.14	4 (7%)	61,113,113	1.09	4 (6%)
32	LHG	a	720	-	38,38,48	0.67	0	39,44,54	1.18	3 (7%)
29	SQD	b	601	-	53,54,54	0.94	3 (5%)	62,65,65	2.17	10 (16%)
27	BCR	b	602	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	7 (12%)
25	CLA	b	607	35	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	b	608	-	57,73,73	1.13	4 (7%)	61,113,113	1.08	6 (9%)
25	CLA	b	609	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	b	610	-	57,73,73	1.13	4 (7%)	61,113,113	1.23	6 (9%)
25	CLA	b	611	-	57,73,73	1.14	5 (8%)	61,113,113	1.08	5 (8%)
25	CLA	b	612	-	57,73,73	1.13	5 (8%)	61,113,113	1.15	5 (8%)
25	CLA	b	613	35	57,73,73	1.13	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	b	614	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	615	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	b	616	35	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	b	617	-	57,73,73	1.12	5 (8%)	61,113,113	1.19	7 (11%)
25	CLA	b	618	-	57,73,73	1.15	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	b	619	-	57,73,73	1.12	4 (7%)	61,113,113	1.19	7 (11%)
25	CLA	b	620	-	57,73,73	1.14	5 (8%)	61,113,113	1.10	4 (6%)
25	CLA	b	621	-	57,73,73	1.13	5 (8%)	61,113,113	1.17	6 (9%)
25	CLA	b	622	-	39,55,73	1.34	4 (10%)	42,91,113	1.37	6 (14%)
27	BCR	b	623	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	8 (14%)
27	BCR	b	624	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
27	BCR	b	625	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	7 (12%)
23	LMG	b	626	-	51,51,55	0.80	3 (5%)	59,59,63	1.53	9 (15%)
23	LMG	b	627	-	51,51,55	0.77	0	59,59,63	1.27	4 (6%)
23	LMG	b	628	-	8,8,55	0.16	0	7,7,63	0.91	0
32	LHG	b	629	-	48,48,48	0.61	1 (2%)	49,54,54	1.24	6 (12%)
25	CLA	c	501	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	c	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	7 (11%)
25	CLA	c	503	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	c	504	35	50,66,73	1.21	4 (8%)	52,104,113	1.21	6 (11%)
25	CLA	c	505	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	7 (11%)
25	CLA	c	506	-	57,73,73	1.13	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	c	507	35	57,73,73	1.13	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	508	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	c	509	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	6 (9%)
25	CLA	c	510	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	5 (8%)
25	CLA	c	511	3	57,73,73	1.13	5 (8%)	61,113,113	1.16	6 (9%)
25	CLA	c	512	-	57,73,73	1.11	4 (7%)	61,113,113	1.21	6 (9%)
25	CLA	c	513	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	6 (9%)
27	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
27	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	5 (8%)
33	DGD	c	516	-	63,63,67	0.85	1 (1%)	77,77,81	1.41	11 (14%)
33	DGD	c	517	-	63,63,67	0.93	2 (3%)	77,77,81	1.42	10 (12%)
33	DGD	c	518	-	63,63,67	0.85	1 (1%)	77,77,81	1.42	10 (12%)
23	LMG	c	519	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
23	LMG	c	520	-	51,51,55	0.81	1 (1%)	59,59,63	1.36	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	d	402	-	57,73,73	1.15	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	d	403	-	57,73,73	1.12	4 (7%)	61,113,113	1.17	6 (9%)
27	BCR	d	404	-	41,41,41	1.15	3 (7%)	56,56,56	1.24	7 (12%)
28	PL9	d	405	-	54,55,55	0.82	2 (3%)	68,69,69	1.43	14 (20%)
32	LHG	d	406	-	48,48,48	0.61	0	49,54,54	1.28	7 (14%)
32	LHG	d	407	-	48,48,48	0.61	0	49,54,54	1.25	6 (12%)
23	LMG	d	408	-	39,39,55	0.53	0	41,41,63	1.27	3 (7%)
32	LHG	e	101	-	41,41,48	0.67	1 (2%)	42,47,54	1.33	7 (16%)
34	HEM	e	102	5,6	24,50,50	2.12	5 (20%)	16,82,82	1.44	2 (12%)
23	LMG	f	101	-	51,51,55	0.70	0	59,59,63	1.36	7 (11%)
29	SQD	f	102	-	40,41,54	1.08	5 (12%)	49,52,65	1.99	9 (18%)
27	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	7 (12%)
33	DGD	h	102	-	63,63,67	0.87	0	77,77,81	1.30	7 (9%)
27	BCR	k	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	2 (3%)
27	BCR	k	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
27	BCR	t	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	7 (12%)
34	HEM	v	201	16	24,50,50	2.04	5 (20%)	16,82,82	1.32	1 (6%)

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	OEX	A	601	1,3,35	-	0/0/68/68	0/0/6/6
23	LMG	A	603	-	-	0/46/66/70	0/1/1/1
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	A	608	-	-	0/53/103/103	0/1/6/6
25	CLA	A	609	-	3/3/17/25	0/24/122/135	0/0/9/9
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
28	PL9	A	611	-	-	0/53/73/73	0/1/1/1
29	SQD	A	612	-	-	0/47/67/69	0/1/1/1
29	SQD	A	614	-	-	0/41/41/69	0/0/0/1
31	BCT	A	615	22	-	0/0/0/0	0/0/0/0
25	CLA	B	602	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	608	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	LMG	B	621	-	-	0/46/66/70	0/1/1/1
29	SQD	B	623	-	-	0/42/62/69	0/1/1/1
32	LHG	B	625	-	-	0/53/53/53	0/0/0/0
29	SQD	B	626	-	-	1/49/69/69	0/1/1/1
23	LMG	C	501	-	-	0/46/66/70	0/1/1/1
25	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	514	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
33	DGD	C	517	-	-	0/51/91/95	0/2/2/2
33	DGD	C	518	-	-	0/51/91/95	0/2/2/2
33	DGD	C	519	-	-	0/51/91/95	0/2/2/2
23	LMG	C	520	-	-	0/46/66/70	0/1/1/1
23	LMG	C	521	-	-	0/46/66/70	0/1/1/1
26	PHO	D	401	-	-	0/53/103/103	0/1/6/6
25	CLA	D	402	35	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	D	404	-	2/2/20/25	0/37/135/135	0/0/9/9
27	BCR	D	405	-	-	0/29/63/63	0/2/2/2
28	PL9	D	406	-	-	0/53/73/73	0/1/1/1
32	LHG	D	407	-	-	0/53/53/53	0/0/0/0
32	LHG	D	408	-	-	0/53/53/53	0/0/0/0
23	LMG	D	409	-	-	0/46/66/70	0/1/1/1
29	SQD	D	410	-	-	0/38/58/69	0/1/1/1
32	LHG	E	101	-	-	0/53/53/53	0/0/0/0
34	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
27	BCR	H	102	-	-	0/29/63/63	0/2/2/2
33	DGD	H	103	-	-	0/51/91/95	0/2/2/2
29	SQD	I	102	-	-	0/41/41/69	0/0/0/1
27	BCR	K	101	-	-	0/29/63/63	0/2/2/2
32	LHG	L	101	-	-	0/53/53/53	0/0/0/0
23	LMG	M	101	-	-	0/46/66/70	0/1/1/1
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
27	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
23	LMG	a	701	-	-	0/46/66/70	0/1/1/1
21	OEX	a	702	1,3,35	-	0/0/68/68	0/0/6/6
31	BCT	a	706	22	-	0/0/0/0	0/0/0/0
25	CLA	a	707	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	708	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	a	709	-	-	0/53/103/103	0/1/6/6
26	PHO	a	710	-	-	0/53/103/103	0/1/6/6
25	CLA	a	711	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	a	712	-	-	0/29/63/63	0/2/2/2
28	PL9	a	713	-	-	0/53/73/73	0/1/1/1
29	SQD	a	714	-	-	0/49/69/69	0/1/1/1
23	LMG	a	715	-	-	0/46/66/70	0/1/1/1
25	CLA	a	719	35	3/3/20/25	0/37/135/135	0/0/9/9
32	LHG	a	720	-	-	0/43/43/53	0/0/0/0
29	SQD	b	601	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	602	-	-	0/29/63/63	0/2/2/2
25	CLA	b	607	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	613	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	615	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	616	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	621	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	622	-	3/3/16/25	0/16/114/135	0/0/9/9
27	BCR	b	623	-	-	0/29/63/63	0/2/2/2
27	BCR	b	624	-	-	0/29/63/63	0/2/2/2
27	BCR	b	625	-	-	0/29/63/63	0/2/2/2
23	LMG	b	626	-	-	0/46/66/70	0/1/1/1
23	LMG	b	627	-	-	0/46/66/70	0/1/1/1
23	LMG	b	628	-	-	0/6/6/70	0/0/0/1
32	LHG	b	629	-	-	0/53/53/53	0/0/0/0
25	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	35	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	c	505	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
33	DGD	c	516	-	-	0/51/91/95	0/2/2/2
33	DGD	c	517	-	-	0/51/91/95	0/2/2/2
33	DGD	c	518	-	-	0/51/91/95	0/2/2/2
23	LMG	c	519	-	-	0/46/66/70	0/1/1/1
23	LMG	c	520	-	-	0/46/66/70	0/1/1/1
25	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
27	BCR	d	404	-	-	0/29/63/63	0/2/2/2
28	PL9	d	405	-	-	0/53/73/73	0/1/1/1
32	LHG	d	406	-	-	0/53/53/53	0/0/0/0
32	LHG	d	407	-	-	0/53/53/53	0/0/0/0
23	LMG	d	408	-	-	0/41/41/70	0/0/0/1
32	LHG	e	101	-	-	0/46/46/53	0/0/0/0
34	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
23	LMG	f	101	-	-	0/46/66/70	0/1/1/1
29	SQD	f	102	-	-	0/36/56/69	0/1/1/1
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
27	BCR	k	101	-	-	0/29/63/63	0/2/2/2
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
27	BCR	t	103	-	-	0/29/63/63	0/2/2/2
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8

All (469) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	e	102	HEM	C3B-C2B	-5.24	1.33	1.40
34	V	201	HEM	C3C-C2C	-5.10	1.33	1.40
34	E	102	HEM	C3C-C2C	-5.02	1.34	1.40
34	v	201	HEM	C3C-C2C	-4.96	1.34	1.40
34	e	102	HEM	C3C-C2C	-4.93	1.34	1.40
34	E	102	HEM	C3B-C2B	-4.09	1.35	1.40
34	v	201	HEM	C3B-C2B	-4.08	1.35	1.40
34	V	201	HEM	C3B-C2B	-4.07	1.35	1.40
27	d	404	BCR	C1-C6	-3.76	1.48	1.53
27	D	405	BCR	C30-C25	-3.70	1.48	1.53
27	D	405	BCR	C1-C6	-3.61	1.48	1.53
27	b	623	BCR	C1-C6	-3.60	1.48	1.53
27	k	101	BCR	C1-C6	-3.52	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	515	BCR	C1-C6	-3.52	1.49	1.53
27	C	516	BCR	C1-C6	-3.50	1.49	1.53
27	Y	101	BCR	C1-C6	-3.47	1.49	1.53
27	t	103	BCR	C1-C6	-3.47	1.49	1.53
27	b	602	BCR	C1-C6	-3.46	1.49	1.53
27	B	620	BCR	C1-C6	-3.46	1.49	1.53
27	a	712	BCR	C1-C6	-3.43	1.49	1.53
27	c	514	BCR	C30-C25	-3.42	1.49	1.53
27	b	624	BCR	C1-C6	-3.41	1.49	1.53
27	B	618	BCR	C1-C6	-3.41	1.49	1.53
27	k	102	BCR	C1-C6	-3.40	1.49	1.53
27	K	101	BCR	C1-C6	-3.40	1.49	1.53
27	b	625	BCR	C1-C6	-3.39	1.49	1.53
27	c	514	BCR	C1-C6	-3.39	1.49	1.53
27	B	619	BCR	C1-C6	-3.36	1.49	1.53
27	b	623	BCR	C30-C25	-3.34	1.49	1.53
27	A	610	BCR	C1-C6	-3.28	1.49	1.53
27	b	625	BCR	C30-C25	-3.21	1.49	1.53
27	C	515	BCR	C30-C25	-3.18	1.49	1.53
27	C	515	BCR	C1-C6	-3.16	1.49	1.53
27	C	516	BCR	C30-C25	-3.13	1.49	1.53
27	B	620	BCR	C30-C25	-3.13	1.49	1.53
27	c	515	BCR	C30-C25	-3.10	1.49	1.53
27	H	102	BCR	C1-C6	-3.09	1.49	1.53
27	b	624	BCR	C30-C25	-3.08	1.49	1.53
27	a	712	BCR	C30-C25	-3.08	1.49	1.53
27	d	404	BCR	C30-C25	-3.08	1.49	1.53
27	Y	101	BCR	C30-C25	-3.08	1.49	1.53
27	B	619	BCR	C30-C25	-3.00	1.49	1.53
27	h	101	BCR	C1-C6	-3.00	1.49	1.53
27	k	102	BCR	C30-C25	-2.99	1.49	1.53
27	A	610	BCR	C30-C25	-2.99	1.49	1.53
27	b	602	BCR	C30-C25	-2.98	1.49	1.53
27	h	101	BCR	C30-C25	-2.97	1.49	1.53
27	B	618	BCR	C30-C25	-2.94	1.49	1.53
27	k	101	BCR	C30-C25	-2.94	1.49	1.53
27	K	101	BCR	C30-C25	-2.91	1.49	1.53
27	H	102	BCR	C30-C25	-2.90	1.49	1.53
27	t	103	BCR	C30-C25	-2.89	1.49	1.53
28	D	406	PL9	C3-C4	-2.68	1.45	1.49
28	A	611	PL9	C3-C4	-2.66	1.45	1.49
25	c	501	CLA	CMB-C2B	-2.55	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	CMB-C2B	-2.54	1.46	1.51
25	b	617	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.50	1.46	1.51
25	a	708	CLA	CMB-C2B	-2.50	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.50	1.46	1.51
25	B	605	CLA	CMB-C2B	-2.49	1.46	1.51
25	B	612	CLA	CMB-C2B	-2.49	1.46	1.51
25	a	711	CLA	CMB-C2B	-2.49	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.48	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.48	1.46	1.51
28	d	405	PL9	C3-C4	-2.47	1.45	1.49
25	B	602	CLA	CMB-C2B	-2.47	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	614	CLA	CMB-C2B	-2.46	1.46	1.51
25	c	510	CLA	CMD-C2D	-2.45	1.46	1.51
25	a	719	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	611	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	506	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.44	1.46	1.51
28	a	713	PL9	C3-C4	-2.44	1.45	1.49
25	A	609	CLA	CMB-C2B	-2.44	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	506	CLA	CMB-C2B	-2.44	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.44	1.46	1.51
25	A	607	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.44	1.46	1.51
25	b	618	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	613	CLA	CMB-C2B	-2.44	1.46	1.51
25	D	404	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	505	CLA	CMD-C2D	-2.43	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	621	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	613	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.43	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.42	1.46	1.51
25	a	707	CLA	CMB-C2B	-2.42	1.46	1.51
25	D	402	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	620	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.42	1.46	1.51
33	c	517	DGD	O1G-C1G	-2.41	1.39	1.45
25	C	513	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.41	1.46	1.51
25	d	402	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.40	1.46	1.51
25	A	606	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.40	1.46	1.51
33	C	518	DGD	O1G-C1G	-2.40	1.39	1.45
25	C	504	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	506	CLA	CMD-C2D	-2.39	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	619	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.38	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	604	CLA	CMD-C2D	-2.38	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	618	CLA	CMD-C2D	-2.37	1.46	1.51
25	B	617	CLA	CMB-C2B	-2.37	1.46	1.51
25	a	707	CLA	CMD-C2D	-2.37	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.36	1.46	1.51
25	A	606	CLA	CMD-C2D	-2.35	1.46	1.51
25	b	609	CLA	CMD-C2D	-2.33	1.46	1.51
25	c	503	CLA	CMD-C2D	-2.33	1.46	1.51
25	C	514	CLA	CMB-C2B	-2.33	1.46	1.51
25	b	622	CLA	CMB-C2B	-2.33	1.46	1.51
25	d	402	CLA	CMD-C2D	-2.33	1.46	1.51
25	D	403	CLA	CMD-C2D	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	CMD-C2D	-2.32	1.46	1.51
25	b	611	CLA	CMD-C2D	-2.32	1.46	1.51
25	c	512	CLA	CMD-C2D	-2.31	1.46	1.51
25	B	609	CLA	CMD-C2D	-2.31	1.46	1.51
25	C	504	CLA	CMD-C2D	-2.30	1.46	1.51
25	C	502	CLA	CMD-C2D	-2.29	1.46	1.51
25	C	503	CLA	CMD-C2D	-2.29	1.46	1.51
25	a	708	CLA	CMD-C2D	-2.29	1.46	1.51
25	B	614	CLA	CMD-C2D	-2.29	1.46	1.51
25	c	502	CLA	CMD-C2D	-2.29	1.46	1.51
25	B	602	CLA	CMD-C2D	-2.28	1.46	1.51
25	B	615	CLA	CMD-C2D	-2.28	1.46	1.51
25	b	619	CLA	CMD-C2D	-2.28	1.46	1.51
25	D	404	CLA	CMD-C2D	-2.28	1.46	1.51
25	C	509	CLA	CMD-C2D	-2.28	1.46	1.51
25	B	610	CLA	CMD-C2D	-2.28	1.46	1.51
25	c	501	CLA	CMD-C2D	-2.27	1.46	1.51
25	C	507	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	613	CLA	CMD-C2D	-2.27	1.46	1.51
25	C	511	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	606	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	608	CLA	CMD-C2D	-2.27	1.46	1.51
25	b	608	CLA	CMD-C2D	-2.27	1.46	1.51
25	b	616	CLA	CMD-C2D	-2.27	1.46	1.51
25	c	504	CLA	CMD-C2D	-2.26	1.46	1.51
25	b	607	CLA	CMD-C2D	-2.26	1.46	1.51
25	a	719	CLA	CMD-C2D	-2.26	1.46	1.51
25	b	613	CLA	CMD-C2D	-2.26	1.46	1.51
25	b	615	CLA	CMD-C2D	-2.26	1.46	1.51
25	C	508	CLA	CMD-C2D	-2.26	1.46	1.51
25	B	605	CLA	CMD-C2D	-2.26	1.46	1.51
25	B	607	CLA	CMD-C2D	-2.26	1.46	1.51
25	C	513	CLA	CMD-C2D	-2.25	1.46	1.51
25	D	402	CLA	CMD-C2D	-2.25	1.46	1.51
25	B	617	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	617	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	622	CLA	CMD-C2D	-2.25	1.46	1.51
25	A	607	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	614	CLA	CMD-C2D	-2.24	1.46	1.51
25	c	513	CLA	CMD-C2D	-2.24	1.46	1.51
25	b	621	CLA	CMD-C2D	-2.24	1.46	1.51
25	d	403	CLA	CMD-C2D	-2.24	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	620	CLA	CMD-C2D	-2.24	1.46	1.51
25	c	508	CLA	CMD-C2D	-2.24	1.46	1.51
25	c	506	CLA	CMD-C2D	-2.24	1.46	1.51
25	C	505	CLA	CMD-C2D	-2.24	1.46	1.51
25	C	512	CLA	CMD-C2D	-2.24	1.46	1.51
25	C	514	CLA	CMD-C2D	-2.24	1.46	1.51
25	B	611	CLA	CMD-C2D	-2.24	1.46	1.51
25	B	612	CLA	CMD-C2D	-2.24	1.46	1.51
25	A	609	CLA	CMD-C2D	-2.24	1.46	1.51
25	b	610	CLA	CMD-C2D	-2.24	1.46	1.51
25	c	507	CLA	CMD-C2D	-2.23	1.46	1.51
25	a	711	CLA	CMD-C2D	-2.23	1.46	1.51
25	B	603	CLA	CMD-C2D	-2.23	1.46	1.51
33	C	517	DGD	O1G-C1G	-2.23	1.40	1.45
29	A	612	SQD	O2-C2	-2.22	1.37	1.43
25	c	509	CLA	CMD-C2D	-2.22	1.46	1.51
25	b	612	CLA	CMD-C2D	-2.22	1.46	1.51
25	C	510	CLA	CMD-C2D	-2.21	1.46	1.51
26	D	401	PHO	C1C-NC	-2.21	1.33	1.38
29	a	714	SQD	O2-C2	-2.20	1.37	1.43
26	A	608	PHO	C1C-NC	-2.20	1.33	1.38
25	B	616	CLA	CMD-C2D	-2.20	1.46	1.51
26	a	709	PHO	C1C-NC	-2.19	1.33	1.38
26	a	710	PHO	C1C-NC	-2.17	1.33	1.38
33	c	516	DGD	O1G-C1G	-2.17	1.40	1.45
29	D	410	SQD	O2-C2	-2.17	1.37	1.43
29	b	601	SQD	O2-C2	-2.17	1.37	1.43
29	f	102	SQD	O2-C2	-2.15	1.37	1.43
29	B	626	SQD	O2-C2	-2.15	1.37	1.43
33	C	518	DGD	O6D-C5D	-2.14	1.39	1.44
33	C	518	DGD	O2G-C2G	-2.11	1.41	1.46
33	c	517	DGD	O2G-C2G	-2.10	1.41	1.46
33	c	518	DGD	O1G-C1G	-2.10	1.40	1.45
23	b	626	LMG	O8-C9	-2.09	1.40	1.45
33	C	519	DGD	O1G-C1G	-2.09	1.40	1.45
25	B	617	CLA	CMC-C2C	-2.08	1.46	1.50
28	d	405	PL9	C53-C6	-2.08	1.46	1.50
29	B	623	SQD	O2-C2	-2.07	1.38	1.43
28	A	611	PL9	C53-C6	-2.06	1.46	1.50
29	a	714	SQD	O3-C3	-2.05	1.38	1.43
28	a	713	PL9	C53-C6	-2.05	1.46	1.50
28	D	406	PL9	C53-C6	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	518	DGD	O5D-C6D	-2.04	1.40	1.43
29	f	102	SQD	O4-C4	-2.04	1.38	1.43
32	b	629	LHG	O7-C5	-2.04	1.41	1.46
29	B	626	SQD	O3-C3	-2.03	1.38	1.43
32	D	407	LHG	O7-C5	-2.03	1.41	1.46
32	L	101	LHG	O7-C5	-2.03	1.41	1.46
27	d	404	BCR	C33-C5	-2.02	1.47	1.51
25	b	621	CLA	CMC-C2C	-2.02	1.46	1.50
29	D	410	SQD	O3-C3	-2.02	1.38	1.43
25	b	612	CLA	CMC-C2C	-2.02	1.46	1.50
29	A	612	SQD	O3-C3	-2.02	1.38	1.43
25	B	613	CLA	CMC-C2C	-2.02	1.46	1.50
33	H	103	DGD	O2G-C2G	-2.02	1.41	1.46
27	b	623	BCR	C33-C5	-2.02	1.47	1.51
29	D	410	SQD	O4-C4	-2.01	1.38	1.43
29	f	102	SQD	O3-C3	-2.01	1.38	1.43
29	A	612	SQD	O4-C4	-2.01	1.38	1.43
27	Y	101	BCR	C33-C5	-2.01	1.47	1.51
29	B	626	SQD	O4-C4	-2.01	1.38	1.43
25	b	617	CLA	C4C-NC	2.00	1.40	1.37
25	A	606	CLA	C4C-NC	2.00	1.40	1.37
25	c	511	CLA	C4C-NC	2.01	1.40	1.37
25	B	603	CLA	C4C-NC	2.01	1.40	1.37
25	c	502	CLA	C4C-NC	2.01	1.40	1.37
26	D	401	PHO	C4B-NB	2.01	1.41	1.36
25	c	501	CLA	C4C-NC	2.01	1.40	1.37
25	C	514	CLA	C4C-NC	2.02	1.40	1.37
25	C	503	CLA	C4C-NC	2.02	1.40	1.37
25	C	505	CLA	C4C-NC	2.02	1.40	1.37
25	D	402	CLA	C4C-NC	2.03	1.40	1.37
25	c	506	CLA	C4C-NC	2.03	1.40	1.37
25	c	509	CLA	C4C-NC	2.03	1.40	1.37
25	C	504	CLA	C4C-NC	2.04	1.40	1.37
25	b	611	CLA	C4C-NC	2.04	1.40	1.37
25	D	403	CLA	C4C-NC	2.05	1.40	1.37
25	B	615	CLA	C4C-NC	2.05	1.40	1.37
25	B	609	CLA	C4C-NC	2.06	1.40	1.37
25	C	511	CLA	C4C-NC	2.06	1.40	1.37
25	b	613	CLA	C4C-NC	2.06	1.40	1.37
32	e	101	LHG	P-O6	2.06	1.68	1.59
25	a	708	CLA	C4C-NC	2.07	1.40	1.37
25	b	614	CLA	C4C-NC	2.07	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	620	CLA	C4C-NC	2.08	1.40	1.37
25	A	607	CLA	C4C-NC	2.09	1.40	1.37
23	B	621	LMG	C7-C8	2.09	1.56	1.50
23	b	626	LMG	C7-C8	2.11	1.56	1.50
34	E	102	HEM	CAD-C3D	2.12	1.55	1.52
23	b	626	LMG	O6-C1	2.16	1.47	1.41
32	E	101	LHG	P-O6	2.19	1.68	1.59
26	a	709	PHO	C4C-C3C	2.27	1.49	1.45
34	v	201	HEM	CAD-C3D	2.28	1.55	1.52
26	A	608	PHO	CHD-C1D	2.28	1.43	1.38
26	a	710	PHO	C4C-C3C	2.28	1.49	1.45
26	D	401	PHO	CHD-C1D	2.28	1.43	1.38
26	A	608	PHO	C4C-C3C	2.30	1.49	1.45
26	a	710	PHO	CHD-C1D	2.30	1.43	1.38
26	a	709	PHO	CHD-C1D	2.36	1.43	1.38
34	e	102	HEM	CAD-C3D	2.36	1.55	1.52
26	D	401	PHO	C4C-C3C	2.36	1.49	1.45
34	V	201	HEM	CAD-C3D	2.37	1.55	1.52
23	C	521	LMG	C1-C2	2.39	1.59	1.52
23	c	520	LMG	C1-C2	2.42	1.59	1.52
26	a	710	PHO	C1A-NA	2.52	1.42	1.37
25	B	605	CLA	CHC-C1C	2.54	1.42	1.35
25	b	621	CLA	CHC-C1C	2.56	1.42	1.35
26	A	608	PHO	C1A-NA	2.57	1.42	1.37
25	C	508	CLA	CHC-C1C	2.58	1.42	1.35
26	a	709	PHO	C1A-NA	2.58	1.43	1.37
26	A	608	PHO	C4C-NC	2.59	1.42	1.36
26	D	401	PHO	C1A-NA	2.59	1.43	1.37
25	b	612	CLA	CHC-C1C	2.60	1.42	1.35
25	D	404	CLA	CHC-C1C	2.60	1.42	1.35
25	c	513	CLA	CHC-C1C	2.60	1.43	1.35
25	B	604	CLA	CHC-C1C	2.61	1.43	1.35
25	c	507	CLA	CHC-C1C	2.61	1.43	1.35
25	c	512	CLA	CHC-C1C	2.61	1.43	1.35
25	B	608	CLA	CHC-C1C	2.62	1.43	1.35
25	b	619	CLA	CHC-C1C	2.63	1.43	1.35
25	c	501	CLA	CHC-C1C	2.63	1.43	1.35
25	b	610	CLA	CHC-C1C	2.63	1.43	1.35
25	b	608	CLA	CHC-C1C	2.63	1.43	1.35
25	B	611	CLA	CHC-C1C	2.63	1.43	1.35
25	b	617	CLA	CHC-C1C	2.63	1.43	1.35
25	B	617	CLA	CHC-C1C	2.64	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	709	PHO	C4C-NC	2.64	1.42	1.36
26	D	401	PHO	C4C-NC	2.64	1.42	1.36
25	B	612	CLA	CHC-C1C	2.64	1.43	1.35
25	b	607	CLA	CHC-C1C	2.64	1.43	1.35
25	b	615	CLA	CHC-C1C	2.64	1.43	1.35
25	C	510	CLA	CHC-C1C	2.64	1.43	1.35
25	c	504	CLA	CHC-C1C	2.64	1.43	1.35
25	a	707	CLA	CHC-C1C	2.64	1.43	1.35
25	C	502	CLA	CHC-C1C	2.64	1.43	1.35
25	c	505	CLA	CHC-C1C	2.64	1.43	1.35
25	b	622	CLA	CHC-C1C	2.64	1.43	1.35
25	B	616	CLA	CHC-C1C	2.65	1.43	1.35
25	B	606	CLA	CHC-C1C	2.65	1.43	1.35
25	B	610	CLA	CHC-C1C	2.65	1.43	1.35
25	c	510	CLA	CHC-C1C	2.65	1.43	1.35
25	a	719	CLA	CHC-C1C	2.65	1.43	1.35
25	C	513	CLA	CHC-C1C	2.65	1.43	1.35
25	a	711	CLA	CHC-C1C	2.65	1.43	1.35
25	D	402	CLA	CHC-C1C	2.66	1.43	1.35
25	a	708	CLA	CHC-C1C	2.66	1.43	1.35
25	C	505	CLA	CHC-C1C	2.66	1.43	1.35
25	c	506	CLA	CHC-C1C	2.66	1.43	1.35
25	c	502	CLA	CHC-C1C	2.67	1.43	1.35
25	d	402	CLA	CHC-C1C	2.67	1.43	1.35
25	D	403	CLA	CHC-C1C	2.67	1.43	1.35
25	A	606	CLA	CHC-C1C	2.67	1.43	1.35
25	C	503	CLA	CHC-C1C	2.67	1.43	1.35
25	C	514	CLA	CHC-C1C	2.67	1.43	1.35
25	C	506	CLA	CHC-C1C	2.67	1.43	1.35
25	b	616	CLA	CHC-C1C	2.67	1.43	1.35
25	c	509	CLA	CHC-C1C	2.67	1.43	1.35
29	b	601	SQD	O47-C7	2.68	1.42	1.34
25	B	603	CLA	CHC-C1C	2.68	1.43	1.35
25	A	609	CLA	CHC-C1C	2.68	1.43	1.35
26	a	710	PHO	C4C-NC	2.68	1.43	1.36
25	b	618	CLA	CHC-C1C	2.68	1.43	1.35
25	C	507	CLA	CHC-C1C	2.68	1.43	1.35
25	B	602	CLA	CHC-C1C	2.68	1.43	1.35
25	B	607	CLA	CHC-C1C	2.68	1.43	1.35
25	b	611	CLA	CHC-C1C	2.68	1.43	1.35
25	c	511	CLA	CHC-C1C	2.69	1.43	1.35
25	B	614	CLA	CHC-C1C	2.69	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	CHC-C1C	2.69	1.43	1.35
25	c	508	CLA	CHC-C1C	2.69	1.43	1.35
25	C	511	CLA	CHC-C1C	2.69	1.43	1.35
25	d	403	CLA	CHC-C1C	2.69	1.43	1.35
25	b	609	CLA	CHC-C1C	2.69	1.43	1.35
25	b	613	CLA	CHC-C1C	2.70	1.43	1.35
25	C	509	CLA	CHC-C1C	2.70	1.43	1.35
25	C	504	CLA	CHC-C1C	2.70	1.43	1.35
25	C	512	CLA	CHC-C1C	2.70	1.43	1.35
25	A	607	CLA	CHC-C1C	2.70	1.43	1.35
29	a	714	SQD	O47-C7	2.71	1.42	1.34
25	B	615	CLA	CHC-C1C	2.72	1.43	1.35
25	b	620	CLA	CHC-C1C	2.72	1.43	1.35
25	B	613	CLA	CHC-C1C	2.72	1.43	1.35
29	A	612	SQD	O47-C7	2.73	1.42	1.34
29	D	410	SQD	O47-C7	2.73	1.42	1.34
25	B	609	CLA	CHC-C1C	2.73	1.43	1.35
25	c	503	CLA	CHC-C1C	2.73	1.43	1.35
29	B	626	SQD	O47-C7	2.74	1.42	1.34
29	f	102	SQD	O47-C7	2.76	1.42	1.34
29	I	102	SQD	O47-C7	2.79	1.42	1.34
26	a	709	PHO	CHC-C1C	2.86	1.44	1.38
29	B	623	SQD	O47-C7	2.87	1.42	1.34
29	A	614	SQD	O47-C7	2.88	1.42	1.34
26	D	401	PHO	CHC-C1C	2.90	1.44	1.38
23	A	603	LMG	C4-C3	2.91	1.60	1.52
26	A	608	PHO	CHC-C1C	2.91	1.44	1.38
26	a	710	PHO	CHC-C1C	2.92	1.44	1.38
29	b	601	SQD	O48-C23	3.03	1.42	1.33
29	A	612	SQD	O48-C23	3.04	1.42	1.33
29	I	102	SQD	O48-C23	3.05	1.42	1.33
29	B	626	SQD	O48-C23	3.05	1.42	1.33
29	f	102	SQD	O48-C23	3.10	1.42	1.33
29	B	623	SQD	O48-C23	3.10	1.42	1.33
29	a	714	SQD	O48-C23	3.11	1.42	1.33
29	D	410	SQD	O48-C23	3.11	1.42	1.33
29	A	614	SQD	O48-C23	3.23	1.42	1.33
23	A	603	LMG	C4-C5	3.40	1.60	1.53
26	a	709	PHO	C3B-C4B	3.44	1.50	1.43
34	e	102	HEM	C3B-CAB	3.46	1.55	1.47
26	D	401	PHO	C3B-C4B	3.47	1.50	1.43
26	a	710	PHO	C3B-C4B	3.52	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C3B-C4B	3.53	1.50	1.43
34	V	201	HEM	C3C-CAC	3.59	1.55	1.47
34	v	201	HEM	C3C-CAC	3.63	1.55	1.47
34	E	102	HEM	C3C-CAC	3.68	1.55	1.47
34	e	102	HEM	C3C-CAC	3.69	1.55	1.47
34	V	201	HEM	C3B-CAB	3.70	1.55	1.47
34	E	102	HEM	C3B-CAB	3.70	1.55	1.47
34	v	201	HEM	C3B-CAB	3.76	1.55	1.47
25	A	609	CLA	CHB-C4A	3.81	1.38	1.33
25	c	505	CLA	CHB-C4A	3.84	1.38	1.33
25	c	507	CLA	CHB-C4A	3.84	1.38	1.33
25	B	608	CLA	CHB-C4A	3.85	1.38	1.33
25	a	708	CLA	CHB-C4A	3.85	1.38	1.33
25	b	616	CLA	CHB-C4A	3.86	1.38	1.33
25	C	505	CLA	CHB-C4A	3.86	1.38	1.33
25	c	509	CLA	CHB-C4A	3.86	1.38	1.33
25	b	614	CLA	CHB-C4A	3.87	1.38	1.33
25	C	507	CLA	CHB-C4A	3.87	1.38	1.33
25	B	611	CLA	CHB-C4A	3.87	1.38	1.33
25	C	508	CLA	CHB-C4A	3.88	1.38	1.33
25	c	506	CLA	CHB-C4A	3.88	1.38	1.33
25	B	609	CLA	CHB-C4A	3.88	1.38	1.33
25	B	603	CLA	CHB-C4A	3.89	1.38	1.33
25	b	613	CLA	CHB-C4A	3.89	1.38	1.33
25	b	622	CLA	CHB-C4A	3.90	1.38	1.33
25	d	403	CLA	CHB-C4A	3.90	1.38	1.33
25	B	617	CLA	CHB-C4A	3.91	1.38	1.33
25	A	607	CLA	CHB-C4A	3.91	1.38	1.33
25	b	620	CLA	CHB-C4A	3.91	1.38	1.33
25	c	512	CLA	CHB-C4A	3.91	1.38	1.33
25	a	711	CLA	CHB-C4A	3.91	1.38	1.33
25	C	506	CLA	CHB-C4A	3.91	1.38	1.33
25	b	609	CLA	CHB-C4A	3.91	1.38	1.33
25	C	509	CLA	CHB-C4A	3.92	1.38	1.33
25	D	402	CLA	CHB-C4A	3.92	1.38	1.33
25	b	617	CLA	CHB-C4A	3.92	1.38	1.33
25	b	615	CLA	CHB-C4A	3.92	1.38	1.33
25	c	502	CLA	CHB-C4A	3.92	1.38	1.33
25	b	611	CLA	CHB-C4A	3.92	1.38	1.33
25	C	513	CLA	CHB-C4A	3.93	1.38	1.33
25	B	616	CLA	CHB-C4A	3.93	1.38	1.33
25	c	508	CLA	CHB-C4A	3.93	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	CHB-C4A	3.94	1.38	1.33
25	b	607	CLA	CHB-C4A	3.94	1.38	1.33
25	C	514	CLA	CHB-C4A	3.94	1.38	1.33
25	B	610	CLA	CHB-C4A	3.95	1.38	1.33
25	D	403	CLA	CHB-C4A	3.95	1.38	1.33
25	C	503	CLA	CHB-C4A	3.96	1.38	1.33
25	c	501	CLA	CHB-C4A	3.96	1.38	1.33
25	b	608	CLA	CHB-C4A	3.96	1.38	1.33
25	B	613	CLA	CHB-C4A	3.98	1.38	1.33
25	c	503	CLA	CHB-C4A	3.98	1.38	1.33
25	B	602	CLA	CHB-C4A	3.98	1.38	1.33
25	d	402	CLA	CHB-C4A	3.98	1.38	1.33
25	B	606	CLA	CHB-C4A	3.99	1.38	1.33
25	B	614	CLA	CHB-C4A	3.99	1.38	1.33
25	C	510	CLA	CHB-C4A	3.99	1.38	1.33
25	C	512	CLA	CHB-C4A	3.99	1.38	1.33
25	D	404	CLA	CHB-C4A	3.99	1.38	1.33
25	C	502	CLA	CHB-C4A	4.00	1.38	1.33
25	b	610	CLA	CHB-C4A	4.00	1.38	1.33
25	B	612	CLA	CHB-C4A	4.01	1.38	1.33
25	B	604	CLA	CHB-C4A	4.01	1.38	1.33
25	b	612	CLA	CHB-C4A	4.01	1.38	1.33
25	b	621	CLA	CHB-C4A	4.02	1.38	1.33
25	C	511	CLA	CHB-C4A	4.02	1.38	1.33
25	a	707	CLA	CHB-C4A	4.03	1.38	1.33
25	b	619	CLA	CHB-C4A	4.03	1.38	1.33
25	B	607	CLA	CHB-C4A	4.03	1.38	1.33
25	c	511	CLA	CHB-C4A	4.03	1.38	1.33
25	B	615	CLA	CHB-C4A	4.04	1.38	1.33
25	a	719	CLA	CHB-C4A	4.04	1.38	1.33
25	c	504	CLA	CHB-C4A	4.04	1.38	1.33
25	c	513	CLA	CHB-C4A	4.05	1.39	1.33
25	c	510	CLA	CHB-C4A	4.06	1.39	1.33
25	A	606	CLA	CHB-C4A	4.08	1.39	1.33
25	B	605	CLA	CHB-C4A	4.12	1.39	1.33
25	b	618	CLA	CHB-C4A	4.14	1.39	1.33

All (945) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	612	SQD	O9-S-O7	-4.75	100.56	113.96
29	B	626	SQD	O9-S-O7	-4.71	100.66	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	623	SQD	O9-S-O7	-4.64	100.84	113.96
29	f	102	SQD	O9-S-O7	-4.54	101.13	113.96
29	D	410	SQD	O9-S-O7	-4.51	101.21	113.96
33	C	519	DGD	O3G-C3G-C2G	-4.48	100.32	110.99
29	a	714	SQD	O9-S-O7	-4.46	101.37	113.96
33	C	517	DGD	O3G-C3G-C2G	-4.38	100.56	110.99
33	c	516	DGD	O3G-C3G-C2G	-4.36	100.60	110.99
33	C	518	DGD	O3G-C3G-C2G	-4.32	100.70	110.99
33	c	518	DGD	O3G-C3G-C2G	-4.29	100.78	110.99
33	c	517	DGD	O3G-C3G-C2G	-4.27	100.82	110.99
29	b	601	SQD	O9-S-O7	-4.02	102.61	113.96
23	c	520	LMG	O6-C1-O1	-3.99	100.42	109.99
33	H	103	DGD	O3G-C3G-C2G	-3.90	101.71	110.99
25	d	403	CLA	CMB-C2B-C1B	-3.81	121.83	128.31
25	b	617	CLA	CMB-C2B-C1B	-3.81	121.83	128.31
23	C	521	LMG	O6-C1-O1	-3.78	100.91	109.99
25	C	514	CLA	CMB-C2B-C1B	-3.77	121.89	128.31
25	B	617	CLA	CMB-C2B-C1B	-3.76	121.92	128.31
25	B	612	CLA	CMB-C2B-C1B	-3.72	121.98	128.31
25	B	613	CLA	CMB-C2B-C1B	-3.71	122.00	128.31
25	c	512	CLA	CMB-C2B-C1B	-3.70	122.01	128.31
25	C	512	CLA	CMB-C2B-C1B	-3.70	122.02	128.31
25	b	622	CLA	CMB-C2B-C1B	-3.67	122.06	128.31
25	b	619	CLA	CMB-C2B-C1B	-3.63	122.14	128.31
25	c	513	CLA	CMB-C2B-C1B	-3.62	122.15	128.31
33	C	518	DGD	O5D-C6D-C5D	-3.56	102.80	109.14
25	c	510	CLA	CMB-C2B-C1B	-3.56	122.26	128.31
33	h	102	DGD	O3G-C3G-C2G	-3.54	102.56	110.99
25	b	612	CLA	CMB-C2B-C1B	-3.53	122.31	128.31
25	c	509	CLA	CMB-C2B-C1B	-3.52	122.32	128.31
25	a	707	CLA	CMB-C2B-C1B	-3.50	122.37	128.31
25	C	511	CLA	CMB-C2B-C1B	-3.48	122.39	128.31
33	C	519	DGD	O6D-C1D-O3G	-3.45	101.72	109.99
25	B	614	CLA	CMB-C2B-C1B	-3.45	122.45	128.31
25	c	503	CLA	CMB-C2B-C1B	-3.40	122.52	128.31
25	C	513	CLA	CMB-C2B-C1B	-3.40	122.53	128.31
25	B	609	CLA	CMB-C2B-C1B	-3.40	122.53	128.31
25	b	613	CLA	CMB-C2B-C1B	-3.40	122.53	128.31
33	c	518	DGD	O6D-C1D-O3G	-3.39	101.85	109.99
25	C	509	CLA	CMB-C2B-C1B	-3.39	122.55	128.31
25	B	604	CLA	CMB-C2B-C1B	-3.39	122.55	128.31
25	D	402	CLA	CMB-C2B-C1B	-3.38	122.56	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	CMB-C2B-C1B	-3.36	122.60	128.31
33	c	517	DGD	O6D-C1D-O3G	-3.36	101.94	109.99
25	b	609	CLA	CMB-C2B-C1B	-3.35	122.61	128.31
25	c	511	CLA	CMB-C2B-C1B	-3.35	122.61	128.31
33	C	518	DGD	O6D-C1D-O3G	-3.32	102.02	109.99
25	C	504	CLA	CMB-C2B-C1B	-3.30	122.71	128.31
33	C	517	DGD	O6D-C1D-O3G	-3.29	102.09	109.99
33	c	516	DGD	O6D-C1D-O3G	-3.29	102.10	109.99
25	A	606	CLA	CMB-C2B-C1B	-3.28	122.72	128.31
25	c	507	CLA	CMB-C2B-C1B	-3.24	122.79	128.31
25	b	614	CLA	CMB-C2B-C1B	-3.24	122.81	128.31
25	b	610	CLA	CMB-C2B-C1B	-3.22	122.83	128.31
25	B	607	CLA	CMB-C2B-C1B	-3.21	122.85	128.31
25	c	504	CLA	CMB-C2B-C1B	-3.21	122.85	128.31
25	C	506	CLA	CMB-C2B-C1B	-3.18	122.90	128.31
23	B	621	LMG	O6-C1-O1	-3.17	102.39	109.99
25	C	510	CLA	CMB-C2B-C1B	-3.16	122.93	128.31
25	B	608	CLA	CMB-C2B-C1B	-3.15	122.95	128.31
25	b	620	CLA	CMB-C2B-C1B	-3.15	122.95	128.31
27	b	602	BCR	C33-C5-C6	-3.12	121.29	124.62
27	t	103	BCR	C33-C5-C6	-3.12	121.30	124.62
25	c	508	CLA	CMB-C2B-C1B	-3.12	123.01	128.31
33	H	103	DGD	O6D-C1D-O3G	-3.10	102.55	109.99
25	C	507	CLA	CMB-C2B-C1B	-3.09	123.05	128.31
25	c	501	CLA	CMB-C2B-C1B	-3.08	123.07	128.31
25	C	505	CLA	CMB-C2B-C1B	-3.07	123.08	128.31
25	B	615	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
25	b	608	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
25	C	503	CLA	CMB-C2B-C1B	-3.05	123.13	128.31
25	C	508	CLA	CMB-C2B-C1B	-3.03	123.15	128.31
25	b	611	CLA	CMB-C2B-C1B	-3.03	123.16	128.31
25	b	607	CLA	CMB-C2B-C1B	-3.01	123.20	128.31
28	A	611	PL9	C22-C23-C24	-3.00	121.13	127.75
27	b	623	BCR	C33-C5-C6	-2.99	121.43	124.62
25	a	708	CLA	CMB-C2B-C1B	-2.98	123.25	128.31
25	b	618	CLA	CMB-C2B-C1B	-2.98	123.25	128.31
25	a	711	CLA	CMB-C2B-C1B	-2.97	123.25	128.31
25	C	502	CLA	CMB-C2B-C1B	-2.96	123.27	128.31
25	A	609	CLA	CMB-C2B-C1B	-2.95	123.29	128.31
25	D	404	CLA	CMB-C2B-C1B	-2.95	123.29	128.31
25	b	616	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
27	B	618	BCR	C33-C5-C6	-2.94	121.49	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	516	BCR	C15-C16-C17	-2.93	116.91	123.23
33	c	518	DGD	O5D-C6D-C5D	-2.93	103.93	109.14
25	b	621	CLA	CMB-C2B-C1B	-2.92	123.35	128.31
33	c	516	DGD	O5D-C6D-C5D	-2.92	103.95	109.14
27	k	101	BCR	C33-C5-C6	-2.91	121.52	124.62
25	B	606	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
33	h	102	DGD	O6D-C1D-O3G	-2.91	103.00	109.99
25	B	611	CLA	CMB-C2B-C1B	-2.90	123.38	128.31
25	a	719	CLA	CMB-C2B-C1B	-2.90	123.39	128.31
25	B	602	CLA	CMB-C2B-C1B	-2.89	123.39	128.31
27	H	102	BCR	C24-C23-C22	-2.89	121.85	126.21
25	B	616	CLA	CMB-C2B-C1B	-2.88	123.41	128.31
27	D	405	BCR	C33-C5-C6	-2.88	121.56	124.62
25	B	610	CLA	CMB-C2B-C1B	-2.87	123.43	128.31
25	c	502	CLA	CMB-C2B-C1B	-2.87	123.43	128.31
28	a	713	PL9	C22-C23-C24	-2.86	121.44	127.75
25	b	615	CLA	CMB-C2B-C1B	-2.86	123.45	128.31
25	b	607	CLA	O2D-CGD-O1D	-2.85	117.76	123.77
25	D	403	CLA	CMB-C2B-C1B	-2.85	123.46	128.31
28	A	611	PL9	C7-C8-C9	-2.85	121.85	126.70
25	B	603	CLA	CMB-C2B-C1B	-2.85	123.46	128.31
28	D	406	PL9	C27-C28-C29	-2.85	121.46	127.75
25	d	402	CLA	CMB-C2B-C1B	-2.85	123.47	128.31
25	B	605	CLA	CMB-C2B-C1B	-2.84	123.47	128.31
25	A	607	CLA	CMB-C2B-C1B	-2.84	123.48	128.31
28	a	713	PL9	C7-C3-C2	-2.84	118.53	122.66
33	C	519	DGD	C3G-C2G-C1G	-2.83	105.48	112.08
28	d	405	PL9	C22-C23-C24	-2.83	121.50	127.75
25	B	602	CLA	O2D-CGD-O1D	-2.83	117.81	123.77
27	B	620	BCR	C33-C5-C6	-2.83	121.61	124.62
27	Y	101	BCR	C33-C5-C6	-2.82	121.62	124.62
25	b	612	CLA	O2D-CGD-O1D	-2.80	117.87	123.77
27	b	625	BCR	C33-C5-C6	-2.80	121.64	124.62
25	B	607	CLA	O2D-CGD-O1D	-2.80	117.88	123.77
28	d	405	PL9	C27-C28-C29	-2.80	121.58	127.75
33	h	102	DGD	CDB-CCB-CBB	-2.79	100.04	114.54
25	c	505	CLA	CMB-C2B-C1B	-2.78	123.59	128.31
23	A	603	LMG	O6-C1-O1	-2.77	103.33	109.99
33	c	517	DGD	CDB-CCB-CBB	-2.77	100.14	114.54
27	t	103	BCR	C15-C14-C13	-2.77	123.19	127.22
27	c	514	BCR	C33-C5-C6	-2.76	121.68	124.62
25	B	604	CLA	O2D-CGD-O1D	-2.76	117.97	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	O2D-CGD-O1D	-2.75	117.98	123.77
25	b	621	CLA	O2D-CGD-O1D	-2.75	117.98	123.77
33	C	519	DGD	CDB-CCB-CBB	-2.74	100.28	114.54
27	C	516	BCR	C33-C5-C6	-2.74	121.71	124.62
27	c	515	BCR	C33-C5-C6	-2.73	121.71	124.62
25	a	708	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
33	C	518	DGD	CDB-CCB-CBB	-2.73	100.38	114.54
33	C	519	DGD	O5D-C6D-C5D	-2.72	104.29	109.14
25	C	502	CLA	O2D-CGD-O1D	-2.72	118.04	123.77
28	A	611	PL9	C27-C28-C29	-2.72	121.75	127.75
28	A	611	PL9	C7-C3-C2	-2.72	118.70	122.66
25	C	508	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
25	D	402	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
25	D	404	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
25	B	605	CLA	O2D-CGD-O1D	-2.71	118.07	123.77
33	c	516	DGD	CDB-CCB-CBB	-2.71	100.48	114.54
25	c	504	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
25	b	613	CLA	O2D-CGD-O1D	-2.70	118.09	123.77
25	C	506	CLA	O2D-CGD-O1D	-2.69	118.10	123.77
25	c	508	CLA	O2D-CGD-O1D	-2.69	118.10	123.77
28	D	406	PL9	C7-C3-C2	-2.69	118.75	122.66
32	D	408	LHG	C11-C10-C9	-2.69	100.59	114.54
27	c	515	BCR	C15-C16-C17	-2.68	117.45	123.23
33	c	518	DGD	C3G-C2G-C1G	-2.68	105.84	112.08
28	d	405	PL9	C7-C3-C2	-2.68	118.77	122.66
27	b	602	BCR	C15-C14-C13	-2.68	123.33	127.22
27	k	102	BCR	C33-C5-C6	-2.67	121.77	124.62
25	c	501	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
33	c	517	DGD	O5D-C6D-C5D	-2.67	104.38	109.14
33	c	518	DGD	CDB-CCB-CBB	-2.67	100.66	114.54
25	c	502	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
25	C	509	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
25	C	513	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
33	H	103	DGD	CDB-CCB-CBB	-2.67	100.69	114.54
23	f	101	LMG	O6-C1-O1	-2.66	103.61	109.99
33	C	517	DGD	O5D-C6D-C5D	-2.66	104.41	109.14
25	A	607	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
25	b	617	CLA	O2D-CGD-O1D	-2.66	118.18	123.77
25	B	616	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
25	C	503	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
33	C	517	DGD	C3G-C2G-C1G	-2.65	105.91	112.08
26	A	608	PHO	CBD-CHA-C4D	-2.64	105.56	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	505	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
25	B	603	CLA	O2D-CGD-O1D	-2.63	118.22	123.77
25	C	505	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
25	a	711	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
23	b	626	LMG	C4-C3-C2	-2.63	105.94	110.79
26	a	710	PHO	O2D-CGD-O1D	-2.63	118.24	123.77
25	B	609	CLA	O2D-CGD-O1D	-2.63	118.24	123.77
25	d	403	CLA	O2D-CGD-O1D	-2.62	118.25	123.77
25	b	609	CLA	O2D-CGD-O1D	-2.62	118.25	123.77
25	b	620	CLA	O2D-CGD-O1D	-2.62	118.25	123.77
25	C	510	CLA	O2D-CGD-O1D	-2.62	118.25	123.77
27	a	712	BCR	C33-C5-C6	-2.62	121.83	124.62
25	a	719	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
25	c	507	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
25	c	512	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
25	C	514	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
25	b	618	CLA	O2D-CGD-O1D	-2.61	118.28	123.77
27	b	624	BCR	C33-C5-C6	-2.61	121.84	124.62
27	B	618	BCR	C15-C16-C17	-2.61	117.61	123.23
25	d	402	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
26	D	401	PHO	CBD-CHA-C4D	-2.60	105.61	108.54
26	A	608	PHO	O2D-CGD-O1D	-2.60	118.29	123.77
27	K	101	BCR	C33-C5-C6	-2.60	121.85	124.62
28	D	406	PL9	C31-C32-C33	-2.60	104.79	111.61
25	B	613	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
25	B	615	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
25	A	609	CLA	O2D-CGD-O1D	-2.60	118.31	123.77
23	b	627	LMG	O6-C1-O1	-2.59	103.77	109.99
23	b	626	LMG	O2-C2-C1	-2.59	104.26	110.01
25	c	511	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
28	D	406	PL9	C22-C23-C24	-2.59	122.03	127.75
27	B	619	BCR	C33-C5-C6	-2.59	121.86	124.62
27	B	618	BCR	C11-C10-C9	-2.58	123.47	127.22
26	a	709	PHO	CBD-CHA-C4D	-2.58	105.63	108.54
23	A	603	LMG	O6-C1-C2	-2.58	104.92	110.28
25	C	511	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
23	a	701	LMG	O6-C1-O1	-2.56	103.84	109.99
33	C	517	DGD	CDB-CCB-CBB	-2.56	101.22	114.54
27	C	515	BCR	C33-C5-C6	-2.56	121.89	124.62
25	b	614	CLA	O2D-CGD-O1D	-2.56	118.38	123.77
27	b	623	BCR	C15-C14-C13	-2.56	123.50	127.22
27	A	610	BCR	C33-C5-C6	-2.56	121.90	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	611	CLA	O2D-CGD-O1D	-2.56	118.38	123.77
25	c	503	CLA	O2D-CGD-O1D	-2.56	118.39	123.77
34	e	102	HEM	CBA-CAA-C2A	-2.55	108.00	112.49
25	b	616	CLA	O2D-CGD-O1D	-2.55	118.40	123.77
28	D	406	PL9	C7-C8-C9	-2.55	122.36	126.70
25	c	510	CLA	O2D-CGD-O1D	-2.55	118.41	123.77
27	b	623	BCR	C15-C16-C17	-2.54	117.75	123.23
25	D	403	CLA	O2D-CGD-O1D	-2.54	118.43	123.77
27	t	103	BCR	C24-C23-C22	-2.53	122.38	126.21
25	b	608	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
27	c	515	BCR	C15-C14-C13	-2.53	123.54	127.22
25	b	622	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
25	B	612	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
26	a	710	PHO	CBD-CHA-C4D	-2.53	105.69	108.54
32	B	625	LHG	C11-C10-C9	-2.53	101.42	114.54
27	C	515	BCR	C11-C10-C9	-2.52	123.55	127.22
25	B	614	CLA	O2D-CGD-O1D	-2.52	118.46	123.77
25	b	619	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
28	a	713	PL9	C27-C28-C29	-2.52	122.20	127.75
23	B	621	LMG	O1-C7-C8	-2.51	105.01	110.99
25	B	608	CLA	O2D-CGD-O1D	-2.51	118.48	123.77
33	c	516	DGD	C3G-C2G-C1G	-2.51	106.23	112.08
32	d	406	LHG	C11-C10-C9	-2.51	101.50	114.54
27	D	405	BCR	C24-C23-C22	-2.51	122.42	126.21
27	t	103	BCR	C15-C16-C17	-2.51	117.83	123.23
23	c	519	LMG	O6-C1-O1	-2.50	103.99	109.99
25	C	504	CLA	O2D-CGD-O1D	-2.50	118.50	123.77
25	c	506	CLA	O2D-CGD-O1D	-2.50	118.50	123.77
26	D	401	PHO	O2D-CGD-O1D	-2.50	118.51	123.77
25	C	512	CLA	O2D-CGD-O1D	-2.50	118.51	123.77
25	B	610	CLA	O2D-CGD-O1D	-2.50	118.51	123.77
27	A	610	BCR	C24-C23-C22	-2.50	122.44	126.21
34	e	102	HEM	CMD-C2D-C1D	-2.49	124.07	128.31
25	B	617	CLA	O2D-CGD-O1D	-2.49	118.53	123.77
27	b	602	BCR	C15-C16-C17	-2.49	117.87	123.23
32	L	101	LHG	C11-C10-C9	-2.49	101.63	114.54
23	a	701	LMG	C38-C37-C36	-2.49	101.63	114.54
23	C	501	LMG	C38-C37-C36	-2.48	101.64	114.54
23	M	101	LMG	O6-C1-O1	-2.48	104.04	109.99
23	a	701	LMG	C40-C39-C38	-2.48	101.67	114.54
23	a	715	LMG	O6-C1-O1	-2.47	104.06	109.99
28	D	406	PL9	C37-C38-C39	-2.47	122.30	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	710	PHO	CMB-C2B-C1B	-2.46	121.13	125.06
23	b	626	LMG	O3-C3-C2	-2.46	104.82	110.36
23	f	101	LMG	O1-C1-C2	-2.46	104.98	108.00
32	b	629	LHG	C11-C10-C9	-2.46	101.78	114.54
23	M	101	LMG	C38-C37-C36	-2.45	101.83	114.54
25	c	513	CLA	O2D-CGD-O1D	-2.45	118.62	123.77
27	C	516	BCR	C15-C14-C13	-2.44	123.67	127.22
28	a	713	PL9	C7-C8-C9	-2.43	122.56	126.70
23	C	501	LMG	O6-C1-O1	-2.43	104.16	109.99
25	b	611	CLA	O2D-CGD-O1D	-2.42	118.67	123.77
32	D	408	LHG	C20-C19-C18	-2.42	101.98	114.54
25	c	509	CLA	O2D-CGD-O1D	-2.42	118.68	123.77
27	K	101	BCR	C24-C23-C22	-2.41	122.56	126.21
25	C	507	CLA	O2D-CGD-O1D	-2.41	118.70	123.77
33	h	102	DGD	C3G-C2G-C1G	-2.41	106.47	112.08
32	D	407	LHG	C20-C19-C18	-2.41	102.03	114.54
32	d	406	LHG	C20-C19-C18	-2.41	102.04	114.54
27	d	404	BCR	C7-C8-C9	-2.41	122.57	126.21
32	D	407	LHG	C11-C10-C9	-2.40	102.06	114.54
23	A	603	LMG	C1-C2-C3	-2.40	105.22	109.98
27	a	712	BCR	C24-C23-C22	-2.40	122.58	126.21
23	M	101	LMG	C40-C39-C38	-2.40	102.08	114.54
32	d	407	LHG	C20-C19-C18	-2.40	102.08	114.54
25	B	606	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
23	D	409	LMG	O6-C1-O1	-2.40	104.24	109.99
27	h	101	BCR	C24-C23-C22	-2.39	122.59	126.21
23	f	101	LMG	C40-C39-C38	-2.39	102.12	114.54
23	C	501	LMG	C40-C39-C38	-2.39	102.15	114.54
32	B	625	LHG	C20-C19-C18	-2.39	102.15	114.54
23	A	603	LMG	C40-C39-C38	-2.39	102.15	114.54
23	B	621	LMG	C38-C37-C36	-2.38	102.18	114.54
26	a	709	PHO	O2D-CGD-O1D	-2.38	118.76	123.77
27	c	514	BCR	C24-C23-C22	-2.38	122.61	126.21
26	D	401	PHO	CMB-C2B-C1B	-2.38	121.26	125.06
23	A	603	LMG	O3-C3-C2	-2.38	104.99	110.36
23	C	520	LMG	O6-C1-O1	-2.37	104.30	109.99
23	C	521	LMG	C40-C39-C38	-2.37	102.23	114.54
27	h	101	BCR	C15-C14-C13	-2.37	123.78	127.22
23	B	621	LMG	C40-C39-C38	-2.37	102.24	114.54
32	e	101	LHG	C11-C10-C9	-2.37	102.24	114.54
23	B	621	LMG	O3-C3-C2	-2.37	105.02	110.36
23	f	101	LMG	O1-C7-C8	-2.36	105.37	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	H	103	DGD	C3G-C2G-C1G	-2.36	106.58	112.08
27	b	624	BCR	C15-C14-C13	-2.36	123.79	127.22
23	a	701	LMG	O1-C7-C8	-2.36	105.38	110.99
23	b	627	LMG	C38-C37-C36	-2.36	102.30	114.54
23	c	520	LMG	C40-C39-C38	-2.36	102.30	114.54
28	a	713	PL9	C37-C38-C39	-2.36	122.55	127.75
23	c	519	LMG	C40-C39-C38	-2.35	102.31	114.54
27	d	404	BCR	C33-C5-C6	-2.35	122.11	124.62
23	C	520	LMG	O3-C3-C2	-2.35	105.06	110.36
27	c	514	BCR	C11-C10-C9	-2.35	123.80	127.22
23	a	715	LMG	C40-C39-C38	-2.35	102.34	114.54
23	D	409	LMG	C40-C39-C38	-2.35	102.35	114.54
28	D	406	PL9	C36-C34-C33	-2.35	116.61	120.98
23	b	627	LMG	C40-C39-C38	-2.35	102.36	114.54
32	L	101	LHG	C20-C19-C18	-2.34	102.36	114.54
32	d	407	LHG	C11-C10-C9	-2.34	102.38	114.54
32	e	101	LHG	C20-C19-C18	-2.34	102.40	114.54
27	H	102	BCR	C3-C4-C5	-2.34	109.99	113.87
32	b	629	LHG	C20-C19-C18	-2.34	102.41	114.54
23	c	519	LMG	C38-C37-C36	-2.33	102.45	114.54
27	b	625	BCR	C24-C23-C22	-2.33	122.69	126.21
23	f	101	LMG	O3-C3-C2	-2.32	105.12	110.36
27	b	624	BCR	C15-C16-C17	-2.32	118.22	123.23
27	B	618	BCR	C15-C14-C13	-2.32	123.86	127.22
23	f	101	LMG	O2-C2-C1	-2.32	104.87	110.01
26	a	709	PHO	CMB-C2B-C1B	-2.32	121.36	125.06
32	E	101	LHG	C20-C19-C18	-2.31	102.53	114.54
25	b	615	CLA	O2D-CGD-O1D	-2.31	118.90	123.77
27	D	405	BCR	C15-C16-C17	-2.31	118.25	123.23
32	e	101	LHG	C5-O7-C7	-2.31	112.20	117.91
23	b	626	LMG	C40-C39-C38	-2.30	102.58	114.54
28	d	405	PL9	C31-C32-C33	-2.30	105.57	111.61
27	c	514	BCR	C15-C14-C13	-2.30	123.88	127.22
23	f	101	LMG	C38-C37-C36	-2.30	102.60	114.54
23	a	701	LMG	O2-C2-C1	-2.30	104.91	110.01
33	c	518	DGD	C3D-C4D-C5D	-2.30	106.13	110.23
33	c	517	DGD	C3G-C2G-C1G	-2.30	106.73	112.08
23	a	715	LMG	C38-C37-C36	-2.29	102.62	114.54
25	A	606	CLA	O2D-CGD-O1D	-2.29	118.94	123.77
27	h	101	BCR	C11-C10-C9	-2.29	123.89	127.22
28	d	405	PL9	C7-C8-C9	-2.29	122.81	126.70
28	A	611	PL9	C46-C47-C48	-2.29	105.61	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	518	DGD	C3G-C2G-C1G	-2.28	106.76	112.08
28	a	713	PL9	C31-C32-C33	-2.28	105.62	111.61
23	C	520	LMG	O2-C2-C1	-2.28	104.95	110.01
27	K	101	BCR	C15-C14-C13	-2.28	123.90	127.22
27	c	514	BCR	C15-C16-C17	-2.28	118.32	123.23
27	d	404	BCR	C1-C6-C5	-2.28	119.45	122.50
28	d	405	PL9	C37-C38-C39	-2.27	122.73	127.75
23	c	519	LMG	O3-C3-C2	-2.27	105.24	110.36
23	M	101	LMG	O2-C2-C1	-2.27	104.97	110.01
23	a	715	LMG	O3-C3-C2	-2.27	105.24	110.36
23	c	520	LMG	C38-C37-C36	-2.27	102.76	114.54
23	C	520	LMG	C38-C37-C36	-2.27	102.76	114.54
23	A	603	LMG	C38-C37-C36	-2.27	102.77	114.54
23	C	521	LMG	C38-C37-C36	-2.27	102.77	114.54
23	C	521	LMG	O3-C3-C2	-2.27	105.25	110.36
27	B	620	BCR	C24-C23-C22	-2.26	122.79	126.21
25	a	707	CLA	O2D-CGD-O1D	-2.26	119.01	123.77
23	b	627	LMG	O2-C2-C1	-2.26	104.99	110.01
23	a	715	LMG	O2-C2-C1	-2.25	105.01	110.01
28	A	611	PL9	C31-C32-C33	-2.25	105.70	111.61
33	c	517	DGD	O3E-C3E-C2E	-2.25	105.28	110.36
33	c	517	DGD	CBB-CAB-C9B	-2.25	102.84	114.54
23	C	520	LMG	C40-C39-C38	-2.25	102.86	114.54
27	b	625	BCR	C38-C26-C25	-2.25	122.23	124.62
23	D	409	LMG	C38-C37-C36	-2.25	102.88	114.54
27	B	618	BCR	C7-C8-C9	-2.24	122.82	126.21
23	C	501	LMG	O3-C3-C2	-2.24	105.30	110.36
27	k	102	BCR	C24-C23-C22	-2.24	122.82	126.21
32	d	406	LHG	C18-C17-C16	-2.24	102.89	114.54
23	D	409	LMG	O2-C2-C1	-2.24	105.04	110.01
28	a	713	PL9	C32-C33-C34	-2.24	122.81	127.75
27	Y	101	BCR	C24-C23-C22	-2.23	122.83	126.21
23	M	101	LMG	O3-C3-C2	-2.23	105.33	110.36
27	b	623	BCR	C11-C10-C9	-2.23	123.98	127.22
33	h	102	DGD	C1D-C2D-C3D	-2.23	105.56	109.98
27	A	610	BCR	C15-C14-C13	-2.23	123.98	127.22
23	C	521	LMG	O2-C2-C3	-2.23	105.34	110.36
27	B	620	BCR	C38-C26-C25	-2.22	122.26	124.62
27	D	405	BCR	C7-C8-C9	-2.22	122.86	126.21
33	C	518	DGD	C3D-C4D-C5D	-2.21	106.28	110.23
27	H	102	BCR	C15-C14-C13	-2.21	124.01	127.22
33	c	518	DGD	O2D-C2D-C1D	-2.21	105.11	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	611	PL9	C37-C38-C39	-2.20	122.89	127.75
23	a	701	LMG	C1-O6-C5	-2.20	109.42	113.74
27	d	404	BCR	C24-C23-C22	-2.20	122.89	126.21
27	b	602	BCR	C11-C10-C9	-2.20	124.03	127.22
27	C	515	BCR	C15-C14-C13	-2.20	124.03	127.22
23	b	626	LMG	C38-C37-C36	-2.19	103.14	114.54
27	h	101	BCR	C33-C5-C6	-2.19	122.28	124.62
34	E	102	HEM	CBA-CAA-C2A	-2.19	108.64	112.49
23	c	519	LMG	O2-C2-C1	-2.19	105.14	110.01
23	c	520	LMG	O2-C2-C3	-2.18	105.43	110.36
33	H	103	DGD	C1D-C2D-C3D	-2.18	105.66	109.98
34	V	201	HEM	C3C-CAC-CBC	-2.18	122.01	126.40
32	D	408	LHG	C18-C17-C16	-2.18	103.22	114.54
23	b	626	LMG	O6-C1-O1	-2.18	104.77	109.99
28	A	611	PL9	C32-C33-C34	-2.18	122.95	127.75
27	a	712	BCR	C15-C14-C13	-2.18	124.06	127.22
23	c	520	LMG	O3-C3-C2	-2.17	105.46	110.36
27	D	405	BCR	C38-C26-C25	-2.17	122.31	124.62
26	A	608	PHO	CMB-C2B-C1B	-2.17	121.60	125.06
32	D	408	LHG	C27-C26-C25	-2.17	103.28	114.54
28	A	611	PL9	C12-C13-C14	-2.17	122.97	127.75
28	a	713	PL9	O2-C1-C2	-2.16	116.90	121.78
32	L	101	LHG	C18-C17-C16	-2.16	103.30	114.54
27	B	619	BCR	C15-C14-C13	-2.16	124.08	127.22
32	e	101	LHG	C27-C26-C25	-2.16	103.32	114.54
32	B	625	LHG	C27-C26-C25	-2.16	103.33	114.54
32	L	101	LHG	C27-C26-C25	-2.16	103.33	114.54
28	d	405	PL9	C46-C47-C48	-2.16	105.95	111.61
28	d	405	PL9	C32-C33-C34	-2.16	122.99	127.75
32	E	101	LHG	C11-C10-C9	-2.16	103.35	114.54
23	a	715	LMG	C1-C2-C3	-2.16	105.71	109.98
32	b	629	LHG	C18-C17-C16	-2.15	103.35	114.54
27	a	712	BCR	C15-C16-C17	-2.15	118.59	123.23
27	B	618	BCR	C24-C23-C22	-2.15	122.96	126.21
32	d	406	LHG	C27-C26-C25	-2.15	103.37	114.54
32	B	625	LHG	C18-C17-C16	-2.15	103.38	114.54
27	b	624	BCR	C38-C26-C25	-2.14	122.34	124.62
33	C	518	DGD	CBB-CAB-C9B	-2.14	103.42	114.54
33	C	518	DGD	O2D-C2D-C1D	-2.14	105.26	110.01
32	a	720	LHG	C27-C26-C25	-2.14	103.43	114.54
28	d	405	PL9	C12-C13-C14	-2.14	123.03	127.75
33	c	516	DGD	O2D-C2D-C1D	-2.14	105.27	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	621	LMG	O2-C2-C1	-2.14	105.27	110.01
28	A	611	PL9	O2-C1-C2	-2.14	116.96	121.78
33	c	516	DGD	CBB-CAB-C9B	-2.13	103.46	114.54
27	d	404	BCR	C11-C10-C9	-2.13	124.12	127.22
23	B	621	LMG	C3-C4-C5	-2.13	106.43	110.23
32	d	407	LHG	C18-C17-C16	-2.13	103.48	114.54
32	e	101	LHG	C18-C17-C16	-2.13	103.48	114.54
33	C	519	DGD	CAB-C9B-C8B	-2.13	103.49	114.54
28	D	406	PL9	O2-C1-C2	-2.13	116.99	121.78
23	C	501	LMG	C1-C2-C3	-2.13	105.76	109.98
23	D	409	LMG	O3-C3-C2	-2.13	105.56	110.36
27	K	101	BCR	C15-C16-C17	-2.13	118.65	123.23
28	a	713	PL9	C46-C47-C48	-2.13	106.03	111.61
23	A	603	LMG	O2-C2-C1	-2.12	105.30	110.01
27	H	102	BCR	C11-C10-C9	-2.12	124.14	127.22
28	D	406	PL9	C42-C43-C44	-2.12	123.07	127.75
33	C	518	DGD	O3E-C3E-C2E	-2.12	105.58	110.36
27	A	610	BCR	C15-C16-C17	-2.11	118.68	123.23
28	d	405	PL9	O2-C1-C2	-2.11	117.02	121.78
33	C	517	DGD	CAB-C9B-C8B	-2.11	103.59	114.54
32	d	407	LHG	C27-C26-C25	-2.11	103.59	114.54
27	Y	101	BCR	C15-C16-C17	-2.11	118.69	123.23
28	D	406	PL9	C46-C47-C48	-2.11	106.08	111.61
29	b	601	SQD	O48-C23-O10	-2.11	117.99	123.51
28	A	611	PL9	C36-C34-C33	-2.10	117.06	120.98
28	a	713	PL9	C12-C13-C14	-2.10	123.12	127.75
27	C	515	BCR	C24-C23-C22	-2.10	123.04	126.21
32	b	629	LHG	C27-C26-C25	-2.10	103.65	114.54
23	d	408	LMG	O7-C10-O9	-2.10	117.97	123.67
33	H	103	DGD	CBB-CAB-C9B	-2.09	103.66	114.54
28	D	406	PL9	C12-C13-C14	-2.09	123.13	127.75
27	C	515	BCR	C7-C8-C9	-2.09	123.05	126.21
23	D	409	LMG	C1-C2-C3	-2.09	105.83	109.98
33	c	518	DGD	CBB-CAB-C9B	-2.09	103.68	114.54
32	D	407	LHG	C27-C26-C25	-2.09	103.69	114.54
27	b	624	BCR	C11-C10-C9	-2.09	124.18	127.22
33	C	519	DGD	O2D-C2D-C1D	-2.09	105.38	110.01
33	c	518	DGD	CAB-C9B-C8B	-2.08	103.72	114.54
27	b	625	BCR	C15-C16-C17	-2.08	118.74	123.23
25	C	504	CLA	O2A-CGA-O1A	-2.08	118.05	123.51
23	C	520	LMG	C1-C2-C3	-2.08	105.85	109.98
32	E	101	LHG	C18-C17-C16	-2.08	103.73	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	101	LMG	C1-C2-C3	-2.08	105.86	109.98
26	A	608	PHO	C2B-C1B-NB	-2.08	106.71	109.81
25	B	605	CLA	O2A-CGA-O1A	-2.08	118.06	123.51
23	a	701	LMG	O3-C3-C2	-2.08	105.67	110.36
25	c	505	CLA	C4B-CHC-C1C	-2.08	125.22	129.34
25	C	509	CLA	O2A-CGA-O1A	-2.07	118.08	123.51
33	C	518	DGD	O2E-C2E-C1E	-2.07	105.41	110.01
34	E	102	HEM	CMD-C2D-C1D	-2.07	124.79	128.31
27	k	102	BCR	C15-C16-C17	-2.07	118.77	123.23
33	h	102	DGD	CBB-CAB-C9B	-2.07	103.78	114.54
32	D	407	LHG	C18-C17-C16	-2.07	103.79	114.54
27	H	102	BCR	C20-C21-C22	-2.07	124.21	127.22
25	C	507	CLA	O2A-CGA-O1A	-2.07	118.09	123.51
28	A	611	PL9	C36-C37-C38	-2.07	106.18	111.61
33	C	519	DGD	O6E-C1E-O5D	-2.07	105.03	109.99
25	b	617	CLA	O2A-CGA-O1A	-2.07	118.09	123.51
27	b	623	BCR	C24-C23-C22	-2.07	123.09	126.21
23	B	621	LMG	O7-C10-O9	-2.06	118.06	123.67
27	C	515	BCR	C15-C16-C17	-2.06	118.79	123.23
23	c	520	LMG	O2-C2-C1	-2.06	105.45	110.01
33	H	103	DGD	CAB-C9B-C8B	-2.05	103.87	114.54
33	C	518	DGD	CAB-C9B-C8B	-2.05	103.88	114.54
33	c	517	DGD	CAB-C9B-C8B	-2.05	103.89	114.54
27	C	516	BCR	C11-C10-C9	-2.05	124.24	127.22
27	b	602	BCR	C7-C8-C9	-2.05	123.12	126.21
33	C	517	DGD	CBB-CAB-C9B	-2.05	103.91	114.54
34	V	201	HEM	CMD-C2D-C1D	-2.05	124.83	128.31
33	c	517	DGD	O2D-C2D-C1D	-2.04	105.47	110.01
27	t	103	BCR	C35-C13-C14	-2.04	119.92	122.89
32	E	101	LHG	C27-C26-C25	-2.04	103.93	114.54
27	b	623	BCR	C7-C8-C9	-2.04	123.12	126.21
25	c	508	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
27	c	515	BCR	C38-C26-C25	-2.04	122.45	124.62
25	C	503	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
33	c	516	DGD	O3E-C3E-C2E	-2.04	105.75	110.36
33	c	517	DGD	C3D-C4D-C5D	-2.04	106.59	110.23
27	h	101	BCR	C38-C26-C25	-2.04	122.45	124.62
25	B	608	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
27	B	619	BCR	C24-C23-C22	-2.04	123.13	126.21
25	B	610	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
25	D	404	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
25	B	612	CLA	O2A-CGA-O1A	-2.04	118.17	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	621	LMG	O1-C1-C2	-2.04	105.50	108.00
25	A	606	CLA	O2A-CGA-O1A	-2.03	118.18	123.51
27	B	619	BCR	C15-C16-C17	-2.03	118.85	123.23
25	b	608	CLA	C4B-CHC-C1C	-2.03	125.31	129.34
23	D	409	LMG	O1-C7-C8	-2.03	106.16	110.99
28	D	406	PL9	C36-C37-C38	-2.03	106.28	111.61
28	d	405	PL9	C42-C43-C44	-2.03	123.27	127.75
25	B	617	CLA	O2A-CGA-O1A	-2.03	118.19	123.51
27	b	625	BCR	C15-C14-C13	-2.03	124.27	127.22
23	C	501	LMG	O2-C2-C1	-2.03	105.51	110.01
27	k	102	BCR	C15-C14-C13	-2.03	124.27	127.22
25	B	614	CLA	O2A-CGA-O1A	-2.03	118.20	123.51
25	C	514	CLA	O2A-CGA-O1A	-2.03	118.20	123.51
25	c	503	CLA	O2A-CGA-O1A	-2.03	118.20	123.51
25	c	502	CLA	O2A-CGA-O1A	-2.02	118.20	123.51
33	c	516	DGD	CAB-C9B-C8B	-2.02	104.03	114.54
23	d	408	LMG	C38-C37-C36	-2.02	104.03	114.54
25	C	511	CLA	O2A-CGA-O1A	-2.02	118.22	123.51
25	b	609	CLA	C4B-CHC-C1C	-2.02	125.33	129.34
32	d	406	LHG	C5-O7-C7	-2.02	112.92	117.91
33	c	518	DGD	O6E-C1E-O5D	-2.02	105.15	109.99
26	a	709	PHO	C2B-C1B-NB	-2.02	106.81	109.81
33	h	102	DGD	CAB-C9B-C8B	-2.02	104.07	114.54
23	d	408	LMG	C40-C39-C38	-2.01	104.08	114.54
33	C	517	DGD	C5B-C4B-C3B	-2.01	104.08	114.54
33	c	516	DGD	C5B-C4B-C3B	-2.01	104.08	114.54
25	C	506	CLA	C4B-CHC-C1C	-2.01	125.34	129.34
27	D	405	BCR	C11-C10-C9	-2.01	124.30	127.22
25	C	512	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
25	b	619	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
34	v	201	HEM	CBA-CAA-C2A	-2.00	108.97	112.49
33	C	519	DGD	O3E-C3E-C2E	-2.00	105.84	110.36
33	C	519	DGD	C5B-C4B-C3B	-2.00	104.15	114.54
25	A	607	CLA	C4A-NA-C1A	2.00	108.92	106.38
25	b	617	CLA	O1D-CGD-CBD	2.00	127.75	124.64
25	c	511	CLA	O1D-CGD-CBD	2.00	127.75	124.64
28	d	405	PL9	C35-C34-C36	2.01	118.42	115.37
25	C	505	CLA	CMD-C2D-C3D	2.01	129.01	125.09
25	b	616	CLA	C4A-NA-C1A	2.01	108.92	106.38
25	B	612	CLA	O1D-CGD-CBD	2.01	127.76	124.64
27	B	620	BCR	C2-C1-C6	2.03	113.49	110.48
25	a	711	CLA	O2D-CGD-CBD	2.03	114.14	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	506	CLA	CMD-C2D-C3D	2.03	129.07	125.09
25	B	605	CLA	CMD-C2D-C3D	2.03	129.07	125.09
25	b	610	CLA	CMD-C2D-C3D	2.03	129.07	125.09
25	b	614	CLA	C4A-NA-C1A	2.04	108.96	106.38
25	c	502	CLA	O2D-CGD-CBD	2.04	114.16	111.22
25	C	507	CLA	O1D-CGD-CBD	2.04	127.81	124.64
25	c	506	CLA	O1D-CGD-CBD	2.04	127.81	124.64
25	b	607	CLA	CMD-C2D-C3D	2.04	129.09	125.09
29	B	623	SQD	O6-C1-C2	2.04	110.52	108.00
25	c	501	CLA	CMD-C2D-C3D	2.05	129.09	125.09
25	B	615	CLA	O2D-CGD-CBD	2.05	114.17	111.22
25	B	606	CLA	CMD-C2D-C3D	2.05	129.09	125.09
25	B	606	CLA	O1D-CGD-CBD	2.05	127.83	124.64
27	b	623	BCR	C4-C5-C6	2.05	124.99	122.73
25	C	513	CLA	O2D-CGD-CBD	2.05	114.18	111.22
25	C	514	CLA	O1D-CGD-CBD	2.05	127.83	124.64
25	B	609	CLA	O2D-CGD-CBD	2.06	114.18	111.22
25	a	708	CLA	CMD-C2D-C3D	2.06	129.11	125.09
25	a	719	CLA	CMD-C2D-C3D	2.06	129.12	125.09
25	c	505	CLA	C4A-NA-C1A	2.06	108.99	106.38
25	B	614	CLA	O1D-CGD-CBD	2.06	127.84	124.64
25	C	510	CLA	CMD-C2D-C3D	2.06	129.12	125.09
27	t	103	BCR	C4-C5-C6	2.06	125.00	122.73
25	b	612	CLA	CMD-C2D-C3D	2.06	129.13	125.09
25	B	603	CLA	O1D-CGD-CBD	2.07	127.85	124.64
25	d	403	CLA	O2D-CGD-CBD	2.07	114.20	111.22
27	d	404	BCR	C2-C3-C4	2.07	116.67	111.42
25	c	507	CLA	C2A-C1A-CHA	2.07	127.14	123.80
25	C	511	CLA	CMD-C2D-C3D	2.08	129.15	125.09
25	B	615	CLA	C4A-NA-C1A	2.08	109.01	106.38
25	c	506	CLA	C4A-NA-C1A	2.08	109.01	106.38
25	c	501	CLA	O1D-CGD-CBD	2.08	127.87	124.64
25	B	604	CLA	C4A-NA-C1A	2.08	109.02	106.38
25	B	611	CLA	C4A-NA-C1A	2.08	109.02	106.38
29	A	614	SQD	C45-O47-C7	2.08	123.05	117.91
27	b	602	BCR	C4-C5-C6	2.08	125.02	122.73
25	b	614	CLA	CMD-C2D-C3D	2.09	129.17	125.09
25	C	508	CLA	O1D-CGD-CBD	2.09	127.88	124.64
25	C	514	CLA	CMD-C2D-C3D	2.09	129.18	125.09
25	d	403	CLA	C4A-NA-C1A	2.09	109.03	106.38
25	C	504	CLA	O1D-CGD-CBD	2.09	127.89	124.64
25	C	503	CLA	O2D-CGD-CBD	2.09	114.24	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	CMD-C2D-C3D	2.09	129.18	125.09
25	B	608	CLA	CMD-C2D-C3D	2.10	129.19	125.09
25	b	620	CLA	CMD-C2D-C3D	2.10	129.19	125.09
33	c	516	DGD	O6E-C5E-C4E	2.10	113.67	109.67
25	c	504	CLA	C4A-NA-C1A	2.10	109.04	106.38
25	C	502	CLA	CMD-C2D-C3D	2.10	129.19	125.09
25	C	504	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	C	512	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	b	613	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	c	504	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	B	603	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	B	613	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	b	611	CLA	O1D-CGD-CBD	2.11	127.91	124.64
25	b	611	CLA	C4A-NA-C1A	2.11	109.05	106.38
25	b	608	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	c	511	CLA	CMD-C2D-C3D	2.11	129.22	125.09
25	b	617	CLA	CMD-C2D-C3D	2.11	129.22	125.09
25	A	607	CLA	O2D-CGD-CBD	2.11	114.26	111.22
25	A	609	CLA	C4A-NA-C1A	2.11	109.06	106.38
25	b	616	CLA	CMD-C2D-C3D	2.12	129.24	125.09
25	c	509	CLA	CMD-C2D-C3D	2.12	129.24	125.09
33	C	517	DGD	O6E-C5E-C4E	2.12	113.71	109.67
27	b	625	BCR	C2-C1-C6	2.12	113.64	110.48
25	c	505	CLA	CMD-C2D-C3D	2.12	129.24	125.09
25	D	403	CLA	C4A-NA-C1A	2.12	109.07	106.38
25	B	614	CLA	CMD-C2D-C3D	2.13	129.25	125.09
26	a	710	PHO	C1B-NB-C4B	2.13	110.54	106.50
25	a	711	CLA	C4A-NA-C1A	2.13	109.08	106.38
25	C	505	CLA	O2D-CGD-CBD	2.13	114.29	111.22
28	D	406	PL9	C35-C34-C36	2.13	118.62	115.37
26	a	709	PHO	C1B-NB-C4B	2.13	110.55	106.50
25	c	507	CLA	CMD-C2D-C3D	2.13	129.26	125.09
25	b	608	CLA	O2D-CGD-CBD	2.14	114.30	111.22
25	B	607	CLA	CMD-C2D-C3D	2.14	129.27	125.09
25	B	611	CLA	CMD-C2D-C3D	2.14	129.28	125.09
25	c	508	CLA	C4A-NA-C1A	2.15	109.10	106.38
25	C	507	CLA	CMD-C2D-C3D	2.15	129.29	125.09
25	B	608	CLA	O1D-CGD-CBD	2.15	127.98	124.64
25	C	512	CLA	O1D-CGD-CBD	2.15	127.98	124.64
25	B	612	CLA	CMD-C2D-C3D	2.15	129.30	125.09
25	B	615	CLA	CMD-C2D-C3D	2.15	129.30	125.09
25	b	615	CLA	O1D-CGD-CBD	2.15	127.99	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	C4A-NA-C1A	2.16	109.11	106.38
25	D	403	CLA	CMD-C2D-C3D	2.16	129.31	125.09
25	b	617	CLA	C4A-NA-C1A	2.16	109.12	106.38
26	D	401	PHO	C1B-NB-C4B	2.17	110.61	106.50
25	b	609	CLA	O2D-CGD-CBD	2.17	114.34	111.22
25	C	511	CLA	C4A-NA-C1A	2.17	109.13	106.38
25	C	510	CLA	O1D-CGD-CBD	2.17	128.01	124.64
25	D	404	CLA	CMD-C2D-C3D	2.17	129.33	125.09
25	a	711	CLA	CMD-C2D-C3D	2.17	129.33	125.09
25	d	403	CLA	CMD-C2D-C3D	2.17	129.34	125.09
25	c	501	CLA	C4A-NA-C1A	2.18	109.14	106.38
25	C	508	CLA	CMD-C2D-C3D	2.18	129.35	125.09
25	c	506	CLA	CMD-C2D-C3D	2.18	129.35	125.09
25	C	514	CLA	C4A-NA-C1A	2.18	109.14	106.38
25	C	507	CLA	C4A-NA-C1A	2.18	109.15	106.38
25	a	708	CLA	O2D-CGD-CBD	2.18	114.36	111.22
25	A	609	CLA	CMD-C2D-C3D	2.18	129.36	125.09
25	b	615	CLA	CMD-C2D-C3D	2.18	129.36	125.09
25	D	404	CLA	O2D-CGD-CBD	2.18	114.37	111.22
25	B	604	CLA	CMD-C2D-C3D	2.18	129.36	125.09
25	B	610	CLA	CMD-C2D-C3D	2.19	129.36	125.09
25	B	607	CLA	O2D-CGD-CBD	2.19	114.38	111.22
25	D	404	CLA	C4A-NA-C1A	2.19	109.16	106.38
25	C	509	CLA	C4A-NA-C1A	2.19	109.16	106.38
29	b	601	SQD	O5-C5-C4	2.19	113.85	109.67
29	D	410	SQD	O48-C23-C24	2.20	118.62	111.85
25	d	402	CLA	CMD-C2D-C3D	2.21	129.40	125.09
25	B	616	CLA	CMD-C2D-C3D	2.21	129.40	125.09
25	B	607	CLA	C4A-NA-C1A	2.21	109.18	106.38
25	C	511	CLA	O1D-CGD-CBD	2.21	128.08	124.64
27	c	514	BCR	C2-C1-C6	2.21	113.77	110.48
26	A	608	PHO	C1B-NB-C4B	2.22	110.71	106.50
25	b	619	CLA	CMD-C2D-C3D	2.22	129.42	125.09
25	b	619	CLA	O1D-CGD-CBD	2.22	128.09	124.64
25	c	510	CLA	C4A-NA-C1A	2.22	109.20	106.38
25	c	513	CLA	CMD-C2D-C3D	2.23	129.44	125.09
25	c	502	CLA	CMD-C2D-C3D	2.23	129.45	125.09
25	d	402	CLA	C4A-NA-C1A	2.23	109.21	106.38
25	C	503	CLA	C4A-NA-C1A	2.24	109.22	106.38
25	B	604	CLA	O2D-CGD-CBD	2.24	114.45	111.22
25	b	622	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	b	618	CLA	O1D-CGD-CBD	2.25	128.14	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	502	CLA	C4A-NA-C1A	2.26	109.24	106.38
25	C	503	CLA	CMD-C2D-C3D	2.26	129.52	125.09
25	B	609	CLA	CMD-C2D-C3D	2.27	129.52	125.09
25	B	614	CLA	C4A-NA-C1A	2.27	109.26	106.38
25	b	622	CLA	C4A-NA-C1A	2.27	109.26	106.38
25	c	508	CLA	O2D-CGD-CBD	2.28	114.50	111.22
25	b	618	CLA	CMD-C2D-C3D	2.28	129.54	125.09
29	a	714	SQD	C44-O6-C1	2.28	118.57	113.81
25	C	509	CLA	CMD-C2D-C3D	2.28	129.54	125.09
25	b	616	CLA	O1D-CGD-CBD	2.28	128.19	124.64
25	B	602	CLA	C4A-NA-C1A	2.29	109.28	106.38
25	C	506	CLA	C4A-NA-C1A	2.29	109.28	106.38
25	B	617	CLA	O1D-CGD-CBD	2.29	128.20	124.64
25	C	506	CLA	O2D-CGD-CBD	2.29	114.53	111.22
25	B	612	CLA	C4A-NA-C1A	2.29	109.29	106.38
29	A	612	SQD	C1-O5-C5	2.30	118.25	113.74
25	c	507	CLA	O1D-CGD-CBD	2.30	128.21	124.64
25	D	402	CLA	O2D-CGD-CBD	2.30	114.54	111.22
25	b	618	CLA	C4A-NA-C1A	2.31	109.31	106.38
25	c	509	CLA	O1D-CGD-CBD	2.31	128.23	124.64
25	c	502	CLA	C4A-NA-C1A	2.31	109.31	106.38
25	B	613	CLA	C4A-NA-C1A	2.31	109.31	106.38
25	B	605	CLA	CMB-C2B-C3B	2.32	129.62	125.09
26	D	401	PHO	C3D-C4D-CHA	2.32	112.78	107.14
25	B	610	CLA	O1D-CGD-CBD	2.32	128.25	124.64
29	f	102	SQD	O48-C23-C24	2.32	119.00	111.85
25	B	617	CLA	C4A-NA-C1A	2.33	109.33	106.38
29	a	714	SQD	O8-S-C6	2.33	109.83	104.99
25	C	502	CLA	O2D-CGD-CBD	2.33	114.58	111.22
25	b	607	CLA	C4A-NA-C1A	2.34	109.34	106.38
25	B	617	CLA	CMD-C2D-C3D	2.34	129.66	125.09
25	C	512	CLA	C4A-NA-C1A	2.34	109.34	106.38
25	b	622	CLA	O1D-CGD-CBD	2.34	128.28	124.64
29	f	102	SQD	O47-C7-C8	2.34	119.18	110.82
26	D	401	PHO	CBD-CHA-C1A	2.34	130.83	126.70
29	f	102	SQD	O8-S-C6	2.35	109.86	104.99
25	B	610	CLA	C4A-NA-C1A	2.35	109.36	106.38
26	a	710	PHO	CBD-CHA-C1A	2.35	130.84	126.70
26	a	709	PHO	C3D-C4D-CHA	2.35	112.85	107.14
25	B	616	CLA	C4A-NA-C1A	2.35	109.36	106.38
25	C	510	CLA	C4A-NA-C1A	2.35	109.36	106.38
28	A	611	PL9	C20-C19-C21	2.35	118.96	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	612	SQD	O8-S-C6	2.36	109.89	104.99
25	B	611	CLA	O1D-CGD-CBD	2.36	128.31	124.64
25	b	615	CLA	C4A-NA-C1A	2.36	109.37	106.38
29	D	410	SQD	C3-C4-C5	2.37	114.45	110.23
25	c	510	CLA	O1D-CGD-CBD	2.37	128.32	124.64
26	A	608	PHO	C3D-C4D-CHA	2.37	112.90	107.14
25	b	612	CLA	O2D-CGD-CBD	2.37	114.64	111.22
25	b	607	CLA	CMB-C2B-C3B	2.37	129.73	125.09
25	c	512	CLA	C4A-NA-C1A	2.37	109.39	106.38
25	C	513	CLA	CMD-C2D-C3D	2.37	129.73	125.09
26	a	710	PHO	C3D-C4D-CHA	2.38	112.93	107.14
25	c	502	CLA	CMB-C2B-C3B	2.38	129.74	125.09
29	f	102	SQD	C44-O6-C1	2.38	118.79	113.81
25	c	505	CLA	O2D-CGD-CBD	2.38	114.65	111.22
25	B	613	CLA	O1D-CGD-CBD	2.38	128.34	124.64
29	D	410	SQD	O8-S-C6	2.39	109.95	104.99
25	c	504	CLA	O2D-CGD-CBD	2.39	114.66	111.22
25	A	607	CLA	CMB-C2B-C3B	2.39	129.76	125.09
25	c	503	CLA	C4A-NA-C1A	2.39	109.42	106.38
25	c	513	CLA	C4A-NA-C1A	2.40	109.42	106.38
28	a	713	PL9	C20-C19-C21	2.40	119.03	115.37
25	c	512	CLA	O1D-CGD-CBD	2.40	128.37	124.64
25	c	511	CLA	C4A-NA-C1A	2.40	109.43	106.38
25	B	610	CLA	CMB-C2B-C3B	2.41	129.79	125.09
25	B	616	CLA	O2D-CGD-CBD	2.41	114.69	111.22
25	C	502	CLA	CMB-C2B-C3B	2.41	129.80	125.09
25	b	616	CLA	CMB-C2B-C3B	2.41	129.80	125.09
25	c	509	CLA	C4A-NA-C1A	2.41	109.44	106.38
25	c	508	CLA	CMD-C2D-C3D	2.41	129.81	125.09
25	C	504	CLA	C4A-NA-C1A	2.41	109.44	106.38
29	a	714	SQD	C4-C3-C2	2.42	115.25	110.79
25	c	507	CLA	C4A-NA-C1A	2.43	109.46	106.38
25	C	509	CLA	O2D-CGD-CBD	2.43	114.72	111.22
29	b	601	SQD	O8-S-C6	2.43	110.05	104.99
25	B	611	CLA	CMB-C2B-C3B	2.43	129.85	125.09
25	B	602	CLA	CMB-C2B-C3B	2.43	129.85	125.09
25	b	613	CLA	O2D-CGD-CBD	2.43	114.73	111.22
25	b	615	CLA	CMB-C2B-C3B	2.43	129.85	125.09
25	c	505	CLA	CMB-C2B-C3B	2.44	129.85	125.09
25	D	403	CLA	CMB-C2B-C3B	2.44	129.85	125.09
25	a	719	CLA	CMB-C2B-C3B	2.44	129.85	125.09
25	b	621	CLA	C4A-NA-C1A	2.44	109.48	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	CLA	CMB-C2B-C3B	2.44	129.87	125.09
25	d	402	CLA	CMB-C2B-C3B	2.44	129.87	125.09
25	B	603	CLA	CMB-C2B-C3B	2.45	129.87	125.09
25	B	616	CLA	CMB-C2B-C3B	2.45	129.88	125.09
25	b	619	CLA	C4A-NA-C1A	2.46	109.50	106.38
32	e	101	LHG	O8-C23-C24	2.46	119.42	111.85
26	a	709	PHO	CBD-CHA-C1A	2.47	131.06	126.70
29	b	601	SQD	C4-C3-C2	2.47	115.33	110.79
25	b	618	CLA	CMB-C2B-C3B	2.48	129.93	125.09
25	B	606	CLA	CMB-C2B-C3B	2.48	129.93	125.09
25	b	611	CLA	CMB-C2B-C3B	2.48	129.94	125.09
25	D	404	CLA	CMB-C2B-C3B	2.48	129.94	125.09
25	b	621	CLA	CMD-C2D-C3D	2.48	129.94	125.09
25	C	513	CLA	C4A-NA-C1A	2.49	109.53	106.38
25	c	513	CLA	O1D-CGD-CBD	2.49	128.51	124.64
25	c	512	CLA	CMD-C2D-C3D	2.49	129.96	125.09
29	B	623	SQD	C44-O6-C1	2.50	119.04	113.81
25	a	708	CLA	CMB-C2B-C3B	2.50	129.99	125.09
25	a	711	CLA	CMB-C2B-C3B	2.51	129.99	125.09
25	c	501	CLA	CMB-C2B-C3B	2.51	129.99	125.09
25	C	508	CLA	C4A-NA-C1A	2.51	109.57	106.38
25	b	610	CLA	C4A-NA-C1A	2.53	109.58	106.38
27	k	102	BCR	C29-C30-C25	2.54	114.27	110.48
25	A	606	CLA	O1D-CGD-CBD	2.55	128.60	124.64
26	A	608	PHO	CBD-CHA-C1A	2.55	131.20	126.70
25	B	615	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	C	503	CLA	CMB-C2B-C3B	2.55	130.08	125.09
32	D	408	LHG	O8-C23-C24	2.56	119.72	111.85
32	b	629	LHG	O8-C23-C24	2.56	119.73	111.85
25	b	610	CLA	O2D-CGD-CBD	2.56	114.91	111.22
25	A	609	CLA	CMB-C2B-C3B	2.56	130.10	125.09
25	C	507	CLA	CMB-C2B-C3B	2.57	130.11	125.09
25	b	621	CLA	O2D-CGD-CBD	2.58	114.94	111.22
29	B	626	SQD	O48-C23-C24	2.59	119.81	111.85
25	B	605	CLA	O2D-CGD-CBD	2.59	114.96	111.22
25	C	505	CLA	CMB-C2B-C3B	2.59	130.16	125.09
25	B	607	CLA	CMB-C2B-C3B	2.60	130.18	125.09
25	B	605	CLA	C4A-NA-C1A	2.60	109.68	106.38
29	A	614	SQD	O48-C23-C24	2.61	119.87	111.85
25	B	608	CLA	CMB-C2B-C3B	2.62	130.21	125.09
25	c	508	CLA	CMB-C2B-C3B	2.62	130.21	125.09
29	a	714	SQD	O48-C23-C24	2.62	119.91	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	623	SQD	C1-C2-C3	2.62	115.18	109.98
25	b	608	CLA	CMB-C2B-C3B	2.62	130.22	125.09
25	C	508	CLA	CMB-C2B-C3B	2.62	130.22	125.09
29	A	612	SQD	O48-C23-C24	2.62	119.92	111.85
25	b	620	CLA	CMB-C2B-C3B	2.62	130.22	125.09
25	a	707	CLA	O1D-CGD-CBD	2.63	128.72	124.64
25	b	614	CLA	CMB-C2B-C3B	2.65	130.27	125.09
25	c	504	CLA	CMB-C2B-C3B	2.65	130.28	125.09
29	B	623	SQD	O48-C23-C24	2.65	120.01	111.85
28	D	406	PL9	C20-C19-C21	2.66	119.43	115.37
32	L	101	LHG	O8-C23-C24	2.67	120.06	111.85
25	C	510	CLA	CMB-C2B-C3B	2.68	130.32	125.09
29	f	102	SQD	O5-C5-C4	2.68	114.79	109.67
25	b	610	CLA	CMB-C2B-C3B	2.69	130.35	125.09
29	I	102	SQD	O48-C23-C24	2.69	120.14	111.85
28	d	405	PL9	C20-C19-C21	2.70	119.48	115.37
23	A	603	LMG	O6-C5-C4	2.71	114.84	109.67
25	C	504	CLA	CMB-C2B-C3B	2.72	130.42	125.09
29	b	601	SQD	C44-O6-C1	2.74	119.54	113.81
25	C	506	CLA	CMB-C2B-C3B	2.75	130.46	125.09
27	B	618	BCR	C27-C26-C25	2.75	125.75	122.73
32	d	407	LHG	O8-C23-C24	2.75	120.33	111.85
27	C	515	BCR	C2-C1-C6	2.76	114.58	110.48
25	A	606	CLA	CMB-C2B-C3B	2.76	130.48	125.09
27	B	618	BCR	C29-C30-C25	2.78	114.61	110.48
32	d	406	LHG	O8-C23-C24	2.79	120.42	111.85
25	c	511	CLA	CMB-C2B-C3B	2.80	130.57	125.09
25	c	506	CLA	CMB-C2B-C3B	2.81	130.59	125.09
32	E	101	LHG	O8-C23-C24	2.81	120.51	111.85
25	b	609	CLA	CMB-C2B-C3B	2.82	130.60	125.09
25	b	613	CLA	CMB-C2B-C3B	2.83	130.63	125.09
25	c	507	CLA	CMB-C2B-C3B	2.84	130.64	125.09
29	B	623	SQD	O8-S-C6	2.84	110.89	104.99
32	D	407	LHG	O8-C23-C24	2.85	120.62	111.85
25	B	602	CLA	O2D-CGD-CBD	2.85	115.33	111.22
25	B	604	CLA	CMB-C2B-C3B	2.86	130.68	125.09
25	c	503	CLA	CMB-C2B-C3B	2.86	130.68	125.09
28	D	406	PL9	C40-C39-C41	2.87	119.74	115.37
25	b	607	CLA	O2D-CGD-CBD	2.87	115.36	111.22
25	B	614	CLA	CMB-C2B-C3B	2.88	130.71	125.09
25	C	509	CLA	CMB-C2B-C3B	2.88	130.72	125.09
29	B	626	SQD	C3-C4-C5	2.88	115.37	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	402	CLA	CMB-C2B-C3B	2.89	130.74	125.09
32	B	625	LHG	O8-C23-C24	2.89	120.76	111.85
32	a	720	LHG	O8-C23-C24	2.90	120.78	111.85
25	B	609	CLA	CMB-C2B-C3B	2.90	130.77	125.09
25	C	513	CLA	CMB-C2B-C3B	2.91	130.79	125.09
28	a	713	PL9	C40-C39-C41	2.92	119.82	115.37
25	b	612	CLA	CMB-C2B-C3B	2.93	130.83	125.09
25	a	707	CLA	CMB-C2B-C3B	2.93	130.83	125.09
25	C	511	CLA	CMB-C2B-C3B	2.96	130.87	125.09
26	A	608	PHO	O1D-CGD-CBD	2.96	129.24	124.64
29	D	410	SQD	O5-C5-C4	2.97	115.33	109.67
25	c	509	CLA	CMB-C2B-C3B	2.97	130.90	125.09
29	B	623	SQD	C1-O5-C5	2.98	119.58	113.74
27	k	102	BCR	C27-C26-C25	3.00	126.03	122.73
23	b	626	LMG	C1-O6-C5	3.01	119.65	113.74
27	b	602	BCR	C27-C26-C25	3.01	126.04	122.73
25	c	510	CLA	CMB-C2B-C3B	3.02	130.99	125.09
27	t	103	BCR	C27-C26-C25	3.02	126.05	122.73
25	B	612	CLA	CMB-C2B-C3B	3.03	131.02	125.09
25	b	619	CLA	CMB-C2B-C3B	3.05	131.05	125.09
29	A	612	SQD	C3-C4-C5	3.05	115.67	110.23
27	h	101	BCR	C2-C1-C6	3.07	115.05	110.48
27	k	101	BCR	C27-C26-C25	3.08	126.12	122.73
25	B	613	CLA	CMB-C2B-C3B	3.09	131.14	125.09
27	C	516	BCR	C27-C26-C25	3.10	126.14	122.73
29	B	626	SQD	C1-O5-C5	3.10	119.82	113.74
28	A	611	PL9	C40-C39-C41	3.11	120.11	115.37
28	d	405	PL9	C40-C39-C41	3.12	120.13	115.37
25	b	617	CLA	CMB-C2B-C3B	3.12	131.19	125.09
25	C	512	CLA	CMB-C2B-C3B	3.13	131.22	125.09
27	A	610	BCR	C27-C26-C25	3.14	126.19	122.73
27	Y	101	BCR	C27-C26-C25	3.16	126.20	122.73
25	c	513	CLA	CMB-C2B-C3B	3.16	131.27	125.09
27	C	515	BCR	C27-C26-C25	3.20	126.25	122.73
26	a	709	PHO	O1D-CGD-CBD	3.20	129.61	124.64
25	b	622	CLA	CMB-C2B-C3B	3.20	131.35	125.09
25	c	512	CLA	CMB-C2B-C3B	3.22	131.38	125.09
26	D	401	PHO	O1D-CGD-CBD	3.23	129.66	124.64
25	d	403	CLA	CMB-C2B-C3B	3.23	131.41	125.09
25	B	617	CLA	CMB-C2B-C3B	3.24	131.42	125.09
27	H	102	BCR	C27-C26-C25	3.24	126.29	122.73
27	K	101	BCR	C27-C26-C25	3.24	126.30	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	712	BCR	C27-C26-C25	3.28	126.34	122.73
25	C	514	CLA	CMB-C2B-C3B	3.29	131.53	125.09
27	c	515	BCR	C27-C26-C25	3.31	126.37	122.73
26	a	710	PHO	O1D-CGD-CBD	3.32	129.80	124.64
29	a	714	SQD	C3-C4-C5	3.32	116.15	110.23
27	h	101	BCR	C27-C26-C25	3.34	126.40	122.73
27	B	619	BCR	C27-C26-C25	3.35	126.42	122.73
27	b	624	BCR	C27-C26-C25	3.42	126.49	122.73
27	D	405	BCR	C27-C26-C25	3.42	126.49	122.73
29	B	626	SQD	O47-C7-C8	3.43	118.75	111.53
27	c	514	BCR	C27-C26-C25	3.44	126.51	122.73
29	b	601	SQD	O47-C7-C8	3.45	118.81	111.53
29	B	623	SQD	C3-C4-C5	3.46	116.41	110.23
23	b	626	LMG	O6-C5-C4	3.47	116.28	109.67
29	B	623	SQD	O5-C5-C4	3.47	116.29	109.67
29	D	410	SQD	O47-C7-C8	3.49	118.89	111.53
27	b	623	BCR	C27-C26-C25	3.50	126.58	122.73
27	B	620	BCR	C27-C26-C25	3.55	126.64	122.73
27	b	625	BCR	C27-C26-C25	3.57	126.66	122.73
29	a	714	SQD	O47-C7-C8	3.58	119.06	111.53
27	d	404	BCR	C27-C26-C25	3.60	126.69	122.73
29	A	614	SQD	O47-C7-C8	3.66	119.24	111.53
29	A	612	SQD	O47-C7-C8	3.77	119.47	111.53
29	B	623	SQD	O47-C7-C8	3.80	119.54	111.53
27	H	102	BCR	C2-C1-C6	3.82	116.16	110.48
29	A	612	SQD	O5-C5-C4	3.84	116.99	109.67
32	E	101	LHG	O4-P-O5	3.86	132.62	112.56
32	e	101	LHG	O4-P-O5	3.89	132.79	112.56
32	D	407	LHG	O4-P-O5	3.91	132.88	112.56
32	a	720	LHG	O4-P-O5	3.91	132.89	112.56
32	b	629	LHG	O4-P-O5	3.91	132.90	112.56
32	d	406	LHG	O4-P-O5	3.91	132.91	112.56
32	d	407	LHG	O4-P-O5	3.91	132.91	112.56
32	L	101	LHG	O4-P-O5	3.92	132.94	112.56
32	B	625	LHG	O4-P-O5	3.92	132.94	112.56
32	D	408	LHG	O4-P-O5	3.93	133.01	112.56
29	a	714	SQD	O5-C5-C4	3.99	117.28	109.67
23	b	626	LMG	O6-C1-C2	4.08	118.76	110.28
29	a	714	SQD	O6-C1-C2	4.14	113.09	108.00
29	I	102	SQD	O47-C7-C8	4.18	120.33	111.53
29	B	623	SQD	C4-C3-C2	4.26	118.64	110.79
29	f	102	SQD	O6-C1-C2	4.29	113.27	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	626	SQD	O5-C5-C4	4.33	117.93	109.67
29	A	612	SQD	O6-C1-C2	4.52	113.56	108.00
29	D	410	SQD	O6-C1-C2	5.25	114.46	108.00
29	B	626	SQD	O6-C1-C2	5.25	114.46	108.00
29	B	623	SQD	O7-S-C6	5.82	111.02	106.92
29	A	612	SQD	O7-S-C6	6.23	111.31	106.92
29	B	623	SQD	O9-S-C6	6.31	111.36	106.92
29	b	601	SQD	O6-C1-C2	6.36	115.82	108.00
29	a	714	SQD	O9-S-C6	6.51	111.51	106.92
29	f	102	SQD	O9-S-C6	6.75	111.68	106.92
29	D	410	SQD	O9-S-C6	6.76	111.68	106.92
29	D	410	SQD	O7-S-C6	6.86	111.75	106.92
29	f	102	SQD	O7-S-C6	6.91	111.79	106.92
29	a	714	SQD	O7-S-C6	7.08	111.91	106.92
29	B	626	SQD	O7-S-C6	7.15	111.96	106.92
29	b	601	SQD	O9-S-C6	7.65	112.31	106.92
29	A	612	SQD	O9-S-C6	8.22	112.71	106.92
29	b	601	SQD	O7-S-C6	9.11	113.34	106.92
29	B	626	SQD	O9-S-C6	9.38	113.53	106.92

All (196) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	513	CLA	NC
25	C	513	CLA	ND
25	C	513	CLA	NA
25	C	508	CLA	NC
25	C	508	CLA	NA
25	C	508	CLA	ND
25	c	508	CLA	NC
25	c	508	CLA	NA
25	B	610	CLA	NC
25	B	610	CLA	NA
25	c	512	CLA	NC
25	c	512	CLA	NA
25	c	512	CLA	ND
25	d	402	CLA	NC
25	d	402	CLA	NA
25	C	503	CLA	NC
25	C	503	CLA	ND
25	C	503	CLA	NA
25	B	614	CLA	NC

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Mol	Chain	Res	Type	Atom
25	B	614	CLA	NA
25	B	614	CLA	ND
25	c	506	CLA	NC
25	c	506	CLA	NA
25	c	507	CLA	NC
25	c	507	CLA	NA
25	c	507	CLA	ND
25	C	509	CLA	NC
25	C	509	CLA	ND
25	C	509	CLA	NA
25	C	511	CLA	NC
25	C	511	CLA	ND
25	C	511	CLA	NA
25	b	609	CLA	NC
25	b	609	CLA	ND
25	b	609	CLA	NA
25	b	620	CLA	NC
25	b	620	CLA	ND
25	b	620	CLA	NA
25	B	612	CLA	NC
25	B	612	CLA	ND
25	B	612	CLA	NA
25	B	608	CLA	NA
25	B	608	CLA	NC
25	B	608	CLA	ND
25	c	511	CLA	NC
25	c	511	CLA	ND
25	c	511	CLA	NA
25	b	611	CLA	NC
25	b	611	CLA	NA
25	B	602	CLA	NC
25	B	602	CLA	ND
25	B	602	CLA	NA
25	D	403	CLA	NC
25	D	403	CLA	NA
25	B	609	CLA	NA
25	B	609	CLA	NC
25	B	609	CLA	ND
25	c	510	CLA	NC
25	c	510	CLA	ND
25	c	510	CLA	NA
25	c	502	CLA	NC

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Mol	Chain	Res	Type	Atom
25	c	502	CLA	ND
25	c	502	CLA	NA
25	b	619	CLA	NC
25	b	619	CLA	NA
25	b	619	CLA	ND
25	B	617	CLA	NC
25	B	617	CLA	NA
25	B	617	CLA	ND
25	B	616	CLA	NC
25	B	616	CLA	ND
25	B	616	CLA	NA
25	C	504	CLA	NC
25	C	504	CLA	ND
25	C	504	CLA	NA
25	c	504	CLA	NC
25	c	504	CLA	ND
25	c	504	CLA	NA
25	C	502	CLA	NC
25	C	502	CLA	ND
25	C	502	CLA	NA
25	B	615	CLA	NC
25	B	615	CLA	ND
25	B	615	CLA	NA
25	A	609	CLA	NC
25	A	609	CLA	ND
25	A	609	CLA	NA
25	B	607	CLA	NC
25	B	607	CLA	ND
25	B	607	CLA	NA
25	D	402	CLA	NA
25	D	402	CLA	NC
25	C	506	CLA	NC
25	C	506	CLA	NA
25	B	611	CLA	NA
25	B	611	CLA	NC
25	B	611	CLA	ND
25	d	403	CLA	NC
25	d	403	CLA	NA
25	b	616	CLA	NA
25	b	616	CLA	NC
25	b	616	CLA	ND
25	c	513	CLA	NC

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Mol	Chain	Res	Type	Atom
25	c	513	CLA	ND
25	c	513	CLA	NA
25	b	614	CLA	NC
25	b	614	CLA	ND
25	b	614	CLA	NA
25	D	404	CLA	NC
25	D	404	CLA	NA
25	C	505	CLA	NA
25	C	505	CLA	NC
25	C	505	CLA	ND
25	b	612	CLA	NC
25	b	612	CLA	ND
25	b	612	CLA	NA
25	a	711	CLA	NC
25	a	711	CLA	ND
25	a	711	CLA	NA
25	c	501	CLA	NC
25	c	501	CLA	ND
25	c	501	CLA	NA
25	b	621	CLA	NC
25	b	621	CLA	ND
25	b	621	CLA	NA
25	C	514	CLA	NC
25	C	514	CLA	ND
25	C	514	CLA	NA
25	B	605	CLA	NC
25	B	605	CLA	ND
25	B	605	CLA	NA
25	c	509	CLA	NC
25	c	509	CLA	ND
25	c	509	CLA	NA
25	b	610	CLA	NC
25	b	610	CLA	ND
25	b	610	CLA	NA
25	B	603	CLA	NC
25	B	603	CLA	NA
25	b	607	CLA	NC
25	b	607	CLA	ND
25	b	607	CLA	NA
25	C	512	CLA	NC
25	C	512	CLA	ND
25	C	512	CLA	NA

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Mol	Chain	Res	Type	Atom
25	B	606	CLA	NC
25	B	606	CLA	ND
25	B	606	CLA	NA
25	b	617	CLA	NC
25	b	617	CLA	ND
25	b	617	CLA	NA
25	a	719	CLA	NA
25	a	719	CLA	NC
25	a	719	CLA	ND
25	b	613	CLA	NA
25	b	613	CLA	NC
25	b	613	CLA	ND
25	a	708	CLA	NA
25	a	708	CLA	NC
25	a	708	CLA	ND
25	b	618	CLA	NC
25	b	618	CLA	ND
25	b	618	CLA	NA
25	A	606	CLA	NA
25	A	606	CLA	NC
25	A	606	CLA	ND
25	C	507	CLA	NC
25	C	507	CLA	NA
25	B	613	CLA	NC
25	B	613	CLA	ND
25	B	613	CLA	NA
25	b	622	CLA	NC
25	b	622	CLA	NA
25	b	622	CLA	ND
25	c	503	CLA	NC
25	c	503	CLA	ND
25	c	503	CLA	NA
25	b	608	CLA	NC
25	b	608	CLA	ND
25	b	608	CLA	NA
25	a	707	CLA	NC
25	a	707	CLA	ND
25	a	707	CLA	NA
25	b	615	CLA	NC
25	b	615	CLA	NA
25	B	604	CLA	NC
25	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	604	CLA	NA
25	c	505	CLA	NC
25	c	505	CLA	NA
25	C	510	CLA	NC
25	C	510	CLA	ND
25	C	510	CLA	NA
25	A	607	CLA	NA
25	A	607	CLA	NC
25	A	607	CLA	ND

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	B	626	SQD	C45-O47-C7-C8

There are no ring outliers.

69 monomers are involved in 200 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	603	LMG	2	0
25	A	606	CLA	1	0
25	A	607	CLA	2	0
26	A	608	PHO	2	0
25	A	609	CLA	1	0
27	A	610	BCR	4	0
28	A	611	PL9	5	0
29	A	612	SQD	2	0
29	A	614	SQD	1	0
25	B	602	CLA	4	0
25	B	603	CLA	1	0
25	B	604	CLA	4	0
25	B	605	CLA	3	0
25	B	606	CLA	1	0
25	B	607	CLA	7	0
25	B	608	CLA	2	0
25	B	609	CLA	3	0
25	B	610	CLA	6	0
25	B	611	CLA	3	0
25	B	612	CLA	8	0
25	B	613	CLA	2	0
25	B	614	CLA	3	0
25	B	615	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	616	CLA	4	0
25	B	617	CLA	6	0
27	B	618	BCR	2	0
27	B	619	BCR	1	0
27	B	620	BCR	1	0
23	B	621	LMG	1	0
29	B	623	SQD	1	0
32	B	625	LHG	2	0
29	B	626	SQD	5	0
25	C	502	CLA	2	0
25	C	503	CLA	2	0
25	C	504	CLA	3	0
25	C	505	CLA	6	0
25	C	506	CLA	3	0
25	C	507	CLA	3	0
25	C	508	CLA	2	0
25	C	509	CLA	10	0
25	C	510	CLA	4	0
25	C	511	CLA	6	0
25	C	512	CLA	6	0
25	C	513	CLA	3	0
25	C	514	CLA	2	0
27	C	515	BCR	2	0
27	C	516	BCR	3	0
33	C	517	DGD	3	0
33	C	518	DGD	4	0
33	C	519	DGD	2	0
23	C	520	LMG	1	0
26	D	401	PHO	3	0
25	D	402	CLA	6	0
25	D	403	CLA	5	0
25	D	404	CLA	1	0
27	D	405	BCR	4	0
28	D	406	PL9	2	0
32	D	407	LHG	4	0
32	D	408	LHG	6	0
23	D	409	LMG	3	0
29	D	410	SQD	4	0
32	E	101	LHG	4	0
34	E	102	HEM	5	0
27	H	102	BCR	3	0
29	I	102	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	K	101	BCR	3	0
32	L	101	LHG	4	0
23	M	101	LMG	3	0
34	V	201	HEM	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	334/344 (97%)	-0.31	2 (0%) 90 86	38, 46, 69, 82	0
1	a	334/344 (97%)	-0.21	4 (1%) 81 73	35, 48, 71, 82	0
2	B	504/510 (98%)	-0.11	10 (1%) 68 58	38, 50, 74, 98	0
2	b	504/510 (98%)	-0.11	25 (4%) 32 21	38, 50, 76, 94	0
3	C	451/461 (97%)	-0.14	3 (0%) 89 84	41, 54, 71, 90	0
3	c	451/461 (97%)	-0.10	3 (0%) 89 84	39, 55, 74, 90	0
4	D	341/352 (96%)	-0.35	1 (0%) 94 92	37, 48, 63, 82	0
4	d	341/352 (96%)	-0.20	3 (0%) 85 79	40, 50, 67, 85	0
5	E	81/84 (96%)	0.30	8 (9%) 9 4	47, 67, 79, 85	0
5	e	82/84 (97%)	0.71	11 (13%) 4 2	52, 70, 85, 87	0
6	F	34/45 (75%)	-0.16	0 100 100	54, 64, 78, 84	0
6	f	34/45 (75%)	-0.35	0 100 100	56, 63, 77, 80	0
7	H	63/63 (100%)	0.13	2 (3%) 51 39	43, 55, 68, 73	0
7	h	63/63 (100%)	0.02	0 100 100	48, 56, 64, 68	0
8	I	35/38 (92%)	0.14	2 (5%) 27 17	43, 53, 83, 94	0
8	i	35/38 (92%)	0.13	2 (5%) 27 17	44, 51, 82, 89	0
9	J	36/40 (90%)	-0.01	2 (5%) 28 18	56, 64, 86, 99	0
9	j	36/40 (90%)	0.12	2 (5%) 28 18	55, 66, 85, 89	0
10	K	37/46 (80%)	0.34	4 (10%) 8 3	62, 68, 83, 89	0
10	k	37/46 (80%)	0.19	0 100 100	60, 70, 84, 89	0
11	L	37/37 (100%)	-0.32	0 100 100	34, 45, 82, 93	0
11	l	37/37 (100%)	-0.43	1 (2%) 58 45	36, 47, 81, 90	0
12	M	32/36 (88%)	-0.40	1 (3%) 52 40	38, 47, 71, 83	0
12	m	32/36 (88%)	-0.30	1 (3%) 52 40	36, 47, 71, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.03	9 (3%) 45 33	42, 57, 87, 106	0
13	o	244/272 (89%)	-0.06	10 (4%) 41 29	43, 56, 89, 116	0
14	T	29/32 (90%)	-0.08	1 (3%) 49 36	37, 46, 69, 87	0
14	t	29/32 (90%)	-0.52	0 100 100	38, 48, 70, 79	0
15	U	97/134 (72%)	0.04	3 (3%) 52 40	45, 58, 75, 86	0
15	u	97/134 (72%)	-0.20	0 100 100	47, 55, 69, 84	0
16	V	137/163 (84%)	-0.13	0 100 100	45, 55, 67, 85	0
16	v	137/163 (84%)	0.18	4 (2%) 55 43	49, 63, 79, 100	0
17	Y	27/46 (58%)	0.35	1 (3%) 45 33	68, 75, 87, 95	0
17	y	30/46 (65%)	0.39	1 (3%) 50 38	69, 79, 89, 90	0
18	X	38/41 (92%)	0.25	2 (5%) 30 20	52, 60, 82, 93	0
18	x	38/41 (92%)	0.25	4 (10%) 8 4	54, 63, 80, 92	0
19	Z	62/62 (100%)	0.87	17 (27%) 1 0	62, 76, 100, 113	0
19	z	62/62 (100%)	0.65	9 (14%) 3 2	67, 82, 101, 112	0
20	R	34/41 (82%)	1.68	14 (41%) 0 0	70, 82, 94, 95	0
20	r	34/41 (82%)	1.58	12 (35%) 0 0	70, 84, 94, 101	0
All	All	5310/5694 (93%)	-0.06	174 (3%) 50 38	34, 53, 81, 116	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	56	PRO	5.5
20	R	28	VAL	5.4
16	v	18	THR	5.4
14	T	30	THR	5.3
3	C	142	GLU	5.1
19	Z	7	LEU	4.7
13	O	35	SER	4.6
19	Z	2	THR	4.6
2	b	487	SER	4.5
13	o	58	ASN	4.4
9	J	5	GLY	4.4
2	B	488	PRO	4.3
13	o	61	GLN	4.2
13	O	63	ALA	4.2
2	b	495	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
19	Z	8	ALA	4.1
19	Z	62	VAL	4.1
20	R	23	ILE	4.1
19	z	34	ASP	3.9
2	b	496	TYR	3.9
19	z	32	ASP	3.8
15	U	8	GLU	3.8
20	R	25	PRO	3.8
20	r	25	PRO	3.7
2	b	504	THR	3.7
12	M	33	GLN	3.7
20	r	3	TRP	3.7
8	i	36	ASP	3.6
9	j	6	GLY	3.6
8	I	36	ASP	3.6
8	I	34	ARG	3.5
13	o	4	THR	3.5
2	b	293	ALA	3.5
3	c	454	GLY	3.5
1	a	13	LEU	3.4
2	B	128	THR	3.4
2	b	294	SER	3.4
20	r	32	GLN	3.4
13	O	61	GLN	3.3
20	R	18	TRP	3.3
10	K	14	ALA	3.3
7	H	2	ALA	3.3
19	z	31	GLN	3.3
19	z	1	MET	3.3
2	b	482	ILE	3.2
18	X	2	THR	3.2
2	b	503	THR	3.2
2	b	485	GLU	3.2
2	b	500	GLY	3.2
13	o	3	GLN	3.2
19	Z	9	LEU	3.2
15	U	73	GLN	3.1
13	O	4	THR	3.1
1	a	12	ASN	3.1
16	v	16	GLY	3.1
19	z	62	VAL	3.1
13	o	5	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
19	Z	1	MET	3.1
16	v	19	ILE	3.1
5	E	15	THR	3.1
20	R	24	LEU	3.0
20	r	26	TYR	3.0
18	x	2	THR	3.0
20	R	26	TYR	3.0
20	r	2	ASP	3.0
19	z	29	SER	3.0
20	r	18	TRP	3.0
13	O	245	PRO	2.9
2	b	497	GLN	2.9
19	Z	3	ILE	2.9
19	z	56	VAL	2.9
20	R	5	VAL	2.9
19	Z	61	VAL	2.9
3	c	453	ALA	2.9
9	J	7	ARG	2.9
20	R	21	ARG	2.9
20	R	27	ALA	2.9
13	o	62	GLU	2.9
2	b	486	LEU	2.8
20	r	22	ASN	2.8
17	y	20	ALA	2.8
19	Z	6	GLN	2.8
2	B	487	SER	2.8
20	R	29	LYS	2.8
5	e	79	PHE	2.8
5	e	4	THR	2.8
5	E	60	GLN	2.8
5	e	16	SER	2.8
19	Z	32	ASP	2.7
5	e	82	GLN	2.7
1	a	243	GLU	2.7
2	b	502	VAL	2.7
9	j	5	GLY	2.7
2	B	126	PRO	2.7
13	O	62	GLU	2.7
2	B	292	LEU	2.7
12	m	33	GLN	2.7
13	o	60	ARG	2.7
4	d	240	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	b	127	ARG	2.6
2	B	127	ARG	2.6
19	Z	30	PRO	2.6
5	e	83	LEU	2.5
1	a	225	ARG	2.5
5	E	13	ILE	2.5
20	r	34	LEU	2.5
5	e	5	THR	2.5
20	r	20	VAL	2.5
2	b	295	GLY	2.5
19	z	35	ARG	2.5
20	R	31	VAL	2.5
20	R	3	TRP	2.5
2	b	489	GLU	2.4
19	Z	4	LEU	2.4
11	l	1	MET	2.4
2	b	85	GLY	2.4
5	e	60	GLN	2.4
10	K	17	ILE	2.4
20	R	30	GLN	2.4
20	r	35	LEU	2.4
19	Z	60	PHE	2.4
2	B	484	PRO	2.4
13	O	180	GLU	2.3
2	b	505	ARG	2.3
20	r	19	ALA	2.3
5	E	20	TRP	2.3
17	Y	43	ARG	2.3
3	c	23	ALA	2.3
13	O	246	ALA	2.3
20	r	14	LEU	2.3
1	A	12	ASN	2.3
4	D	238	THR	2.3
19	z	2	THR	2.2
13	o	6	THR	2.2
16	v	106	ASN	2.2
2	b	501	ASP	2.2
19	Z	59	PHE	2.2
5	E	17	VAL	2.2
2	b	84	THR	2.2
5	E	16	SER	2.2
2	B	489	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
18	x	37	VAL	2.2
10	K	20	PRO	2.2
19	Z	33	TRP	2.1
2	b	129	GLY	2.1
10	K	13	GLU	2.1
18	x	36	LYS	2.1
19	Z	57	LEU	2.1
2	b	239[A]	SER	2.1
20	R	33	LYS	2.1
5	e	78	THR	2.1
5	e	77	GLU	2.1
8	i	31	ASN	2.1
7	H	23	PRO	2.1
13	O	37	THR	2.1
18	X	34	ILE	2.1
5	e	81	GLU	2.1
1	A	228	THR	2.1
4	d	17	ILE	2.1
3	C	192	GLY	2.1
18	x	38	GLN	2.0
19	Z	52	LEU	2.0
5	e	11	SER	2.0
5	E	14	ILE	2.0
15	U	53	ALA	2.0
3	C	191	PRO	2.0
2	b	478	VAL	2.0
5	E	61	ARG	2.0
2	B	485	GLU	2.0
13	o	54	GLU	2.0
2	b	477	ASP	2.0
2	b	494	GLY	2.0
4	d	238	THR	2.0
2	B	223	GLN	2.0

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

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(\AA^2)	Q<0.9
8	FME	I	1	10/11	0.90	0.28	-	50,60,70,76	0
12	FME	M	1	10/11	0.92	0.30	-	54,63,77,87	0
12	FME	m	1	10/11	0.94	0.12	-	52,59,74,79	0
14	FME	t	1	10/11	0.94	0.12	-	42,56,71,77	0
14	FME	T	1	10/11	0.92	0.15	-	51,58,70,77	0
8	FME	i	1	10/11	0.90	0.34	-	49,61,69,69	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
30	UNL	b	606	13/-	0.80	0.25	7.03	45,51,57,59	0
23	LMG	c	520	51/55	0.82	0.40	6.84	61,75,95,100	0
29	SQD	I	102	40/54	0.65	0.49	6.35	44,69,94,102	0
23	LMG	c	519	51/55	0.82	0.30	4.44	42,75,90,91	0
30	UNL	b	604	11/-	0.85	0.27	4.01	38,48,57,59	0
23	LMG	b	626	51/55	0.80	0.30	3.65	38,56,72,77	0
27	BCR	D	405	40/40	0.87	0.24	3.41	48,61,77,81	0
23	LMG	C	501	51/55	0.77	0.31	3.41	46,67,81,88	0
30	UNL	z	101	11/-	0.81	0.29	3.32	48,65,72,72	0
23	LMG	C	521	51/55	0.81	0.34	3.23	49,71,81,91	0
23	LMG	b	627	51/55	0.84	0.31	3.22	51,70,80,82	0
25	CLA	c	512	65/65	0.87	0.25	3.20	60,67,89,91	0
30	UNL	b	605	13/-	0.87	0.21	3.15	42,54,62,62	0
32	LHG	E	101	49/49	0.80	0.28	3.15	48,77,92,95	0
28	PL9	A	611	55/55	0.82	0.29	3.01	46,68,78,83	0
23	LMG	B	621	51/55	0.80	0.25	2.83	52,70,78,88	0
29	SQD	B	623	47/54	0.74	0.27	2.64	44,61,109,124	0
30	UNL	t	102	5/-	0.93	0.20	2.58	32,38,43,47	0
23	LMG	A	603	51/55	0.81	0.26	2.39	40,62,77,83	0
32	LHG	D	407	49/49	0.94	0.23	2.30	34,49,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	LHG	e	101	42/49	0.76	0.31	2.21	57,76,98,101	0
29	SQD	b	601	54/54	0.83	0.24	2.20	45,66,94,105	0
30	UNL	t	101	10/-	0.92	0.17	2.18	26,44,49,50	0
29	SQD	B	626	54/54	0.88	0.25	2.08	46,67,90,99	0
27	BCR	t	103	40/40	0.88	0.23	2.07	36,47,60,63	0
23	LMG	D	409	51/55	0.91	0.20	2.06	39,61,82,88	0
28	PL9	a	713	55/55	0.86	0.25	2.01	57,68,77,84	0
25	CLA	b	607	65/65	0.86	0.26	1.99	48,63,81,91	0
25	CLA	c	513	65/65	0.87	0.24	1.85	57,68,82,96	0
30	UNL	d	401	22/-	0.82	0.23	1.85	39,54,63,66	0
29	SQD	A	614	40/54	0.84	0.22	1.73	47,59,68,72	0
23	LMG	C	520	51/55	0.78	0.27	1.64	43,74,86,89	0
28	PL9	D	406	55/55	0.91	0.22	1.64	31,43,52,55	0
27	BCR	B	618	40/40	0.93	0.18	1.62	37,52,60,63	0
27	BCR	d	404	40/40	0.90	0.23	1.58	45,59,70,77	0
25	CLA	D	404	65/65	0.89	0.22	1.51	34,44,80,84	0
27	BCR	b	602	40/40	0.89	0.22	1.50	45,53,70,76	0
27	BCR	k	102	40/40	0.86	0.26	1.49	53,65,81,84	0
33	DGD	c	517	62/66	0.89	0.22	1.46	54,61,81,92	0
23	LMG	d	408	40/55	0.79	0.24	1.46	47,61,84,89	0
27	BCR	B	619	40/40	0.93	0.20	1.45	35,47,51,52	0
27	BCR	k	101	40/40	0.84	0.24	1.43	53,69,78,78	0
28	PL9	d	405	55/55	0.93	0.20	1.38	32,41,53,56	0
25	CLA	C	514	65/65	0.86	0.24	1.37	44,73,81,89	0
30	UNL	a	717	7/-	0.84	0.26	1.31	48,53,61,67	0
27	BCR	b	623	40/40	0.92	0.19	1.23	42,53,60,61	0
25	CLA	A	607	65/65	0.93	0.19	1.15	31,46,91,99	0
25	CLA	C	513	65/65	0.88	0.23	1.13	52,66,80,86	0
23	LMG	a	701	51/55	0.85	0.23	1.13	42,64,87,90	0
23	LMG	a	715	51/55	0.82	0.24	1.07	47,65,85,91	0
32	LHG	D	408	49/49	0.92	0.21	1.05	42,59,72,84	0
25	CLA	C	505	65/65	0.89	0.22	1.05	48,63,71,79	0
25	CLA	b	613	65/65	0.92	0.19	1.04	37,44,55,58	0
30	UNL	B	624	11/-	0.92	0.20	1.02	34,49,52,53	0
23	LMG	f	101	51/55	0.90	0.20	1.02	48,58,84,93	0
29	SQD	f	102	41/54	0.87	0.30	0.99	54,73,85,89	0
27	BCR	c	514	40/40	0.89	0.25	0.98	61,67,74,75	0
23	LMG	M	101	51/55	0.88	0.20	0.92	34,58,74,77	0
25	CLA	c	503	65/65	0.90	0.21	0.92	48,61,68,73	0
25	CLA	B	606	65/65	0.93	0.18	0.91	37,45,52,53	0
27	BCR	b	624	40/40	0.90	0.20	0.90	38,49,58,59	0
26	PHO	a	710	64/64	0.93	0.22	0.89	38,46,55,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	B	602	65/65	0.87	0.21	0.89	44,62,75,80	0
25	CLA	C	509	65/65	0.92	0.21	0.88	46,55,91,100	0
33	DGD	c	518	62/66	0.92	0.19	0.88	44,57,76,81	0
25	CLA	B	609	65/65	0.93	0.25	0.84	32,45,51,59	0
25	CLA	c	505	65/65	0.92	0.19	0.76	41,52,60,69	0
30	UNL	m	102	12/-	0.91	0.19	0.76	41,47,50,52	0
32	LHG	d	406	49/49	0.94	0.19	0.73	32,53,61,65	0
27	BCR	Y	101	40/40	0.91	0.20	0.73	46,66,71,72	0
29	SQD	A	612	52/54	0.92	0.20	0.71	45,67,80,92	0
25	CLA	B	607	65/65	0.90	0.20	0.71	41,50,64,75	0
25	CLA	c	510	65/65	0.92	0.21	0.69	43,54,63,68	0
25	CLA	a	707	65/65	0.91	0.18	0.69	33,47,51,53	0
25	CLA	A	606	65/65	0.91	0.19	0.68	29,43,48,53	0
25	CLA	C	511	65/65	0.89	0.24	0.68	44,57,64,70	0
29	SQD	D	410	43/54	0.88	0.29	0.66	56,75,87,96	0
26	PHO	D	401	64/64	0.94	0.20	0.63	37,46,55,59	0
32	LHG	B	625	49/49	0.93	0.20	0.63	41,51,58,61	0
25	CLA	C	503	65/65	0.92	0.23	0.60	43,56,62,68	0
27	BCR	c	515	40/40	0.91	0.18	0.58	38,53,64,72	0
25	CLA	a	711	65/65	0.92	0.19	0.57	34,46,79,87	0
27	BCR	h	101	40/40	0.88	0.22	0.56	40,54,68,71	0
27	BCR	H	102	40/40	0.84	0.25	0.56	41,54,62,62	0
25	CLA	C	506	65/65	0.91	0.19	0.55	41,51,57,60	0
27	BCR	C	516	40/40	0.91	0.20	0.54	42,51,58,58	0
25	CLA	c	506	65/65	0.91	0.21	0.52	47,57,79,92	0
25	CLA	C	510	65/65	0.92	0.20	0.51	45,57,64,68	0
25	CLA	b	609	65/65	0.94	0.19	0.51	34,45,55,61	0
33	DGD	C	517	62/66	0.92	0.20	0.50	36,46,65,71	0
25	CLA	b	616	65/65	0.92	0.20	0.48	34,42,50,56	0
32	LHG	d	407	49/49	0.94	0.18	0.47	36,46,54,61	0
33	DGD	C	518	62/66	0.91	0.19	0.46	51,62,81,88	0
33	DGD	h	102	62/66	0.90	0.23	0.46	41,55,63,66	0
29	SQD	a	714	54/54	0.92	0.22	0.46	48,68,83,90	0
33	DGD	c	516	62/66	0.92	0.20	0.46	34,50,68,76	0
25	CLA	b	620	65/65	0.93	0.17	0.46	35,52,61,64	0
25	CLA	b	610	65/65	0.91	0.22	0.45	37,47,59,62	0
25	CLA	B	604	65/65	0.93	0.20	0.45	33,44,54,57	0
27	BCR	a	712	40/40	0.93	0.16	0.44	26,44,53,54	0
25	CLA	B	603	65/65	0.93	0.21	0.44	42,52,59,62	0
26	PHO	a	709	64/64	0.95	0.19	0.43	26,41,47,50	0
32	LHG	b	629	49/49	0.94	0.16	0.40	36,50,57,64	0
32	LHG	a	720	39/49	0.92	0.20	0.40	41,54,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	UNL	M	103	16/-	0.88	0.21	0.40	41,51,57,58	0
27	BCR	B	620	40/40	0.91	0.18	0.39	39,48,56,71	0
25	CLA	D	402	65/65	0.92	0.18	0.39	31,41,47,51	0
33	DGD	C	519	62/66	0.92	0.17	0.36	43,56,67,76	0
25	CLA	d	403	65/65	0.89	0.20	0.36	45,54,65,66	0
25	CLA	c	504	58/65	0.90	0.19	0.36	52,59,66,67	0
25	CLA	B	608	65/65	0.93	0.17	0.35	30,42,52,56	0
25	CLA	C	507	65/65	0.91	0.20	0.35	44,55,75,88	0
25	CLA	B	611	65/65	0.94	0.19	0.34	40,47,55,60	0
25	CLA	b	612	65/65	0.91	0.17	0.31	32,46,56,69	0
25	CLA	A	609	54/65	0.94	0.16	0.29	34,43,60,71	0
25	CLA	C	502	65/65	0.93	0.20	0.29	38,50,57,64	0
27	BCR	b	625	40/40	0.92	0.16	0.28	36,49,55,58	0
25	CLA	C	508	65/65	0.89	0.20	0.28	41,50,57,66	0
25	CLA	B	610	65/65	0.90	0.19	0.27	36,51,58,63	0
25	CLA	B	615	65/65	0.92	0.17	0.27	38,48,67,73	0
25	CLA	C	504	65/65	0.93	0.20	0.25	43,57,62,68	0
33	DGD	H	103	62/66	0.91	0.21	0.24	39,49,59,62	0
27	BCR	C	515	40/40	0.88	0.23	0.23	53,63,72,76	0
26	PHO	A	608	64/64	0.95	0.18	0.21	32,40,46,50	0
25	CLA	b	618	65/65	0.95	0.20	0.19	32,43,50,52	0
25	CLA	a	719	65/65	0.94	0.16	0.17	32,43,49,54	0
25	CLA	b	619	65/65	0.94	0.20	0.16	31,42,59,67	0
32	LHG	L	101	49/49	0.94	0.17	0.16	39,50,57,64	0
25	CLA	b	608	65/65	0.93	0.19	0.15	39,49,60,64	0
25	CLA	c	502	65/65	0.93	0.21	0.15	45,55,67,81	0
25	CLA	B	614	65/65	0.93	0.20	0.12	34,43,57,69	0
34	HEM	V	201	43/43	0.95	0.16	0.12	41,51,57,63	0
25	CLA	b	611	65/65	0.95	0.16	0.07	30,46,52,56	0
25	CLA	c	508	65/65	0.93	0.19	0.06	46,57,72,82	0
25	CLA	C	512	65/65	0.91	0.19	0.06	52,60,69,71	0
25	CLA	B	605	65/65	0.92	0.22	0.04	35,47,62,73	0
25	CLA	b	617	65/65	0.93	0.19	0.02	36,45,50,57	0
25	CLA	B	613	65/65	0.94	0.19	0.02	36,43,55,59	0
25	CLA	c	501	65/65	0.94	0.19	0.01	37,49,55,59	0
27	BCR	K	101	40/40	0.90	0.20	0.01	51,60,70,75	0
25	CLA	a	708	65/65	0.95	0.16	-0.02	37,47,89,101	0
25	CLA	b	615	65/65	0.92	0.17	-0.11	42,50,55,60	0
25	CLA	c	509	65/65	0.93	0.19	-0.12	49,57,70,73	0
25	CLA	D	403	65/65	0.94	0.16	-0.17	33,42,54,61	0
25	CLA	b	614	65/65	0.94	0.22	-0.17	39,48,58,60	0
25	CLA	d	402	65/65	0.93	0.16	-0.20	35,45,51,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	B	617	65/65	0.89	0.20	-0.25	39,52,80,84	0
34	HEM	E	102	43/43	0.93	0.21	-0.26	52,66,76,80	0
30	UNL	I	101	9/-	0.84	0.20	-0.26	44,52,61,61	0
25	CLA	B	612	65/65	0.93	0.19	-0.31	32,42,49,54	0
25	CLA	b	621	65/65	0.92	0.17	-0.40	38,49,55,60	0
25	CLA	c	507	65/65	0.93	0.17	-0.54	41,50,61,67	0
25	CLA	B	616	65/65	0.92	0.16	-0.56	42,51,60,64	0
27	BCR	A	610	40/40	0.94	0.15	-0.57	31,44,52,56	0
34	HEM	e	102	43/43	0.93	0.20	-0.58	60,71,81,91	0
25	CLA	b	622	47/65	0.93	0.16	-0.67	40,48,58,64	0
25	CLA	c	511	65/65	0.90	0.18	-0.74	50,62,71,74	0
34	HEM	v	201	43/43	0.95	0.15	-0.87	46,58,64,72	0
24	CL	A	605	1/1	0.94	0.14	-1.27	51,51,51,51	0
31	BCT	a	706	4/4	0.98	0.09	-1.49	50,56,56,59	0
31	BCT	A	615	4/4	0.97	0.10	-1.72	46,49,51,54	0
24	CL	a	705	1/1	0.97	0.12	-2.05	50,50,50,50	0
21	OEX	A	601	10/10	0.98	0.11	-2.11	42,54,59,60	0
21	OEX	a	702	10/10	0.97	0.11	-2.52	44,52,59,60	0
24	CL	a	704	1/1	0.93	0.12	-3.34	59,59,59,59	0
22	FE2	A	602	1/1	0.97	0.03	-3.97	60,60,60,60	0
24	CL	A	604	1/1	0.99	0.06	-5.11	39,39,39,39	0
22	FE2	a	703	1/1	0.95	0.03	-7.24	60,60,60,60	0
30	UNL	j	101	9/-	0.85	0.24	-	52,61,65,65	0
30	UNL	a	718	13/-	0.85	0.21	-	45,54,61,62	0
30	UNL	i	101	22/-	0.85	0.22	-	36,50,58,62	0
30	UNL	M	102	6/-	0.88	0.31	-	45,51,51,53	0
30	UNL	m	101	5/-	0.88	0.23	-	36,39,42,45	0
30	UNL	a	716	4/-	0.82	0.31	-	31,46,50,51	0
30	UNL	B	622	6/-	0.85	0.26	-	40,51,56,56	0
30	UNL	B	601	12/-	0.85	0.18	-	31,49,56,56	0
30	UNL	b	603	11/-	0.83	0.24	-	44,54,62,62	0
30	UNL	A	613	7/-	0.89	0.18	-	34,49,53,55	0
23	LMG	b	628	9/55	0.87	0.22	-	36,50,54,54	0
30	UNL	H	101	8/-	0.87	0.18	-	43,53,58,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.