



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2016 – 02:46 PM EST

PDB ID : 5B1B  
Title : Bovine heart cytochrome c oxidase in the fully reduced state at 1.6 angstrom resolution  
Authors : Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2015-12-01  
Resolution : 1.60 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](mailto: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.

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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-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

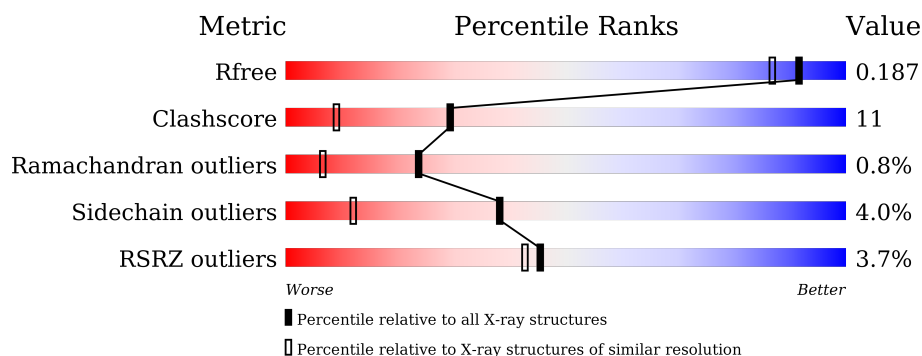
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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  $\geq 3$ , 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	514	<div> <div>66%</div> <div>31%</div> <div>.</div> </div>
1	N	514	<div> <div>68%</div> <div>27%</div> <div>..</div> </div>
2	B	227	<div> <div>%</div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
2	O	227	<div> <div>2%</div> <div>68%</div> <div>25%</div> <div>7%</div> </div>
3	C	261	<div> <div>68%</div> <div>26%</div> <div>5%</div> <div>.</div> </div>
3	P	261	<div> <div>67%</div> <div>28%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-
14	HEA	N	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
16	MG	N	604	-	-	-	X
18	PGV	A	607	-	-	-	X
18	PGV	C	309	-	-	-	X
18	PGV	N	606	-	-	-	X
18	PGV	P	301	-	-	-	X
19	TGL	B	301	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	L	101	-	-	-	X
19	TGL	N	608	-	-	-	X
19	TGL	N	609	-	-	-	X
19	TGL	Q	201	-	-	-	X
2	FME	B	1	-	-	X	-
21	CHD	C	306	-	-	-	X
21	CHD	J	101	-	-	-	X
21	CHD	P	306	-	-	-	X
21	CHD	W	101	-	-	-	X
23	DMU	C	301	-	-	-	X
23	DMU	P	302	-	-	-	X
23	DMU	Z	101	-	-	-	X
26	CDL	C	305	-	-	X	X
26	CDL	G	101	-	-	X	X
26	CDL	P	305	-	-	X	X
26	CDL	T	104	-	-	X	X

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 34897 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4131	2757	639	694	41			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	6	0
			1874	1216	289	350	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			609	395	108	101	5			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

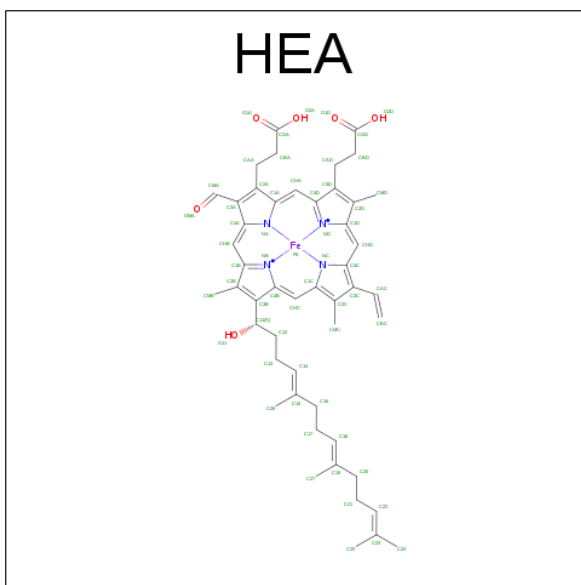
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

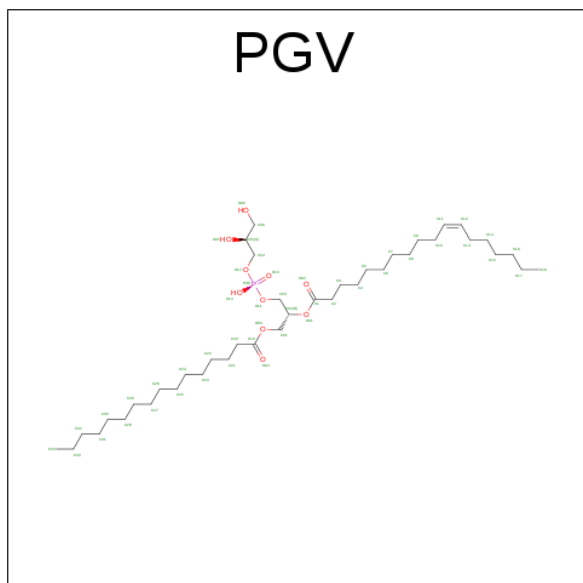
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).



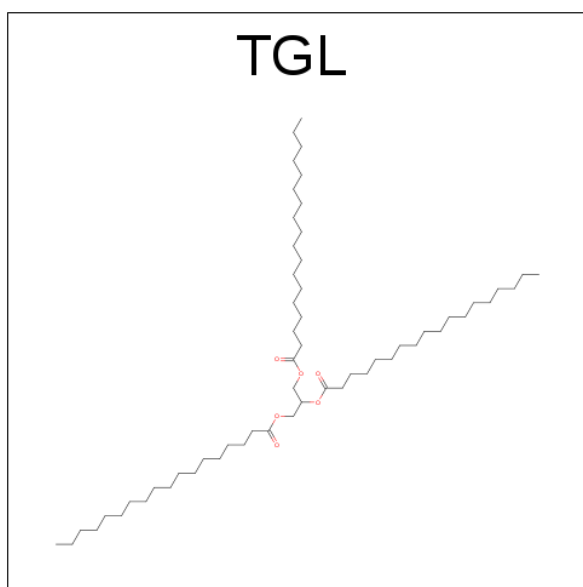
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL|OXY}}(HYDROXY)PHOSPHORYL|OXY}}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



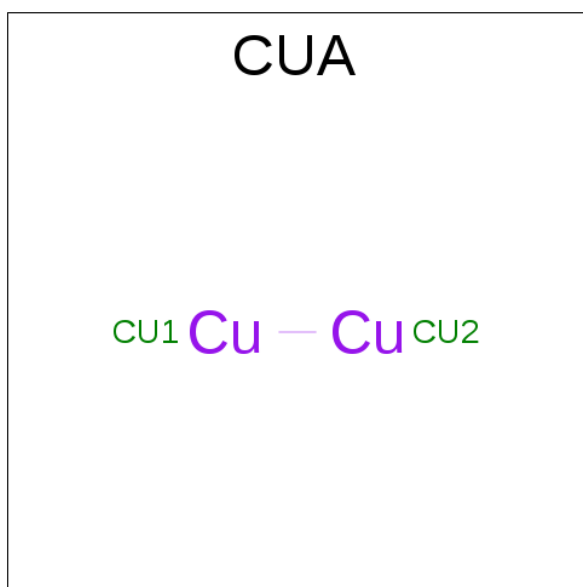
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



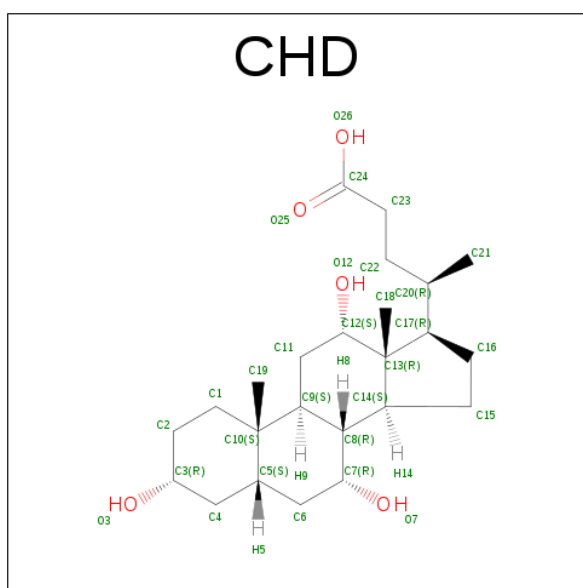
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Cu	0	0
			2	2		
20	O	1	Total	Cu	0	0
			2	2		

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



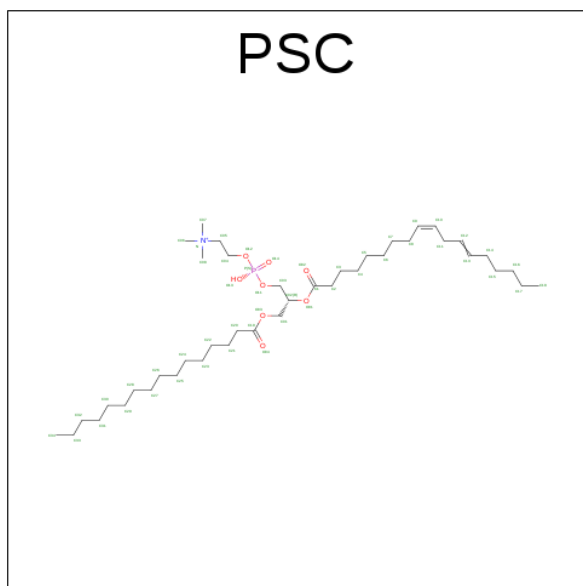
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		

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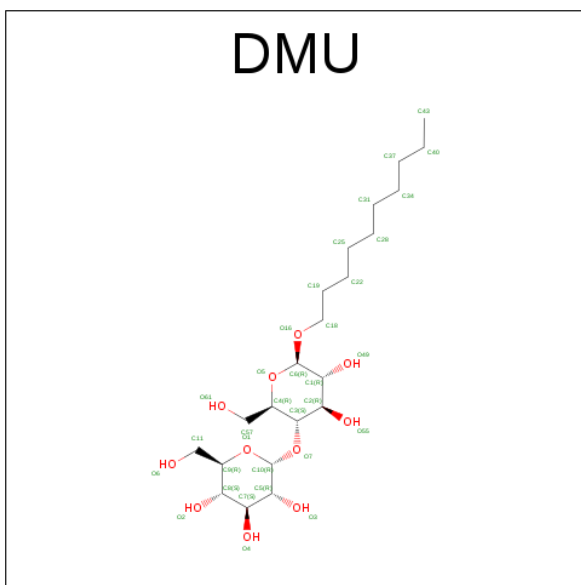
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	C	1	Total	C	O	0	0
			29	24	5		
21	G	1	Total	C	O	0	0
			29	24	5		
21	J	1	Total	C	O	0	0
			29	24	5		
21	P	1	Total	C	O	0	0
			29	24	5		
21	P	1	Total	C	O	0	0
			29	24	5		
21	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).

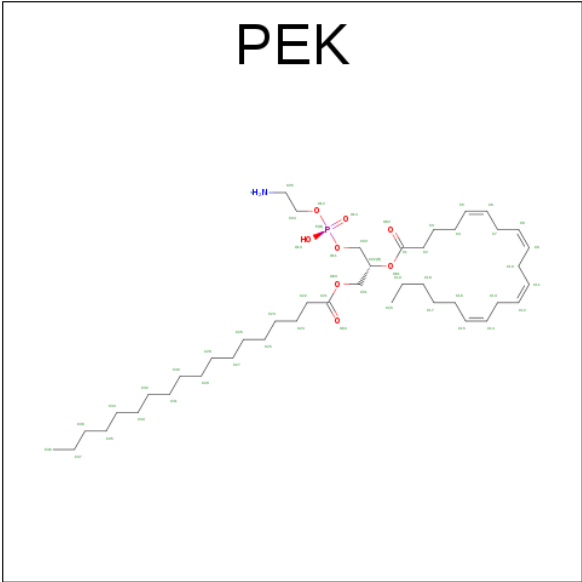


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total 33	C 22	O 11	0	0
23	M	1	Total 33	C 22	O 11	0	0
23	P	1	Total 33	C 22	O 11	0	0
23	Z	1	Total 33	C 22	O 11	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

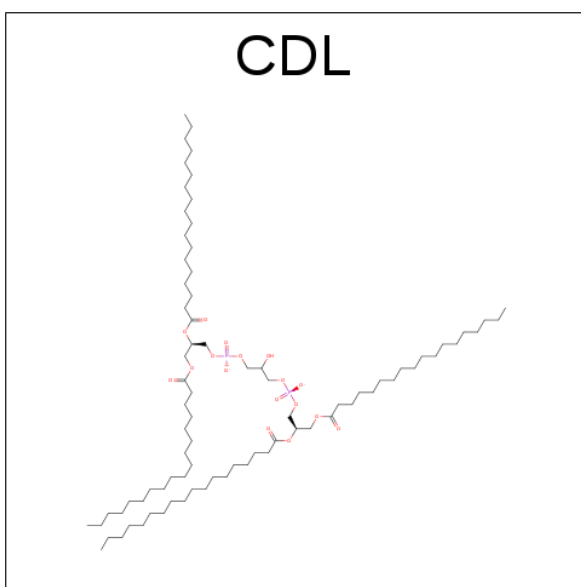
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	S	1	Total	Zn	0	0
			1	1		
27	F	1	Total	Zn	0	0
			1	1		

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	289	Total	O	0	0
			289	289		
28	B	254	Total	O	0	1
			255	255		
28	C	181	Total	O	0	0
			181	181		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	256	Total 256	O 256	0	0
28	E	169	Total 169	O 169	0	0
28	F	200	Total 200	O 200	0	0
28	G	108	Total 108	O 108	0	0
28	H	129	Total 129	O 129	0	0
28	I	78	Total 78	O 78	0	0
28	J	64	Total 64	O 64	0	0
28	K	68	Total 68	O 68	0	0
28	L	47	Total 47	O 47	0	0
28	M	50	Total 50	O 50	0	0
28	N	286	Total 286	O 286	0	0
28	O	225	Total 226	O 226	0	1
28	P	194	Total 194	O 194	0	0
28	Q	143	Total 143	O 143	0	0
28	R	156	Total 156	O 156	0	0
28	S	187	Total 187	O 187	0	0
28	T	97	Total 97	O 97	0	0
28	U	113	Total 113	O 113	0	0
28	V	73	Total 73	O 73	0	0
28	W	72	Total 72	O 72	0	0
28	X	48	Total 48	O 48	0	0

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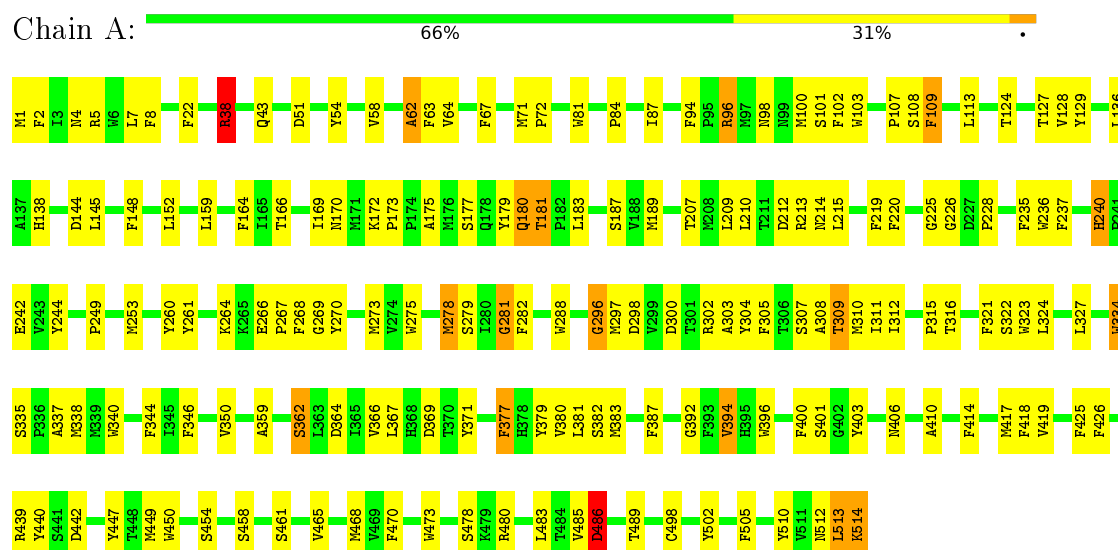
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Y	31	Total 31	O 31	0	0
28	Z	36	Total 36	O 36	0	0

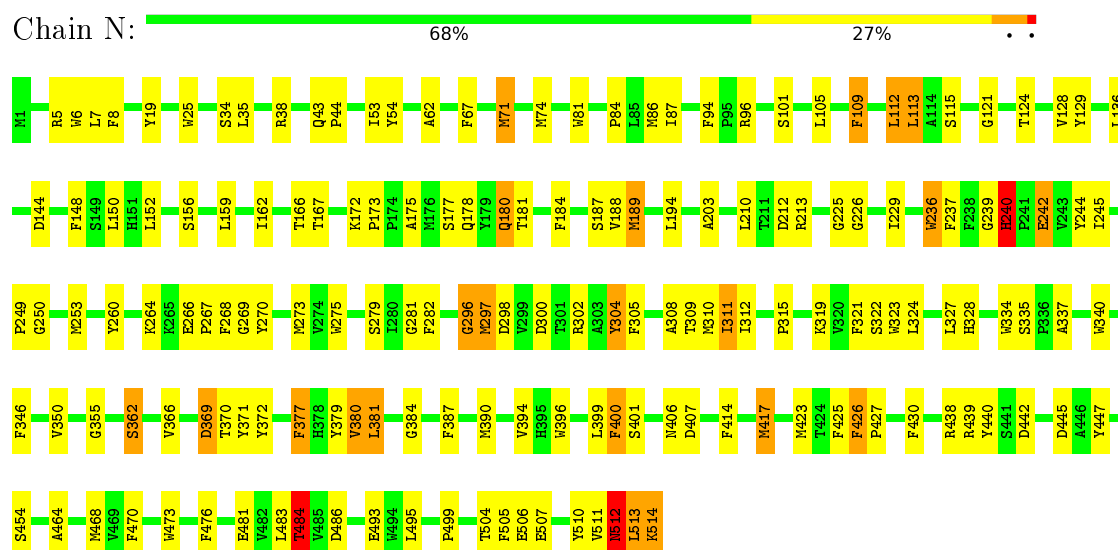
### 3 Residue-property plots

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

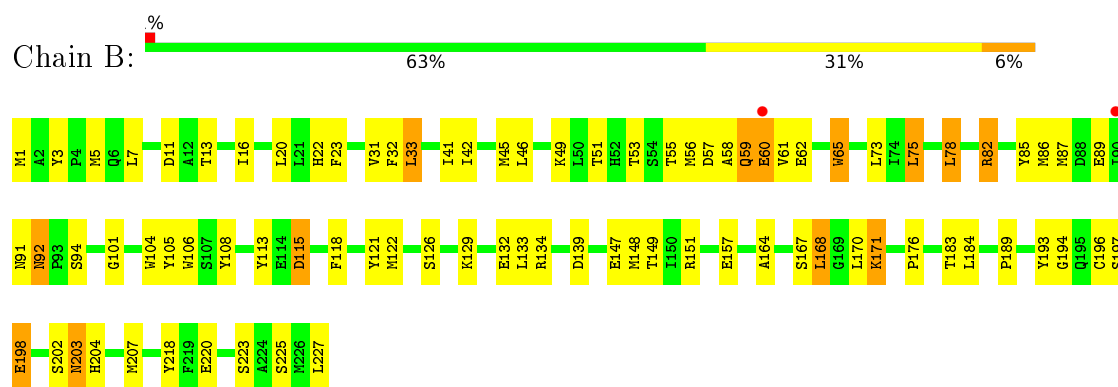
#### • Molecule 1: Cytochrome c oxidase subunit 1



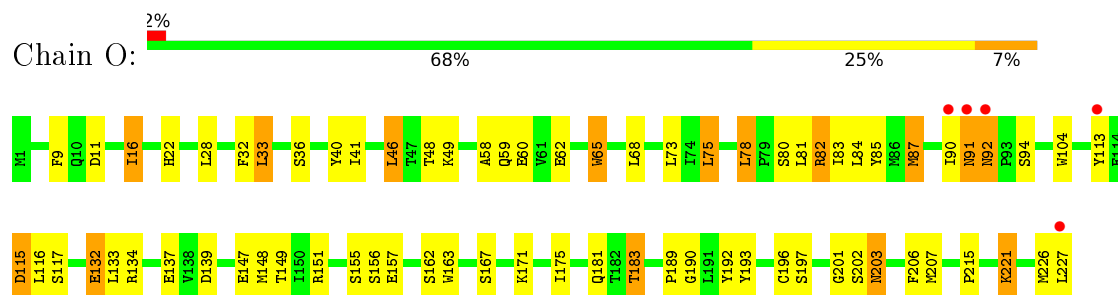
#### • Molecule 1: Cytochrome c oxidase subunit 1



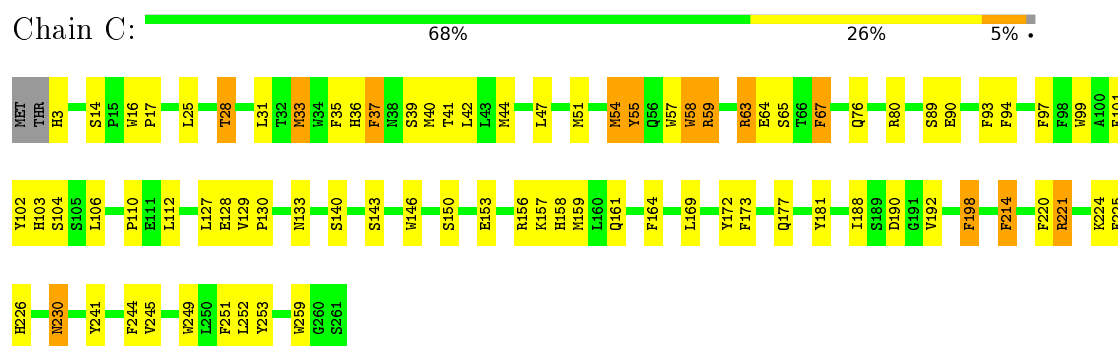
#### • Molecule 2: Cytochrome c oxidase subunit 2



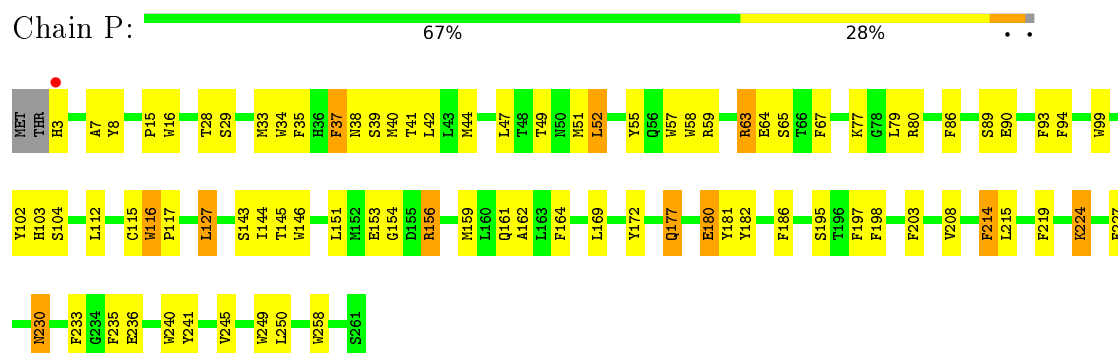
- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3

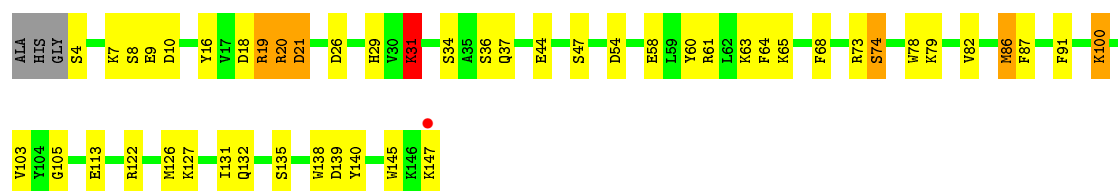


- Molecule 3: Cytochrome c oxidase subunit 3

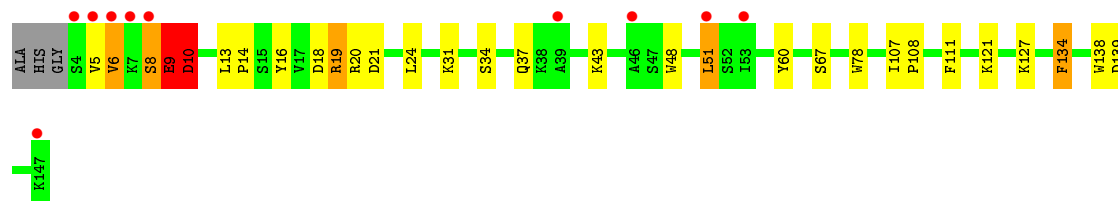
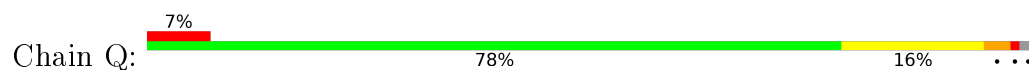


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

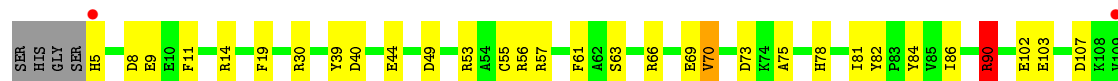




- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



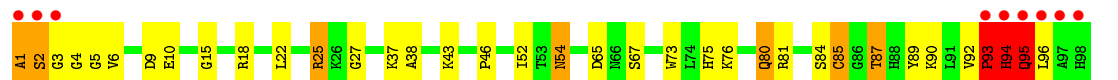
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

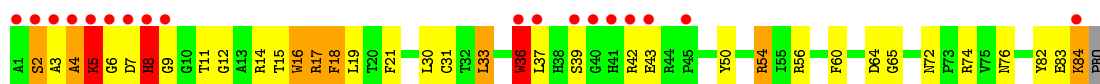


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

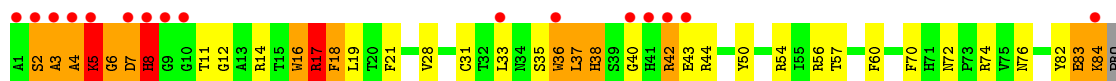


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

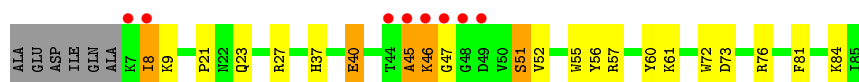




- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



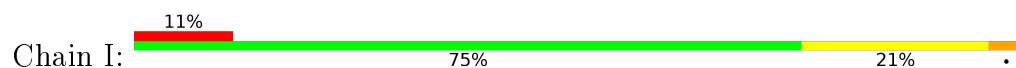
- Molecule 8: Cytochrome c oxidase subunit 6B1



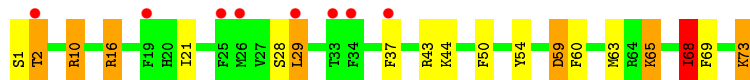
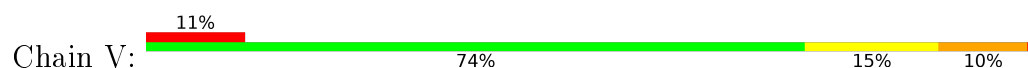
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

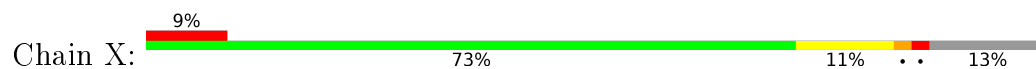




- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



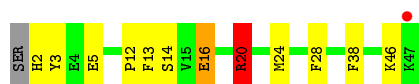
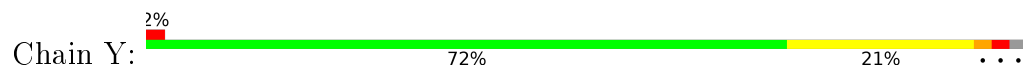
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



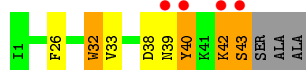
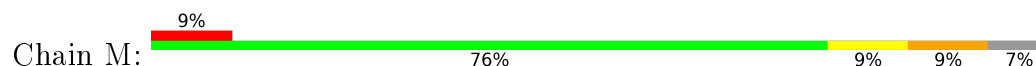
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.61Å 204.14Å 177.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 88.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-1.60) 96.5 (88.98-1.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.161 , 0.186 0.161 , 0.187	Depositor DCC
$R_{free}$ test set	41997 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

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	2.03	91/4253 (2.1%)	1.92	121/5805 (2.1%)
1	N	2.02	93/4260 (2.2%)	1.80	93/5814 (1.6%)
2	B	1.98	42/1912 (2.2%)	1.70	36/2603 (1.4%)
2	O	1.77	26/1908 (1.4%)	1.52	27/2599 (1.0%)
3	C	1.96	45/2261 (2.0%)	1.77	39/3090 (1.3%)
3	P	1.99	54/2260 (2.4%)	1.79	48/3088 (1.6%)
4	D	2.07	36/1284 (2.8%)	2.16	25/1730 (1.4%)
4	Q	1.64	11/1237 (0.9%)	1.67	16/1668 (1.0%)
5	E	2.03	23/882 (2.6%)	2.13	31/1196 (2.6%)
5	R	1.88	19/871 (2.2%)	1.69	19/1182 (1.6%)
6	F	1.75	13/806 (1.6%)	1.65	16/1093 (1.5%)
6	S	1.89	19/772 (2.5%)	1.65	11/1048 (1.0%)
7	G	2.08	19/702 (2.7%)	1.73	15/953 (1.6%)
7	T	1.94	16/724 (2.2%)	2.18	20/984 (2.0%)
8	H	1.72	4/682 (0.6%)	1.51	8/921 (0.9%)
8	U	1.63	7/682 (1.0%)	1.24	1/921 (0.1%)
9	I	1.84	10/605 (1.7%)	1.63	11/802 (1.4%)
9	V	1.58	2/613 (0.3%)	1.65	8/812 (1.0%)
10	J	1.85	9/471 (1.9%)	1.61	7/636 (1.1%)
10	W	1.74	8/471 (1.7%)	1.66	10/636 (1.6%)
11	K	1.80	7/405 (1.7%)	1.49	4/556 (0.7%)
11	X	1.66	4/405 (1.0%)	1.57	5/556 (0.9%)
12	L	2.08	6/393 (1.5%)	2.28	12/526 (2.3%)
12	Y	2.03	11/393 (2.8%)	1.70	3/526 (0.6%)
13	M	1.74	5/345 (1.4%)	1.53	2/470 (0.4%)
13	Z	1.72	5/345 (1.4%)	1.36	0/470
All	All	1.92	585/29942 (2.0%)	1.78	588/40685 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is



detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	N	0	4
2	B	0	1
2	O	0	1
3	C	0	1
4	D	0	1
4	Q	0	2
5	E	0	1
6	F	0	1
6	S	0	4
7	T	0	1
8	U	0	1
9	V	0	1
10	W	0	1
12	L	0	1
All	All	0	26

All (585) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	TRP	CB-CG	-18.39	1.17	1.50
1	N	512	ASN	CA-CB	17.27	1.98	1.53
12	L	5	GLU	CD-OE2	-15.61	1.08	1.25
2	O	65	TRP	CB-CG	-14.85	1.23	1.50
4	D	100	LYS	CE-NZ	14.62	1.85	1.49
12	L	26	THR	CB-CG2	-14.60	1.04	1.52
4	D	58	GLU	CD-OE2	13.94	1.41	1.25
1	N	189	MET	CB-CG	13.68	1.95	1.51
2	O	167	SER	CB-OG	-13.05	1.25	1.42
5	R	90	ARG	CD-NE	11.85	1.66	1.46
11	K	54	ARG	CZ-NH2	11.33	1.47	1.33
11	X	54	ARG	CZ-NH2	10.96	1.47	1.33
9	I	61	GLU	CD-OE1	-10.94	1.13	1.25
1	A	362	SER	CA-CB	10.84	1.69	1.52
5	E	84	TYR	CG-CD1	10.82	1.53	1.39
4	D	20	ARG	CD-NE	-10.37	1.28	1.46
3	C	90	GLU	CD-OE1	10.32	1.37	1.25
1	A	335	SER	CB-OG	10.30	1.55	1.42
2	O	167	SER	CA-CB	10.25	1.68	1.52
1	A	486	ASP	CB-CG	-10.13	1.30	1.51
4	D	36	SER	CB-OG	-10.03	1.29	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	266	GLU	CD-OE2	9.92	1.36	1.25
3	C	104	SER	CB-OG	9.84	1.55	1.42
2	O	59	GLN	CG-CD	9.69	1.73	1.51
12	Y	5	GLU	CD-OE2	-9.68	1.15	1.25
4	D	61	ARG	CZ-NH2	9.65	1.45	1.33
7	G	36	TRP	CB-CG	9.64	1.67	1.50
1	N	512	ASN	CB-CG	-9.63	1.28	1.51
11	K	31	TYR	CG-CD1	9.58	1.51	1.39
6	F	1	ALA	C-O	9.48	1.41	1.23
2	O	59	GLN	CD-OE1	9.47	1.44	1.24
7	T	17	ARG	CZ-NH2	9.42	1.45	1.33
1	N	281	GLY	N-CA	9.31	1.60	1.46
3	P	153	GLU	CG-CD	9.18	1.65	1.51
3	C	102	TYR	CG-CD2	-9.14	1.27	1.39
3	C	104	SER	CA-CB	9.06	1.66	1.52
5	E	90	ARG	CZ-NH1	8.97	1.44	1.33
1	A	447	TYR	CG-CD1	8.93	1.50	1.39
3	C	90	GLU	CD-OE2	8.89	1.35	1.25
1	N	279	SER	CA-CB	8.87	1.66	1.52
1	N	71	MET	CG-SD	8.86	2.04	1.81
7	T	36[A]	TRP	CB-CG	8.83	1.66	1.50
7	T	36[B]	TRP	CB-CG	8.83	1.66	1.50
12	Y	20	ARG	CZ-NH2	8.81	1.44	1.33
2	B	59	GLN	CG-CD	8.77	1.71	1.51
3	P	143	SER	CA-CB	8.77	1.66	1.52
3	P	102	TYR	CG-CD2	-8.76	1.27	1.39
1	A	242	GLU	CD-OE1	8.74	1.35	1.25
2	B	115	ASP	CB-CG	8.73	1.70	1.51
1	N	84	PRO	CA-CB	8.73	1.71	1.53
7	T	17	ARG	CD-NE	-8.71	1.31	1.46
4	D	60	TYR	CE1-CZ	8.71	1.49	1.38
1	N	447	TYR	CE1-CZ	8.71	1.49	1.38
3	P	172	TYR	CG-CD1	8.69	1.50	1.39
2	B	220	GLU	CD-OE1	-8.66	1.16	1.25
7	G	17	ARG	CZ-NH2	8.56	1.44	1.33
13	M	40	TYR	CG-CD1	8.53	1.50	1.39
2	O	36	SER	CA-CB	8.51	1.65	1.52
7	T	16	TRP	CZ3-CH2	8.40	1.53	1.40
3	P	90	GLU	CD-OE1	8.38	1.34	1.25
10	W	7	GLU	CD-OE1	8.34	1.34	1.25
2	B	59	GLN	CD-OE1	8.31	1.42	1.24
3	C	99	TRP	CE3-CZ3	8.27	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	192	TYR	CE1-CZ	8.27	1.49	1.38
5	R	63	SER	CB-OG	8.24	1.52	1.42
6	S	1	ALA	C-O	8.24	1.39	1.23
1	A	382	SER	CB-OG	8.20	1.52	1.42
7	T	83	GLU	CD-OE1	8.19	1.34	1.25
8	H	40	GLU	CD-OE2	8.11	1.34	1.25
3	P	35	PHE	CE1-CZ	8.10	1.52	1.37
1	A	394	VAL	CB-CG2	-8.09	1.35	1.52
6	S	67	SER	CB-OG	8.00	1.52	1.42
3	P	89	SER	CB-OG	7.96	1.52	1.42
11	X	20	SER	CB-OG	-7.95	1.31	1.42
5	E	19	PHE	CE2-CZ	7.89	1.52	1.37
3	C	89	SER	CB-OG	7.84	1.52	1.42
13	Z	40	TYR	CE2-CZ	7.83	1.48	1.38
3	C	143	SER	CA-CB	7.79	1.64	1.52
4	D	44	GLU	CD-OE1	7.77	1.34	1.25
1	N	25	TRP	CE3-CZ3	7.71	1.51	1.38
1	N	505	PHE	CE2-CZ	7.68	1.51	1.37
1	N	323	TRP	CZ3-CH2	7.66	1.52	1.40
5	R	19	PHE	CE2-CZ	7.66	1.51	1.37
1	A	266	GLU	CD-OE2	7.62	1.34	1.25
5	E	9	GLU	CG-CD	7.62	1.63	1.51
12	Y	16	GLU	CD-OE1	7.61	1.34	1.25
2	B	82	ARG	CZ-NH2	7.55	1.42	1.33
1	N	476	PHE	CG-CD2	7.53	1.50	1.38
3	P	99	TRP	CD1-NE1	7.50	1.50	1.38
1	A	260	TYR	CE1-CZ	7.45	1.48	1.38
1	N	473	TRP	CE3-CZ3	7.44	1.51	1.38
1	N	242	GLU	CD-OE1	7.43	1.33	1.25
1	A	512	ASN	CA-CB	7.42	1.72	1.53
3	C	172	TYR	CG-CD1	7.42	1.48	1.39
3	P	64	GLU	CD-OE2	7.41	1.33	1.25
1	A	96	ARG	CZ-NH1	7.40	1.42	1.33
1	A	2	PHE	CG-CD2	7.31	1.49	1.38
1	N	5	ARG	CZ-NH2	7.29	1.42	1.33
4	Q	20	ARG	CD-NE	-7.27	1.34	1.46
4	Q	6	VAL	C-N	7.26	1.50	1.34
13	Z	40	TYR	CG-CD1	7.15	1.48	1.39
4	D	135	SER	CB-OG	7.15	1.51	1.42
1	A	71	MET	CG-SD	7.13	1.99	1.81
1	A	450	TRP	CE3-CZ3	7.11	1.50	1.38
2	O	132	GLU	CD-OE2	7.10	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	58	TRP	CZ3-CH2	7.08	1.51	1.40
3	C	44	MET	CA-CB	7.07	1.69	1.53
3	P	198	PHE	CG-CD1	7.07	1.49	1.38
2	B	65	TRP	CD2-CE2	7.06	1.49	1.41
3	P	180[A]	GLU	CD-OE1	-7.04	1.18	1.25
3	P	180[B]	GLU	CD-OE1	-7.04	1.18	1.25
1	A	458	SER	CA-CB	7.03	1.63	1.52
3	P	58	TRP	CZ3-CH2	7.00	1.51	1.40
4	D	19[A]	ARG	CZ-NH2	6.99	1.42	1.33
4	D	19[B]	ARG	CZ-NH2	6.99	1.42	1.33
2	O	85	TYR	CG-CD1	6.99	1.48	1.39
1	N	335	SER	CB-OG	6.98	1.51	1.42
5	E	44	GLU	CD-OE2	-6.98	1.18	1.25
2	B	108	TYR	CE2-CZ	6.97	1.47	1.38
3	C	58	TRP	CG-CD1	6.95	1.46	1.36
1	N	244	TYR	CG-CD1	6.95	1.48	1.39
12	Y	13	PHE	CE1-CZ	6.94	1.50	1.37
12	Y	5	GLU	CD-OE1	-6.93	1.18	1.25
6	F	56	ARG	CZ-NH1	6.92	1.42	1.33
1	N	380	VAL	CB-CG1	6.90	1.67	1.52
1	N	362	SER	CB-OG	-6.89	1.33	1.42
1	N	305	PHE	CG-CD2	6.88	1.49	1.38
8	U	40	GLU	CD-OE2	6.85	1.33	1.25
7	G	56	ARG	CZ-NH1	6.82	1.42	1.33
3	C	16	TRP	CE3-CZ3	6.81	1.50	1.38
2	O	147	GLU	CD-OE1	-6.80	1.18	1.25
1	A	281	GLY	N-CA	6.79	1.56	1.46
5	R	69	GLU	CD-OE2	-6.79	1.18	1.25
4	D	65	LYS	CE-NZ	6.76	1.66	1.49
3	P	161	GLN	CG-CD	6.75	1.66	1.51
1	A	480	ARG	CZ-NH2	6.74	1.41	1.33
5	E	9	GLU	CD-OE2	6.73	1.33	1.25
3	P	162	ALA	CA-CB	6.73	1.66	1.52
2	B	197	SER	CB-OG	6.72	1.50	1.42
2	B	51	THR	C-O	6.68	1.36	1.23
1	N	470	PHE	CE2-CZ	6.66	1.50	1.37
1	N	322	SER	CA-CB	6.66	1.62	1.52
1	N	362	SER	CA-CB	6.63	1.62	1.52
9	I	4	LEU	CA-CB	6.63	1.69	1.53
2	B	225	SER	CA-CB	6.62	1.62	1.52
1	A	43	GLN	CG-CD	6.61	1.66	1.51
5	E	56	ARG	CZ-NH2	6.61	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	90	ARG	NE-CZ	6.61	1.41	1.33
1	N	476	PHE	CG-CD1	6.59	1.48	1.38
3	C	245	VAL	CB-CG1	-6.58	1.39	1.52
1	A	371	TYR	CE1-CZ	6.58	1.47	1.38
4	D	47	SER	CA-CB	6.57	1.62	1.52
1	A	260	TYR	CG-CD2	6.54	1.47	1.39
1	A	152	LEU	CB-CG	6.53	1.71	1.52
6	S	93	PRO	CA-CB	6.52	1.66	1.53
2	B	147	GLU	CG-CD	6.51	1.61	1.51
5	R	32	GLY	N-CA	6.51	1.55	1.46
2	B	121	TYR	CG-CD1	6.51	1.47	1.39
7	G	82	TYR	CG-CD1	6.50	1.47	1.39
3	P	90	GLU	CD-OE2	6.49	1.32	1.25
1	N	43	GLN	CG-CD	6.49	1.66	1.51
5	E	78	HIS	N-CA	6.47	1.59	1.46
9	I	28	SER	CB-OG	6.46	1.50	1.42
1	A	401	SER	CB-OG	6.46	1.50	1.42
4	D	16	TYR	CD2-CE2	6.45	1.49	1.39
1	N	275	TRP	CZ3-CH2	6.45	1.50	1.40
1	A	307	SER	CB-OG	6.45	1.50	1.42
1	A	226	GLY	CA-C	6.44	1.62	1.51
1	N	439	ARG	CZ-NH1	6.44	1.41	1.33
2	O	9	PHE	CG-CD1	6.43	1.48	1.38
1	A	458	SER	CB-OG	6.43	1.50	1.42
6	S	18	ARG	CZ-NH1	6.43	1.41	1.33
3	C	169	LEU	CA-CB	6.42	1.68	1.53
3	C	65	SER	CA-CB	6.42	1.62	1.52
5	E	69	GLU	CA-CB	6.41	1.68	1.53
5	R	84	TYR	CE1-CZ	-6.41	1.30	1.38
1	N	54	TYR	CG-CD1	6.40	1.47	1.39
1	N	423[A]	MET	C-O	6.40	1.35	1.23
1	N	423[B]	MET	C-O	6.40	1.35	1.23
1	A	322	SER	CA-CB	6.39	1.62	1.52
3	P	57	TRP	CD1-NE1	6.38	1.48	1.38
1	N	86	MET	N-CA	6.37	1.59	1.46
3	P	16	TRP	CE3-CZ3	6.36	1.49	1.38
12	L	6	GLY	N-CA	6.35	1.55	1.46
2	B	147	GLU	CD-OE1	-6.34	1.18	1.25
1	N	514	LYS	N-CA	6.34	1.59	1.46
3	P	35	PHE	CA-CB	6.33	1.67	1.53
2	O	40	TYR	CE1-CZ	6.33	1.46	1.38
11	K	20	SER	CB-OG	-6.32	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	27	GLY	N-CA	6.31	1.55	1.46
3	P	153	GLU	CD-OE1	-6.30	1.18	1.25
3	P	146	TRP	CE3-CZ3	6.30	1.49	1.38
7	T	21	PHE	CG-CD2	-6.29	1.29	1.38
4	Q	8	SER	C-O	6.29	1.35	1.23
4	D	63	LYS	CA-CB	6.28	1.67	1.53
1	N	371	TYR	CD2-CE2	6.28	1.48	1.39
9	I	61	GLU	CD-OE2	-6.28	1.18	1.25
2	O	65	TRP	CD2-CE3	6.27	1.49	1.40
3	C	55	TYR	CG-CD2	6.26	1.47	1.39
1	N	387	PHE	CG-CD2	6.26	1.48	1.38
7	G	16	TRP	CA-C	6.26	1.69	1.52
3	C	65	SER	CB-OG	6.25	1.50	1.42
5	E	39	TYR	CG-CD2	-6.25	1.31	1.39
1	A	396	TRP	CZ3-CH2	6.25	1.50	1.40
1	N	203	ALA	C-O	6.25	1.35	1.23
2	O	65	TRP	CE3-CZ3	6.24	1.49	1.38
5	R	90	ARG	CZ-NH1	6.24	1.41	1.33
9	I	60	PHE	CG-CD1	6.23	1.48	1.38
3	P	104	SER	CB-OG	6.22	1.50	1.42
5	R	80	GLU	CD-OE2	6.22	1.32	1.25
1	N	148	PHE	CG-CD2	6.22	1.48	1.38
5	E	82	TYR	CG-CD1	6.21	1.47	1.39
10	J	33	ARG	CA-CB	6.21	1.67	1.53
7	G	12	GLY	CA-C	6.20	1.61	1.51
6	S	89	TYR	CE2-CZ	6.20	1.46	1.38
3	C	64	GLU	CD-OE2	6.19	1.32	1.25
5	R	44	GLU	CD-OE2	-6.19	1.18	1.25
3	C	241	TYR	CE1-CZ	-6.17	1.30	1.38
1	N	189	MET	CG-SD	-6.17	1.65	1.81
9	I	19	PHE	CG-CD2	6.17	1.48	1.38
1	N	328	HIS	N-CA	6.17	1.58	1.46
13	M	40	TYR	CE2-CZ	6.16	1.46	1.38
7	G	39	SER	CB-OG	6.16	1.50	1.42
1	N	484	THR	CB-CG2	-6.15	1.32	1.52
1	A	84	PRO	CA-CB	6.14	1.65	1.53
1	N	396	TRP	CD2-CE2	6.14	1.48	1.41
6	S	89	TYR	CG-CD1	6.12	1.47	1.39
5	R	9	GLU	CG-CD	6.12	1.61	1.51
5	E	57	ARG	CZ-NH1	6.12	1.41	1.33
11	K	40	TRP	CE3-CZ3	6.11	1.48	1.38
1	N	54	TYR	CD2-CE2	6.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	CB-CG2	6.11	1.65	1.52
6	F	67	SER	CB-OG	6.11	1.50	1.42
1	A	244	TYR	CG-CD1	6.11	1.47	1.39
10	W	27	THR	CB-OG1	6.11	1.55	1.43
10	W	25	GLY	N-CA	6.10	1.55	1.46
1	A	38	ARG	NE-CZ	6.10	1.41	1.33
8	H	56	TYR	CE1-CZ	6.10	1.46	1.38
4	D	135	SER	CA-CB	6.10	1.62	1.52
7	T	50	TYR	CG-CD2	6.09	1.47	1.39
1	A	450	TRP	CD2-CE2	6.09	1.48	1.41
2	O	59	GLN	CD-NE2	6.08	1.48	1.32
3	P	186	PHE	CA-CB	6.08	1.67	1.53
2	B	60	GLU	CD-OE1	6.08	1.32	1.25
6	S	5	GLY	N-CA	6.08	1.55	1.46
13	M	26	PHE	CE1-CZ	6.08	1.48	1.37
3	P	104	SER	CA-CB	6.07	1.62	1.52
1	N	38	ARG	CZ-NH2	6.04	1.41	1.33
6	S	46	PRO	N-CA	6.04	1.57	1.47
2	B	157	GLU	CD-OE2	-6.03	1.19	1.25
1	N	340	TRP	CE2-CZ2	6.03	1.50	1.39
11	K	24	PHE	CG-CD2	6.03	1.47	1.38
1	N	396	TRP	CE3-CZ3	6.03	1.48	1.38
6	F	73	TRP	CE3-CZ3	6.02	1.48	1.38
1	A	129	TYR	CD1-CE1	6.01	1.48	1.39
12	Y	20	ARG	CD-NE	6.01	1.56	1.46
7	G	5	LYS	CA-C	6.00	1.68	1.52
3	C	172	TYR	CE2-CZ	6.00	1.46	1.38
8	H	72	TRP	CD2-CE2	6.00	1.48	1.41
1	A	512	ASN	CB-CG	-6.00	1.37	1.51
12	Y	38	PHE	CG-CD1	6.00	1.47	1.38
3	P	230	ASN	CB-CG	-5.99	1.37	1.51
4	Q	138	TRP	CE3-CZ3	5.99	1.48	1.38
1	A	219	PHE	CE1-CZ	5.98	1.48	1.37
4	D	8	SER	CB-OG	-5.98	1.34	1.42
10	W	7	GLU	CG-CD	5.97	1.60	1.51
1	A	214	ASN	C-O	5.97	1.34	1.23
3	P	227	PHE	CE2-CZ	5.97	1.48	1.37
3	C	57	TRP	CZ3-CH2	5.96	1.49	1.40
1	N	226	GLY	N-CA	5.95	1.54	1.46
3	C	14	SER	CA-CB	5.95	1.61	1.52
2	O	85	TYR	CE1-CZ	5.94	1.46	1.38
3	P	55	TYR	CG-CD2	5.93	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	140	TYR	CB-CG	5.92	1.60	1.51
12	Y	46	LYS	CD-CE	-5.92	1.36	1.51
2	B	65	TRP	CZ2-CH2	5.92	1.48	1.37
1	A	403	TYR	CG-CD1	5.92	1.46	1.39
1	A	249	PRO	CA-CB	5.91	1.65	1.53
1	A	220	PHE	CG-CD1	5.90	1.47	1.38
3	P	203	PHE	CE2-CZ	5.90	1.48	1.37
11	K	54	ARG	NE-CZ	5.89	1.40	1.33
1	N	260	TYR	CG-CD2	5.89	1.46	1.39
1	N	304	TYR	CE1-CZ	5.89	1.46	1.38
1	A	267	PRO	N-CD	5.88	1.56	1.47
1	A	410	ALA	CA-CB	5.88	1.64	1.52
13	M	40	TYR	CG-CD2	5.88	1.46	1.39
7	T	16	TRP	CD2-CE2	5.88	1.48	1.41
1	A	101	SER	CB-OG	5.87	1.49	1.42
1	N	67	PHE	CG-CD1	5.87	1.47	1.38
1	N	8	PHE	CD1-CE1	5.87	1.50	1.39
3	P	16	TRP	CZ3-CH2	5.87	1.49	1.40
3	C	35	PHE	CE1-CZ	5.85	1.48	1.37
5	E	102	GLU	CD-OE1	5.84	1.32	1.25
1	N	440	TYR	CE2-CZ	5.83	1.46	1.38
2	B	121	TYR	CD1-CE1	5.83	1.48	1.39
3	P	37	PHE	CG-CD2	5.82	1.47	1.38
10	W	5	VAL	CB-CG1	5.82	1.65	1.52
1	A	334	TRP	CB-CG	5.82	1.60	1.50
1	A	305	PHE	CG-CD2	5.80	1.47	1.38
1	A	244	TYR	CE1-CZ	5.80	1.46	1.38
2	B	132	GLU	CD-OE2	5.79	1.32	1.25
2	B	106	TRP	CE2-CZ2	5.78	1.49	1.39
4	D	91	PHE	CG-CD2	5.78	1.47	1.38
3	P	15	PRO	CA-CB	5.78	1.65	1.53
12	Y	16	GLU	CG-CD	5.78	1.60	1.51
1	N	377	PHE	CE1-CZ	5.78	1.48	1.37
11	X	39	GLU	CD-OE2	5.78	1.32	1.25
1	A	323	TRP	CZ3-CH2	5.77	1.49	1.40
1	N	372	TYR	CD1-CE1	5.77	1.48	1.39
8	H	72	TRP	CZ3-CH2	5.76	1.49	1.40
6	S	93	PRO	CA-C	5.74	1.64	1.52
6	F	84	SER	CA-CB	5.74	1.61	1.52
3	P	197	PHE	CE2-CZ	5.74	1.48	1.37
4	Q	24	LEU	CB-CG	5.74	1.69	1.52
8	U	16	PHE	CG-CD1	5.74	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	7	ALA	C-O	5.74	1.34	1.23
1	N	19	TYR	CG-CD2	5.72	1.46	1.39
2	B	60	GLU	CG-CD	5.72	1.60	1.51
1	A	485	VAL	CB-CG2	5.72	1.64	1.52
1	N	387	PHE	CE1-CZ	5.72	1.48	1.37
1	A	270	TYR	N-CA	5.71	1.57	1.46
5	E	103	GLU	CB-CG	5.71	1.62	1.52
3	P	79	LEU	CA-CB	5.71	1.66	1.53
4	Q	16	TYR	CD2-CE2	5.71	1.48	1.39
5	R	30	ARG	CZ-NH2	5.71	1.40	1.33
7	G	36	TRP	CG-CD2	5.70	1.53	1.43
2	O	9	PHE	CE2-CZ	5.70	1.48	1.37
3	C	146	TRP	CE3-CZ3	5.70	1.48	1.38
5	R	39	TYR	CG-CD2	-5.70	1.31	1.39
3	C	39	SER	C-O	5.69	1.34	1.23
13	Z	9	PRO	CA-CB	5.68	1.65	1.53
1	A	419	VAL	CB-CG1	5.68	1.64	1.52
3	C	35	PHE	CG-CD1	5.68	1.47	1.38
3	P	241	TYR	CG-CD1	5.68	1.46	1.39
8	U	78	GLU	CD-OE2	5.67	1.31	1.25
10	J	17	GLY	CA-C	5.67	1.60	1.51
1	A	2	PHE	CE1-CZ	5.66	1.48	1.37
4	D	20	ARG	N-CA	5.66	1.57	1.46
1	A	108	SER	CA-CB	5.66	1.61	1.52
6	F	18	ARG	CZ-NH2	5.66	1.40	1.33
1	N	493	GLU	CG-CD	5.66	1.60	1.51
10	W	24	GLY	N-CA	5.66	1.54	1.46
10	J	50	LEU	N-CA	5.66	1.57	1.46
5	E	30	ARG	CA-CB	5.65	1.66	1.53
4	D	29	HIS	C-O	5.64	1.34	1.23
1	A	498	CYS	C-O	5.63	1.34	1.23
10	J	1	PHE	CG-CD2	5.63	1.47	1.38
3	C	153	GLU	CD-OE1	-5.62	1.19	1.25
7	T	28	VAL	CB-CG2	5.62	1.64	1.52
1	A	323	TRP	CD1-NE1	5.62	1.47	1.38
2	B	113	TYR	CG-CD2	5.61	1.46	1.39
2	B	202	SER	CB-OG	-5.61	1.34	1.42
4	D	73	ARG	CZ-NH2	5.61	1.40	1.33
3	C	244	PHE	CD2-CE2	5.61	1.50	1.39
1	A	269	GLY	CA-C	5.61	1.60	1.51
9	I	16	ARG	NE-CZ	5.61	1.40	1.33
5	E	84	TYR	CE2-CZ	5.61	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	32	TRP	CG-CD1	5.60	1.44	1.36
10	J	26	ALA	CA-CB	5.60	1.64	1.52
6	S	85	CYS	CB-SG	5.59	1.91	1.82
2	B	167	SER	CB-OG	-5.59	1.34	1.42
1	N	188	VAL	CB-CG1	5.58	1.64	1.52
3	C	102	TYR	CG-CD1	5.58	1.46	1.39
8	U	36	PHE	CG-CD1	5.58	1.47	1.38
3	P	219	PHE	CE1-CZ	5.58	1.48	1.37
1	A	264	LYS	CD-CE	5.57	1.65	1.51
1	N	264	LYS	CD-CE	5.57	1.65	1.51
1	A	440	TYR	CD1-CE1	5.57	1.47	1.39
12	L	33	PHE	CE1-CZ	5.56	1.48	1.37
6	S	93	PRO	C-O	5.56	1.34	1.23
4	D	64	PHE	CA-CB	5.56	1.66	1.53
7	T	82	TYR	CG-CD1	5.56	1.46	1.39
9	V	50	PHE	CE1-CZ	5.56	1.48	1.37
7	G	65	GLY	N-CA	5.56	1.54	1.46
1	A	144	ASP	CA-CB	5.55	1.66	1.53
1	N	510	TYR	CG-CD1	5.55	1.46	1.39
10	W	26	ALA	CA-CB	5.55	1.64	1.52
6	F	60	CYS	CB-SG	5.54	1.91	1.82
2	O	156	SER	CB-OG	5.54	1.49	1.42
10	J	34	VAL	CB-CG2	5.53	1.64	1.52
2	O	206	PHE	CG-CD2	5.52	1.47	1.38
2	B	223	SER	CB-OG	-5.52	1.35	1.42
3	C	230	ASN	CB-CG	-5.52	1.38	1.51
1	N	94	PHE	CG-CD1	5.52	1.47	1.38
6	S	81	ARG	CA-CB	5.51	1.66	1.53
1	N	438	ARG	CG-CD	5.51	1.65	1.51
1	N	506	GLU	CD-OE2	-5.51	1.19	1.25
1	A	387	PHE	CA-CB	5.50	1.66	1.53
3	C	33	MET	N-CA	5.50	1.57	1.46
10	J	32	TYR	CE1-CZ	5.50	1.45	1.38
1	N	401	SER	CA-CB	5.50	1.61	1.52
1	A	98	ASN	CG-ND2	-5.49	1.19	1.32
1	N	297[A]	MET	N-CA	5.48	1.57	1.46
1	N	297[B]	MET	N-CA	5.48	1.57	1.46
3	P	240	TRP	CE3-CZ3	5.48	1.47	1.38
3	C	35	PHE	CG-CD2	5.48	1.47	1.38
4	D	79	LYS	CD-CE	5.48	1.65	1.51
7	G	56	ARG	CD-NE	5.47	1.55	1.46
5	E	73	ASP	CB-CG	5.47	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	16	TRP	CD1-NE1	5.47	1.47	1.38
1	A	461	SER	CB-OG	5.47	1.49	1.42
3	P	16	TRP	CE2-CZ2	5.47	1.49	1.39
5	R	88	GLU	CD-OE1	-5.46	1.19	1.25
4	D	113	GLU	CD-OE2	-5.46	1.19	1.25
1	A	346	PHE	CD1-CE1	5.45	1.50	1.39
3	C	249	TRP	CE3-CZ3	5.45	1.47	1.38
2	B	85	TYR	CG-CD2	5.45	1.46	1.39
12	L	33	PHE	CG-CD1	5.45	1.47	1.38
1	N	81	TRP	CZ3-CH2	5.44	1.48	1.40
1	A	94	PHE	CG-CD2	5.44	1.47	1.38
1	N	414	PHE	CG-CD1	5.44	1.47	1.38
6	F	4	GLY	N-CA	5.43	1.54	1.46
6	F	87	THR	CB-CG2	-5.43	1.34	1.52
5	E	61	PHE	CE2-CZ	5.42	1.47	1.37
3	P	8	TYR	CD2-CE2	5.42	1.47	1.39
1	A	315	PRO	CA-CB	5.42	1.64	1.53
1	A	379	TYR	CG-CD2	5.42	1.46	1.39
2	B	82	ARG	CZ-NH1	5.41	1.40	1.33
1	N	175	ALA	C-O	5.41	1.33	1.23
7	T	12	GLY	CA-C	5.41	1.60	1.51
2	B	59	GLN	CB-CG	5.41	1.67	1.52
1	A	102	PHE	CE1-CZ	5.41	1.47	1.37
1	A	486	ASP	CG-OD2	5.41	1.37	1.25
2	O	201	GLY	N-CA	5.40	1.54	1.46
6	S	73	TRP	CE3-CZ3	5.39	1.47	1.38
1	A	210	LEU	N-CA	5.39	1.57	1.46
3	P	258	TRP	CG-CD1	5.39	1.44	1.36
1	N	244	TYR	CE2-CZ	5.38	1.45	1.38
3	P	208	VAL	CB-CG2	5.37	1.64	1.52
1	N	101	SER	CB-OG	5.37	1.49	1.42
3	C	99	TRP	CD2-CE2	5.36	1.47	1.41
4	D	105	GLY	N-CA	5.36	1.54	1.46
1	A	303	ALA	CA-CB	5.36	1.63	1.52
2	B	202	SER	CA-CB	5.36	1.60	1.52
6	S	3	GLY	N-CA	5.36	1.54	1.46
1	A	414	PHE	CE1-CZ	5.34	1.47	1.37
3	C	150	SER	CA-CB	5.34	1.60	1.52
4	D	58	GLU	CD-OE1	5.34	1.31	1.25
1	A	81	TRP	CE2-CZ2	5.34	1.48	1.39
4	D	54	ASP	N-CA	5.34	1.57	1.46
2	O	163	TRP	CE3-CZ3	5.34	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	36	HIS	CA-CB	-5.33	1.42	1.53
1	N	250	GLY	CA-C	5.33	1.60	1.51
1	A	425	PHE	CD1-CE1	5.33	1.50	1.39
2	O	134	ARG	CZ-NH1	5.33	1.40	1.33
3	P	233	PHE	CG-CD1	5.32	1.46	1.38
1	N	184	PHE	CE1-CZ	5.32	1.47	1.37
6	S	18	ARG	CD-NE	5.32	1.55	1.46
5	R	18	TYR	CZ-OH	5.32	1.46	1.37
2	O	197	SER	CB-OG	5.32	1.49	1.42
1	A	58	VAL	N-CA	5.31	1.56	1.46
7	G	21	PHE	CG-CD2	-5.31	1.30	1.38
3	C	67	PHE	CG-CD2	5.30	1.46	1.38
1	N	150	LEU	N-CA	5.30	1.56	1.46
2	B	220	GLU	CG-CD	5.30	1.59	1.51
10	J	32	TYR	CG-CD2	5.30	1.46	1.39
2	B	121	TYR	CE1-CZ	5.30	1.45	1.38
2	B	218	TYR	CE2-CZ	5.29	1.45	1.38
3	P	169	LEU	CA-CB	5.29	1.66	1.53
1	A	94	PHE	CG-CD1	5.29	1.46	1.38
3	P	156	ARG	CG-CD	5.29	1.65	1.51
3	C	17	PRO	CG-CD	5.28	1.68	1.50
1	A	170	ASN	CG-ND2	5.28	1.46	1.32
8	U	27	ARG	CZ-NH2	5.28	1.40	1.33
4	D	9	GLU	CD-OE2	5.28	1.31	1.25
6	S	3	GLY	CA-C	5.28	1.60	1.51
6	F	64	GLU	C-N	-5.28	1.22	1.34
3	P	195	SER	CB-OG	5.28	1.49	1.42
9	I	54	TYR	CD1-CE1	5.27	1.47	1.39
4	Q	14	PRO	N-CA	5.27	1.56	1.47
1	N	384	GLY	N-CA	5.26	1.53	1.46
1	A	72	PRO	CA-CB	5.26	1.64	1.53
1	A	392	GLY	N-CA	5.26	1.53	1.46
2	B	85	TYR	CE1-CZ	5.25	1.45	1.38
7	G	60	PHE	CG-CD1	5.25	1.46	1.38
3	P	65	SER	CB-OG	5.25	1.49	1.42
1	A	207	THR	N-CA	5.25	1.56	1.46
1	A	473	TRP	CZ3-CH2	5.25	1.48	1.40
1	A	382	SER	CA-C	-5.24	1.39	1.52
6	F	2	SER	N-CA	5.24	1.56	1.46
3	P	94	PHE	CD2-CE2	5.24	1.49	1.39
3	C	57	TRP	CD1-NE1	5.24	1.46	1.38
6	F	4	GLY	CA-C	5.24	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	SER	CA-CB	5.23	1.60	1.52
3	C	140	SER	CB-OG	5.23	1.49	1.42
4	D	58	GLU	CG-CD	5.22	1.59	1.51
1	N	440	TYR	CG-CD1	5.22	1.46	1.39
6	S	4	GLY	N-CA	5.22	1.53	1.46
2	B	106	TRP	CE3-CZ3	5.22	1.47	1.38
1	N	249	PRO	CA-CB	5.22	1.64	1.53
12	Y	3	TYR	CG-CD1	5.22	1.46	1.39
4	D	103	VAL	CA-CB	5.22	1.65	1.54
5	E	63	SER	CB-OG	5.22	1.49	1.42
1	N	260	TYR	CE1-CZ	5.22	1.45	1.38
2	O	115	ASP	CB-CG	5.22	1.62	1.51
1	N	430	PHE	CE2-CZ	5.21	1.47	1.37
5	R	47	ILE	C-O	5.21	1.33	1.23
8	U	19	ARG	CZ-NH1	5.21	1.39	1.33
9	I	61	GLU	CG-CD	5.21	1.59	1.51
5	R	29	LEU	N-CA	5.21	1.56	1.46
3	P	116	TRP	CE3-CZ3	5.21	1.47	1.38
3	P	249	TRP	CE3-CZ3	5.21	1.47	1.38
2	B	23	PHE	CG-CD1	5.20	1.46	1.38
1	A	454	SER	CA-CB	5.20	1.60	1.52
3	C	259	TRP	CE3-CZ3	5.20	1.47	1.38
9	V	28	SER	CB-OG	5.19	1.49	1.42
1	N	167	THR	CB-OG1	5.18	1.53	1.43
5	E	66	ARG	CD-NE	5.18	1.55	1.46
7	G	15	THR	CA-CB	5.18	1.66	1.53
1	N	269	GLY	CA-C	5.18	1.60	1.51
2	B	176	PRO	CA-CB	5.18	1.64	1.53
1	N	6	TRP	CE3-CZ3	5.17	1.47	1.38
1	A	175	ALA	CA-CB	5.17	1.63	1.52
3	P	161	GLN	CD-OE1	-5.17	1.12	1.24
1	A	270	TYR	CZ-OH	5.16	1.46	1.37
11	X	29	TRP	CE3-CZ3	5.16	1.47	1.38
2	B	126	SER	CA-CB	5.16	1.60	1.52
2	O	162	SER	C-O	5.16	1.33	1.23
2	B	122	MET	C-O	5.16	1.33	1.23
5	R	82	TYR	CG-CD1	5.16	1.45	1.39
1	N	236	TRP	CZ3-CH2	5.16	1.48	1.40
5	R	84	TYR	CE2-CZ	5.16	1.45	1.38
1	A	275	TRP	CE3-CZ3	5.15	1.47	1.38
4	D	9	GLU	CG-CD	5.15	1.59	1.51
7	T	17	ARG	CZ-NH1	5.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	17	VAL	N-CA	5.15	1.56	1.46
7	G	21	PHE	CD2-CE2	5.14	1.49	1.39
3	P	86	PHE	CD2-CE2	5.14	1.49	1.39
1	N	355	GLY	N-CA	5.14	1.53	1.46
7	G	16	TRP	CZ3-CH2	5.14	1.48	1.40
6	F	31	TYR	CG-CD2	5.13	1.45	1.39
5	E	55	CYS	N-CA	5.13	1.56	1.46
1	N	371	TYR	CG-CD1	5.13	1.45	1.39
4	Q	60	TYR	CE1-CZ	5.13	1.45	1.38
8	U	68	TRP	CZ3-CH2	5.12	1.48	1.40
13	Z	32	TRP	CE3-CZ3	5.12	1.47	1.38
5	R	84	TYR	CG-CD1	5.12	1.45	1.39
7	G	5	LYS	CA-CB	5.12	1.65	1.53
2	B	108	TYR	CE1-CZ	-5.12	1.31	1.38
12	L	38	PHE	N-CA	5.12	1.56	1.46
3	C	37	PHE	CG-CD1	5.11	1.46	1.38
4	D	138	TRP	CZ3-CH2	5.11	1.48	1.40
6	S	2	SER	N-CA	5.11	1.56	1.46
4	D	60	TYR	CG-CD1	5.10	1.45	1.39
7	T	5	LYS	CA-CB	5.10	1.65	1.53
1	A	359	ALA	CA-CB	5.10	1.63	1.52
3	P	115	CYS	CB-SG	5.10	1.91	1.82
4	Q	18	ASP	N-CA	5.10	1.56	1.46
1	N	298[A]	ASP	N-CA	5.09	1.56	1.46
1	N	298[B]	ASP	N-CA	5.09	1.56	1.46
2	B	203	ASN	CG-OD1	-5.09	1.12	1.24
5	E	82	TYR	CE2-CZ	5.09	1.45	1.38
1	A	502	TYR	CD2-CE2	5.09	1.47	1.39
3	C	220	PHE	CE2-CZ	5.08	1.47	1.37
2	B	171	LYS	C-O	5.08	1.33	1.23
7	G	7	ASP	N-CA	5.08	1.56	1.46
10	W	33	ARG	CA-CB	5.08	1.65	1.53
1	A	418	PHE	CD1-CE1	5.08	1.49	1.39
4	Q	134	PHE	CG-CD2	5.08	1.46	1.38
7	T	56	ARG	CZ-NH1	5.08	1.39	1.33
12	Y	38	PHE	CE1-CZ	5.08	1.47	1.37
1	N	236	TRP	CE3-CZ3	5.08	1.47	1.38
4	D	145	TRP	CE3-CZ3	5.07	1.47	1.38
1	N	267	PRO	N-CD	5.07	1.54	1.47
10	J	48	TYR	CG-CD1	5.07	1.45	1.39
1	N	323	TRP	CD2-CE2	5.07	1.47	1.41
3	P	57	TRP	CB-CG	5.05	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	40	TYR	CD2-CE2	5.05	1.47	1.39
1	A	344	PHE	CG-CD2	5.05	1.46	1.38
9	I	35	TYR	CG-CD2	5.05	1.45	1.39
4	Q	67	SER	CA-CB	5.05	1.60	1.52
1	A	288	TRP	CD2-CE2	5.04	1.47	1.41
1	N	315	PRO	CA-CB	5.04	1.63	1.53
1	N	454	SER	CA-CB	5.04	1.60	1.52
2	O	155	SER	CA-CB	5.04	1.60	1.52
1	A	129	TYR	CD2-CE2	5.03	1.46	1.39
4	D	126	MET	CG-SD	5.02	1.94	1.81
7	G	50	TYR	CD2-CE2	5.02	1.46	1.39
4	D	68	PHE	CG-CD1	5.02	1.46	1.38
1	A	362	SER	C-O	5.01	1.32	1.23
1	N	372	TYR	CE2-CZ	5.01	1.45	1.38
3	P	186	PHE	CD1-CE1	5.01	1.49	1.39
2	B	55	THR	C-O	5.00	1.32	1.23
3	C	173	PHE	CG-CD1	5.00	1.46	1.38
1	N	319	LYS	CA-CB	5.00	1.65	1.53

All (588) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-43.20	98.70	120.30
7	T	17	ARG	NE-CZ-NH1	35.11	137.86	120.30
4	D	20	ARG	NE-CZ-NH1	32.62	136.61	120.30
4	Q	20	ARG	NE-CZ-NH2	-29.37	105.62	120.30
7	T	17	ARG	NE-CZ-NH2	-25.91	107.34	120.30
1	N	71	MET	CG-SD-CE	-25.78	58.95	100.20
12	L	20	ARG	NE-CZ-NH2	-24.20	108.20	120.30
1	A	71	MET	CG-SD-CE	-23.77	62.17	100.20
4	Q	20	ARG	NE-CZ-NH1	22.60	131.60	120.30
5	E	90	ARG	NE-CZ-NH1	21.11	130.86	120.30
12	L	20	ARG	NE-CZ-NH1	18.06	129.33	120.30
9	V	10	ARG	NE-CZ-NH2	-17.38	111.61	120.30
9	I	16	ARG	NE-CZ-NH2	-16.64	111.98	120.30
11	X	54	ARG	NE-CZ-NH2	15.45	128.03	120.30
4	D	20	ARG	CD-NE-CZ	15.39	145.15	123.60
11	X	54	ARG	NE-CZ-NH1	-15.39	112.61	120.30
12	Y	20	ARG	NE-CZ-NH1	-14.99	112.81	120.30
3	P	63	ARG	NE-CZ-NH1	14.96	127.78	120.30
11	K	54	ARG	NE-CZ-NH1	-14.89	112.85	120.30
12	Y	20	ARG	NE-CZ-NH2	13.90	127.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH2	-13.84	113.38	120.30
7	T	17	ARG	CD-NE-CZ	13.71	142.79	123.60
2	B	134	ARG	NE-CZ-NH2	-13.42	113.59	120.30
5	E	40	ASP	CB-CG-OD1	13.13	130.12	118.30
9	V	10	ARG	NE-CZ-NH1	12.44	126.52	120.30
3	P	63	ARG	NE-CZ-NH2	-12.32	114.14	120.30
2	O	82	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	A	129	TYR	CB-CG-CD2	-11.97	113.81	121.00
12	L	5	GLU	OE1-CD-OE2	-11.75	109.20	123.30
1	A	38	ARG	NE-CZ-NH1	11.55	126.08	120.30
4	D	21	ASP	CB-CG-OD2	11.33	128.49	118.30
10	W	27	THR	OG1-CB-CG2	-11.21	84.22	110.00
2	B	151	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	346	PHE	CB-CG-CD2	-10.92	113.15	120.80
1	A	8	PHE	CB-CG-CD2	-10.79	113.24	120.80
8	H	73	ASP	CB-CG-OD2	-10.72	108.65	118.30
1	A	442	ASP	CB-CG-OD1	10.67	127.90	118.30
1	A	51	ASP	CB-CG-OD2	-10.64	108.72	118.30
4	D	31	LYS	CD-CE-NZ	-10.48	87.59	111.70
6	S	25	ARG	NE-CZ-NH2	-10.43	115.08	120.30
11	K	47	ARG	NE-CZ-NH2	10.41	125.50	120.30
1	A	486	ASP	CB-CG-OD1	-10.30	109.03	118.30
3	C	63	ARG	NE-CZ-NH2	-10.23	115.18	120.30
12	L	20	ARG	CG-CD-NE	-10.21	90.35	111.80
1	N	486	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	213	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	A	302[A]	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	302[B]	ARG	NE-CZ-NH1	10.15	125.38	120.30
4	Q	20	ARG	CD-NE-CZ	10.13	137.79	123.60
1	N	96	ARG	NE-CZ-NH2	-10.12	115.24	120.30
5	R	90	ARG	NE-CZ-NH2	-10.01	115.30	120.30
3	P	80	ARG	CG-CD-NE	-9.96	90.89	111.80
7	T	17	ARG	CB-CG-CD	-9.80	86.12	111.60
5	E	66	ARG	NE-CZ-NH2	-9.77	115.41	120.30
5	E	49	ASP	CB-CG-OD1	9.77	127.09	118.30
5	E	107	ASP	CB-CG-OD1	9.71	127.04	118.30
3	C	214	PHE	CB-CG-CD1	9.70	127.59	120.80
1	A	38	ARG	NE-CZ-NH2	-9.69	115.45	120.30
9	V	43	ARG	NE-CZ-NH1	9.66	125.13	120.30
3	P	59	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	N	96	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	A	51	ASP	CB-CG-OD1	9.57	126.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	90	GLU	OE1-CD-OE2	9.50	134.70	123.30
3	C	214	PHE	CB-CG-CD2	-9.36	114.25	120.80
3	C	181	TYR	CZ-CE2-CD2	-9.34	111.39	119.80
1	N	237	PHE	CB-CG-CD1	-9.30	114.29	120.80
1	N	400	PHE	CB-CG-CD2	-9.29	114.29	120.80
3	C	31	LEU	CB-CG-CD1	-9.28	95.22	111.00
3	C	156	ARG	NE-CZ-NH1	9.23	124.92	120.30
5	E	53	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	377	PHE	CB-CG-CD1	-9.13	114.41	120.80
1	N	189	MET	CG-SD-CE	9.01	114.62	100.20
5	E	56	ARG	NE-CZ-NH2	-8.97	115.81	120.30
4	Q	121	LYS	CD-CE-NZ	-8.95	91.11	111.70
2	B	133	LEU	CB-CG-CD1	-8.91	95.85	111.00
1	N	512	ASN	CB-CG-ND2	-8.76	95.68	116.70
1	A	152	LEU	CB-CG-CD1	-8.73	96.16	111.00
5	E	90	ARG	CD-NE-CZ	8.72	135.80	123.60
2	O	75	LEU	CB-CG-CD1	8.67	125.73	111.00
1	A	439	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	N	512	ASN	CA-CB-CG	-8.66	94.35	113.40
1	N	212	ASP	CB-CG-OD2	-8.57	110.59	118.30
2	B	87	MET	CA-CB-CG	8.56	127.86	113.30
3	C	44	MET	CG-SD-CE	8.44	113.70	100.20
12	L	20	ARG	CD-NE-CZ	8.41	135.37	123.60
1	A	417	MET	CG-SD-CE	-8.38	86.80	100.20
1	N	439	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	387	PHE	CB-CG-CD2	-8.33	114.97	120.80
1	A	63	PHE	CB-CG-CD2	-8.32	114.97	120.80
2	O	134	ARG	NE-CZ-NH2	-8.31	116.14	120.30
5	R	36	LEU	CB-CG-CD2	-8.28	96.93	111.00
2	B	75	LEU	CB-CG-CD1	8.27	125.06	111.00
5	E	19	PHE	CZ-CE2-CD2	-8.24	110.21	120.10
10	J	44	LEU	CB-CG-CD1	-8.20	97.05	111.00
3	P	219	PHE	CB-CG-CD2	-8.20	115.06	120.80
1	N	505	PHE	CB-CG-CD2	-8.20	115.06	120.80
3	P	153	GLU	OE1-CD-OE2	8.20	133.14	123.30
5	R	30	ARG	NE-CZ-NH1	8.19	124.39	120.30
4	Q	16	TYR	CB-CG-CD1	-8.12	116.13	121.00
2	O	36	SER	CB-CA-C	8.10	125.48	110.10
8	H	52	VAL	CB-CA-C	-8.09	96.03	111.40
1	N	425	PHE	CB-CG-CD1	-8.08	115.14	120.80
2	O	65	TRP	CB-CA-C	8.07	126.54	110.40
5	E	70	VAL	CA-CB-CG1	-8.03	98.85	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	59	ARG	NE-CZ-NH2	8.03	124.31	120.30
2	O	75	LEU	CB-CG-CD2	-8.01	97.38	111.00
1	N	442	ASP	CB-CG-OD1	7.96	125.46	118.30
1	N	366	VAL	CG1-CB-CG2	-7.94	98.20	110.90
1	A	270	TYR	CZ-CE2-CD2	-7.92	112.67	119.80
10	J	28	ASP	CB-CG-OD2	-7.89	111.20	118.30
7	G	14	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	A	366	VAL	CG1-CB-CG2	-7.86	98.32	110.90
2	B	139	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	480	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	N	144	ASP	CB-CG-OD2	-7.84	111.25	118.30
2	O	134	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	270	TYR	CB-CG-CD1	-7.82	116.31	121.00
3	P	90	GLU	OE1-CD-OE2	7.82	132.68	123.30
1	N	440	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	A	7	LEU	CB-CG-CD1	7.81	124.28	111.00
5	E	84	TYR	CG-CD1-CE1	-7.74	115.11	121.30
3	C	59	ARG	NE-CZ-NH1	-7.68	116.46	120.30
2	O	36	SER	CA-CB-OG	-7.67	90.48	111.20
1	N	426	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	A	268	PHE	CB-CG-CD2	-7.63	115.46	120.80
3	P	214	PHE	CB-CG-CD2	-7.61	115.47	120.80
3	P	80	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	O	133	LEU	CB-CG-CD2	-7.56	98.14	111.00
10	W	18	LEU	CB-CG-CD1	-7.54	98.19	111.00
9	I	15	ARG	NE-CZ-NH2	-7.53	116.53	120.30
6	S	1	ALA	C-N-CA	7.53	140.52	121.70
1	A	400	PHE	CB-CG-CD2	-7.52	115.54	120.80
10	W	50	LEU	CB-CG-CD2	7.51	123.77	111.00
2	O	59	GLN	CB-CG-CD	7.50	131.09	111.60
1	N	268	PHE	CG-CD1-CE1	-7.49	112.56	120.80
11	K	20	SER	CB-CA-C	7.44	124.24	110.10
7	T	18	PHE	CB-CG-CD2	-7.41	115.61	120.80
5	E	73	ASP	CB-CG-OD1	-7.40	111.64	118.30
7	T	5	LYS	CB-CA-C	7.40	125.20	110.40
1	A	179	TYR	CB-CG-CD2	-7.38	116.57	121.00
5	E	30	ARG	NE-CZ-NH2	-7.38	116.61	120.30
3	P	181	TYR	CG-CD1-CE1	-7.33	115.43	121.30
1	A	8	PHE	CB-CG-CD1	7.30	125.91	120.80
1	N	440	TYR	CD1-CE1-CZ	-7.30	113.23	119.80
11	K	54	ARG	NE-CZ-NH2	7.29	123.95	120.30
6	F	87	THR	OG1-CB-CG2	-7.29	93.23	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	55	ASP	CB-CG-OD1	7.27	124.84	118.30
7	G	5	LYS	CB-CA-C	7.26	124.93	110.40
1	A	512	ASN	CB-CA-C	-7.26	95.88	110.40
3	C	94	PHE	CB-CG-CD1	-7.25	115.72	120.80
1	A	5	ARG	NE-CZ-NH2	-7.25	116.67	120.30
2	B	82	ARG	NE-CZ-NH2	-7.19	116.70	120.30
3	C	40	MET	CG-SD-CE	-7.17	88.73	100.20
3	C	101	PHE	CB-CG-CD1	-7.16	115.78	120.80
5	E	56	ARG	NE-CZ-NH1	7.16	123.88	120.30
6	F	74	LEU	CB-CG-CD2	-7.14	98.87	111.00
5	E	84	TYR	CZ-CE2-CD2	-7.13	113.38	119.80
5	R	23	ASP	CB-CG-OD2	-7.13	111.88	118.30
6	F	1	ALA	C-N-CA	7.11	139.49	121.70
1	N	152	LEU	CB-CG-CD2	7.11	123.09	111.00
3	C	44	MET	CA-CB-CG	-7.11	101.22	113.30
1	A	237	PHE	CB-CG-CD2	-7.10	115.83	120.80
2	B	134	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	N	148	PHE	CB-CG-CD2	-7.10	115.83	120.80
3	C	221	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	364	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	A	340	TRP	CH2-CZ2-CE2	-7.07	110.33	117.40
2	O	11	ASP	CB-CG-OD1	7.05	124.65	118.30
3	P	224	LYS	CD-CE-NZ	7.05	127.91	111.70
5	R	30	ARG	NE-CZ-NH2	-7.03	116.79	120.30
12	L	5	GLU	CG-CD-OE1	7.02	132.34	118.30
2	B	115	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	96	ARG	NE-CZ-NH2	-6.96	116.82	120.30
4	D	16	TYR	CB-CG-CD1	-6.95	116.83	121.00
5	E	49	ASP	OD1-CG-OD2	-6.95	110.10	123.30
1	N	270	TYR	CB-CG-CD1	-6.94	116.84	121.00
6	F	65	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	N	484	THR	N-CA-CB	-6.93	97.13	110.30
1	N	512	ASN	CB-CG-OD1	6.93	135.46	121.60
3	P	57	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	N	311	ILE	CA-CB-CG1	-6.90	97.89	111.00
1	A	300	ASP	CB-CG-OD2	-6.89	112.10	118.30
3	C	251	PHE	CB-CG-CD2	-6.88	115.99	120.80
3	C	102	TYR	CB-CG-CD1	-6.87	116.88	121.00
3	P	214	PHE	CB-CG-CD1	6.86	125.60	120.80
5	R	80	GLU	OE1-CD-OE2	6.85	131.51	123.30
2	B	133	LEU	CB-CG-CD2	-6.84	99.38	111.00
12	L	26	THR	N-CA-CB	-6.84	97.31	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	139	ASP	CB-CG-OD1	6.83	124.44	118.30
4	Q	18	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	212	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	270	TYR	CG-CD1-CE1	-6.77	115.89	121.30
1	N	512	ASN	CB-CA-C	-6.76	96.87	110.40
4	Q	8	SER	C-N-CA	6.75	138.57	121.70
2	B	82	ARG	CG-CD-NE	-6.74	97.64	111.80
1	A	296	GLY	O-C-N	-6.73	111.93	122.70
3	P	49	THR	CA-CB-CG2	-6.72	102.99	112.40
3	P	182	TYR	CB-CG-CD1	-6.72	116.97	121.00
3	C	181	TYR	CB-CG-CD2	-6.72	116.97	121.00
4	D	18	ASP	CB-CG-OD2	6.72	124.35	118.30
1	N	113[A]	LEU	CB-CA-C	6.71	122.95	110.20
1	N	113[B]	LEU	CB-CA-C	6.71	122.95	110.20
3	C	93	PHE	CB-CG-CD2	-6.68	116.13	120.80
3	P	151	LEU	CB-CG-CD2	-6.67	99.66	111.00
5	R	90	ARG	CG-CD-NE	-6.65	97.83	111.80
7	T	18	PHE	CB-CG-CD1	6.63	125.44	120.80
5	E	19	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	N	240	HIS	CA-CB-CG	-6.63	102.33	113.60
6	S	1	ALA	O-C-N	6.63	133.31	122.70
1	N	156	SER	O-C-N	6.62	133.29	122.70
1	N	327	LEU	O-C-N	6.62	133.29	122.70
2	B	3	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	505	PHE	CB-CG-CD1	-6.59	116.18	120.80
1	N	74	MET	CA-CB-CG	-6.59	102.10	113.30
3	P	181	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	A	480	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	425	PHE	CB-CG-CD1	-6.57	116.20	120.80
1	A	270	TYR	CE1-CZ-CE2	6.56	130.29	119.80
1	A	212	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	400	PHE	CZ-CE2-CD2	-6.54	112.25	120.10
7	G	33	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	164	PHE	CB-CG-CD1	-6.53	116.23	120.80
1	N	109	PHE	CB-CG-CD2	-6.52	116.24	120.80
3	C	97	PHE	CB-CG-CD2	-6.51	116.25	120.80
5	E	61	PHE	CG-CD2-CE2	6.49	127.94	120.80
5	R	84	TYR	CB-CG-CD2	6.48	124.89	121.00
1	N	189	MET	CB-CG-SD	-6.47	93.00	112.40
10	W	32	TYR	CG-CD2-CE2	6.47	126.47	121.30
1	N	324	LEU	CB-CG-CD2	6.43	121.94	111.00
6	F	1	ALA	O-C-N	6.42	132.98	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	23	ASP	CB-CG-OD1	6.41	124.07	118.30
3	C	181	TYR	CG-CD1-CE1	-6.39	116.19	121.30
1	A	22	PHE	CB-CG-CD2	-6.39	116.33	120.80
8	H	76	ARG	NE-CZ-NH1	6.37	123.48	120.30
2	B	11	ASP	CB-CG-OD1	6.36	124.03	118.30
9	V	21	ILE	CG1-CB-CG2	-6.36	97.41	111.40
2	B	65	TRP	CB-CA-C	6.35	123.11	110.40
1	N	159	LEU	CB-CG-CD1	-6.35	100.21	111.00
3	P	181	TYR	CZ-CE2-CD2	-6.34	114.09	119.80
7	G	18[A]	PHE	CB-CG-CD1	6.34	125.24	120.80
7	G	18[B]	PHE	CB-CG-CD1	6.34	125.24	120.80
4	D	10	ASP	CB-CG-OD2	-6.34	112.60	118.30
4	D	16	TYR	CG-CD2-CE2	-6.31	116.25	121.30
9	I	61	GLU	OE1-CD-OE2	-6.29	115.76	123.30
5	E	70	VAL	CB-CA-C	6.28	123.34	111.40
9	I	49	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	54	TYR	CG-CD1-CE1	-6.27	116.28	121.30
10	J	33	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	N	212	ASP	CB-CG-OD1	6.27	123.94	118.30
1	N	407	ASP	CB-CG-OD1	6.25	123.93	118.30
2	B	31	VAL	CA-CB-CG2	-6.25	101.53	110.90
1	N	387	PHE	CG-CD2-CE2	-6.24	113.94	120.80
1	N	19	TYR	CD1-CE1-CZ	-6.24	114.19	119.80
5	E	63	SER	O-C-N	6.23	132.66	122.70
1	A	270	TYR	CD1-CG-CD2	6.23	124.75	117.90
3	P	58	TRP	CD1-NE1-CE2	6.21	114.59	109.00
1	N	296	GLY	O-C-N	-6.21	112.76	122.70
1	A	253	MET	CA-CB-CG	-6.21	102.74	113.30
1	A	379	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	N	268	PHE	CZ-CE2-CD2	-6.20	112.66	120.10
2	B	59	GLN	N-CA-CB	6.20	121.75	110.60
5	R	18	TYR	CB-CG-CD2	-6.20	117.28	121.00
7	T	57	THR	CA-CB-CG2	-6.20	103.73	112.40
4	D	74	SER	CA-CB-OG	-6.19	94.48	111.20
7	G	7	ASP	N-CA-C	6.18	127.68	111.00
10	W	23	LYS	CG-CD-CE	-6.16	93.41	111.90
4	D	61	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	P	86	PHE	CE1-CZ-CE2	6.15	131.07	120.00
4	Q	10	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	B	151	ARG	NE-CZ-NH2	-6.14	117.23	120.30
6	S	15	GLY	O-C-N	6.13	132.51	122.70
5	R	53	ARG	NE-CZ-NH1	6.13	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	THR	CA-CB-CG2	-6.13	103.82	112.40
7	G	16	TRP	O-C-N	6.13	132.50	122.70
1	N	268	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	A	244	TYR	CD1-CE1-CZ	6.12	125.31	119.80
3	C	93	PHE	CG-CD2-CE2	-6.12	114.06	120.80
3	P	241	TYR	CB-CG-CD1	-6.12	117.33	121.00
3	P	233	PHE	CB-CG-CD2	-6.12	116.52	120.80
7	G	21	PHE	CB-CG-CD1	-6.11	116.52	120.80
6	S	1	ALA	CA-C-N	-6.11	103.76	117.20
1	A	400	PHE	CG-CD1-CE1	-6.11	114.08	120.80
3	P	102	TYR	CB-CG-CD1	-6.11	117.34	121.00
3	P	233	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	N	513	LEU	C-N-CA	-6.09	106.48	121.70
1	A	371	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	N	181	THR	CA-CB-OG1	-6.08	96.23	109.00
6	F	31	TYR	CG-CD2-CE2	-6.08	116.44	121.30
1	N	445	ASP	CB-CG-OD1	6.07	123.76	118.30
1	N	381	LEU	CB-CG-CD2	-6.06	100.69	111.00
1	A	244	TYR	CG-CD1-CE1	-6.06	116.45	121.30
2	B	11	ASP	CB-CG-OD2	-6.06	112.85	118.30
2	O	132	GLU	CG-CD-OE1	-6.06	106.18	118.30
3	C	244	PHE	CB-CG-CD2	-6.05	116.56	120.80
3	C	181	TYR	CE1-CZ-CE2	6.05	129.48	119.80
6	F	87	THR	N-CA-CB	6.05	121.79	110.30
13	M	33	VAL	CG1-CB-CG2	-6.05	101.22	110.90
1	A	240	HIS	CA-CB-CG	-6.03	103.35	113.60
2	B	73	LEU	CB-CG-CD1	-6.03	100.75	111.00
7	G	8	HIS	N-CA-C	6.03	127.28	111.00
3	P	86	PHE	CZ-CE2-CD2	-6.01	112.89	120.10
6	S	90	LYS	CB-CG-CD	6.00	127.21	111.60
1	A	181	THR	OG1-CB-CG2	-6.00	96.19	110.00
1	A	242	GLU	CG-CD-OE2	6.00	130.29	118.30
5	R	52	LEU	CB-CG-CD2	6.00	121.19	111.00
4	D	31	LYS	CB-CG-CD	-5.99	96.03	111.60
6	F	37[A]	LYS	CD-CE-NZ	-5.99	97.92	111.70
6	F	37[B]	LYS	CD-CE-NZ	-5.99	97.92	111.70
10	J	12	PHE	CG-CD1-CE1	-5.99	114.21	120.80
1	N	370	THR	CA-CB-CG2	-5.98	104.03	112.40
3	P	28	THR	CA-CB-CG2	-5.97	104.04	112.40
2	O	82	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	N	371	TYR	CB-CG-CD2	-5.96	117.42	121.00
5	E	61	PHE	CB-CG-CD2	5.96	124.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	193	TYR	CZ-CE2-CD2	-5.96	114.44	119.80
7	T	7	ASP	N-CA-C	5.95	127.05	111.00
4	Q	127	LYS	CD-CE-NZ	5.94	125.37	111.70
1	A	67	PHE	CB-CG-CD1	-5.92	116.65	120.80
6	S	93	PRO	CB-CA-C	5.92	126.80	112.00
2	B	16	ILE	CA-CB-CG1	-5.91	99.77	111.00
3	C	225	PHE	CB-CG-CD2	-5.91	116.66	120.80
2	B	198	GLU	CA-C-N	-5.91	104.21	117.20
1	N	129	TYR	CB-CG-CD2	-5.90	117.46	121.00
4	Q	19	ARG	NE-CZ-NH1	-5.89	117.36	120.30
6	F	45	ASP	CB-CG-OD1	5.88	123.59	118.30
5	R	79	LYS	CD-CE-NZ	-5.88	98.17	111.70
3	P	241	TYR	CG-CD1-CE1	-5.87	116.60	121.30
1	N	210	LEU	CB-CG-CD2	-5.87	101.02	111.00
9	V	68	ILE	CB-CG1-CD1	-5.86	97.48	113.90
5	E	19	PHE	CG-CD2-CE2	5.86	127.25	120.80
4	Q	8	SER	O-C-N	5.86	132.07	122.70
7	G	56	ARG	NE-CZ-NH2	5.86	123.23	120.30
5	R	39	TYR	CG-CD2-CE2	5.86	125.98	121.30
1	N	390	MET	CG-SD-CE	5.85	109.56	100.20
3	C	63	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	340	TRP	CZ3-CH2-CZ2	5.84	128.60	121.60
1	N	270	TYR	CE1-CZ-CE2	5.83	129.12	119.80
8	U	8	ILE	CB-CA-C	5.82	123.24	111.60
10	J	18	LEU	CB-CG-CD1	-5.81	101.13	111.00
5	R	88	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	310	MET	CA-CB-CG	-5.80	103.43	113.30
1	A	510	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	346	PHE	CD1-CG-CD2	5.80	125.83	118.30
1	A	513	LEU	CA-CB-CG	-5.79	101.98	115.30
1	A	344	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	A	124	THR	CA-CB-CG2	-5.79	104.30	112.40
1	A	346	PHE	CD1-CE1-CZ	-5.78	113.16	120.10
3	P	161	GLN	CB-CG-CD	-5.77	96.59	111.60
2	B	105	TYR	CB-CG-CD2	-5.77	117.54	121.00
2	B	89	GLU	CA-CB-CG	5.76	126.06	113.40
2	O	16	ILE	CG1-CB-CG2	-5.75	98.74	111.40
9	V	29	LEU	CB-CG-CD1	5.75	120.78	111.00
6	S	84	SER	N-CA-CB	-5.75	101.88	110.50
1	A	261	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	N	270	TYR	CZ-CE2-CD2	-5.73	114.64	119.80
4	D	122	ARG	NE-CZ-NH2	-5.72	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	184	LEU	N-CA-CB	-5.72	98.96	110.40
3	P	86	PHE	CD1-CE1-CZ	-5.72	113.24	120.10
3	P	8	TYR	CG-CD1-CE1	-5.72	116.73	121.30
3	C	54[A]	MET	CG-SD-CE	5.71	109.33	100.20
3	C	54[B]	MET	CG-SD-CE	5.71	109.33	100.20
10	W	44	LEU	CB-CG-CD2	5.70	120.69	111.00
3	P	181	TYR	CD1-CG-CD2	5.69	124.16	117.90
3	P	52	LEU	CB-CG-CD2	-5.69	101.32	111.00
3	C	181	TYR	CD1-CG-CD2	5.69	124.16	117.90
1	A	309	THR	O-C-N	5.69	131.80	122.70
1	N	194	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	A	310	MET	CG-SD-CE	-5.68	91.11	100.20
1	N	379	TYR	CB-CG-CD2	-5.68	117.59	121.00
3	P	236	GLU	CA-CB-CG	-5.68	100.90	113.40
9	V	16	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	109	PHE	CB-CG-CD2	-5.67	116.83	120.80
10	W	33	ARG	NE-CZ-NH2	-5.67	117.46	120.30
10	J	33	ARG	CA-CB-CG	-5.66	100.95	113.40
7	T	44	ARG	NE-CZ-NH1	5.66	123.13	120.30
7	T	5	LYS	CB-CG-CD	5.66	126.31	111.60
1	N	8	PHE	CB-CG-CD2	-5.64	116.85	120.80
5	R	14	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	B	204	HIS	N-CA-CB	-5.64	100.45	110.60
4	D	79	LYS	CD-CE-NZ	-5.64	98.74	111.70
8	H	81	PHE	CB-CG-CD1	-5.64	116.86	120.80
8	H	76	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	N	181	THR	OG1-CB-CG2	-5.63	97.06	110.00
1	A	327	LEU	O-C-N	5.62	131.69	122.70
3	C	80	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	387	PHE	CB-CG-CD1	5.62	124.73	120.80
1	N	369	ASP	CB-CG-OD2	-5.61	113.25	118.30
3	C	198	PHE	CB-CG-CD1	-5.61	116.88	120.80
7	T	36[A]	TRP	CA-CB-CG	5.60	124.35	113.70
7	T	36[B]	TRP	CA-CB-CG	5.60	124.35	113.70
12	L	28	PHE	CG-CD2-CE2	-5.60	114.64	120.80
4	D	127	LYS	CD-CE-NZ	5.60	124.58	111.70
12	Y	28	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	A	486	ASP	CB-CA-C	-5.58	99.23	110.40
1	N	5	ARG	CG-CD-NE	-5.58	100.08	111.80
1	A	152	LEU	CD1-CG-CD2	5.58	127.23	110.50
1	A	442	ASP	CB-CG-OD2	-5.57	113.29	118.30
3	C	192	VAL	CG1-CB-CG2	5.57	119.81	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	71	VAL	CG1-CB-CG2	5.57	119.80	110.90
6	S	3	GLY	N-CA-C	-5.54	99.26	113.10
6	F	48	LEU	CB-CG-CD1	5.53	120.41	111.00
5	E	73	ASP	OD1-CG-OD2	5.53	133.81	123.30
1	N	187	SER	O-C-N	5.53	131.54	122.70
2	B	82	ARG	NH1-CZ-NH2	5.52	125.48	119.40
1	A	213	ARG	NE-CZ-NH1	5.52	123.06	120.30
4	D	19[A]	ARG	NE-CZ-NH1	-5.52	117.54	120.30
4	D	19[B]	ARG	NE-CZ-NH1	-5.52	117.54	120.30
12	L	16	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	A	159	LEU	CB-CG-CD1	-5.51	101.63	111.00
9	I	10	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	N	213	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	94	PHE	CG-CD2-CE2	-5.49	114.76	120.80
1	A	327	LEU	CB-CA-C	-5.49	99.76	110.20
7	G	16	TRP	CA-CB-CG	-5.49	103.27	113.70
1	N	270	TYR	CD1-CG-CD2	5.49	123.94	117.90
4	Q	20	ARG	CG-CD-NE	-5.49	100.27	111.80
1	A	129	TYR	CG-CD1-CE1	-5.48	116.92	121.30
4	D	64	PHE	CB-CG-CD2	-5.48	116.96	120.80
2	O	73	LEU	CB-CG-CD1	-5.48	101.68	111.00
2	B	101	GLY	O-C-N	5.48	131.46	122.70
10	J	21	HIS	O-C-N	5.47	131.45	122.70
2	O	87	MET	CA-CB-CG	5.47	122.60	113.30
6	F	87	THR	CA-CB-CG2	-5.46	104.75	112.40
12	L	44	LEU	CB-CG-CD2	-5.46	101.71	111.00
3	P	245	VAL	CA-CB-CG1	5.46	119.08	110.90
1	N	109	PHE	CB-CG-CD1	5.45	124.62	120.80
8	H	21	PRO	C-N-CA	-5.45	108.07	121.70
1	A	316	THR	C-N-CA	-5.45	110.86	122.30
2	O	167	SER	CB-CA-C	-5.45	99.75	110.10
4	D	21	ASP	CB-CG-OD1	-5.44	113.40	118.30
2	O	82	ARG	CG-CD-NE	-5.44	100.37	111.80
1	N	362	SER	N-CA-CB	-5.44	102.34	110.50
13	M	26	PHE	CB-CA-C	-5.44	99.52	110.40
7	T	19	LEU	CB-CG-CD2	-5.43	101.76	111.00
2	O	148	MET	CA-CB-CG	-5.42	104.09	113.30
3	P	93	PHE	CG-CD2-CE2	-5.41	114.85	120.80
1	A	403	TYR	CZ-CE2-CD2	-5.41	114.94	119.80
1	N	105	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	A	113[A]	LEU	CB-CA-C	5.39	120.45	110.20
1	A	113[B]	LEU	CB-CA-C	5.39	120.45	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	102	TYR	CZ-CE2-CD2	-5.39	114.94	119.80
3	P	215	LEU	O-C-N	5.39	131.33	122.70
4	Q	51	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	62	ALA	N-CA-CB	-5.38	102.57	110.10
1	N	156	SER	N-CA-CB	-5.38	102.43	110.50
1	A	145	LEU	O-C-N	5.38	131.31	122.70
3	P	16	TRP	NE1-CE2-CZ2	-5.38	124.49	130.40
5	E	90	ARG	CB-CG-CD	5.37	125.57	111.60
1	A	129	TYR	CD1-CG-CD2	5.37	123.81	117.90
6	F	81	ARG	CG-CD-NE	-5.37	100.53	111.80
5	E	61	PHE	CD1-CE1-CZ	5.36	126.53	120.10
3	C	253	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	N	442	ASP	CB-CG-OD2	-5.35	113.48	118.30
7	T	28	VAL	CA-CB-CG2	-5.35	102.87	110.90
5	E	102	GLU	OE1-CD-OE2	-5.35	116.88	123.30
11	X	47	ARG	CB-CG-CD	5.35	125.51	111.60
1	N	323	TRP	O-C-N	5.35	131.26	122.70
1	A	383	MET	CB-CA-C	-5.34	99.71	110.40
1	N	253	MET	CA-CB-CG	-5.34	104.23	113.30
3	C	190	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	N	124	THR	CA-CB-CG2	-5.33	104.93	112.40
7	G	64	ASP	CB-CG-OD1	5.33	123.09	118.30
1	N	162	ILE	CA-CB-CG1	-5.32	100.89	111.00
1	A	470	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	N	310	MET	CA-CB-CG	-5.32	104.26	113.30
2	B	65	TRP	CA-CB-CG	5.31	123.79	113.70
7	G	5	LYS	CD-CE-NZ	-5.31	99.48	111.70
1	A	63	PHE	CG-CD2-CE2	-5.31	114.96	120.80
9	I	12	LEU	CB-CG-CD1	-5.31	101.98	111.00
12	L	28	PHE	CB-CG-CD2	-5.31	117.08	120.80
3	P	233	PHE	CG-CD1-CE1	-5.30	114.97	120.80
1	A	323	TRP	O-C-N	5.30	131.18	122.70
4	D	139	ASP	CB-CG-OD1	5.30	123.07	118.30
2	O	157	GLU	CA-CB-CG	-5.30	101.75	113.40
3	P	104	SER	CA-CB-OG	-5.30	96.90	111.20
1	A	183	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	A	278	MET	CB-CG-SD	-5.29	96.52	112.40
6	F	52	ILE	CG1-CB-CG2	5.29	123.04	111.40
1	N	148	PHE	CG-CD2-CE2	-5.29	114.98	120.80
3	C	28	THR	CA-CB-CG2	-5.29	105.00	112.40
1	N	511	VAL	C-N-CA	5.28	134.90	121.70
2	B	168	LEU	CB-CG-CD2	-5.27	102.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	43	LYS	CD-CE-NZ	-5.26	99.59	111.70
1	N	310	MET	CG-SD-CE	-5.26	91.78	100.20
5	E	73	ASP	CB-CG-OD2	-5.26	113.57	118.30
9	I	10	ARG	NE-CZ-NH1	5.26	122.93	120.30
9	I	16	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	N	7	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	473	TRP	CD1-CG-CD2	5.25	110.50	106.30
1	A	486	ASP	OD1-CG-OD2	5.25	133.28	123.30
7	T	14	ARG	NE-CZ-NH1	-5.25	117.67	120.30
9	I	47	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	P	86	PHE	CD1-CG-CD2	5.23	125.09	118.30
3	C	181	TYR	CD1-CE1-CZ	-5.22	115.10	119.80
1	N	269	GLY	O-C-N	5.22	131.05	122.70
7	T	42	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	C	173	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	A	215	LEU	CB-CG-CD1	-5.22	102.13	111.00
6	F	1	ALA	CA-C-N	-5.22	105.72	117.20
11	X	47	ARG	CD-NE-CZ	5.22	130.90	123.60
1	A	403	TYR	CB-CG-CD1	-5.21	117.88	121.00
4	D	26	ASP	CB-CG-OD1	5.21	122.98	118.30
7	G	19	LEU	CB-CG-CD1	-5.20	102.16	111.00
10	W	24	GLY	C-N-CA	-5.20	111.38	122.30
1	A	379	TYR	CB-CG-CD1	5.20	124.12	121.00
9	I	47	TYR	CB-CG-CD1	5.20	124.12	121.00
1	A	371	TYR	CD1-CG-CD2	5.19	123.61	117.90
2	O	82	ARG	CD-NE-CZ	5.19	130.87	123.60
3	P	145	THR	CA-CB-CG2	-5.19	105.13	112.40
1	N	239	GLY	CA-C-O	-5.18	111.27	120.60
6	S	9	ASP	CB-CG-OD1	5.18	122.96	118.30
1	N	346	PHE	CD1-CE1-CZ	-5.18	113.89	120.10
1	A	514	LYS	CA-C-O	-5.17	109.24	120.10
5	E	75	ALA	C-N-CA	-5.17	111.44	122.30
1	N	152	LEU	CD1-CG-CD2	5.17	126.01	110.50
1	A	366	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	N	387	PHE	CD1-CE1-CZ	-5.17	113.90	120.10
9	V	59	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	103	TRP	CA-CB-CG	-5.16	103.90	113.70
4	Q	24	LEU	CB-CG-CD1	-5.16	102.23	111.00
11	X	52	GLU	CA-CB-CG	5.16	124.74	113.40
2	O	183	THR	N-CA-CB	5.16	120.10	110.30
1	A	298[A]	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	298[B]	ASP	CB-CG-OD1	-5.15	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	300	ASP	CB-CG-OD2	-5.15	113.66	118.30
3	P	127[A]	LEU	CB-CG-CD2	-5.15	102.24	111.00
3	P	127[B]	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	A	128	VAL	CG1-CB-CG2	-5.15	102.66	110.90
7	T	37	LEU	CB-CG-CD1	5.15	119.75	111.00
1	A	346	PHE	CG-CD2-CE2	-5.14	115.14	120.80
3	C	164	PHE	CZ-CE2-CD2	-5.14	113.93	120.10
1	N	166	THR	CA-CB-CG2	-5.14	105.20	112.40
1	A	209	LEU	O-C-N	5.14	130.93	122.70
1	A	426	PHE	CB-CG-CD1	-5.14	117.20	120.80
6	S	25	ARG	CG-CD-NE	-5.14	101.01	111.80
10	W	18	LEU	CA-CB-CG	-5.14	103.48	115.30
3	C	127	LEU	CB-CG-CD2	5.14	119.73	111.00
1	A	228	PRO	O-C-N	5.13	130.92	122.70
7	T	8	HIS	N-CA-C	5.13	124.85	111.00
1	N	35	LEU	CA-CB-CG	-5.12	103.52	115.30
1	A	100	MET	CA-CB-CG	-5.12	104.59	113.30
1	A	189[A]	MET	CG-SD-CE	-5.12	92.01	100.20
1	A	189[B]	MET	CG-SD-CE	-5.12	92.01	100.20
4	D	86[A]	MET	CA-CB-CG	-5.12	104.59	113.30
4	D	86[B]	MET	CA-CB-CG	-5.12	104.59	113.30
12	L	46	LYS	CG-CD-CE	-5.12	96.53	111.90
1	A	235	PHE	O-C-N	5.12	130.89	122.70
4	D	16	TYR	CD1-CG-CD2	5.11	123.52	117.90
2	B	73	LEU	CA-CB-CG	-5.11	103.56	115.30
3	P	86	PHE	CB-CG-CD1	-5.11	117.23	120.80
3	C	252	LEU	CB-CA-C	-5.10	100.50	110.20
2	B	170	LEU	CB-CG-CD2	5.10	119.67	111.00
6	F	65	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	367	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	A	179	TYR	CG-CD2-CE2	-5.09	117.22	121.30
1	N	510	TYR	CG-CD1-CE1	-5.09	117.22	121.30
5	E	103	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	324	LEU	CB-CG-CD2	5.09	119.65	111.00
1	A	478	SER	CB-CA-C	-5.08	100.44	110.10
2	B	118	PHE	CG-CD1-CE1	-5.08	115.21	120.80
1	N	417[A]	MET	CG-SD-CE	5.08	108.33	100.20
1	N	417[B]	MET	CG-SD-CE	5.08	108.33	100.20
5	R	39	TYR	CB-CG-CD1	5.08	124.05	121.00
2	O	80	SER	N-CA-CB	-5.07	102.89	110.50
3	P	164	PHE	CB-CG-CD1	-5.07	117.25	120.80
3	P	235	PHE	CB-CG-CD2	-5.07	117.25	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	GLU	CG-CD-OE2	5.06	128.43	118.30
1	A	502	TYR	CG-CD2-CE2	-5.06	117.25	121.30
4	Q	139	ASP	CB-CG-OD2	-5.06	113.75	118.30
2	B	92	ASN	N-CA-CB	5.06	119.71	110.60
1	N	128	VAL	CG1-CB-CG2	-5.06	102.80	110.90
8	H	57	ARG	NE-CZ-NH1	5.04	122.82	120.30
7	G	54	ARG	NE-CZ-NH2	-5.04	117.78	120.30
4	D	73	ARG	CB-CG-CD	-5.04	98.50	111.60
2	O	46	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	N	507	GLU	OE1-CD-OE2	-5.04	117.26	123.30
2	B	75	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	N	350	VAL	C-N-CA	-5.03	111.73	122.30
5	E	84	TYR	CB-CG-CD1	-5.03	117.98	121.00
8	H	27	ARG	NE-CZ-NH2	5.02	122.81	120.30
2	O	33	LEU	CB-CG-CD1	5.02	119.53	111.00
10	W	22	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	209	LEU	CB-CG-CD2	-5.02	102.47	111.00
2	B	82	ARG	NE-CZ-NH1	-5.01	117.79	120.30
7	T	5	LYS	CA-C-N	5.01	126.22	116.20
1	N	387	PHE	CB-CG-CD2	-5.01	117.30	120.80
5	R	84	TYR	CD1-CE1-CZ	5.00	124.30	119.80
1	A	187	SER	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ILE	Mainchain
1	A	296	GLY	Mainchain
1	A	304	TYR	Sidechain
1	A	38	ARG	Sidechain
1	A	96	ARG	Sidechain
2	B	198	GLU	Mainchain
3	C	76	GLN	Sidechain
4	D	31	LYS	Mainchain
5	E	81	ILE	Mainchain
6	F	93	PRO	Peptide
12	L	20	ARG	Sidechain
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
1	N	304	TYR	Sidechain
1	N	512	ASN	Sidechain

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Mol	Chain	Res	Type	Group
2	O	91	ASN	Peptide
4	Q	10	ASP	Peptide
4	Q	9	GLU	Peptide
6	S	93	PRO	Mainchain,Peptide
6	S	94	HIS	Peptide
6	S	95	GLN	Peptide
7	T	40	GLY	Peptide
8	U	9	LYS	Peptide
9	V	1	SAC	Peptide
10	W	57	HIS	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	4124	0	4102	50	0
1	N	4131	0	4107	97	0
2	B	1874	0	1869	51	0
2	O	1870	0	1867	51	0
3	C	2174	0	2082	54	0
3	P	2173	0	2083	43	0
4	D	1249	0	1242	25	0
4	Q	1203	0	1191	15	0
5	E	863	0	857	8	0
5	R	852	0	845	5	0
6	F	789	0	769	24	0
6	S	755	0	734	30	0
7	G	686	0	651	31	0
7	T	706	0	664	46	0
8	H	662	0	623	10	0
8	U	662	0	623	15	0
9	I	601	0	613	9	0
9	V	609	0	621	18	0
10	J	460	0	459	7	0
10	W	460	0	459	8	0
11	K	391	0	374	1	0
11	X	391	0	374	5	0
12	L	380	0	380	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	380	0	380	7	0
13	M	335	0	352	4	0
13	Z	335	0	352	6	0
14	A	120	0	108	10	0
14	N	120	0	108	9	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	102	0	152	10	0
18	C	102	0	152	7	0
18	N	102	0	152	7	0
18	P	102	0	152	8	0
19	B	63	0	110	4	0
19	D	63	0	110	10	0
19	L	63	0	110	12	0
19	N	126	0	218	18	0
19	Q	63	0	110	10	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	0	0
21	C	58	0	77	3	0
21	G	29	0	39	1	0
21	J	29	0	38	5	0
21	P	58	0	77	4	0
21	W	29	0	37	2	0
22	B	52	0	80	14	0
22	R	52	0	80	17	0
23	C	33	0	42	12	0
23	M	33	0	42	0	0
23	P	33	0	42	4	0
23	Z	33	0	42	0	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	23	0
25	G	53	0	77	12	0
25	T	159	0	231	29	0
26	C	100	0	156	25	0
26	G	100	0	156	27	0
26	P	100	0	156	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	T	100	0	156	26	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	289	0	0	11	0
28	B	255	0	0	9	0
28	C	181	0	0	7	0
28	D	256	0	0	11	0
28	E	169	0	0	1	0
28	F	200	0	0	10	0
28	G	108	0	0	4	0
28	H	129	0	0	4	0
28	I	78	0	0	1	0
28	J	64	0	0	2	0
28	K	68	0	0	0	0
28	L	47	0	0	4	0
28	M	50	0	0	0	0
28	N	286	0	0	14	0
28	O	226	0	0	6	0
28	P	194	0	0	6	0
28	Q	143	0	0	3	0
28	R	156	0	0	2	0
28	S	187	0	0	8	0
28	T	97	0	0	3	0
28	U	113	0	0	5	0
28	V	73	0	0	4	0
28	W	72	0	0	2	0
28	X	48	0	0	1	0
28	Y	31	0	0	1	0
28	Z	36	0	0	1	0
All	All	34897	0	31876	713	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 11.

All (713) 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)
2:B:1:FME:CB	2:B:1:FME:CG	1.76	1.61
1:N:71:MET:CE	1:N:71:MET:CG	1.86	1.53
1:N:512:ASN:CA	1:N:512:ASN:ND2	1.72	1.49
1:N:512:ASN:CA	1:N:512:ASN:HD22	1.26	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:MET:CG	1:N:71:MET:HE3	1.41	1.47
1:N:71:MET:CG	1:N:71:MET:SD	2.04	1.45
1:N:189:MET:CB	1:N:189:MET:CG	1.95	1.42
1:N:512:ASN:CB	1:N:512:ASN:CA	1.98	1.42
25:C:308:PEK:H383	26:G:101:CDL:C27	1.47	1.42
2:B:1:FME:CN	2:B:1:FME:N	1.84	1.40
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.85	1.39
2:B:1:FME:N	2:B:1:FME:O1	1.58	1.34
1:N:297[B]:MET:HB2	28:N:746:HOH:O	1.24	1.31
1:N:512:ASN:HA	1:N:512:ASN:ND2	1.33	1.25
25:T:103:PEK:H383	26:T:104:CDL:C27	1.74	1.17
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.18	1.17
25:C:308:PEK:H383	26:G:101:CDL:H273	1.17	1.16
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.11	1.14
19:L:101:TGL:HC62	19:L:101:TGL:HC22	1.15	1.13
25:C:308:PEK:C38	26:G:101:CDL:H273	1.78	1.12
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.89	1.12
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG2	1.91	1.11
22:R:201:PSC:C34	22:R:201:PSC:H141	1.82	1.10
7:G:84:LYS:HD2	7:G:84:LYS:H	0.95	1.08
1:N:297[B]:MET:CB	28:N:746:HOH:O	1.82	1.08
6:S:95:GLN:HB2	28:S:201:HOH:O	1.50	1.08
7:G:5:LYS:HG3	25:G:102:PEK:H371	1.34	1.08
25:T:103:PEK:H383	26:T:104:CDL:H273	1.17	1.08
25:T:103:PEK:C38	26:T:104:CDL:C27	2.31	1.08
18:C:304:PGV:H11	18:C:304:PGV:H151	1.35	1.06
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.86	1.05
19:L:101:TGL:CC6	19:L:101:TGL:HC22	1.72	1.05
7:T:84:LYS:N	7:T:84:LYS:HD2	1.72	1.04
1:N:400:PHE:HB3	19:N:609:TGL:H283	1.37	1.03
1:N:513:LEU:O	1:N:514:LYS:HB2	1.56	1.03
26:G:101:CDL:H201	26:G:101:CDL:H511	1.36	1.03
2:B:129:LYS:HE3	28:B:591:HOH:O	1.57	1.03
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.41	1.03
7:T:84:LYS:H	7:T:84:LYS:HD2	0.89	1.02
22:R:201:PSC:H141	22:R:201:PSC:H341	1.36	1.02
5:E:90:ARG:HD2	28:E:312:HOH:O	1.60	1.01
25:C:308:PEK:H383	26:G:101:CDL:H272	1.41	1.01
7:T:84:LYS:H	7:T:84:LYS:CD	1.71	1.01
1:N:297[B]:MET:O	1:N:302[B]:ARG:NE	1.93	0.99
19:N:608:TGL:C28	19:N:608:TGL:H101	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:H	7:G:84:LYS:CD	1.74	0.98
4:D:19[B]:ARG:HG2	4:D:21:ASP:OD1	1.63	0.98
1:A:297[A]:MET:HG2	28:A:933:HOH:O	1.63	0.98
25:C:308:PEK:C38	26:G:101:CDL:C27	2.37	0.98
6:S:1:ALA:HB2	28:T:206:HOH:O	1.63	0.98
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.78	0.98
1:N:71:MET:CE	1:N:71:MET:HG2	1.67	0.97
1:N:513:LEU:O	1:N:514:LYS:CB	2.10	0.97
1:N:417[A]:MET:CE	28:N:851:HOH:O	2.12	0.97
19:N:608:TGL:HC21	28:V:157:HOH:O	1.65	0.97
6:S:95:GLN:HG3	28:S:202:HOH:O	1.64	0.96
7:G:2:SER:OG	25:G:102:PEK:H291	1.66	0.96
7:G:84:LYS:N	7:G:84:LYS:HD2	1.78	0.96
2:O:41:ILE:HD13	22:R:201:PSC:H342	1.45	0.96
25:T:103:PEK:C38	26:T:104:CDL:H273	1.95	0.95
7:T:5:LYS:HB2	25:T:102:PEK:H371	1.46	0.95
9:I:1:SAC:HA	28:I:138:HOH:O	1.66	0.95
22:R:201:PSC:O01	22:R:201:PSC:H212	1.66	0.95
3:C:67:PHE:HE2	26:C:305:CDL:H1	1.30	0.94
7:G:5:LYS:CG	25:G:102:PEK:H371	1.98	0.94
6:F:1:ALA:HB3	6:S:65:ASP:OD2	1.68	0.93
12:L:20:ARG:HH12	19:L:101:TGL:HC61	1.29	0.93
26:P:305:CDL:HB21	26:P:305:CDL:OB6	1.67	0.93
2:O:82:ARG:HD2	28:O:413:HOH:O	1.69	0.92
12:L:14:SER:H	19:L:101:TGL:HC31	1.33	0.92
3:P:63:ARG:HE	26:P:305:CDL:HA22	1.35	0.91
1:N:112:LEU:HD23	1:N:112:LEU:O	1.70	0.91
4:D:31:LYS:HG2	28:D:318:HOH:O	1.71	0.90
3:C:188[B]:ILE:HD13	3:C:198:PHE:HB2	1.54	0.90
7:T:72:ASN:H	7:T:76:ASN:HD22	1.20	0.90
3:C:33:MET:HE1	3:C:42:LEU:H	1.36	0.90
3:P:67:PHE:HE2	26:P:305:CDL:H1	1.37	0.90
28:N:841:HOH:O	2:O:87:MET:SD	2.29	0.89
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	1.72	0.89
18:C:304:PGV:H151	18:C:304:PGV:C11	1.96	0.89
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	2.61	0.89
1:N:189:MET:CB	1:N:189:MET:SD	2.61	0.88
1:N:512:ASN:HA	1:N:512:ASN:HD22	0.83	0.87
7:T:31:CYS:SG	26:T:104:CDL:H532	2.14	0.87
26:G:101:CDL:H351	2:O:78:LEU:HD12	1.57	0.87
3:C:63:ARG:HE	26:C:305:CDL:HA21	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:LYS:CD	26:C:305:CDL:HB31	2.05	0.86
1:A:136[B]:LEU:HD11	28:A:978:HOH:O	1.74	0.86
7:G:72:ASN:H	7:G:76:ASN:HD22	1.22	0.86
5:E:14[B]:ARG:O	5:E:14[B]:ARG:HD2	1.76	0.86
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.39	0.85
3:C:161[B]:GLN:HE22	25:C:308:PEK:H22	1.41	0.85
26:P:305:CDL:H262	26:P:305:CDL:H392	1.55	0.85
1:N:512:ASN:CG	1:N:512:ASN:CA	2.44	0.85
7:G:5:LYS:HG3	25:G:102:PEK:C37	2.05	0.85
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.56	0.85
19:N:609:TGL:HC41	12:Y:14:SER:H	1.41	0.84
2:O:41:ILE:CD1	22:R:201:PSC:H342	2.06	0.84
3:P:127[B]:LEU:HD13	26:T:104:CDL:OB3	1.77	0.84
3:P:63:ARG:HE	26:P:305:CDL:CA2	1.91	0.84
19:L:101:TGL:CC2	19:L:101:TGL:HC62	2.06	0.84
1:N:297[B]:MET:O	1:N:302[B]:ARG:NH2	2.09	0.84
2:O:190:GLY:HA2	9:V:63[B]:MET:HE1	1.59	0.84
9:V:63[B]:MET:HE2	9:V:69:PHE:CZ	2.13	0.84
19:Q:201:TGL:H361	28:V:151:HOH:O	1.78	0.83
7:G:4:ALA:CB	1:N:282:PHE:HA	2.08	0.83
3:P:33:MET:HE1	3:P:42:LEU:H	1.44	0.82
4:D:34:SER:H	4:D:37:GLN:HE21	1.27	0.82
2:B:1:FME:HCN	2:B:193:TYR:H	1.44	0.82
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.61	0.82
2:B:1:FME:CN	2:B:1:FME:CA	2.57	0.81
7:G:5:LYS:HB2	25:G:102:PEK:H371	1.62	0.81
7:T:5:LYS:HB2	25:T:102:PEK:C37	2.10	0.81
2:B:1:FME:CB	2:B:1:FME:SD	2.67	0.81
22:B:304:PSC:H212	22:B:304:PSC:O01	1.80	0.81
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.62	0.81
6:S:52:ILE:O	6:S:94:HIS:CE1	2.33	0.81
3:C:67:PHE:CE2	26:C:305:CDL:H1	2.15	0.81
22:R:201:PSC:H141	22:R:201:PSC:H343	1.63	0.81
6:S:95:GLN:HA	28:S:300:HOH:O	1.80	0.81
1:N:113[A]:LEU:HD12	19:N:609:TGL:H141	1.63	0.80
1:A:406:ASN:HD21	18:A:607:PGV:H22	1.47	0.80
25:T:103:PEK:H382	26:T:104:CDL:H272	1.64	0.80
4:D:19[B]:ARG:CG	4:D:21:ASP:OD1	2.30	0.80
2:B:49:LYS:HE2	28:D:488:HOH:O	1.82	0.79
2:B:53:THR:HG21	28:D:309:HOH:O	1.81	0.79
19:B:301:TGL:H101	19:B:301:TGL:H281	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:567:HOH:O	19:Q:201:TGL:HC72	1.82	0.79
1:N:71:MET:HE3	1:N:71:MET:HG2	0.81	0.79
26:T:104:CDL:H541	26:T:104:CDL:H242	1.64	0.79
25:C:303:PEK:HN2	7:G:76:ASN:HD21	1.30	0.78
22:B:304:PSC:H063	9:I:10:ARG:HH21	1.49	0.78
1:N:297[B]:MET:O	1:N:302[B]:ARG:CZ	2.31	0.78
26:T:104:CDL:H571	26:T:104:CDL:H782	1.63	0.78
3:P:40[B]:MET:O	3:P:44[B]:MET:HG3	1.83	0.78
1:A:486:ASP:OD2	4:D:19[A]:ARG:HD2	1.82	0.78
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.30	0.78
7:G:5:LYS:CB	25:G:102:PEK:H371	2.14	0.77
7:T:5:LYS:CD	25:T:102:PEK:H381	2.14	0.77
18:P:304:PGV:H151	18:P:304:PGV:H11	1.64	0.77
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.50	0.77
3:C:63:ARG:HE	26:C:305:CDL:CA2	1.97	0.77
6:S:75:HIS:H	6:S:80:GLN:HE22	1.30	0.77
3:P:67:PHE:CE2	26:P:305:CDL:H1	2.19	0.76
5:E:14[B]:ARG:C	5:E:14[B]:ARG:HD2	2.06	0.76
25:C:303:PEK:H11	25:C:303:PEK:H172	1.67	0.76
12:L:20:ARG:HH22	19:L:101:TGL:CC3	1.94	0.76
1:N:112:LEU:HD23	1:N:112:LEU:C	2.06	0.76
3:C:157:LYS:NZ	25:C:308:PEK:H051	2.01	0.76
7:G:2:SER:OG	25:G:102:PEK:C29	2.35	0.75
18:A:606:PGV:H183	25:C:303:PEK:H332	1.66	0.75
26:C:305:CDL:OB9	26:C:305:CDL:H522	1.86	0.75
2:O:117:SER:HB2	28:O:560:HOH:O	1.84	0.74
25:T:103:PEK:H382	26:T:104:CDL:C27	2.16	0.74
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.52	0.74
7:T:76:ASN:HD21	25:T:101:PEK:HN2	1.34	0.74
8:U:43:MET:HE3	8:U:49:ASP:N	2.03	0.73
3:C:224:LYS:HE3	26:C:305:CDL:HB31	1.70	0.73
1:A:282:PHE:HA	7:T:4:ALA:CB	2.18	0.73
28:C:481:HOH:O	26:G:101:CDL:H801	1.89	0.73
25:C:303:PEK:C20	28:C:566:HOH:O	2.37	0.73
18:A:607:PGV:H061	18:A:607:PGV:P	2.30	0.72
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.22	0.72
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.24	0.72
1:A:513:LEU:O	1:A:514:LYS:HB2	1.90	0.72
18:C:304:PGV:C11	18:C:304:PGV:C15	2.68	0.72
1:N:297[B]:MET:C	1:N:302[B]:ARG:HE	1.92	0.72
25:C:303:PEK:H201	28:C:566:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:297[B]:MET:HB3	1:N:302[B]:ARG:HD3	1.70	0.72
3:C:128:GLU:HG2	28:G:235:HOH:O	1.89	0.72
1:N:297[B]:MET:HB3	1:N:302[B]:ARG:CD	2.19	0.72
1:N:417[A]:MET:HE2	28:N:851:HOH:O	1.81	0.72
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.72	0.71
19:Q:201:TGL:HG32	28:Q:363:HOH:O	1.89	0.71
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.24	0.71
3:P:180[B]:GLU:OE2	28:P:401:HOH:O	2.08	0.71
2:B:227:LEU:HD21	28:B:555:HOH:O	1.89	0.71
9:V:59:ASP:O	9:V:63[B]:MET:HG3	1.91	0.71
9:V:63[A]:MET:HB3	9:V:68:ILE:HG12	1.73	0.71
1:A:177:SER:H	1:A:180:GLN:HE21	1.39	0.71
9:V:63[B]:MET:CE	9:V:68:ILE:HD11	2.21	0.71
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.73	0.70
2:B:41:ILE:HD13	22:B:304:PSC:H342	1.72	0.70
2:O:84:LEU:HA	2:O:87:MET:HE2	1.73	0.70
19:N:608:TGL:H281	19:N:608:TGL:H101	1.73	0.70
6:F:85:CYS:SG	6:F:87:THR:HG23	2.32	0.70
3:P:33:MET:HB2	23:P:302:DMU:H8	1.74	0.70
6:F:30:PRO:O	6:F:96:LEU:HD11	1.91	0.70
1:A:468:MET:HG3	28:A:944:HOH:O	1.91	0.70
12:Y:2:HIS:N	28:Y:101:HOH:O	2.24	0.70
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.75	0.69
7:T:31:CYS:SG	26:T:104:CDL:H551	2.32	0.69
1:N:417[A]:MET:HE3	28:N:851:HOH:O	1.80	0.69
19:D:201:TGL:HC31	28:D:346:HOH:O	1.92	0.69
8:U:47:GLY:HA2	28:U:187:HOH:O	1.92	0.69
18:P:304:PGV:C15	18:P:304:PGV:H11	2.21	0.69
4:D:19[B]:ARG:HE	4:D:21:ASP:CG	1.95	0.69
3:C:224:LYS:CE	26:C:305:CDL:HB31	2.23	0.68
26:G:101:CDL:H241	26:G:101:CDL:C54	2.22	0.68
28:B:457:HOH:O	7:T:17:ARG:HD2	1.92	0.68
8:U:43:MET:HE3	8:U:49:ASP:H	1.58	0.68
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.09	0.68
3:C:33:MET:HE1	3:C:42:LEU:N	2.08	0.67
7:G:4:ALA:HB1	1:N:282:PHE:HA	1.74	0.67
2:O:183:THR:HG22	28:O:472:HOH:O	1.93	0.67
6:S:92:VAL:O	6:S:93:PRO:O	2.12	0.67
1:N:512:ASN:CB	1:N:512:ASN:C	2.62	0.67
28:L:228:HOH:O	13:M:32:TRP:CH2	2.46	0.67
2:B:1:FME:CA	2:B:1:FME:CG	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:92[A]:VAL:HG21	28:F:384:HOH:O	1.95	0.67
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.22	0.67
7:T:2:SER:OG	25:T:102:PEK:H301	1.95	0.67
2:B:56:MET:HG2	22:B:304:PSC:H211	1.77	0.67
18:C:304:PGV:H11	18:C:304:PGV:C15	2.19	0.67
25:T:103:PEK:C38	26:T:104:CDL:H272	2.18	0.67
2:B:22[B]:HIS:NE2	9:I:44:LYS:HE2	2.10	0.66
28:L:228:HOH:O	13:M:32:TRP:HH2	1.78	0.66
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.78	0.66
14:A:602:HEA:HMD1	14:A:602:HEA:HBD2	1.77	0.66
1:N:302[A]:ARG:HH22	2:O:87:MET:CE	2.08	0.66
22:B:304:PSC:C06	9:I:10:ARG:HH21	2.08	0.65
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.36	0.65
13:M:39:ASN:O	13:M:43:SER:HB3	1.95	0.65
18:N:607:PGV:H183	25:T:101:PEK:H341	1.78	0.65
18:N:606:PGV:H231	13:Z:12:PRO:HG3	1.78	0.65
1:N:71:MET:CB	1:N:71:MET:CE	2.74	0.65
1:A:297[A]:MET:CG	28:A:933:HOH:O	2.29	0.65
21:P:306:CHD:H231	28:P:551:HOH:O	1.95	0.65
2:B:78:LEU:HD12	26:T:104:CDL:H351	1.78	0.65
4:D:7:LYS:HG3	28:D:315:HOH:O	1.95	0.65
25:C:308:PEK:H381	26:G:101:CDL:H273	1.73	0.65
7:T:5:LYS:HD2	25:T:102:PEK:H381	1.78	0.65
8:U:43:MET:CE	8:U:49:ASP:H	2.09	0.65
18:A:606:PGV:C18	25:C:303:PEK:H332	2.26	0.65
3:C:33:MET:CG	23:C:301:DMU:H8	2.26	0.64
1:N:302[A]:ARG:HH22	2:O:87:MET:HE1	1.63	0.64
8:U:48:GLY:HA2	28:U:135:HOH:O	1.97	0.64
1:N:400:PHE:CB	19:N:609:TGL:H283	2.22	0.64
4:D:78:TRP:N	19:D:201:TGL:HB21	2.13	0.64
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.27	0.64
8:H:46:LYS:HD2	28:U:108:HOH:O	1.98	0.64
1:A:513:LEU:O	1:A:514:LYS:CB	2.46	0.64
1:N:297[B]:MET:CG	1:N:302[B]:ARG:HG3	2.28	0.64
19:B:301:TGL:C28	19:B:301:TGL:H101	2.26	0.64
18:A:607:PGV:H322	18:A:607:PGV:H152	1.78	0.63
25:T:101:PEK:H101	25:T:101:PEK:H161	1.79	0.63
28:B:457:HOH:O	7:T:17:ARG:CD	2.46	0.63
3:C:55:TYR:CE1	26:C:305:CDL:H532	2.33	0.63
3:P:33:MET:CE	3:P:41:THR:HB	2.29	0.63
10:J:7:GLU:HG3	28:J:238:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:224:LYS:CD	26:P:305:CDL:CB3	2.77	0.63
1:N:273:MET:HE2	28:N:762:HOH:O	1.98	0.63
10:W:7:GLU:HG3	28:W:238:HOH:O	1.98	0.63
3:P:127[A]:LEU:HD22	3:P:127[A]:LEU:N	2.14	0.63
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:HG3	1.80	0.62
9:V:65:LYS:O	11:X:54:ARG:NH1	2.32	0.62
12:Y:20:ARG:HH21	12:Y:24:MET:HG3	1.62	0.62
1:A:273:MET:HE2	28:A:830:HOH:O	1.98	0.62
7:T:3:ALA:O	7:T:4:ALA:HB2	1.98	0.62
26:G:101:CDL:H341	26:G:101:CDL:OA7	1.97	0.62
3:P:33:MET:HE1	3:P:42:LEU:N	2.13	0.62
1:N:71:MET:CB	1:N:71:MET:SD	2.88	0.62
22:R:201:PSC:H12	22:R:201:PSC:H343	1.81	0.62
2:O:190:GLY:HA2	9:V:63[B]:MET:CE	2.28	0.62
1:N:302[A]:ARG:NH2	2:O:87:MET:CE	2.63	0.62
26:P:305:CDL:OB9	26:P:305:CDL:H522	1.99	0.62
4:D:7:LYS:NZ	28:D:301:HOH:O	2.23	0.62
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	1.80	0.61
1:N:53:ILE:HG12	28:N:938:HOH:O	2.00	0.61
9:V:2:THR:HA	28:V:134:HOH:O	1.99	0.61
1:N:177:SER:H	1:N:180:GLN:HE21	1.48	0.61
19:N:609:TGL:HC41	12:Y:14:SER:N	2.15	0.61
6:S:95:GLN:CG	28:S:202:HOH:O	2.34	0.61
23:P:302:DMU:H11	10:W:49:CYS:HB3	1.81	0.61
4:D:19[B]:ARG:NH2	28:D:302:HOH:O	2.33	0.61
1:N:400:PHE:HB3	19:N:609:TGL:C28	2.23	0.61
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.30	0.61
18:A:607:PGV:H302	18:A:607:PGV:H141	1.81	0.61
12:L:2:HIS:CG	12:L:3:TYR:H	2.19	0.61
3:P:224:LYS:CD	26:P:305:CDL:HB31	2.31	0.61
26:C:305:CDL:OB6	26:C:305:CDL:HB21	2.00	0.61
22:R:201:PSC:C12	22:R:201:PSC:H343	2.31	0.61
3:C:33:MET:HB2	23:C:301:DMU:H8	1.83	0.60
26:G:101:CDL:C51	26:G:101:CDL:H201	2.23	0.60
1:N:302[A]:ARG:NH2	2:O:87:MET:HE1	2.15	0.60
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.31	0.60
25:G:102:PEK:H222	28:G:270:HOH:O	2.01	0.60
3:C:157:LYS:HZ1	25:C:308:PEK:H051	1.63	0.60
6:F:54[B]:ASN:HD22	6:F:54[B]:ASN:H	1.48	0.60
4:D:31:LYS:HB3	28:D:494:HOH:O	2.01	0.60
6:F:94:HIS:ND1	28:F:201:HOH:O	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161[B]:GLN:HE22	25:C:308:PEK:C2	2.11	0.60
6:F:92[A]:VAL:HG23	6:F:92[A]:VAL:O	2.01	0.60
1:N:112:LEU:CD2	1:N:112:LEU:C	2.69	0.60
7:T:72:ASN:H	7:T:76:ASN:ND2	1.96	0.60
28:C:481:HOH:O	26:G:101:CDL:C80	2.50	0.60
3:P:33:MET:CE	3:P:42:LEU:H	2.15	0.60
10:J:32:TYR:OH	21:J:101:CHD:H213	2.00	0.59
18:P:304:PGV:H181	26:P:305:CDL:H652	1.84	0.59
1:N:297[B]:MET:HB3	28:N:746:HOH:O	1.74	0.59
1:N:468:MET:HG3	28:N:946:HOH:O	2.02	0.59
26:T:104:CDL:C54	26:T:104:CDL:H242	2.32	0.59
3:C:59:ARG:HG3	26:C:305:CDL:H512	1.85	0.59
1:N:71:MET:CG	1:N:71:MET:HE2	2.21	0.59
1:N:136[B]:LEU:HD11	28:N:964:HOH:O	2.02	0.59
6:S:1:ALA:HA	7:T:17:ARG:NH1	2.18	0.58
5:R:7:THR:HB	5:R:9:GLU:OE2	2.04	0.58
1:A:309:THR:O	1:A:312[B]:ILE:HG22	2.04	0.58
7:T:38:HIS:HE1	26:T:104:CDL:H122	1.69	0.58
6:S:22:LEU:HD12	28:S:332:HOH:O	2.02	0.58
19:L:101:TGL:HC52	28:L:239:HOH:O	2.04	0.58
1:N:362:SER:HA	2:O:87:MET:HE1	1.86	0.58
7:T:5:LYS:CG	25:T:102:PEK:C38	2.82	0.57
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.85	0.57
28:N:710:HOH:O	3:P:77:LYS:HE3	2.03	0.57
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.18	0.57
7:G:5:LYS:HG3	25:G:102:PEK:C38	2.35	0.57
22:B:304:PSC:H212	22:B:304:PSC:C02	2.34	0.57
3:P:29:SER:HB2	23:P:302:DMU:H21	1.85	0.57
1:A:321:PHE:CD1	22:B:304:PSC:H341	2.40	0.57
7:G:9:GLY:HA3	28:N:831:HOH:O	2.03	0.57
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.86	0.57
4:D:31:LYS:CG	28:D:318:HOH:O	2.38	0.57
22:R:201:PSC:C07	9:V:10:ARG:HH21	2.18	0.57
3:C:33:MET:CB	23:C:301:DMU:H8	2.34	0.57
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.70	0.57
28:A:903:HOH:O	25:C:303:PEK:H381	2.05	0.57
18:P:304:PGV:C11	18:P:304:PGV:C15	2.81	0.57
2:B:1:FME:CN	2:B:1:FME:HA	2.34	0.56
1:N:484:THR:HG21	28:Z:221:HOH:O	2.05	0.56
6:S:52:ILE:HA	6:S:94:HIS:CG	2.40	0.56
26:G:101:CDL:H372	2:O:78:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:33:ARG:HG2	21:J:101:CHD:H152	1.87	0.56
28:B:572:HOH:O	19:D:201:TGL:HC72	2.04	0.56
18:N:606:PGV:H011	18:N:606:PGV:C2	2.35	0.56
26:P:305:CDL:C26	26:P:305:CDL:H392	2.30	0.56
3:P:224:LYS:HE3	26:P:305:CDL:HB31	1.88	0.56
6:S:2:SER:HB2	28:S:270:HOH:O	2.06	0.56
1:N:177:SER:H	1:N:180:GLN:NE2	2.04	0.55
5:R:8:ASP:OD1	22:R:201:PSC:H061	2.06	0.55
6:S:76:LYS:HE2	6:S:93:PRO:CG	2.12	0.55
3:C:224:LYS:HD3	26:C:305:CDL:HB31	1.84	0.55
3:C:33:MET:HB2	23:C:301:DMU:H11	1.87	0.55
2:B:13:THR:HB	2:B:168:LEU:HD23	1.88	0.55
7:G:83:GLU:HA	7:G:84:LYS:HD2	1.88	0.55
6:F:95:GLN:HA	28:F:311:HOH:O	2.06	0.55
21:C:306:CHD:H231	21:C:306:CHD:H162	1.88	0.55
3:C:37:PHE:HB3	23:C:301:DMU:C1	2.37	0.55
18:P:304:PGV:C11	18:P:304:PGV:H151	2.36	0.55
1:N:189:MET:CB	1:N:189:MET:CE	2.84	0.54
25:C:303:PEK:C11	25:C:303:PEK:H172	2.36	0.54
2:O:92:ASN:HB3	28:U:156:HOH:O	2.08	0.54
7:T:5:LYS:CB	25:T:102:PEK:H371	2.31	0.54
26:G:101:CDL:H371	2:O:81:LEU:HD12	1.90	0.54
1:N:406:ASN:HD21	18:N:606:PGV:H21	1.71	0.54
26:T:104:CDL:H161	26:T:104:CDL:H391	1.89	0.54
6:S:10:GLU:OE2	6:S:25:ARG:NH2	2.40	0.54
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.43	0.54
18:A:607:PGV:H201	28:A:963:HOH:O	2.08	0.54
2:B:1:FME:HCN	2:B:193:TYR:HB2	1.90	0.54
22:R:201:PSC:H343	22:R:201:PSC:C14	2.34	0.54
7:T:5:LYS:HG3	25:T:102:PEK:H383	1.90	0.54
12:L:22:LEU:O	12:L:26:THR:HB	2.07	0.54
3:P:33:MET:HG2	3:P:39:SER:O	2.07	0.54
3:C:33:MET:HB2	23:C:301:DMU:C19	2.37	0.53
6:F:1:ALA:CB	6:S:65:ASP:OD2	2.49	0.53
2:B:22[B]:HIS:HD2	28:B:405:HOH:O	1.90	0.53
26:G:101:CDL:C20	26:G:101:CDL:H511	2.24	0.53
8:H:55:TRP:H	8:U:46:LYS:HZ1	1.56	0.53
1:N:377:PHE:HA	1:N:380:VAL:HG12	1.91	0.53
22:R:201:PSC:C34	22:R:201:PSC:C14	2.71	0.53
19:N:609:TGL:HG2	12:Y:12:PRO:HB2	1.91	0.53
8:H:45:ALA:O	8:H:47:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:417[A]:MET:HE1	1:N:464:ALA:HB3	1.91	0.53
1:A:362:SER:HB3	2:B:20:LEU:HD21	1.91	0.53
5:E:14[B]:ARG:CD	5:E:14[B]:ARG:O	2.52	0.53
3:P:156:ARG:HE	21:P:306:CHD:C23	2.21	0.53
3:C:33:MET:HE1	3:C:41:THR:HB	1.91	0.53
19:N:609:TGL:H282	19:N:609:TGL:C24	2.33	0.53
6:S:76:LYS:CE	6:S:93:PRO:CG	2.75	0.52
10:W:32:TYR:OH	21:W:101:CHD:H213	2.09	0.52
1:A:297[A]:MET:SD	28:A:933:HOH:O	2.59	0.52
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.06	0.52
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.49	0.52
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.44	0.52
12:L:14:SER:N	19:L:101:TGL:HC31	2.14	0.52
3:C:103:HIS:HA	18:C:309:PGV:H012	1.90	0.52
12:L:14:SER:H	19:L:101:TGL:CC3	2.16	0.52
26:T:104:CDL:H762	26:T:104:CDL:H562	1.92	0.52
7:T:3:ALA:O	7:T:4:ALA:CB	2.58	0.52
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.39	0.52
2:O:49:LYS:HD3	19:Q:201:TGL:HC71	1.92	0.52
7:T:72:ASN:N	7:T:76:ASN:HD22	2.00	0.52
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.91	0.52
26:G:101:CDL:H542	26:G:101:CDL:H241	1.90	0.52
1:N:87:ILE:O	1:N:173:PRO:HD3	2.10	0.52
1:N:189:MET:CA	1:N:189:MET:CG	2.85	0.52
6:F:87:THR:HG21	28:F:346:HOH:O	2.10	0.52
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.92	0.52
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.52
18:N:606:PGV:H302	13:Z:19:LEU:HD23	1.91	0.52
3:P:224:LYS:CE	26:P:305:CDL:HB31	2.40	0.52
18:C:309:PGV:H21	18:C:309:PGV:H62	1.91	0.51
3:C:33:MET:CE	3:C:41:THR:HB	2.40	0.51
6:S:52:ILE:O	6:S:94:HIS:NE2	2.43	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.05	0.51
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.92	0.51
21:G:103:CHD:H12	21:G:103:CHD:H212	1.92	0.51
3:P:37:PHE:CD2	23:P:302:DMU:H13	2.44	0.51
26:C:305:CDL:H131	26:C:305:CDL:HA4	1.91	0.51
4:D:34:SER:H	4:D:37:GLN:NE2	2.00	0.51
6:F:1:ALA:HA	7:G:17:ARG:NH1	2.25	0.51
3:C:33:MET:CE	3:C:42:LEU:H	2.15	0.51
1:N:377:PHE:CD2	14:N:602:HEA:HAD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:608:TGL:HA52	2:O:32[A]:PHE:CE1	2.46	0.51
23:C:301:DMU:H6	10:J:49:CYS:HB3	1.92	0.51
3:C:224:LYS:HE3	26:C:305:CDL:CB3	2.38	0.51
3:C:224:LYS:HD2	26:C:305:CDL:HB31	1.90	0.51
2:O:221:LYS:HD3	28:O:622:HOH:O	2.10	0.51
19:N:608:TGL:H283	19:N:608:TGL:H101	1.86	0.51
2:B:129:LYS:CE	28:B:591:HOH:O	2.34	0.51
28:A:973:HOH:O	25:C:303:PEK:H381	2.10	0.51
7:G:72:ASN:H	7:G:76:ASN:ND2	1.99	0.51
8:H:23:GLN:NE2	28:H:103:HOH:O	2.44	0.51
18:P:304:PGV:C18	26:P:305:CDL:H652	2.40	0.51
7:T:8:HIS:O	7:T:8:HIS:CD2	2.64	0.51
6:S:43:LYS:HD3	28:S:305:HOH:O	2.09	0.50
2:O:203[B]:ASN:ND2	28:O:404:HOH:O	2.44	0.50
3:C:226:HIS:CE1	26:C:305:CDL:HB32	2.47	0.50
6:F:54[B]:ASN:ND2	28:F:203:HOH:O	2.43	0.50
8:H:8:ILE:HG22	28:H:101:HOH:O	2.10	0.50
2:B:91:ASN:HB3	2:B:149:THR:HG21	1.92	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.12	0.50
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.12	0.50
9:V:63[B]:MET:HE2	9:V:68:ILE:HD11	1.92	0.50
1:A:281:GLY:C	7:T:4:ALA:HB1	2.32	0.50
6:F:97:ALA:HB1	28:F:318:HOH:O	2.12	0.50
2:B:183:THR:HG22	28:B:626:HOH:O	2.11	0.50
3:C:55:TYR:CD1	26:C:305:CDL:H532	2.47	0.50
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.94	0.50
3:P:156:ARG:HE	21:P:306:CHD:C24	2.24	0.50
1:A:278:MET:HB3	7:T:5:LYS:HB3	1.94	0.49
2:B:1:FME:CN	2:B:193:TYR:H	2.19	0.49
26:G:101:CDL:H541	26:G:101:CDL:H241	1.94	0.49
26:P:305:CDL:H241	26:P:305:CDL:H661	1.94	0.49
3:C:3:HIS:N	28:C:404:HOH:O	2.44	0.49
1:N:381:LEU:HA	14:N:602:HEA:CBC	2.43	0.49
19:D:201:TGL:CC3	28:D:346:HOH:O	2.55	0.49
6:S:87[A]:THR:HG21	28:S:239:HOH:O	2.13	0.49
3:C:106:LEU:HD13	18:C:309:PGV:H22	1.94	0.49
7:T:5:LYS:HB2	25:T:102:PEK:C38	2.42	0.49
2:B:7:LEU:HD11	19:B:301:TGL:H152	1.95	0.49
7:T:11:TPO:O	7:T:11:TPO:CG2	2.61	0.49
2:B:33:LEU:CD1	9:I:31:PHE:CD2	2.97	0.48
2:B:78:LEU:O	26:T:104:CDL:H331	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLY:O	7:T:4:ALA:HB1	2.13	0.48
3:C:33:MET:HG3	23:C:301:DMU:H8	1.94	0.48
4:D:131[A]:ILE:HG22	4:D:132:GLN:HG3	1.95	0.48
18:N:606:PGV:H302	13:Z:19:LEU:CD2	2.43	0.48
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.48
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.13	0.48
6:S:94:HIS:HB2	6:S:95:GLN:O	2.13	0.48
3:C:33:MET:HB2	23:C:301:DMU:C22	2.44	0.48
25:C:308:PEK:H041	6:F:1:ALA:H2	1.78	0.48
2:B:13:THR:HB	2:B:168:LEU:CD2	2.43	0.48
7:G:3:ALA:HB1	25:G:102:PEK:H383	1.96	0.48
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.95	0.48
2:B:183:THR:CG2	28:B:626:HOH:O	2.61	0.48
4:D:7:LYS:CE	28:D:301:HOH:O	2.61	0.48
7:G:3:ALA:CB	25:G:102:PEK:H383	2.44	0.48
12:L:41:ARG:HD2	13:M:40:TYR:CZ	2.49	0.48
3:P:33:MET:HE1	3:P:41:THR:HB	1.96	0.48
22:R:201:PSC:C02	22:R:201:PSC:H212	2.44	0.48
3:C:158:HIS:HD2	3:C:161[A]:GLN:OE1	1.97	0.47
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.44	0.47
1:N:302[A]:ARG:NH2	2:O:87:MET:HE3	2.29	0.47
18:P:304:PGV:H182	26:P:305:CDL:H671	1.96	0.47
3:P:63:ARG:NE	26:P:305:CDL:HA22	2.15	0.47
2:B:57:ASP:H	22:B:304:PSC:H201	1.80	0.47
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.95	0.47
26:P:305:CDL:H642	26:P:305:CDL:H242	1.95	0.47
1:N:297[B]:MET:CG	1:N:302[B]:ARG:CG	2.91	0.47
12:L:2:HIS:CG	12:L:3:TYR:N	2.82	0.47
7:T:84:LYS:NZ	28:T:202:HOH:O	2.46	0.47
23:C:301:DMU:H10	10:J:49:CYS:HB3	1.97	0.47
6:F:54[A]:ASN:ND2	28:F:205:HOH:O	2.47	0.47
2:O:104:TRP:CG	2:O:203[A]:ASN:HB2	2.49	0.47
10:W:50:LEU:HD22	10:W:54:SER:HG	1.80	0.47
19:N:609:TGL:H282	19:N:609:TGL:H241	1.97	0.47
1:A:240:HIS:CD2	1:A:240:HIS:C	2.88	0.47
6:F:54[B]:ASN:HD22	6:F:54[B]:ASN:N	2.12	0.47
6:F:94:HIS:CE1	28:F:239:HOH:O	2.67	0.47
2:O:22[B]:HIS:CE1	9:V:44:LYS:CE	2.95	0.47
23:C:301:DMU:H30	28:J:237:HOH:O	2.14	0.47
25:T:101:PEK:H221	25:T:101:PEK:H251	1.37	0.46
1:N:334:TRP:CD1	19:Q:201:TGL:HC41	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CG	25:T:102:PEK:H383	2.44	0.46
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.98	0.46
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.97	0.46
3:P:103:HIS:HA	18:P:301:PGV:H012	1.97	0.46
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.15	0.46
26:G:101:CDL:H561	26:G:101:CDL:H782	1.97	0.46
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.46
2:B:32[B]:PHE:CD1	9:I:31:PHE:CZ	3.04	0.46
21:C:306:CHD:H12A	21:C:306:CHD:H112	1.71	0.46
25:C:308:PEK:H041	6:F:1:ALA:N	2.31	0.46
3:P:63:ARG:HE	26:P:305:CDL:HA21	1.73	0.46
3:P:224:LYS:HD2	26:P:305:CDL:CB3	2.45	0.46
21:P:307:CHD:H12	21:P:307:CHD:H212	1.98	0.46
3:C:224:LYS:HD3	26:C:305:CDL:CB3	2.45	0.46
7:G:3:ALA:O	7:G:4:ALA:CB	2.63	0.46
26:C:305:CDL:H261	26:C:305:CDL:H661	1.98	0.46
3:C:157:LYS:HZ2	25:C:308:PEK:H051	1.79	0.46
7:G:42:ARG:NH1	28:G:203:HOH:O	2.49	0.46
19:N:609:TGL:H282	19:N:609:TGL:H252	1.45	0.46
2:O:116:LEU:HD13	2:O:226:MET:HG3	1.98	0.46
3:P:3:HIS:HB2	28:P:567:HOH:O	2.16	0.46
8:H:37:HIS:HD2	8:H:40:GLU:OE2	1.99	0.46
1:N:309:THR:HG22	14:N:602:HEA:HMB2	1.97	0.46
2:O:104:TRP:CG	2:O:203[B]:ASN:HB2	2.50	0.46
3:C:37:PHE:HB3	23:C:301:DMU:H1	1.97	0.45
4:D:87[B]:PHE:HZ	11:K:20:SER:HG	1.64	0.45
26:G:101:CDL:H341	26:G:101:CDL:H311	1.84	0.45
1:A:350:VAL:HG13	19:B:301:TGL:HB81	1.97	0.45
7:G:36:TRP:HD1	28:G:272:HOH:O	2.00	0.45
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.98	0.45
6:S:94:HIS:HB2	6:S:95:GLN:C	2.36	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.45
18:A:607:PGV:C06	28:A:701:HOH:O	2.65	0.45
26:G:101:CDL:H541	26:G:101:CDL:C24	2.46	0.45
4:Q:10:ASP:HB3	4:Q:13:LEU:HB2	1.98	0.45
8:U:60:TYR:CD1	8:U:60:TYR:C	2.90	0.45
26:P:305:CDL:H222	26:P:305:CDL:H651	1.97	0.45
7:G:30:LEU:CD2	26:G:101:CDL:H461	2.47	0.45
1:N:308:ALA:HA	1:N:311:ILE:HD12	1.98	0.45
18:N:606:PGV:H21	18:N:606:PGV:H011	1.99	0.45
25:T:102:PEK:H282	25:T:102:PEK:H312	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:HD1	22:B:304:PSC:H341	1.83	0.44
2:B:58:ALA:O	2:B:62:GLU:HG3	2.16	0.44
26:P:305:CDL:CB5	26:P:305:CDL:HB21	2.46	0.44
3:P:38:ASN:HA	28:P:482:HOH:O	2.16	0.44
7:T:5:LYS:HG3	25:T:102:PEK:C38	2.47	0.44
1:A:377:PHE:HA	1:A:380:VAL:HG12	1.99	0.44
1:N:321:PHE:CD1	22:R:201:PSC:H332	2.52	0.44
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.99	0.44
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.17	0.44
7:G:31:CYS:SG	26:G:101:CDL:H532	2.57	0.44
3:P:116:TRP:HA	3:P:117:PRO:C	2.37	0.44
3:P:51[B]:MET:SD	26:P:305:CDL:H261	2.57	0.44
5:R:46:LYS:NZ	28:R:303:HOH:O	2.49	0.44
26:T:104:CDL:H192	26:T:104:CDL:H152	2.00	0.44
7:T:11:TPO:O	7:T:11:TPO:HG22	2.18	0.44
2:B:1:FME:HCN	2:B:193:TYR:N	2.22	0.44
26:G:101:CDL:H222	26:G:101:CDL:H531	1.99	0.44
12:L:24:MET:HG3	28:L:231:HOH:O	2.16	0.44
2:O:58:ALA:O	2:O:62:GLU:HG3	2.18	0.44
3:P:34:TRP:CD1	3:P:40[A]:MET:HG2	2.53	0.44
3:P:250:LEU:HD22	26:T:104:CDL:H661	1.99	0.44
26:T:104:CDL:H592	26:T:104:CDL:H561	1.34	0.44
22:B:304:PSC:H072	5:E:11:PHE:CB	2.48	0.44
26:P:305:CDL:HB22	26:P:305:CDL:PA1	2.56	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.80	0.44
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.99	0.44
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.99	0.44
2:O:48:THR:HB	9:V:16:ARG:CZ	2.48	0.44
10:W:3:ASN:C	10:W:3:ASN:OD1	2.55	0.44
4:Q:134:PHE:CE1	11:X:44:PRO:HG2	2.52	0.44
2:O:16:ILE:HG23	2:O:16:ILE:HD12	1.60	0.43
3:C:157:LYS:HZ2	25:C:308:PEK:C05	2.31	0.43
19:L:101:TGL:HB82	19:L:101:TGL:H361	2.00	0.43
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.17	0.43
26:T:104:CDL:C24	26:T:104:CDL:C54	2.96	0.43
1:A:381:LEU:HB2	14:A:602:HEA:CAC	2.48	0.43
2:B:56:MET:HA	22:B:304:PSC:C20	2.47	0.43
7:T:5:LYS:CG	25:T:102:PEK:H381	2.47	0.43
8:U:45:ALA:O	8:U:47:GLY:N	2.52	0.43
8:U:7:LYS:O	8:U:8:ILE:HB	2.18	0.43
22:R:201:PSC:H042	22:R:201:PSC:H063	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CD2	14:A:602:HEA:HAD1	2.53	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.54	0.43
10:W:15:ASP:OD2	28:W:201:HOH:O	2.21	0.43
26:P:305:CDL:CB2	26:P:305:CDL:OB6	2.54	0.43
4:Q:31:LYS:HD2	28:Q:442:HOH:O	2.17	0.43
18:A:607:PGV:H221	18:A:607:PGV:H011	2.00	0.43
28:A:733:HOH:O	12:L:7:PRO:HG3	2.19	0.43
1:N:302[A]:ARG:HH22	2:O:87:MET:HE3	1.83	0.43
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	2.01	0.43
7:T:3:ALA:HB1	25:T:102:PEK:C38	2.49	0.43
7:G:11:TPO:CG2	7:G:11:TPO:O	2.67	0.43
1:N:483:LEU:HD23	4:Q:8:SER:HA	2.00	0.43
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.54	0.43
7:G:2:SER:O	25:G:102:PEK:H331	2.19	0.43
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.66	0.43
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.92	0.43
1:A:514:LYS:CD	28:F:243:HOH:O	2.66	0.43
10:J:32:TYR:CE2	21:J:101:CHD:H213	2.54	0.43
3:P:52:LEU:HD21	26:P:305:CDL:H402	2.01	0.43
7:T:31:CYS:SG	26:T:104:CDL:C55	3.06	0.43
7:T:83:GLU:HA	7:T:84:LYS:HD2	2.00	0.43
8:U:44:THR:O	8:U:45:ALA:O	2.36	0.43
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.18	0.43
2:B:82:ARG:HG2	2:B:86:MET:HE3	2.00	0.42
3:C:133:ASN:ND2	28:C:401:HOH:O	2.39	0.42
3:P:224:LYS:HD3	26:P:305:CDL:CB3	2.47	0.42
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.84	0.42
2:B:61:VAL:HG22	2:B:65:TRP:CE3	2.54	0.42
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.19	0.42
2:O:83:ILE:O	2:O:87:MET:HG3	2.19	0.42
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.72	0.42
2:B:42:ILE:HG21	19:D:201:TGL:H231	2.01	0.42
21:C:307:CHD:H12	21:C:307:CHD:H212	2.00	0.42
1:N:514:LYS:HE3	28:N:701:HOH:O	2.19	0.42
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.00	0.42
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.50	0.42
4:Q:8:SER:HB2	4:Q:9:GLU:OE1	2.19	0.42
2:O:22[B]:HIS:ND1	9:V:44:LYS:HE2	2.33	0.42
2:O:49:LYS:HE3	28:R:309:HOH:O	2.18	0.42
3:P:144[A]:ILE:HD13	3:P:144[A]:ILE:HG21	1.77	0.42
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:608:TGL:H282	19:N:608:TGL:H101	1.91	0.42
1:A:377:PHE:O	1:A:381:LEU:HB3	2.19	0.42
6:F:92[A]:VAL:CG2	6:F:92[A]:VAL:O	2.67	0.42
12:L:44:LEU:HA	12:L:44:LEU:HD23	1.87	0.42
1:A:148:PHE:HB3	3:C:28:THR:HB	2.01	0.42
1:A:514:LYS:HD3	28:F:243:HOH:O	2.19	0.42
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	2.01	0.42
2:B:56:MET:HA	22:B:304:PSC:H202	2.01	0.42
2:B:94:SER:HB2	2:B:148[B]:MET:SD	2.59	0.42
2:B:227:LEU:HA	2:B:227:LEU:HD23	1.86	0.42
22:B:304:PSC:H212	22:B:304:PSC:H02	2.02	0.42
3:C:54[A]:MET:HB3	3:C:58:TRP:CZ3	2.55	0.42
1:A:489:THR:HA	6:F:71:TRP:O	2.20	0.42
8:H:55:TRP:H	8:U:46:LYS:NZ	2.18	0.42
1:N:426:PHE:N	1:N:427:PRO:CD	2.82	0.42
2:O:28:LEU:HD23	28:V:115:HOH:O	2.20	0.42
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.79	0.42
19:Q:201:TGL:CG3	28:Q:363:HOH:O	2.57	0.42
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.55	0.42
1:A:311[B]:ILE:HG22	26:T:104:CDL:H441	2.02	0.41
26:C:305:CDL:OA3	26:C:305:CDL:OB7	2.38	0.41
14:N:602:HEA:HMC1	14:N:602:HEA:CBC	2.50	0.41
3:P:3:HIS:HD2	28:P:524:HOH:O	2.03	0.41
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.18	0.41
26:T:104:CDL:H791	26:T:104:CDL:H821	1.76	0.41
10:W:29:ASN:HD22	10:W:29:ASN:H	1.68	0.41
18:A:607:PGV:H151	4:D:87[A]:PHE:CZ	2.55	0.41
19:D:201:TGL:H351	9:I:16:ARG:HE	1.85	0.41
2:O:22[B]:HIS:HE1	9:V:44:LYS:NZ	2.18	0.41
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.02	0.41
5:E:86:ILE:O	5:E:90:ARG:HG2	2.20	0.41
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.19	0.41
3:P:224:LYS:HD2	26:P:305:CDL:HB31	2.00	0.41
22:R:201:PSC:H232	22:R:201:PSC:H201	1.43	0.41
3:C:221:ARG:HG2	26:C:305:CDL:HB61	2.03	0.41
3:C:63:ARG:HE	26:C:305:CDL:HA22	1.80	0.41
26:G:101:CDL:H161	26:G:101:CDL:H391	2.02	0.41
1:N:189:MET:HB3	1:N:189:MET:CE	2.50	0.41
7:T:6:GLY:O	25:T:102:PEK:H311	2.21	0.41
9:V:69:PHE:O	9:V:73:LYS:HD2	2.21	0.41
4:D:100:LYS:CD	4:D:100:LYS:NZ	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:575:HOH:O	6:F:33:ILE:HD13	2.20	0.41
10:J:32:TYR:OH	21:J:101:CHD:C21	2.67	0.41
1:N:513:LEU:O	1:N:514:LYS:CG	2.68	0.41
25:T:102:PEK:H041	25:T:102:PEK:H011	2.02	0.41
7:T:60:PHE:HE1	28:T:203:HOH:O	2.02	0.41
22:B:304:PSC:H081	5:E:8:ASP:OD1	2.21	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
1:N:399:LEU:O	1:N:499:PRO:HA	2.20	0.41
14:A:602:HEA:HMC1	14:A:602:HEA:CBC	2.51	0.41
26:G:101:CDL:H252	26:G:101:CDL:H221	1.88	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.03	0.41
1:A:236:TRP:CH2	14:A:602:HEA:HBD1	2.56	0.41
3:C:59:ARG:HB2	26:C:305:CDL:H531	2.03	0.41
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.56	0.41
19:N:608:TGL:H282	19:N:608:TGL:H252	1.89	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.61	0.41
28:P:542:HOH:O	7:T:11:TPO:CG2	2.68	0.41
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.20	0.41
7:T:70[B]:PHE:HB2	25:T:101:PEK:H041	2.02	0.41
8:U:37:HIS:HE1	28:U:119:HOH:O	2.03	0.41
21:W:101:CHD:H111	21:W:101:CHD:H193	1.82	0.41
1:A:87:ILE:O	1:A:173:PRO:HD3	2.21	0.41
1:A:465:VAL:HG21	14:A:601:HEA:H261	2.03	0.41
6:F:85:CYS:SG	6:F:87:THR:CG2	3.07	0.41
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.03	0.41
1:N:312:ILE:O	1:N:312:ILE:HG22	2.21	0.41
7:T:3:ALA:HB1	25:T:102:PEK:H383	2.03	0.41
26:T:104:CDL:H111	26:T:104:CDL:HA21	2.02	0.41
26:P:305:CDL:H201	26:P:305:CDL:H631	2.03	0.41
3:C:55:TYR:HA	26:C:305:CDL:H572	2.03	0.40
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.40
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	2.03	0.40
2:O:202:SER:C	2:O:203[A]:ASN:HD22	2.23	0.40
2:O:203[A]:ASN:HD22	2:O:203[A]:ASN:N	2.19	0.40
10:W:29:ASN:ND2	10:W:29:ASN:H	2.19	0.40
19:N:609:TGL:H152	12:Y:24:MET:SD	2.61	0.40
26:G:101:CDL:H362	26:G:101:CDL:H121	2.02	0.40
8:H:23:GLN:NE2	28:H:105:HOH:O	2.54	0.40
5:R:76:GLY:O	5:R:79:LYS:HE3	2.21	0.40
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:8:ASP:HB2	28:X:109:HOH:O	2.21	0.40
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.40
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.95	0.40
1:A:1:FME:CE	1:A:4:ASN:HD22	2.34	0.40
3:C:63:ARG:NE	26:C:305:CDL:HA21	2.22	0.40
4:D:82:VAL:O	4:D:86[A]:MET:HG3	2.21	0.40
5:E:86:ILE:HD13	5:E:86:ILE:HA	1.87	0.40
8:H:37:HIS:HE1	28:H:114:HOH:O	2.05	0.40
21:J:101:CHD:H192	21:J:101:CHD:H3	2.02	0.40
8:U:43:MET:CE	8:U:48:GLY:HA3	2.50	0.40
2:B:41:ILE:O	2:B:45:MET:HG2	2.21	0.40
22:R:201:PSC:C13	22:R:201:PSC:H343	2.51	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	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	525/514 (102%)	510 (97%)	15 (3%)	0	100	100
2	B	231/227 (102%)	224 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	222 (96%)	6 (3%)	2 (1%)	21	5
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/261 (102%)	259 (98%)	6 (2%)	0	100	100
4	D	148/147 (101%)	143 (97%)	5 (3%)	0	100	100
4	Q	143/147 (97%)	134 (94%)	8 (6%)	1 (1%)	26	8
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	101/98 (103%)	97 (96%)	1 (1%)	3 (3%)	5	0
6	S	97/98 (99%)	90 (93%)	5 (5%)	2 (2%)	9	1
7	G	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	3	0
7	T	84/85 (99%)	71 (84%)	6 (7%)	7 (8%)	1	0
8	H	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	0
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	4	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	72/73 (99%)	70 (97%)	1 (1%)	1 (1%)	14	2
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	44 (100%)	0	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	7	1
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3577/3614 (99%)	3447 (96%)	102 (3%)	28 (1%)	24	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	97	ALA
7	G	5	LYS
7	G	8	HIS
8	H	8	ILE
8	H	45	ALA
8	H	46	LYS
13	M	42	LYS
6	S	93	PRO
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	5	LYS
7	T	7	ASP
7	T	8	HIS

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Mol	Chain	Res	Type
8	U	8	ILE
8	U	45	ALA
8	U	46	LYS
7	G	4	ALA
8	H	51	SER
4	Q	5	VAL
9	V	2	THR
6	F	95	GLN
7	T	6	GLY
7	T	2	SER
7	G	6	GLY
2	O	90	ILE
2	O	92	ASN

### 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	438/426 (103%)	430 (98%)	8 (2%)	66	41
1	N	439/426 (103%)	431 (98%)	8 (2%)	66	41
2	B	216/210 (103%)	208 (96%)	8 (4%)	41	13
2	O	215/210 (102%)	202 (94%)	13 (6%)	24	5
3	C	232/226 (103%)	228 (98%)	4 (2%)	68	44
3	P	232/226 (103%)	228 (98%)	4 (2%)	68	44
4	D	134/129 (104%)	130 (97%)	4 (3%)	48	19
4	Q	129/129 (100%)	126 (98%)	3 (2%)	58	29
5	E	93/95 (98%)	90 (97%)	3 (3%)	46	18
5	R	92/95 (97%)	89 (97%)	3 (3%)	45	17
6	F	86/81 (106%)	83 (96%)	3 (4%)	43	16
6	S	82/81 (101%)	74 (90%)	8 (10%)	10	1
7	G	68/68 (100%)	57 (84%)	11 (16%)	3	0
7	T	70/68 (103%)	56 (80%)	14 (20%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	71/75 (95%)	67 (94%)	4 (6%)	26	6
8	U	71/75 (95%)	64 (90%)	7 (10%)	10	1
9	I	57/57 (100%)	56 (98%)	1 (2%)	66	41
9	V	58/57 (102%)	53 (91%)	5 (9%)	13	2
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	36
11	K	40/46 (87%)	39 (98%)	1 (2%)	55	26
11	X	40/46 (87%)	38 (95%)	2 (5%)	30	7
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	25
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	7
13	M	37/38 (97%)	34 (92%)	3 (8%)	15	2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	5	0
All	All	3113/3082 (101%)	2987 (96%)	126 (4%)	38	12

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	127	THR
1	A	138	HIS
1	A	180	GLN
1	A	338	MET
1	A	369	ASP
1	A	486	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	92	ASN
2	B	115	ASP
2	B	171	LYS
3	C	110	PRO
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	4	SER

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Mol	Chain	Res	Type
4	D	20	ARG
4	D	74	SER
4	D	147	LYS
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	96	LEU
6	F	98	HIS
7	G	2	SER
7	G	8	HIS
7	G	18[A]	PHE
7	G	18[B]	PHE
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	43	GLU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
8	H	84	LYS
9	I	8	GLN
11	K	20	SER
12	L	5	GLU
13	M	38	ASP
13	M	42	LYS
13	M	43	SER
1	N	109	PHE
1	N	112	LEU
1	N	180	GLN
1	N	369	ASP
1	N	484	THR
1	N	495	LEU
1	N	504	THR
1	N	512	ASN
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU

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Mol	Chain	Res	Type
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	115	ASP
2	O	171	LYS
2	O	203[A]	ASN
2	O	203[B]	ASN
2	O	221	LYS
2	O	227	LEU
3	P	159	MET
3	P	177	GLN
3	P	214	PHE
3	P	230	ASN
4	Q	9	GLU
4	Q	10	ASP
4	Q	51	LEU
5	R	79	LYS
5	R	83	PRO
5	R	91	PRO
6	S	37	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	5	LYS
7	T	17	ARG
7	T	18	PHE
7	T	33	LEU
7	T	35	SER
7	T	36[A]	TRP
7	T	36[B]	TRP
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE

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Mol	Chain	Res	Type
8	U	9	LYS
8	U	29	CYS
8	U	46	LYS
8	U	51	SER
8	U	60	TYR
8	U	61	LYS
9	V	29	LEU
9	V	37	PHE
9	V	65	LYS
9	V	68	ILE
9	V	73	LYS
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	16	GLU
12	Y	20	ARG
13	Z	13	LYS
13	Z	38	ASP
13	Z	39	ASN
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	94	ASN

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Mol	Chain	Res	Type
7	G	34	ASN
7	G	76	ASN
8	H	31	GLN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
1	N	80	ASN
1	N	98	ASN
1	N	99	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	8	HIS
7	T	76	ASN
8	U	23	GLN
8	U	37	HIS
10	W	29	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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$
1	FME	A	1	1	8,9,10	1.02	1 (12%)	5,9,11	2.62	2 (40%)
2	FME	B	1	2	8,9,10	6.17	5 (62%)	5,9,11	19.48	3 (60%)
7	TPO	G	11	7	7,10,11	2.63	4 (57%)	10,14,16	3.15	6 (60%)
9	SAC	I	1	9	7,8,9	2.60	3 (42%)	7,9,11	2.80	3 (42%)
1	FME	N	1	1	8,9,10	0.76	0	5,9,11	2.87	5 (100%)
2	FME	O	1	2	8,9,10	1.67	2 (25%)	5,9,11	2.57	3 (60%)
7	TPO	T	11	7	7,10,11	2.02	1 (14%)	10,14,16	2.15	3 (30%)
9	SAC	V	1	9	7,8,9	3.11	2 (28%)	7,9,11	2.17	2 (28%)

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
1	FME	A	1	1	-	0/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	0/6/9/11	0/0/0/0
2	FME	O	1	2	-	0/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.68	1.62	1.81
2	O	1	FME	CG-SD	-2.69	1.67	1.81
9	I	1	SAC	CB-CA	2.09	1.57	1.53
7	G	11	TPO	P-O2P	2.26	1.62	1.54
1	A	1	FME	O-C	2.35	1.30	1.19
7	G	11	TPO	CG2-CB	2.55	1.57	1.51
2	O	1	FME	CB-CG	3.29	1.65	1.51
7	G	11	TPO	P-O1P	3.57	1.62	1.50
9	V	1	SAC	OAC-C1A	4.16	1.33	1.23
7	T	11	TPO	P-O1P	4.22	1.64	1.50
9	I	1	SAC	OAC-C1A	4.32	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	CB-CA	4.39	1.61	1.54
9	I	1	SAC	CA-N	4.69	1.52	1.46
2	B	1	FME	CA-N	5.06	1.53	1.46
2	B	1	FME	CB-CA	5.74	1.64	1.53
2	B	1	FME	CB-CG	6.16	1.76	1.51
9	V	1	SAC	CA-N	6.82	1.55	1.46
2	B	1	FME	CN-N	13.78	1.84	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	-43.28	58.59	124.80
9	I	1	SAC	CB-CA-N	-5.13	99.44	110.70
7	G	11	TPO	C-CA-N	-4.56	99.88	109.95
2	O	1	FME	O1-CN-N	-4.38	118.09	124.80
7	G	11	TPO	O2P-P-O1P	-3.79	98.27	110.63
1	N	1	FME	O-C-CA	-3.52	116.06	125.69
1	N	1	FME	CE-SD-CG	-3.49	88.22	100.36
2	B	1	FME	O-C-CA	-3.33	116.59	125.69
1	N	1	FME	CG-CB-CA	-2.83	104.57	113.07
7	G	11	TPO	O-C-CA	-2.75	118.18	125.69
7	T	11	TPO	O-C-CA	-2.64	118.47	125.69
2	O	1	FME	CG-CB-CA	-2.53	105.47	113.07
1	A	1	FME	O-C-CA	-2.47	118.94	125.69
2	B	1	FME	CG-CB-CA	-2.40	105.87	113.07
9	V	1	SAC	OAC-C1A-C2A	-2.38	117.69	122.07
2	O	1	FME	O-C-CA	-2.33	119.32	125.69
1	N	1	FME	O1-CN-N	-2.10	121.58	124.80
1	N	1	FME	CB-CG-SD	2.04	122.00	113.07
7	T	11	TPO	P-OG1-CB	2.67	133.12	121.42
7	G	11	TPO	OG1-P-O1P	3.31	115.38	107.48
9	I	1	SAC	OG-CB-CA	3.31	118.82	111.18
9	I	1	SAC	CA-N-C1A	3.53	133.45	121.32
7	G	11	TPO	O2P-P-OG1	4.18	119.13	106.62
9	V	1	SAC	CA-N-C1A	4.37	136.34	121.32
1	A	1	FME	CE-SD-CG	4.91	117.41	100.36
7	G	11	TPO	P-OG1-CB	4.96	143.14	121.42
7	T	11	TPO	OG1-P-O1P	5.11	119.68	107.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FME	O1-CN-N-CA

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	B	1	FME	11	0
7	G	11	TPO	2	0
9	I	1	SAC	1	0
7	T	11	TPO	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 44 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	$\# Z  > 2$
14	HEA	A	601	1	40,67,67	2.34	19 (47%)	36,103,103	3.44	19 (52%)
14	HEA	A	602	1	40,67,67	1.74	13 (32%)	36,103,103	2.69	17 (47%)
18	PGV	A	606	-	50,50,50	1.40	6 (12%)	51,56,56	1.48	8 (15%)
18	PGV	A	607	-	50,50,50	1.59	5 (10%)	51,56,56	2.00	13 (25%)
19	TGL	B	301	-	62,62,62	1.41	7 (11%)	65,65,65	2.57	17 (26%)
20	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
21	CHD	B	303	-	29,32,32	2.90	17 (58%)	48,51,51	2.98	26 (54%)
22	PSC	B	304	-	51,51,51	1.33	3 (5%)	55,59,59	1.54	10 (18%)
23	DMU	C	301	-	34,34,34	0.67	0	45,45,45	2.42	15 (33%)
25	PEK	C	303	-	51,52,52	1.31	6 (11%)	52,57,57	2.00	17 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	PGV	C	304	-	50,50,50	1.02	2 (4%)	51,56,56	1.24	5 (9%)
26	CDL	C	305	-	99,99,99	1.64	21 (21%)	101,111,111	1.96	26 (25%)
21	CHD	C	306	-	29,32,32	1.21	4 (13%)	48,51,51	3.91	26 (54%)
21	CHD	C	307	-	29,32,32	2.82	14 (48%)	48,51,51	3.33	28 (58%)
25	PEK	C	308	-	51,52,52	1.58	4 (7%)	52,57,57	1.82	13 (25%)
18	PGV	C	309	-	50,50,50	1.30	4 (8%)	51,56,56	2.03	11 (21%)
19	TGL	D	201	-	62,62,62	2.12	9 (14%)	65,65,65	2.90	17 (26%)
26	CDL	G	101	-	99,99,99	1.54	15 (15%)	101,111,111	1.80	25 (24%)
25	PEK	G	102	-	51,52,52	1.21	2 (3%)	52,57,57	1.60	7 (13%)
21	CHD	G	103	-	29,32,32	2.75	14 (48%)	48,51,51	3.11	24 (50%)
21	CHD	J	101	-	29,32,32	1.87	8 (27%)	48,51,51	4.06	32 (66%)
19	TGL	L	101	-	62,62,62	1.95	11 (17%)	65,65,65	2.75	22 (33%)
23	DMU	M	101	-	34,34,34	1.06	1 (2%)	45,45,45	1.84	11 (24%)
14	HEA	N	601	1	40,67,67	1.63	9 (22%)	36,103,103	3.58	19 (52%)
14	HEA	N	602	1	40,67,67	1.90	11 (27%)	36,103,103	2.23	12 (33%)
18	PGV	N	606	-	50,50,50	1.29	2 (4%)	51,56,56	1.97	9 (17%)
18	PGV	N	607	-	50,50,50	1.46	7 (14%)	51,56,56	1.58	8 (15%)
19	TGL	N	608	-	62,62,62	1.49	8 (12%)	65,65,65	2.57	18 (27%)
19	TGL	N	609	-	62,62,62	1.70	9 (14%)	65,65,65	2.22	17 (26%)
20	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
18	PGV	P	301	-	50,50,50	1.21	3 (6%)	51,56,56	1.72	10 (19%)
23	DMU	P	302	-	34,34,34	0.79	1 (2%)	45,45,45	1.53	7 (15%)
18	PGV	P	304	-	50,50,50	1.10	2 (4%)	51,56,56	1.41	10 (19%)
26	CDL	P	305	-	99,99,99	1.71	17 (17%)	101,111,111	2.10	27 (26%)
21	CHD	P	306	-	29,32,32	1.39	5 (17%)	48,51,51	3.20	24 (50%)
21	CHD	P	307	-	29,32,32	2.10	12 (41%)	48,51,51	2.85	22 (45%)
19	TGL	Q	201	-	62,62,62	1.89	7 (11%)	65,65,65	2.28	13 (20%)
22	PSC	R	201	-	51,51,51	1.60	5 (9%)	55,59,59	1.81	10 (18%)
25	PEK	T	101	-	51,52,52	1.10	3 (5%)	52,57,57	1.59	12 (23%)
25	PEK	T	102	-	51,52,52	1.26	3 (5%)	52,57,57	1.34	7 (13%)
25	PEK	T	103	-	51,52,52	1.91	9 (17%)	52,57,57	2.18	11 (21%)
26	CDL	T	104	-	99,99,99	1.42	14 (14%)	101,111,111	1.84	22 (21%)
21	CHD	W	101	-	29,32,32	1.72	9 (31%)	48,51,51	4.42	26 (54%)
23	DMU	Z	101	-	34,34,34	1.19	3 (8%)	45,45,45	1.66	12 (26%)

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
14	HEA	A	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1	2/2/7/16	0/24/76/76	0/0/8/8
18	PGV	A	606	-	-	0/55/55/55	0/0/0/0
18	PGV	A	607	-	-	1/55/55/55	0/0/0/0
19	TGL	B	301	-	-	0/65/65/65	0/0/0/0
20	CUA	B	302	2	-	0/0/0/0	0/0/0/0
21	CHD	B	303	-	-	0/7/74/74	0/4/4/4
22	PSC	B	304	-	-	0/55/55/55	0/0/0/0
23	DMU	C	301	-	-	0/19/59/59	0/2/2/2
25	PEK	C	303	-	-	0/56/56/56	0/0/0/0
18	PGV	C	304	-	-	0/55/55/55	0/0/0/0
26	CDL	C	305	-	-	0/110/110/110	0/0/0/0
21	CHD	C	306	-	-	0/7/74/74	0/4/4/4
21	CHD	C	307	-	-	0/7/74/74	0/4/4/4
25	PEK	C	308	-	-	0/56/56/56	0/0/0/0
18	PGV	C	309	-	-	1/55/55/55	0/0/0/0
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0
26	CDL	G	101	-	-	0/110/110/110	0/0/0/0
25	PEK	G	102	-	-	0/56/56/56	0/0/0/0
21	CHD	G	103	-	-	0/7/74/74	0/4/4/4
21	CHD	J	101	-	-	0/7/74/74	0/4/4/4
19	TGL	L	101	-	-	0/65/65/65	0/0/0/0
23	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	HEA	N	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1	3/3/7/16	0/24/76/76	0/0/8/8
18	PGV	N	606	-	-	3/55/55/55	0/0/0/0
18	PGV	N	607	-	-	0/55/55/55	0/0/0/0
19	TGL	N	608	-	-	0/65/65/65	0/0/0/0
19	TGL	N	609	-	-	0/65/65/65	0/0/0/0
20	CUA	O	301	2	-	0/0/0/0	0/0/0/0
18	PGV	P	301	-	-	1/55/55/55	0/0/0/0
23	DMU	P	302	-	-	0/19/59/59	0/2/2/2
18	PGV	P	304	-	-	0/55/55/55	0/0/0/0
26	CDL	P	305	-	-	2/110/110/110	0/0/0/0
21	CHD	P	306	-	-	0/7/74/74	0/4/4/4
21	CHD	P	307	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
22	PSC	R	201	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	T	101	-	-	0/56/56/56	0/0/0/0
25	PEK	T	102	-	-	0/56/56/56	0/0/0/0
25	PEK	T	103	-	-	2/56/56/56	0/0/0/0
26	CDL	T	104	-	-	0/110/110/110	0/0/0/0
21	CHD	W	101	-	-	0/7/74/74	1/4/4/4
23	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

All (324) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	307	CHD	C13-C12	-5.24	1.46	1.54
14	A	601	HEA	C3C-C2C	-5.24	1.33	1.40
21	B	303	CHD	C10-C5	-4.09	1.48	1.55
21	G	103	CHD	C10-C5	-3.91	1.48	1.55
14	A	601	HEA	C4B-NB	-3.65	1.31	1.36
19	N	609	TGL	C20-CA9	-3.64	1.30	1.51
25	C	303	PEK	C23-C22	-3.62	1.38	1.52
19	L	101	TGL	C20-CA9	-3.49	1.31	1.51
26	G	101	CDL	C59-C58	-3.46	1.31	1.51
14	N	602	HEA	C3C-C2C	-3.46	1.36	1.40
14	A	602	HEA	C3C-C2C	-3.37	1.36	1.40
19	B	301	TGL	OC1-CC1	-3.34	1.12	1.22
26	C	305	CDL	C82-C81	-3.27	1.32	1.51
26	T	104	CDL	C59-C58	-3.26	1.32	1.51
26	C	305	CDL	C79-C78	-3.26	1.32	1.51
14	A	601	HEA	C1D-ND	-3.22	1.32	1.36
26	T	104	CDL	C62-C61	-3.17	1.33	1.51
26	C	305	CDL	C59-C58	-3.11	1.33	1.51
19	B	301	TGL	C10-CB9	-3.07	1.34	1.51
14	N	601	HEA	C4B-NB	-3.07	1.32	1.36
14	A	601	HEA	C3B-C2B	-3.06	1.30	1.41
26	C	305	CDL	C19-C18	-3.04	1.34	1.51
19	N	608	TGL	C10-CB9	-3.04	1.34	1.51
26	P	305	CDL	C62-C61	-3.04	1.34	1.51
26	P	305	CDL	C19-C18	-3.00	1.34	1.51
26	T	104	CDL	C42-C41	-2.99	1.34	1.51
26	P	305	CDL	C22-C21	-2.96	1.34	1.51
14	N	601	HEA	C3C-C2C	-2.91	1.36	1.40
19	N	608	TGL	C20-CA9	-2.91	1.34	1.51
26	P	305	CDL	C82-C81	-2.91	1.34	1.51
26	P	305	CDL	C59-C58	-2.90	1.35	1.51
19	B	301	TGL	C20-CA9	-2.89	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	305	CDL	C79-C78	-2.88	1.35	1.51
19	L	101	TGL	C10-CB9	-2.87	1.35	1.51
21	B	303	CHD	C13-C14	-2.85	1.50	1.55
26	G	101	CDL	C62-C61	-2.84	1.35	1.51
19	D	201	TGL	C15-CC9	-2.81	1.35	1.51
19	Q	201	TGL	C10-CB9	-2.81	1.35	1.51
19	Q	201	TGL	C15-CC9	-2.79	1.35	1.51
26	G	101	CDL	C19-C18	-2.79	1.35	1.51
26	G	101	CDL	C79-C78	-2.72	1.36	1.51
26	C	305	CDL	C22-C21	-2.69	1.36	1.51
26	T	104	CDL	C22-C21	-2.66	1.36	1.51
26	T	104	CDL	C79-C78	-2.63	1.36	1.51
26	C	305	CDL	C39-C38	-2.58	1.36	1.51
19	N	609	TGL	C15-CC9	-2.53	1.37	1.51
26	C	305	CDL	C62-C61	-2.51	1.37	1.51
19	D	201	TGL	C20-CA9	-2.50	1.37	1.51
21	G	103	CHD	C13-C14	-2.46	1.51	1.55
19	N	608	TGL	C15-CC9	-2.45	1.37	1.51
26	G	101	CDL	C82-C81	-2.44	1.37	1.51
26	T	104	CDL	C39-C38	-2.43	1.37	1.51
26	T	104	CDL	C19-C18	-2.42	1.37	1.51
26	C	305	CDL	C42-C41	-2.41	1.37	1.51
26	T	104	CDL	C82-C81	-2.38	1.37	1.51
19	L	101	TGL	C15-CC9	-2.38	1.37	1.51
14	N	601	HEA	C3A-C2A	-2.38	1.37	1.40
26	G	101	CDL	C22-C21	-2.37	1.38	1.51
19	D	201	TGL	C10-CB9	-2.35	1.38	1.51
25	C	303	PEK	O02-C1	-2.32	1.15	1.22
26	G	101	CDL	C42-C41	-2.30	1.38	1.51
18	N	607	PGV	O02-C1	-2.29	1.15	1.22
26	G	101	CDL	C39-C38	-2.22	1.38	1.51
19	B	301	TGL	C15-CC9	-2.21	1.38	1.51
21	B	303	CHD	C10-C9	-2.19	1.51	1.56
26	P	305	CDL	OA2-CA2	-2.18	1.36	1.44
26	P	305	CDL	C42-C41	-2.17	1.39	1.51
14	A	601	HEA	C16-C17	-2.17	1.46	1.53
14	A	602	HEA	C26-C15	-2.16	1.44	1.50
19	Q	201	TGL	C20-CA9	-2.15	1.39	1.51
18	A	607	PGV	C3-C2	-2.14	1.44	1.52
19	N	608	TGL	OC1-CC1	-2.09	1.16	1.22
14	N	601	HEA	C16-C17	-2.07	1.46	1.53
18	A	606	PGV	O01-C02	-2.03	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	304	PGV	O01-C02	-2.03	1.41	1.46
26	C	305	CDL	OB6-CB4	-2.01	1.41	1.46
18	A	606	PGV	C5-C4	2.00	1.62	1.51
21	C	307	CHD	C19-C10	2.01	1.58	1.54
19	N	609	TGL	OG2-CG2	2.01	1.52	1.46
14	A	601	HEA	C20-C21	2.02	1.60	1.53
14	N	601	HEA	C13-C14	2.02	1.57	1.50
21	W	101	CHD	C13-C14	2.02	1.59	1.55
25	T	103	PEK	C01-C02	2.03	1.56	1.50
18	C	309	PGV	C03-C02	2.05	1.56	1.50
21	W	101	CHD	C8-C7	2.05	1.57	1.53
21	B	303	CHD	O3-C3	2.05	1.49	1.43
14	A	601	HEA	C1A-NA	2.05	1.39	1.36
18	N	607	PGV	C5-C4	2.07	1.63	1.51
25	T	102	PEK	C01-C02	2.07	1.56	1.50
21	C	307	CHD	C6-C5	2.08	1.57	1.53
21	P	307	CHD	C18-C13	2.08	1.57	1.54
18	A	606	PGV	C20-C19	2.09	1.56	1.50
14	A	601	HEA	CMB-C2B	2.09	1.56	1.51
14	N	602	HEA	C24-C23	2.10	1.56	1.50
14	N	602	HEA	C4B-NB	2.11	1.39	1.36
14	N	602	HEA	C1C-CHC	2.11	1.45	1.40
25	C	303	PEK	O01-C1	2.13	1.40	1.34
19	N	609	TGL	OA1-CA1	2.14	1.28	1.22
21	B	303	CHD	C4-C5	2.14	1.57	1.53
21	P	306	CHD	C11-C12	2.16	1.57	1.53
26	T	104	CDL	O1-C1	2.16	1.49	1.43
26	C	305	CDL	PA1-OA2	2.16	1.68	1.59
26	G	101	CDL	CB3-CB4	2.17	1.56	1.50
14	N	602	HEA	OMA-CMA	2.19	1.29	1.21
21	P	307	CHD	C16-C15	2.19	1.60	1.54
14	N	602	HEA	C1B-CHB	2.21	1.46	1.40
21	W	101	CHD	C16-C17	2.22	1.59	1.54
14	A	602	HEA	C21-C22	2.22	1.58	1.50
19	D	201	TGL	CG3-CG2	2.23	1.57	1.50
18	N	607	PGV	C20-C19	2.23	1.57	1.50
14	A	602	HEA	C16-C17	2.24	1.61	1.53
25	T	103	PEK	P-O12	2.24	1.68	1.59
21	B	303	CHD	O7-C7	2.25	1.48	1.43
21	C	306	CHD	C10-C5	2.26	1.59	1.55
21	P	307	CHD	C22-C20	2.26	1.60	1.54
14	A	602	HEA	C14-C15	2.28	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	101	CHD	C13-C12	2.28	1.58	1.54
19	L	101	TGL	OB1-CB1	2.29	1.29	1.22
26	C	305	CDL	CA2-C1	2.30	1.60	1.51
21	J	101	CHD	C8-C9	2.30	1.58	1.53
21	P	307	CHD	C16-C17	2.32	1.59	1.54
26	C	305	CDL	OB2-CB2	2.32	1.54	1.44
21	P	307	CHD	O12-C12	2.32	1.47	1.43
21	C	307	CHD	O12-C12	2.34	1.47	1.43
21	G	103	CHD	O3-C3	2.35	1.50	1.43
19	L	101	TGL	CG1-CG2	2.36	1.57	1.50
21	P	307	CHD	C19-C10	2.36	1.58	1.54
18	P	301	PGV	P-O11	2.37	1.69	1.59
21	W	101	CHD	C13-C12	2.37	1.58	1.54
26	C	305	CDL	PB2-OB2	2.37	1.69	1.59
26	T	104	CDL	CB6-CB4	2.38	1.57	1.50
26	G	101	CDL	C11-CA5	2.39	1.57	1.50
21	B	303	CHD	C13-C12	2.41	1.58	1.54
14	A	602	HEA	C24-C23	2.42	1.57	1.50
19	N	609	TGL	OB1-CB1	2.43	1.29	1.22
18	A	606	PGV	O01-C1	2.44	1.41	1.34
18	P	304	PGV	O05-C05	2.44	1.50	1.43
14	A	602	HEA	C3A-C2A	2.44	1.43	1.40
21	C	306	CHD	C8-C9	2.44	1.58	1.53
14	A	601	HEA	C4C-CHD	2.46	1.46	1.40
14	A	602	HEA	C4B-NB	2.47	1.40	1.36
21	W	101	CHD	C11-C9	2.48	1.57	1.53
25	C	303	PEK	P-O14	2.49	1.60	1.51
18	C	309	PGV	P-O11	2.49	1.69	1.59
18	A	607	PGV	P-O12	2.50	1.69	1.59
21	P	306	CHD	C10-C5	2.51	1.59	1.55
19	D	201	TGL	OC1-CC1	2.51	1.30	1.22
25	T	103	PEK	C03-C02	2.51	1.57	1.50
21	C	307	CHD	C2-C3	2.51	1.58	1.51
22	R	201	PSC	C01-C02	2.54	1.58	1.50
14	A	602	HEA	CMC-C2C	2.54	1.56	1.51
26	C	305	CDL	PA1-OA5	2.56	1.70	1.59
14	N	601	HEA	C14-C15	2.57	1.39	1.32
14	A	601	HEA	C14-C15	2.57	1.39	1.32
21	J	101	CHD	C11-C9	2.59	1.58	1.53
21	G	103	CHD	C20-C17	2.59	1.59	1.54
21	C	306	CHD	C8-C14	2.59	1.58	1.53
21	C	307	CHD	C16-C17	2.60	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CAA-C2A	2.60	1.55	1.52
23	Z	101	DMU	O55-C2	2.61	1.49	1.43
14	A	601	HEA	C24-C23	2.61	1.58	1.50
26	P	305	CDL	PB2-OB2	2.62	1.70	1.59
25	C	303	PEK	O11-C03	2.64	1.55	1.44
23	Z	101	DMU	C2-C1	2.64	1.59	1.52
14	A	602	HEA	OMA-CMA	2.66	1.30	1.21
19	N	609	TGL	CG1-CG2	2.66	1.58	1.50
23	Z	101	DMU	O16-C6	2.67	1.45	1.40
19	L	101	TGL	CC2-CC1	2.67	1.58	1.50
14	A	601	HEA	C20-C19	2.68	1.57	1.51
21	C	306	CHD	C20-C17	2.68	1.59	1.54
21	P	306	CHD	C11-C9	2.70	1.58	1.53
26	G	101	CDL	CB6-CB4	2.70	1.58	1.50
19	N	608	TGL	CG1-CG2	2.70	1.58	1.50
14	N	602	HEA	C12-C13	2.71	1.62	1.53
14	A	602	HEA	C12-C13	2.72	1.62	1.53
25	T	101	PEK	C3-C4	2.72	1.62	1.52
21	C	307	CHD	C16-C15	2.73	1.61	1.54
21	P	307	CHD	C6-C5	2.75	1.58	1.53
26	P	305	CDL	PA1-OA5	2.78	1.71	1.59
14	N	601	HEA	C12-C13	2.78	1.62	1.53
14	A	601	HEA	C12-C13	2.79	1.62	1.53
18	N	607	PGV	O01-C1	2.79	1.42	1.34
21	B	303	CHD	C16-C17	2.79	1.60	1.54
14	A	602	HEA	C18-C19	2.79	1.40	1.32
14	N	602	HEA	C1A-NA	2.83	1.40	1.36
25	T	103	PEK	C2-C1	2.83	1.58	1.50
18	A	606	PGV	C3-C2	2.83	1.62	1.52
21	C	307	CHD	C10-C9	2.83	1.61	1.56
21	P	307	CHD	C2-C3	2.84	1.59	1.51
21	P	307	CHD	C10-C9	2.85	1.61	1.56
23	P	302	DMU	O16-C6	2.87	1.45	1.40
21	C	307	CHD	C8-C7	2.88	1.58	1.53
25	C	308	PEK	C22-C21	2.88	1.59	1.50
14	N	602	HEA	CMB-C2B	2.92	1.57	1.51
22	R	201	PSC	C2-C1	2.93	1.59	1.50
21	P	306	CHD	C8-C9	2.95	1.59	1.53
23	M	101	DMU	O7-C3	2.96	1.51	1.43
21	P	306	CHD	C8-C14	2.96	1.59	1.53
21	W	101	CHD	C8-C14	2.97	1.59	1.53
18	C	304	PGV	O05-C05	3.00	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C17-C18	3.00	1.61	1.50
25	T	101	PEK	C2-C1	3.02	1.59	1.50
21	W	101	CHD	C20-C17	3.03	1.59	1.54
21	J	101	CHD	C10-C5	3.03	1.60	1.55
21	G	103	CHD	C18-C13	3.04	1.59	1.54
25	T	103	PEK	O02-C1	3.05	1.31	1.22
25	C	308	PEK	P-O11	3.05	1.72	1.59
21	J	101	CHD	C8-C14	3.06	1.59	1.53
21	W	101	CHD	C8-C9	3.09	1.59	1.53
21	J	101	CHD	C8-C7	3.10	1.58	1.53
25	C	303	PEK	C2-C1	3.11	1.59	1.50
25	T	103	PEK	P-O11	3.12	1.72	1.59
18	C	309	PGV	O03-C19	3.13	1.42	1.33
14	A	601	HEA	C27-C19	3.14	1.59	1.50
21	G	103	CHD	C16-C17	3.25	1.61	1.54
19	L	101	TGL	CG3-CG2	3.27	1.60	1.50
26	P	305	CDL	O1-C1	3.27	1.53	1.43
21	J	101	CHD	C13-C17	3.28	1.61	1.55
19	B	301	TGL	OG3-CC1	3.29	1.43	1.33
25	T	101	PEK	O11-C03	3.31	1.58	1.44
21	C	307	CHD	C6-C7	3.36	1.58	1.52
19	L	101	TGL	OG2-CG2	3.37	1.55	1.46
21	P	307	CHD	C13-C17	3.38	1.61	1.55
21	B	303	CHD	C19-C10	3.41	1.60	1.54
14	A	601	HEA	C13-C14	3.43	1.62	1.50
26	P	305	CDL	CB2-C1	3.46	1.65	1.51
19	N	609	TGL	OG3-CC1	3.48	1.43	1.33
14	N	601	HEA	CMB-C2B	3.53	1.58	1.51
26	C	305	CDL	OB6-CB5	3.60	1.44	1.34
14	N	601	HEA	CMC-C2C	3.60	1.59	1.51
21	C	307	CHD	C4-C3	3.61	1.58	1.51
21	G	103	CHD	C19-C10	3.63	1.61	1.54
21	G	103	CHD	C6-C7	3.64	1.58	1.52
21	W	101	CHD	C13-C17	3.67	1.62	1.55
18	P	304	PGV	C01-C02	3.72	1.61	1.50
14	A	602	HEA	CAA-C2A	3.79	1.57	1.52
21	C	307	CHD	C13-C17	3.79	1.62	1.55
26	C	305	CDL	CB2-C1	3.83	1.66	1.51
18	N	607	PGV	O03-C01	3.83	1.53	1.45
18	A	607	PGV	O01-C1	3.85	1.45	1.34
18	N	607	PGV	C3-C2	3.86	1.66	1.52
21	B	303	CHD	C8-C9	3.91	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	103	CHD	C4-C3	3.94	1.59	1.51
21	B	303	CHD	C6-C7	3.98	1.59	1.52
25	T	103	PEK	C22-C21	3.99	1.62	1.50
21	B	303	CHD	C1-C10	4.00	1.61	1.54
19	N	608	TGL	OG3-CC1	4.02	1.45	1.33
21	G	103	CHD	C6-C5	4.02	1.60	1.53
22	B	304	PSC	C13-C12	4.07	1.55	1.31
19	B	301	TGL	OG2-CB1	4.07	1.46	1.34
21	B	303	CHD	C15-C14	4.11	1.63	1.54
19	Q	201	TGL	OG3-CC1	4.12	1.45	1.33
14	A	601	HEA	O11-C11	4.15	1.52	1.42
18	N	607	PGV	C01-C02	4.15	1.62	1.50
26	P	305	CDL	OB6-CB5	4.20	1.46	1.34
21	B	303	CHD	C6-C5	4.23	1.61	1.53
21	P	307	CHD	C6-C7	4.29	1.59	1.52
22	B	304	PSC	O03-C19	4.34	1.46	1.33
26	T	104	CDL	OA6-CA5	4.36	1.47	1.34
26	T	104	CDL	OB6-CB5	4.38	1.47	1.34
21	J	101	CHD	C20-C17	4.38	1.62	1.54
21	G	103	CHD	C13-C12	4.41	1.61	1.54
26	C	305	CDL	OA6-CA5	4.42	1.47	1.34
26	T	104	CDL	OA8-CA7	4.44	1.46	1.33
14	N	602	HEA	O11-C11	4.44	1.53	1.42
21	B	303	CHD	C11-C12	4.47	1.61	1.53
14	N	602	HEA	CAA-C2A	4.57	1.58	1.52
25	T	102	PEK	O01-C1	4.58	1.47	1.34
26	T	104	CDL	OB8-CB7	4.58	1.47	1.33
22	R	201	PSC	C13-C12	4.60	1.59	1.31
19	D	201	TGL	OG3-CC1	4.61	1.47	1.33
14	A	601	HEA	CAD-C3D	4.62	1.59	1.52
21	G	103	CHD	C4-C5	4.65	1.61	1.53
26	C	305	CDL	PB2-OB3	4.68	1.68	1.51
18	P	301	PGV	O01-C1	4.70	1.48	1.34
18	P	301	PGV	O03-C19	4.71	1.47	1.33
26	G	101	CDL	OA8-CA7	4.72	1.47	1.33
21	C	307	CHD	C22-C20	4.78	1.67	1.54
25	G	102	PEK	O01-C1	4.78	1.48	1.34
26	C	305	CDL	O1-C1	4.78	1.57	1.43
18	N	606	PGV	O01-C1	4.80	1.48	1.34
26	C	305	CDL	OB8-CB7	4.81	1.47	1.33
21	P	307	CHD	C11-C12	4.82	1.61	1.53
22	B	304	PSC	O01-C1	4.89	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	201	TGL	OG1-CA1	4.95	1.48	1.33
21	G	103	CHD	C8-C9	5.01	1.63	1.53
21	G	103	CHD	C15-C14	5.04	1.65	1.54
19	D	201	TGL	OG1-CA1	5.06	1.48	1.33
25	G	102	PEK	O03-C21	5.08	1.48	1.33
19	N	608	TGL	OG2-CB1	5.09	1.49	1.34
21	B	303	CHD	C18-C13	5.12	1.62	1.54
26	C	305	CDL	OA8-CA7	5.15	1.48	1.33
18	A	606	PGV	C01-C02	5.15	1.65	1.50
26	P	305	CDL	OA8-CA7	5.16	1.48	1.33
18	A	607	PGV	O02-C1	5.20	1.38	1.22
26	P	305	CDL	OB8-CB7	5.22	1.48	1.33
26	G	101	CDL	OB6-CB5	5.30	1.49	1.34
26	P	305	CDL	OA6-CA5	5.37	1.50	1.34
26	G	101	CDL	OA6-CA5	5.39	1.50	1.34
25	T	102	PEK	O03-C21	5.41	1.49	1.33
18	N	606	PGV	O03-C19	5.42	1.49	1.33
26	G	101	CDL	OB8-CB7	5.49	1.49	1.33
19	L	101	TGL	OG3-CC1	5.49	1.49	1.33
21	B	303	CHD	C4-C3	5.57	1.62	1.51
19	L	101	TGL	OG1-CA1	5.62	1.50	1.33
22	R	201	PSC	O03-C19	5.66	1.50	1.33
19	N	608	TGL	OG1-CA1	5.72	1.50	1.33
19	B	301	TGL	OG1-CA1	5.76	1.50	1.33
25	C	308	PEK	O01-C1	5.80	1.51	1.34
22	R	201	PSC	O01-C1	5.80	1.51	1.34
26	P	305	CDL	PB2-OB3	5.84	1.72	1.51
18	C	309	PGV	O01-C1	6.29	1.52	1.34
18	A	607	PGV	O03-C19	6.49	1.52	1.33
25	C	308	PEK	O03-C21	6.50	1.52	1.33
19	Q	201	TGL	OG2-CB1	6.55	1.53	1.34
19	N	609	TGL	OG2-CB1	6.63	1.53	1.34
25	T	103	PEK	O03-C21	6.69	1.53	1.33
19	N	609	TGL	OG1-CA1	6.93	1.54	1.33
25	T	103	PEK	O01-C1	7.23	1.55	1.34
19	D	201	TGL	OG2-CB1	7.30	1.55	1.34
19	L	101	TGL	OG2-CB1	8.13	1.58	1.34
21	C	307	CHD	C11-C12	8.48	1.68	1.53
19	Q	201	TGL	OB1-CB1	9.39	1.50	1.22
19	D	201	TGL	OB1-CB1	10.53	1.53	1.22

All (685) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C13-C12-C11	-14.55	97.63	114.74
19	D	201	TGL	OG2-CB1-CB2	-14.46	81.04	111.53
21	W	101	CHD	C18-C13-C12	-12.63	96.45	109.09
19	Q	201	TGL	OG2-CB1-CB2	-11.88	86.49	111.53
19	L	101	TGL	CC4-CC3-CC2	-10.79	73.35	113.30
14	A	601	HEA	C13-C12-C11	-10.18	102.76	114.74
14	A	602	HEA	C13-C12-C11	-9.78	103.24	114.74
21	C	306	CHD	C6-C5-C4	-9.36	101.02	111.07
21	G	103	CHD	C6-C5-C4	-9.35	101.04	111.07
19	N	609	TGL	CC5-CC4-CC3	-9.26	66.46	114.54
21	P	307	CHD	C23-C22-C20	-9.09	103.56	114.79
21	P	306	CHD	C6-C5-C4	-9.03	101.38	111.07
21	C	307	CHD	C23-C22-C20	-7.62	105.37	114.79
21	J	101	CHD	C18-C13-C12	-7.56	101.52	109.09
21	W	101	CHD	C17-C13-C14	-7.53	92.46	100.08
14	N	602	HEA	C13-C12-C11	-7.39	106.05	114.74
26	P	305	CDL	C52-C51-CB5	-7.22	85.41	113.57
26	C	305	CDL	C52-C51-CB5	-7.21	85.44	113.57
21	G	103	CHD	C5-C4-C3	-7.08	102.39	112.88
21	C	306	CHD	C23-C22-C20	-6.95	106.20	114.79
21	C	307	CHD	C17-C13-C12	-6.81	111.70	117.68
21	G	103	CHD	C11-C12-C13	-6.81	104.36	111.22
25	C	303	PEK	C24-C23-C22	-6.79	88.18	113.30
21	B	303	CHD	C6-C5-C4	-6.72	103.85	111.07
21	P	307	CHD	C6-C7-C8	-6.61	104.45	111.46
21	J	101	CHD	C6-C5-C4	-6.58	104.01	111.07
21	C	306	CHD	C18-C13-C12	-6.49	102.60	109.09
19	B	301	TGL	OG3-CC1-OC1	-6.34	106.89	123.51
21	B	303	CHD	C5-C4-C3	-6.24	103.64	112.88
21	J	101	CHD	C19-C10-C9	-6.14	103.08	111.20
19	N	608	TGL	OG3-CC1-OC1	-6.09	107.54	123.51
26	P	305	CDL	OB4-PB2-OB2	-6.05	79.38	108.24
14	A	601	HEA	C13-C14-C15	-5.96	114.59	127.75
19	L	101	TGL	C22-C21-C20	-5.80	84.44	114.54
14	A	601	HEA	CMB-C2B-C1B	-5.53	118.90	128.31
21	P	307	CHD	C11-C12-C13	-5.47	105.70	111.22
14	N	601	HEA	CAA-CBA-CGA	-5.38	102.31	112.78
14	N	601	HEA	C13-C14-C15	-5.26	116.14	127.75
21	P	306	CHD	C18-C13-C12	-5.26	103.83	109.09
26	T	104	CDL	CB2-C1-CA2	-5.22	95.82	112.42
21	C	307	CHD	C13-C14-C8	-5.17	107.93	114.73
21	B	303	CHD	C2-C1-C10	-5.08	103.69	112.81
14	A	601	HEA	C16-C15-C14	-5.02	111.62	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	306	CHD	C19-C10-C1	-4.98	99.79	108.23
25	T	103	PEK	C36-C35-C34	-4.93	88.93	114.54
21	C	306	CHD	C19-C10-C1	-4.88	99.96	108.23
21	G	103	CHD	C2-C1-C10	-4.87	104.07	112.81
14	N	602	HEA	CBA-CAA-C2A	-4.84	103.98	112.47
19	L	101	TGL	CA9-CA8-CA7	-4.82	89.50	114.54
25	T	103	PEK	O03-C21-O04	-4.82	110.88	123.51
14	A	601	HEA	CBA-CAA-C2A	-4.77	104.10	112.47
21	C	307	CHD	C14-C8-C7	-4.69	105.06	111.77
21	C	307	CHD	C9-C11-C12	-4.62	108.58	114.38
23	M	101	DMU	C22-C25-C28	-4.56	90.84	114.54
21	C	307	CHD	C11-C9-C10	-4.55	109.04	113.77
26	P	305	CDL	C57-C56-C55	-4.52	91.05	114.54
19	D	201	TGL	OG3-CG3-CG2	-4.49	96.59	108.70
19	L	101	TGL	OG3-CC1-OC1	-4.47	111.80	123.51
14	A	601	HEA	C12-C11-C3B	-4.46	103.37	112.59
21	G	103	CHD	C19-C10-C1	-4.45	100.70	108.23
25	C	308	PEK	O03-C21-O04	-4.36	112.09	123.51
26	C	305	CDL	C76-C75-C74	-4.35	91.93	114.54
21	B	303	CHD	O12-C12-C13	-4.33	103.89	111.12
21	P	307	CHD	C22-C20-C17	-4.33	101.13	110.24
21	C	306	CHD	C17-C13-C12	-4.31	113.90	117.68
19	N	609	TGL	OG3-CC1-OC1	-4.30	112.23	123.51
21	P	307	CHD	C21-C20-C22	-4.28	103.37	110.33
19	N	608	TGL	CG3-CG2-CG1	-4.27	102.14	112.08
21	G	103	CHD	O3-C3-C4	-4.21	101.35	109.86
18	A	606	PGV	C4-C3-C2	-4.15	97.95	113.30
14	A	601	HEA	CAA-CBA-CGA	-4.14	104.73	112.78
19	B	301	TGL	OB1-CB1-CB2	-4.12	107.98	123.76
21	B	303	CHD	C11-C9-C8	-4.12	104.83	110.77
23	C	301	DMU	C2-C3-C4	-4.10	101.47	110.85
21	C	307	CHD	C11-C12-C13	-4.09	107.09	111.22
18	A	607	PGV	C8-C9-C10	-4.06	97.28	113.79
26	G	101	CDL	OA8-CA7-OA9	-4.06	112.86	123.51
18	P	301	PGV	O04-C19-C20	-4.01	108.42	123.76
14	A	602	HEA	CBA-CAA-C2A	-4.00	105.45	112.47
23	C	301	DMU	O49-C1-C2	-3.96	101.42	110.36
21	P	306	CHD	C22-C23-C24	-3.90	97.13	113.05
21	C	307	CHD	C22-C20-C17	-3.87	102.09	110.24
18	N	607	PGV	O01-C1-O02	-3.83	113.26	123.67
18	P	304	PGV	C03-C02-C01	-3.81	103.20	112.08
18	N	606	PGV	C8-C9-C10	-3.81	98.32	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	303	CHD	C13-C17-C20	-3.80	114.80	119.44
21	G	103	CHD	C13-C17-C20	-3.75	114.87	119.44
21	C	307	CHD	C4-C5-C10	-3.71	108.67	112.66
14	N	601	HEA	C27-C19-C18	-3.71	116.41	123.58
23	M	101	DMU	C6-C1-C2	-3.67	102.69	109.98
18	P	301	PGV	C03-C02-C01	-3.67	103.53	112.08
14	N	601	HEA	C12-C11-C3B	-3.66	105.03	112.59
21	C	307	CHD	C6-C7-C8	-3.63	107.61	111.46
21	G	103	CHD	C15-C14-C8	-3.62	112.99	118.34
14	N	601	HEA	C17-C18-C19	-3.61	119.78	127.75
25	C	303	PEK	C29-C28-C27	-3.61	95.79	114.54
14	N	602	HEA	CAA-CBA-CGA	-3.60	105.77	112.78
18	C	309	PGV	O03-C19-O04	-3.59	114.09	123.51
21	B	303	CHD	C11-C12-C13	-3.58	107.61	111.22
22	B	304	PSC	C32-C31-C30	-3.55	96.09	114.54
23	Z	101	DMU	O55-C2-C1	-3.55	102.35	110.36
26	T	104	CDL	OA6-CA5-OA7	-3.54	114.03	123.67
21	P	306	CHD	C19-C10-C9	-3.53	106.53	111.20
21	B	303	CHD	C15-C14-C8	-3.52	113.13	118.34
21	P	307	CHD	C22-C23-C24	-3.50	98.78	113.05
23	C	301	DMU	O61-C57-C4	-3.49	99.64	111.30
21	B	303	CHD	C9-C8-C7	-3.46	107.70	111.89
14	N	601	HEA	CMB-C2B-C1B	-3.45	122.45	128.31
23	Z	101	DMU	C11-C9-C8	-3.44	104.36	112.99
19	Q	201	TGL	OG3-CC1-OC1	-3.43	114.52	123.51
18	A	606	PGV	O01-C1-O02	-3.38	114.47	123.67
14	A	602	HEA	C3C-CAC-CBC	-3.38	119.60	126.40
18	N	606	PGV	O01-C1-O02	-3.38	114.49	123.67
23	M	101	DMU	C18-O16-C6	-3.37	108.10	114.00
26	P	305	CDL	OB8-CB7-OB9	-3.36	114.70	123.51
21	C	307	CHD	C19-C10-C1	-3.36	102.54	108.23
14	N	601	HEA	C20-C21-C22	-3.35	102.82	111.61
23	M	101	DMU	O49-C1-C2	-3.34	102.83	110.36
25	T	101	PEK	C27-C26-C25	-3.34	97.21	114.54
21	P	307	CHD	C5-C4-C3	-3.33	107.95	112.88
14	A	602	HEA	C16-C15-C14	-3.32	114.80	120.98
21	G	103	CHD	O12-C12-C13	-3.28	105.64	111.12
21	B	303	CHD	C19-C10-C1	-3.25	102.72	108.23
14	A	601	HEA	CBD-CAD-C3D	-3.24	106.79	112.49
19	Q	201	TGL	CC4-CC3-CC2	-3.23	101.33	113.30
19	B	301	TGL	CB7-CB6-CB5	-3.23	97.77	114.54
25	T	101	PEK	C24-C23-C22	-3.21	101.41	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	103	CHD	C17-C13-C12	-3.21	114.86	117.68
23	M	101	DMU	O3-C5-C10	-3.20	102.92	110.01
26	C	305	CDL	OB8-CB6-CB4	-3.19	100.08	108.70
18	N	607	PGV	C22-C21-C20	-3.19	101.49	113.30
23	M	101	DMU	O2-C8-C9	-3.19	100.83	109.23
21	P	307	CHD	C17-C13-C14	-3.18	96.86	100.08
25	C	303	PEK	O03-C21-C22	-3.18	102.07	111.85
21	P	306	CHD	O7-C7-C6	-3.17	102.28	110.02
14	A	602	HEA	C20-C19-C18	-3.17	115.07	120.98
19	Q	201	TGL	CG3-CG2-CG1	-3.16	104.71	112.08
14	A	601	HEA	CMC-C2C-C1C	-3.13	122.98	128.31
18	C	304	PGV	C30-C29-C28	-3.09	98.49	114.54
19	B	301	TGL	OG2-CB1-OB1	-3.08	115.30	123.67
18	A	607	PGV	C23-C22-C21	-3.08	98.57	114.54
26	C	305	CDL	OB4-PB2-OB5	-3.07	93.61	108.24
14	A	602	HEA	OMA-CMA-C3A	-3.07	118.00	125.03
19	D	201	TGL	OG1-CA1-OA1	-3.06	115.48	123.51
18	N	607	PGV	C4-C3-C2	-3.04	102.03	113.30
21	J	101	CHD	C11-C9-C8	-3.04	106.38	110.77
14	A	602	HEA	C12-C13-C14	-3.04	103.76	112.42
21	W	101	CHD	C9-C11-C12	-3.02	110.59	114.38
19	N	609	TGL	CA4-CA3-CA2	-3.02	102.11	113.30
18	P	304	PGV	O03-C01-C02	-3.02	100.54	108.70
22	R	201	PSC	C27-C26-C25	-3.02	98.87	114.54
22	R	201	PSC	C21-C20-C19	-3.00	101.85	113.57
23	M	101	DMU	C22-C19-C18	-3.00	99.93	113.47
26	P	305	CDL	CB4-OB6-CB5	-2.99	110.52	117.91
21	B	303	CHD	O3-C3-C4	-2.99	103.82	109.86
14	A	601	HEA	CAD-C3D-C2D	-2.98	120.51	129.00
19	N	609	TGL	CB9-CB8-CB7	-2.97	99.09	114.54
19	L	101	TGL	OC1-CC1-CC2	-2.97	112.38	123.76
21	J	101	CHD	O12-C12-C11	-2.97	102.94	109.09
21	J	101	CHD	C14-C8-C9	-2.96	105.45	109.63
18	C	304	PGV	C10-C11-C12	-2.96	101.34	124.66
23	Z	101	DMU	O49-C1-C6	-2.96	103.45	110.01
14	A	601	HEA	C20-C21-C22	-2.94	103.88	111.61
26	C	305	CDL	C73-C72-C71	-2.94	102.42	113.30
14	A	602	HEA	C12-C11-C3B	-2.94	106.51	112.59
21	C	306	CHD	C13-C17-C20	-2.94	115.86	119.44
26	P	305	CDL	OB4-PB2-OB5	-2.93	94.25	108.24
14	A	602	HEA	C1A-C2A-C3A	-2.93	104.14	107.07
21	B	303	CHD	C16-C15-C14	-2.93	99.23	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	307	CHD	C10-C9-C8	-2.91	108.71	111.86
21	B	303	CHD	C5-C6-C7	-2.91	111.13	114.44
18	P	304	PGV	C21-C20-C19	-2.90	102.24	113.57
23	C	301	DMU	C6-O5-C4	-2.89	108.08	113.74
22	R	201	PSC	C32-C31-C30	-2.88	99.60	114.54
21	C	306	CHD	O3-C3-C4	-2.87	104.06	109.86
21	C	306	CHD	C22-C23-C24	-2.87	101.35	113.05
21	C	307	CHD	C22-C23-C24	-2.87	101.35	113.05
25	T	101	PEK	C29-C28-C27	-2.87	99.65	114.54
26	G	101	CDL	OA6-CA5-OA7	-2.86	115.89	123.67
19	D	201	TGL	C26-C25-C24	-2.86	99.71	114.54
26	C	305	CDL	OB4-PB2-OB2	-2.83	94.76	108.24
26	T	104	CDL	OB8-CB7-OB9	-2.82	116.12	123.51
21	G	103	CHD	C18-C13-C12	-2.81	106.28	109.09
14	A	601	HEA	CAD-CBD-CGD	-2.79	107.36	112.78
21	J	101	CHD	C19-C10-C1	-2.78	103.51	108.23
25	C	303	PEK	C2-C3-C4	-2.78	108.55	113.65
18	N	607	PGV	C3-C2-C1	-2.78	102.72	113.57
26	T	104	CDL	OB6-CB5-OB7	-2.78	116.11	123.67
18	N	606	PGV	C23-C22-C21	-2.78	100.11	114.54
14	N	602	HEA	OMA-CMA-C3A	-2.78	118.66	125.03
19	L	101	TGL	CA7-CA6-CA5	-2.77	100.14	114.54
18	A	607	PGV	C27-C26-C25	-2.77	100.14	114.54
23	Z	101	DMU	O7-C10-O1	-2.77	103.47	110.69
25	C	303	PEK	C02-O01-C1	-2.76	111.08	117.91
26	C	305	CDL	C53-C52-C51	-2.76	103.08	113.30
21	C	307	CHD	C16-C15-C14	-2.76	99.57	105.11
14	A	602	HEA	CMD-C2D-C3D	-2.75	119.49	125.24
25	C	303	PEK	C27-C26-C25	-2.75	100.27	114.54
21	C	306	CHD	C11-C9-C10	-2.74	110.92	113.77
21	C	307	CHD	C21-C20-C22	-2.72	105.90	110.33
26	C	305	CDL	OB8-CB7-OB9	-2.72	116.37	123.51
25	T	103	PEK	C33-C32-C31	-2.71	100.45	114.54
21	C	307	CHD	C17-C13-C14	-2.71	97.34	100.08
19	N	609	TGL	C25-C24-C23	-2.70	100.50	114.54
25	C	303	PEK	C25-C24-C23	-2.68	100.60	114.54
14	N	601	HEA	C16-C15-C14	-2.68	116.00	120.98
14	A	602	HEA	CAA-CBA-CGA	-2.67	107.60	112.78
21	C	307	CHD	C10-C9-C8	-2.66	108.97	111.86
19	N	609	TGL	CB4-CB3-CB2	-2.65	103.48	113.30
25	C	308	PEK	O02-C1-C2	-2.65	113.63	123.76
26	T	104	CDL	OA8-CA7-OA9	-2.64	116.59	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	101	DMU	O5-C4-C3	-2.62	104.18	109.78
14	A	602	HEA	C13-C14-C15	-2.62	121.97	127.75
26	T	104	CDL	OB5-PB2-OB3	-2.61	98.53	109.21
23	Z	101	DMU	C22-C19-C18	-2.61	101.69	113.47
18	N	607	PGV	C5-C4-C3	-2.60	101.05	114.54
21	G	103	CHD	C16-C15-C14	-2.60	99.90	105.11
18	A	606	PGV	C5-C4-C3	-2.59	101.09	114.54
21	B	303	CHD	C18-C13-C12	-2.58	106.51	109.09
21	C	307	CHD	C1-C10-C9	-2.58	107.33	111.43
22	R	201	PSC	O01-C1-O02	-2.58	116.66	123.67
18	C	309	PGV	C01-O03-C19	-2.56	109.36	117.00
18	C	309	PGV	O04-C19-C20	-2.56	113.97	123.76
25	T	101	PEK	O11-P-O14	-2.55	98.78	109.21
18	A	606	PGV	C3-C2-C1	-2.55	103.63	113.57
25	C	303	PEK	C26-C25-C24	-2.54	101.32	114.54
23	Z	101	DMU	O5-C6-O16	-2.53	103.91	109.99
22	B	304	PSC	C26-C25-C24	-2.53	101.39	114.54
21	C	307	CHD	C19-C10-C9	-2.52	107.86	111.20
19	B	301	TGL	CB9-CB8-CB7	-2.50	101.56	114.54
23	C	301	DMU	O5-C4-C3	-2.49	104.46	109.78
14	N	601	HEA	C3C-CAC-CBC	-2.48	121.40	126.40
25	T	101	PEK	C25-C24-C23	-2.48	101.66	114.54
25	C	303	PEK	O01-C02-C03	-2.48	99.65	108.36
14	N	602	HEA	C16-C15-C14	-2.48	116.37	120.98
18	C	309	PGV	O02-C1-C2	-2.47	114.29	123.76
25	T	101	PEK	O01-C02-C01	-2.47	99.67	108.36
23	Z	101	DMU	C18-O16-C6	-2.45	109.72	114.00
19	N	608	TGL	OG2-CB1-OB1	-2.45	117.01	123.67
19	D	201	TGL	CC3-CC2-CC1	-2.44	104.05	113.57
26	P	305	CDL	CA6-CA4-CA3	-2.43	106.41	112.08
22	B	304	PSC	C27-C26-C25	-2.43	101.92	114.54
26	T	104	CDL	C58-C57-C56	-2.42	101.95	114.54
21	G	103	CHD	C14-C8-C9	-2.42	106.21	109.63
19	N	608	TGL	OB1-CB1-CB2	-2.42	114.49	123.76
14	N	602	HEA	C1A-C2A-C3A	-2.41	104.66	107.07
18	P	301	PGV	C21-C20-C19	-2.40	104.20	113.57
23	C	301	DMU	O1-C10-C5	-2.39	105.32	110.28
18	A	607	PGV	O04-C19-C20	-2.37	114.69	123.76
19	D	201	TGL	CC4-CC3-CC2	-2.36	104.55	113.30
14	A	602	HEA	CMB-C2B-C1B	-2.36	124.30	128.31
18	A	607	PGV	C22-C21-C20	-2.36	104.57	113.30
26	G	101	CDL	OB7-CB5-C51	-2.35	114.76	123.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	305	CDL	C13-C12-C11	-2.35	104.61	113.30
23	C	301	DMU	C18-O16-C6	-2.34	109.91	114.00
21	P	306	CHD	C14-C8-C9	-2.34	106.33	109.63
21	P	307	CHD	C13-C17-C20	-2.34	116.59	119.44
18	A	607	PGV	C30-C29-C28	-2.34	102.40	114.54
14	N	601	HEA	CMC-C2C-C1C	-2.33	124.35	128.31
14	N	602	HEA	C13-C14-C15	-2.32	122.62	127.75
18	P	304	PGV	C22-C21-C20	-2.32	104.70	113.30
18	C	309	PGV	C22-C21-C20	-2.31	104.74	113.30
18	P	304	PGV	O01-C02-C03	-2.31	100.25	108.36
18	A	606	PGV	C03-C02-C01	-2.30	106.72	112.08
19	N	609	TGL	CA7-CA6-CA5	-2.30	102.60	114.54
18	N	607	PGV	O01-C02-C01	-2.30	100.28	108.36
25	T	102	PEK	C13-C14-C15	-2.30	110.52	124.38
19	L	101	TGL	C21-C20-CA9	-2.30	102.61	114.54
26	P	305	CDL	C78-C77-C76	-2.27	102.72	114.54
18	P	304	PGV	C10-C11-C12	-2.25	106.93	124.66
21	C	307	CHD	O3-C3-C2	-2.25	104.60	110.04
19	L	101	TGL	C14-C13-C12	-2.25	102.86	114.54
26	C	305	CDL	OA6-CA5-OA7	-2.25	117.55	123.67
26	G	101	CDL	OB8-CB7-OB9	-2.24	117.65	123.51
25	T	101	PEK	C23-C22-C21	-2.23	104.88	113.57
18	A	607	PGV	C10-C11-C12	-2.23	107.14	124.66
19	N	609	TGL	CA8-CA7-CA6	-2.23	102.98	114.54
21	J	101	CHD	C13-C14-C8	-2.22	111.81	114.73
18	P	301	PGV	C01-O03-C19	-2.22	110.39	117.00
19	L	101	TGL	CA4-CA3-CA2	-2.21	105.11	113.30
18	A	606	PGV	C34-C33-C32	-2.20	96.24	113.49
26	P	305	CDL	OB8-CB6-CB4	-2.20	102.77	108.70
26	G	101	CDL	CB2-C1-CA2	-2.19	105.45	112.42
14	N	601	HEA	CBA-CAA-C2A	-2.19	108.62	112.47
25	C	303	PEK	O01-C02-C01	-2.17	100.73	108.36
21	W	101	CHD	C1-C10-C9	-2.16	107.99	111.43
18	C	304	PGV	C7-C6-C5	-2.16	103.30	114.54
14	A	601	HEA	C1A-C2A-C3A	-2.15	104.92	107.07
21	P	307	CHD	C17-C13-C12	-2.14	115.80	117.68
19	L	101	TGL	OA1-CA1-CA2	-2.14	115.57	123.76
23	M	101	DMU	O5-C6-O16	-2.13	104.88	109.99
18	P	301	PGV	O03-C19-O04	-2.13	117.93	123.51
26	P	305	CDL	OB9-CB7-C71	-2.13	115.62	123.76
19	N	609	TGL	OA1-CA1-CA2	-2.12	115.64	123.76
18	C	304	PGV	C8-C9-C10	-2.11	105.21	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	302	DMU	O6-C11-C9	-2.10	104.30	111.30
25	C	303	PEK	O11-P-O14	-2.10	100.62	109.21
21	G	103	CHD	C21-C20-C17	-2.09	109.77	112.99
21	P	307	CHD	C19-C10-C1	-2.08	104.70	108.23
19	Q	201	TGL	OG3-CG3-CG2	-2.08	103.09	108.70
26	P	305	CDL	OB6-CB5-OB7	-2.08	118.02	123.67
18	P	304	PGV	C24-C23-C22	-2.08	103.75	114.54
21	C	306	CHD	O7-C7-C6	-2.08	104.95	110.02
25	T	101	PEK	O04-C21-C22	-2.07	115.82	123.76
21	P	307	CHD	C11-C9-C10	-2.06	111.62	113.77
19	B	301	TGL	OA1-CA1-CA2	-2.06	115.87	123.76
18	N	606	PGV	C27-C26-C25	-2.06	103.84	114.54
26	C	305	CDL	C54-C53-C52	-2.06	103.84	114.54
25	C	308	PEK	O12-P-O14	-2.06	100.78	109.21
14	N	602	HEA	C12-C11-C3B	-2.06	108.34	112.59
26	C	305	CDL	CB4-OB6-CB5	-2.05	112.84	117.91
21	P	307	CHD	C19-C10-C9	-2.05	108.48	111.20
14	N	601	HEA	OMA-CMA-C3A	-2.05	120.33	125.03
25	C	308	PEK	C2-C3-C4	-2.05	109.90	113.65
21	P	307	CHD	C16-C17-C20	-2.04	108.86	112.12
23	Z	101	DMU	C22-C25-C28	-2.04	103.96	114.54
26	P	305	CDL	OA7-CA5-C11	-2.04	115.96	123.76
23	Z	101	DMU	C25-C28-C31	-2.03	103.99	114.54
26	P	305	CDL	C73-C72-C71	-2.02	105.82	113.30
18	C	309	PGV	O01-C1-O02	-2.02	118.17	123.67
18	C	304	PGV	C21-C20-C19	-2.02	105.71	113.57
26	G	101	CDL	OB2-PB2-OB3	-2.01	100.97	109.21
25	C	303	PEK	C3-C2-C1	-2.01	105.72	113.57
18	A	606	PGV	C14-C13-C12	-2.01	100.02	112.08
25	C	303	PEK	C37-C36-C35	-2.01	95.74	115.41
25	G	102	PEK	C2-C3-C4	-2.01	109.97	113.65
21	B	303	CHD	C21-C20-C22	-2.00	107.08	110.33
23	P	302	DMU	O1-C10-C5	-2.00	106.12	110.28
21	B	303	CHD	C23-C22-C20	2.00	117.27	114.79
19	D	201	TGL	OB1-CB1-CB2	2.01	131.44	123.76
19	N	608	TGL	C19-C18-C17	2.01	124.96	114.54
21	P	306	CHD	C4-C3-C2	2.02	113.11	110.53
26	T	104	CDL	O1-C1-CB2	2.02	116.89	109.32
26	G	101	CDL	OB8-CB7-C71	2.03	118.08	111.85
25	C	303	PEK	C01-O03-C21	2.03	123.05	117.00
26	C	305	CDL	C82-C81-C80	2.04	125.11	114.54
23	P	302	DMU	O16-C18-C19	2.04	115.50	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	101	CHD	C21-C20-C17	2.05	116.14	112.99
19	N	608	TGL	C16-C15-CC9	2.05	125.18	114.54
14	N	601	HEA	O11-C11-C12	2.05	114.74	109.73
14	A	602	HEA	C26-C15-C14	2.06	127.58	123.58
18	P	304	PGV	C28-C27-C26	2.06	125.25	114.54
25	T	102	PEK	C11-C10-C9	2.07	119.05	112.17
21	C	306	CHD	C9-C8-C7	2.08	114.40	111.89
26	T	104	CDL	C44-C43-C42	2.08	125.35	114.54
25	C	308	PEK	C11-C10-C9	2.08	119.08	112.17
21	P	306	CHD	O12-C12-C13	2.09	114.60	111.12
19	Q	201	TGL	C21-C20-CA9	2.09	125.38	114.54
14	A	601	HEA	C27-C19-C20	2.09	118.55	115.37
21	B	303	CHD	C10-C9-C8	2.09	114.12	111.86
18	N	606	PGV	O01-C02-C01	2.09	115.71	108.36
19	L	101	TGL	C11-C10-CB9	2.10	125.43	114.54
26	C	305	CDL	C23-C22-C21	2.10	125.44	114.54
26	C	305	CDL	CA4-OA6-CA5	2.10	123.10	117.91
19	N	608	TGL	C15-CC9-CC8	2.10	125.46	114.54
26	T	104	CDL	C80-C79-C78	2.11	125.50	114.54
19	D	201	TGL	C11-C10-CB9	2.13	125.61	114.54
21	B	303	CHD	C6-C7-C8	2.13	113.72	111.46
19	L	101	TGL	C29-C14-C13	2.14	125.63	114.54
14	N	602	HEA	CMC-C2C-C3C	2.14	129.28	125.09
21	W	101	CHD	C11-C9-C10	2.15	116.00	113.77
26	P	305	CDL	C39-C38-C37	2.17	125.82	114.54
18	P	301	PGV	O01-C02-C03	2.18	116.02	108.36
26	T	104	CDL	C72-C71-CB7	2.20	122.13	113.57
25	G	102	PEK	C01-O03-C21	2.20	123.55	117.00
21	B	303	CHD	O7-C7-C8	2.20	114.29	109.28
21	C	306	CHD	C16-C17-C13	2.20	105.71	103.59
26	G	101	CDL	C40-C39-C38	2.22	126.05	114.54
23	Z	101	DMU	C7-C8-C9	2.23	114.20	110.23
21	W	101	CHD	C6-C5-C10	2.23	115.05	112.66
19	N	608	TGL	CC3-CC2-CC1	2.25	122.33	113.57
21	J	101	CHD	C23-C22-C20	2.25	117.57	114.79
26	C	305	CDL	C83-C82-C81	2.25	126.22	114.54
21	W	101	CHD	C4-C3-C2	2.25	113.41	110.53
25	T	102	PEK	C02-O01-C1	2.27	123.51	117.91
26	G	101	CDL	OA6-CA4-CA6	2.27	116.34	108.36
26	G	101	CDL	C82-C81-C80	2.28	126.37	114.54
21	C	307	CHD	C11-C9-C8	2.28	114.05	110.77
22	R	201	PSC	C31-C30-C29	2.28	126.41	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C21-C20-C19	2.29	120.18	112.61
19	Q	201	TGL	OG1-CA1-CA2	2.29	118.90	111.85
23	P	302	DMU	O1-C9-C8	2.29	114.04	109.67
25	C	308	PEK	C02-O01-C1	2.30	123.58	117.91
22	B	304	PSC	C08-N-C05	2.30	119.23	109.92
26	G	101	CDL	C44-C43-C42	2.30	126.48	114.54
26	P	305	CDL	C62-C61-C60	2.31	126.52	114.54
26	T	104	CDL	C85-C84-C83	2.32	126.57	114.54
19	D	201	TGL	OG2-CG2-CG3	2.32	116.52	108.36
26	G	101	CDL	C13-C12-C11	2.32	121.90	113.30
26	G	101	CDL	CA4-OA6-CA5	2.33	123.67	117.91
25	T	103	PEK	C01-O03-C21	2.33	123.95	117.00
21	W	101	CHD	C6-C7-C8	2.34	113.94	111.46
21	P	306	CHD	C18-C13-C14	2.34	114.89	111.20
25	T	103	PEK	C11-C10-C9	2.35	119.96	112.17
26	C	305	CDL	OA2-PA1-OA3	2.35	118.84	109.21
21	W	101	CHD	C2-C1-C10	2.35	117.03	112.81
19	D	201	TGL	C20-CA9-CA8	2.37	126.83	114.54
25	C	308	PEK	C30-C29-C28	2.37	126.84	114.54
21	C	307	CHD	C2-C1-C10	2.37	117.06	112.81
19	B	301	TGL	OG2-CG2-CG1	2.38	116.72	108.36
26	C	305	CDL	OB5-PB2-OB3	2.38	118.97	109.21
22	B	304	PSC	C3-C2-C1	2.39	122.89	113.57
25	T	102	PEK	O03-C01-C02	2.40	115.18	108.70
19	B	301	TGL	CG1-OG1-CA1	2.40	124.15	117.00
18	A	607	PGV	O01-C02-C03	2.40	116.80	108.36
26	P	305	CDL	C53-C52-C51	2.40	122.19	113.30
25	C	308	PEK	O03-C01-C02	2.43	115.25	108.70
19	N	609	TGL	C15-CC9-CC8	2.45	127.26	114.54
26	C	305	CDL	C43-C42-C41	2.46	127.30	114.54
21	C	306	CHD	C15-C14-C13	2.46	105.96	103.59
21	W	101	CHD	C4-C5-C10	2.46	115.30	112.66
23	P	302	DMU	O7-C10-C5	2.46	114.23	108.12
22	B	304	PSC	C22-C21-C20	2.46	122.42	113.30
25	C	308	PEK	C14-C13-C12	2.46	120.36	112.17
21	P	307	CHD	C18-C13-C12	2.48	111.57	109.09
19	L	101	TGL	OG3-CG3-CG2	2.48	115.39	108.70
21	C	306	CHD	O7-C7-C8	2.48	114.93	109.28
26	G	101	CDL	C80-C79-C78	2.48	127.43	114.54
22	R	201	PSC	O01-C02-C01	2.49	117.13	108.36
18	P	304	PGV	C29-C28-C27	2.51	127.58	114.54
25	T	103	PEK	C2-C3-C4	2.52	118.28	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	101	CDL	C39-C38-C37	2.52	127.64	114.54
22	B	304	PSC	O03-C19-C20	2.52	119.62	111.85
21	G	103	CHD	C4-C5-C10	2.53	115.37	112.66
19	Q	201	TGL	CG2-OG2-CB1	2.54	124.18	117.91
19	Q	201	TGL	C20-CA9-CA8	2.54	127.72	114.54
21	W	101	CHD	C9-C10-C5	2.54	112.30	108.68
19	N	609	TGL	OG1-CA1-CA2	2.55	119.70	111.85
21	W	101	CHD	O7-C7-C8	2.55	115.09	109.28
21	J	101	CHD	O7-C7-C8	2.55	115.09	109.28
21	G	103	CHD	C1-C10-C5	2.56	110.58	107.76
21	P	306	CHD	C11-C9-C8	2.57	114.47	110.77
21	W	101	CHD	C16-C17-C13	2.57	106.06	103.59
19	B	301	TGL	C15-CC9-CC8	2.58	127.94	114.54
19	Q	201	TGL	CG1-OG1-CA1	2.58	124.69	117.00
22	B	304	PSC	O01-C02-C03	2.61	117.52	108.36
26	G	101	CDL	C23-C22-C21	2.61	128.08	114.54
19	B	301	TGL	CC3-CC2-CC1	2.62	123.77	113.57
26	T	104	CDL	C19-C18-C17	2.63	128.20	114.54
21	J	101	CHD	C1-C10-C5	2.63	110.66	107.76
21	G	103	CHD	O3-C3-C2	2.66	116.45	110.04
18	C	309	PGV	C25-C24-C23	2.66	128.34	114.54
18	P	304	PGV	C9-C10-C11	2.66	128.03	112.08
21	P	306	CHD	C5-C6-C7	2.66	117.47	114.44
26	G	101	CDL	C72-C71-CB7	2.67	123.97	113.57
25	T	101	PEK	C03-C02-C01	2.68	118.32	112.08
21	P	307	CHD	C4-C3-C2	2.68	113.95	110.53
19	B	301	TGL	OG2-CG2-CG3	2.68	117.77	108.36
21	J	101	CHD	C2-C1-C10	2.70	117.64	112.81
21	J	101	CHD	C21-C20-C22	2.70	114.71	110.33
23	M	101	DMU	O7-C10-C5	2.70	114.84	108.12
23	Z	101	DMU	C10-O1-C9	2.71	119.06	113.74
25	T	101	PEK	O03-C01-C02	2.72	116.04	108.70
21	G	103	CHD	C9-C10-C5	2.72	112.55	108.68
19	L	101	TGL	OG2-CG2-CG1	2.73	117.95	108.36
19	N	609	TGL	OG3-CC1-CC2	2.74	120.27	111.85
14	A	601	HEA	CMC-C2C-C3C	2.74	130.44	125.09
21	P	306	CHD	C16-C17-C20	2.76	116.53	112.12
18	A	607	PGV	O01-C02-C01	2.77	118.09	108.36
26	C	305	CDL	OA8-CA7-C31	2.78	120.39	111.85
21	P	306	CHD	C21-C20-C17	2.78	117.28	112.99
14	N	602	HEA	C3A-C4A-NA	2.79	116.21	110.94
18	P	301	PGV	C02-O01-C1	2.79	124.81	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	103	CHD	C11-C9-C10	2.79	116.67	113.77
14	A	602	HEA	CMB-C2B-C3B	2.80	130.86	125.14
26	T	104	CDL	C40-C39-C38	2.80	129.08	114.54
21	W	101	CHD	C18-C13-C14	2.80	115.62	111.20
25	C	308	PEK	C24-C23-C22	2.82	123.74	113.30
26	G	101	CDL	C22-C21-C20	2.83	129.22	114.54
21	B	303	CHD	O3-C3-C2	2.83	116.88	110.04
21	P	306	CHD	C17-C13-C14	2.85	102.96	100.08
26	C	305	CDL	C42-C41-C40	2.87	129.42	114.54
23	C	301	DMU	O16-C18-C19	2.87	117.88	109.63
25	C	303	PEK	C14-C13-C12	2.87	121.71	112.17
26	T	104	CDL	C22-C21-C20	2.87	129.47	114.54
14	N	601	HEA	C3C-C4C-NC	2.88	112.94	109.21
21	C	307	CHD	C21-C20-C17	2.91	117.47	112.99
18	P	301	PGV	O01-C1-C2	2.91	117.67	111.53
18	N	607	PGV	C26-C25-C24	2.92	129.72	114.54
25	C	308	PEK	C01-O03-C21	2.93	125.73	117.00
26	G	101	CDL	C19-C18-C17	2.94	129.79	114.54
26	T	104	CDL	OB8-CB6-CB4	2.94	116.64	108.70
26	P	305	CDL	OA4-PA1-OA3	2.95	127.91	112.56
21	W	101	CHD	C21-C20-C22	2.96	115.14	110.33
23	C	301	DMU	C7-C8-C9	2.97	115.52	110.23
19	L	101	TGL	C15-CC9-CC8	2.97	129.96	114.54
26	P	305	CDL	OB6-CB5-C51	2.98	117.80	111.53
21	C	306	CHD	C4-C3-C2	2.98	114.34	110.53
18	P	301	PGV	O03-C01-C02	2.98	116.75	108.70
18	N	606	PGV	O03-C19-C20	2.99	121.05	111.85
19	L	101	TGL	OG2-CB1-CB2	2.99	117.84	111.53
19	N	609	TGL	OG2-CG2-CG3	3.00	118.92	108.36
21	P	306	CHD	C4-C5-C10	3.00	115.88	112.66
25	T	101	PEK	C11-C10-C9	3.03	122.22	112.17
19	Q	201	TGL	OG3-CC1-CC2	3.03	121.16	111.85
26	T	104	CDL	O1-C1-CA2	3.04	120.68	109.32
19	L	101	TGL	CG3-OG3-CC1	3.04	126.05	117.00
19	N	608	TGL	CG1-OG1-CA1	3.04	126.06	117.00
14	N	601	HEA	CMB-C2B-C3B	3.05	131.37	125.14
21	C	307	CHD	C15-C14-C13	3.10	106.57	103.59
25	T	101	PEK	O03-C21-C22	3.13	121.49	111.85
18	N	607	PGV	O02-C1-C2	3.14	135.77	123.76
14	A	602	HEA	C27-C19-C20	3.15	120.16	115.37
21	P	307	CHD	C11-C9-C8	3.15	115.30	110.77
21	G	103	CHD	O7-C7-C8	3.15	116.45	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	305	CDL	O1-C1-CB2	3.15	121.10	109.32
21	G	103	CHD	C9-C11-C12	3.15	118.34	114.38
26	P	305	CDL	C42-C41-C40	3.15	130.92	114.54
21	W	101	CHD	C1-C2-C3	3.16	114.61	110.41
26	G	101	CDL	C83-C82-C81	3.19	131.10	114.54
18	A	606	PGV	O02-C1-C2	3.20	136.00	123.76
23	P	302	DMU	C1-C2-C3	3.22	116.74	109.63
23	C	301	DMU	C1-C2-C3	3.22	116.74	109.63
25	T	102	PEK	O03-C21-C22	3.25	121.86	111.85
21	J	101	CHD	C11-C9-C10	3.27	117.16	113.77
18	C	309	PGV	C02-O01-C1	3.27	126.00	117.91
21	J	101	CHD	C16-C17-C13	3.28	106.75	103.59
19	N	608	TGL	CB3-CB2-CB1	3.28	126.37	113.57
26	C	305	CDL	CA6-OA8-CA7	3.30	126.84	117.00
19	L	101	TGL	OG2-CG2-CG3	3.31	120.01	108.36
19	B	301	TGL	C16-C15-CC9	3.32	131.79	114.54
21	P	306	CHD	C10-C9-C8	3.34	115.47	111.86
22	R	201	PSC	C3-C2-C1	3.34	126.61	113.57
26	G	101	CDL	OA8-CA7-C31	3.35	122.15	111.85
21	W	101	CHD	C22-C20-C17	3.37	117.33	110.24
25	G	102	PEK	O01-C02-C01	3.39	120.29	108.36
21	J	101	CHD	C14-C13-C12	3.43	110.47	107.37
14	A	602	HEA	CAD-C3D-C2D	3.44	138.82	129.00
26	T	104	CDL	OA8-CA7-C31	3.47	122.52	111.85
14	A	601	HEA	C26-C15-C14	3.48	130.33	123.58
23	C	301	DMU	C10-O1-C9	3.48	120.58	113.74
26	T	104	CDL	C83-C82-C81	3.50	132.74	114.54
19	N	609	TGL	OG2-CB1-OB1	3.51	133.23	123.67
26	P	305	CDL	C40-C39-C38	3.52	132.82	114.54
21	J	101	CHD	C22-C20-C17	3.52	117.65	110.24
26	P	305	CDL	OB2-PB2-OB3	3.53	123.64	109.21
21	J	101	CHD	C1-C2-C3	3.53	115.11	110.41
26	P	305	CDL	C54-C53-C52	3.54	132.93	114.54
25	G	102	PEK	O03-C21-C22	3.55	122.78	111.85
23	M	101	DMU	O4-C7-C8	3.55	118.36	110.36
14	N	601	HEA	C16-C17-C18	3.55	120.94	111.61
19	D	201	TGL	C10-CB9-CB8	3.58	133.12	114.54
25	C	303	PEK	O04-C21-C22	3.61	137.59	123.76
21	B	303	CHD	C1-C2-C3	3.62	115.23	110.41
19	D	201	TGL	CB5-CB4-CB3	3.63	133.38	114.54
21	P	306	CHD	C16-C17-C13	3.63	107.09	103.59
19	L	101	TGL	OG1-CA1-CA2	3.63	123.03	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	201	TGL	OG1-CA1-CA2	3.64	123.05	111.85
21	C	307	CHD	C6-C5-C4	3.66	114.99	111.07
21	G	103	CHD	C6-C5-C10	3.67	116.59	112.66
21	W	101	CHD	C10-C9-C8	3.67	115.83	111.86
25	G	102	PEK	O03-C01-C02	3.70	118.69	108.70
21	J	101	CHD	C9-C10-C5	3.71	113.96	108.68
26	C	305	CDL	C39-C38-C37	3.71	133.81	114.54
22	R	201	PSC	C02-O01-C1	3.71	127.09	117.91
25	T	102	PEK	C01-O03-C21	3.73	128.10	117.00
21	G	103	CHD	C4-C3-C2	3.74	115.32	110.53
21	P	307	CHD	C9-C8-C7	3.75	116.42	111.89
21	B	303	CHD	C9-C11-C12	3.75	119.09	114.38
23	C	301	DMU	O1-C9-C8	3.76	116.83	109.67
18	C	309	PGV	O03-C01-C02	3.81	119.00	108.70
21	C	306	CHD	C14-C8-C7	3.83	117.24	111.77
21	C	307	CHD	C18-C13-C12	3.84	112.93	109.09
19	N	608	TGL	OG1-CA1-CA2	3.85	123.69	111.85
18	A	607	PGV	O03-C19-C20	3.85	123.70	111.85
25	C	303	PEK	C8-C7-C6	3.85	124.97	112.17
21	C	306	CHD	C4-C5-C10	3.86	116.80	112.66
21	W	101	CHD	C15-C14-C13	3.87	107.31	103.59
21	J	101	CHD	C5-C6-C7	3.87	118.85	114.44
25	T	102	PEK	O01-C1-C2	3.91	119.77	111.53
21	J	101	CHD	C15-C14-C13	3.92	107.37	103.59
19	N	608	TGL	OG2-CG2-CG3	3.94	122.21	108.36
21	B	303	CHD	C15-C14-C13	3.96	107.41	103.59
21	P	307	CHD	C15-C14-C13	3.97	107.41	103.59
22	B	304	PSC	O01-C1-C2	3.99	119.93	111.53
14	A	601	HEA	CMD-C2D-C3D	4.00	133.60	125.24
26	P	305	CDL	OB5-PB2-OB3	4.05	125.80	109.21
19	D	201	TGL	CG1-OG1-CA1	4.06	129.09	117.00
21	W	101	CHD	O12-C12-C13	4.06	117.90	111.12
26	P	305	CDL	CA6-OA8-CA7	4.09	129.19	117.00
23	Z	101	DMU	O1-C9-C8	4.11	117.51	109.67
14	N	602	HEA	CBD-CAD-C3D	4.15	119.80	112.49
21	C	306	CHD	C21-C20-C17	4.16	119.39	112.99
19	B	301	TGL	OG3-CC1-CC2	4.16	124.64	111.85
26	T	104	CDL	CB6-OB8-CB7	4.17	129.41	117.00
21	W	101	CHD	C1-C10-C5	4.18	112.36	107.76
23	C	301	DMU	C57-C4-C3	4.18	125.53	113.25
22	B	304	PSC	C02-O01-C1	4.18	128.25	117.91
14	A	601	HEA	O11-C11-C12	4.21	120.01	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	609	TGL	CG1-OG1-CA1	4.21	129.55	117.00
14	N	601	HEA	C27-C19-C20	4.26	121.85	115.37
26	C	305	CDL	OB2-PB2-OB3	4.26	126.66	109.21
18	A	607	PGV	C01-O03-C19	4.27	129.72	117.00
18	N	606	PGV	C02-O01-C1	4.33	128.62	117.91
26	G	101	CDL	OB8-CB6-CB4	4.35	120.45	108.70
19	N	608	TGL	OG1-CG1-CG2	4.38	120.53	108.70
21	C	307	CHD	C4-C3-C2	4.40	116.16	110.53
19	N	609	TGL	OG1-CG1-CG2	4.41	120.60	108.70
25	T	103	PEK	O03-C01-C02	4.42	120.64	108.70
19	B	301	TGL	OG1-CA1-CA2	4.45	125.53	111.85
26	T	104	CDL	OA6-CA5-C11	4.46	120.92	111.53
23	C	301	DMU	C6-C1-C2	4.46	118.83	109.98
21	P	306	CHD	C15-C14-C13	4.47	107.89	103.59
21	B	303	CHD	C4-C5-C10	4.48	117.46	112.66
26	G	101	CDL	CB6-OB8-CB7	4.52	130.47	117.00
26	C	305	CDL	OB8-CB7-C71	4.53	125.81	111.85
21	P	306	CHD	C14-C8-C7	4.63	118.39	111.77
22	R	201	PSC	O03-C01-C02	4.64	121.24	108.70
19	D	201	TGL	CG3-OG3-CC1	4.76	131.17	117.00
25	T	103	PEK	C24-C23-C22	4.76	130.92	113.30
26	G	101	CDL	OA6-CA5-C11	4.81	121.66	111.53
21	J	101	CHD	C4-C5-C10	4.84	117.85	112.66
21	P	307	CHD	C14-C13-C12	4.87	111.78	107.37
25	G	102	PEK	C02-O01-C1	4.90	130.03	117.91
19	N	608	TGL	CG3-OG3-CC1	4.93	131.68	117.00
21	P	307	CHD	C1-C10-C5	4.97	113.24	107.76
21	B	303	CHD	C4-C3-C2	5.04	116.98	110.53
23	P	302	DMU	O16-C6-C1	5.06	114.23	108.00
19	L	101	TGL	OG1-CG1-CG2	5.07	122.38	108.70
21	G	103	CHD	C23-C22-C20	5.08	121.08	114.79
14	N	601	HEA	C26-C15-C16	5.08	123.11	115.37
25	T	103	PEK	O01-C1-C2	5.08	122.24	111.53
19	Q	201	TGL	CB3-CB2-CB1	5.12	133.53	113.57
25	T	103	PEK	C02-O01-C1	5.14	130.61	117.91
18	N	606	PGV	C01-O03-C19	5.25	132.64	117.00
21	J	101	CHD	C6-C7-C8	5.29	117.06	111.46
21	C	306	CHD	C5-C6-C7	5.30	120.47	114.44
19	N	608	TGL	OG2-CG2-CG1	5.36	127.20	108.36
26	P	305	CDL	OA6-CA5-C11	5.50	123.11	111.53
18	A	607	PGV	C3-C2-C1	5.51	135.06	113.57
25	C	308	PEK	O03-C21-C22	5.51	128.82	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	306	CHD	C1-C10-C5	5.53	113.85	107.76
21	J	101	CHD	C9-C8-C7	5.53	118.57	111.89
18	A	607	PGV	C02-O01-C1	5.59	131.72	117.91
21	W	101	CHD	C14-C8-C7	5.62	119.80	111.77
19	B	301	TGL	CG2-OG2-CB1	5.70	132.00	117.91
21	P	306	CHD	C6-C5-C10	5.72	118.79	112.66
21	J	101	CHD	C15-C14-C8	5.78	126.90	118.34
26	P	305	CDL	OB8-CB7-C71	5.79	129.67	111.85
25	G	102	PEK	O01-C1-C2	5.87	123.90	111.53
25	T	103	PEK	O03-C21-C22	5.95	130.16	111.85
21	J	101	CHD	C6-C5-C10	6.00	119.09	112.66
21	P	306	CHD	C15-C14-C8	6.02	127.26	118.34
21	W	101	CHD	C15-C14-C8	6.13	127.42	118.34
19	N	608	TGL	OG3-CC1-CC2	6.17	130.85	111.85
25	C	308	PEK	O01-C1-C2	6.18	124.56	111.53
21	C	306	CHD	C16-C17-C20	6.23	122.08	112.12
19	B	301	TGL	CG3-OG3-CC1	6.27	135.66	117.00
26	C	305	CDL	OA6-CA5-C11	6.29	124.77	111.53
21	C	307	CHD	C14-C13-C12	6.32	113.09	107.37
18	C	309	PGV	O03-C19-C20	6.34	131.37	111.85
26	G	101	CDL	OB6-CB5-C51	6.35	124.92	111.53
19	N	609	TGL	CG2-OG2-CB1	6.44	133.83	117.91
21	C	306	CHD	C15-C14-C8	6.48	127.94	118.34
21	J	101	CHD	C10-C9-C8	6.60	119.00	111.86
14	A	601	HEA	CMB-C2B-C3B	6.67	138.77	125.14
21	C	306	CHD	C1-C10-C5	6.73	115.17	107.76
21	C	306	CHD	C14-C13-C12	6.75	113.48	107.37
21	B	303	CHD	C1-C10-C5	6.80	115.25	107.76
21	C	306	CHD	C10-C9-C8	6.81	119.22	111.86
18	P	301	PGV	O03-C19-C20	7.07	133.60	111.85
19	Q	201	TGL	OG2-CB1-OB1	7.08	142.94	123.67
21	J	101	CHD	C17-C13-C12	7.09	123.89	117.68
22	R	201	PSC	O01-C1-C2	7.19	126.69	111.53
21	C	306	CHD	C6-C5-C10	7.40	120.60	112.66
21	W	101	CHD	C11-C12-C13	7.42	118.70	111.22
19	L	101	TGL	CG2-OG2-CB1	7.42	136.25	117.91
26	T	104	CDL	OB6-CB5-C51	7.51	127.35	111.53
18	C	309	PGV	O01-C1-C2	7.57	127.48	111.53
19	D	201	TGL	CB3-CB2-CB1	7.59	143.18	113.57
19	N	608	TGL	OG2-CB1-CB2	7.75	127.86	111.53
21	C	307	CHD	C1-C10-C5	7.76	116.31	107.76
19	L	101	TGL	OG3-CC1-CC2	7.78	135.80	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	606	PGV	O01-C1-C2	7.83	128.02	111.53
23	C	301	DMU	O16-C6-C1	7.93	117.75	108.00
21	J	101	CHD	C13-C17-C20	8.01	129.20	119.44
21	C	306	CHD	C6-C7-C8	8.21	120.16	111.46
21	P	306	CHD	C6-C7-C8	8.30	120.25	111.46
21	J	101	CHD	C14-C8-C7	8.46	123.87	111.77
19	D	201	TGL	OG2-CB1-OB1	8.74	147.45	123.67
19	N	608	TGL	CG2-OG2-CB1	8.93	139.98	117.91
21	J	101	CHD	C11-C12-C13	8.93	120.23	111.22
21	W	101	CHD	C13-C17-C20	9.51	131.02	119.44
19	B	301	TGL	OG2-CB1-CB2	11.52	135.81	111.53
21	W	101	CHD	C17-C13-C12	17.62	133.13	117.68

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NA

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	309	PGV	C02-O01-C1-C2
18	A	607	PGV	C02-O01-C1-C2
25	T	103	PEK	C02-O01-C1-O02
18	P	301	PGV	P-O11-C03-C02
18	N	606	PGV	P-O11-C03-C02
25	T	103	PEK	C02-O01-C1-C2
18	N	606	PGV	C02-O01-C1-O02
26	P	305	CDL	CA4-OA6-CA5-OA7
26	P	305	CDL	CA4-OA6-CA5-C11
18	N	606	PGV	C02-O01-C1-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	W	101	CHD	C11-C12-C13-C14-C8-C9

39 monomers are involved in 319 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	3	0
14	A	602	HEA	7	0
18	A	606	PGV	2	0
18	A	607	PGV	8	0
19	B	301	TGL	4	0
22	B	304	PSC	14	0
23	C	301	DMU	12	0
25	C	303	PEK	9	0
18	C	304	PGV	4	0
26	C	305	CDL	25	0
21	C	306	CHD	2	0
21	C	307	CHD	1	0
25	C	308	PEK	14	0
18	C	309	PGV	3	0
19	D	201	TGL	10	0
26	G	101	CDL	27	0
25	G	102	PEK	12	0
21	G	103	CHD	1	0
21	J	101	CHD	5	0
19	L	101	TGL	12	0
14	N	601	HEA	3	0
14	N	602	HEA	6	0
18	N	606	PGV	6	0
18	N	607	PGV	1	0
19	N	608	TGL	7	0
19	N	609	TGL	11	0
18	P	301	PGV	1	0
23	P	302	DMU	4	0
18	P	304	PGV	7	0
26	P	305	CDL	29	0
21	P	306	CHD	3	0
21	P	307	CHD	1	0
19	Q	201	TGL	10	0
22	R	201	PSC	17	0
25	T	101	PEK	5	0
25	T	102	PEK	17	0
25	T	103	PEK	7	0
26	T	104	CDL	26	0
21	W	101	CHD	2	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.65	0 <a href="#">100</a> <a href="#">100</a>	16, 20, 28, 70	0
1	N	513/514 (99%)	-0.61	0 <a href="#">100</a> <a href="#">100</a>	17, 24, 31, 63	0
2	B	226/227 (99%)	-0.62	2 (0%) <a href="#">85</a> <a href="#">85</a>	19, 28, 48, 90	0
2	O	226/227 (99%)	-0.52	5 (2%) <a href="#">65</a> <a href="#">64</a>	23, 34, 61, 99	0
3	C	259/261 (99%)	-0.86	0 <a href="#">100</a> <a href="#">100</a>	19, 24, 36, 77	0
3	P	259/261 (99%)	-0.81	1 (0%) <a href="#">93</a> <a href="#">93</a>	19, 24, 37, 65	0
4	D	144/147 (97%)	-0.84	1 (0%) <a href="#">89</a> <a href="#">89</a>	23, 29, 42, 72	0
4	Q	144/147 (97%)	0.36	10 (6%) <a href="#">20</a> <a href="#">18</a>	28, 42, 74, 152	0
5	E	105/109 (96%)	-0.70	2 (1%) <a href="#">70</a> <a href="#">68</a>	23, 29, 51, 123	0
5	R	105/109 (96%)	-0.14	3 (2%) <a href="#">55</a> <a href="#">53</a>	26, 36, 58, 130	0
6	F	98/98 (100%)	-0.09	7 (7%) <a href="#">19</a> <a href="#">17</a>	20, 31, 98, 153	0
6	S	98/98 (100%)	-0.08	9 (9%) <a href="#">11</a> <a href="#">9</a>	20, 29, 72, 146	0
7	G	83/85 (97%)	0.41	18 (21%) <a href="#">1</a> <a href="#">1</a>	22, 31, 92, 134	0
7	T	83/85 (97%)	0.21	16 (19%) <a href="#">2</a> <a href="#">1</a>	22, 33, 103, 143	0
8	H	79/85 (92%)	-0.14	8 (10%) <a href="#">9</a> <a href="#">7</a>	25, 35, 95, 127	0
8	U	79/85 (92%)	-0.24	9 (11%) <a href="#">7</a> <a href="#">5</a>	30, 39, 95, 118	0
9	I	72/73 (98%)	0.25	8 (11%) <a href="#">7</a> <a href="#">6</a>	26, 41, 62, 79	0
9	V	72/73 (98%)	0.32	8 (11%) <a href="#">7</a> <a href="#">6</a>	26, 46, 68, 86	0
10	J	58/59 (98%)	0.22	5 (8%) <a href="#">13</a> <a href="#">11</a>	25, 33, 64, 120	0
10	W	58/59 (98%)	-0.10	4 (6%) <a href="#">20</a> <a href="#">18</a>	24, 35, 68, 141	0
11	K	49/56 (87%)	-0.41	0 <a href="#">100</a> <a href="#">100</a>	27, 34, 50, 61	0
11	X	49/56 (87%)	0.71	5 (10%) <a href="#">9</a> <a href="#">7</a>	34, 43, 65, 81	0
12	L	46/47 (97%)	-0.91	0 <a href="#">100</a> <a href="#">100</a>	21, 26, 41, 89	0
12	Y	46/47 (97%)	-0.76	1 (2%) <a href="#">65</a> <a href="#">64</a>	25, 32, 53, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.43	4 (9%) 11 9	23, 27, 64, 116	0
13	Z	43/46 (93%)	-0.16	6 (13%) 4 3	30, 36, 78, 136	0
All	All	3550/3614 (98%)	-0.43	132 (3%) 45 43	16, 28, 60, 153	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	35.6
4	Q	5	VAL	32.0
4	Q	6	VAL	15.9
6	F	97	ALA	14.9
4	Q	4	SER	11.6
6	F	98	HIS	10.4
5	R	5	HIS	9.5
5	R	109	VAL	9.1
10	J	1	PHE	8.5
6	F	96	LEU	8.4
9	I	37	PHE	7.4
6	S	98	HIS	7.1
6	F	2	SER	6.9
8	U	7	LYS	6.7
2	O	90	ILE	6.6
4	Q	8	SER	6.6
9	V	37	PHE	6.5
4	Q	7	LYS	6.4
6	S	96	LEU	6.4
6	F	1	ALA	6.4
8	H	44	THR	6.4
6	S	94	HIS	6.2
10	W	58	LYS	6.0
7	G	3	ALA	5.8
11	X	6	ALA	5.8
8	U	8	ILE	5.7
7	T	3	ALA	5.7
6	S	2	SER	5.5
8	H	8	ILE	5.2
10	J	58	LYS	5.0
7	G	36	TRP	4.9
7	G	5	LYS	4.9
8	H	46	LYS	4.9
8	H	7	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
4	Q	51	LEU	4.9
10	W	1	PHE	4.8
7	G	1	ALA	4.8
7	G	8	HIS	4.7
9	I	25	PHE	4.6
8	H	45	ALA	4.6
5	E	5	HIS	4.3
7	G	84	LYS	4.2
11	X	7	PRO	4.2
7	T	2	SER	4.2
8	H	47	GLY	4.2
7	T	1	ALA	4.1
13	M	43	SER	4.1
6	S	1	ALA	4.1
9	V	2	THR	4.0
8	U	10	ASN	4.0
7	T	36[A]	TRP	3.9
6	F	95	GLN	3.9
6	S	95	GLN	3.9
7	G	9	GLY	3.9
8	H	48	GLY	3.8
13	Z	40	TYR	3.8
3	P	3	HIS	3.8
6	F	94	HIS	3.8
13	Z	42	LYS	3.8
9	I	29	LEU	3.7
13	Z	43	SER	3.7
7	G	2	SER	3.7
7	G	40	GLY	3.7
7	T	84	LYS	3.7
7	T	42	ARG	3.6
8	U	47	GLY	3.6
9	V	25	PHE	3.5
11	X	13	TYR	3.5
7	T	10	GLY	3.5
13	M	42	LYS	3.4
7	T	40	GLY	3.4
7	T	4	ALA	3.4
13	M	40	TYR	3.3
2	O	91	ASN	3.3
4	Q	147	LYS	3.2
8	U	46	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
8	U	45	ALA	3.1
13	Z	39	ASN	3.0
7	G	43	GLU	3.0
7	G	41	HIS	3.0
2	O	92	ASN	2.9
7	G	42	ARG	2.9
7	T	43	GLU	2.8
7	T	5	LYS	2.8
7	T	41	HIS	2.8
9	I	33	THR	2.8
7	G	6	GLY	2.8
13	Z	41	LYS	2.8
7	T	8	HIS	2.7
10	J	2	GLU	2.7
10	J	4	ARG	2.6
7	G	7	ASP	2.6
4	D	147	LYS	2.6
2	O	113	TYR	2.6
4	Q	39	ALA	2.5
7	G	4	ALA	2.5
8	U	9	LYS	2.5
9	V	34	PHE	2.5
4	Q	53	ILE	2.5
9	V	33	THR	2.4
9	I	30	GLY	2.4
13	M	39	ASN	2.4
10	W	48	TYR	2.4
7	G	37	LEU	2.3
10	W	2	GLU	2.3
5	R	108	LYS	2.3
6	S	93	PRO	2.3
6	S	3	GLY	2.3
9	I	21	ILE	2.3
8	U	44	THR	2.3
2	B	60	GLU	2.3
9	I	34	PHE	2.3
9	V	29	LEU	2.2
9	I	19	PHE	2.2
12	Y	47	LYS	2.2
9	V	26	MET	2.2
5	E	109	VAL	2.2
7	T	9	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
13	Z	35	TYR	2.1
7	T	33	LEU	2.1
11	X	34	THR	2.1
4	Q	46	ALA	2.1
7	G	39	SER	2.1
8	U	48	GLY	2.1
9	V	19	PHE	2.1
7	T	7	ASP	2.1
2	B	90	ILE	2.1
7	G	45	PRO	2.1
8	H	49	ASP	2.0
11	X	12	LYS	2.0
10	J	48	TYR	2.0
2	O	227	LEU	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	FME	A	1	10/11	0.97	0.09	-	31,38,64,86	0
9	SAC	I	1	9/10	0.82	0.29	-	63,91,107,108	0
9	SAC	V	1	9/10	0.67	0.53	-	108,123,136,136	0
7	TPO	G	11	11/12	0.49	0.23	-	68,82,133,143	0
2	FME	O	1	10/11	0.97	0.06	-	33,33,40,47	0
2	FME	B	1	10/11	0.96	0.08	-	20,26,38,51	0
1	FME	N	1	10/11	0.97	0.11	-	32,37,56,66	0
7	TPO	T	11	11/12	0.49	0.24	-	74,84,143,151	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
21	CHD	W	101	29/29	0.52	0.43	12.70	62,129,154,158	0
26	CDL	P	305	100/100	0.85	0.30	10.24	34,76,126,142	0
21	CHD	J	101	29/29	0.61	0.45	9.67	54,125,148,152	0
26	CDL	C	305	100/100	0.84	0.35	7.74	33,74,131,147	0
18	PGV	A	607	51/51	0.86	0.17	6.48	34,73,109,140	0
19	TGL	D	201	63/63	0.83	0.15	6.16	29,61,90,99	0
26	CDL	T	104	100/100	0.67	0.26	5.98	50,87,137,163	0
19	TGL	N	608	63/63	0.85	0.20	5.60	47,73,106,120	0
18	PGV	N	606	51/51	0.82	0.25	5.49	39,75,149,165	0
19	TGL	L	101	63/63	0.85	0.18	5.48	28,54,93,94	0
26	CDL	G	101	100/100	0.62	0.28	4.51	49,89,146,161	0
16	MG	N	604	1/1	0.98	0.13	4.20	24,24,24,24	0
19	TGL	N	609	63/63	0.79	0.20	4.02	40,61,94,100	0
23	DMU	C	301	33/33	0.77	0.21	3.60	33,123,149,150	0
21	CHD	P	306	29/29	0.79	0.31	3.38	51,89,103,106	0
19	TGL	Q	201	63/63	0.76	0.18	3.13	41,69,93,97	0
19	TGL	B	301	63/63	0.87	0.15	3.08	38,67,95,99	0
21	CHD	C	306	29/29	0.73	0.38	2.83	52,101,116,126	0
23	DMU	Z	101	33/33	0.80	0.19	2.67	38,44,61,64	0
18	PGV	C	309	51/51	0.85	0.23	2.65	46,78,152,155	0
23	DMU	P	302	33/33	0.75	0.16	2.37	38,103,146,150	0
18	PGV	P	301	51/51	0.79	0.23	2.27	50,79,135,157	0
23	DMU	M	101	33/33	0.89	0.12	1.71	34,37,52,59	0
22	PSC	B	304	52/52	0.82	0.21	1.57	39,93,160,161	0
25	PEK	T	102	53/53	0.77	0.25	1.50	41,91,153,157	0
25	PEK	T	103	53/53	0.76	0.22	1.49	38,73,125,130	0
18	PGV	C	304	51/51	0.98	0.07	1.25	21,26,67,77	0
22	PSC	R	201	52/52	0.84	0.21	1.16	35,80,159,164	0
16	MG	A	604	1/1	0.99	0.09	1.12	19,19,19,19	0
25	PEK	T	101	53/53	0.97	0.08	1.11	26,38,86,89	0
18	PGV	A	606	51/51	0.98	0.07	1.06	18,25,54,62	0
25	PEK	G	102	53/53	0.82	0.24	1.00	43,91,139,153	0
25	PEK	C	308	53/53	0.75	0.18	0.91	43,71,122,155	0
25	PEK	C	303	53/53	0.98	0.07	0.91	23,38,73,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
18	PGV	P	304	51/51	0.98	0.06	0.64	20,26,69,77	0
14	HEA	N	601	60/60	0.99	0.07	0.54	20,22,38,41	0
21	CHD	C	307	29/29	0.95	0.09	0.32	23,26,31,34	0
14	HEA	N	602	60/60	0.99	0.08	0.27	18,21,26,30	0
27	ZN	F	101	1/1	1.00	0.05	0.26	25,25,25,25	0
18	PGV	N	607	51/51	0.99	0.07	0.24	19,27,59,65	0
21	CHD	P	307	29/29	0.96	0.09	0.06	25,28,31,34	0
21	CHD	G	103	29/29	0.95	0.07	-0.17	22,24,27,31	0
21	CHD	B	303	29/29	0.95	0.07	-0.32	23,25,28,34	0
14	HEA	A	601	60/60	0.99	0.06	-0.48	16,18,31,34	0
14	HEA	A	602	60/60	0.99	0.06	-0.68	16,18,24,28	0
27	ZN	S	101	1/1	0.99	0.05	-0.81	25,25,25,25	0
20	CUA	B	302	2/2	1.00	0.07	-1.03	21,21,21,21	0
20	CUA	O	301	2/2	1.00	0.06	-1.77	26,26,26,26	0
17	NA	N	605	1/1	1.00	0.02	-1.95	30,30,30,30	0
17	NA	A	605	1/1	0.99	0.02	-2.98	24,24,24,24	0
24	UNX	C	302	1/1	0.45	0.81	-	38,38,38,38	1
24	UNX	P	303	1/1	0.42	0.91	-	34,34,34,34	1
15	CU	A	603	1/1	1.00	0.07	-	18,18,18,18	0
15	CU	N	603	1/1	1.00	0.07	-	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.