



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:58 am GMT

PDB ID : 3ABK  
Title : Bovine heart cytochrome c oxidase at the NO-bound fully reduced state (50K)  
Authors : Ohta, K.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.;  
Tsukihara, T.  
Deposited on : 2009-12-16  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

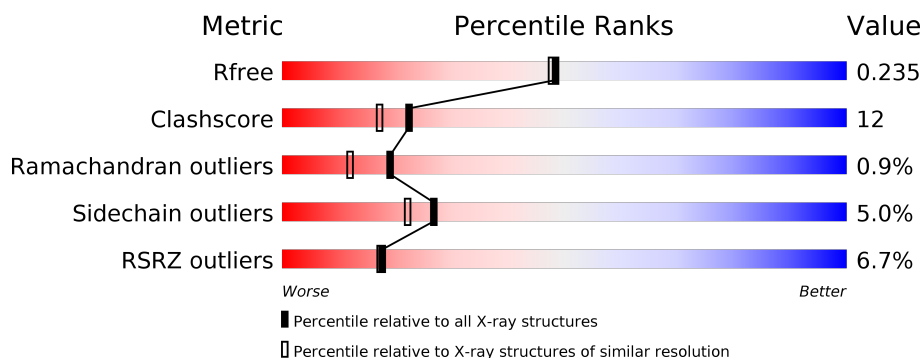
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
1	N	514	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
2	B	227	<div> <div></div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
2	O	227	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div>
3	C	261	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>•••</div> </div> </div>
3	P	261	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <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	515	X	-	-	-
14	HEA	A	516	X	-	-	-
14	HEA	N	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
19	PGV	U	1268	-	-	-	X
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1059	X	-	-	X
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	PEK	G	1263	-	-	-	X
25	PEK	T	263	-	-	-	X
26	CDL	G	269	-	-	X	-
26	CDL	P	1270	-	-	X	-
26	CDL	T	1269	-	-	X	-
27	DMU	C	272	X	-	-	-
27	DMU	M	526	X	-	-	-
27	DMU	P	272	X	-	-	X
27	DMU	Z	1526	X	-	-	-
9	SAC	V	1	-	-	-	X

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32382 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	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	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	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

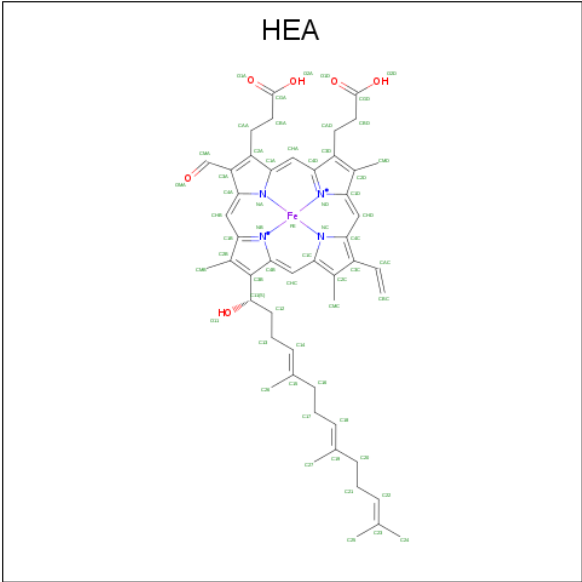
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

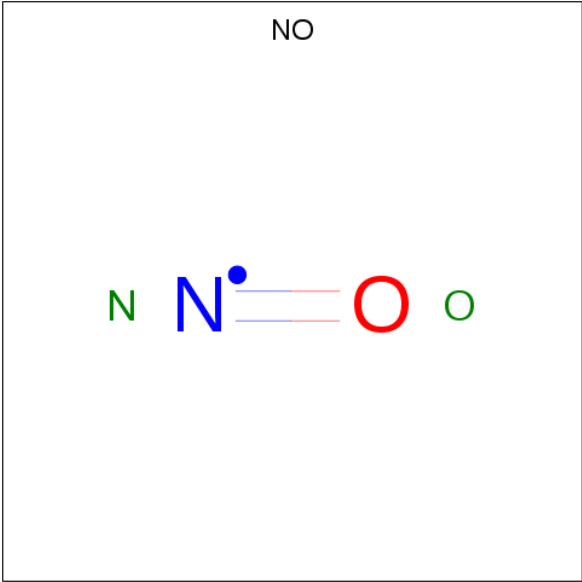
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- 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 NITRIC OXIDE (three-letter code: NO) (formula: NO).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total N O 2 1 1	0	0
15	N	1	Total N O 2 1 1	0	0

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

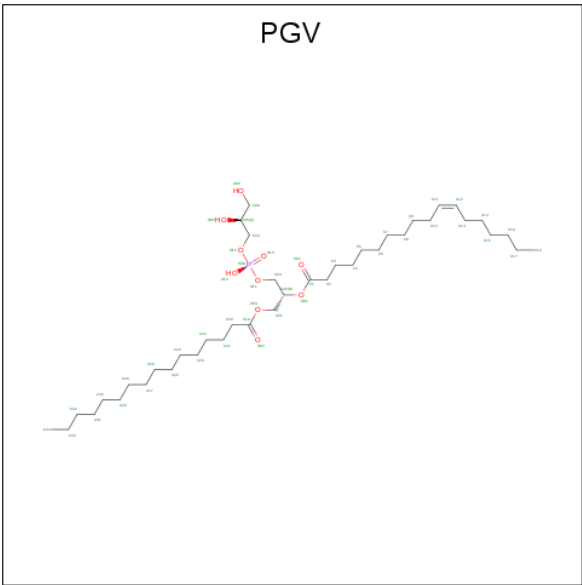
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

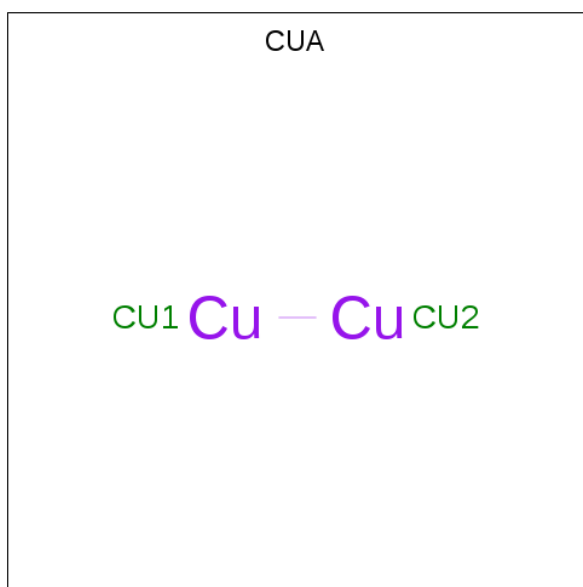
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 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).



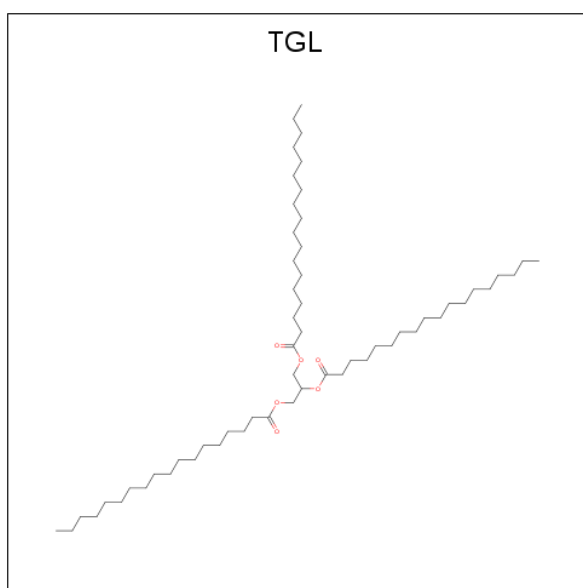
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

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



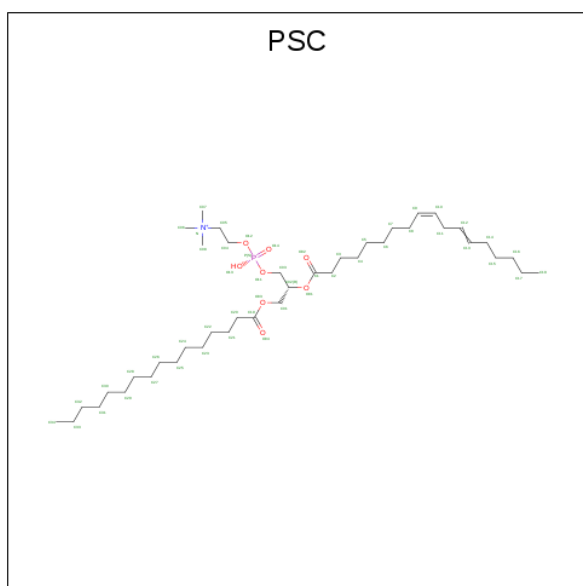
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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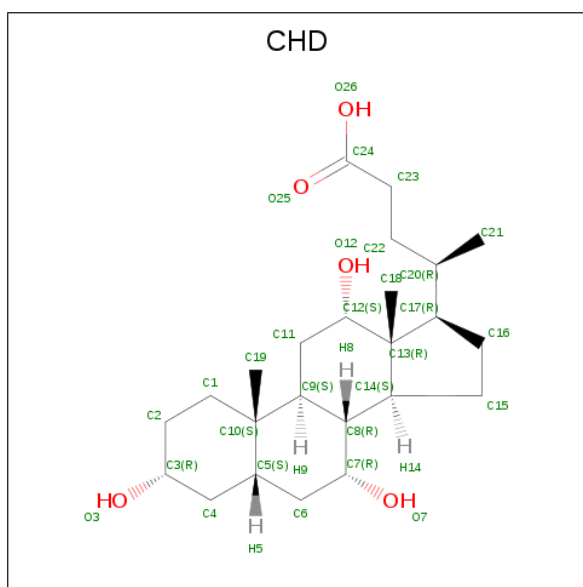
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- 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:  $C_{42}H_{81}NO_8P$ ).



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 CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).

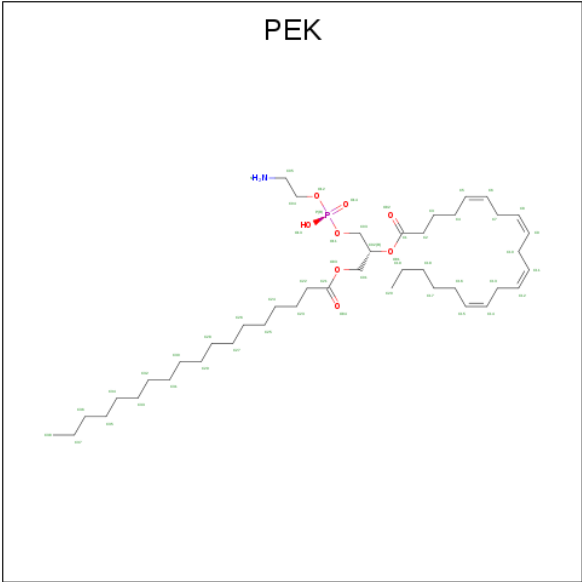


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	O	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

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

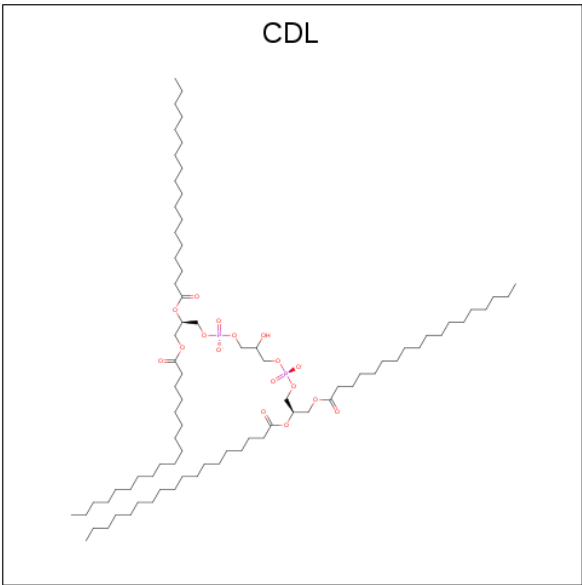
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- 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).



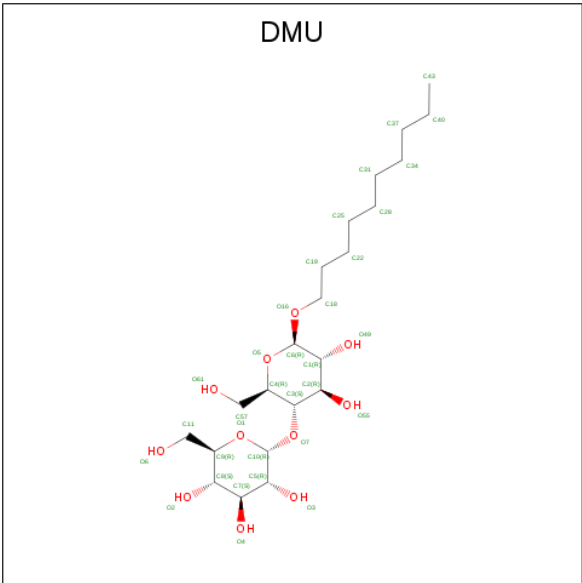
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- 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 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
27	C	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	217	Total O 217 217	0	0
29	B	127	Total O 127 127	0	0
29	C	93	Total O 93 93	0	0
29	D	86	Total O 86 86	0	0
29	E	52	Total O 52 52	0	0
29	F	72	Total O 72 72	0	0
29	G	42	Total O 42 42	0	0
29	H	46	Total O 46 46	0	0
29	I	31	Total O 31 31	0	0
29	J	28	Total O 28 28	0	0
29	K	27	Total O 27 27	0	0
29	L	16	Total O 16 16	0	0

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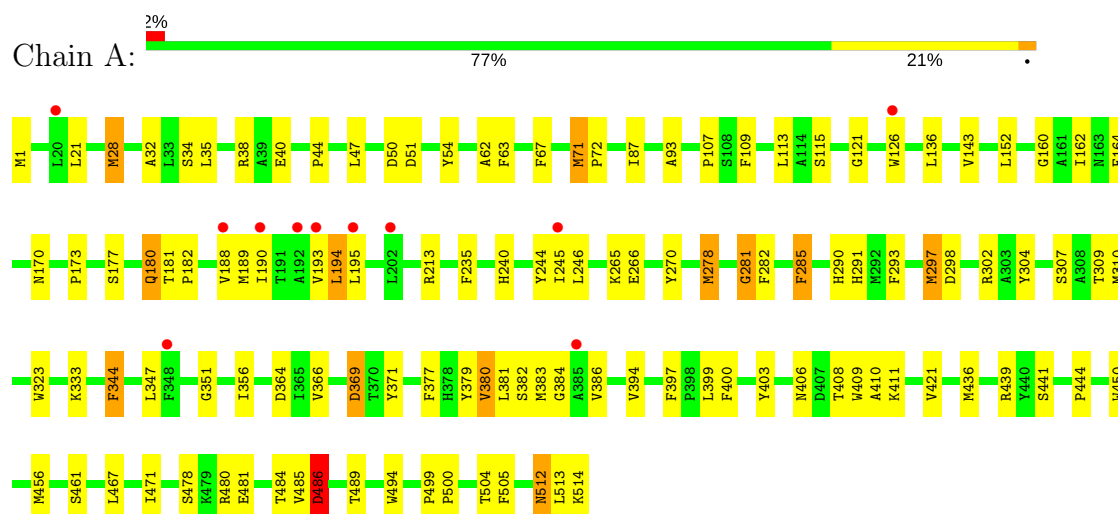
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	M	20	Total 20	O 20	0	0
29	N	207	Total 207	O 207	0	0
29	O	105	Total 105	O 105	0	0
29	P	96	Total 96	O 96	0	0
29	Q	57	Total 57	O 57	0	0
29	R	35	Total 35	O 35	0	0
29	S	63	Total 63	O 63	0	0
29	T	44	Total 44	O 44	0	0
29	U	43	Total 43	O 43	0	0
29	V	20	Total 20	O 20	0	0
29	W	17	Total 17	O 17	0	0
29	X	13	Total 13	O 13	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	11	Total 11	O 11	0	0

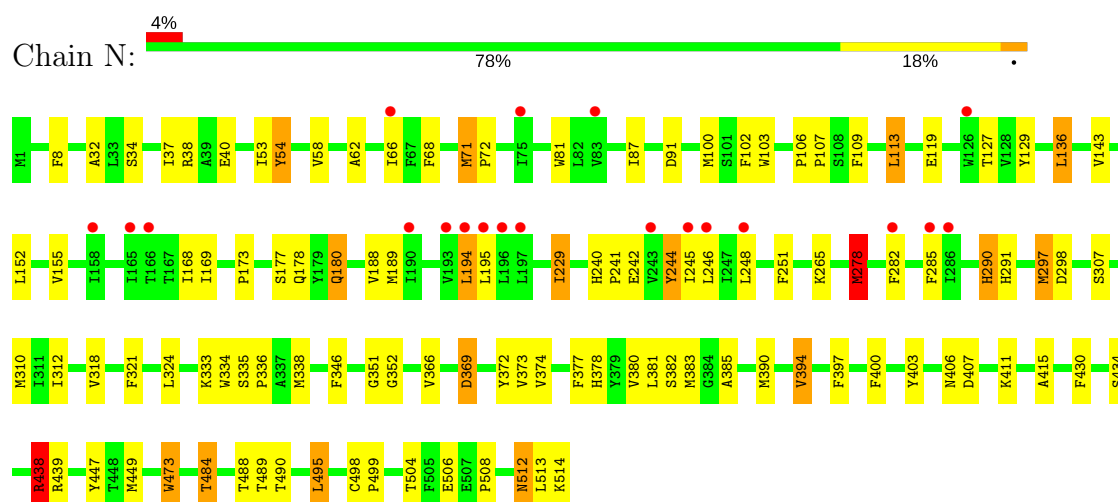
### 3 Residue-property plots

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

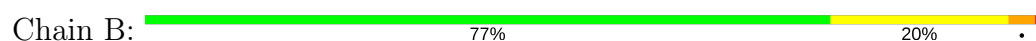
#### • Molecule 1: Cytochrome c oxidase subunit 1

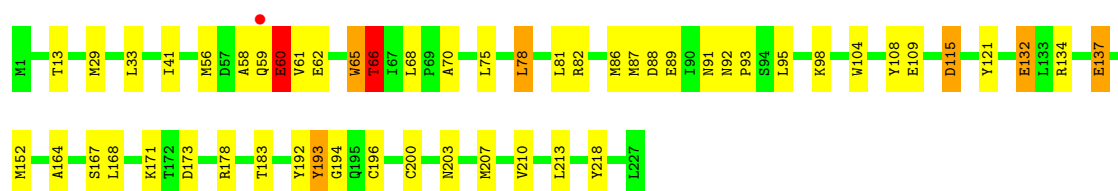


#### • Molecule 1: Cytochrome c oxidase subunit 1

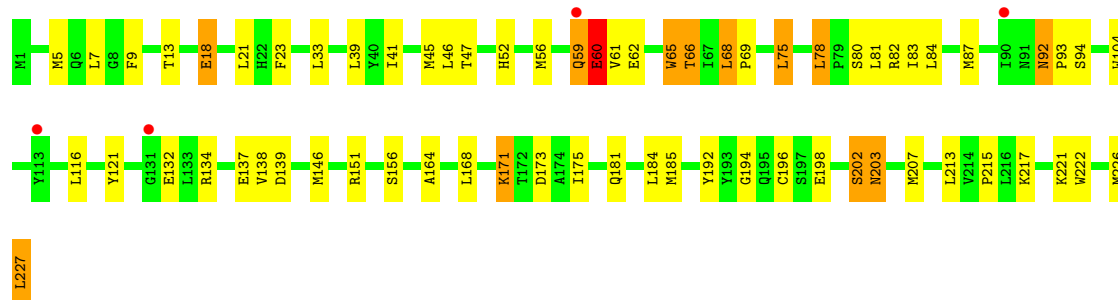


#### • Molecule 2: Cytochrome c oxidase subunit 2

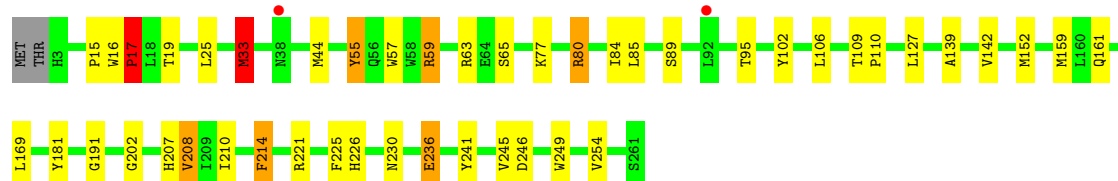
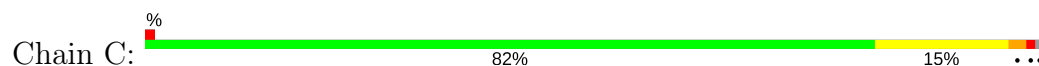




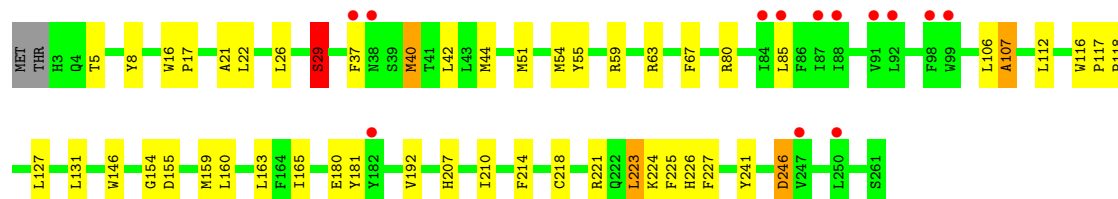
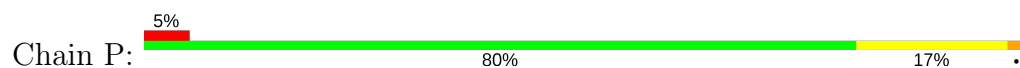
• Molecule 2: Cytochrome c oxidase subunit 2



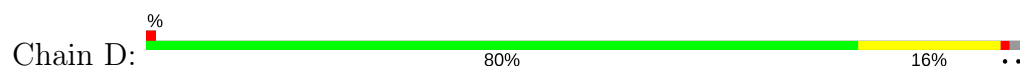
• Molecule 3: Cytochrome c oxidase subunit 3



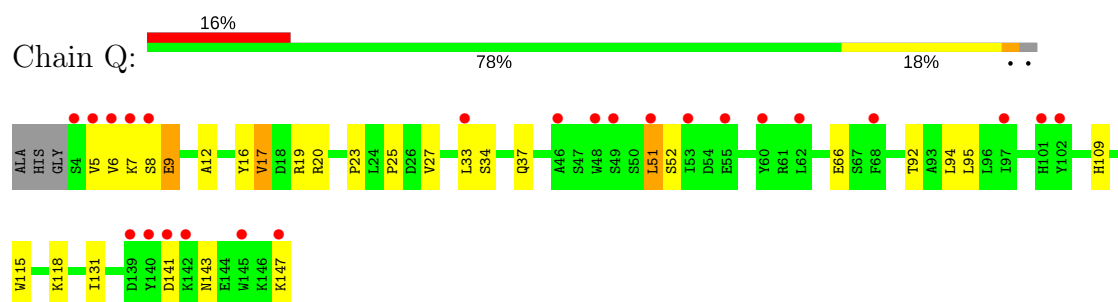
• Molecule 3: Cytochrome c oxidase subunit 3



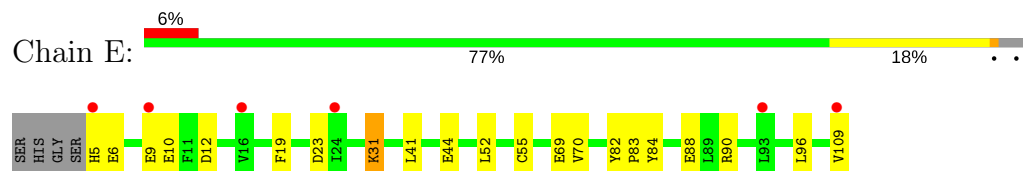
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



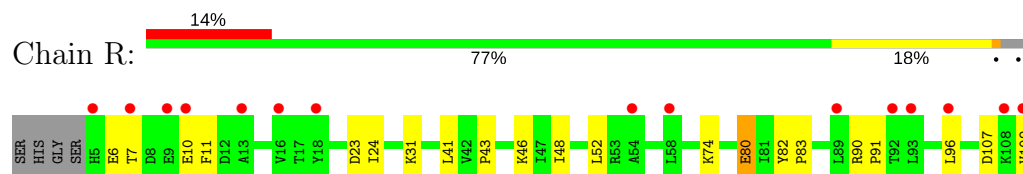
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



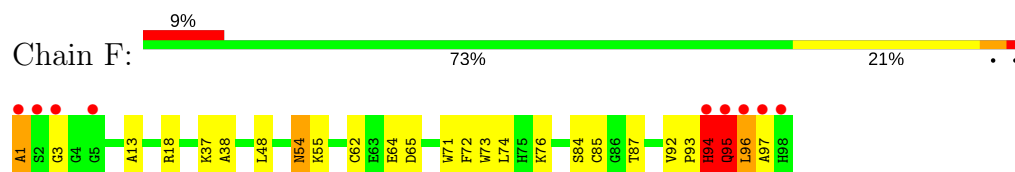
- Molecule 5: Cytochrome c oxidase subunit 5A



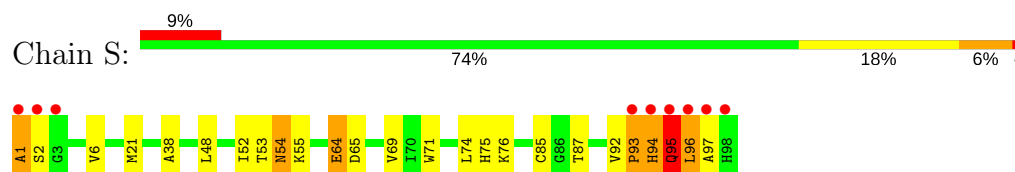
- Molecule 5: Cytochrome c oxidase subunit 5A



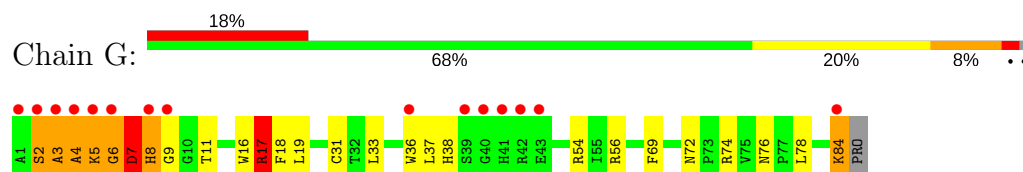
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

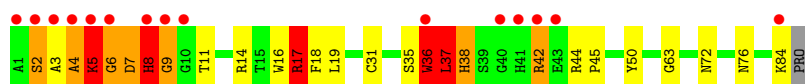


- Molecule 7: Cytochrome c oxidase subunit 6A2

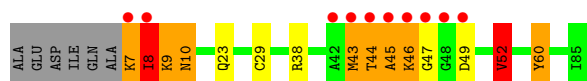
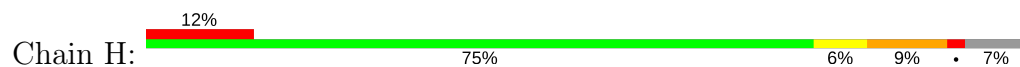


- Molecule 7: Cytochrome c oxidase subunit 6A2

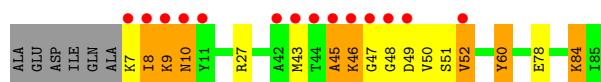
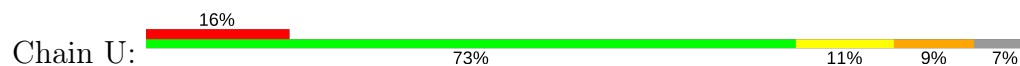




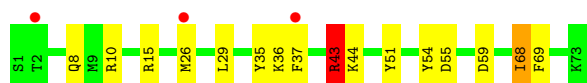
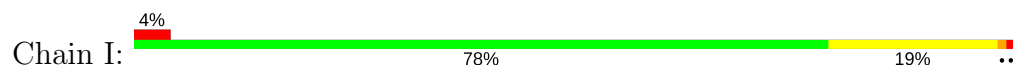
• Molecule 8: Cytochrome c oxidase subunit 6B1



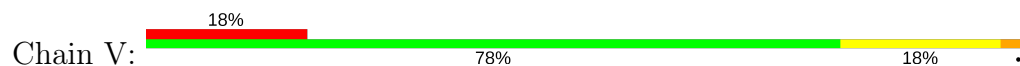
• Molecule 8: Cytochrome c oxidase subunit 6B1



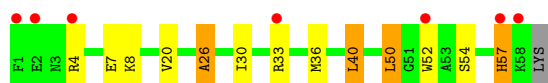
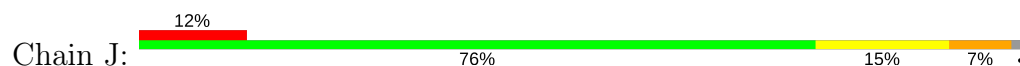
• Molecule 9: Cytochrome c oxidase subunit 6C



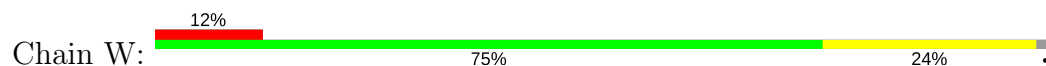
• Molecule 9: Cytochrome c oxidase subunit 6C



• Molecule 10: Cytochrome c oxidase polypeptide 7A1



• Molecule 10: Cytochrome c oxidase polypeptide 7A1

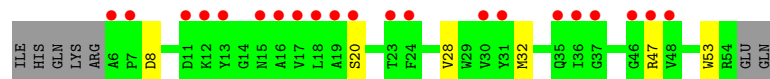
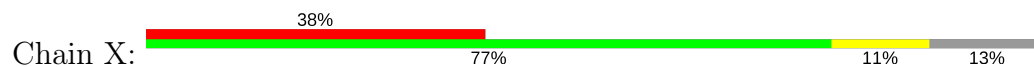


• Molecule 11: Cytochrome c oxidase subunit 7B





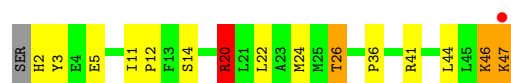
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



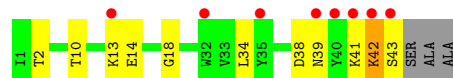
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.25Å 207.94Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 75.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.00) 98.7 (75.57-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.183 , 0.219 0.201 , 0.235	Depositor DCC
$R_{free}$ test set	22073 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 69.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: PEK, ZN, CHD, HEA, SAC, CDL, PSC, NO, 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	1.64	40/4189 (1.0%)	1.27	19/5722 (0.3%)
1	N	1.46	26/4189 (0.6%)	1.20	22/5722 (0.4%)
2	B	1.54	15/1860 (0.8%)	1.32	11/2534 (0.4%)
2	O	1.32	7/1860 (0.4%)	1.14	9/2534 (0.4%)
3	C	1.43	15/2197 (0.7%)	1.13	10/3005 (0.3%)
3	P	1.36	9/2197 (0.4%)	1.16	11/3005 (0.4%)
4	D	1.33	2/1229 (0.2%)	1.11	5/1658 (0.3%)
4	Q	1.24	5/1229 (0.4%)	1.04	5/1658 (0.3%)
5	E	1.32	4/871 (0.5%)	0.98	0/1182
5	R	1.15	0/871	0.98	1/1182 (0.1%)
6	F	1.44	6/765 (0.8%)	1.23	1/1038 (0.1%)
6	S	1.33	3/765 (0.4%)	1.17	1/1038 (0.1%)
7	G	1.38	3/690 (0.4%)	1.28	7/937 (0.7%)
7	T	1.36	3/690 (0.4%)	1.21	6/937 (0.6%)
8	H	1.34	0/682	1.12	2/921 (0.2%)
8	U	1.16	0/682	0.97	0/921
9	I	1.32	3/605 (0.5%)	1.20	5/802 (0.6%)
9	V	1.22	1/605 (0.2%)	0.97	1/802 (0.1%)
10	J	1.26	2/471 (0.4%)	1.09	2/636 (0.3%)
10	W	1.25	0/471	1.10	2/636 (0.3%)
11	K	1.36	0/398	1.19	4/546 (0.7%)
11	X	1.11	0/398	0.95	1/546 (0.2%)
12	L	1.42	2/393 (0.5%)	1.09	0/526
12	Y	1.35	1/393 (0.3%)	1.00	1/526 (0.2%)
13	M	1.41	1/345 (0.3%)	1.23	2/470 (0.4%)
13	Z	1.17	0/345	0.99	0/470
All	All	1.41	148/29390 (0.5%)	1.16	128/39954 (0.3%)

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
5	E	0	1
6	F	0	1
6	S	0	2
12	Y	0	1
All	All	0	5

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	10.56	1.69	1.50
7	T	36	TRP	CB-CG	10.45	1.69	1.50
1	A	380[A]	VAL	CB-CG1	-9.14	1.33	1.52
1	A	380[B]	VAL	CB-CG1	-9.14	1.33	1.52
3	P	180	GLU	CD-OE1	8.86	1.35	1.25
2	O	198	GLU	C-O	8.77	1.40	1.23
2	B	59	GLN	CG-CD	8.68	1.71	1.51
1	A	371	TYR	CD1-CE1	8.39	1.51	1.39
1	N	54	TYR	CD1-CE1	8.15	1.51	1.39
1	A	394	VAL	CB-CG2	-8.09	1.35	1.52
1	A	371	TYR	CD2-CE2	8.00	1.51	1.39
1	A	189	MET	CG-SD	-7.71	1.61	1.81
1	A	285	PHE	CE1-CZ	7.71	1.51	1.37
3	C	57	TRP	CB-CG	7.58	1.63	1.50
2	B	200	CYS	CB-SG	7.56	1.95	1.82
3	C	181	TYR	CD1-CE1	7.56	1.50	1.39
2	B	132	GLU	CD-OE2	7.54	1.33	1.25
2	B	65	TRP	CB-CG	-7.53	1.36	1.50
3	P	218	CYS	CB-SG	7.53	1.95	1.82
3	C	142	VAL	CB-CG2	7.36	1.68	1.52
1	N	188	VAL	N-CA	7.05	1.60	1.46
3	C	102	TYR	CE1-CZ	7.03	1.47	1.38
12	L	16	GLU	CG-CD	7.03	1.62	1.51
1	A	512	ASN	CB-CG	-6.93	1.35	1.51
5	E	9	GLU	CG-CD	6.88	1.62	1.51
1	N	54	TYR	CD2-CE2	6.87	1.49	1.39
1	N	403	TYR	CD1-CE1	6.80	1.49	1.39
2	B	60	GLU	CG-CD	6.71	1.62	1.51
1	N	394	VAL	CB-CG2	-6.70	1.38	1.52
6	F	72	PHE	CE2-CZ	6.63	1.50	1.37
1	A	189	MET	CB-CG	6.62	1.72	1.51
1	N	434	SER	CB-OG	6.60	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	225	PHE	CE2-CZ	6.58	1.49	1.37
1	A	436	MET	N-CA	6.54	1.59	1.46
1	N	473	TRP	CE3-CZ3	6.51	1.49	1.38
1	A	113	LEU	CB-CG	6.48	1.71	1.52
2	B	115	ASP	CB-CG	6.45	1.65	1.51
3	C	57	TRP	CD1-NE1	6.43	1.48	1.38
2	B	218	TYR	CD1-CE1	6.41	1.49	1.39
1	N	102	PHE	CD2-CE2	-6.39	1.26	1.39
1	A	323	TRP	CB-CG	6.34	1.61	1.50
3	P	181	TYR	CD1-CE1	6.33	1.48	1.39
2	O	65	TRP	CB-CG	-6.33	1.38	1.50
1	A	439	ARG	C-O	6.30	1.35	1.23
2	B	108	TYR	CD2-CE2	6.22	1.48	1.39
2	B	59	GLN	CB-CG	6.17	1.69	1.52
2	O	192	TYR	CD1-CE1	6.16	1.48	1.39
7	G	17	ARG	CD-NE	-6.16	1.35	1.46
2	B	60	GLU	CB-CG	6.13	1.63	1.52
4	Q	9	GLU	CB-CG	6.12	1.63	1.52
1	A	297	MET	CB-CG	6.10	1.70	1.51
3	C	208	VAL	CB-CG2	6.10	1.65	1.52
3	C	254	VAL	CB-CG2	6.09	1.65	1.52
13	M	32	TRP	CG-CD1	6.03	1.45	1.36
3	C	55	TYR	CD2-CE2	6.02	1.48	1.39
10	J	20	VAL	CB-CG1	6.02	1.65	1.52
1	N	397	PHE	CE2-CZ	5.99	1.48	1.37
2	B	167	SER	CB-OG	-5.97	1.34	1.42
1	A	270	TYR	CB-CG	5.94	1.60	1.51
4	Q	17	VAL	CB-CG1	-5.94	1.40	1.52
1	A	397	PHE	CD2-CE2	5.84	1.50	1.39
9	I	69	PHE	CG-CD2	5.84	1.47	1.38
1	N	438	ARG	CB-CG	-5.83	1.36	1.52
1	A	93	ALA	CA-CB	5.80	1.64	1.52
1	N	372	TYR	CB-CG	5.79	1.60	1.51
3	C	214	PHE	CE2-CZ	5.78	1.48	1.37
1	N	297	MET	SD-CE	5.75	2.10	1.77
1	A	164	PHE	CE1-CZ	5.73	1.48	1.37
2	O	221	LYS	CD-CE	5.72	1.65	1.51
6	F	1	ALA	C-O	5.71	1.34	1.23
1	A	293	PHE	CE2-CZ	5.67	1.48	1.37
1	N	113	LEU	CB-CG	5.67	1.69	1.52
6	F	3	GLY	C-O	5.66	1.32	1.23
1	N	244	TYR	CD2-CE2	-5.66	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	VAL	CB-CG1	5.65	1.64	1.52
7	T	17	ARG	CD-NE	-5.62	1.36	1.46
3	P	16	TRP	CE3-CZ3	5.61	1.48	1.38
1	A	467	LEU	N-CA	-5.61	1.35	1.46
4	Q	115	TRP	CE3-CZ3	5.58	1.48	1.38
10	J	26	ALA	CA-CB	5.58	1.64	1.52
2	O	18	GLU	CB-CG	-5.58	1.41	1.52
5	E	84	TYR	CG-CD1	5.57	1.46	1.39
6	F	72	PHE	CE1-CZ	5.56	1.48	1.37
1	N	168	ILE	CB-CG2	5.55	1.70	1.52
4	Q	9	GLU	CG-CD	5.55	1.60	1.51
1	N	415	ALA	CA-CB	5.54	1.64	1.52
2	O	156	SER	CB-OG	5.54	1.49	1.42
3	P	246	ASP	CG-OD2	5.54	1.38	1.25
1	A	266	GLU	CB-CG	5.53	1.62	1.52
1	A	411	LYS	CE-NZ	5.53	1.62	1.49
1	N	189	MET	CB-CG	5.52	1.69	1.51
1	A	213	ARG	CG-CD	5.50	1.65	1.51
4	D	104	TYR	CD1-CE1	5.50	1.47	1.39
3	P	8	TYR	CD1-CE1	-5.46	1.31	1.39
1	N	372	TYR	CD2-CE2	5.46	1.47	1.39
1	N	8	PHE	CD2-CE2	5.45	1.50	1.39
1	A	281	GLY	C-O	5.43	1.32	1.23
3	C	249	TRP	CB-CG	5.42	1.60	1.50
12	L	5	GLU	CD-OE2	-5.42	1.19	1.25
12	Y	20	ARG	CG-CD	5.42	1.65	1.51
6	F	54	ASN	CB-CG	5.42	1.63	1.51
2	B	193	TYR	CD1-CE1	5.42	1.47	1.39
3	C	17	PRO	CG-CD	5.41	1.68	1.50
4	D	64	PHE	CE1-CZ	5.40	1.47	1.37
1	A	244	TYR	CD1-CE1	5.40	1.47	1.39
6	F	73	TRP	CE3-CZ3	5.40	1.47	1.38
5	E	88	GLU	CG-CD	5.37	1.60	1.51
1	A	379	TYR	CE2-CZ	5.36	1.45	1.38
2	B	137	GLU	C-O	5.35	1.33	1.23
7	G	5	LYS	CB-CG	5.33	1.67	1.52
3	C	89	SER	CB-OG	5.32	1.49	1.42
3	C	139	ALA	CA-CB	5.28	1.63	1.52
1	A	113	LEU	CG-CD1	5.27	1.71	1.51
9	I	69	PHE	CE2-CZ	5.27	1.47	1.37
1	A	126	TRP	CG-CD1	5.26	1.44	1.36
3	P	107	ALA	CA-CB	5.24	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	6	VAL	CA-CB	5.23	1.65	1.54
1	N	244	TYR	CE2-CZ	5.22	1.45	1.38
1	A	410	ALA	CA-CB	5.22	1.63	1.52
1	A	160	GLY	N-CA	5.22	1.53	1.46
1	A	304	TYR	CD2-CE2	5.22	1.47	1.39
1	A	505	PHE	CG-CD2	5.20	1.46	1.38
1	N	373	VAL	CB-CG2	5.20	1.63	1.52
2	B	121	TYR	CE1-CZ	-5.19	1.31	1.38
6	S	1	ALA	C-O	5.19	1.33	1.23
1	N	81	TRP	CD1-NE1	5.17	1.46	1.38
1	N	506	GLU	CB-CG	-5.16	1.42	1.52
6	S	2	SER	N-CA	5.14	1.56	1.46
1	A	193	VAL	CA-CB	5.13	1.65	1.54
1	A	63	PHE	CD1-CE1	5.12	1.49	1.39
1	N	447	TYR	CD2-CE2	5.12	1.47	1.39
1	A	67	PHE	CE2-CZ	5.12	1.47	1.37
1	A	494	TRP	CZ3-CH2	5.12	1.48	1.40
3	C	236	GLU	CG-CD	5.11	1.59	1.51
1	A	344	PHE	CD2-CE2	5.10	1.49	1.39
1	A	162	ILE	CA-CB	5.10	1.66	1.54
1	N	143	VAL	CB-CG2	5.10	1.63	1.52
7	T	50	TYR	CE1-CZ	5.09	1.45	1.38
5	E	19	PHE	CD1-CE1	5.07	1.49	1.39
9	V	51	TYR	CD1-CE1	5.07	1.47	1.39
3	P	181	TYR	CD2-CE2	5.07	1.47	1.39
1	A	235	PHE	CG-CD1	5.05	1.46	1.38
9	I	15	ARG	CG-CD	5.04	1.64	1.51
3	P	227	PHE	CE2-CZ	5.04	1.47	1.37
6	S	69	VAL	CA-CB	-5.04	1.44	1.54
2	B	192	TYR	CG-CD1	5.03	1.45	1.39
2	O	171	LYS	CB-CG	5.01	1.66	1.52
1	N	447	TYR	CD1-CE1	5.00	1.46	1.39

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	17	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	A	71	MET	CG-SD-CE	-14.02	77.77	100.20
7	G	17	ARG	NE-CZ-NH1	12.88	126.74	120.30
3	P	246	ASP	CB-CG-OD1	-12.27	107.26	118.30
1	N	278	MET	CG-SD-CE	-11.92	81.12	100.20
1	N	71	MET	CG-SD-CE	-11.66	81.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	221	ARG	NE-CZ-NH1	-10.62	114.99	120.30
1	A	136	LEU	CB-CG-CD1	-10.11	93.81	111.00
1	N	310	MET	CG-SD-CE	-9.35	85.24	100.20
9	I	43	ARG	NE-CZ-NH2	9.15	124.88	120.30
7	T	17	ARG	NE-CZ-NH2	-9.12	115.74	120.30
7	T	17	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	N	298	ASP	CB-CG-OD1	-8.56	110.59	118.30
4	D	20	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	N	298	ASP	CB-CG-OD2	8.40	125.86	118.30
8	H	38	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	A	298	ASP	CB-CG-OD2	8.29	125.76	118.30
1	N	113	LEU	CB-CG-CD2	8.07	124.71	111.00
2	B	173	ASP	CB-CG-OD1	7.96	125.47	118.30
2	B	65	TRP	CB-CA-C	7.75	125.90	110.40
4	D	51	LEU	CA-CB-CG	7.67	132.94	115.30
2	B	178	ARG	NE-CZ-NH1	-7.64	116.48	120.30
4	Q	20	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	278	MET	CG-SD-CE	-7.51	88.19	100.20
9	I	68	ILE	CG1-CB-CG2	7.30	127.45	111.40
4	Q	17	VAL	CB-CA-C	-7.20	97.72	111.40
1	A	512	ASN	CB-CA-C	-7.16	96.09	110.40
4	D	19	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	486	ASP	CB-CG-OD2	-7.04	111.97	118.30
3	P	29	SER	CB-CA-C	-6.96	96.88	110.10
2	B	152	MET	CG-SD-CE	6.95	111.31	100.20
13	M	34	LEU	CB-CG-CD1	6.86	122.66	111.00
1	N	136	LEU	CA-CB-CG	6.83	131.01	115.30
1	A	302	ARG	NE-CZ-NH2	-6.81	116.89	120.30
3	P	80	ARG	CG-CD-NE	-6.79	97.55	111.80
1	A	366	VAL	CG1-CB-CG2	-6.78	100.06	110.90
1	A	189	MET	CG-SD-CE	-6.77	89.37	100.20
1	N	438	ARG	NE-CZ-NH1	-6.76	116.92	120.30
8	H	52	VAL	CB-CA-C	-6.75	98.57	111.40
1	A	369	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	439	ARG	NE-CZ-NH1	-6.72	116.94	120.30
2	O	139	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	456	MET	CG-SD-CE	-6.65	89.56	100.20
10	W	44	LEU	CB-CG-CD1	-6.60	99.78	111.00
11	K	47	ARG	NE-CZ-NH1	-6.59	117.01	120.30
6	S	21	MET	CG-SD-CE	6.57	110.72	100.20
1	N	136	LEU	CB-CG-CD2	-6.50	99.95	111.00
4	Q	20	ARG	NE-CZ-NH2	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	91	ASP	CB-CG-OD1	6.40	124.06	118.30
2	B	134	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	N	244	TYR	CG-CD2-CE2	6.29	126.33	121.30
1	A	35	LEU	CB-CG-CD1	-6.26	100.35	111.00
3	C	152	MET	CG-SD-CE	6.24	110.18	100.20
1	A	113	LEU	CB-CG-CD2	6.24	121.60	111.00
2	O	184	LEU	CA-CB-CG	6.22	129.60	115.30
4	D	20	ARG	NE-CZ-NH1	6.20	123.40	120.30
4	Q	51	LEU	CA-CB-CG	6.18	129.52	115.30
9	I	55	ASP	CB-CG-OD1	6.18	123.86	118.30
2	O	185	MET	CG-SD-CE	6.17	110.08	100.20
2	B	82	ARG	CG-CD-NE	-6.16	98.87	111.80
11	K	54	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	B	95	LEU	CB-CG-CD1	6.13	121.42	111.00
1	N	244	TYR	CZ-CE2-CD2	-6.11	114.30	119.80
1	A	188	VAL	CG1-CB-CG2	-6.03	101.26	110.90
3	P	163	LEU	CB-CG-CD2	-6.02	100.76	111.00
2	B	88	ASP	CB-CG-OD2	6.02	123.72	118.30
3	P	221	ARG	NE-CZ-NH2	6.01	123.31	120.30
7	G	78	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	A	194	LEU	CB-CG-CD1	5.97	121.16	111.00
1	N	189	MET	CA-CB-CG	-5.95	103.18	113.30
3	C	59	ARG	NE-CZ-NH1	-5.95	117.33	120.30
10	J	40	LEU	CB-CG-CD2	5.94	121.10	111.00
3	P	180	GLU	OE1-CD-OE2	5.89	130.36	123.30
2	O	173	ASP	CB-CG-OD1	5.88	123.59	118.30
6	F	95	GLN	N-CA-C	5.87	126.85	111.00
1	N	438	ARG	CG-CD-NE	-5.81	99.61	111.80
1	A	189	MET	CA-CB-CG	-5.80	103.43	113.30
3	C	80	ARG	CG-CD-NE	-5.76	99.71	111.80
1	N	38	ARG	NE-CZ-NH1	5.73	123.17	120.30
11	X	32	MET	CG-SD-CE	5.68	109.30	100.20
7	T	44	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	G	56	ARG	NE-CZ-NH2	-5.65	117.47	120.30
13	M	27	LEU	CB-CG-CD1	-5.63	101.44	111.00
2	O	202	SER	CB-CA-C	-5.62	99.42	110.10
3	P	192	VAL	CG1-CB-CG2	5.62	119.89	110.90
7	G	19	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	N	369	ASP	CB-CG-OD2	5.62	123.36	118.30
1	N	438	ARG	CB-CA-C	-5.61	99.19	110.40
7	T	14	ARG	NE-CZ-NH1	-5.60	117.50	120.30
9	I	15	ARG	NE-CZ-NH2	5.59	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	43	ARG	NE-CZ-NH1	-5.59	117.50	120.30
12	Y	41	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	N	366	VAL	CG1-CB-CG2	-5.49	102.11	110.90
3	C	221	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	28	MET	CG-SD-CE	5.47	108.96	100.20
2	O	134	ARG	NE-CZ-NH1	-5.47	117.56	120.30
2	O	92	ASN	CB-CA-C	5.47	121.34	110.40
10	J	57	HIS	CB-CA-C	5.46	121.31	110.40
2	B	87	MET	CA-CB-CG	5.46	122.57	113.30
7	T	17	ARG	CB-CG-CD	-5.43	97.47	111.60
1	N	438	ARG	N-CA-CB	-5.39	100.89	110.60
4	D	137	LYS	CD-CE-NZ	-5.35	99.40	111.70
2	O	75	LEU	CB-CG-CD1	5.34	120.07	111.00
1	N	113	LEU	CB-CG-CD1	5.33	120.06	111.00
3	P	155	ASP	CB-CG-OD1	5.33	123.09	118.30
3	C	33	MET	CG-SD-CE	5.32	108.72	100.20
3	C	169	LEU	CB-CG-CD2	-5.31	101.97	111.00
2	O	82	ARG	NE-CZ-NH2	-5.28	117.66	120.30
7	G	7	ASP	N-CA-C	5.27	125.24	111.00
3	P	223	LEU	CB-CG-CD1	-5.22	102.12	111.00
2	B	66	THR	OG1-CB-CG2	5.22	122.01	110.00
4	Q	19	ARG	NE-CZ-NH1	-5.22	117.69	120.30
5	R	96	LEU	CA-CB-CG	5.21	127.29	115.30
3	C	33	MET	CB-CG-SD	5.18	127.93	112.40
3	C	44	MET	CG-SD-CE	5.18	108.48	100.20
7	G	17	ARG	CB-CG-CD	-5.17	98.16	111.60
1	A	152	LEU	CA-CB-CG	5.13	127.11	115.30
3	C	102	TYR	CB-CG-CD2	-5.12	117.92	121.00
11	K	39	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	N	229	ILE	CG1-CB-CG2	-5.12	100.13	111.40
7	T	19	LEU	CB-CG-CD2	-5.12	102.30	111.00
2	B	213	LEU	CB-CG-CD1	-5.10	102.32	111.00
3	C	85	LEU	CA-CB-CG	-5.10	103.56	115.30
3	P	40	MET	CB-CG-SD	-5.10	97.10	112.40
9	V	64	ARG	NE-CZ-NH1	5.09	122.85	120.30
11	K	47	ARG	CG-CD-NE	-5.09	101.12	111.80
1	N	194	LEU	CB-CG-CD1	5.07	119.61	111.00
10	W	44	LEU	CB-CG-CD2	5.02	119.54	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	5	HIS	Peptide
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide
12	Y	46	LYS	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	4060	0	4037	74	0
1	N	4060	0	4037	86	0
2	B	1824	0	1833	25	0
2	O	1824	0	1833	50	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	35	0
4	D	1195	0	1183	19	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	10	0
5	R	852	0	845	19	0
6	F	748	0	728	22	0
6	S	748	0	728	40	0
7	G	675	0	643	45	0
7	T	675	0	643	43	0
8	H	662	0	623	19	0
8	U	662	0	623	20	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	13	0
10	W	460	0	459	12	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	16	0
12	Y	380	0	380	20	0
13	M	335	0	352	13	0
13	Z	335	0	352	6	0
14	A	120	0	108	16	0
14	N	120	0	108	9	0
15	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	2	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	1	0	0	0	0
18	N	1	0	0	0	0
19	A	102	0	152	16	0
19	C	102	0	152	10	0
19	N	102	0	152	7	0
19	P	51	0	76	3	0
19	U	51	0	76	4	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	4	0
21	D	63	0	110	10	0
21	L	63	0	110	15	0
21	N	63	0	110	14	0
21	O	63	0	110	5	0
21	Y	63	0	110	20	0
22	B	52	0	80	20	0
22	R	52	0	80	20	0
23	B	29	0	37	4	0
23	C	58	0	71	4	0
23	J	29	0	36	8	0
23	O	29	0	37	3	0
23	P	58	0	72	5	0
23	W	29	0	35	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	22	0
25	G	53	0	77	19	0
25	P	53	0	77	6	0
25	T	106	0	154	34	0
26	C	100	0	156	20	0
26	G	100	0	156	33	0
26	P	100	0	156	27	0
26	T	100	0	156	30	0
27	C	33	0	39	4	0
27	M	33	0	39	0	0
27	P	33	0	38	1	0
27	Z	33	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	217	0	0	5	0
29	B	127	0	0	3	0
29	C	93	0	0	4	0
29	D	86	0	0	6	0
29	E	52	0	0	0	0
29	F	72	0	0	3	0
29	G	42	0	0	7	0
29	H	46	0	0	1	0
29	I	31	0	0	3	0
29	J	28	0	0	4	0
29	K	27	0	0	2	0
29	L	16	0	0	1	0
29	M	20	0	0	0	0
29	N	207	0	0	6	0
29	O	105	0	0	2	0
29	P	96	0	0	3	0
29	Q	57	0	0	4	0
29	R	35	0	0	1	0
29	S	63	0	0	5	0
29	T	44	0	0	5	0
29	U	43	0	0	5	0
29	V	20	0	0	0	0
29	W	17	0	0	2	0
29	X	13	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	1	0
All	All	32382	0	31350	777	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 12.

All (777) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:1265:PEK:H383	26:T:1269:CDL:C27	1.34	1.51
1:N:297:MET:CE	1:N:297:MET:SD	2.10	1.40
25:T:1265:PEK:C38	26:T:1269:CDL:H273	1.51	1.36
10:W:2:GLU:HB2	10:W:4:ARG:NH1	1.50	1.26
25:T:1265:PEK:C38	26:T:1269:CDL:C27	2.12	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:HD2	25:G:1263:PEK:C37	1.73	1.18
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.24	1.16
19:U:1268:PGV:H032	29:U:4495:HOH:O	1.43	1.14
25:C:264:PEK:H162	25:C:264:PEK:H101	1.17	1.14
7:G:5:LYS:CD	25:G:1263:PEK:H371	1.78	1.13
26:C:270:CDL:HB22	10:J:8:LYS:NZ	1.62	1.13
29:B:2562:HOH:O	21:D:523:TGL:HC61	1.50	1.11
26:C:270:CDL:HB22	10:J:8:LYS:HZ2	1.09	1.10
7:G:84:LYS:HD2	7:G:84:LYS:H	1.03	1.10
12:L:20:ARG:NH2	21:L:522:TGL:HC32	1.64	1.10
25:T:1265:PEK:H383	26:T:1269:CDL:H271	1.23	1.10
26:G:269:CDL:H561	26:G:269:CDL:H762	1.33	1.09
8:H:52:VAL:HG12	8:U:46:LYS:HB2	1.17	1.09
21:N:1523:TGL:HC21	21:N:1523:TGL:HG11	1.31	1.08
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.26	1.06
26:G:269:CDL:H222	26:G:269:CDL:H522	1.39	1.04
1:N:513:LEU:O	1:N:514:LYS:HB2	1.55	1.04
7:G:5:LYS:CG	25:G:1263:PEK:H371	1.88	1.03
6:S:94:HIS:CD2	6:S:95:GLN:N	2.26	1.03
26:C:270:CDL:H212	26:C:270:CDL:H631	1.05	1.02
1:A:513:LEU:O	1:A:514:LYS:HB2	1.60	1.02
8:U:9:LYS:HG3	8:U:10:ASN:H	1.21	1.01
2:O:59:GLN:O	2:O:59:GLN:HG3	1.59	0.98
6:S:94:HIS:CD2	6:S:95:GLN:H	1.80	0.98
22:R:1229:PSC:C34	22:R:1229:PSC:H142	1.94	0.98
19:N:1524:PGV:H012	19:N:1524:PGV:H221	1.45	0.97
7:G:84:LYS:N	7:G:84:LYS:HD2	1.78	0.95
19:N:1524:PGV:H221	19:N:1524:PGV:C01	1.96	0.94
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	1.98	0.94
10:W:2:GLU:HB2	10:W:4:ARG:HH12	1.32	0.94
22:B:229:PSC:O01	22:B:229:PSC:H212	1.67	0.94
19:C:267:PGV:H181	26:C:270:CDL:H652	1.48	0.93
7:G:2:SER:OG	25:G:1263:PEK:H291	1.66	0.93
6:F:94:HIS:HB3	6:F:95:GLN:OE1	1.68	0.93
7:G:72:ASN:H	7:G:76:ASN:HD22	0.99	0.93
26:P:1270:CDL:HB21	26:P:1270:CDL:HB32	1.49	0.93
25:T:1265:PEK:H383	26:T:1269:CDL:H273	1.00	0.92
6:F:85:CYS:SG	6:F:87:THR:HG23	2.09	0.92
26:G:269:CDL:HA21	26:G:269:CDL:H112	1.52	0.92
25:T:1265:PEK:H381	26:T:1269:CDL:H273	1.48	0.92
10:W:2:GLU:HB2	10:W:4:ARG:HH11	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.32	0.91
6:S:85:CYS:SG	6:S:87:THR:HG23	2.10	0.91
26:T:1269:CDL:H241	26:T:1269:CDL:H531	1.53	0.90
25:P:1264:PEK:H32	25:P:1264:PEK:H71	1.55	0.89
3:P:29:SER:HB2	3:P:42:LEU:HD13	1.53	0.89
25:T:1265:PEK:H71	29:T:4407:HOH:O	1.73	0.89
8:H:9:LYS:O	8:H:10:ASN:HB2	1.71	0.88
7:T:7:ASP:O	7:T:8:HIS:HB2	1.73	0.88
1:A:513:LEU:O	1:A:514:LYS:CB	2.22	0.87
7:G:84:LYS:H	7:G:84:LYS:CD	1.87	0.87
1:A:282:PHE:HA	7:T:4:ALA:CB	2.04	0.87
26:C:270:CDL:H212	26:C:270:CDL:C63	1.99	0.87
12:L:20:ARG:HH22	21:L:522:TGL:HC32	1.38	0.87
1:N:513:LEU:O	1:N:514:LYS:CB	2.23	0.86
7:G:2:SER:OG	25:G:1263:PEK:C29	2.22	0.86
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.41	0.86
12:Y:20:ARG:HH21	21:Y:1522:TGL:HC32	1.39	0.86
19:A:524:PGV:H011	19:A:524:PGV:H22	1.59	0.85
3:C:63:ARG:HH21	26:C:270:CDL:HA21	1.38	0.85
2:B:81:LEU:HD12	26:T:1269:CDL:H351	1.57	0.85
7:G:2:SER:O	25:G:1263:PEK:H331	1.77	0.84
9:I:44:LYS:HE2	29:I:4717:HOH:O	1.77	0.84
8:H:52:VAL:HG12	8:U:46:LYS:CB	2.06	0.83
19:A:524:PGV:H311	13:M:19:LEU:CD2	2.09	0.83
21:D:523:TGL:HG32	29:D:4105:HOH:O	1.76	0.83
6:F:97:ALA:CB	29:F:4782:HOH:O	2.26	0.83
7:G:5:LYS:HG3	25:G:1263:PEK:H371	1.60	0.82
7:G:3:ALA:HB1	25:G:1263:PEK:H383	1.61	0.82
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.60	0.82
12:Y:20:ARG:HH21	21:Y:1522:TGL:CC3	1.93	0.82
3:C:246:ASP:HB2	29:C:4124:HOH:O	1.81	0.81
7:G:72:ASN:H	7:G:76:ASN:ND2	1.78	0.81
8:U:9:LYS:HG3	8:U:10:ASN:N	1.94	0.81
6:S:76:LYS:HE2	29:S:4790:HOH:O	1.80	0.81
7:T:2:SER:OG	25:T:263:PEK:H301	1.79	0.81
5:R:7:THR:OG1	5:R:10:GLU:HG3	1.80	0.81
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.62	0.81
22:B:229:PSC:C07	9:I:10:ARG:HH21	1.93	0.81
4:D:45:LYS:HB3	29:D:4504:HOH:O	1.81	0.81
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.63	0.80
22:B:229:PSC:H142	22:B:229:PSC:H343	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:45:ALA:O	8:U:47:GLY:N	2.14	0.80
6:S:94:HIS:HD2	6:S:95:GLN:N	1.80	0.80
26:C:270:CDL:C21	26:C:270:CDL:H631	2.01	0.80
21:N:1523:TGL:HC21	21:N:1523:TGL:CG1	2.12	0.80
25:C:264:PEK:H162	25:C:264:PEK:C10	2.07	0.79
26:T:1269:CDL:H111	26:T:1269:CDL:CA2	2.11	0.79
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.61	0.79
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.48	0.79
19:N:1524:PGV:H321	19:N:1524:PGV:H151	1.64	0.79
7:G:31:CYS:SG	26:G:269:CDL:H532	2.22	0.78
8:H:43:MET:HE3	8:H:49:ASP:H	1.47	0.78
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.63	0.78
22:R:1229:PSC:H142	22:R:1229:PSC:H343	1.63	0.78
12:L:20:ARG:HH21	21:L:522:TGL:HC32	1.48	0.78
8:U:9:LYS:O	8:U:10:ASN:HB2	1.82	0.77
10:W:33:ARG:HG2	23:W:1059:CHD:H152	1.66	0.77
6:F:97:ALA:HB3	29:F:4782:HOH:O	1.84	0.77
6:S:94:HIS:HD2	6:S:95:GLN:CA	1.97	0.77
3:P:107:ALA:HB2	19:U:1268:PGV:H031	1.66	0.77
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.67	0.77
1:A:351:GLY:HA3	1:A:380[A]:VAL:HG13	1.67	0.76
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.65	0.76
21:Y:1522:TGL:CA9	21:Y:1522:TGL:H231	2.14	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.33	0.76
25:C:264:PEK:H101	25:C:264:PEK:C16	2.08	0.76
2:O:227:LEU:OXT	2:O:227:LEU:HD13	1.86	0.76
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.21	0.75
26:G:269:CDL:H372	2:O:78:LEU:CD1	2.16	0.75
22:B:229:PSC:O02	22:B:229:PSC:H032	1.85	0.75
1:A:484:THR:HB	13:M:2:THR:OG1	1.87	0.75
22:B:229:PSC:H142	22:B:229:PSC:C34	2.17	0.75
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.84	0.74
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.87	0.74
4:D:20:ARG:HG3	29:D:4132:HOH:O	1.86	0.74
2:B:56:MET:HA	22:B:229:PSC:H201	1.68	0.74
19:A:521:PGV:H183	25:C:264:PEK:H332	1.68	0.74
26:T:1269:CDL:H111	26:T:1269:CDL:HA22	1.67	0.74
22:R:1229:PSC:H22	22:R:1229:PSC:H221	1.70	0.74
7:G:5:LYS:HD2	25:G:1263:PEK:H372	1.69	0.73
2:B:70:ALA:HB1	26:T:1269:CDL:H451	1.70	0.73
26:G:269:CDL:C22	26:G:269:CDL:H522	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:95:GLN:CG	29:S:4728:HOH:O	2.36	0.73
19:C:267:PGV:C18	26:C:270:CDL:H652	2.18	0.72
8:H:43:MET:HE3	8:H:49:ASP:N	2.04	0.72
21:N:1523:TGL:HA81	21:N:1523:TGL:H231	1.71	0.72
19:C:268:PGV:H061	29:C:4333:HOH:O	1.89	0.72
3:C:95:THR:HG21	19:C:268:PGV:H282	1.71	0.72
26:G:269:CDL:H171	29:G:4479:HOH:O	1.90	0.71
7:G:72:ASN:N	7:G:76:ASN:HD22	1.83	0.71
22:R:1229:PSC:H343	22:R:1229:PSC:C14	2.20	0.71
9:V:61:GLU:HG3	9:V:65:LYS:NZ	2.06	0.71
12:Y:20:ARG:NH2	21:Y:1522:TGL:HC32	2.05	0.71
6:S:52:ILE:O	6:S:94:HIS:ND1	2.25	0.70
12:Y:20:ARG:NH2	21:Y:1522:TGL:CC3	2.54	0.70
26:C:270:CDL:HA22	29:J:4496:HOH:O	1.92	0.70
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.27	0.70
7:G:3:ALA:CB	25:G:1263:PEK:H383	2.22	0.69
25:C:265:PEK:H041	7:G:17:ARG:HH22	1.57	0.69
19:N:1524:PGV:H012	19:N:1524:PGV:C22	2.22	0.69
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.21	0.69
6:S:94:HIS:HD2	6:S:95:GLN:HA	1.57	0.69
12:Y:12:PRO:HB2	21:Y:1522:TGL:HG11	1.72	0.69
22:B:229:PSC:H041	5:E:41:LEU:HD23	1.73	0.69
21:B:521:TGL:H252	21:B:521:TGL:HA91	1.75	0.69
7:T:3:ALA:CB	25:T:263:PEK:H383	2.22	0.69
21:D:523:TGL:H242	21:D:523:TGL:HA91	1.74	0.69
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.39	0.68
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.75	0.68
10:J:26:ALA:O	10:J:30:ILE:HD12	1.94	0.68
10:J:4:ARG:HD3	10:J:7:GLU:OE2	1.94	0.68
7:T:2:SER:O	25:T:263:PEK:H331	1.93	0.68
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.68
7:T:45:PRO:HD2	29:T:3099:HOH:O	1.94	0.68
26:C:270:CDL:H222	26:C:270:CDL:H661	1.76	0.68
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.76	0.67
6:S:94:HIS:CD2	6:S:95:GLN:CA	2.73	0.67
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.75	0.67
21:N:1523:TGL:HG11	21:N:1523:TGL:CC2	2.18	0.67
7:T:37:LEU:HD21	26:T:1269:CDL:H361	1.76	0.67
7:G:7:ASP:O	7:G:9:GLY:N	2.22	0.67
1:N:378:HIS:HA	1:N:382[A]:SER:OG	1.93	0.67
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:268:PGV:H102	29:C:4697:HOH:O	1.94	0.67
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.82	0.67
1:N:351:GLY:C	1:N:380[A]:VAL:CG1	2.62	0.66
29:A:4171:HOH:O	22:B:229:PSC:H32	1.96	0.66
2:O:52:HIS:CE1	22:R:1229:PSC:H202	2.31	0.66
21:Y:1522:TGL:OC1	21:Y:1522:TGL:HC51	1.96	0.66
2:B:183:THR:CG2	29:B:4424:HOH:O	2.43	0.66
25:C:265:PEK:H371	26:G:269:CDL:C27	2.26	0.66
2:O:227:LEU:HB2	29:O:4695:HOH:O	1.96	0.66
10:J:33:ARG:HG2	23:J:60:CHD:C15	2.25	0.66
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.76	0.66
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.77	0.66
25:C:265:PEK:H042	6:F:1:ALA:H1	1.61	0.66
22:B:229:PSC:H31	22:B:229:PSC:H221	1.78	0.66
8:H:9:LYS:O	8:H:10:ASN:CB	2.43	0.65
29:N:4633:HOH:O	2:O:87:MET:SD	2.53	0.65
26:G:269:CDL:H752	1:N:282:PHE:HZ	1.62	0.65
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.79	0.65
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.78	0.65
6:S:94:HIS:CG	6:S:95:GLN:H	2.12	0.65
6:F:87:THR:HG21	29:F:4730:HOH:O	1.97	0.65
19:P:1267:PGV:H181	26:P:1270:CDL:H651	1.79	0.65
4:D:86:MET:CE	29:K:4243:HOH:O	2.44	0.64
12:L:11:ILE:CG2	21:L:522:TGL:H272	2.27	0.64
1:N:407:ASP:O	1:N:411:LYS:HG3	1.97	0.64
12:Y:47:LYS:OXT	12:Y:47:LYS:HE2	1.97	0.64
25:C:265:PEK:H222	25:C:265:PEK:H6	1.80	0.64
26:T:1269:CDL:H241	26:T:1269:CDL:C53	2.27	0.64
7:T:7:ASP:CG	7:T:8:HIS:N	2.51	0.64
1:A:51:ASP:OD1	1:A:441:SER:OG	2.12	0.64
12:Y:22:LEU:O	12:Y:26:THR:HB	1.96	0.64
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	1.79	0.64
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.63	0.63
1:N:87:ILE:O	1:N:173:PRO:HD3	1.99	0.63
8:H:43:MET:CE	8:H:49:ASP:H	2.11	0.63
1:N:113:LEU:HD12	21:Y:1522:TGL:C13	2.28	0.63
8:H:46:LYS:HE2	8:U:8:ILE:CG2	2.27	0.63
2:O:59:GLN:C	2:O:60:GLU:HG3	2.19	0.63
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.46	0.63
6:F:64:GLU:O	6:F:65:ASP:HB2	1.97	0.63
4:Q:92:THR:O	4:Q:95:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:2:GLU:HG2	29:W:4564:HOH:O	1.98	0.63
4:D:78:TRP:HB3	21:D:523:TGL:HB22	1.81	0.62
10:J:33:ARG:HG2	23:J:60:CHD:H151	1.80	0.62
1:A:485:VAL:HG22	13:M:1:ILE:HG13	1.82	0.62
25:P:1264:PEK:H12	25:P:1264:PEK:H242	1.80	0.62
6:S:94:HIS:CG	6:S:95:GLN:N	2.66	0.62
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.17	0.62
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.82	0.62
13:M:10:THR:HA	13:M:14:GLU:OE2	2.00	0.62
26:P:1270:CDL:HB22	26:P:1270:CDL:PA1	2.40	0.62
22:R:1229:PSC:H071	9:V:10:ARG:HE	1.65	0.62
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.80	0.61
3:P:29:SER:CB	3:P:42:LEU:HD13	2.28	0.61
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.83	0.61
1:N:488:THR:HB	1:N:495:LEU:HD13	1.82	0.61
23:P:1271:CHD:C16	23:P:1271:CHD:H232	2.31	0.61
14:A:516:HEA:HMC1	14:A:516:HEA:HBC1	1.81	0.61
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.15	0.61
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.21	0.61
26:T:1269:CDL:H751	26:T:1269:CDL:H582	1.83	0.61
1:A:514:LYS:NZ	29:A:2645:HOH:O	2.34	0.61
19:A:524:PGV:H221	19:A:524:PGV:H012	1.82	0.61
3:C:63:ARG:NH2	26:C:270:CDL:HA21	2.15	0.61
2:O:62:GLU:O	2:O:66:THR:HB	2.01	0.61
3:C:33:MET:HE3	29:J:4237:HOH:O	2.01	0.60
10:W:2:GLU:CB	10:W:4:ARG:HH12	2.10	0.60
26:G:269:CDL:H362	2:O:81:LEU:HD12	1.83	0.60
8:U:48:GLY:HA2	29:U:4792:HOH:O	2.00	0.60
1:N:113:LEU:HD12	21:Y:1522:TGL:C14	2.31	0.60
1:N:484:THR:HB	13:Z:2:THR:OG1	2.02	0.60
4:Q:66:GLU:HG2	29:Q:4646:HOH:O	2.02	0.60
7:G:2:SER:OG	25:G:1263:PEK:H292	2.00	0.60
2:O:66:THR:HG21	23:O:229:CHD:H3	1.84	0.60
6:F:1:ALA:CB	6:S:65:ASP:OD1	2.49	0.60
12:L:2:HIS:CG	12:L:3:TYR:H	2.19	0.59
1:A:351:GLY:C	1:A:380[A]:VAL:CG1	2.70	0.59
7:G:6:GLY:O	25:G:1263:PEK:H311	2.03	0.59
29:A:2527:HOH:O	12:L:7:PRO:HG3	2.03	0.59
1:A:351:GLY:CA	1:A:380[A]:VAL:HG13	2.33	0.59
3:P:210:ILE:HG12	19:P:1267:PGV:H132	1.85	0.59
21:B:521:TGL:C28	21:B:521:TGL:H101	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.38	0.58
2:O:56:MET:HA	22:R:1229:PSC:H201	1.83	0.58
3:C:80:ARG:NH1	3:C:236:GLU:OE2	2.34	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.58
1:N:377:PHE:O	1:N:381[A]:LEU:HB3	2.03	0.58
25:G:1263:PEK:H221	25:G:1263:PEK:HN1	1.68	0.58
21:N:1523:TGL:H231	21:N:1523:TGL:CA9	2.33	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.84	0.58
1:N:113:LEU:CD1	21:Y:1522:TGL:H292	2.33	0.58
21:N:1523:TGL:HC61	29:O:3562:HOH:O	2.03	0.58
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.86	0.58
26:C:270:CDL:O1	26:C:270:CDL:OA3	2.11	0.58
1:N:377:PHE:O	1:N:381[B]:LEU:HB2	2.04	0.58
2:O:59:GLN:O	2:O:59:GLN:CG	2.40	0.58
1:A:400:PHE:HB3	21:L:522:TGL:H283	1.86	0.58
19:A:524:PGV:H142	19:A:524:PGV:C30	2.34	0.58
23:O:229:CHD:H212	23:O:229:CHD:H12	1.85	0.58
23:C:525:CHD:H152	19:C:268:PGV:H11	1.86	0.58
3:C:55:TYR:CE1	26:C:270:CDL:H512	2.38	0.58
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.39	0.58
9:V:10:ARG:HG3	9:V:10:ARG:HH11	1.68	0.58
9:V:61:GLU:HG3	9:V:65:LYS:HZ1	1.69	0.58
1:N:113:LEU:HD13	21:Y:1522:TGL:H292	1.85	0.57
25:C:265:PEK:H371	26:G:269:CDL:H273	1.86	0.57
26:C:270:CDL:CB2	10:J:8:LYS:HZ2	2.01	0.57
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.69	0.57
21:B:521:TGL:HC21	29:I:2606:HOH:O	2.04	0.57
25:C:265:PEK:H042	6:F:1:ALA:N	2.20	0.57
1:N:400:PHE:HB3	21:Y:1522:TGL:H283	1.87	0.57
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.87	0.57
1:N:449:MET:SD	2:O:5:MET:HG2	2.44	0.57
25:T:1265:PEK:C37	26:T:1269:CDL:C27	2.82	0.57
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.57
9:V:2:THR:HG22	9:V:3:ALA:H	1.69	0.57
7:G:7:ASP:HB3	29:N:4167:HOH:O	2.02	0.57
8:H:45:ALA:O	8:H:47:GLY:N	2.37	0.57
3:P:223:LEU:HD21	23:P:1271:CHD:H183	1.87	0.57
1:N:514:LYS:HA	6:S:38:ALA:CB	2.35	0.56
26:C:270:CDL:HB22	10:J:8:LYS:HZ1	1.65	0.56
1:A:307:SER:HB3	26:T:1269:CDL:H171	1.86	0.56
22:R:1229:PSC:H011	22:R:1229:PSC:C2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:TPO:CG2	7:G:11:TPO:O	2.53	0.56
29:N:4604:HOH:O	11:X:8:ASP:HB2	2.05	0.56
2:O:13:THR:HB	2:O:168:LEU:HD23	1.88	0.56
21:O:1521:TGL:H241	21:O:1521:TGL:H201	1.87	0.56
19:C:268:PGV:C06	29:C:4333:HOH:O	2.52	0.56
2:O:52:HIS:HE1	22:R:1229:PSC:H202	1.68	0.56
6:S:64:GLU:O	6:S:65:ASP:HB2	2.05	0.56
19:A:524:PGV:H312	13:M:16:ALA:HA	1.88	0.56
2:O:146:MET:HA	2:O:213:LEU:HD12	1.88	0.56
9:V:52:ARG:CZ	9:V:52:ARG:HB2	2.36	0.55
23:P:1271:CHD:H232	23:P:1271:CHD:H162	1.87	0.55
7:T:35:SER:HB3	7:T:36:TRP:CE3	2.42	0.55
6:S:54:ASN:HD22	6:S:54:ASN:C	2.09	0.55
7:T:5:LYS:CG	25:T:263:PEK:H371	2.36	0.55
7:G:2:SER:HG	25:G:1263:PEK:H291	1.71	0.55
12:L:14:SER:H	21:L:522:TGL:HC31	1.72	0.55
25:P:1264:PEK:C3	25:P:1264:PEK:H71	2.26	0.55
22:B:229:PSC:H42	29:I:2588:HOH:O	2.07	0.55
2:O:84:LEU:HA	2:O:87:MET:CE	2.36	0.55
3:P:40:MET:O	3:P:44:MET:HG2	2.07	0.55
6:S:92:VAL:HG23	6:S:92:VAL:O	2.06	0.55
1:A:382[A]:SER:O	1:A:386:VAL:HB	2.06	0.55
26:G:269:CDL:C11	26:G:269:CDL:HA21	2.33	0.55
2:O:164:ALA:O	2:O:194:GLY:HA3	2.07	0.55
21:D:523:TGL:HG31	21:D:523:TGL:OA1	2.07	0.55
14:A:516:HEA:HMC1	14:A:516:HEA:CBC	2.37	0.55
21:N:1523:TGL:CA8	21:N:1523:TGL:H231	2.36	0.55
25:T:1265:PEK:C38	26:T:1269:CDL:H271	2.11	0.55
4:D:34:SER:O	4:D:38:LYS:HG3	2.07	0.54
7:G:7:ASP:CB	29:N:4167:HOH:O	2.55	0.54
8:H:23:GLN:HG3	29:H:4128:HOH:O	2.07	0.54
5:R:48:ILE:O	5:R:52:LEU:HG	2.07	0.54
19:U:1268:PGV:C03	29:U:4495:HOH:O	2.22	0.54
6:S:1:ALA:N	25:T:1265:PEK:H041	2.22	0.54
7:T:5:LYS:HG3	25:T:263:PEK:H371	1.90	0.54
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.22	0.54
6:S:95:GLN:HG2	29:S:4728:HOH:O	2.05	0.54
23:W:1059:CHD:H41	29:W:4647:HOH:O	2.07	0.54
1:A:381[A]:LEU:HB2	14:A:516:HEA:CAC	2.38	0.54
6:S:95:GLN:HG3	29:S:4728:HOH:O	2.03	0.54
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.54
7:T:7:ASP:O	7:T:8:HIS:CB	2.53	0.54
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.43	0.53
3:C:59:ARG:HA	26:C:270:CDL:H522	1.90	0.53
9:V:1:SAC:OAC	9:V:1:SAC:HB3	2.09	0.53
21:D:523:TGL:CG3	29:D:4105:HOH:O	2.42	0.53
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.44	0.53
26:P:1270:CDL:H352	26:P:1270:CDL:H162	1.90	0.53
3:P:51:MET:HB3	26:P:1270:CDL:H392	1.90	0.53
1:N:297:MET:CE	1:N:297:MET:HB2	2.39	0.53
26:T:1269:CDL:C11	26:T:1269:CDL:HA22	2.36	0.53
8:U:43:MET:HE3	8:U:49:ASP:N	2.23	0.53
7:T:8:HIS:O	7:T:9:GLY:C	2.46	0.53
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.91	0.53
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.85	0.53
21:N:1523:TGL:HA92	21:N:1523:TGL:H231	1.91	0.53
3:C:106:LEU:HD13	19:C:268:PGV:H22	1.90	0.53
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.91	0.53
1:A:47:LEU:O	13:M:41:LYS:HE3	2.09	0.53
7:T:42:ARG:HB2	29:T:4747:HOH:O	2.09	0.53
2:B:58:ALA:O	2:B:62:GLU:HG3	2.09	0.53
25:C:265:PEK:C37	26:G:269:CDL:C27	2.86	0.53
12:L:20:ARG:HH12	21:L:522:TGL:HC61	1.74	0.53
6:S:1:ALA:N	25:T:1265:PEK:C04	2.72	0.53
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.69	0.52
26:G:269:CDL:H471	29:G:4791:HOH:O	2.08	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.56	0.52
1:A:28:MET:HE2	14:A:515:HEA:H271	1.92	0.52
19:A:524:PGV:C22	19:A:524:PGV:H012	2.39	0.52
2:B:183:THR:HG23	29:B:4424:HOH:O	2.04	0.52
1:N:352:GLY:N	1:N:380[A]:VAL:CG1	2.72	0.52
1:A:87:ILE:O	1:A:173:PRO:HD3	2.10	0.52
8:H:45:ALA:C	8:H:47:GLY:H	2.12	0.52
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.52
2:B:89:GLU:O	2:B:91:ASN:ND2	2.42	0.52
7:G:11:TPO:CG2	7:G:16:TRP:HE1	2.19	0.52
26:C:270:CDL:PA1	26:C:270:CDL:HB21	2.50	0.52
5:E:52:LEU:O	5:E:55:CYS:HB2	2.09	0.52
2:O:222:TRP:O	2:O:226:MET:HB2	2.10	0.52
6:F:55:LYS:HA	6:F:74:LEU:O	2.10	0.52
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:524:PGV:H142	19:A:524:PGV:H301	1.90	0.52
8:U:9:LYS:CG	8:U:10:ASN:H	2.09	0.52
2:O:84:LEU:HA	2:O:87:MET:HE3	1.92	0.51
25:C:264:PEK:H71	25:C:264:PEK:H32	1.93	0.51
4:D:61:ARG:HD2	29:D:2674:HOH:O	2.10	0.51
29:L:4557:HOH:O	13:M:32:TRP:HH2	1.94	0.51
6:S:76:LYS:HG3	6:S:93:PRO:HG2	1.92	0.51
6:S:94:HIS:O	6:S:95:GLN:HB2	2.09	0.51
5:R:23:ASP:O	5:R:24:ILE:C	2.49	0.51
6:S:95:GLN:O	6:S:97:ALA:N	2.43	0.51
7:G:3:ALA:HB3	25:G:1263:PEK:H362	1.91	0.51
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.26	0.51
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.98	0.51
12:L:20:ARG:HH22	21:L:522:TGL:CC3	2.19	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.92	0.51
8:H:7:LYS:O	8:H:8:ILE:HG22	2.10	0.51
1:N:381[A]:LEU:O	1:N:385:ALA:HB3	2.11	0.51
6:S:55:LYS:HA	6:S:74:LEU:O	2.11	0.51
3:P:131:LEU:HD21	26:T:1269:CDL:HB61	1.91	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
2:B:62:GLU:O	2:B:66:THR:HB	2.11	0.51
3:P:59:ARG:HA	26:P:1270:CDL:H522	1.93	0.51
7:T:38:HIS:NE2	26:T:1269:CDL:HA21	2.26	0.51
8:U:43:MET:HG3	8:U:49:ASP:O	2.11	0.51
8:H:46:LYS:HE2	8:U:8:ILE:HG21	1.92	0.51
26:P:1270:CDL:OB7	26:P:1270:CDL:H112	2.10	0.51
25:C:265:PEK:C04	6:F:1:ALA:N	2.74	0.51
7:T:17:ARG:NH1	25:T:1265:PEK:O13	2.43	0.51
5:E:31:LYS:HE3	6:F:84:SER:O	2.12	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.11	0.50
25:G:1263:PEK:H281	3:P:85:LEU:HD21	1.93	0.50
1:A:351:GLY:HA3	1:A:380[A]:VAL:CG1	2.39	0.50
26:G:269:CDL:C37	2:O:78:LEU:CD1	2.88	0.50
3:C:65:SER:HB2	19:C:267:PGV:H041	1.94	0.50
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.93	0.50
26:G:269:CDL:CA2	26:G:269:CDL:H112	2.33	0.50
8:U:27:ARG:HG2	29:U:4672:HOH:O	2.12	0.50
1:A:377:PHE:O	1:A:381[A]:LEU:HB3	2.11	0.50
1:N:381[A]:LEU:HD13	14:N:516:HEA:HBC2	1.94	0.50
6:S:1:ALA:H1	25:T:1265:PEK:C04	2.24	0.50
9:V:61:GLU:HG3	9:V:65:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:LEU:HD12	26:T:1269:CDL:H352	1.93	0.50
12:Y:2:HIS:N	29:Y:4665:HOH:O	2.44	0.50
7:T:8:HIS:O	7:T:9:GLY:O	2.30	0.49
12:Y:14:SER:H	21:Y:1522:TGL:HC31	1.77	0.49
3:P:59:ARG:HG3	26:P:1270:CDL:H511	1.93	0.49
1:A:347:LEU:HD22	1:A:383[B]:MET:SD	2.51	0.49
2:B:68:LEU:HB3	22:B:229:PSC:H182	1.92	0.49
7:G:5:LYS:HB2	25:G:1263:PEK:H351	1.95	0.49
10:J:36:MET:HG2	23:J:60:CHD:H221	1.95	0.49
21:N:1523:TGL:HG32	21:N:1523:TGL:OB1	2.11	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
26:G:269:CDL:H182	1:N:307:SER:CB	2.42	0.49
8:H:7:LYS:O	8:H:8:ILE:HB	2.12	0.49
1:A:21:LEU:CD2	21:L:522:TGL:HA81	2.43	0.49
7:T:5:LYS:HG3	25:T:263:PEK:C37	2.42	0.49
10:W:3:ASN:C	10:W:3:ASN:OD1	2.51	0.49
1:A:115:SER:O	1:A:121:GLY:HA2	2.12	0.49
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.12	0.49
1:N:489:THR:HA	6:S:71:TRP:O	2.12	0.49
29:N:4743:HOH:O	23:W:1059:CHD:H212	2.12	0.49
1:A:489:THR:HA	6:F:71:TRP:O	2.12	0.49
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.94	0.49
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.77	0.49
3:C:191:GLY:HA3	29:G:2132:HOH:O	2.13	0.49
12:Y:20:ARG:NH2	21:Y:1522:TGL:HC31	2.25	0.49
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.95	0.49
7:G:17:ARG:HD2	29:G:2446:HOH:O	2.12	0.49
3:C:84:ILE:HD13	25:T:263:PEK:H241	1.95	0.49
3:C:210:ILE:HG21	19:C:267:PGV:H282	1.95	0.49
4:D:86:MET:HE2	29:K:4243:HOH:O	2.10	0.49
25:C:265:PEK:C36	26:G:269:CDL:H271	2.42	0.49
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.22	0.48
21:N:1523:TGL:HC81	2:O:47:THR:HA	1.95	0.48
5:R:41:LEU:HD22	22:R:1229:PSC:H072	1.95	0.48
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	1.95	0.48
1:A:310:MET:CE	1:A:356:ILE:HG23	2.43	0.48
1:A:383[A]:MET:O	1:A:384[A]:GLY:C	2.48	0.48
1:N:381[A]:LEU:HB2	14:N:516:HEA:CAC	2.43	0.48
7:T:5:LYS:HG3	25:T:263:PEK:C38	2.42	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.06	0.48
7:G:11:TPO:HG23	7:G:11:TPO:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:1522:TGL:OC1	21:Y:1522:TGL:CC5	2.61	0.48
1:A:478:SER:O	13:M:6:ALA:HB1	2.13	0.48
22:B:229:PSC:H041	5:E:41:LEU:CD2	2.41	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.13	0.48
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.61	0.48
19:A:524:PGV:H011	19:A:524:PGV:C2	2.38	0.48
7:G:17:ARG:CD	29:G:2446:HOH:O	2.60	0.48
27:C:272:DMU:H1	7:G:69:PHE:HZ	1.79	0.48
1:N:248:LEU:O	1:N:251:PHE:HB2	2.13	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.48
7:T:38:HIS:HE1	26:T:1269:CDL:OA7	1.95	0.48
1:A:281:GLY:O	7:T:4:ALA:HB1	2.14	0.48
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.95	0.48
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.96	0.48
5:R:41:LEU:HD23	22:R:1229:PSC:H041	1.95	0.48
26:G:269:CDL:H762	26:G:269:CDL:C56	2.25	0.48
1:N:390:MET:O	1:N:394:VAL:HG13	2.13	0.48
1:N:155:VAL:CG2	25:P:1264:PEK:H382	2.44	0.48
4:Q:12:ALA:O	6:S:75:HIS:NE2	2.46	0.48
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.78	0.47
25:C:265:PEK:H362	26:G:269:CDL:C27	2.44	0.47
7:G:5:LYS:HG3	25:G:1263:PEK:C37	2.40	0.47
3:P:22:LEU:O	3:P:26:LEU:HG	2.14	0.47
1:A:28:MET:CE	14:A:515:HEA:H271	2.45	0.47
21:O:1521:TGL:HA82	21:O:1521:TGL:H301	1.96	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
6:F:62:CYS:HB3	6:F:85:CYS:HB3	1.96	0.47
1:N:498:CYS:HA	1:N:499:PRO:HA	1.74	0.47
2:B:41:ILE:HD13	22:B:229:PSC:H342	1.97	0.47
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.97	0.47
14:N:515:HEA:HHC	14:N:515:HEA:H11	1.63	0.47
3:P:63:ARG:HE	26:P:1270:CDL:CA2	2.28	0.47
7:T:17:ARG:HD2	29:T:3446:HOH:O	2.13	0.47
27:C:272:DMU:O1	27:C:272:DMU:H29	2.15	0.47
8:U:45:ALA:C	8:U:47:GLY:H	2.13	0.47
2:B:13:THR:HB	2:B:168:LEU:HD23	1.97	0.47
25:C:265:PEK:C36	26:G:269:CDL:C27	2.93	0.47
10:J:40:LEU:HD12	23:J:60:CHD:H183	1.97	0.47
26:C:270:CDL:HA4	26:C:270:CDL:H131	1.97	0.47
4:D:109:HIS:HD2	29:D:2122:HOH:O	1.97	0.47
1:N:240:HIS:O	1:N:241:PRO:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:1229:PSC:O01	22:R:1229:PSC:H212	2.15	0.47
1:N:321:PHE:CD2	22:R:1229:PSC:H341	2.49	0.47
7:T:6:GLY:O	7:T:7:ASP:O	2.32	0.47
21:B:521:TGL:H211	21:B:521:TGL:H241	1.59	0.47
8:H:43:MET:O	8:H:44:THR:C	2.53	0.47
10:J:52:TRP:O	10:J:57:HIS:HE1	1.98	0.47
21:Y:1522:TGL:CC4	21:Y:1522:TGL:OC1	2.63	0.47
2:B:196:CYS:CB	2:B:207:MET:HG3	2.45	0.47
26:T:1269:CDL:H732	26:T:1269:CDL:H541	1.97	0.47
10:W:36:MET:HG3	10:W:40:LEU:HD12	1.97	0.47
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.50	0.46
1:N:62:ALA:HB1	14:N:515:HEA:HMD3	1.96	0.46
21:Y:1522:TGL:H231	21:Y:1522:TGL:HA92	1.92	0.46
1:A:380[A]:VAL:HG23	1:A:381[A]:LEU:N	2.30	0.46
1:A:383[B]:MET:HG2	1:A:421:VAL:HG21	1.95	0.46
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.15	0.46
25:C:265:PEK:H362	26:G:269:CDL:H272	1.97	0.46
1:N:430:PHE:HE1	21:O:1521:TGL:HB21	1.79	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.46
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.67	0.46
12:Y:47:LYS:HE3	13:Z:42:LYS:NZ	2.30	0.46
26:P:1270:CDL:H152	26:P:1270:CDL:H202	1.97	0.46
6:S:94:HIS:CD2	6:S:95:GLN:HA	2.44	0.46
1:A:309:THR:CG2	14:A:516:HEA:HMB2	2.45	0.46
2:B:66:THR:HG21	23:B:1085:CHD:H42	1.97	0.46
26:C:270:CDL:C13	26:C:270:CDL:HA4	2.45	0.46
27:C:272:DMU:H1	7:G:69:PHE:CZ	2.51	0.46
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.46
8:U:78:GLU:O	8:U:78:GLU:HG2	2.15	0.46
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.16	0.46
12:Y:2:HIS:NE2	12:Y:5:GLU:OE1	2.48	0.46
5:E:23:ASP:N	5:E:23:ASP:OD2	2.49	0.46
2:O:65:TRP:O	2:O:69:PRO:HG2	2.15	0.46
3:P:54:MET:HE3	26:P:1270:CDL:H601	1.97	0.46
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.78	0.46
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.46	0.46
19:P:1267:PGV:C18	26:P:1270:CDL:H651	2.46	0.46
3:P:55:TYR:OH	26:P:1270:CDL:H121	2.15	0.46
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.87	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.46
3:P:116:TRP:HA	3:P:117:PRO:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.15	0.46
1:N:346:PHE:CE2	21:O:1521:TGL:H271	2.50	0.46
7:T:2:SER:O	25:T:263:PEK:C33	2.62	0.46
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.98	0.46
1:A:309:THR:HG22	14:A:516:HEA:HMB2	1.99	0.45
26:P:1270:CDL:H181	26:P:1270:CDL:H632	1.97	0.45
4:Q:94:LEU:CD2	11:X:28:VAL:HG21	2.46	0.45
1:A:382[A]:SER:HB3	14:A:515:HEA:HMC2	1.98	0.45
1:A:399:LEU:O	1:A:499:PRO:HA	2.17	0.45
4:D:34:SER:H	4:D:37:GLN:NE2	2.14	0.45
23:J:60:CHD:H12A	23:J:60:CHD:H112	1.54	0.45
2:O:226:MET:O	2:O:227:LEU:C	2.55	0.45
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.32	0.45
5:R:23:ASP:N	5:R:23:ASP:OD2	2.34	0.45
1:A:170:ASN:OD1	3:C:77:LYS:HD2	2.17	0.45
5:R:11:PHE:CG	22:R:1229:PSC:H073	2.51	0.45
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.52	0.45
14:A:516:HEA:HHA	14:A:516:HEA:HAD2	1.79	0.45
25:C:265:PEK:C37	26:G:269:CDL:H271	2.45	0.45
5:R:31:LYS:O	5:R:31:LYS:HD2	2.16	0.45
1:A:240:HIS:C	1:A:240:HIS:CD2	2.89	0.45
7:G:84:LYS:NZ	29:G:4536:HOH:O	2.48	0.45
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.45
3:C:226:HIS:CE1	26:C:270:CDL:HB31	2.52	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.45
29:P:4419:HOH:O	25:T:1265:PEK:H41	2.17	0.45
7:T:17:ARG:CD	29:T:3446:HOH:O	2.65	0.45
1:A:71:MET:N	1:A:72:PRO:CD	2.80	0.45
26:G:269:CDL:C47	29:G:4791:HOH:O	2.64	0.45
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.79	0.45
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.99	0.45
1:A:461:SER:HB2	29:A:2700:HOH:O	2.16	0.45
2:B:66:THR:HG21	23:B:1085:CHD:H3	1.97	0.45
4:D:34:SER:H	4:D:37:GLN:HE21	1.65	0.45
21:L:522:TGL:H202	21:L:522:TGL:H231	1.27	0.45
26:P:1270:CDL:H652	26:P:1270:CDL:H612	1.98	0.45
3:P:51:MET:HG3	26:P:1270:CDL:H672	1.99	0.45
25:T:1265:PEK:H6	25:T:1265:PEK:H222	1.99	0.45
1:A:50:ASP:OD1	1:A:50:ASP:C	2.54	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.51	0.45
3:P:63:ARG:HE	26:P:1270:CDL:HA21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:3:ALA:O	7:G:4:ALA:HB2	2.16	0.44
13:Z:39:ASN:O	13:Z:43:SER:OG	2.27	0.44
1:N:100:MET:N	3:P:17:PRO:HB3	2.32	0.44
2:O:121:TYR:O	2:O:138:VAL:HA	2.17	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.44
19:A:524:PGV:H152	4:D:87:PHE:CZ	2.53	0.44
2:O:7:LEU:HD12	21:O:1521:TGL:HC31	1.98	0.44
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.98	0.44
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.18	0.44
1:N:113:LEU:HD12	21:Y:1522:TGL:H131	1.98	0.44
26:P:1270:CDL:H432	26:P:1270:CDL:H362	1.99	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.47	0.44
8:H:7:LYS:O	8:H:8:ILE:CB	2.65	0.44
3:C:16:TRP:N	3:C:17:PRO:CD	2.80	0.44
1:A:351:GLY:C	1:A:380[A]:VAL:HG13	2.38	0.44
2:B:56:MET:CA	22:B:229:PSC:H201	2.42	0.44
23:C:271:CHD:H232	23:C:271:CHD:H162	1.98	0.44
12:L:2:HIS:CG	12:L:3:TYR:N	2.85	0.44
21:N:1523:TGL:H181	2:O:47:THR:HB	2.00	0.44
26:P:1270:CDL:HB32	26:P:1270:CDL:CB2	2.36	0.44
5:R:80:GLU:CD	5:R:80:GLU:H	2.21	0.44
1:A:377:PHE:CD1	14:A:516:HEA:HAD1	2.52	0.44
22:B:229:PSC:C02	22:B:229:PSC:H212	2.46	0.44
8:H:49:ASP:O	8:H:52:VAL:HG22	2.18	0.44
9:I:54:TYR:OH	9:I:59:ASP:OD1	2.27	0.44
3:P:37:PHE:HD1	29:P:4771:HOH:O	2.00	0.44
1:A:486:ASP:HB2	29:A:2142:HOH:O	2.18	0.44
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.99	0.44
3:C:15:PRO:O	3:C:19:THR:HG23	2.18	0.44
26:G:269:CDL:CA2	26:G:269:CDL:C11	2.95	0.44
1:N:378:HIS:O	1:N:382[A]:SER:HB2	2.18	0.44
19:A:524:PGV:H12	4:D:87:PHE:CD2	2.53	0.43
9:I:43:ARG:HD3	9:I:43:ARG:HH11	1.62	0.43
11:K:6:ALA:HA	11:K:7:PRO:HD2	1.78	0.43
4:Q:12:ALA:CB	6:S:55:LYS:HE3	2.48	0.43
22:B:229:PSC:H062	22:B:229:PSC:H042	1.75	0.43
3:C:33:MET:CE	29:J:4237:HOH:O	2.61	0.43
26:G:269:CDL:H182	1:N:307:SER:HB2	2.00	0.43
25:P:1264:PEK:H32	25:P:1264:PEK:C7	2.38	0.43
1:A:181:THR:HA	1:A:182:PRO:HD3	1.78	0.43
1:A:34:SER:HB2	14:A:515:HEA:C2B	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:521:PGV:C18	25:C:264:PEK:H332	2.42	0.43
27:C:272:DMU:H29	27:C:272:DMU:C10	2.47	0.43
21:N:1523:TGL:H222	2:O:39:LEU:CD1	2.48	0.43
1:N:514:LYS:H	6:S:38:ALA:H	1.67	0.43
3:P:224:LYS:O	3:P:225:PHE:HB2	2.18	0.43
1:A:408:THR:HB	19:A:524:PGV:H32	2.01	0.43
3:C:109:THR:HB	3:C:110:PRO:CD	2.48	0.43
21:L:522:TGL:HC22	21:L:522:TGL:HC62	1.99	0.43
3:P:165:ILE:HG12	25:T:1265:PEK:H102	2.01	0.43
5:R:107:ASP:N	5:R:107:ASP:OD2	2.45	0.43
8:U:49:ASP:O	8:U:52:VAL:HG13	2.18	0.43
6:F:65:ASP:OD1	6:S:1:ALA:HB3	2.18	0.43
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
1:N:512:ASN:HB2	29:N:4003:HOH:O	2.18	0.43
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.53	0.43
21:Y:1522:TGL:C23	21:Y:1522:TGL:HA92	2.49	0.43
1:A:450:TRP:CE3	1:A:450:TRP:HA	2.54	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.18	0.43
26:P:1270:CDL:H222	26:P:1270:CDL:H191	1.77	0.43
12:Y:2:HIS:CG	12:Y:3:TYR:N	2.85	0.43
1:N:473:TRP:CZ3	13:Z:18:GLY:HA3	2.53	0.43
6:F:13:ALA:O	6:F:18:ARG:HD2	2.19	0.43
9:I:51:TYR:HA	9:I:54:TYR:HB2	2.00	0.43
1:N:312:ILE:HG22	1:N:312:ILE:O	2.17	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.76	0.43
27:P:272:DMU:H34	7:T:63:GLY:HA2	2.00	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.92	0.43
1:A:500:PRO:HB2	1:A:504:THR:HG21	2.00	0.43
26:G:269:CDL:H241	26:G:269:CDL:H531	1.99	0.43
5:R:41:LEU:CD2	22:R:1229:PSC:H041	2.48	0.43
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.85	0.43
6:S:1:ALA:H2	25:T:1265:PEK:H041	1.83	0.43
6:S:1:ALA:N	25:T:1265:PEK:H042	2.33	0.43
1:A:344:PHE:CD2	1:A:384[B]:GLY:O	2.72	0.43
23:B:1085:CHD:H212	23:B:1085:CHD:H12	2.00	0.43
21:D:523:TGL:OG1	21:D:523:TGL:HB31	2.18	0.43
1:A:21:LEU:HD23	21:L:522:TGL:HA81	2.00	0.43
12:Y:11:ILE:CG2	21:Y:1522:TGL:H272	2.48	0.43
23:B:1085:CHD:H12A	23:B:1085:CHD:H112	1.69	0.42
1:N:382[A]:SER:O	1:N:383[A]:MET:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:109:HIS:CD2	29:Q:3122:HOH:O	2.68	0.42
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.42
23:J:60:CHD:H211	23:J:60:CHD:H232	1.74	0.42
2:O:68:LEU:HA	2:O:68:LEU:HD12	1.73	0.42
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	2.01	0.42
22:R:1229:PSC:H042	29:R:3664:HOH:O	2.19	0.42
5:R:11:PHE:CD1	22:R:1229:PSC:H073	2.54	0.42
1:A:246:LEU:HD13	1:A:381[A]:LEU:HD11	2.01	0.42
2:B:78:LEU:CD1	26:T:1269:CDL:H352	2.50	0.42
3:C:109:THR:HB	3:C:110:PRO:HD2	1.99	0.42
3:C:202:GLY:HA3	25:C:264:PEK:H21	2.01	0.42
2:O:202:SER:HB3	2:O:203:ASN:HD22	1.84	0.42
4:Q:7:LYS:HB3	4:Q:8:SER:H	1.68	0.42
5:R:80:GLU:N	5:R:80:GLU:CD	2.73	0.42
26:T:1269:CDL:H581	26:T:1269:CDL:H552	1.94	0.42
10:W:57:HIS:O	10:W:58:LYS:HB2	2.18	0.42
1:A:382[B]:SER:OG	14:A:515:HEA:H121	2.20	0.42
1:N:438:ARG:O	1:N:439:ARG:HB2	2.19	0.42
2:O:52:HIS:HE1	22:R:1229:PSC:H02	1.84	0.42
26:P:1270:CDL:CB2	26:P:1270:CDL:CB3	2.85	0.42
7:T:3:ALA:O	7:T:4:ALA:CB	2.67	0.42
12:L:20:ARG:HH22	21:L:522:TGL:CC5	2.33	0.42
3:P:106:LEU:HD13	19:U:1268:PGV:H21	2.01	0.42
7:G:3:ALA:O	7:G:4:ALA:CB	2.67	0.42
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.00	0.42
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.02	0.42
5:R:90:ARG:HB3	5:R:91:PRO:CD	2.43	0.42
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.55	0.42
21:D:523:TGL:HA91	21:D:523:TGL:C24	2.47	0.42
1:A:1:FME:CE	12:L:3:TYR:HE1	2.33	0.42
13:M:13:LYS:HD2	13:M:13:LYS:C	2.40	0.42
4:D:101:HIS:CD2	4:D:102:TYR:CE2	3.08	0.42
1:N:127:THR:HB	1:N:129:TYR:CE2	2.55	0.42
1:N:514:LYS:HE2	29:S:3514:HOH:O	2.18	0.42
14:N:515:HEA:HMC1	14:N:515:HEA:CBC	2.46	0.42
6:F:92:VAL:O	6:F:92:VAL:HG23	2.18	0.41
26:G:269:CDL:OA7	26:G:269:CDL:H311	2.20	0.41
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.85	0.41
10:J:50:LEU:HD22	10:J:54:SER:OG	2.20	0.41
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.42	0.41
13:Z:41:LYS:NZ	29:Z:3672:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:OD2	14:A:516:HEA:O1A	2.38	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.41
21:D:523:TGL:HB71	21:D:523:TGL:HA52	2.01	0.41
12:L:24:MET:SD	21:L:522:TGL:H161	2.60	0.41
6:S:54:ASN:ND2	6:S:54:ASN:C	2.73	0.41
29:P:4425:HOH:O	7:T:11:TPO:CG2	2.68	0.41
7:T:7:ASP:CG	7:T:8:HIS:H	2.24	0.41
1:N:119:GLU:O	12:Y:46:LYS:HE2	2.21	0.41
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	2.02	0.41
8:U:84:LYS:HA	29:U:3538:HOH:O	2.21	0.41
10:W:31:LEU:HA	10:W:31:LEU:HD12	1.88	0.41
1:A:177:SER:H	1:A:180:GLN:HE21	1.68	0.41
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.81	0.41
4:D:39:ALA:O	4:D:42:GLU:HB2	2.21	0.41
26:G:269:CDL:C24	26:G:269:CDL:H542	2.51	0.41
26:G:269:CDL:H571	26:G:269:CDL:H782	2.01	0.41
26:G:269:CDL:H821	26:G:269:CDL:H791	1.50	0.41
1:A:382[A]:SER:HB3	14:A:515:HEA:C2C	2.50	0.41
12:L:20:ARG:HH22	21:L:522:TGL:CC6	2.33	0.41
13:M:17:ILE:HD13	13:M:17:ILE:HG21	1.87	0.41
22:B:229:PSC:H242	22:B:229:PSC:H271	1.01	0.41
8:H:46:LYS:HE2	8:U:8:ILE:HG22	1.99	0.41
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.74	0.41
4:Q:52:SER:HB2	29:Q:4686:HOH:O	2.19	0.41
7:T:3:ALA:HB1	25:T:263:PEK:H383	2.00	0.41
8:U:50:VAL:O	8:U:51:SER:C	2.57	0.41
10:W:55:PHE:HA	10:W:56:PRO:HD3	1.83	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.02	0.41
1:N:334:TRP:CE3	21:N:1523:TGL:HA31	2.56	0.41
1:N:318:VAL:HG22	2:O:65:TRP:HD1	1.85	0.41
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.51	0.41
5:R:90:ARG:CB	5:R:91:PRO:HD3	2.44	0.41
6:F:92:VAL:O	6:F:92:VAL:CG2	2.69	0.41
21:N:1523:TGL:OB1	21:N:1523:TGL:CG3	2.68	0.41
22:R:1229:PSC:H063	22:R:1229:PSC:H042	1.76	0.41
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.02	0.41
1:A:190:ILE:CD1	1:A:278:MET:HG2	2.51	0.41
19:A:524:PGV:C21	19:A:524:PGV:H012	2.51	0.41
23:J:60:CHD:H161	29:J:4539:HOH:O	2.21	0.41
1:N:66:ILE:HG23	1:N:246:LEU:HD21	2.03	0.41
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.02	0.41
2:O:226:MET:O	2:O:227:LEU:O	2.38	0.41
26:P:1270:CDL:HB21	26:P:1270:CDL:CB4	2.51	0.41
1:N:103:TRP:O	3:P:21:ALA:HB1	2.21	0.41
6:S:1:ALA:H1	25:T:1265:PEK:H042	1.86	0.41
25:T:1265:PEK:H311	25:T:1265:PEK:H282	1.84	0.41
7:T:3:ALA:CB	25:T:263:PEK:C38	2.95	0.41
25:C:264:PEK:C7	25:C:264:PEK:H32	2.51	0.40
22:R:1229:PSC:C02	22:R:1229:PSC:H212	2.51	0.40
26:T:1269:CDL:OA7	26:T:1269:CDL:H342	2.21	0.40
22:B:229:PSC:H341	22:B:229:PSC:H142	2.00	0.40
10:J:33:ARG:HG2	23:J:60:CHD:H152	2.01	0.40
19:N:1524:PGV:H22	19:N:1524:PGV:C01	2.52	0.40
3:P:226:HIS:CE1	26:P:1270:CDL:HB31	2.57	0.40
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.56	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H383	2.01	0.40
4:D:92:THR:O	4:D:95:LEU:HB2	2.21	0.40
1:N:374:VAL:HG13	1:N:378:HIS:CE1	2.56	0.40
1:N:37:ILE:HD11	1:N:58:VAL:HA	2.03	0.40
1:N:68:PHE:HA	1:N:72:PRO:HG2	2.03	0.40
2:O:116:LEU:HD13	2:O:226:MET:HG3	2.03	0.40
2:B:98:LYS:HB2	2:B:109:GLU:HB2	2.02	0.40
2:B:164:ALA:O	2:B:194:GLY:HA3	2.21	0.40
21:D:523:TGL:H231	21:D:523:TGL:CA9	2.51	0.40
1:N:34:SER:HB2	14:N:515:HEA:C2B	2.51	0.40
23:P:1271:CHD:H12A	23:P:1271:CHD:H112	1.54	0.40
4:Q:16:TYR:HB2	4:Q:27:VAL:HG23	2.04	0.40
1:A:403:TYR:HA	1:A:480:ARG:O	2.21	0.40
3:C:207:HIS:HD2	3:C:241:TYR:OH	2.05	0.40
4:D:48:TRP:HB2	5:E:96:LEU:O	2.21	0.40
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.93	0.40
1:N:240:HIS:CE1	1:N:244:TYR:OH	2.74	0.40
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.85	0.40
3:P:131:LEU:CD2	26:T:1269:CDL:HB61	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	517/514 (101%)	502 (97%)	15 (3%)	0	100	100
1	N	517/514 (101%)	495 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	36	31
2	O	225/227 (99%)	219 (97%)	5 (2%)	1 (0%)	36	31
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	2 (2%)	1 (1%)	17	10
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	1
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	4	1
7	G	81/85 (95%)	68 (84%)	7 (9%)	6 (7%)	1	0
7	T	81/85 (95%)	67 (83%)	6 (7%)	8 (10%)	1	0
8	H	77/85 (91%)	68 (88%)	3 (4%)	6 (8%)	1	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3514/3614 (97%)	3356 (96%)	125 (4%)	33 (1%)	19	12

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	8	ILE
8	H	44	THR
8	H	46	LYS
2	O	60	GLU
5	R	6	GLU
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	37	LEU
7	T	38	HIS
8	U	10	ASN
8	U	45	ALA
8	U	46	LYS
7	G	3	ALA
7	G	37	LEU
7	T	9	GLY
8	U	8	ILE
2	B	60	GLU
6	F	96	LEU
8	H	10	ASN
8	H	43	MET
7	T	5	LYS
7	G	6	GLY
8	H	45	ALA
7	T	6	GLY

### 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	430/426 (101%)	419 (97%)	11 (3%)	49	50
1	N	430/426 (101%)	414 (96%)	16 (4%)	37	35
2	B	210/210 (100%)	200 (95%)	10 (5%)	28	24
2	O	210/210 (100%)	196 (93%)	14 (7%)	18	13
3	C	224/226 (99%)	217 (97%)	7 (3%)	43	42
3	P	224/226 (99%)	219 (98%)	5 (2%)	55	58
4	D	128/129 (99%)	124 (97%)	4 (3%)	43	42
4	Q	128/129 (99%)	121 (94%)	7 (6%)	24	19
5	E	92/95 (97%)	88 (96%)	4 (4%)	32	28
5	R	92/95 (97%)	89 (97%)	3 (3%)	41	39
6	F	81/81 (100%)	76 (94%)	5 (6%)	20	15
6	S	81/81 (100%)	77 (95%)	4 (5%)	27	23
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	3
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	2
8	H	71/75 (95%)	65 (92%)	6 (8%)	12	7
8	U	71/75 (95%)	66 (93%)	5 (7%)	16	11
9	I	57/57 (100%)	50 (88%)	7 (12%)	5	3
9	V	57/57 (100%)	48 (84%)	9 (16%)	3	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	58	61
10	W	49/50 (98%)	48 (98%)	1 (2%)	58	61
11	K	39/46 (85%)	36 (92%)	3 (8%)	14	9
11	X	39/46 (85%)	37 (95%)	2 (5%)	26	21
12	L	39/40 (98%)	38 (97%)	1 (3%)	49	50
12	Y	39/40 (98%)	36 (92%)	3 (8%)	14	9
13	M	37/38 (97%)	33 (89%)	4 (11%)	7	4
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3048/3082 (99%)	2895 (95%)	153 (5%)	27	22

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	44	PRO
1	A	109	PHE
1	A	180	GLN
1	A	265	LYS
1	A	297	MET
1	A	333	LYS
1	A	369	ASP
1	A	444	PRO
1	A	486	ASP
1	A	512	ASN
2	B	33	LEU
2	B	60	GLU
2	B	61	VAL
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	115	ASP
2	B	171	LYS
3	C	17	PRO
3	C	33	MET
3	C	127	LEU
3	C	159	MET
3	C	161	GLN
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	20	ARG
4	D	31	LYS
4	D	51	LEU
5	E	31	LYS
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	37	LYS

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Mol	Chain	Res	Type
6	F	48	LEU
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	8	HIS
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	52	VAL
8	H	60	TYR
9	I	8	GLN
9	I	26	MET
9	I	29	LEU
9	I	36	LYS
9	I	37	PHE
9	I	43	ARG
9	I	68	ILE
10	J	50	LEU
11	K	20	SER
11	K	47	ARG
11	K	54	ARG
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	109	PHE
1	N	136	LEU
1	N	152	LEU
1	N	169	ILE
1	N	180	GLN
1	N	278	MET
1	N	290	HIS
1	N	333	LYS

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Mol	Chain	Res	Type
1	N	338	MET
1	N	369	ASP
1	N	438	ARG
1	N	484	THR
1	N	495	LEU
1	N	504	THR
1	N	508	PRO
1	N	512	ASN
2	O	18	GLU
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	171	LYS
2	O	203	ASN
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	246	ASP
4	Q	5	VAL
4	Q	9	GLU
4	Q	17	VAL
4	Q	51	LEU
4	Q	141	ASP
4	Q	143	ASN
4	Q	147	LYS
5	R	46	LYS
5	R	80	GLU
5	R	109	VAL
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	64	GLU
7	T	2	SER

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Mol	Chain	Res	Type
7	T	5	LYS
7	T	8	HIS
7	T	17	ARG
7	T	18	PHE
7	T	36	TRP
7	T	37	LEU
7	T	42	ARG
7	T	84	LYS
8	U	7	LYS
8	U	9	LYS
8	U	52	VAL
8	U	60	TYR
8	U	84	LYS
9	V	2	THR
9	V	18	ARG
9	V	26	MET
9	V	29	LEU
9	V	37	PHE
9	V	61	GLU
9	V	65	LYS
9	V	70	GLN
9	V	73	LYS
10	W	50	LEU
11	X	20	SER
11	X	47	ARG
12	Y	20	ARG
12	Y	26	THR
12	Y	47	LYS
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	70	HIS
3	C	207	HIS
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	23	GLN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	328	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	207	HIS
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
6	S	95	GLN

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Mol	Chain	Res	Type
6	S	98	HIS
7	T	8	HIS
7	T	76	ASN
8	U	12	GLN
9	V	8	GLN
13	Z	36	HIS

### 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	9,9,10	1.05	1 (11%)	7,9,11	5.42	3 (42%)
2	FME	B	1	2	9,9,10	2.06	3 (33%)	7,9,11	8.14	4 (57%)
7	TPO	G	11	7	9,10,11	2.72	5 (55%)	11,14,16	1.49	2 (18%)
9	SAC	I	1	9	8,8,9	2.53	2 (25%)	7,9,11	2.04	2 (28%)
1	FME	N	1	1	9,9,10	0.67	0	7,9,11	6.28	3 (42%)
2	FME	O	1	2	9,9,10	1.33	2 (22%)	7,9,11	5.22	3 (42%)
7	TPO	T	11	7	9,10,11	3.33	4 (44%)	11,14,16	1.92	4 (36%)
9	SAC	V	1	9	8,8,9	3.38	3 (37%)	7,9,11	1.96	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	-	0/5/9/11	0/0/0/0
2	FME	B	1	2	-	0/5/9/11	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	-	0/5/9/11	0/0/0/0
2	FME	O	1	2	-	0/5/9/11	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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.57	1.08	1.22
2	B	1	FME	CG-SD	-2.31	1.68	1.81
2	O	1	FME	CA-C	-2.22	1.47	1.50
2	O	1	FME	O1-CN	-2.20	1.15	1.22
7	G	11	TPO	CG2-CB	2.02	1.56	1.51
7	T	11	TPO	P-O3P	2.16	1.63	1.54
7	G	11	TPO	CA-C	2.32	1.53	1.50
7	G	11	TPO	P-O2P	2.39	1.64	1.54
1	A	1	FME	CA-C	2.49	1.53	1.50
2	B	1	FME	CA-N	2.71	1.50	1.46
7	T	11	TPO	P-O1P	3.45	1.62	1.50
9	V	1	SAC	CA-C	3.57	1.54	1.50
7	G	11	TPO	P-O1P	3.97	1.64	1.50
9	I	1	SAC	CA-N	4.13	1.52	1.46
9	I	1	SAC	OAC-C1A	5.15	1.35	1.23
7	T	11	TPO	CA-C	5.28	1.57	1.50
7	G	11	TPO	P-OG1	5.37	1.69	1.59
9	V	1	SAC	OAC-C1A	5.59	1.36	1.23
9	V	1	SAC	CA-N	6.30	1.55	1.46
7	T	11	TPO	P-OG1	6.58	1.71	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.70	90.98	122.82
1	N	1	FME	CA-N-CN	-15.77	98.57	122.82
1	A	1	FME	CA-N-CN	-13.36	102.27	122.82
2	O	1	FME	CA-N-CN	-13.30	102.36	122.82
2	B	1	FME	CG-CB-CA	-4.09	101.51	112.97
9	I	1	SAC	OG-CB-CA	-3.22	102.83	111.00
2	B	1	FME	CB-CG-SD	-2.83	99.92	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	O-C-CA	-2.73	118.74	125.09
2	B	1	FME	O-C-CA	-2.70	118.80	125.09
7	T	11	TPO	O-C-CA	-2.60	119.03	125.09
7	T	11	TPO	C-CA-N	-2.46	104.90	109.86
9	V	1	SAC	O-C-CA	-2.45	119.37	125.09
1	A	1	FME	O-C-CA	-2.38	119.55	125.09
1	N	1	FME	O-C-CA	-2.28	119.78	125.09
2	O	1	FME	CG-CB-CA	-2.12	107.04	112.97
2	O	1	FME	O-C-CA	-2.11	120.18	125.09
7	G	11	TPO	O2P-P-OG1	2.54	117.36	105.99
7	T	11	TPO	P-OG1-CB	3.06	132.46	123.21
9	I	1	SAC	CA-N-C1A	3.07	128.84	123.24
7	T	11	TPO	O3P-P-OG1	3.32	120.87	105.99
9	V	1	SAC	CA-N-C1A	4.10	130.73	123.24
1	N	1	FME	CB-CA-C	4.27	120.00	111.85
1	A	1	FME	CE-SD-CG	4.46	116.22	100.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 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	515	1	43,67,67	1.42	9 (20%)	37,103,103	2.07	13 (35%)
14	HEA	A	516	1	43,67,67	1.36	7 (16%)	37,103,103	2.21	11 (29%)
15	NO	A	520	16	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	521	-	50,50,50	1.27	6 (12%)	53,56,56	1.75	12 (22%)
19	PGV	A	524	-	50,50,50	1.35	4 (8%)	53,56,56	1.70	11 (20%)
23	CHD	B	1085	-	29,32,32	1.84	5 (17%)	47,51,51	5.73	34 (72%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	229	-	51,51,51	1.22	3 (5%)	57,59,59	1.38	10 (17%)
21	TGL	B	521	-	62,62,62	1.30	6 (9%)	65,65,65	1.97	13 (20%)
25	PEK	C	264	-	52,52,52	0.93	2 (3%)	55,57,57	1.84	16 (29%)
25	PEK	C	265	-	52,52,52	1.62	6 (11%)	55,57,57	1.68	8 (14%)
19	PGV	C	267	-	50,50,50	0.88	3 (6%)	53,56,56	1.36	8 (15%)
19	PGV	C	268	-	50,50,50	1.41	4 (8%)	53,56,56	1.70	7 (13%)
26	CDL	C	270	-	99,99,99	1.48	13 (13%)	105,111,111	1.46	15 (14%)
23	CHD	C	271	-	29,32,32	0.73	0	47,51,51	5.03	33 (70%)
27	DMU	C	272	-	34,34,34	1.49	4 (11%)	45,45,45	3.37	25 (55%)
23	CHD	C	525	-	29,32,32	1.57	6 (20%)	47,51,51	5.57	37 (78%)
21	TGL	D	523	-	62,62,62	1.61	8 (12%)	65,65,65	1.56	15 (23%)
25	PEK	G	1263	-	52,52,52	1.34	4 (7%)	55,57,57	1.51	7 (12%)
26	CDL	G	269	-	99,99,99	1.43	12 (12%)	105,111,111	1.54	19 (18%)
23	CHD	J	60	-	29,32,32	0.96	0	47,51,51	5.35	35 (74%)
21	TGL	L	522	-	62,62,62	1.57	8 (12%)	65,65,65	2.14	16 (24%)
27	DMU	M	526	-	34,34,34	1.10	4 (11%)	45,45,45	3.32	25 (55%)
19	PGV	N	1266	-	50,50,50	0.98	2 (4%)	53,56,56	1.55	9 (16%)
21	TGL	N	1523	-	62,62,62	1.40	7 (11%)	65,65,65	1.47	10 (15%)
19	PGV	N	1524	-	50,50,50	1.10	2 (4%)	53,56,56	1.34	6 (11%)
14	HEA	N	515	1	43,67,67	1.12	4 (9%)	37,103,103	1.84	9 (24%)
14	HEA	N	516	1,15	43,67,67	1.14	5 (11%)	37,103,103	2.44	14 (37%)
15	NO	N	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
21	TGL	O	1521	-	62,62,62	1.36	6 (9%)	65,65,65	1.65	11 (16%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.62	5 (17%)	47,51,51	5.71	32 (68%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PEK	P	1264	-	52,52,52	0.93	3 (5%)	55,57,57	1.84	14 (25%)
19	PGV	P	1267	-	50,50,50	0.93	3 (6%)	53,56,56	1.54	8 (15%)
26	CDL	P	1270	-	99,99,99	1.45	12 (12%)	105,111,111	1.71	20 (19%)
23	CHD	P	1271	-	29,32,32	0.80	1 (3%)	47,51,51	5.12	33 (70%)
23	CHD	P	1525	-	29,32,32	1.68	6 (20%)	47,51,51	5.60	38 (80%)
27	DMU	P	272	-	34,34,34	1.65	6 (17%)	45,45,45	3.32	25 (55%)
22	PSC	R	1229	-	51,51,51	1.35	3 (5%)	57,59,59	1.34	5 (8%)
25	PEK	T	1265	-	52,52,52	1.43	6 (11%)	55,57,57	1.59	6 (10%)
26	CDL	T	1269	-	99,99,99	1.42	13 (13%)	105,111,111	1.55	16 (15%)
25	PEK	T	263	-	52,52,52	1.47	4 (7%)	55,57,57	1.42	7 (12%)
19	PGV	U	1268	-	50,50,50	1.56	3 (6%)	53,56,56	1.91	7 (13%)
23	CHD	W	1059	-	29,32,32	1.24	3 (10%)	47,51,51	5.45	32 (68%)
21	TGL	Y	1522	-	62,62,62	1.69	10 (16%)	65,65,65	2.25	17 (26%)
27	DMU	Z	1526	-	34,34,34	1.11	2 (5%)	45,45,45	3.11	25 (55%)

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	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	A	520	16	-	0/0/0/0	0/0/0/0
19	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	229	-	-	0/55/55/55	0/0/0/0
21	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
21	TGL	D	523	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
21	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
21	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	N	520	14,16	-	0/0/0/0	0/0/0/0
21	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	-	0/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	2/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	P	1525	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	P	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
25	PEK	T	1265	-	-	0/56/56/56	0/0/0/0
26	CDL	T	1269	-	-	3/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
19	PGV	U	1268	-	-	0/55/55/55	0/0/0/0
23	CHD	W	1059	-	1/1/12/12	0/7/74/74	0/4/4/4
21	TGL	Y	1522	-	-	2/65/65/65	0/0/0/0
27	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1085	CHD	C10-C5	-4.73	1.47	1.55
23	P	1525	CHD	C13-C12	-4.51	1.47	1.54
23	O	229	CHD	C13-C14	-3.98	1.48	1.55
21	L	522	TGL	C20-CA9	-3.53	1.31	1.51
23	B	1085	CHD	C13-C14	-3.47	1.49	1.55
27	Z	1526	DMU	C3-C4	-3.47	1.43	1.52
26	G	269	CDL	C59-C58	-3.41	1.32	1.51
21	Y	1522	TGL	C20-CA9	-3.35	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	C59-C58	-3.25	1.33	1.51
23	O	229	CHD	C10-C5	-3.20	1.50	1.55
26	T	1269	CDL	C62-C61	-3.13	1.33	1.51
21	O	1521	TGL	C10-CB9	-3.13	1.33	1.51
21	O	1521	TGL	C20-CA9	-3.13	1.33	1.51
26	P	1270	CDL	C59-C58	-3.10	1.33	1.51
21	B	521	TGL	C10-CB9	-3.10	1.33	1.51
27	M	526	DMU	C3-C4	-3.08	1.44	1.52
26	T	1269	CDL	C59-C58	-3.06	1.34	1.51
26	C	270	CDL	C79-C78	-3.02	1.34	1.51
26	G	269	CDL	C42-C41	-2.99	1.34	1.51
26	P	1270	CDL	C22-C21	-2.97	1.34	1.51
26	G	269	CDL	C62-C61	-2.95	1.34	1.51
26	T	1269	CDL	C79-C78	-2.95	1.34	1.51
26	P	1270	CDL	C19-C18	-2.94	1.34	1.51
21	L	522	TGL	C10-CB9	-2.93	1.34	1.51
23	P	1525	CHD	C6-C5	-2.93	1.48	1.53
21	N	1523	TGL	C10-CB9	-2.91	1.35	1.51
26	C	270	CDL	C39-C38	-2.90	1.35	1.51
26	C	270	CDL	C62-C61	-2.89	1.35	1.51
21	N	1523	TGL	C20-CA9	-2.89	1.35	1.51
21	Y	1522	TGL	C10-CB9	-2.87	1.35	1.51
26	C	270	CDL	C82-C81	-2.86	1.35	1.51
26	P	1270	CDL	C82-C81	-2.85	1.35	1.51
26	G	269	CDL	C39-C38	-2.84	1.35	1.51
26	P	1270	CDL	C39-C38	-2.83	1.35	1.51
26	G	269	CDL	C22-C21	-2.82	1.35	1.51
26	T	1269	CDL	C82-C81	-2.82	1.35	1.51
26	G	269	CDL	C19-C18	-2.80	1.35	1.51
26	C	270	CDL	C22-C21	-2.79	1.35	1.51
26	G	269	CDL	C79-C78	-2.79	1.35	1.51
21	D	523	TGL	C15-CC9	-2.78	1.35	1.51
26	P	1270	CDL	C62-C61	-2.78	1.35	1.51
26	T	1269	CDL	C42-C41	-2.78	1.35	1.51
21	N	1523	TGL	C15-CC9	-2.75	1.35	1.51
26	T	1269	CDL	C39-C38	-2.71	1.36	1.51
26	T	1269	CDL	C19-C18	-2.66	1.36	1.51
26	C	270	CDL	C19-C18	-2.65	1.36	1.51
21	D	523	TGL	C20-CA9	-2.63	1.36	1.51
14	A	516	HEA	C3C-C2C	-2.63	1.36	1.40
26	T	1269	CDL	C22-C21	-2.62	1.36	1.51
23	O	229	CHD	C1-C2	-2.61	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	521	TGL	C20-CA9	-2.61	1.36	1.51
26	P	1270	CDL	C79-C78	-2.57	1.37	1.51
21	O	1521	TGL	C15-CC9	-2.56	1.37	1.51
26	P	1270	CDL	C42-C41	-2.55	1.37	1.51
26	C	270	CDL	C42-C41	-2.53	1.37	1.51
21	L	522	TGL	C15-CC9	-2.49	1.37	1.51
21	Y	1522	TGL	C15-CC9	-2.48	1.37	1.51
26	G	269	CDL	C82-C81	-2.48	1.37	1.51
23	C	525	CHD	C13-C12	-2.46	1.50	1.54
14	A	515	HEA	C4B-C3B	-2.43	1.37	1.42
23	O	229	CHD	C6-C7	-2.40	1.48	1.52
19	A	521	PGV	P-O14	-2.39	1.43	1.55
23	P	1525	CHD	C10-C5	-2.37	1.51	1.55
27	M	526	DMU	C6-C1	-2.35	1.45	1.52
19	A	521	PGV	O01-C02	-2.34	1.40	1.46
21	D	523	TGL	C10-CB9	-2.33	1.38	1.51
23	B	1085	CHD	C8-C7	-2.29	1.49	1.53
21	B	521	TGL	C15-CC9	-2.27	1.38	1.51
19	C	268	PGV	O04-C19	-2.25	1.15	1.22
23	C	525	CHD	C1-C2	-2.24	1.48	1.53
14	A	515	HEA	C3A-C2A	-2.20	1.37	1.40
23	C	525	CHD	C1-C10	-2.16	1.50	1.54
23	P	1525	CHD	C13-C14	-2.11	1.51	1.55
27	M	526	DMU	O49-C1	-2.10	1.37	1.43
27	C	272	DMU	C3-C4	-2.04	1.47	1.52
14	A	516	HEA	C3A-C2A	-2.03	1.37	1.40
27	P	272	DMU	C3-C4	-2.01	1.47	1.52
14	A	515	HEA	C1A-C2A	-2.01	1.38	1.42
27	M	526	DMU	C8-C9	-2.00	1.48	1.53
19	C	267	PGV	O01-C1	2.01	1.40	1.34
14	A	515	HEA	O11-C11	2.01	1.47	1.42
14	N	516	HEA	C14-C15	2.02	1.38	1.33
19	P	1267	PGV	C03-C02	2.03	1.56	1.50
25	T	263	PEK	O12-C04	2.04	1.53	1.45
14	N	515	HEA	OMA-CMA	2.04	1.28	1.21
21	D	523	TGL	CB2-CB1	2.05	1.56	1.50
21	N	1523	TGL	OB1-CB1	2.06	1.28	1.22
25	T	1265	PEK	C22-C21	2.06	1.56	1.50
19	U	1268	PGV	P-O11	2.06	1.67	1.59
25	G	1263	PEK	C03-C02	2.08	1.56	1.50
26	T	1269	CDL	CA3-CA4	2.10	1.56	1.50
25	C	264	PEK	C2-C1	2.11	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	1263	PEK	P-O11	2.11	1.67	1.59
19	A	524	PGV	C01-C02	2.12	1.56	1.50
21	L	522	TGL	CG1-CG2	2.12	1.56	1.50
23	P	1525	CHD	C16-C17	2.13	1.58	1.54
25	P	1264	PEK	C2-C1	2.13	1.56	1.50
14	A	516	HEA	C1B-CHB	2.13	1.45	1.40
14	N	515	HEA	C1C-CHC	2.14	1.45	1.40
27	P	272	DMU	O7-C10	2.16	1.47	1.41
14	N	516	HEA	OMA-CMA	2.16	1.29	1.21
25	T	1265	PEK	C03-C02	2.20	1.57	1.50
21	Y	1522	TGL	CB2-CB1	2.22	1.57	1.50
19	A	524	PGV	C20-C19	2.23	1.57	1.50
14	A	515	HEA	C4D-CHA	2.27	1.46	1.40
27	P	272	DMU	O1-C10	2.32	1.47	1.41
14	A	515	HEA	C12-C13	2.33	1.61	1.53
14	A	515	HEA	CMC-C2C	2.33	1.56	1.51
14	A	516	HEA	C20-C19	2.34	1.56	1.51
25	C	265	PEK	C22-C21	2.34	1.57	1.50
27	C	272	DMU	O1-C10	2.34	1.47	1.41
27	P	272	DMU	O5-C4	2.36	1.50	1.44
14	N	516	HEA	CAD-C3D	2.37	1.56	1.52
21	L	522	TGL	CC2-CC1	2.42	1.57	1.50
14	A	515	HEA	C1B-CHB	2.42	1.46	1.40
23	C	525	CHD	C4-C3	2.43	1.56	1.51
14	N	515	HEA	C4C-CHD	2.43	1.46	1.40
19	C	267	PGV	C03-C02	2.46	1.57	1.50
14	A	516	HEA	CAD-C3D	2.48	1.56	1.52
14	A	516	HEA	C3C-CAC	2.50	1.52	1.47
25	P	1264	PEK	O03-C21	2.51	1.40	1.33
23	W	1059	CHD	C13-C17	2.51	1.60	1.55
23	P	1525	CHD	C11-C9	2.58	1.58	1.53
19	C	267	PGV	O03-C19	2.63	1.40	1.33
14	N	516	HEA	C4C-CHD	2.64	1.47	1.40
19	A	521	PGV	C01-C02	2.67	1.58	1.50
27	C	272	DMU	O5-C6	2.72	1.48	1.41
19	P	1267	PGV	O03-C19	2.72	1.41	1.33
27	P	272	DMU	O5-C6	2.74	1.48	1.41
23	B	1085	CHD	C11-C12	2.75	1.58	1.53
14	N	516	HEA	C1C-CHC	2.75	1.47	1.40
25	T	1265	PEK	P-O11	2.80	1.70	1.59
21	Y	1522	TGL	OG2-CG2	2.80	1.53	1.46
21	Y	1522	TGL	CG3-CG2	2.82	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	1267	PGV	O01-C1	2.82	1.42	1.34
23	W	1059	CHD	C11-C9	2.89	1.58	1.53
21	Y	1522	TGL	CG1-CG2	2.89	1.59	1.50
23	P	1271	CHD	C20-C17	2.90	1.59	1.54
14	A	516	HEA	CMD-C2D	2.96	1.58	1.51
25	T	1265	PEK	P-O12	2.98	1.71	1.59
14	A	515	HEA	C1C-CHC	3.07	1.48	1.40
25	C	265	PEK	P-O11	3.08	1.71	1.59
19	A	521	PGV	C03-C02	3.12	1.59	1.50
14	N	515	HEA	C4D-CHA	3.13	1.48	1.40
25	C	265	PEK	P-O12	3.23	1.72	1.59
27	Z	1526	DMU	O16-C6	3.28	1.45	1.40
25	P	1264	PEK	O01-C1	3.32	1.43	1.34
19	N	1266	PGV	O03-C19	3.36	1.43	1.33
19	N	1524	PGV	O01-C1	3.36	1.44	1.34
23	C	525	CHD	C18-C13	3.37	1.60	1.54
26	C	270	CDL	C18-C17	3.39	1.70	1.51
25	C	264	PEK	O01-C1	3.40	1.44	1.34
19	C	268	PGV	P-O11	3.40	1.73	1.59
21	B	521	TGL	OG3-CC1	3.47	1.43	1.33
19	N	1266	PGV	O01-C1	3.56	1.44	1.34
23	C	525	CHD	O12-C12	3.59	1.49	1.43
25	C	265	PEK	O03-C01	3.71	1.53	1.45
22	B	229	PSC	C13-C12	3.75	1.52	1.31
21	L	522	TGL	OG3-CC1	3.85	1.44	1.33
21	Y	1522	TGL	OG1-CA1	3.98	1.44	1.33
23	W	1059	CHD	C20-C17	4.03	1.61	1.54
21	O	1521	TGL	OG3-CC1	4.04	1.45	1.33
26	G	269	CDL	OB8-CB7	4.07	1.45	1.33
23	O	229	CHD	C18-C13	4.08	1.61	1.54
19	A	521	PGV	O03-C19	4.17	1.45	1.33
19	A	521	PGV	O01-C1	4.20	1.46	1.34
19	C	268	PGV	O03-C19	4.25	1.45	1.33
22	R	1229	PSC	O03-C19	4.26	1.45	1.33
26	C	270	CDL	OA6-CA5	4.27	1.46	1.34
22	R	1229	PSC	C13-C12	4.27	1.55	1.31
21	N	1523	TGL	OG3-CC1	4.31	1.45	1.33
19	A	524	PGV	O01-C1	4.31	1.46	1.34
22	B	229	PSC	O01-C1	4.37	1.46	1.34
26	C	270	CDL	OB6-CB5	4.44	1.47	1.34
26	T	1269	CDL	OA8-CA7	4.49	1.46	1.33
25	T	263	PEK	O01-C1	4.59	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	521	TGL	OG2-CB1	4.60	1.47	1.34
22	B	229	PSC	O03-C19	4.65	1.46	1.33
26	T	1269	CDL	OB8-CB7	4.71	1.47	1.33
26	T	1269	CDL	OB6-CB5	4.73	1.47	1.34
21	D	523	TGL	OG3-CC1	4.76	1.47	1.33
21	N	1523	TGL	OG1-CA1	4.79	1.47	1.33
26	P	1270	CDL	OB6-CB5	4.83	1.48	1.34
21	O	1521	TGL	OG2-CB1	4.83	1.48	1.34
21	L	522	TGL	OG1-CA1	4.90	1.47	1.33
26	G	269	CDL	OB6-CB5	4.99	1.48	1.34
26	G	269	CDL	OA8-CA7	4.99	1.47	1.33
21	B	521	TGL	OG1-CA1	5.00	1.47	1.33
26	P	1270	CDL	OB8-CB7	5.04	1.47	1.33
26	C	270	CDL	OB8-CB7	5.09	1.48	1.33
19	U	1268	PGV	O03-C19	5.19	1.48	1.33
21	D	523	TGL	OB1-CB1	5.23	1.38	1.22
19	N	1524	PGV	O03-C19	5.24	1.48	1.33
21	Y	1522	TGL	OG3-CC1	5.27	1.48	1.33
25	T	263	PEK	C05-C04	5.28	1.71	1.50
21	O	1521	TGL	OG1-CA1	5.29	1.48	1.33
21	N	1523	TGL	OG2-CB1	5.29	1.49	1.34
21	D	523	TGL	OG2-CB1	5.33	1.49	1.34
26	P	1270	CDL	OA8-CA7	5.35	1.48	1.33
21	D	523	TGL	OG1-CA1	5.42	1.49	1.33
25	G	1263	PEK	O01-C1	5.42	1.49	1.34
22	R	1229	PSC	O01-C1	5.44	1.50	1.34
26	T	1269	CDL	OA6-CA5	5.45	1.50	1.34
25	T	263	PEK	O03-C21	5.46	1.49	1.33
26	G	269	CDL	OA6-CA5	5.51	1.50	1.34
26	P	1270	CDL	OA6-CA5	5.51	1.50	1.34
25	T	1265	PEK	O03-C21	5.55	1.49	1.33
25	T	1265	PEK	O01-C1	5.60	1.50	1.34
25	G	1263	PEK	O03-C21	5.60	1.49	1.33
23	B	1085	CHD	C18-C13	5.62	1.63	1.54
19	A	524	PGV	O03-C19	5.64	1.49	1.33
25	C	265	PEK	O01-C1	5.67	1.50	1.34
26	C	270	CDL	OA8-CA7	5.67	1.49	1.33
27	C	272	DMU	O16-C6	5.93	1.50	1.40
19	C	268	PGV	O01-C1	6.42	1.52	1.34
25	C	265	PEK	O03-C21	6.50	1.52	1.33
27	P	272	DMU	O16-C6	6.90	1.52	1.40
21	L	522	TGL	OG2-CB1	7.08	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	U	1268	PGV	O01-C1	7.09	1.54	1.34
21	Y	1522	TGL	OG2-CB1	7.70	1.56	1.34

All (714) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C18-C13-C12	-13.70	94.92	109.07
23	P	1525	CHD	C18-C13-C12	-11.80	96.87	109.07
23	B	1085	CHD	C18-C13-C12	-11.00	97.70	109.07
23	C	525	CHD	C23-C22-C20	-10.23	100.94	114.72
23	W	1059	CHD	C6-C5-C4	-9.84	99.98	111.13
23	O	229	CHD	C19-C10-C9	-8.93	98.53	111.17
23	C	525	CHD	C19-C10-C9	-8.86	98.63	111.17
23	P	1271	CHD	C18-C13-C12	-8.69	100.09	109.07
23	P	1525	CHD	C19-C10-C9	-8.61	98.98	111.17
23	J	60	CHD	C18-C13-C12	-8.30	100.49	109.07
23	W	1059	CHD	C1-C10-C9	-8.08	98.51	111.36
23	C	525	CHD	C18-C13-C17	-8.00	98.60	111.23
23	B	1085	CHD	C19-C10-C9	-7.58	100.44	111.17
23	C	271	CHD	C18-C13-C12	-7.55	101.27	109.07
21	L	522	TGL	OG3-CC1-OC1	-7.38	105.58	123.58
23	B	1085	CHD	C18-C13-C17	-7.18	99.91	111.23
23	O	229	CHD	O12-C12-C13	-6.97	99.35	111.08
23	J	60	CHD	C6-C5-C4	-6.43	103.84	111.13
23	O	229	CHD	C6-C5-C4	-6.40	103.88	111.13
23	B	1085	CHD	O12-C12-C13	-6.33	100.43	111.08
23	J	60	CHD	C1-C10-C9	-6.01	101.80	111.36
23	P	1525	CHD	C6-C5-C4	-5.99	104.34	111.13
23	B	1085	CHD	C6-C5-C4	-5.83	104.52	111.13
23	C	525	CHD	C18-C13-C12	-5.82	103.06	109.07
23	C	525	CHD	C6-C5-C4	-5.75	104.62	111.13
23	B	1085	CHD	C4-C5-C10	-5.65	106.56	112.66
23	C	525	CHD	O12-C12-C13	-5.59	101.66	111.08
21	L	522	TGL	CA4-CA3-CA2	-5.59	92.94	113.23
14	N	515	HEA	C13-C12-C11	-5.57	106.03	114.46
23	P	1525	CHD	O12-C12-C13	-5.45	101.91	111.08
14	A	515	HEA	C13-C12-C11	-5.22	106.56	114.46
23	O	229	CHD	O12-C12-C11	-5.15	98.55	109.12
23	P	1525	CHD	C18-C13-C14	-5.15	103.11	111.23
14	N	516	HEA	C13-C12-C11	-5.00	106.89	114.46
23	C	271	CHD	C19-C10-C9	-5.00	104.09	111.17
23	O	229	CHD	C18-C13-C17	-4.94	103.44	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	264	PEK	O01-C1-O02	-4.92	111.55	123.69
19	A	521	PGV	C8-C9-C10	-4.89	94.96	113.70
25	T	1265	PEK	O03-C21-O04	-4.89	111.66	123.58
19	A	524	PGV	C4-C3-C2	-4.87	95.54	113.23
23	B	1085	CHD	O7-C7-C6	-4.84	97.82	109.95
23	P	1271	CHD	O7-C7-C6	-4.84	97.82	109.95
25	P	1264	PEK	O03-C01-C02	-4.84	96.58	108.64
14	A	516	HEA	C20-C19-C18	-4.79	111.34	121.10
23	C	525	CHD	C19-C10-C5	-4.74	102.14	110.35
23	O	229	CHD	O7-C7-C6	-4.65	98.30	109.95
21	B	521	TGL	OG3-CC1-OC1	-4.65	112.23	123.58
23	P	1271	CHD	C19-C10-C9	-4.63	104.62	111.17
23	P	1525	CHD	C1-C10-C9	-4.52	104.17	111.36
19	P	1267	PGV	O12-P-O13	-4.47	91.61	109.07
21	Y	1522	TGL	OG1-CA1-OA1	-4.45	112.71	123.58
23	C	525	CHD	O7-C7-C6	-4.44	98.83	109.95
23	P	1525	CHD	O7-C7-C6	-4.41	98.91	109.95
26	P	1270	CDL	CB4-OB6-CB5	-4.33	107.64	117.88
19	N	1266	PGV	O01-C1-O02	-4.30	113.08	123.69
23	P	1271	CHD	C18-C13-C17	-4.27	104.49	111.23
23	O	229	CHD	C18-C13-C14	-4.25	104.53	111.23
21	N	1523	TGL	CG3-CG2-CG1	-4.24	102.28	111.86
23	P	1525	CHD	C18-C13-C17	-4.19	104.62	111.23
19	P	1267	PGV	O03-C19-O04	-4.18	113.37	123.58
23	J	60	CHD	C19-C10-C5	-4.18	103.12	110.35
19	U	1268	PGV	O04-C19-C20	-4.14	107.54	123.70
14	N	516	HEA	CAD-CBD-CGD	-4.11	105.64	112.66
19	N	1524	PGV	C4-C3-C2	-4.10	98.33	113.23
14	A	516	HEA	C4B-C3B-C2B	-4.07	104.03	106.87
25	P	1264	PEK	O01-C1-O02	-4.06	113.67	123.69
21	N	1523	TGL	OG3-CC1-OC1	-4.01	113.80	123.58
19	A	524	PGV	C8-C9-C10	-4.00	98.37	113.70
25	C	265	PEK	O03-C21-O04	-3.99	113.85	123.58
25	C	264	PEK	O03-C01-C02	-3.94	98.83	108.64
23	C	271	CHD	C23-C22-C20	-3.91	109.45	114.72
23	C	525	CHD	O12-C12-C11	-3.86	101.20	109.12
26	T	1269	CDL	CB6-CB4-CB3	-3.83	103.21	111.86
23	P	1525	CHD	C21-C20-C22	-3.83	104.32	110.34
23	C	525	CHD	C18-C13-C14	-3.78	105.27	111.23
14	A	515	HEA	CMB-C2B-C1B	-3.70	122.77	128.46
27	M	526	DMU	O7-C10-C5	-3.69	98.30	108.08
14	N	516	HEA	CAD-C3D-C2D	-3.65	118.58	129.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C23-C22-C20	-3.65	109.81	114.72
14	N	515	HEA	C1B-C2B-C3B	-3.62	104.47	107.00
14	N	516	HEA	C13-C14-C15	-3.60	118.75	127.66
21	L	522	TGL	CA8-CA7-CA6	-3.60	94.88	114.41
23	C	525	CHD	C22-C20-C17	-3.58	102.79	110.28
23	J	60	CHD	O12-C12-C11	-3.58	101.78	109.12
19	C	268	PGV	O04-C19-C20	-3.57	109.74	123.70
25	P	1264	PEK	C03-C02-C01	-3.56	103.82	111.86
19	A	524	PGV	O03-C19-O04	-3.56	114.90	123.58
23	B	1085	CHD	O12-C12-C11	-3.55	101.84	109.12
26	G	269	CDL	OB8-CB7-OB9	-3.48	115.10	123.58
26	P	1270	CDL	C53-C52-C51	-3.46	100.67	113.23
21	O	1521	TGL	OG3-CC1-OC1	-3.45	115.17	123.58
23	C	271	CHD	O7-C7-C6	-3.45	101.32	109.95
14	N	516	HEA	C4B-C3B-C2B	-3.43	104.47	106.87
23	P	1271	CHD	O12-C12-C11	-3.43	102.07	109.12
25	T	263	PEK	O03-C21-O04	-3.40	115.28	123.58
25	P	1264	PEK	O01-C02-C01	-3.35	96.31	108.43
25	C	264	PEK	C03-C02-C01	-3.33	104.34	111.86
23	P	1271	CHD	C19-C10-C5	-3.31	104.62	110.35
23	B	1085	CHD	C23-C22-C20	-3.30	110.27	114.72
14	A	515	HEA	CAA-CBA-CGA	-3.28	107.05	112.66
26	C	270	CDL	OB8-CB7-OB9	-3.27	115.59	123.58
14	N	516	HEA	C1B-C2B-C3B	-3.27	104.72	107.00
19	U	1268	PGV	O02-C1-C2	-3.27	110.95	123.70
23	P	1525	CHD	O12-C12-C11	-3.26	102.43	109.12
27	Z	1526	DMU	O7-C10-C5	-3.25	99.47	108.08
25	C	264	PEK	C3-C2-C1	-3.23	101.95	113.60
19	C	267	PGV	O12-P-O13	-3.23	96.46	109.07
26	P	1270	CDL	OA8-CA7-OA9	-3.22	115.72	123.58
14	N	515	HEA	C21-C20-C19	-3.22	102.22	112.85
14	A	516	HEA	C12-C13-C14	-3.19	103.97	112.33
14	A	516	HEA	CAA-CBA-CGA	-3.16	107.27	112.66
23	C	271	CHD	O3-C3-C4	-3.15	103.56	109.86
26	T	1269	CDL	OA6-CA5-OA7	-3.13	115.96	123.69
23	C	271	CHD	C6-C5-C4	-3.11	107.61	111.13
19	A	521	PGV	O01-C1-O02	-3.09	116.05	123.69
22	B	229	PSC	C30-C29-C28	-3.09	97.65	114.41
23	C	271	CHD	C19-C10-C1	-3.07	103.26	108.25
19	A	521	PGV	O03-C19-O04	-3.06	116.12	123.58
14	A	515	HEA	C17-C18-C19	-2.97	120.30	127.66
19	A	521	PGV	C7-C6-C5	-2.94	98.44	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	OA8-CA7-OA9	-2.93	116.42	123.58
23	O	229	CHD	C1-C10-C9	-2.93	106.69	111.36
26	P	1270	CDL	OA6-CA5-OA7	-2.93	116.45	123.69
19	C	267	PGV	O03-C19-O04	-2.91	116.48	123.58
21	D	523	TGL	OG1-CA1-OA1	-2.91	116.48	123.58
14	N	515	HEA	OMA-CMA-C3A	-2.91	118.48	125.09
23	W	1059	CHD	C18-C13-C14	-2.91	106.64	111.23
23	C	271	CHD	O12-C12-C11	-2.90	103.17	109.12
25	C	264	PEK	C25-C24-C23	-2.89	98.72	114.41
14	N	516	HEA	C27-C19-C18	-2.89	116.11	123.70
23	J	60	CHD	C18-C13-C14	-2.88	106.69	111.23
23	P	1525	CHD	C22-C20-C17	-2.87	104.28	110.28
23	B	1085	CHD	C19-C10-C5	-2.85	105.41	110.35
19	N	1266	PGV	C15-C14-C13	-2.84	102.82	113.70
23	B	1085	CHD	C1-C10-C9	-2.83	106.86	111.36
23	W	1059	CHD	C18-C13-C12	-2.83	106.14	109.07
25	G	1263	PEK	O01-C1-O02	-2.83	116.71	123.69
21	L	522	TGL	CB4-CB3-CB2	-2.82	103.00	113.23
26	T	1269	CDL	OB5-PB2-OB3	-2.81	98.08	109.07
27	M	526	DMU	C25-C28-C31	-2.80	99.21	114.41
26	P	1270	CDL	OB8-CB7-OB9	-2.80	116.75	123.58
26	G	269	CDL	OB6-CB5-OB7	-2.78	116.81	123.69
19	A	521	PGV	C15-C14-C13	-2.78	103.06	113.70
14	A	516	HEA	CBA-CAA-C2A	-2.77	107.19	112.47
14	N	515	HEA	C13-C14-C15	-2.77	120.81	127.66
23	B	1085	CHD	C18-C13-C14	-2.75	106.89	111.23
14	A	516	HEA	O11-C11-C3B	-2.75	104.07	112.00
22	B	229	PSC	C32-C31-C30	-2.75	99.49	114.41
22	R	1229	PSC	O01-C1-O02	-2.74	116.92	123.69
25	P	1264	PEK	O11-P-O14	-2.74	98.36	109.07
14	A	515	HEA	O11-C11-C3B	-2.72	104.15	112.00
21	B	521	TGL	OG1-CG1-CG2	-2.72	101.86	108.64
19	N	1524	PGV	O03-C19-O04	-2.71	116.97	123.58
21	Y	1522	TGL	OG3-CC1-OC1	-2.71	116.98	123.58
14	A	515	HEA	CAD-CBD-CGD	-2.69	108.06	112.66
19	N	1524	PGV	O01-C1-O02	-2.69	117.05	123.69
19	N	1266	PGV	C23-C22-C21	-2.66	99.96	114.41
27	M	526	DMU	O4-C7-C5	-2.66	104.13	110.34
19	C	267	PGV	C30-C29-C28	-2.65	100.01	114.41
19	A	521	PGV	C23-C22-C21	-2.64	100.09	114.41
23	J	60	CHD	O7-C7-C6	-2.63	103.37	109.95
23	C	525	CHD	C1-C10-C9	-2.62	107.19	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	CMB-C2B-C1B	-2.62	124.44	128.46
21	D	523	TGL	OG2-CB1-CB2	-2.60	106.07	111.55
27	P	272	DMU	O55-C2-C3	-2.59	102.94	109.93
14	A	515	HEA	C26-C15-C14	-2.59	116.90	123.70
14	A	515	HEA	C21-C20-C19	-2.58	104.34	112.85
21	L	522	TGL	C22-C21-C20	-2.57	100.49	114.41
27	M	526	DMU	C22-C19-C18	-2.56	101.94	113.51
19	C	268	PGV	O03-C19-O04	-2.56	117.34	123.58
23	P	1271	CHD	C6-C5-C4	-2.55	108.25	111.13
23	O	229	CHD	C19-C10-C5	-2.55	105.94	110.35
27	M	526	DMU	O7-C10-O1	-2.54	103.47	110.66
21	Y	1522	TGL	OB1-CB1-CB2	-2.54	113.80	123.70
19	C	267	PGV	O03-C01-C02	-2.53	102.32	108.64
26	C	270	CDL	OA6-CA5-OA7	-2.53	117.45	123.69
25	T	1265	PEK	C2-C3-C4	-2.52	108.82	113.28
21	Y	1522	TGL	OG2-CB1-OB1	-2.52	117.48	123.69
25	C	264	PEK	C32-C31-C30	-2.50	100.85	114.41
23	C	271	CHD	C18-C13-C17	-2.49	107.30	111.23
25	T	263	PEK	O01-C1-O02	-2.49	117.55	123.69
23	W	1059	CHD	C23-C22-C20	-2.47	111.39	114.72
26	C	270	CDL	C18-C17-C16	-2.46	101.04	114.41
21	O	1521	TGL	OG2-CB1-OB1	-2.43	117.69	123.69
23	W	1059	CHD	C19-C10-C1	-2.43	104.30	108.25
19	P	1267	PGV	C03-C02-C01	-2.43	106.39	111.86
26	T	1269	CDL	OB8-CB7-OB9	-2.42	117.68	123.58
21	L	522	TGL	C26-C25-C24	-2.41	101.31	114.41
19	A	521	PGV	C6-C5-C4	-2.41	101.33	114.41
21	D	523	TGL	CC4-CC3-CC2	-2.41	104.49	113.23
26	G	269	CDL	CB2-C1-CA2	-2.40	105.57	112.75
19	A	521	PGV	C01-O03-C19	-2.37	110.05	117.13
21	N	1523	TGL	OG1-CA1-OA1	-2.34	117.86	123.58
22	B	229	PSC	C11-C12-C13	-2.34	111.05	124.90
22	B	229	PSC	O01-C1-O02	-2.34	117.91	123.69
21	L	522	TGL	CA9-CA8-CA7	-2.33	101.75	114.41
21	B	521	TGL	OB1-CB1-CB2	-2.33	114.62	123.70
26	G	269	CDL	OA6-CA5-OA7	-2.33	117.95	123.69
26	C	270	CDL	C53-C52-C51	-2.32	104.79	113.23
21	L	522	TGL	OB1-CB1-CB2	-2.32	114.63	123.70
25	P	1264	PEK	C24-C23-C22	-2.32	104.80	113.23
19	N	1266	PGV	O03-C19-O04	-2.32	117.93	123.58
23	W	1059	CHD	C19-C10-C5	-2.31	106.36	110.35
19	N	1266	PGV	O14-P-O12	-2.29	97.12	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	CB6-CB4-CB3	-2.28	106.70	111.86
25	C	264	PEK	O03-C21-O04	-2.28	118.01	123.58
27	Z	1526	DMU	O7-C10-O1	-2.26	104.26	110.66
19	N	1266	PGV	O01-C02-C01	-2.26	100.26	108.43
19	C	268	PGV	O02-C1-C2	-2.25	114.90	123.70
14	A	516	HEA	C13-C14-C15	-2.25	122.09	127.66
19	P	1267	PGV	C7-C6-C5	-2.24	102.23	114.41
25	C	265	PEK	O04-C21-C22	-2.24	114.96	123.70
26	C	270	CDL	O1-C1-CA2	-2.24	101.28	109.42
14	N	516	HEA	O11-C11-C3B	-2.23	105.56	112.00
22	B	229	PSC	C27-C26-C25	-2.23	102.30	114.41
25	P	1264	PEK	O03-C21-C22	-2.22	105.49	111.92
19	P	1267	PGV	C4-C3-C2	-2.21	105.20	113.23
26	P	1270	CDL	CA6-CA4-CA3	-2.21	106.88	111.86
14	N	516	HEA	C20-C19-C18	-2.20	116.61	121.10
21	Y	1522	TGL	C26-C25-C24	-2.20	102.49	114.41
25	C	264	PEK	C26-C25-C24	-2.20	102.50	114.41
23	J	60	CHD	O12-C12-C13	-2.19	107.39	111.08
25	P	1264	PEK	C3-C2-C1	-2.19	105.71	113.60
14	A	516	HEA	OMA-CMA-C3A	-2.19	120.12	125.09
19	A	524	PGV	C8-C7-C6	-2.17	102.65	114.41
23	C	525	CHD	O7-C7-C8	-2.17	104.51	109.33
19	N	1266	PGV	C6-C5-C4	-2.17	102.66	114.41
23	P	1525	CHD	C4-C5-C10	-2.16	110.33	112.66
25	P	1264	PEK	C33-C32-C31	-2.14	102.80	114.41
25	C	264	PEK	C24-C23-C22	-2.13	105.48	113.23
21	Y	1522	TGL	CG3-CG2-CG1	-2.13	107.04	111.86
27	P	272	DMU	O49-C1-C2	-2.13	105.37	110.34
23	P	1525	CHD	C19-C10-C5	-2.12	106.69	110.35
19	P	1267	PGV	C22-C21-C20	-2.12	105.55	113.23
27	C	272	DMU	O2-C8-C7	-2.11	105.42	110.34
26	P	1270	CDL	C54-C53-C52	-2.11	102.97	114.41
21	B	521	TGL	OG2-CB1-OB1	-2.11	118.49	123.69
23	P	1271	CHD	C1-C10-C9	-2.09	108.03	111.36
26	P	1270	CDL	C56-C55-C54	-2.09	103.08	114.41
23	C	271	CHD	C22-C20-C17	-2.08	105.93	110.28
26	P	1270	CDL	OA7-CA5-C11	-2.08	115.59	123.70
19	C	267	PGV	C21-C20-C19	-2.06	106.18	113.60
25	C	264	PEK	C35-C34-C33	-2.03	103.38	114.41
22	B	229	PSC	O03-C19-O04	-2.02	118.64	123.58
23	C	271	CHD	C19-C10-C5	-2.01	106.87	110.35
14	A	515	HEA	OMA-CMA-C3A	-2.00	120.54	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	524	PGV	C21-C20-C19	2.01	120.85	113.60
22	R	1229	PSC	O03-C01-C02	2.01	113.65	108.64
26	C	270	CDL	C22-C21-C20	2.02	125.35	114.41
26	P	1270	CDL	C40-C39-C38	2.02	125.36	114.41
21	N	1523	TGL	C21-C20-CA9	2.02	125.36	114.41
27	C	272	DMU	O7-C10-C5	2.02	113.44	108.08
22	R	1229	PSC	C01-O03-C19	2.02	123.18	117.13
21	O	1521	TGL	OG2-CG2-CG1	2.03	115.77	108.43
27	P	272	DMU	O7-C3-C2	2.03	112.73	107.27
23	B	1085	CHD	C1-C2-C3	2.03	113.04	110.45
27	C	272	DMU	O55-C2-C3	2.04	115.43	109.93
21	D	523	TGL	C21-C20-CA9	2.04	125.50	114.41
26	T	1269	CDL	C20-C19-C18	2.05	125.53	114.41
21	D	523	TGL	CB5-CB4-CB3	2.05	125.53	114.41
21	D	523	TGL	C13-C12-C11	2.05	125.56	114.41
26	G	269	CDL	C23-C22-C21	2.06	125.57	114.41
21	O	1521	TGL	OG2-CG2-CG3	2.06	115.88	108.43
21	Y	1522	TGL	C10-CB9-CB8	2.06	125.58	114.41
26	T	1269	CDL	OB8-CB6-CB4	2.06	113.77	108.64
26	T	1269	CDL	C39-C38-C37	2.07	125.66	114.41
26	G	269	CDL	OB8-CB6-CB4	2.08	113.81	108.64
14	N	515	HEA	C12-C11-C3B	2.08	118.19	112.68
25	T	1265	PEK	C24-C23-C22	2.09	120.84	113.23
27	Z	1526	DMU	O61-C57-C4	2.10	118.61	111.29
22	B	229	PSC	C01-O03-C19	2.10	123.39	117.13
21	D	523	TGL	C20-CA9-CA8	2.10	125.83	114.41
26	C	270	CDL	C39-C38-C37	2.11	125.85	114.41
26	C	270	CDL	C83-C82-C81	2.11	125.86	114.41
14	N	515	HEA	CMB-C2B-C3B	2.11	128.98	124.92
27	Z	1526	DMU	O7-C3-C4	2.12	115.29	109.42
23	B	1085	CHD	C13-C14-C8	2.12	117.50	114.77
27	Z	1526	DMU	O55-C2-C3	2.13	115.67	109.93
23	C	525	CHD	C2-C1-C10	2.14	116.50	112.79
26	T	1269	CDL	CA6-OA8-CA7	2.14	123.53	117.13
26	C	270	CDL	OB4-PB2-OB3	2.14	123.04	112.14
25	G	1263	PEK	C2-C3-C4	2.17	117.11	113.28
25	C	264	PEK	O13-P-O14	2.19	123.28	112.14
19	C	267	PGV	O14-P-O13	2.19	123.29	112.14
27	C	272	DMU	C11-C9-C8	2.20	118.19	112.99
25	C	265	PEK	P-O11-C03	2.20	134.60	121.68
21	Y	1522	TGL	C15-CC9-CC8	2.21	126.39	114.41
26	P	1270	CDL	C42-C41-C40	2.21	126.42	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	523	TGL	CG3-OG3-CC1	2.21	123.74	117.13
21	N	1523	TGL	OG2-CG2-CG3	2.23	116.51	108.43
26	T	1269	CDL	CA4-OA6-CA5	2.23	123.15	117.88
26	G	269	CDL	O1-C1-CB2	2.24	117.57	109.42
23	O	229	CHD	C2-C1-C10	2.24	116.68	112.79
27	Z	1526	DMU	C6-C1-C2	2.25	114.67	109.98
25	T	263	PEK	O03-C01-C02	2.25	114.23	108.64
21	D	523	TGL	OG2-CG2-CG3	2.25	116.58	108.43
23	J	60	CHD	C14-C8-C9	2.26	112.71	109.64
25	G	1263	PEK	C11-C10-C9	2.26	119.52	111.84
25	C	265	PEK	O13-P-O11	2.26	118.25	107.75
21	N	1523	TGL	OG2-CB1-CB2	2.27	116.33	111.55
19	A	524	PGV	C02-O01-C1	2.27	123.23	117.88
26	G	269	CDL	C82-C81-C80	2.27	126.72	114.41
21	D	523	TGL	C11-C10-CB9	2.28	126.76	114.41
19	A	524	PGV	C01-O03-C19	2.28	123.94	117.13
21	O	1521	TGL	C15-CC9-CC8	2.30	126.88	114.41
26	P	1270	CDL	OB4-PB2-OB3	2.30	123.83	112.14
26	T	1269	CDL	C82-C81-C80	2.31	126.93	114.41
21	L	522	TGL	C15-CC9-CC8	2.31	126.97	114.41
14	N	515	HEA	C3C-C4C-NC	2.31	112.20	109.21
23	C	525	CHD	C9-C11-C12	2.32	117.39	114.33
19	C	268	PGV	O01-C02-C03	2.33	116.86	108.43
14	N	516	HEA	C16-C15-C14	2.35	125.87	121.10
21	D	523	TGL	CG1-OG1-CA1	2.35	124.14	117.13
19	U	1268	PGV	O01-C02-C01	2.35	116.94	108.43
26	C	270	CDL	O1-C1-CB2	2.35	117.97	109.42
19	A	524	PGV	O14-P-O13	2.35	124.09	112.14
27	Z	1526	DMU	O16-C18-C19	2.35	118.07	109.68
19	C	267	PGV	O03-C19-C20	2.37	118.78	111.92
26	G	269	CDL	OA8-CA6-CA4	2.40	114.62	108.64
26	P	1270	CDL	CA6-OA8-CA7	2.42	124.36	117.13
21	L	522	TGL	OG2-CG2-CG1	2.42	117.21	108.43
22	B	229	PSC	C16-C15-C14	2.43	123.03	113.70
19	U	1268	PGV	C01-O03-C19	2.47	124.50	117.13
26	G	269	CDL	CB6-OB8-CB7	2.48	124.55	117.13
25	C	265	PEK	C24-C23-C22	2.50	122.30	113.23
23	P	1525	CHD	C2-C1-C10	2.50	117.12	112.79
26	P	1270	CDL	OB6-CB5-C51	2.50	116.81	111.55
25	C	265	PEK	O12-C04-C05	2.50	118.44	109.10
23	J	60	CHD	C9-C8-C7	2.50	114.85	111.92
14	A	515	HEA	C3C-C4C-NC	2.52	112.47	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	272	DMU	O7-C10-O1	2.52	117.80	110.66
27	C	272	DMU	O16-C18-C19	2.53	118.70	109.68
19	A	521	PGV	C9-C8-C7	2.53	128.15	114.41
25	P	1264	PEK	O04-C21-C22	2.53	133.59	123.70
26	G	269	CDL	OB8-CB7-C71	2.53	119.25	111.92
27	Z	1526	DMU	O5-C6-O16	2.57	116.05	109.96
25	C	264	PEK	C14-C13-C12	2.58	120.60	111.84
19	U	1268	PGV	C15-C14-C13	2.58	123.59	113.70
21	B	521	TGL	CC3-CC2-CC1	2.61	123.01	113.60
27	M	526	DMU	C1-C2-C3	2.61	115.68	109.68
26	G	269	CDL	OA6-CA4-CA6	2.62	117.92	108.43
27	P	272	DMU	C11-C9-C8	2.62	119.19	112.99
26	T	1269	CDL	C43-C42-C41	2.63	128.66	114.41
27	Z	1526	DMU	O3-C5-C7	2.64	116.51	110.34
19	A	521	PGV	C8-C7-C6	2.65	128.77	114.41
27	M	526	DMU	O49-C1-C2	2.65	116.54	110.34
14	N	515	HEA	C26-C15-C16	2.67	119.89	115.29
27	M	526	DMU	C10-C5-C7	2.67	115.56	109.98
21	N	1523	TGL	OG1-CA1-CA2	2.67	119.65	111.92
26	P	1270	CDL	C79-C78-C77	2.68	128.95	114.41
21	Y	1522	TGL	OG2-CG2-CG3	2.69	118.18	108.43
27	M	526	DMU	C11-C9-C8	2.70	119.37	112.99
23	P	1525	CHD	C1-C2-C3	2.70	113.89	110.45
26	G	269	CDL	OA8-CA7-C31	2.71	119.75	111.92
19	C	267	PGV	O14-P-O12	2.71	120.35	107.75
27	C	272	DMU	C10-O1-C9	2.71	119.06	113.71
26	T	1269	CDL	CB6-OB8-CB7	2.71	125.24	117.13
14	A	515	HEA	CMB-C2B-C3B	2.72	130.13	124.92
21	L	522	TGL	OG1-CA1-CA2	2.72	119.78	111.92
23	C	525	CHD	C15-C16-C17	2.72	110.55	105.13
26	P	1270	CDL	OA8-CA6-CA4	2.72	115.43	108.64
26	G	269	CDL	C83-C82-C81	2.73	129.22	114.41
27	P	272	DMU	O5-C6-C1	2.74	116.23	110.34
26	C	270	CDL	C42-C41-C40	2.75	129.31	114.41
14	N	516	HEA	CBD-CAD-C3D	2.75	117.74	112.48
26	G	269	CDL	C80-C79-C78	2.75	129.35	114.41
25	P	1264	PEK	C8-C7-C6	2.77	121.27	111.84
23	B	1085	CHD	C16-C17-C20	2.78	116.58	112.15
27	Z	1526	DMU	C57-C4-C3	2.80	121.54	113.31
23	P	1525	CHD	C13-C14-C8	2.81	118.38	114.77
27	Z	1526	DMU	C11-C9-C8	2.84	119.70	112.99
27	P	272	DMU	C10-O1-C9	2.87	119.36	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C14-C8-C7	2.87	115.68	111.80
27	Z	1526	DMU	O7-C3-C2	2.89	115.03	107.27
25	T	1265	PEK	O03-C01-C02	2.90	115.87	108.64
26	C	270	CDL	CA6-OA8-CA7	2.91	125.81	117.13
25	C	264	PEK	O01-C1-C2	2.92	117.70	111.55
21	Y	1522	TGL	CG3-OG3-CC1	2.92	125.85	117.13
23	J	60	CHD	C16-C17-C20	2.92	116.81	112.15
21	B	521	TGL	C15-CC9-CC8	2.94	130.34	114.41
23	J	60	CHD	C11-C9-C10	2.96	116.87	113.74
23	B	1085	CHD	C16-C17-C13	2.97	106.53	103.57
19	A	524	PGV	O03-C01-C02	2.98	116.06	108.64
23	C	525	CHD	C15-C14-C8	2.98	122.54	118.33
27	Z	1526	DMU	C10-C5-C7	2.99	116.24	109.98
27	M	526	DMU	O55-C2-C1	3.01	117.36	110.34
27	C	272	DMU	O7-C3-C4	3.03	117.81	109.42
26	C	270	CDL	OA8-CA7-C31	3.07	120.78	111.92
14	N	516	HEA	CMB-C2B-C3B	3.07	130.81	124.92
23	B	1085	CHD	C11-C9-C10	3.07	116.98	113.74
23	O	229	CHD	C16-C17-C13	3.07	106.64	103.57
27	P	272	DMU	O16-C18-C19	3.07	120.64	109.68
21	D	523	TGL	C10-CB9-CB8	3.08	131.11	114.41
23	O	229	CHD	C6-C7-C8	3.09	114.81	111.51
14	A	515	HEA	C16-C17-C18	3.09	122.22	111.87
21	B	521	TGL	CG2-OG2-CB1	3.11	125.22	117.88
25	C	264	PEK	C11-C10-C9	3.12	122.44	111.84
27	Z	1526	DMU	C1-C2-C3	3.16	116.94	109.68
23	P	1525	CHD	C16-C17-C13	3.17	106.73	103.57
23	O	229	CHD	C11-C9-C10	3.19	117.10	113.74
23	C	271	CHD	C17-C13-C14	3.20	103.36	100.08
23	C	525	CHD	C19-C10-C1	3.21	113.48	108.25
23	C	525	CHD	C5-C6-C7	3.24	118.02	114.44
22	B	229	PSC	O03-C19-C20	3.25	121.31	111.92
25	G	1263	PEK	O03-C21-C22	3.25	121.32	111.92
21	N	1523	TGL	CG3-OG3-CC1	3.25	126.85	117.13
21	O	1521	TGL	CG1-OG1-CA1	3.26	126.86	117.13
21	B	521	TGL	CG1-OG1-CA1	3.27	126.89	117.13
21	O	1521	TGL	CG3-OG3-CC1	3.27	126.89	117.13
23	P	1525	CHD	C6-C7-C8	3.28	115.02	111.51
26	G	269	CDL	CA6-OA8-CA7	3.31	127.02	117.13
19	C	268	PGV	P-O11-C03	3.31	141.11	121.68
27	C	272	DMU	C10-C5-C7	3.32	116.92	109.98
27	M	526	DMU	O3-C5-C7	3.32	118.09	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C14-C8-C7	3.32	116.29	111.80
25	C	264	PEK	C01-O03-C21	3.33	127.09	117.13
23	P	1271	CHD	C11-C12-C13	3.34	114.69	111.23
19	A	524	PGV	O01-C02-C01	3.34	120.54	108.43
25	G	1263	PEK	C01-O03-C21	3.35	127.15	117.13
23	P	1525	CHD	C16-C17-C20	3.35	117.50	112.15
25	T	263	PEK	C2-C3-C4	3.37	119.23	113.28
27	P	272	DMU	C10-C5-C7	3.38	117.04	109.98
23	J	60	CHD	C9-C10-C5	3.40	113.50	108.61
14	A	516	HEA	CBD-CAD-C3D	3.40	118.99	112.48
19	N	1524	PGV	O01-C1-C2	3.40	118.73	111.55
23	O	229	CHD	C16-C17-C20	3.42	117.60	112.15
23	P	1525	CHD	C11-C12-C13	3.45	114.80	111.23
22	R	1229	PSC	O03-C19-C20	3.47	121.94	111.92
23	P	1525	CHD	C14-C8-C9	3.48	114.37	109.64
27	P	272	DMU	C2-C3-C4	3.49	119.03	110.93
21	L	522	TGL	OG1-CG1-CG2	3.49	117.34	108.64
19	N	1524	PGV	O03-C01-C02	3.50	117.35	108.64
23	B	1085	CHD	C11-C9-C8	3.51	115.97	110.81
21	Y	1522	TGL	CB3-CB2-CB1	3.51	126.28	113.60
23	P	1525	CHD	C13-C17-C20	3.52	123.78	119.50
27	P	272	DMU	O7-C3-C4	3.54	119.21	109.42
25	T	263	PEK	O03-C21-C22	3.55	122.17	111.92
27	M	526	DMU	O5-C4-C3	3.55	117.30	109.76
25	P	1264	PEK	O13-P-O14	3.55	130.21	112.14
23	C	525	CHD	C5-C4-C3	3.56	118.09	112.83
25	T	263	PEK	C01-O03-C21	3.58	127.83	117.13
23	C	271	CHD	C21-C20-C17	3.59	118.53	112.94
25	P	1264	PEK	O01-C1-C2	3.60	119.13	111.55
27	Z	1526	DMU	C6-O5-C4	3.60	120.80	113.71
21	D	523	TGL	OG1-CA1-CA2	3.61	122.35	111.92
19	A	521	PGV	O01-C1-C2	3.62	119.19	111.55
27	C	272	DMU	O5-C6-O16	3.62	118.53	109.96
21	B	521	TGL	OG1-CA1-CA2	3.63	122.42	111.92
25	C	264	PEK	C2-C3-C4	3.63	119.70	113.28
21	Y	1522	TGL	OG2-CG2-CG1	3.64	121.61	108.43
19	N	1266	PGV	O01-C1-C2	3.65	119.24	111.55
23	B	1085	CHD	C9-C11-C12	3.65	119.15	114.33
23	C	525	CHD	C1-C2-C3	3.65	115.11	110.45
22	B	229	PSC	O01-C1-C2	3.69	119.33	111.55
27	C	272	DMU	C1-C2-C3	3.71	118.20	109.68
23	P	1525	CHD	O3-C3-C4	3.72	117.30	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C21-C20-C17	3.73	118.75	112.94
21	O	1521	TGL	CG2-OG2-CB1	3.76	126.77	117.88
27	C	272	DMU	O61-C57-C4	3.77	124.44	111.29
27	P	272	DMU	C7-C8-C9	3.77	116.99	110.24
27	C	272	DMU	O5-C4-C3	3.78	117.79	109.76
19	P	1267	PGV	O03-C19-C20	3.79	122.89	111.92
23	P	1271	CHD	C9-C10-C5	3.80	114.08	108.61
23	O	229	CHD	C5-C6-C7	3.82	118.67	114.44
26	P	1270	CDL	CA4-OA6-CA5	3.83	126.93	117.88
23	P	1525	CHD	C17-C13-C14	3.83	104.01	100.08
23	W	1059	CHD	C9-C11-C12	3.84	119.40	114.33
23	C	271	CHD	C17-C13-C12	3.84	121.22	117.67
25	T	1265	PEK	O01-C1-C2	3.86	119.68	111.55
23	J	60	CHD	C4-C5-C10	3.86	116.83	112.66
19	N	1266	PGV	O03-C19-C20	3.89	123.16	111.92
23	P	1271	CHD	C13-C17-C20	3.89	124.22	119.50
23	W	1059	CHD	C21-C20-C17	3.89	119.00	112.94
25	G	1263	PEK	O03-C01-C02	3.90	118.36	108.64
23	O	229	CHD	O3-C3-C4	3.90	117.67	109.86
23	C	271	CHD	C11-C12-C13	3.91	115.28	111.23
23	J	60	CHD	C11-C9-C8	3.91	116.56	110.81
27	C	272	DMU	O5-C6-C1	3.96	118.85	110.34
19	N	1524	PGV	O03-C19-C20	3.98	123.43	111.92
27	M	526	DMU	C7-C8-C9	3.98	117.37	110.24
27	Z	1526	DMU	C7-C8-C9	3.99	117.37	110.24
27	Z	1526	DMU	O5-C4-C3	3.99	118.23	109.76
14	A	515	HEA	C26-C15-C16	3.99	122.17	115.29
27	M	526	DMU	O7-C3-C2	4.00	118.02	107.27
21	O	1521	TGL	OG1-CA1-CA2	4.01	123.52	111.92
27	P	272	DMU	C1-C2-C3	4.01	118.91	109.68
23	W	1059	CHD	C11-C9-C10	4.02	117.98	113.74
23	P	1525	CHD	C5-C6-C7	4.03	118.90	114.44
23	C	525	CHD	C11-C9-C8	4.03	116.74	110.81
23	P	1525	CHD	C5-C4-C3	4.06	118.83	112.83
27	M	526	DMU	O1-C9-C11	4.07	116.66	106.43
27	C	272	DMU	C7-C8-C9	4.07	117.52	110.24
23	P	1271	CHD	C17-C13-C14	4.07	104.25	100.08
23	W	1059	CHD	C11-C9-C8	4.09	116.82	110.81
23	B	1085	CHD	C2-C1-C10	4.09	119.88	112.79
27	P	272	DMU	O7-C10-C5	4.09	118.94	108.08
27	Z	1526	DMU	O16-C6-C1	4.10	114.87	108.24
21	L	522	TGL	OG2-CB1-CB2	4.10	120.20	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C6-C7-C8	4.12	115.91	111.51
21	N	1523	TGL	OG1-CG1-CG2	4.13	118.93	108.64
27	P	272	DMU	C6-O5-C4	4.13	121.85	113.71
27	M	526	DMU	O55-C2-C3	4.14	121.10	109.93
27	C	272	DMU	C6-C1-C2	4.15	118.66	109.98
27	Z	1526	DMU	O1-C9-C11	4.15	116.87	106.43
19	P	1267	PGV	O14-P-O13	4.17	133.32	112.14
21	Y	1522	TGL	OG3-CC1-CC2	4.21	124.10	111.92
21	B	521	TGL	OG2-CG2-CG3	4.23	123.75	108.43
27	C	272	DMU	O7-C3-C2	4.23	118.64	107.27
21	L	522	TGL	CC3-CC2-CC1	4.23	128.87	113.60
23	J	60	CHD	C22-C20-C17	4.24	119.16	110.28
23	P	1271	CHD	C21-C20-C17	4.27	119.60	112.94
23	P	1525	CHD	C9-C11-C12	4.27	119.98	114.33
23	C	525	CHD	C9-C8-C7	4.30	116.96	111.92
25	T	263	PEK	O01-C1-C2	4.30	120.62	111.55
27	P	272	DMU	O1-C9-C11	4.32	117.30	106.43
23	W	1059	CHD	C22-C20-C17	4.33	119.34	110.28
27	M	526	DMU	C6-C1-C2	4.35	119.09	109.98
27	P	272	DMU	O5-C6-O16	4.38	120.31	109.96
19	A	521	PGV	O03-C19-C20	4.45	124.79	111.92
21	D	523	TGL	CG2-OG2-CB1	4.46	128.42	117.88
21	N	1523	TGL	OG3-CC1-CC2	4.51	124.97	111.92
26	T	1269	CDL	OA8-CA7-C31	4.52	124.98	111.92
23	C	271	CHD	C9-C11-C12	4.53	120.32	114.33
26	P	1270	CDL	OB8-CB7-C71	4.54	125.06	111.92
27	Z	1526	DMU	C8-C7-C5	4.54	118.80	110.83
27	M	526	DMU	O5-C6-C1	4.57	120.16	110.34
21	O	1521	TGL	OG3-CC1-CC2	4.59	125.19	111.92
23	C	525	CHD	C11-C9-C10	4.61	118.60	113.74
21	D	523	TGL	CB3-CB2-CB1	4.63	130.31	113.60
26	P	1270	CDL	OA8-CA7-C31	4.67	125.44	111.92
25	P	1264	PEK	C2-C3-C4	4.70	121.59	113.28
23	P	1525	CHD	C9-C8-C7	4.71	117.44	111.92
23	B	1085	CHD	C15-C14-C8	4.72	124.98	118.33
21	Y	1522	TGL	OG1-CA1-CA2	4.75	125.65	111.92
23	W	1059	CHD	C17-C13-C12	4.78	122.09	117.67
23	P	1271	CHD	C4-C5-C10	4.81	117.86	112.66
23	P	1525	CHD	C11-C9-C8	4.81	117.89	110.81
23	J	60	CHD	C13-C14-C8	4.82	120.97	114.77
27	C	272	DMU	O1-C9-C11	4.83	118.58	106.43
27	C	272	DMU	C2-C3-C4	4.88	122.25	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	526	DMU	C6-O5-C4	4.90	123.36	113.71
23	O	229	CHD	C15-C14-C13	4.92	108.49	103.57
21	L	522	TGL	CG2-OG2-CB1	4.93	129.53	117.88
19	C	268	PGV	O01-C1-C2	4.94	121.96	111.55
23	W	1059	CHD	C9-C8-C7	4.96	117.74	111.92
23	C	525	CHD	C14-C8-C9	5.00	116.44	109.64
27	M	526	DMU	O16-C6-C1	5.03	116.37	108.24
23	O	229	CHD	C17-C13-C14	5.04	105.24	100.08
27	M	526	DMU	C8-C7-C5	5.07	119.72	110.83
21	B	521	TGL	CG3-OG3-CC1	5.07	132.29	117.13
19	A	524	PGV	O03-C19-C20	5.07	126.60	111.92
23	P	1271	CHD	C15-C14-C13	5.08	108.64	103.57
26	T	1269	CDL	OB6-CB5-C51	5.13	122.36	111.55
27	P	272	DMU	C8-C7-C5	5.14	119.85	110.83
21	B	521	TGL	OG3-CC1-CC2	5.15	126.81	111.92
26	C	270	CDL	OB8-CB7-C71	5.18	126.91	111.92
27	P	272	DMU	O16-C6-C1	5.20	116.65	108.24
27	C	272	DMU	C8-C7-C5	5.22	119.98	110.83
14	A	516	HEA	C27-C19-C20	5.30	124.43	115.29
27	C	272	DMU	C6-O5-C4	5.33	124.21	113.71
27	C	272	DMU	C18-O16-C6	5.33	122.94	113.85
23	O	229	CHD	C4-C3-C2	5.36	117.11	110.56
23	P	1271	CHD	C9-C11-C12	5.36	121.42	114.33
25	C	265	PEK	O01-C1-C2	5.38	122.90	111.55
27	M	526	DMU	C2-C3-C4	5.40	123.46	110.93
23	C	271	CHD	C2-C1-C10	5.41	122.16	112.79
23	W	1059	CHD	C4-C5-C10	5.41	118.51	112.66
26	G	269	CDL	OA6-CA5-C11	5.43	123.01	111.55
21	L	522	TGL	OG3-CC1-CC2	5.44	127.64	111.92
23	J	60	CHD	C15-C14-C8	5.47	126.05	118.33
27	Z	1526	DMU	O5-C4-C57	5.49	120.22	106.43
23	C	525	CHD	C15-C14-C13	5.52	109.08	103.57
23	B	1085	CHD	C11-C12-C13	5.55	116.98	111.23
23	P	1271	CHD	C5-C6-C7	5.60	120.63	114.44
21	Y	1522	TGL	CG2-OG2-CB1	5.61	131.12	117.88
23	J	60	CHD	C2-C1-C10	5.61	122.52	112.79
26	G	269	CDL	OB6-CB5-C51	5.65	123.46	111.55
27	P	272	DMU	O5-C4-C57	5.65	120.64	106.43
23	P	1271	CHD	C2-C1-C10	5.66	122.60	112.79
23	J	60	CHD	C15-C14-C13	5.66	109.22	103.57
23	C	525	CHD	O3-C3-C4	5.66	121.18	109.86
23	O	229	CHD	C11-C9-C8	5.70	119.19	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	272	DMU	C6-C1-C2	5.70	121.91	109.98
23	P	1271	CHD	C17-C13-C12	5.74	122.97	117.67
23	P	1525	CHD	C11-C9-C10	5.75	119.80	113.74
27	P	272	DMU	O5-C4-C3	5.77	122.02	109.76
23	W	1059	CHD	C14-C13-C12	5.78	112.88	107.39
23	W	1059	CHD	C1-C10-C5	5.86	116.76	107.77
26	C	270	CDL	OA6-CA5-C11	5.93	124.05	111.55
27	Z	1526	DMU	C2-C3-C4	5.95	124.74	110.93
27	P	272	DMU	O1-C10-C5	5.95	123.12	110.34
23	W	1059	CHD	C6-C5-C10	5.99	119.13	112.66
27	C	272	DMU	O1-C10-C5	5.99	123.21	110.34
22	R	1229	PSC	O01-C1-C2	6.03	124.26	111.55
23	W	1059	CHD	C4-C3-C2	6.05	117.95	110.56
23	O	229	CHD	C5-C4-C3	6.08	121.81	112.83
14	A	516	HEA	C3C-C4C-NC	6.09	117.09	109.21
23	B	1085	CHD	C17-C13-C14	6.11	106.34	100.08
23	J	60	CHD	C1-C2-C3	6.11	118.24	110.45
25	G	1263	PEK	O01-C1-C2	6.11	124.43	111.55
23	J	60	CHD	C14-C13-C12	6.12	113.20	107.39
23	O	229	CHD	C15-C14-C8	6.14	126.99	118.33
21	O	1521	TGL	OG2-CB1-CB2	6.15	124.52	111.55
23	O	229	CHD	C9-C8-C7	6.19	119.19	111.92
23	C	271	CHD	C11-C9-C8	6.20	119.93	110.81
23	C	271	CHD	C4-C3-C2	6.32	118.28	110.56
23	W	1059	CHD	C9-C10-C5	6.35	117.75	108.61
23	C	271	CHD	C1-C10-C5	6.36	117.51	107.77
23	J	60	CHD	C9-C11-C12	6.36	122.73	114.33
23	C	271	CHD	C4-C5-C10	6.37	119.55	112.66
23	B	1085	CHD	C15-C14-C13	6.39	109.95	103.57
25	T	1265	PEK	O03-C21-C22	6.40	130.44	111.92
23	C	271	CHD	C15-C14-C13	6.47	110.03	103.57
23	B	1085	CHD	C14-C8-C9	6.47	118.44	109.64
23	C	525	CHD	C14-C13-C12	6.48	113.55	107.39
23	W	1059	CHD	C2-C1-C10	6.48	124.03	112.79
23	P	1271	CHD	C16-C17-C13	6.48	110.05	103.57
27	P	272	DMU	C18-O16-C6	6.50	124.95	113.85
27	Z	1526	DMU	O5-C6-C1	6.51	124.31	110.34
23	J	60	CHD	C5-C4-C3	6.51	122.44	112.83
23	P	1271	CHD	C5-C4-C3	6.51	122.45	112.83
23	P	1271	CHD	C14-C8-C7	6.52	120.62	111.80
23	J	60	CHD	C14-C8-C7	6.54	120.65	111.80
23	C	271	CHD	C6-C7-C8	6.57	118.53	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C5-C4-C3	6.57	122.53	112.83
26	T	1269	CDL	OA6-CA5-C11	6.60	125.47	111.55
23	C	271	CHD	C16-C17-C20	6.61	122.69	112.15
25	C	265	PEK	O03-C21-C22	6.66	131.19	111.92
23	P	1271	CHD	C4-C3-C2	6.68	118.72	110.56
23	W	1059	CHD	C1-C2-C3	6.72	119.01	110.45
23	P	1271	CHD	C11-C9-C8	6.81	120.83	110.81
23	C	271	CHD	C14-C13-C12	6.82	113.87	107.39
23	P	1271	CHD	C1-C2-C3	6.84	119.17	110.45
14	N	516	HEA	C27-C19-C20	6.88	127.16	115.29
27	C	272	DMU	O16-C6-C1	6.91	119.42	108.24
27	M	526	DMU	O5-C4-C57	6.94	123.89	106.43
23	J	60	CHD	C6-C7-C8	7.01	119.01	111.51
23	W	1059	CHD	C6-C7-C8	7.02	119.01	111.51
23	O	229	CHD	C14-C8-C9	7.02	119.19	109.64
21	Y	1522	TGL	OG1-CG1-CG2	7.04	126.18	108.64
19	U	1268	PGV	O01-C1-C2	7.04	126.40	111.55
23	C	271	CHD	C1-C2-C3	7.05	119.44	110.45
27	M	526	DMU	O1-C10-C5	7.09	125.56	110.34
23	P	1271	CHD	C16-C17-C20	7.18	123.60	112.15
21	B	521	TGL	OG2-CB1-CB2	7.20	126.72	111.55
23	J	60	CHD	C11-C12-C13	7.20	118.70	111.23
19	C	268	PGV	O03-C19-C20	7.24	132.85	111.92
27	Z	1526	DMU	O1-C10-C5	7.26	125.93	110.34
23	P	1271	CHD	C15-C14-C8	7.27	128.58	118.33
23	P	1271	CHD	C1-C10-C5	7.30	118.96	107.77
27	C	272	DMU	O5-C4-C57	7.30	124.79	106.43
23	J	60	CHD	C5-C6-C7	7.31	122.53	114.44
23	W	1059	CHD	C5-C4-C3	7.34	123.67	112.83
19	U	1268	PGV	O03-C19-C20	7.34	133.16	111.92
27	C	272	DMU	O1-C9-C8	7.35	123.18	109.69
23	B	1085	CHD	C6-C7-C8	7.41	119.43	111.51
23	P	1271	CHD	C6-C5-C10	7.42	120.68	112.66
27	Z	1526	DMU	O1-C9-C8	7.43	123.35	109.69
27	P	272	DMU	O1-C9-C8	7.52	123.50	109.69
23	J	60	CHD	C6-C5-C10	7.54	120.81	112.66
23	C	271	CHD	C16-C17-C13	7.59	111.15	103.57
23	C	525	CHD	C17-C13-C14	7.59	107.85	100.08
27	M	526	DMU	O1-C9-C8	7.72	123.87	109.69
23	O	229	CHD	C11-C12-C13	7.72	119.24	111.23
26	P	1270	CDL	OA6-CA5-C11	7.78	127.95	111.55
23	J	60	CHD	C4-C3-C2	7.78	120.06	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1059	CHD	C5-C6-C7	7.79	123.06	114.44
23	C	525	CHD	C13-C17-C20	7.79	128.97	119.50
23	J	60	CHD	C16-C17-C13	7.82	111.39	103.57
23	J	60	CHD	C1-C10-C5	7.84	119.79	107.77
23	B	1085	CHD	C5-C4-C3	7.85	124.42	112.83
23	C	271	CHD	C5-C6-C7	7.86	123.14	114.44
23	P	1271	CHD	C14-C13-C12	7.88	114.88	107.39
23	O	229	CHD	C1-C2-C3	7.95	120.58	110.45
23	W	1059	CHD	C15-C14-C8	7.99	129.59	118.33
23	O	229	CHD	C17-C13-C12	8.05	125.11	117.67
23	C	271	CHD	C6-C5-C10	8.09	121.40	112.66
21	Y	1522	TGL	OG2-CB1-CB2	8.14	128.72	111.55
23	C	271	CHD	C15-C14-C8	8.19	129.88	118.33
23	C	525	CHD	C17-C13-C12	8.32	125.36	117.67
23	J	60	CHD	C17-C13-C12	8.33	125.37	117.67
23	W	1059	CHD	C16-C17-C13	8.39	111.95	103.57
23	W	1059	CHD	C15-C14-C13	8.41	111.97	103.57
23	P	1525	CHD	C10-C9-C8	8.44	120.95	111.87
23	W	1059	CHD	C11-C12-C13	8.49	120.03	111.23
23	P	1525	CHD	C15-C14-C13	8.51	112.07	103.57
23	B	1085	CHD	C4-C3-C2	8.52	120.97	110.56
23	B	1085	CHD	C14-C13-C12	8.80	115.75	107.39
23	O	229	CHD	C10-C9-C8	8.81	121.34	111.87
23	C	525	CHD	C11-C12-C13	8.85	120.41	111.23
23	P	1271	CHD	C6-C7-C8	8.93	121.06	111.51
23	C	525	CHD	C10-C9-C8	9.40	121.97	111.87
23	C	525	CHD	C4-C3-C2	9.45	122.10	110.56
23	B	1085	CHD	C17-C13-C12	9.77	126.70	117.67
23	J	60	CHD	C13-C17-C20	9.89	131.51	119.50
23	W	1059	CHD	C14-C8-C7	9.96	125.27	111.80
23	P	1525	CHD	C17-C13-C12	10.22	127.12	117.67
23	W	1059	CHD	C10-C9-C8	10.29	122.93	111.87
23	W	1059	CHD	C13-C17-C20	10.39	132.12	119.50
23	P	1525	CHD	C14-C13-C12	10.47	117.34	107.39
23	O	229	CHD	C1-C10-C5	10.83	124.36	107.77
23	P	1525	CHD	C4-C3-C2	11.29	124.35	110.56
23	B	1085	CHD	C10-C9-C8	11.36	124.08	111.87
23	C	525	CHD	C1-C10-C5	11.49	125.38	107.77
23	B	1085	CHD	C1-C10-C5	12.05	126.24	107.77
23	C	525	CHD	C6-C5-C10	12.35	126.01	112.66
23	P	1525	CHD	C1-C10-C5	12.51	126.94	107.77
23	P	1525	CHD	C6-C5-C10	12.62	126.30	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C10-C9-C8	12.67	125.48	111.87
23	O	229	CHD	C6-C5-C10	12.69	126.37	112.66
23	O	229	CHD	C14-C13-C12	12.71	119.47	107.39
23	J	60	CHD	C10-C9-C8	12.95	125.79	111.87
23	C	271	CHD	C10-C9-C8	14.58	127.55	111.87
23	B	1085	CHD	C6-C5-C10	15.04	128.91	112.66

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
27	Z	1526	DMU	C2
27	Z	1526	DMU	C4
27	Z	1526	DMU	C9
27	Z	1526	DMU	C6
27	Z	1526	DMU	C5
27	P	272	DMU	C5
27	P	272	DMU	C6
27	P	272	DMU	C9
27	P	272	DMU	C4
27	P	272	DMU	C2
27	P	272	DMU	C10
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
23	J	60	CHD	C17
23	J	60	CHD	C9
23	P	1271	CHD	C9
27	C	272	DMU	C5
27	C	272	DMU	C6
27	C	272	DMU	C9
27	C	272	DMU	C4
27	C	272	DMU	C2
27	C	272	DMU	C3
23	W	1059	CHD	C17
23	C	271	CHD	C9
23	P	1525	CHD	C9

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Mol	Chain	Res	Type	Atom
27	M	526	DMU	C2
27	M	526	DMU	C4
27	M	526	DMU	C9
27	M	526	DMU	C5
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	Y	1522	TGL	CG2-OG2-CB1-OB1
19	N	1524	PGV	C02-O01-C1-C2
26	T	1269	CDL	PB2-OB2-CB2-C1
21	Y	1522	TGL	CG2-OG2-CB1-CB2
26	T	1269	CDL	CA4-OA6-CA5-OA7
26	P	1270	CDL	CA4-OA6-CA5-OA7
26	T	1269	CDL	CA4-OA6-CA5-C11
26	P	1270	CDL	CA4-OA6-CA5-C11

There are no ring outliers.

38 monomers are involved in 373 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	8	0
14	A	516	HEA	8	0
19	A	521	PGV	2	0
19	A	524	PGV	14	0
23	B	1085	CHD	4	0
22	B	229	PSC	20	0
21	B	521	TGL	4	0
25	C	264	PEK	9	0
25	C	265	PEK	13	0
19	C	267	PGV	4	0
19	C	268	PGV	6	0
26	C	270	CDL	20	0
23	C	271	CHD	2	0
27	C	272	DMU	4	0
23	C	525	CHD	2	0
21	D	523	TGL	10	0
25	G	1263	PEK	19	0
26	G	269	CDL	33	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	60	CHD	8	0
21	L	522	TGL	15	0
21	N	1523	TGL	14	0
19	N	1524	PGV	7	0
14	N	515	HEA	6	0
14	N	516	HEA	3	0
21	O	1521	TGL	5	0
23	O	229	CHD	3	0
25	P	1264	PEK	6	0
19	P	1267	PGV	3	0
26	P	1270	CDL	27	0
23	P	1271	CHD	5	0
27	P	272	DMU	1	0
22	R	1229	PSC	20	0
25	T	1265	PEK	20	0
26	T	1269	CDL	30	0
25	T	263	PEK	14	0
19	U	1268	PGV	4	0
23	W	1059	CHD	3	0
21	Y	1522	TGL	20	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.30	11 (2%) 63 62	23, 29, 38, 65	0
1	N	513/514 (99%)	0.23	20 (3%) 39 39	29, 35, 44, 71	0
2	B	226/227 (99%)	-0.25	1 (0%) 92 92	24, 33, 53, 72	0
2	O	226/227 (99%)	-0.14	4 (1%) 68 67	31, 42, 64, 81	0
3	C	259/261 (99%)	-0.17	2 (0%) 86 85	26, 32, 43, 66	0
3	P	259/261 (99%)	0.05	13 (5%) 29 28	30, 36, 48, 67	0
4	D	144/147 (97%)	-0.17	1 (0%) 87 87	30, 40, 53, 66	0
4	Q	144/147 (97%)	1.06	24 (16%) 1 1	39, 50, 71, 105	0
5	E	105/109 (96%)	0.36	6 (5%) 24 23	33, 40, 64, 97	0
5	R	105/109 (96%)	0.97	15 (14%) 2 2	36, 46, 70, 97	0
6	F	98/98 (100%)	0.44	9 (9%) 9 8	30, 41, 80, 117	0
6	S	98/98 (100%)	0.30	9 (9%) 9 8	34, 46, 80, 113	0
7	G	83/85 (97%)	0.83	15 (18%) 1 1	29, 38, 90, 106	0
7	T	83/85 (97%)	1.00	15 (18%) 1 1	32, 41, 91, 106	0
8	H	79/85 (92%)	0.27	10 (12%) 3 3	29, 41, 81, 101	0
8	U	79/85 (92%)	0.62	14 (17%) 1 1	37, 47, 85, 106	0
9	I	72/73 (98%)	0.25	3 (4%) 36 35	31, 46, 65, 70	0
9	V	72/73 (98%)	0.96	13 (18%) 1 1	36, 52, 67, 77	0
10	J	58/59 (98%)	0.52	7 (12%) 4 4	32, 41, 66, 95	0
10	W	58/59 (98%)	0.54	7 (12%) 4 4	36, 45, 67, 97	0
11	K	49/56 (87%)	0.03	2 (4%) 37 37	31, 39, 54, 64	0
11	X	49/56 (87%)	1.79	21 (42%) 0 0	42, 50, 66, 78	0
12	L	46/47 (97%)	-0.24	2 (4%) 35 34	29, 34, 51, 77	0
12	Y	46/47 (97%)	-0.06	1 (2%) 62 60	35, 43, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.04	4 (9%) 8 8	31, 34, 72, 96	0
13	Z	43/46 (93%)	0.74	8 (18%) 1 1	39, 44, 81, 104	0
All	All	3550/3614 (98%)	0.27	237 (6%) 18 17	23, 38, 64, 117	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	14.9
6	F	1	ALA	10.4
6	S	98	HIS	9.8
6	S	1	ALA	9.6
6	S	97	ALA	9.1
7	G	1	ALA	8.9
4	Q	4	SER	8.5
6	F	97	ALA	8.2
7	T	1	ALA	7.4
6	F	96	LEU	7.2
6	S	2	SER	6.5
5	R	109	VAL	6.5
13	Z	42	LYS	6.3
6	F	98	HIS	6.3
5	E	5	HIS	6.3
8	U	7	LYS	5.9
4	Q	51	LEU	5.8
10	J	1	PHE	5.6
6	S	94	HIS	5.6
7	T	3	ALA	5.6
7	G	36	TRP	5.5
7	T	36	TRP	5.4
4	Q	48	TRP	5.4
9	I	37	PHE	5.3
6	S	96	LEU	5.3
7	T	84	LYS	5.2
8	U	8	ILE	5.2
4	Q	5	VAL	5.1
13	Z	43	SER	4.9
7	G	40	GLY	4.9
9	V	37	PHE	4.9
11	X	7	PRO	4.9
8	U	44	THR	4.9
10	J	58	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
7	G	8	HIS	4.8
13	Z	41	LYS	4.8
9	V	2	THR	4.7
7	G	2	SER	4.7
7	T	42	ARG	4.6
11	X	19	ALA	4.6
6	F	94	HIS	4.6
8	H	45	ALA	4.5
8	H	48	GLY	4.5
5	R	5	HIS	4.5
13	M	43	SER	4.5
13	M	42	LYS	4.4
7	G	41	HIS	4.3
7	G	42	ARG	4.3
2	O	113	TYR	4.3
10	W	57	HIS	4.2
7	T	41	HIS	4.2
7	T	5	LYS	4.2
10	W	58	LYS	4.2
4	Q	33	LEU	4.1
7	G	84	LYS	4.1
7	G	6	GLY	4.1
11	X	16	ALA	4.1
4	Q	46	ALA	4.0
2	O	90	ILE	4.0
8	U	10	ASN	4.0
7	T	4	ALA	3.9
10	W	55	PHE	3.9
8	H	8	ILE	3.9
7	T	40	GLY	3.9
13	Z	40	TYR	3.9
5	R	96	LEU	3.8
4	Q	145	TRP	3.8
13	Z	35	TYR	3.8
5	R	7	THR	3.7
8	H	44	THR	3.7
12	L	47	LYS	3.7
4	Q	49	SER	3.7
6	F	2	SER	3.7
12	Y	47	LYS	3.7
10	J	57	HIS	3.7
13	Z	39	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	59	GLN	3.5
3	P	88	ILE	3.5
11	X	13	TYR	3.4
7	T	10	GLY	3.4
8	U	49	ASP	3.4
13	M	39	ASN	3.4
11	X	47	ARG	3.4
5	R	108	LYS	3.4
3	P	91	VAL	3.4
8	U	48	GLY	3.4
13	M	40	TYR	3.3
7	G	5	LYS	3.3
11	X	24	PHE	3.3
4	Q	141	ASP	3.3
4	Q	102	TYR	3.3
10	W	52	TRP	3.3
7	G	3	ALA	3.3
11	X	6	ALA	3.3
8	U	52	VAL	3.2
11	X	17	VAL	3.2
8	U	11	TYR	3.2
7	T	8	HIS	3.2
6	F	95	GLN	3.1
6	S	93	PRO	3.1
7	G	43	GLU	3.1
5	E	109	VAL	3.1
10	W	1	PHE	3.0
11	X	46	GLY	3.0
4	Q	7	LYS	3.0
9	V	36	LYS	3.0
7	T	9	GLY	3.0
5	R	58	LEU	3.0
10	J	2	GLU	3.0
8	U	9	LYS	3.0
7	G	4	ALA	3.0
1	N	193	VAL	2.9
12	L	2	HIS	2.9
8	H	7	LYS	2.9
10	J	52	TRP	2.9
7	T	6	GLY	2.9
4	Q	139	ASP	2.9
9	I	2	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	P	37	PHE	2.8
11	K	7	PRO	2.8
9	V	68	ILE	2.8
11	X	23	THR	2.8
9	V	3	ALA	2.7
7	T	43	GLU	2.7
13	Z	32	TRP	2.7
4	Q	53	ILE	2.7
7	G	39	SER	2.7
4	Q	147	LYS	2.7
9	V	7	PRO	2.7
8	H	47	GLY	2.7
5	R	93	LEU	2.7
7	T	2	SER	2.7
11	K	19	ALA	2.7
4	Q	142	LYS	2.7
11	X	18	LEU	2.7
9	V	53	ASN	2.7
5	R	54	ALA	2.7
1	N	195	LEU	2.6
8	H	46	LYS	2.6
11	X	11	ASP	2.6
1	N	190	ILE	2.6
3	C	92	LEU	2.6
3	P	182	TYR	2.6
10	W	2	GLU	2.6
1	N	165	ILE	2.6
3	P	99	TRP	2.6
9	I	26	MET	2.5
5	R	9	GLU	2.5
13	Z	13	LYS	2.5
8	U	43	MET	2.5
5	R	89	LEU	2.5
4	D	147	LYS	2.5
4	Q	140	TYR	2.5
8	U	45	ALA	2.5
3	P	84	ILE	2.5
3	P	92	LEU	2.4
3	P	38	ASN	2.4
11	X	20	SER	2.4
5	R	92	THR	2.4
2	O	59	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	196	LEU	2.4
1	N	282	PHE	2.4
1	N	245	ILE	2.4
8	U	47	GLY	2.4
1	A	193	VAL	2.4
10	J	4	ARG	2.4
3	P	247	VAL	2.3
4	Q	101	HIS	2.3
8	H	43	MET	2.3
11	X	15	ASN	2.3
11	X	36	ILE	2.3
4	Q	60	TYR	2.3
8	U	42	ALA	2.3
1	A	126	TRP	2.3
11	X	30	VAL	2.3
5	R	10	GLU	2.3
1	N	126	TRP	2.3
9	V	45	LYS	2.3
10	W	4	ARG	2.3
1	N	286	ILE	2.3
1	N	246	LEU	2.2
11	X	12	LYS	2.2
10	J	33	ARG	2.2
11	X	35	GLN	2.2
1	N	66	ILE	2.2
1	A	20	LEU	2.2
1	A	195	LEU	2.2
5	R	13	ALA	2.2
9	V	48	ALA	2.2
7	G	9	GLY	2.2
8	H	49	ASP	2.2
3	P	250	LEU	2.2
4	Q	62	LEU	2.2
1	N	285	PHE	2.2
1	A	192	ALA	2.2
4	Q	97	ILE	2.2
8	H	42	ALA	2.2
4	Q	55	GLU	2.2
2	O	131	GLY	2.2
3	P	87	ILE	2.2
6	S	3	GLY	2.2
4	Q	8	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	2.1
1	N	248	LEU	2.1
3	P	85	LEU	2.1
1	N	83	VAL	2.1
3	P	98	PHE	2.1
5	R	16	VAL	2.1
6	F	5	GLY	2.1
1	A	245	ILE	2.1
11	X	48	VAL	2.1
5	R	18	TYR	2.1
6	F	3	GLY	2.1
8	U	46	LYS	2.1
5	E	9	GLU	2.1
1	N	166	THR	2.1
9	V	33	THR	2.1
1	A	190	ILE	2.1
1	N	75	ILE	2.1
1	N	158	ILE	2.1
1	N	197	LEU	2.1
5	E	93	LEU	2.1
1	A	188	VAL	2.1
5	E	16	VAL	2.1
11	X	31	TYR	2.1
6	S	95	GLN	2.1
9	V	65	LYS	2.1
1	N	194	LEU	2.1
9	V	19	PHE	2.1
11	X	37	GLY	2.1
1	A	348	PHE	2.0
9	V	4	LEU	2.0
1	A	385	ALA	2.0
1	N	243	VAL	2.0
4	Q	68	PHE	2.0
3	C	38	ASN	2.0
5	E	24	ILE	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SAC	V	1	9/10	0.44	0.47	83,84,85,86	0
7	TPO	T	11	11/12	0.61	0.28	75,82,102,103	0
9	SAC	I	1	9/10	0.67	0.28	73,76,78,80	0
7	TPO	G	11	11/12	0.68	0.27	69,76,102,102	0
1	FME	A	1	10/11	0.91	0.18	44,51,71,75	0
1	FME	N	1	10/11	0.93	0.18	46,53,78,82	0
2	FME	O	1	10/11	0.96	0.11	40,42,47,55	0
2	FME	B	1	10/11	0.97	0.12	33,33,41,48	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
24	UNX	C	262	1/1	0.08	0.56	80,80,80,80	0
27	DMU	P	272	33/33	0.33	0.44	77,107,124,124	0
27	DMU	C	272	33/33	0.35	0.39	68,100,115,116	0
25	PEK	T	1265	53/53	0.52	0.32	49,79,110,118	0
24	UNX	P	262	1/1	0.55	0.53	79,79,79,79	0
25	PEK	C	265	53/53	0.58	0.31	49,83,106,107	0
26	CDL	G	269	100/100	0.58	0.31	62,86,116,120	0
25	PEK	G	1263	53/53	0.62	0.51	52,103,133,134	0
22	PSC	R	1229	52/52	0.63	0.33	48,99,136,139	0
21	TGL	Y	1522	63/63	0.64	0.30	51,73,89,92	0
26	CDL	T	1269	100/100	0.65	0.30	58,86,114,118	0
23	CHD	W	1059	29/29	0.65	0.45	101,109,113,115	0
25	PEK	T	263	53/53	0.65	0.42	52,103,125,127	0
22	PSC	B	229	52/52	0.68	0.34	43,92,139,143	0
19	PGV	U	1268	51/51	0.69	0.41	60,84,103,105	0
21	TGL	N	1523	63/63	0.72	0.24	61,79,97,99	0
19	PGV	C	268	51/51	0.72	0.38	53,81,98,102	0
19	PGV	N	1524	51/51	0.72	0.28	54,74,103,105	0
26	CDL	P	1270	100/100	0.74	0.30	36,94,119,119	0
23	CHD	J	60	29/29	0.74	0.46	99,105,108,110	0
21	TGL	L	522	63/63	0.76	0.26	43,66,82,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	TGL	D	523	63/63	0.76	0.22	48,69,91,91	0
19	PGV	A	524	51/51	0.76	0.23	44,72,112,114	0
27	DMU	Z	1526	33/33	0.79	0.28	49,57,70,70	0
26	CDL	C	270	100/100	0.79	0.33	41,91,129,130	0
21	TGL	O	1521	63/63	0.80	0.21	58,80,95,96	0
23	CHD	C	271	29/29	0.86	0.25	79,83,85,85	0
21	TGL	B	521	63/63	0.86	0.22	53,74,88,90	0
23	CHD	P	1271	29/29	0.87	0.29	78,92,94,95	0
27	DMU	M	526	33/33	0.90	0.15	33,47,65,71	0
25	PEK	P	1264	53/53	0.92	0.16	35,50,86,88	0
17	MG	N	518	1/1	0.93	0.17	34,34,34,34	0
19	PGV	P	1267	51/51	0.93	0.17	29,40,82,87	0
25	PEK	C	264	53/53	0.94	0.14	30,46,78,80	0
18	NA	N	519	1/1	0.95	0.11	39,39,39,39	0
19	PGV	C	267	51/51	0.95	0.14	28,40,73,76	0
15	NO	N	520	2/2	0.95	0.14	39,39,39,42	0
19	PGV	N	1266	51/51	0.95	0.20	30,42,65,69	0
23	CHD	C	525	29/29	0.96	0.19	26,33,39,41	0
23	CHD	P	1525	29/29	0.96	0.18	32,37,43,47	0
18	NA	A	519	1/1	0.97	0.08	32,32,32,32	0
19	PGV	A	521	51/51	0.97	0.14	23,35,63,67	0
20	CUA	O	228	2/2	0.97	0.09	34,34,34,36	0
15	NO	A	520	2/2	0.97	0.10	32,32,32,36	0
23	CHD	O	229	29/29	0.97	0.10	27,32,38,40	0
23	CHD	B	1085	29/29	0.97	0.10	27,31,36,42	0
14	HEA	N	515	60/60	0.97	0.14	28,36,45,49	0
17	MG	A	518	1/1	0.98	0.18	23,23,23,23	0
14	HEA	N	516	60/60	0.98	0.18	27,33,37,40	0
14	HEA	A	515	60/60	0.98	0.15	22,28,41,42	0
28	ZN	F	99	1/1	0.99	0.08	37,37,37,37	0
20	CUA	B	228	2/2	0.99	0.13	27,27,27,28	0
16	CU	N	517	1/1	0.99	0.15	35,35,35,35	0
28	ZN	S	99	1/1	0.99	0.08	43,43,43,43	0
14	HEA	A	516	60/60	0.99	0.17	18,26,31,36	0
16	CU	A	517	1/1	1.00	0.15	29,29,29,29	0

## 6.5 Other polymers

There are no such residues in this entry.