



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:23 AM GMT

PDB ID : 3ABM
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (200-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-12-16
Resolution : 1.95 Å(reported)

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

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

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

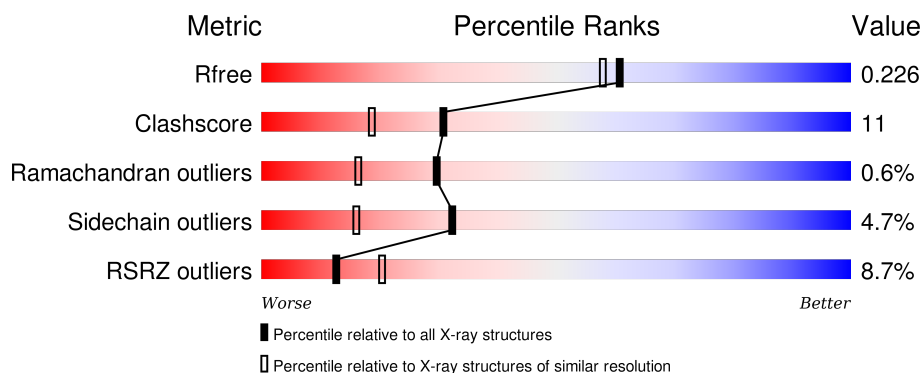
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>11%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
2	O	227	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div>
3	C	261	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
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
17	NA	N	1519	-	-	-	X
18	HEA	A	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	O	1521	-	-	-	X
19	TGL	O	1523	-	-	-	X
19	TGL	Y	1522	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	H	268	-	-	-	X
20	PGV	N	1268	-	-	-	X
20	PGV	N	1524	-	-	-	X
22	CHD	B	1086	X	-	-	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	X
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	X
24	PEK	T	263	-	-	X	-
25	CDL	C	270	-	-	-	X
25	CDL	G	269	-	-	X	X
25	CDL	P	1270	-	-	X	X
26	PSC	E	230	-	-	X	X
26	PSC	R	1230	-	-	-	X
28	DMU	G	272	X	-	-	X
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	X
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32113 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	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			

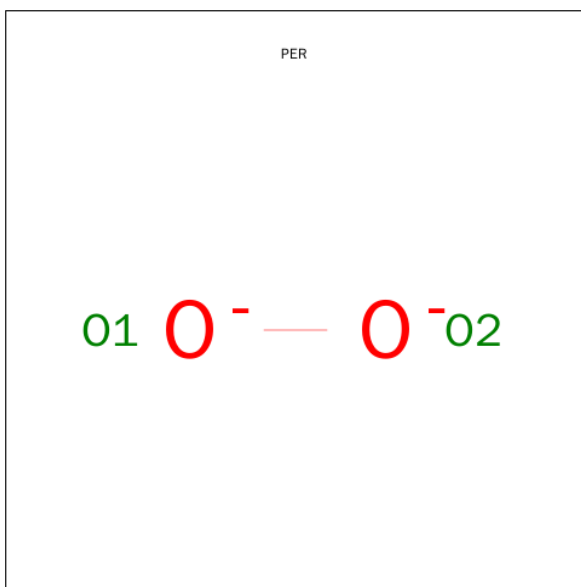
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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

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

- Molecule 15 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

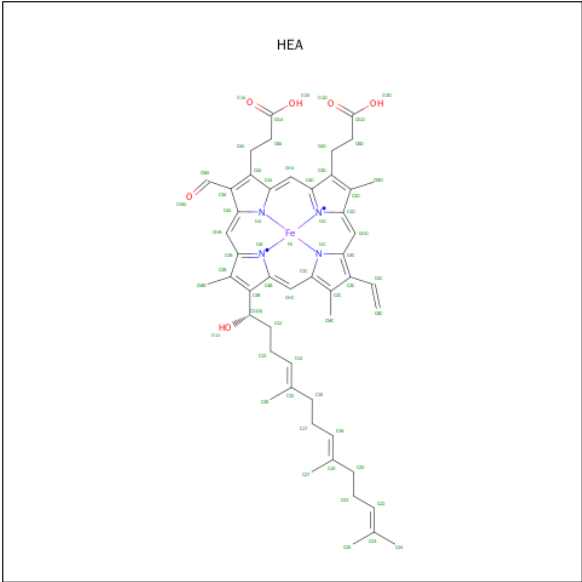
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

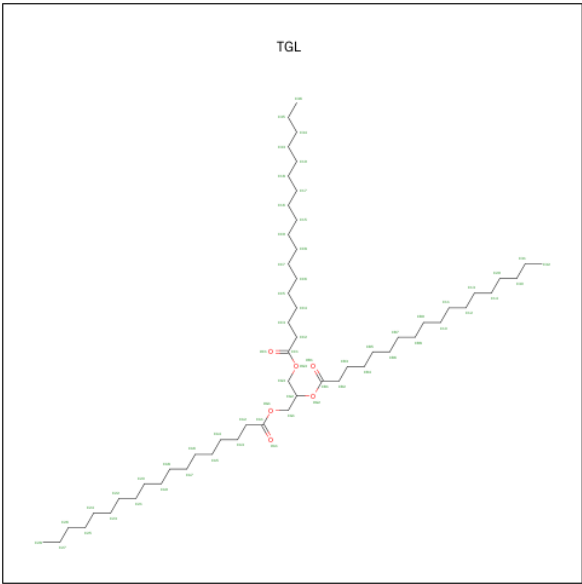
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



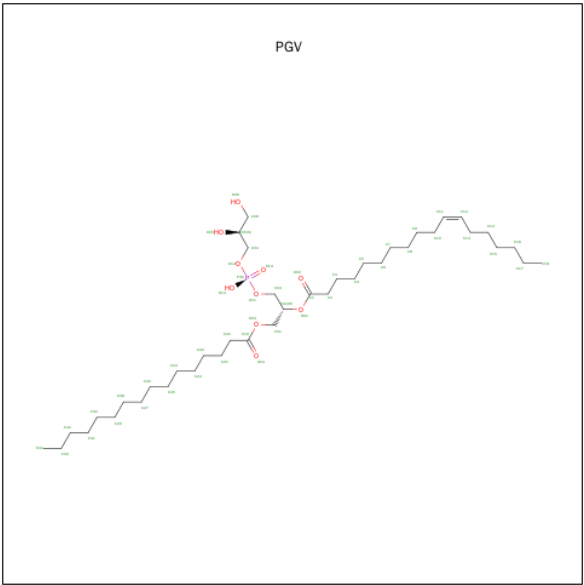
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



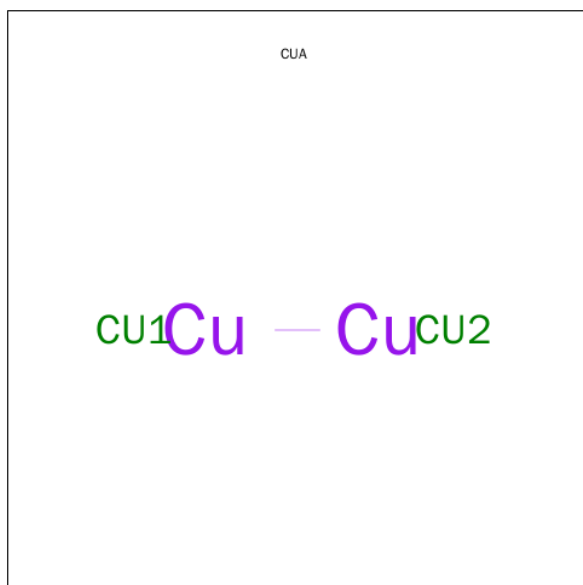
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	H	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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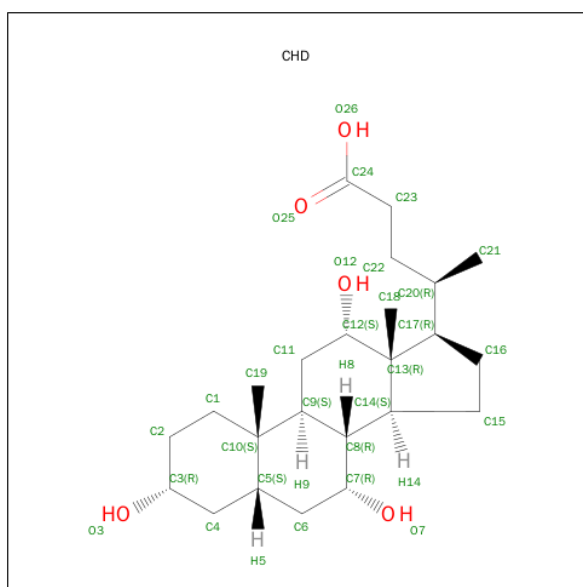
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).

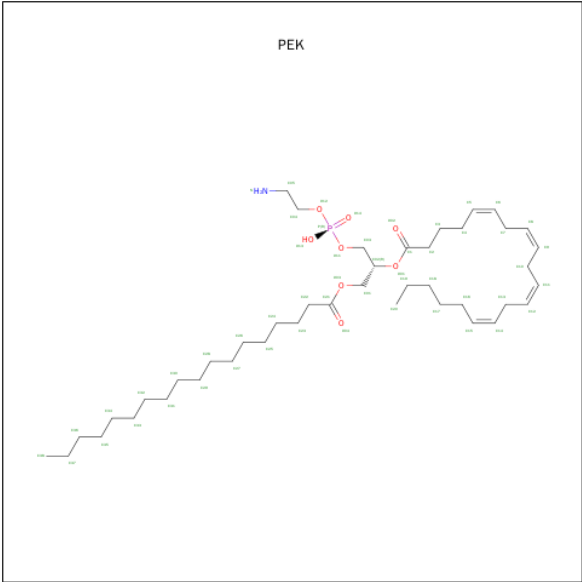


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

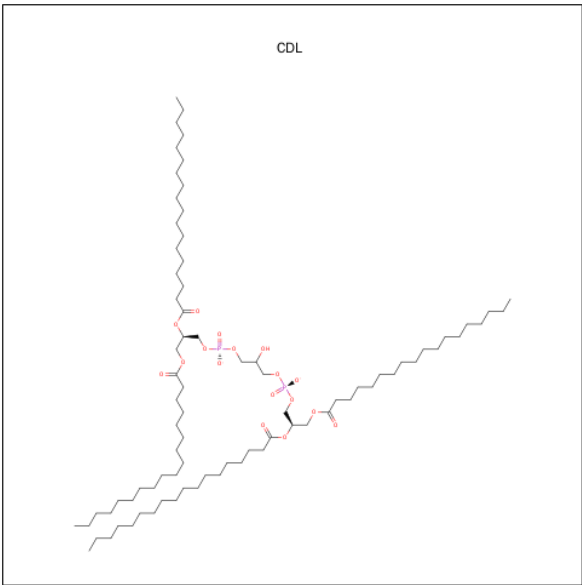
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- Molecule 24 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: C₄₃H₇₈NO₈P).



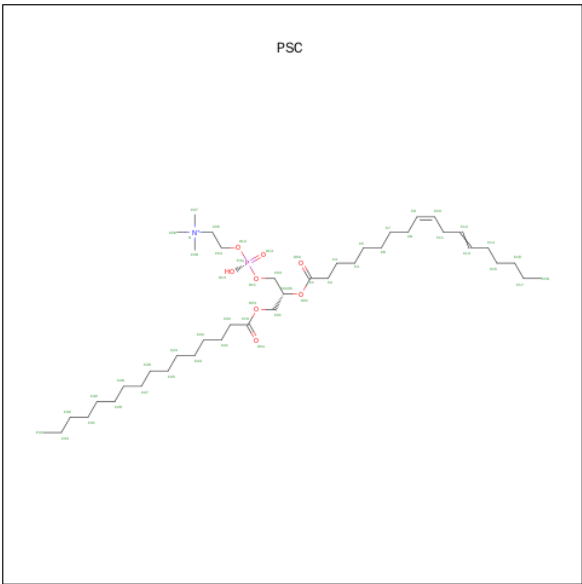
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 26 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: C₄₂H₈₁NO₈P).

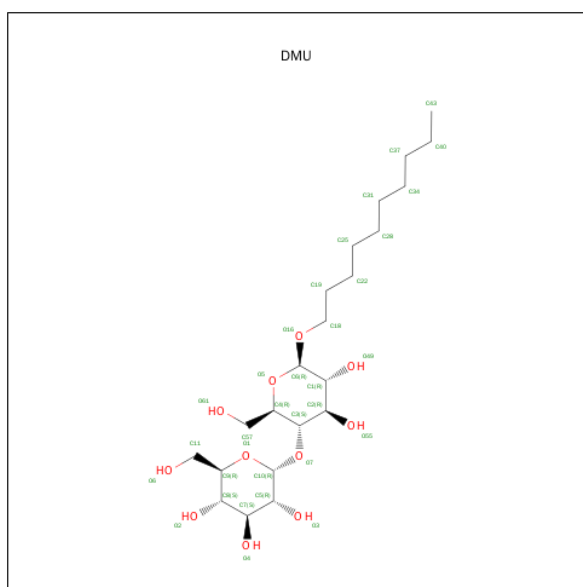


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	203	Total O 203 203	0	0
29	B	131	Total O 131 131	0	0
29	C	90	Total O 90 90	0	0
29	D	96	Total O 96 96	0	0
29	E	62	Total O 62 62	0	0
29	F	70	Total O 70 70	0	0
29	G	41	Total O 41 41	0	0
29	H	46	Total O 46 46	0	0
29	I	44	Total O 44 44	0	0
29	J	17	Total O 17 17	0	0
29	K	22	Total O 22 22	0	0
29	L	23	Total O 23 23	0	0
29	M	19	Total O 19 19	0	0
29	N	196	Total O 196 196	0	0
29	O	106	Total O 106 106	0	0
29	P	89	Total O 89 89	0	0
29	Q	54	Total O 54 54	0	0
29	R	52	Total O 52 52	0	0
29	S	62	Total O 62 62	0	0
29	T	39	Total O 39 39	0	0
29	U	39	Total O 39 39	0	0
29	V	16	Total O 16 16	0	0

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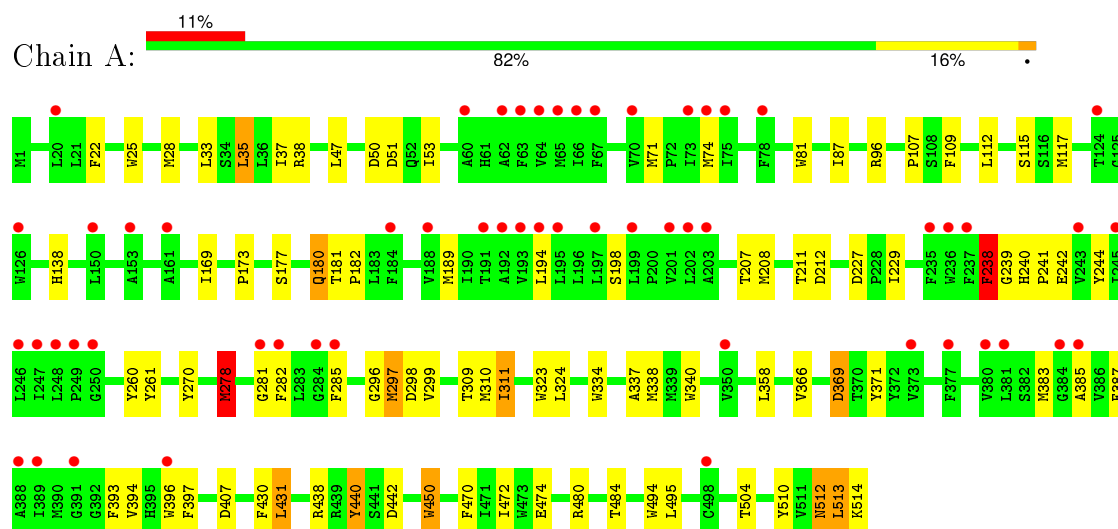
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	W	15	Total 15	O 15	0	0
29	X	16	Total 16	O 16	0	0
29	Y	19	Total 19	O 19	0	0
29	Z	10	Total 10	O 10	0	0

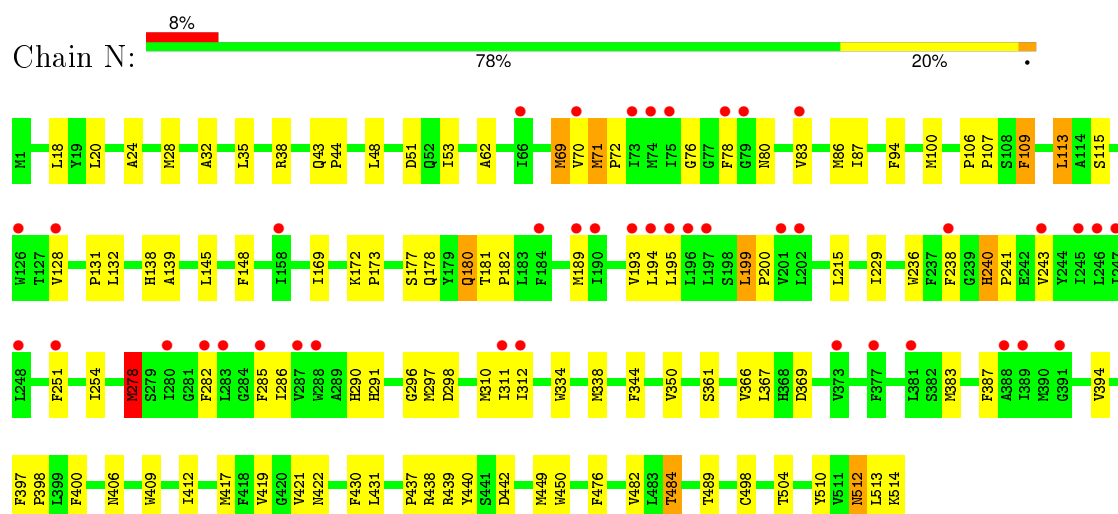
3 Residue-property plots [i](#)

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

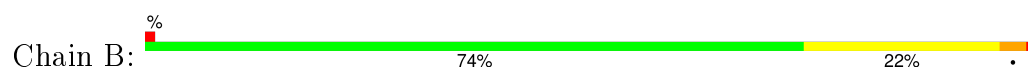
• Molecule 1: Cytochrome c oxidase subunit 1

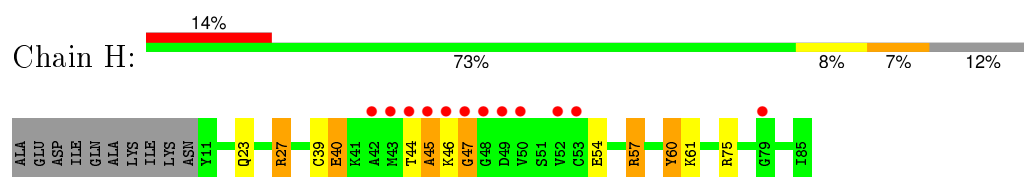


• Molecule 1: Cytochrome c oxidase subunit 1

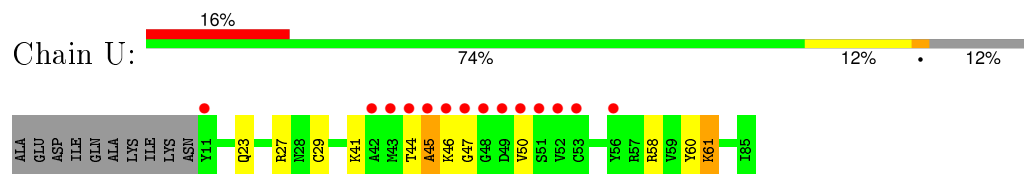


• Molecule 2: Cytochrome c oxidase subunit 2

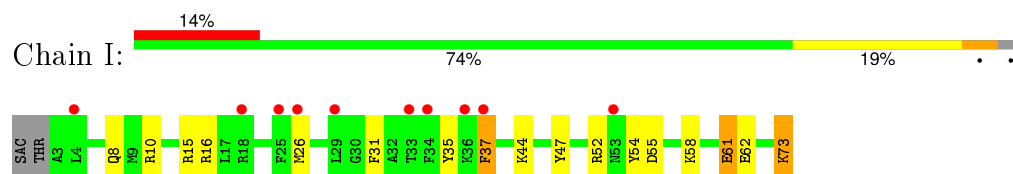




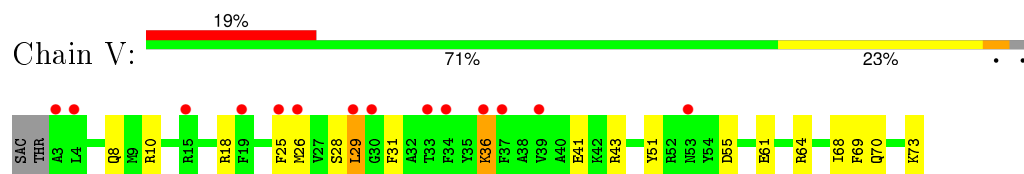
- Molecule 8: Cytochrome c oxidase subunit 6B1



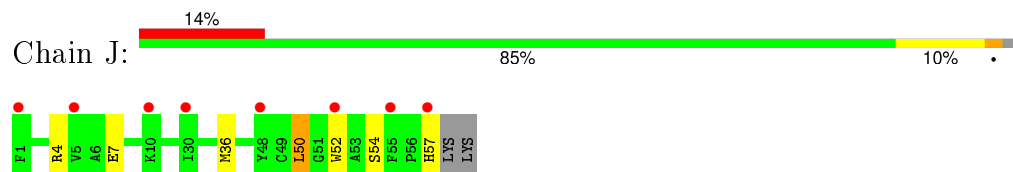
- Molecule 9: Cytochrome c oxidase subunit 6C



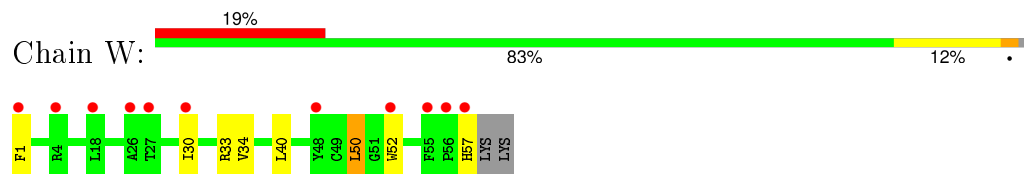
- Molecule 9: Cytochrome c oxidase subunit 6C



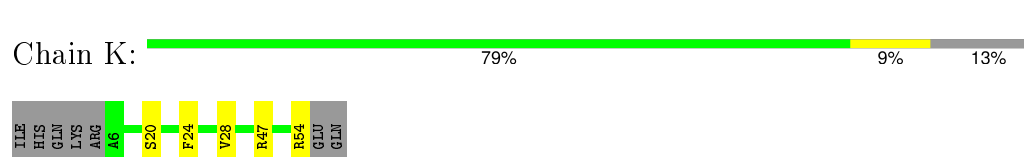
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



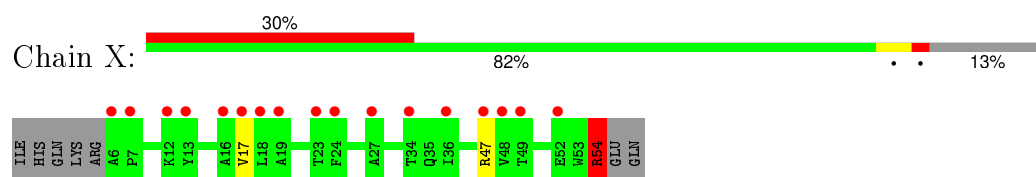
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



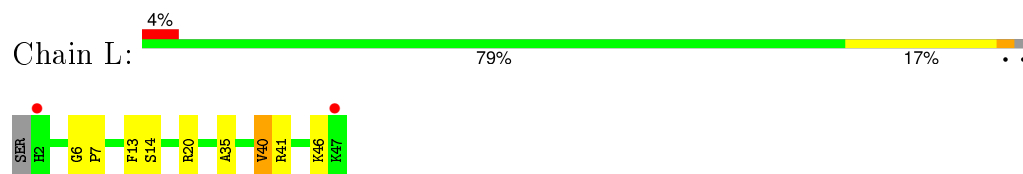
- Molecule 11: Cytochrome c oxidase subunit 7B



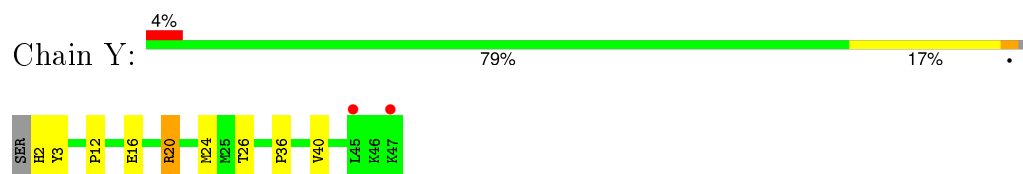
- Molecule 11: Cytochrome c oxidase subunit 7B



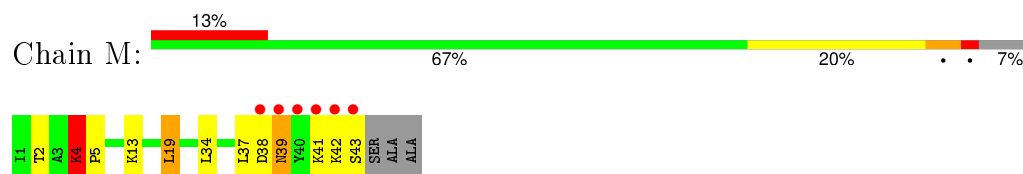
- Molecule 12: Cytochrome c oxidase subunit 7C



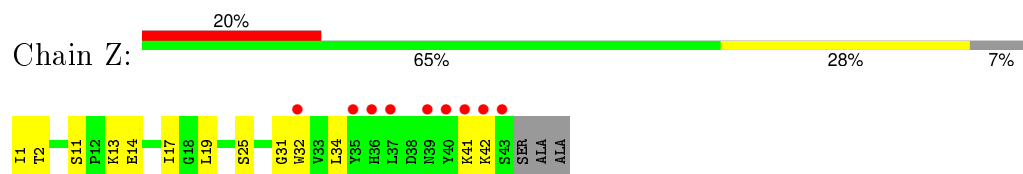
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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, α , β , γ	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 64.10 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.95) 96.4 (64.10-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.181 , 0.214 0.196 , 0.226	Depositor DCC
R_{free} test set	16433 reflections (3.61%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.0	EDS
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 471933 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32113	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.48	26/4156 (0.6%)	1.30	34/5678 (0.6%)
1	N	1.34	13/4156 (0.3%)	1.18	22/5678 (0.4%)
2	B	1.37	10/1860 (0.5%)	1.29	12/2534 (0.5%)
2	O	1.19	9/1860 (0.5%)	1.16	11/2534 (0.4%)
3	C	1.31	8/2197 (0.4%)	1.19	12/3005 (0.4%)
3	P	1.34	13/2197 (0.6%)	1.11	10/3005 (0.3%)
4	D	1.37	5/1229 (0.4%)	1.32	10/1658 (0.6%)
4	Q	1.07	3/1229 (0.2%)	1.08	4/1658 (0.2%)
5	E	1.20	3/860 (0.3%)	1.13	4/1167 (0.3%)
5	R	1.06	0/860	0.99	2/1167 (0.2%)
6	F	1.30	2/733 (0.3%)	1.16	2/996 (0.2%)
6	S	1.28	2/733 (0.3%)	1.29	7/996 (0.7%)
7	G	1.27	2/690 (0.3%)	1.10	3/937 (0.3%)
7	T	1.29	3/690 (0.4%)	1.22	4/937 (0.4%)
8	H	1.27	0/648	1.13	3/877 (0.3%)
8	U	1.03	0/648	0.99	0/877
9	I	1.23	3/598 (0.5%)	1.12	2/792 (0.3%)
9	V	1.09	1/598 (0.2%)	1.00	1/792 (0.1%)
10	J	1.10	0/462	1.04	1/625 (0.2%)
10	W	1.01	0/462	0.94	1/625 (0.2%)
11	K	1.30	1/398 (0.3%)	1.09	0/546
11	X	0.93	0/398	0.97	1/546 (0.2%)
12	L	1.41	2/393 (0.5%)	1.13	1/526 (0.2%)
12	Y	1.19	0/393	0.98	0/526
13	M	1.32	1/345 (0.3%)	1.15	1/470 (0.2%)
13	Z	0.92	0/345	0.95	0/470
All	All	1.29	107/29138 (0.4%)	1.17	148/39622 (0.4%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	2

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	54	ASN	CB-CG	-10.95	1.25	1.51
1	A	270	TYR	CD1-CE1	9.75	1.53	1.39
4	D	17	VAL	CB-CG1	-9.37	1.33	1.52
1	A	396	TRP	CE3-CZ3	9.08	1.53	1.38
1	A	371	TYR	CD1-CE1	8.87	1.52	1.39
7	T	36	TRP	CB-CG	8.51	1.65	1.50
3	P	29	SER	CB-OG	-8.36	1.31	1.42
1	A	371	TYR	CD2-CE2	8.16	1.51	1.39
3	P	214	PHE	CD1-CE1	7.77	1.54	1.39
2	B	200	CYS	CB-SG	7.66	1.95	1.82
1	A	440	TYR	CE1-CZ	7.55	1.48	1.38
3	C	29	SER	CB-OG	-7.41	1.32	1.42
1	A	393	PHE	CE1-CZ	7.39	1.51	1.37
3	P	253	TYR	CD2-CE2	7.38	1.50	1.39
3	P	172	TYR	CD1-CE1	7.27	1.50	1.39
1	A	494	TRP	CZ3-CH2	7.26	1.51	1.40
7	G	36	TRP	CB-CG	7.19	1.63	1.50
3	P	236	GLU	CG-CD	-6.99	1.41	1.51
2	O	200	CYS	CB-SG	6.93	1.94	1.82
13	M	4	LYS	CB-CG	-6.92	1.33	1.52
7	T	5	LYS	CB-CG	6.85	1.71	1.52
6	F	31	TYR	CE1-CZ	6.78	1.47	1.38
3	P	238	ALA	CA-CB	6.72	1.66	1.52
9	I	61	GLU	CG-CD	-6.68	1.42	1.51
3	C	236	GLU	CG-CD	-6.55	1.42	1.51
1	A	261	TYR	CZ-OH	6.51	1.49	1.37
2	B	19	GLU	CB-CG	-6.50	1.39	1.52
2	O	110	TYR	CD1-CE1	6.43	1.49	1.39
11	K	20	SER	CB-OG	-6.39	1.33	1.42
1	A	260	TYR	CE2-CZ	6.36	1.46	1.38
7	G	5	LYS	CB-CG	6.33	1.69	1.52
2	O	198	GLU	C-O	6.33	1.35	1.23
1	N	298	ASP	CB-CG	6.32	1.65	1.51
3	P	180	GLU	CD-OE1	6.21	1.32	1.25
1	A	474	GLU	CB-CG	6.19	1.64	1.52
4	Q	121	LYS	CE-NZ	6.11	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	8	TYR	CD1-CE1	6.09	1.48	1.39
3	P	89	SER	CB-OG	6.06	1.50	1.42
5	E	61	PHE	CE2-CZ	6.05	1.48	1.37
2	O	19	GLU	CB-CG	-6.05	1.40	1.52
12	L	35	ALA	CA-CB	6.04	1.65	1.52
12	L	40	VAL	CB-CG2	-5.97	1.40	1.52
1	A	81	TRP	CE3-CZ3	5.95	1.48	1.38
1	A	239	GLY	C-O	5.91	1.33	1.23
2	B	98	LYS	CD-CE	5.88	1.66	1.51
2	B	115	ASP	CB-CG	5.87	1.64	1.51
1	A	242	GLU	CG-CD	5.81	1.60	1.51
1	N	195	LEU	C-O	5.80	1.34	1.23
6	F	71	TRP	CB-CG	5.79	1.60	1.50
3	P	236	GLU	CB-CG	-5.79	1.41	1.52
1	N	78	PHE	CD1-CE1	5.78	1.50	1.39
3	P	74	ALA	CA-CB	5.78	1.64	1.52
1	A	261	TYR	CD1-CE1	5.78	1.48	1.39
1	A	189	MET	CB-CG	5.75	1.69	1.51
5	E	70	VAL	CB-CG2	5.74	1.65	1.52
4	Q	16	TYR	CD1-CE1	5.74	1.48	1.39
9	I	47	TYR	CD1-CE1	5.67	1.47	1.39
5	E	9	GLU	CG-CD	5.64	1.60	1.51
4	D	19	ARG	CZ-NH2	5.62	1.40	1.33
1	A	244	TYR	CD2-CE2	5.60	1.47	1.39
3	C	90	GLU	CB-CG	-5.59	1.41	1.52
4	D	58	GLU	CD-OE1	5.58	1.31	1.25
1	A	323	TRP	CB-CG	5.54	1.60	1.50
1	A	261	TYR	CE2-CZ	5.52	1.45	1.38
2	B	18	GLU	CG-CD	5.51	1.60	1.51
7	T	17	ARG	CD-NE	-5.50	1.37	1.46
1	A	470	PHE	CD1-CE1	5.47	1.50	1.39
1	N	251	PHE	CE2-CZ	5.43	1.47	1.37
1	N	148	PHE	CD1-CE1	5.42	1.50	1.39
3	C	16	TRP	CB-CG	5.40	1.59	1.50
2	O	196	CYS	CB-SG	5.40	1.91	1.82
2	B	156	SER	CA-CB	5.39	1.61	1.52
1	N	94	PHE	CE2-CZ	5.38	1.47	1.37
9	I	54	TYR	CD2-CE2	5.37	1.47	1.39
1	N	193	VAL	CB-CG1	5.35	1.64	1.52
2	O	113	TYR	CD2-CE2	5.35	1.47	1.39
2	O	65	TRP	CB-CG	-5.34	1.40	1.50
1	N	236	TRP	CB-CG	5.34	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	159	VAL	CB-CG2	5.34	1.64	1.52
2	B	192	TYR	CE2-CZ	5.33	1.45	1.38
2	B	167	SER	CB-OG	-5.33	1.35	1.42
3	P	236	GLU	CD-OE1	-5.28	1.19	1.25
1	A	450	TRP	CB-CG	5.27	1.59	1.50
1	A	385	ALA	CA-CB	5.25	1.63	1.52
3	C	57	TRP	CB-CG	5.25	1.59	1.50
3	C	102	TYR	CB-CG	5.24	1.59	1.51
4	D	11	TYR	CB-CG	5.24	1.59	1.51
4	D	58	GLU	CD-OE2	5.23	1.31	1.25
1	N	128	VAL	N-CA	5.22	1.56	1.46
3	C	197	PHE	CE1-CZ	5.20	1.47	1.37
1	A	297	MET	CB-CG	5.19	1.68	1.51
1	N	476	PHE	CD1-CE1	5.19	1.49	1.39
1	N	419	VAL	CA-CB	5.16	1.65	1.54
2	B	163	TRP	CB-CG	5.15	1.59	1.50
1	N	139	ALA	CA-CB	5.14	1.63	1.52
1	A	22	PHE	CD2-CE2	5.12	1.49	1.39
3	C	113	GLY	C-O	-5.10	1.15	1.23
6	S	92	VAL	CB-CG2	-5.09	1.42	1.52
1	A	340	TRP	CE3-CZ3	5.08	1.47	1.38
2	O	35	SER	CB-OG	-5.07	1.35	1.42
1	A	324	LEU	N-CA	5.05	1.56	1.46
9	V	51	TYR	CD2-CE2	5.04	1.47	1.39
4	Q	81	VAL	CB-CG1	5.02	1.63	1.52
3	P	172	TYR	CD2-CE2	5.01	1.46	1.39
1	A	397	PHE	CG-CD1	5.01	1.46	1.38
1	N	83	VAL	CB-CG2	5.00	1.63	1.52
2	O	121	TYR	CB-CG	-5.00	1.44	1.51

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	ARG	NE-CZ-NH2	-17.04	111.78	120.30
4	D	20	ARG	NE-CZ-NH2	-16.31	112.14	120.30
4	Q	20	ARG	NE-CZ-NH1	14.03	127.31	120.30
4	D	20	ARG	NE-CZ-NH1	13.62	127.11	120.30
4	D	19	ARG	NE-CZ-NH1	-13.50	113.55	120.30
4	Q	20	ARG	NE-CZ-NH2	-13.39	113.60	120.30
3	C	80	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	310	MET	CG-SD-CE	-11.74	81.42	100.20
7	T	17	ARG	NE-CZ-NH2	-10.91	114.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	B	188	ARG	NE-CZ-NH2	-10.35	115.12	120.30
4	D	19	ARG	NE-CZ-NH2	9.81	125.20	120.30
1	A	35	LEU	CA-CB-CG	-9.53	93.39	115.30
5	E	90	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	N	71	MET	CG-SD-CE	-9.35	85.24	100.20
1	A	117	MET	CG-SD-CE	-9.28	85.35	100.20
7	T	33	LEU	CA-CB-CG	8.88	135.72	115.30
3	C	156	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	N	278	MET	CG-SD-CE	-8.28	86.95	100.20
2	O	11	ASP	CB-CG-OD2	8.27	125.75	118.30
1	A	227	ASP	CB-CG-OD2	8.17	125.65	118.30
2	B	139	ASP	CB-CG-OD2	8.06	125.55	118.30
3	P	80	ARG	CG-CD-NE	-7.76	95.51	111.80
1	A	512	ASN	CB-CA-C	-7.70	95.00	110.40
1	N	286	ILE	CG1-CB-CG2	-7.61	94.67	111.40
1	A	278	MET	CG-SD-CE	-7.60	88.05	100.20
1	A	438	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	33	LEU	CB-CG-CD1	-7.47	98.31	111.00
1	A	480	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	71	MET	CG-SD-CE	-7.38	88.39	100.20
1	A	442	ASP	CB-CG-OD2	7.28	124.85	118.30
1	N	298	ASP	CB-CG-OD2	7.15	124.73	118.30
12	L	41	ARG	NE-CZ-NH1	7.14	123.87	120.30
9	I	73	LYS	CD-CE-NZ	-7.01	95.58	111.70
1	N	51	ASP	CB-CG-OD2	6.98	124.58	118.30
3	C	29	SER	CB-CA-C	-6.94	96.92	110.10
8	H	27	ARG	NE-CZ-NH1	6.88	123.74	120.30
8	H	75	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	208	MET	CG-SD-CE	6.84	111.14	100.20
3	C	221	ARG	NE-CZ-NH1	-6.82	116.89	120.30
6	S	54	ASN	CB-CA-C	-6.66	97.07	110.40
2	B	171	LYS	CD-CE-NZ	-6.65	96.41	111.70
3	C	80	ARG	CG-CD-NE	-6.62	97.90	111.80
3	P	127	LEU	CA-CB-CG	6.62	130.52	115.30
2	B	173	ASP	CB-CG-OD1	6.58	124.23	118.30
2	O	188	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	227	ASP	CB-CG-OD1	-6.57	112.39	118.30
3	P	214	PHE	CB-CG-CD1	6.52	125.36	120.80
2	B	82	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	N	366	VAL	CG1-CB-CG2	-6.42	100.62	110.90
1	A	96	ARG	NE-CZ-NH2	-6.38	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	50	LEU	CB-CG-CD1	-6.32	100.26	111.00
1	A	442	ASP	CB-CG-OD1	-6.28	112.65	118.30
3	C	236	GLU	CA-CB-CG	-6.26	99.62	113.40
6	S	25	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	51	ASP	CB-CG-OD2	6.25	123.92	118.30
9	V	55	ASP	CB-CG-OD1	6.25	123.92	118.30
11	X	54	ARG	NE-CZ-NH1	-6.24	117.18	120.30
2	B	152	MET	CG-SD-CE	6.22	110.15	100.20
1	N	310	MET	CG-SD-CE	-6.22	90.25	100.20
2	B	65	TRP	CB-CA-C	6.21	122.82	110.40
1	N	278	MET	CA-CB-CG	-6.21	102.75	113.30
1	A	278	MET	CA-CB-CG	-6.09	102.95	113.30
3	P	80	ARG	NE-CZ-NH1	-6.08	117.26	120.30
3	C	156	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	N	512	ASN	CB-CA-C	-6.01	98.38	110.40
3	C	214	PHE	CB-CG-CD1	5.98	124.99	120.80
3	P	223	LEU	CB-CG-CD1	-5.97	100.84	111.00
2	O	227	LEU	CB-CG-CD1	-5.94	100.90	111.00
6	S	56	ARG	NE-CZ-NH1	-5.90	117.35	120.30
3	C	214	PHE	CB-CG-CD2	-5.90	116.67	120.80
7	G	8	HIS	N-CA-C	5.88	126.86	111.00
1	A	298	ASP	CB-CG-OD2	5.87	123.58	118.30
1	N	28	MET	CG-SD-CE	5.86	109.58	100.20
9	I	55	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	B	139	ASP	CB-CG-OD1	-5.84	113.04	118.30
3	P	214	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	A	513	LEU	CB-CG-CD1	-5.82	101.11	111.00
6	S	94	HIS	N-CA-C	5.82	126.71	111.00
3	P	127	LEU	CB-CG-CD1	5.79	120.83	111.00
2	B	178	ARG	NE-CZ-NH2	5.78	123.19	120.30
6	S	53	THR	CB-CA-C	-5.77	96.03	111.60
4	D	59	LEU	CB-CG-CD2	-5.76	101.21	111.00
2	B	119	ASP	CB-CG-OD2	5.72	123.45	118.30
1	N	169	ILE	CB-CA-C	-5.70	100.19	111.60
1	N	189	MET	CA-CB-CG	-5.68	103.65	113.30
2	B	112	ASP	CB-CG-OD2	-5.67	113.19	118.30
6	S	65	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	212	ASP	CB-CG-OD2	5.60	123.34	118.30
4	D	51	LEU	CA-CB-CG	5.60	128.17	115.30
3	C	44	MET	CG-SD-CE	5.59	109.15	100.20
1	A	50	ASP	CB-CG-OD1	5.59	123.33	118.30
1	N	199	LEU	CB-CG-CD1	-5.58	101.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	21	ASP	CB-CG-OD2	5.58	123.32	118.30
3	C	47	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	N	498	CYS	CA-CB-SG	-5.56	103.99	114.00
4	Q	19	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	407	ASP	CB-CG-OD2	5.56	123.30	118.30
5	R	36	LEU	CB-CG-CD2	-5.54	101.58	111.00
7	G	54	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	N	240	HIS	N-CA-CB	5.52	120.53	110.60
1	A	35	LEU	CB-CG-CD1	5.51	120.37	111.00
2	O	185	MET	CG-SD-CE	5.51	109.02	100.20
4	D	17	VAL	CB-CA-C	-5.51	100.94	111.40
2	O	82	ARG	NE-CZ-NH2	-5.48	117.56	120.30
6	S	45	ASP	CB-CG-OD1	-5.47	113.38	118.30
5	E	21	LYS	CD-CE-NZ	-5.47	99.12	111.70
6	F	18	ARG	NE-CZ-NH2	-5.44	117.58	120.30
7	T	56	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	358	LEU	CB-CG-CD2	-5.39	101.83	111.00
3	P	60	ASP	CB-CG-OD1	5.38	123.14	118.30
2	O	173	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	311	ILE	CG1-CB-CG2	-5.34	99.66	111.40
2	O	65	TRP	CB-CA-C	5.33	121.06	110.40
1	N	100	MET	CG-SD-CE	5.32	108.71	100.20
1	N	312	ILE	CG1-CB-CG2	-5.31	99.72	111.40
5	R	40	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	98	LYS	CD-CE-NZ	-5.31	99.50	111.70
5	E	90	ARG	CG-CD-NE	-5.30	100.66	111.80
1	N	113	LEU	CB-CG-CD2	5.29	120.00	111.00
4	D	13	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	495	LEU	CB-CG-CD2	-5.28	102.03	111.00
10	W	50	LEU	CA-CB-CG	5.26	127.41	115.30
7	T	5	LYS	CB-CA-C	5.25	120.91	110.40
1	A	74	MET	CB-CG-SD	-5.23	96.70	112.40
1	A	238	PHE	CD1-CE1-CZ	-5.23	113.82	120.10
10	J	36	MET	CG-SD-CE	-5.22	91.85	100.20
8	H	57	ARG	NE-CZ-NH1	5.18	122.89	120.30
7	G	54	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	366	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	N	442	ASP	CB-CG-OD2	5.17	122.95	118.30
4	Q	17	VAL	CG1-CB-CG2	-5.15	102.67	110.90
1	N	367	LEU	CB-CG-CD2	-5.14	102.26	111.00
6	F	93	PRO	C-N-CA	5.13	134.52	121.70
2	O	78	LEU	CB-CG-CD1	5.12	119.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	29	SER	CB-CA-C	-5.12	100.36	110.10
1	A	431	LEU	CA-CB-CG	-5.08	103.61	115.30
1	A	270	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	A	369	ASP	CB-CG-OD2	5.07	122.86	118.30
13	M	19	LEU	CB-CG-CD2	-5.07	102.39	111.00
3	P	155	ASP	CB-CG-OD1	5.07	122.86	118.30
2	O	178	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	O	46	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	N	69	MET	CG-SD-CE	5.04	108.26	100.20
1	N	145	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	244	TYR	CA-CB-CG	-5.02	103.87	113.40
4	D	125	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	169	ILE	CB-CA-C	-5.00	101.60	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide
6	S	95	GLN	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	4027	0	4001	47	0
1	N	4027	0	4001	75	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	45	0
3	C	2110	0	2027	37	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	27	0
5	E	842	0	838	5	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	675	0	643	38	0
7	T	675	0	643	45	0
8	H	628	0	580	9	0
8	U	628	0	580	8	0
9	I	585	0	597	13	0
9	V	585	0	597	15	0
10	J	451	0	446	5	0
10	W	451	0	446	6	0
11	K	384	0	366	1	0
11	X	384	0	366	5	0
12	L	380	0	380	11	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	1	0
17	N	1	0	0	0	0
18	A	120	0	108	11	0
18	N	120	0	108	14	0
19	A	63	0	110	13	0
19	D	63	0	110	9	0
19	L	63	0	110	15	0
19	O	126	0	220	23	0
19	Y	63	0	110	18	0
20	A	102	0	152	8	0
20	C	51	0	76	4	0
20	H	51	0	76	3	0
20	N	153	0	228	12	0
20	P	51	0	76	11	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	2	0
22	C	58	0	70	5	0
22	J	29	0	36	1	0
22	O	29	0	36	0	0
22	P	58	0	71	1	0
22	W	29	0	36	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	7	0
24	G	106	0	154	31	0
24	P	53	0	77	7	0
24	T	106	0	154	30	0
25	C	100	0	156	19	0
25	G	100	0	156	27	0
25	P	100	0	156	24	0
25	T	100	0	156	19	0
26	E	52	0	80	22	0
26	R	52	0	80	15	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	5	0
28	M	33	0	39	0	0
28	P	33	0	40	1	0
28	Z	33	0	38	3	0
29	A	203	0	0	3	0
29	B	131	0	0	2	0
29	C	90	0	0	4	0
29	D	96	0	0	8	0
29	E	62	0	0	0	0
29	F	70	0	0	1	0
29	G	41	0	0	6	0
29	H	46	0	0	2	0
29	I	44	0	0	3	0
29	J	17	0	0	1	0
29	K	22	0	0	2	0
29	L	23	0	0	1	0
29	M	19	0	0	0	0
29	N	196	0	0	3	0
29	O	106	0	0	3	0
29	P	89	0	0	1	0
29	Q	54	0	0	4	0
29	R	52	0	0	0	0
29	S	62	0	0	6	0
29	T	39	0	0	7	0
29	U	39	0	0	2	0
29	V	16	0	0	3	0
29	W	15	0	0	1	0
29	X	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Y	19	0	0	1	0
29	Z	10	0	0	1	0
All	All	32113	0	31062	673	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (673) 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)
24:G:265:PEK:C8	24:G:265:PEK:C7	1.75	1.56
24:G:265:PEK:C9	24:G:265:PEK:C8	1.77	1.55
24:G:265:PEK:C10	24:G:265:PEK:C9	1.81	1.50
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.48
24:G:265:PEK:H383	25:G:269:CDL:C27	1.46	1.44
1:N:297:MET:CE	1:N:297:MET:SD	2.04	1.44
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.35	1.37
7:G:5:LYS:HD2	24:G:1263:PEK:C37	1.59	1.33
24:T:1265:PEK:H383	25:T:1269:CDL:C27	1.60	1.28
7:G:5:LYS:CD	24:G:1263:PEK:H371	1.65	1.25
24:G:265:PEK:C38	25:G:269:CDL:C27	2.19	1.21
12:L:20:ARG:HH22	19:L:522:TGL:CC3	1.59	1.15
24:G:265:PEK:H383	25:G:269:CDL:H273	1.26	1.14
7:G:5:LYS:CG	24:G:1263:PEK:H371	1.82	1.10
15:A:520:PER:O1	15:A:520:PER:O2	1.70	1.09
7:T:5:LYS:HD2	24:T:263:PEK:H381	1.28	1.09
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.13	1.09
2:O:41:ILE:HD13	26:R:1230:PSC:H342	1.35	1.08
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.12	1.08
26:E:230:PSC:H072	9:I:10:ARG:HH21	1.19	1.08
24:P:1264:PEK:H71	24:P:1264:PEK:H32	1.30	1.08
29:N:4407:HOH:O	19:O:1523:TGL:HC32	1.52	1.06
7:T:84:LYS:HD2	7:T:84:LYS:N	1.70	1.06
15:N:520:PER:O2	15:N:520:PER:O1	1.70	1.06
24:T:1265:PEK:C38	25:T:1269:CDL:C27	2.35	1.03
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.19	1.03
25:G:269:CDL:H242	25:G:269:CDL:H542	1.40	1.02
26:R:1230:PSC:O01	26:R:1230:PSC:H212	1.58	1.01
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.19	1.01
7:T:84:LYS:HD2	7:T:84:LYS:H	1.20	1.01
7:G:5:LYS:HD2	24:G:1263:PEK:H371	1.14	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:2:SER:OG	24:T:263:PEK:H302	1.60	1.01
2:O:116:LEU:HD12	2:O:117:SER:N	1.75	1.01
25:G:269:CDL:C54	25:G:269:CDL:H242	1.91	1.00
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.78	0.99
20:N:1524:PGV:H221	20:N:1524:PGV:H31	1.40	0.99
24:T:1265:PEK:C38	25:T:1269:CDL:H272	1.91	0.99
1:N:113:LEU:HD12	19:Y:1522:TGL:H292	1.43	0.99
24:T:1265:PEK:H383	25:T:1269:CDL:H272	1.01	0.99
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.44	0.99
20:P:1267:PGV:H182	25:P:1270:CDL:H662	1.42	0.98
18:N:515:HEA:C27	18:N:515:HEA:C16	2.41	0.98
24:G:265:PEK:C38	25:G:269:CDL:H272	1.93	0.98
19:Y:1522:TGL:HC22	19:Y:1522:TGL:HC62	1.45	0.98
6:S:95:GLN:HE21	6:S:95:GLN:HA	1.27	0.97
7:T:5:LYS:CD	24:T:263:PEK:H381	1.95	0.97
18:N:515:HEA:H161	18:N:515:HEA:H272	1.47	0.97
7:G:5:LYS:HB3	1:N:278:MET:SD	2.07	0.95
6:S:95:GLN:HG2	29:S:4406:HOH:O	1.63	0.94
24:G:265:PEK:H383	25:G:269:CDL:H271	1.47	0.94
26:E:230:PSC:C07	9:I:10:ARG:HH21	1.80	0.93
25:G:269:CDL:HA21	25:G:269:CDL:H112	1.50	0.91
19:A:521:TGL:H281	19:A:521:TGL:H101	1.51	0.91
7:G:5:LYS:HD2	24:G:1263:PEK:H372	1.54	0.90
18:N:515:HEA:H272	18:N:515:HEA:C16	1.99	0.88
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	1.73	0.88
7:T:84:LYS:H	7:T:84:LYS:CD	1.85	0.88
20:P:1267:PGV:C18	25:P:1270:CDL:H662	2.04	0.88
6:S:85:CYS:SG	6:S:87:THR:HG23	2.14	0.88
7:T:5:LYS:HD2	24:T:263:PEK:C38	2.03	0.87
26:R:1230:PSC:C07	9:V:10:ARG:HH21	1.87	0.87
7:G:5:LYS:HB2	24:G:1263:PEK:H351	1.54	0.86
24:G:265:PEK:H382	25:G:269:CDL:H272	1.55	0.86
24:G:265:PEK:C6	24:G:265:PEK:C8	2.53	0.86
24:T:1265:PEK:C38	25:T:1269:CDL:H273	2.03	0.86
24:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.24	0.85
26:E:230:PSC:H343	26:E:230:PSC:H142	1.57	0.85
1:A:296:GLY:HA2	8:H:23:GLN:OE1	1.77	0.84
7:T:5:LYS:CD	24:T:263:PEK:C38	2.55	0.84
10:W:33:ARG:HG2	22:W:1060:CHD:H151	1.59	0.84
7:T:5:LYS:HB2	24:T:263:PEK:H371	1.60	0.83
19:O:1521:TGL:HB92	19:O:1521:TGL:H281	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HB2	24:T:263:PEK:C37	2.09	0.82
13:M:39:ASN:O	13:M:43:SER:HB2	1.80	0.82
19:Y:1522:TGL:H231	19:Y:1522:TGL:HA92	1.62	0.81
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.15	0.81
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.62	0.81
18:N:515:HEA:H273	18:N:515:HEA:H162	1.60	0.81
20:A:524:PGV:H02	20:A:524:PGV:O14	1.81	0.81
7:G:5:LYS:HG3	24:G:1263:PEK:H371	1.63	0.80
6:S:95:GLN:NE2	6:S:95:GLN:HA	1.96	0.80
19:O:1521:TGL:H101	19:O:1521:TGL:H281	1.63	0.80
3:C:3:HIS:HE1	6:F:96:LEU:CD2	1.93	0.80
19:L:522:TGL:HC62	19:L:522:TGL:CC2	2.10	0.80
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.46	0.80
19:O:1521:TGL:H101	19:O:1521:TGL:C28	2.12	0.79
7:T:2:SER:OG	24:T:263:PEK:C30	2.29	0.79
8:H:45:ALA:O	8:H:47:GLY:N	2.14	0.79
24:C:264:PEK:C10	24:C:264:PEK:H161	2.11	0.79
7:G:72:ASN:H	7:G:76:ASN:HD22	1.26	0.79
10:J:7:GLU:HG3	29:J:4441:HOH:O	1.83	0.79
9:V:73:LYS:HB2	29:V:4544:HOH:O	1.81	0.79
3:P:224:LYS:CD	25:P:1270:CDL:HB31	2.13	0.78
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.78
9:I:73:LYS:HB3	29:I:4590:HOH:O	1.84	0.78
7:G:5:LYS:CD	24:G:1263:PEK:C37	2.40	0.78
1:N:400:PHE:HB3	19:Y:1522:TGL:H283	1.66	0.78
6:S:52:ILE:O	6:S:94:HIS:CE1	2.36	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.66	0.78
6:F:85:CYS:SG	6:F:87:THR:HG23	2.23	0.78
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.78
4:Q:72:ASN:HB3	29:Q:3133:HOH:O	1.83	0.78
29:O:4115:HOH:O	8:U:61:LYS:HD2	1.83	0.78
4:D:34:SER:H	4:D:37:GLN:HE21	1.32	0.77
19:O:1523:TGL:HA91	19:O:1523:TGL:H231	1.67	0.76
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.67	0.76
2:O:226:MET:O	2:O:227:LEU:O	2.03	0.76
3:C:3:HIS:HE1	6:F:96:LEU:HD22	1.47	0.76
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.68	0.76
20:P:1267:PGV:H182	25:P:1270:CDL:C66	2.15	0.75
1:A:484:THR:HB	13:M:2:THR:OG1	1.86	0.75
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.69	0.75
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.27	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:521:TGL:H322	19:A:521:TGL:HA92	1.68	0.75
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.51	0.74
24:P:1264:PEK:H161	24:P:1264:PEK:C10	2.16	0.74
24:C:264:PEK:H71	24:C:264:PEK:H32	1.68	0.74
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.87	0.74
3:C:3:HIS:CE1	6:F:96:LEU:HD22	2.22	0.74
4:D:86:MET:HE3	29:K:4663:HOH:O	1.87	0.74
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.21	0.74
24:T:1265:PEK:H381	25:T:1269:CDL:H273	1.69	0.74
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.67	0.74
7:G:84:LYS:HD2	7:G:84:LYS:H	1.53	0.74
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.00	0.73
20:C:267:PGV:H172	25:C:270:CDL:H652	1.69	0.73
4:D:31:LYS:HE2	29:D:4577:HOH:O	1.87	0.73
4:D:31:LYS:NZ	29:D:4577:HOH:O	2.22	0.73
3:C:80:ARG:NH1	24:T:263:PEK:H032	2.04	0.73
7:T:17:ARG:HD3	29:T:3302:HOH:O	1.88	0.73
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.69	0.73
2:O:226:MET:O	2:O:227:LEU:C	2.28	0.72
2:B:56:MET:HA	26:E:230:PSC:H202	1.71	0.72
4:D:31:LYS:CE	29:D:4577:HOH:O	2.37	0.72
29:N:4424:HOH:O	26:R:1230:PSC:H21	1.90	0.72
19:L:522:TGL:HC81	29:L:4545:HOH:O	1.89	0.72
19:A:521:TGL:HA82	19:A:521:TGL:H282	1.69	0.72
18:N:515:HEA:C27	18:N:515:HEA:H162	2.17	0.72
7:G:38:HIS:HE1	25:G:269:CDL:H111	1.53	0.71
25:G:269:CDL:H332	2:O:78:LEU:HD12	1.73	0.71
10:J:52:TRP:O	10:J:57:HIS:HE1	1.74	0.71
1:N:113:LEU:CD1	19:Y:1522:TGL:H292	2.19	0.71
24:C:264:PEK:H102	24:C:264:PEK:H161	1.70	0.71
19:A:521:TGL:H281	19:A:521:TGL:C10	2.21	0.71
26:E:230:PSC:H212	26:E:230:PSC:H02	1.73	0.70
25:G:269:CDL:H201	1:N:311:ILE:CD1	2.22	0.70
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.73	0.70
6:S:75:HIS:H	6:S:80:GLN:HE22	1.39	0.70
19:O:1521:TGL:CB9	19:O:1521:TGL:H281	2.21	0.70
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.72	0.70
19:O:1523:TGL:HC21	19:O:1523:TGL:HG11	1.74	0.70
24:C:264:PEK:H101	24:C:264:PEK:H161	1.74	0.70
24:P:1264:PEK:H161	24:P:1264:PEK:H101	1.73	0.70
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:ARG:HD2	10:J:7:GLU:OE2	1.92	0.69
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.22	0.69
2:B:81:LEU:HD12	25:T:1269:CDL:H351	1.74	0.69
18:N:515:HEA:H273	18:N:515:HEA:C16	2.17	0.69
7:T:8:HIS:CE1	24:T:263:PEK:H321	2.28	0.69
3:P:224:LYS:HD2	25:P:1270:CDL:HB31	1.74	0.69
11:X:54:ARG:NH2	11:X:54:ARG:HG3	1.91	0.69
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.55	0.69
3:C:63:ARG:NE	25:C:270:CDL:HA22	2.01	0.69
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.93	0.69
26:R:1230:PSC:H071	9:V:10:ARG:HH21	1.58	0.69
19:A:521:TGL:OB1	19:A:521:TGL:HB42	1.91	0.69
10:W:33:ARG:HG2	22:W:1060:CHD:C15	2.22	0.68
24:G:265:PEK:C38	25:G:269:CDL:H273	2.06	0.68
7:T:5:LYS:CB	24:T:263:PEK:H371	2.23	0.68
29:G:4754:HOH:O	20:N:1268:PGV:H341	1.91	0.68
3:C:55:TYR:CE1	25:C:270:CDL:H521	2.28	0.68
20:N:1524:PGV:C22	20:N:1524:PGV:H31	2.19	0.68
24:G:1263:PEK:H222	29:G:4660:HOH:O	1.93	0.68
20:A:522:PGV:H183	24:C:264:PEK:H332	1.74	0.68
7:T:72:ASN:H	7:T:76:ASN:HD22	1.40	0.67
26:R:1230:PSC:O02	26:R:1230:PSC:H032	1.94	0.67
20:N:1524:PGV:H221	20:N:1524:PGV:C3	2.20	0.67
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.76	0.67
25:G:269:CDL:CA2	25:G:269:CDL:H112	2.23	0.66
25:G:269:CDL:H201	1:N:311:ILE:HD11	1.76	0.66
1:A:278:MET:SD	7:T:5:LYS:HB3	2.35	0.66
24:G:265:PEK:C10	24:G:265:PEK:C8	2.73	0.66
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.77	0.66
7:T:5:LYS:CG	24:T:263:PEK:H383	2.26	0.66
3:P:226:HIS:CE1	25:P:1270:CDL:HB32	2.31	0.66
26:E:230:PSC:H212	26:E:230:PSC:C02	2.26	0.66
26:R:1230:PSC:H072	9:V:10:ARG:HH21	1.61	0.65
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.00	0.65
19:Y:1522:TGL:CC2	19:Y:1522:TGL:HC62	2.06	0.65
1:A:430:PHE:CE1	19:A:521:TGL:HB21	2.29	0.65
4:Q:109:HIS:HD2	29:Q:3152:HOH:O	1.79	0.65
20:N:1524:PGV:H032	20:N:1524:PGV:H22	1.78	0.65
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.43	0.65
25:C:270:CDL:H661	25:C:270:CDL:H241	1.79	0.65
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HD12	19:Y:1522:TGL:C29	2.24	0.65
25:G:269:CDL:H181	25:G:269:CDL:H511	1.78	0.64
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.27	0.64
2:B:129:LYS:HE3	29:B:4594:HOH:O	1.97	0.64
3:P:213:THR:HG21	20:P:1267:PGV:H11	1.78	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.98	0.64
1:A:311:ILE:HD12	25:T:1269:CDL:H201	1.79	0.64
7:G:84:LYS:N	7:G:84:LYS:HD2	2.13	0.64
25:C:270:CDL:H522	25:C:270:CDL:OB9	1.98	0.63
10:J:50:LEU:HD22	10:J:50:LEU:O	1.99	0.63
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.66	0.63
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.96	0.63
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.34	0.63
25:T:1269:CDL:H571	25:T:1269:CDL:C78	2.25	0.63
6:S:94:HIS:CD2	6:S:95:GLN:H	2.16	0.63
1:N:177:SER:H	1:N:180:GLN:NE2	1.95	0.63
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.31	0.63
20:C:267:PGV:H182	25:C:270:CDL:H671	1.79	0.62
1:N:513:LEU:O	1:N:514:LYS:HB2	1.98	0.62
24:G:265:PEK:C9	24:G:265:PEK:C11	2.75	0.62
3:P:111:GLU:HG3	29:U:4773:HOH:O	1.98	0.62
18:N:516:HEA:HBC1	18:N:516:HEA:HMC1	1.81	0.62
7:T:5:LYS:HB2	24:T:263:PEK:C36	2.29	0.62
3:P:55:TYR:CE1	25:P:1270:CDL:H521	2.34	0.62
6:S:94:HIS:CD2	6:S:95:GLN:N	2.68	0.62
3:C:210:ILE:HG12	20:C:267:PGV:H12	1.81	0.62
1:N:87:ILE:O	1:N:173:PRO:HD3	1.99	0.62
2:O:32:PHE:HE2	19:O:1521:TGL:HA52	1.64	0.62
2:O:116:LEU:HD12	2:O:116:LEU:C	2.20	0.62
19:O:1521:TGL:C10	19:O:1521:TGL:H281	2.28	0.61
2:B:62:GLU:O	2:B:66:THR:HB	1.99	0.61
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.18	0.61
2:O:116:LEU:HD12	2:O:117:SER:H	1.62	0.61
25:P:1270:CDL:H222	25:P:1270:CDL:H632	1.83	0.61
19:O:1523:TGL:HG31	29:Q:4568:HOH:O	2.00	0.61
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.65	0.61
1:A:513:LEU:O	1:A:514:LYS:HB2	1.99	0.61
25:T:1269:CDL:C11	25:T:1269:CDL:HA21	2.28	0.61
3:P:210:ILE:HD13	20:P:1267:PGV:H301	1.83	0.61
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.61
4:D:34:SER:H	4:D:37:GLN:NE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.81	0.61
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.83	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.49	0.60
26:E:230:PSC:H072	9:I:10:ARG:NH2	2.04	0.60
26:E:230:PSC:H212	26:E:230:PSC:O01	2.01	0.60
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.37	0.60
7:G:72:ASN:H	7:G:76:ASN:ND2	1.98	0.60
17:A:519:NA:NA	29:A:2026:HOH:O	1.73	0.60
24:P:1264:PEK:H102	24:P:1264:PEK:H161	1.83	0.60
3:P:63:ARG:NE	25:P:1270:CDL:HA22	1.99	0.59
25:G:269:CDL:C63	25:G:269:CDL:H592	2.31	0.59
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.83	0.59
6:S:26:LYS:HB3	6:S:28:GLN:NE2	2.17	0.59
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.03	0.59
3:C:52:LEU:HD23	25:C:270:CDL:H362	1.84	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.31	0.59
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.38	0.59
2:O:41:ILE:HD13	26:R:1230:PSC:C34	2.22	0.59
20:N:1524:PGV:H062	29:Z:3153:HOH:O	2.01	0.59
3:C:3:HIS:N	29:C:4573:HOH:O	2.36	0.59
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.38	0.59
24:G:265:PEK:C9	24:G:265:PEK:C7	2.81	0.59
19:L:522:TGL:HC41	19:L:522:TGL:OC1	2.02	0.59
26:E:230:PSC:H231	26:E:230:PSC:H42	1.84	0.59
12:Y:12:PRO:HG2	19:Y:1522:TGL:HG11	1.84	0.59
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.85	0.59
4:D:107:ILE:HB	4:D:108:PRO:CD	2.32	0.59
7:T:5:LYS:CG	24:T:263:PEK:C38	2.81	0.58
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.58
2:O:42:ILE:HG21	19:O:1523:TGL:H232	1.84	0.58
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.68	0.58
3:C:80:ARG:HH11	24:T:263:PEK:H032	1.67	0.58
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.69	0.58
8:H:45:ALA:C	8:H:47:GLY:H	2.05	0.58
7:G:3:ALA:O	7:G:4:ALA:CB	2.51	0.58
1:A:281:GLY:C	7:T:4:ALA:HB1	2.25	0.58
7:G:45:PRO:HD2	29:G:2145:HOH:O	2.03	0.58
3:C:3:HIS:N	29:C:4600:HOH:O	2.37	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.57
12:L:14:SER:H	19:L:522:TGL:HC31	1.69	0.57
3:P:210:ILE:HG21	20:P:1267:PGV:H282	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.57
2:B:41:ILE:HD13	26:E:230:PSC:H342	1.87	0.57
19:D:523:TGL:HB42	19:D:523:TGL:HA32	1.87	0.57
4:Q:109:HIS:CD2	29:Q:3152:HOH:O	2.54	0.57
7:G:5:LYS:HG3	24:G:1263:PEK:C37	2.32	0.56
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.87	0.56
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.40	0.56
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.40	0.56
3:C:224:LYS:CD	25:C:270:CDL:HB31	2.36	0.56
7:T:36:TRP:HE1	24:T:1265:PEK:C20	2.19	0.56
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.93	0.56
9:V:36:LYS:O	9:V:41:GLU:HG2	2.06	0.56
24:G:1263:PEK:H382	29:G:4355:HOH:O	2.06	0.55
3:C:48:THR:HG23	25:C:270:CDL:H402	1.88	0.55
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.46	0.55
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.55
7:T:45:PRO:HD2	29:T:3145:HOH:O	2.05	0.55
2:B:164:ALA:O	2:B:194:GLY:HA3	2.06	0.55
25:G:269:CDL:H601	25:G:269:CDL:H761	1.89	0.55
26:E:230:PSC:C07	9:I:10:ARG:NH2	2.61	0.55
19:Y:1522:TGL:HC22	19:Y:1522:TGL:CC6	2.28	0.55
1:N:240:HIS:O	1:N:243:VAL:HG22	2.07	0.55
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.55
7:T:37:LEU:HD23	7:T:38:HIS:HD1	1.72	0.55
6:S:64:GLU:O	6:S:65:ASP:HB2	2.06	0.55
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.89	0.54
1:A:311:ILE:CD1	25:T:1269:CDL:H201	2.38	0.54
29:A:4231:HOH:O	26:E:230:PSC:H21	2.08	0.54
1:N:430:PHE:CE1	19:O:1521:TGL:HB21	2.43	0.54
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.64	0.54
19:D:523:TGL:H352	9:I:16:ARG:HH21	1.72	0.54
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.89	0.54
26:R:1230:PSC:H221	26:R:1230:PSC:H42	1.89	0.54
1:N:412:ILE:HD13	4:Q:84:ALA:CB	2.38	0.54
3:P:254:VAL:HG23	25:T:1269:CDL:H672	1.90	0.54
1:N:62:ALA:HB1	18:N:515:HEA:HMD3	1.88	0.54
6:S:25:ARG:HD3	29:S:4659:HOH:O	2.07	0.54
1:N:417:MET:O	1:N:421:VAL:HG22	2.07	0.54
7:G:69:PHE:HZ	28:G:272:DMU:H1	1.72	0.54
1:A:297:MET:CE	1:A:297:MET:CB	2.86	0.53
25:P:1270:CDL:C63	25:P:1270:CDL:H222	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:22:LEU:HD23	6:S:25:ARG:NH1	2.23	0.53
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.89	0.53
8:U:45:ALA:O	8:U:47:GLY:N	2.41	0.53
1:N:438:ARG:O	1:N:439:ARG:HB2	2.07	0.53
25:C:270:CDL:H661	25:C:270:CDL:C24	2.38	0.53
19:A:521:TGL:HC22	29:D:2376:HOH:O	2.08	0.53
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.91	0.53
1:A:112:LEU:HG	29:A:2073:HOH:O	2.08	0.53
19:A:521:TGL:H322	19:A:521:TGL:CA9	2.37	0.53
4:D:78:TRP:HA	19:D:523:TGL:HB22	1.90	0.53
18:A:515:HEA:H122	18:A:515:HEA:HHC	1.89	0.53
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.08	0.53
7:G:5:LYS:HD2	24:G:1263:PEK:C38	2.36	0.52
20:A:524:PGV:H152	20:A:524:PGV:C32	2.39	0.52
4:D:86:MET:CE	29:K:4663:HOH:O	2.51	0.52
4:D:31:LYS:NZ	29:D:4344:HOH:O	2.40	0.52
28:G:272:DMU:O1	28:G:272:DMU:H29	2.09	0.52
26:E:230:PSC:C06	9:I:10:ARG:HE	2.22	0.52
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.52
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.90	0.52
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.52
3:P:112:LEU:CD2	29:T:3156:HOH:O	2.57	0.52
2:O:129:LYS:O	2:O:132:GLU:HB2	2.09	0.52
1:A:514:LYS:OXT	6:F:37:LYS:HE2	2.09	0.52
19:O:1523:TGL:HC21	19:O:1523:TGL:CG1	2.40	0.52
19:Y:1522:TGL:OA1	19:Y:1522:TGL:H171	2.10	0.52
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.07	0.52
9:V:18:ARG:HG3	29:V:3367:HOH:O	2.08	0.52
3:P:213:THR:CG2	20:P:1267:PGV:H11	2.39	0.52
26:E:230:PSC:C14	26:E:230:PSC:H343	2.36	0.52
1:N:430:PHE:HE1	19:O:1521:TGL:HB21	1.75	0.52
3:C:59:ARG:HG3	25:C:270:CDL:H512	1.92	0.52
2:O:139:ASP:OD2	2:O:140:ASN:N	2.41	0.52
9:I:58:LYS:O	9:I:62:GLU:HG3	2.10	0.52
19:O:1523:TGL:H121	19:O:1523:TGL:HB81	1.92	0.51
2:O:128:LEU:HD22	2:O:132:GLU:HB3	1.92	0.51
2:O:221:LYS:NZ	29:O:4469:HOH:O	2.43	0.51
8:H:27:ARG:NH1	29:H:2296:HOH:O	2.43	0.51
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.92	0.51
24:P:1264:PEK:H32	24:P:1264:PEK:C7	2.19	0.51
2:O:41:ILE:CD1	26:R:1230:PSC:H342	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:37:LEU:HD23	7:T:38:HIS:ND1	2.25	0.51
20:A:524:PGV:H152	20:A:524:PGV:H322	1.92	0.51
1:N:199:LEU:N	1:N:200:PRO:CD	2.74	0.51
4:D:58:GLU:HG3	4:D:58:GLU:O	2.10	0.51
25:G:269:CDL:H752	1:N:282:PHE:HZ	1.76	0.51
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.51
25:G:269:CDL:H632	25:G:269:CDL:H592	1.92	0.50
12:Y:24:MET:SD	19:Y:1522:TGL:H162	2.51	0.50
19:Y:1522:TGL:H311	29:Y:4350:HOH:O	2.10	0.50
6:S:94:HIS:CG	6:S:95:GLN:H	2.24	0.50
24:C:264:PEK:H102	24:C:264:PEK:C16	2.40	0.50
2:O:32:PHE:CE2	19:O:1521:TGL:HA52	2.46	0.50
6:S:22:LEU:CD2	6:S:25:ARG:NH1	2.75	0.50
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.08	0.50
8:U:27:ARG:NH1	29:U:3296:HOH:O	2.43	0.50
1:N:20:LEU:HB3	19:Y:1522:TGL:H221	1.93	0.50
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.65	0.50
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.50
9:V:25:PHE:O	9:V:28:SER:HB2	2.11	0.49
19:O:1521:TGL:H101	19:O:1521:TGL:H283	1.90	0.49
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	1.94	0.49
2:B:59:GLN:C	2:B:60:GLU:HG3	2.33	0.49
1:A:28:MET:CE	18:A:515:HEA:H271	2.41	0.49
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.25	0.49
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.94	0.49
7:G:2:SER:O	24:G:1263:PEK:H322	2.13	0.49
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.43	0.49
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.76	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.49
1:N:383:MET:O	1:N:387:PHE:HB2	2.12	0.48
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.61	0.48
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.43	0.48
28:G:272:DMU:C10	28:G:272:DMU:H29	2.43	0.48
7:T:36:TRP:HD1	29:T:4758:HOH:O	1.96	0.48
6:S:52:ILE:O	6:S:94:HIS:HE1	1.91	0.48
18:N:516:HEA:CBC	18:N:516:HEA:HMC1	2.42	0.48
6:S:43:LYS:HE3	29:S:3347:HOH:O	2.13	0.48
1:A:47:LEU:O	13:M:41:LYS:HD2	2.14	0.48
20:A:524:PGV:O02	20:A:524:PGV:P	2.72	0.48
7:G:84:LYS:N	7:G:84:LYS:CD	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:THR:HG21	22:B:1086:CHD:H3	1.96	0.48
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.48
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.59	0.48
1:N:48:LEU:HB2	29:N:3109:HOH:O	2.14	0.48
6:S:95:GLN:CA	6:S:95:GLN:HE21	2.14	0.48
6:S:26:LYS:HB3	6:S:28:GLN:HE22	1.79	0.48
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.40	0.48
7:T:36:TRP:HE1	24:T:1265:PEK:H201	1.79	0.48
10:J:50:LEU:HD22	10:J:54:SER:HG	1.79	0.48
9:I:35:TYR:C	9:I:37:PHE:H	2.17	0.48
26:E:230:PSC:H232	26:E:230:PSC:H201	1.51	0.48
1:N:422:ASN:OD1	19:O:1521:TGL:H262	2.14	0.48
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.48
25:G:269:CDL:H782	25:G:269:CDL:H571	1.96	0.48
3:C:246:ASP:HB2	29:C:4215:HOH:O	2.13	0.48
5:E:11:PHE:CB	26:E:230:PSC:H073	2.44	0.47
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.47	0.47
3:C:106:LEU:HD13	20:H:268:PGV:H22	1.95	0.47
26:R:1230:PSC:H071	9:V:10:ARG:NH2	2.28	0.47
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.41	0.47
2:B:59:GLN:O	2:B:60:GLU:HG3	2.14	0.47
2:O:1:FME:HCN	2:O:193:TYR:HB2	1.96	0.47
1:A:198:SER:HB2	1:A:238:PHE:HA	1.96	0.47
1:A:281:GLY:O	7:T:4:ALA:HB1	2.15	0.47
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.96	0.47
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.14	0.47
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.29	0.47
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.96	0.47
3:C:210:ILE:HD13	20:C:267:PGV:H301	1.97	0.47
7:G:2:SER:OG	24:G:1263:PEK:H291	2.14	0.47
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.96	0.47
7:G:45:PRO:CD	29:G:2145:HOH:O	2.62	0.47
22:C:271:CHD:H212	22:C:271:CHD:H12	1.97	0.47
3:P:254:VAL:CG2	25:T:1269:CDL:H672	2.45	0.47
18:N:515:HEA:H261	18:N:515:HEA:H172	1.36	0.47
1:A:25:TRP:CE3	19:L:522:TGL:HB91	2.49	0.47
5:E:8:ASP:HA	26:E:230:PSC:H071	1.95	0.47
2:B:52:HIS:CE1	26:E:230:PSC:H211	2.49	0.47
1:N:24:ALA:HA	18:N:515:HEA:H22	1.96	0.47
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.30	0.47
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.47
20:P:1267:PGV:H182	25:P:1270:CDL:C67	2.45	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.80	0.46
2:B:65:TRP:HZ3	26:E:230:PSC:H322	1.79	0.46
7:G:69:PHE:CZ	28:G:272:DMU:H1	2.50	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.46
4:D:127:LYS:HD2	29:I:2384:HOH:O	2.14	0.46
25:P:1270:CDL:H362	25:P:1270:CDL:H411	1.97	0.46
10:W:52:TRP:O	10:W:57:HIS:HE1	1.98	0.46
19:A:521:TGL:HA91	19:A:521:TGL:H241	1.96	0.46
18:A:515:HEA:H11	18:A:515:HEA:HMB1	1.76	0.46
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.16	0.46
13:Z:31:GLY:C	28:Z:1526:DMU:H1	2.36	0.46
7:G:37:LEU:HD21	25:G:269:CDL:H341	1.98	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.46
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.46	0.46
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.46	0.46
28:P:1272:DMU:H40	7:T:63:GLY:H	1.80	0.46
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	1.97	0.46
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.61	0.46
25:G:269:CDL:H201	1:N:311:ILE:HD12	1.96	0.46
19:O:1521:TGL:H241	19:O:1521:TGL:H322	1.98	0.46
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.51	0.46
7:T:79:PRO:HD2	29:T:3129:HOH:O	2.16	0.46
6:F:26:LYS:HE3	29:F:4627:HOH:O	2.16	0.46
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	1.96	0.46
7:G:84:LYS:H	7:G:84:LYS:CE	2.28	0.46
1:N:514:LYS:HE2	29:S:3332:HOH:O	2.15	0.46
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.97	0.46
1:N:113:LEU:CD1	19:Y:1522:TGL:C29	2.92	0.46
4:Q:88:PHE:HZ	13:Z:19:LEU:HD21	1.80	0.46
6:S:94:HIS:CG	6:S:95:GLN:N	2.82	0.46
1:N:350:VAL:HG13	19:O:1521:TGL:HB81	1.98	0.46
3:C:3:HIS:CE1	6:F:96:LEU:CD2	2.83	0.46
6:S:94:HIS:HD2	6:S:95:GLN:N	2.13	0.45
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.52	0.45
4:D:109:HIS:HD2	29:D:2152:HOH:O	1.99	0.45
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.42	0.45
1:N:131:PRO:O	1:N:132:LEU:C	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:11:PHE:HB3	26:R:1230:PSC:H073	1.98	0.45
1:A:430:PHE:CE1	19:A:521:TGL:CB2	2.97	0.45
5:R:67:ILE:O	5:R:70:VAL:HG12	2.16	0.45
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.97	0.45
1:N:254:ILE:HG23	1:N:254:ILE:HD12	1.60	0.45
2:B:78:LEU:CB	2:B:79:PRO:CD	2.95	0.45
22:J:60:CHD:H112	22:J:60:CHD:H12A	1.44	0.45
25:T:1269:CDL:H562	25:T:1269:CDL:H762	1.98	0.45
9:V:73:LYS:HA	9:V:73:LYS:HD2	1.64	0.45
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.51	0.45
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.52	0.45
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.45
7:T:2:SER:CB	24:T:263:PEK:H302	2.43	0.45
26:R:1230:PSC:C1	26:R:1230:PSC:H212	2.45	0.45
1:N:215:LEU:HD11	24:P:1264:PEK:H271	1.98	0.45
18:N:515:HEA:H122	18:N:515:HEA:HHC	1.99	0.45
22:C:525:CHD:H112	22:C:525:CHD:H12A	1.56	0.45
3:P:22:LEU:O	3:P:26:LEU:HG	2.17	0.45
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.45
1:A:297:MET:CE	1:A:297:MET:HB2	2.47	0.45
26:E:230:PSC:H061	9:I:10:ARG:HE	1.80	0.45
22:B:1086:CHD:H12A	22:B:1086:CHD:H112	1.68	0.45
3:P:226:HIS:HE1	25:P:1270:CDL:HB32	1.81	0.44
4:D:107:ILE:HG21	4:D:107:ILE:HD13	1.75	0.44
24:T:263:PEK:H5	24:T:263:PEK:H21	1.83	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.17	0.44
12:L:13:PHE:HB3	19:L:522:TGL:HG12	2.00	0.44
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.53	0.44
1:N:69:MET:HE3	1:N:70:VAL:HG23	1.99	0.44
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.65	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.44
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.99	0.44
9:V:68:ILE:HD11	9:V:69:PHE:CZ	2.53	0.44
25:C:270:CDL:HB21	25:C:270:CDL:PA1	2.57	0.44
8:H:44:THR:O	8:H:45:ALA:O	2.36	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.58	0.44
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.00	0.44
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.83	0.44
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.52	0.44
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.18	0.44
3:C:224:LYS:HD2	25:C:270:CDL:HB31	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:524:PGV:C02	20:A:524:PGV:O14	2.61	0.44
6:S:55:LYS:HA	6:S:74:LEU:O	2.18	0.44
24:G:1263:PEK:O13	3:P:80:ARG:HD2	2.17	0.44
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.26	0.44
1:A:309:THR:HG22	18:A:516:HEA:HMB2	1.99	0.44
18:A:516:HEA:HMC1	18:A:516:HEA:HBC1	2.00	0.44
6:F:76:LYS:HD2	6:F:93:PRO:HG3	2.00	0.44
4:Q:88:PHE:CZ	13:Z:19:LEU:HD21	2.53	0.44
19:O:1521:TGL:H251	19:O:1521:TGL:H222	1.44	0.43
4:D:31:LYS:HG2	29:D:4601:HOH:O	2.18	0.43
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.00	0.43
1:N:449:MET:SD	2:O:5:MET:HG2	2.58	0.43
9:I:52:ARG:NH1	29:I:4726:HOH:O	2.51	0.43
5:R:11:PHE:CB	26:R:1230:PSC:H073	2.48	0.43
25:C:270:CDL:H242	25:C:270:CDL:H642	2.00	0.43
7:G:83:GLU:HG2	7:G:84:LYS:HZ2	1.83	0.43
29:B:2353:HOH:O	19:D:523:TGL:HC61	2.18	0.43
6:F:92:VAL:O	6:F:92:VAL:HG23	2.17	0.43
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.19	0.43
2:B:22:HIS:CE1	9:I:44:LYS:HG3	2.53	0.43
24:G:265:PEK:H361	25:G:269:CDL:H273	2.00	0.43
19:O:1523:TGL:HB22	4:Q:78:TRP:HA	2.01	0.43
1:A:299:VAL:CG2	2:B:84:LEU:HG	2.48	0.43
7:T:17:ARG:CD	29:T:3302:HOH:O	2.58	0.43
1:N:240:HIS:O	1:N:241:PRO:C	2.55	0.43
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.59	0.43
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.00	0.43
3:P:55:TYR:HE1	25:P:1270:CDL:H521	1.81	0.43
12:Y:20:ARG:HH21	19:Y:1522:TGL:HC32	1.84	0.43
19:A:521:TGL:H121	19:A:521:TGL:H292	1.79	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.60	0.43
3:C:91:VAL:HG22	24:T:263:PEK:H132	2.01	0.43
22:W:1060:CHD:H232	22:W:1060:CHD:H211	1.69	0.43
10:W:40:LEU:HD12	22:W:1060:CHD:H183	2.01	0.43
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.19	0.43
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.19	0.43
3:P:249:TRP:HD1	29:P:3171:HOH:O	2.00	0.43
1:A:383:MET:O	1:A:387:PHE:HB2	2.17	0.43
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.01	0.43
24:G:265:PEK:H361	25:G:269:CDL:C27	2.49	0.43
20:H:268:PGV:H202	20:H:268:PGV:H231	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:32:TRP:N	28:Z:1526:DMU:H1	2.34	0.43
5:R:31:LYS:HE3	6:S:83:PRO:O	2.18	0.43
20:P:1267:PGV:H12	20:P:1267:PGV:C16	2.45	0.43
1:N:406:ASN:HD21	20:N:1524:PGV:C2	2.32	0.43
18:N:515:HEA:HAD1	18:N:515:HEA:HHA	1.79	0.43
6:S:87:THR:HG21	29:S:4604:HOH:O	2.19	0.43
2:O:161:HIS:HB2	2:O:174:ALA:HB3	2.00	0.43
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.54	0.43
18:A:515:HEA:H272	18:A:515:HEA:C16	2.48	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.43
29:O:3250:HOH:O	4:Q:129:ALA:HB2	2.18	0.42
3:C:19:THR:O	3:C:23:SER:HB3	2.19	0.42
2:O:116:LEU:HD21	2:O:226:MET:HG2	2.01	0.42
7:G:63:GLY:HA2	28:G:272:DMU:H34	2.01	0.42
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.17	0.42
2:O:82:ARG:HH11	2:O:86:MET:CE	2.32	0.42
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.35	0.42
8:U:50:VAL:CG1	8:U:50:VAL:O	2.68	0.42
2:B:108:TYR:O	2:B:117:SER:HA	2.18	0.42
24:T:263:PEK:H361	24:T:263:PEK:H332	1.61	0.42
25:P:1270:CDL:H612	25:P:1270:CDL:H641	1.75	0.42
26:E:230:PSC:H221	26:E:230:PSC:H251	1.70	0.42
1:N:18:LEU:CD2	19:Y:1522:TGL:HB21	2.49	0.42
3:P:8:TYR:CE1	3:P:74:ALA:HB1	2.54	0.42
19:A:521:TGL:OB1	19:A:521:TGL:CB4	2.53	0.42
13:Z:17:ILE:HG21	13:Z:17:ILE:HD13	1.73	0.42
10:W:1:PHE:N	29:W:4539:HOH:O	2.52	0.42
20:N:1524:PGV:H92	4:Q:84:ALA:HB2	2.01	0.42
8:U:50:VAL:O	8:U:50:VAL:HG12	2.20	0.42
1:N:86:MET:HB3	1:N:182:PRO:HG2	2.02	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.94	0.42
4:D:20:ARG:HG3	29:D:4139:HOH:O	2.19	0.42
5:R:8:ASP:HA	26:R:1230:PSC:H071	2.02	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.93	0.42
18:A:515:HEA:HAD1	18:A:515:HEA:HHA	1.73	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.20	0.42
5:E:23:ASP:N	5:E:23:ASP:OD2	2.48	0.42
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.01	0.41
22:C:525:CHD:H42	3:P:127:LEU:HD21	2.02	0.41
3:C:191:GLY:HA3	29:G:2156:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.51	0.41
6:S:95:GLN:CG	29:S:4406:HOH:O	2.41	0.41
7:T:37:LEU:HD23	7:T:38:HIS:CE1	2.56	0.41
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.52	0.41
1:N:69:MET:CE	1:N:70:VAL:CG2	2.98	0.41
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.85	0.41
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.20	0.41
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.41
25:C:270:CDL:H861	25:C:270:CDL:H831	1.92	0.41
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.55	0.41
3:C:246:ASP:HB2	29:C:4076:HOH:O	2.20	0.41
1:A:207:THR:O	1:A:211:THR:HG23	2.19	0.41
3:P:144:ILE:HD13	3:P:144:ILE:HG21	1.80	0.41
11:K:24:PHE:O	11:K:28:VAL:HG12	2.21	0.41
20:H:268:PGV:H21	20:H:268:PGV:H52	1.94	0.41
1:N:35:LEU:HB3	28:Z:1526:DMU:H24	2.03	0.41
3:C:103:HIS:ND1	22:C:525:CHD:O26	2.54	0.41
6:F:53:THR:HB	6:F:54:ASN:H	1.66	0.41
2:B:91:ASN:C	2:B:91:ASN:HD22	2.24	0.41
3:P:65:SER:HB2	20:P:1267:PGV:H041	2.03	0.41
26:E:230:PSC:H042	26:E:230:PSC:H062	1.67	0.41
25:C:270:CDL:PA1	25:C:270:CDL:CB2	3.09	0.41
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.84	0.41
2:O:16:ILE:HG23	2:O:16:ILE:HD12	1.82	0.41
4:Q:130:PRO:HA	4:Q:135:SER:HB2	2.02	0.41
19:O:1523:TGL:CG3	19:O:1523:TGL:OB1	2.68	0.41
1:N:437:PRO:HG2	1:N:440:TYR:CE1	2.55	0.41
9:V:29:LEU:HD12	9:V:29:LEU:HA	1.79	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
3:P:224:LYS:CE	25:P:1270:CDL:HB31	2.49	0.41
1:N:109:PHE:HB3	19:Y:1522:TGL:H122	2.03	0.41
6:F:64:GLU:O	6:F:65:ASP:CB	2.69	0.41
7:T:5:LYS:CB	24:T:263:PEK:C37	2.89	0.41
20:A:522:PGV:H251	20:A:522:PGV:H42	2.02	0.41
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.41
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.55	0.41
1:A:37:ILE:HG21	18:A:515:HEA:HMA	2.02	0.41
4:Q:127:LYS:HD2	29:V:3384:HOH:O	2.20	0.41
3:C:16:TRP:N	3:C:17:PRO:CD	2.84	0.41
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.21	0.41
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:46:ALA:HB1	29:T:4681:HOH:O	2.21	0.41
1:N:106:PRO:N	1:N:107:PRO:CD	2.84	0.41
2:O:139:ASP:N	2:O:139:ASP:OD2	2.52	0.40
1:N:69:MET:CE	1:N:70:VAL:HG23	2.51	0.40
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.03	0.40
5:R:65:VAL:HG13	5:R:101:PRO:HG3	2.03	0.40
1:N:76:GLY:O	1:N:80:ASN:HB2	2.21	0.40
25:G:269:CDL:C53	25:G:269:CDL:H242	2.47	0.40
1:A:311:ILE:HD13	1:A:311:ILE:HG21	1.85	0.40
7:T:8:HIS:O	7:T:9:GLY:C	2.60	0.40
7:G:7:ASP:HA	1:N:178:GLN:HG2	2.03	0.40
1:A:181:THR:HA	1:A:182:PRO:HD3	1.94	0.40
1:N:344:PHE:C	1:N:344:PHE:CD1	2.95	0.40
3:P:59:ARG:HG3	25:P:1270:CDL:H512	2.03	0.40
12:L:6:GLY:O	12:L:7:PRO:C	2.59	0.40
3:C:173:PHE:CD2	3:C:173:PHE:C	2.94	0.40
19:Y:1522:TGL:CC2	19:Y:1522:TGL:CC6	2.82	0.40
8:H:23:GLN:HG3	29:H:4130:HOH:O	2.21	0.40
19:D:523:TGL:HB92	19:D:523:TGL:H121	1.47	0.40
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.40
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.56	0.40
3:P:149:HIS:O	3:P:153:GLU:HG3	2.22	0.40
13:M:4:LYS:HB2	13:M:5:PRO:HD2	2.03	0.40
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.57	0.40
20:N:1524:PGV:H02	20:N:1524:PGV:O14	2.21	0.40
18:A:515:HEA:C12	18:A:515:HEA:HHC	2.51	0.40
8:H:39:CYS:O	8:H:40:GLU:C	2.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	490 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	39	27
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	39	27
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	26	14
5	E	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
5	R	102/109 (94%)	102 (100%)	0	0	100	100
6	F	91/98 (93%)	87 (96%)	2 (2%)	2 (2%)	8	2
6	S	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	17	6
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	2	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	2	0
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	3	0
8	U	73/85 (86%)	66 (90%)	5 (7%)	2 (3%)	6	1
9	I	69/73 (94%)	66 (96%)	3 (4%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	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%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	7	1
All	All	3478/3614 (96%)	3328 (96%)	128 (4%)	22 (1%)	30	16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA

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Mol	Chain	Res	Type
7	G	7	ASP
7	G	8	HIS
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	45	ALA
6	F	94	HIS
8	H	47	GLY
8	U	46	LYS
13	Z	41	LYS
7	G	6	GLY
7	G	37	LEU
4	Q	34	SER
7	T	3	ALA
7	T	6	GLY
2	O	92	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	54	43
1	N	426/426 (100%)	413 (97%)	13 (3%)	47	34
2	B	210/210 (100%)	198 (94%)	12 (6%)	25	11
2	O	210/210 (100%)	197 (94%)	13 (6%)	23	8
3	C	224/226 (99%)	217 (97%)	7 (3%)	47	34
3	P	224/226 (99%)	215 (96%)	9 (4%)	38	23
4	D	128/129 (99%)	127 (99%)	1 (1%)	86	85
4	Q	128/129 (99%)	121 (94%)	7 (6%)	27	12
5	E	91/95 (96%)	90 (99%)	1 (1%)	80	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	91/95 (96%)	88 (97%)	3 (3%)	45	32
6	F	79/81 (98%)	73 (92%)	6 (8%)	16	5
6	S	79/81 (98%)	73 (92%)	6 (8%)	16	5
7	G	67/68 (98%)	58 (87%)	9 (13%)	5	1
7	T	67/68 (98%)	58 (87%)	9 (13%)	5	1
8	H	67/75 (89%)	64 (96%)	3 (4%)	34	18
8	U	67/75 (89%)	62 (92%)	5 (8%)	17	5
9	I	56/57 (98%)	51 (91%)	5 (9%)	12	3
9	V	56/57 (98%)	52 (93%)	4 (7%)	18	6
10	J	48/50 (96%)	47 (98%)	1 (2%)	61	53
10	W	48/50 (96%)	47 (98%)	1 (2%)	61	53
11	K	39/46 (85%)	37 (95%)	2 (5%)	29	13
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	13
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	43
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	13
13	M	37/38 (97%)	31 (84%)	6 (16%)	3	0
13	Z	37/38 (97%)	34 (92%)	3 (8%)	15	4
All	All	3022/3082 (98%)	2880 (95%)	142 (5%)	32	16

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	109	PHE
1	A	115	SER
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	278	MET
1	A	338	MET
1	A	369	ASP
1	A	504	THR
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU

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Mol	Chain	Res	Type
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	158	ASP
2	B	167	SER
2	B	171	LYS
3	C	23	SER
3	C	77	LYS
3	C	80	ARG
3	C	127	LEU
3	C	159	MET
3	C	223	LEU
3	C	230	ASN
4	D	51	LEU
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	53	THR
6	F	78	GLU
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	40	GLU
8	H	60	TYR
8	H	61	LYS
9	I	8	GLN
9	I	15	ARG
9	I	26	MET
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU

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Mol	Chain	Res	Type
11	K	47	ARG
11	K	54	ARG
12	L	46	LYS
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	278	MET
1	N	338	MET
1	N	361	SER
1	N	369	ASP
1	N	394	VAL
1	N	484	THR
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	116	LEU
2	O	148	MET
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	33	MET
3	P	40	MET
3	P	127	LEU
3	P	159	MET
3	P	161	GLN
3	P	214	PHE

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Mol	Chain	Res	Type
3	P	223	LEU
3	P	230	ASN
4	Q	5	VAL
4	Q	9	GLU
4	Q	10	ASP
4	Q	19	ARG
4	Q	31	LYS
4	Q	51	LEU
4	Q	63	LYS
5	R	79	LYS
5	R	90	ARG
5	R	108	LYS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	87	THR
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	18	PHE
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	29	CYS
8	U	41	LYS
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	26	MET
9	V	29	LEU
9	V	36	LYS
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	16	GLU
12	Y	20	ARG
13	Z	13	LYS

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Mol	Chain	Res	Type
13	Z	34	LEU
13	Z	42	LYS

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	22	HIS
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	68	GLN
3	C	149	HIS
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	195	GLN
3	P	68	GLN
3	P	76	GLN
3	P	149	HIS
3	P	161	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	101	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	28	GLN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
10	W	29	ASN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	FME	A	1	1	8,9,10	0.90	1 (12%)	6,9,11	5.39	3 (50%)
2	FME	B	1	2	8,9,10	1.80	3 (37%)	6,9,11	8.12	3 (50%)
7	TPO	G	11	7	8,10,11	2.02	2 (25%)	7,14,16	2.56	4 (57%)
1	FME	N	1	1	8,9,10	0.83	0	6,9,11	6.89	4 (66%)
2	FME	O	1	2	8,9,10	0.88	1 (12%)	6,9,11	6.05	4 (66%)
7	TPO	T	11	7	8,10,11	1.88	4 (50%)	7,14,16	2.21	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	-	1/6/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.50	1.11	1.22
1	A	1	FME	O1-CN	-2.18	1.15	1.22
2	B	1	FME	CG-SD	-2.15	1.69	1.81
2	O	1	FME	O1-CN	-2.01	1.16	1.22
7	T	11	TPO	CG2-CB	2.03	1.56	1.51
2	B	1	FME	CB-CG	2.16	1.60	1.51
7	T	11	TPO	P-O2P	2.22	1.62	1.54
7	T	11	TPO	P-O3P	2.37	1.63	1.54
7	G	11	TPO	P-O2P	2.55	1.63	1.54
7	T	11	TPO	P-O1P	3.08	1.61	1.51
7	G	11	TPO	P-O1P	3.74	1.63	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.38	97.64	122.82
1	N	1	FME	CA-N-CN	-15.33	99.25	122.82
2	O	1	FME	CA-N-CN	-13.71	101.73	122.82
1	A	1	FME	CA-N-CN	-12.21	104.05	122.82
2	B	1	FME	CB-CG-SD	-4.66	93.50	113.17
2	O	1	FME	CG-CB-CA	-4.09	101.06	113.06
2	O	1	FME	O1-CN-N	-2.84	120.66	124.76
7	T	11	TPO	O-C-CA	-2.72	118.25	125.44
7	G	11	TPO	C-CA-N	-2.71	104.16	109.83
1	A	1	FME	O-C-CA	-2.53	118.75	125.44
7	G	11	TPO	OG1-P-O1P	-2.37	101.19	107.11
7	G	11	TPO	O-C-CA	-2.32	119.31	125.44
1	N	1	FME	O-C-CA	-2.25	119.49	125.44
2	O	1	FME	CE-SD-CG	2.20	107.88	100.37
1	A	1	FME	CE-SD-CG	4.28	114.99	100.37
1	N	1	FME	O1-CN-N	4.44	131.15	124.76
7	G	11	TPO	CG2-CB-CA	4.53	122.37	113.17
7	T	11	TPO	CG2-CB-CA	4.76	122.86	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CE-SD-CG	4.86	116.95	100.37
2	B	1	FME	O1-CN-N	9.99	139.14	124.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
2	O	1	FME	1	0
7	T	11	TPO	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	$\# Z > 2$
18	HEA	A	515	1	40,67,67	1.44	8 (20%)	41,103,103	2.94	22 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	HEA	A	516	1,15	40,67,67	1.82	8 (20%)	41,103,103	2.43	14 (34%)
15	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.19	7 (11%)	65,65,65	2.03	12 (18%)
20	PGV	A	522	-	50,50,50	1.07	3 (6%)	51,56,56	1.51	6 (11%)
20	PGV	A	524	-	50,50,50	1.19	3 (6%)	51,56,56	1.66	10 (19%)
22	CHD	B	1086	-	29,32,32	1.25	4 (13%)	48,51,51	5.73	33 (68%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
24	PEK	C	264	-	51,52,52	0.95	3 (5%)	52,57,57	1.54	13 (25%)
20	PGV	C	267	-	50,50,50	0.95	2 (4%)	51,56,56	1.31	7 (13%)
25	CDL	C	270	-	99,99,99	1.34	13 (13%)	101,111,111	1.59	15 (14%)
22	CHD	C	271	-	29,32,32	1.12	2 (6%)	48,51,51	5.31	33 (68%)
22	CHD	C	525	-	29,32,32	1.63	6 (20%)	48,51,51	5.52	37 (77%)
19	TGL	D	523	-	62,62,62	1.56	7 (11%)	65,65,65	1.69	14 (21%)
26	PSC	E	230	-	51,51,51	1.29	3 (5%)	55,59,59	1.20	5 (9%)
24	PEK	G	1263	-	51,52,52	1.15	2 (3%)	52,57,57	1.37	5 (9%)
24	PEK	G	265	-	51,52,52	1.90	5 (9%)	52,57,57	1.57	6 (11%)
25	CDL	G	269	-	99,99,99	1.43	13 (13%)	101,111,111	1.55	17 (16%)
28	DMU	G	272	-	34,34,34	1.29	3 (8%)	45,45,45	3.59	24 (53%)
20	PGV	H	268	-	50,50,50	1.29	2 (4%)	51,56,56	1.52	9 (17%)
22	CHD	J	60	-	29,32,32	0.75	0	48,51,51	4.91	36 (75%)
19	TGL	L	522	-	62,62,62	1.55	7 (11%)	65,65,65	1.96	18 (27%)
28	DMU	M	526	-	34,34,34	0.93	1 (2%)	45,45,45	3.24	24 (53%)
20	PGV	N	1266	-	50,50,50	0.87	2 (4%)	51,56,56	1.60	6 (11%)
20	PGV	N	1268	-	50,50,50	1.18	2 (4%)	51,56,56	1.49	6 (11%)
20	PGV	N	1524	-	50,50,50	1.04	2 (4%)	51,56,56	1.54	6 (11%)
18	HEA	N	515	1	40,67,67	1.41	6 (15%)	41,103,103	2.65	12 (29%)
18	HEA	N	516	1,15	40,67,67	1.35	6 (15%)	41,103,103	2.88	17 (41%)
15	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	O	1521	-	62,62,62	1.29	6 (9%)	65,65,65	1.65	12 (18%)
19	TGL	O	1523	-	62,62,62	1.37	6 (9%)	65,65,65	1.47	10 (15%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	1.35	5 (17%)	48,51,51	5.56	35 (72%)
24	PEK	P	1264	-	51,52,52	1.02	4 (7%)	52,57,57	1.80	10 (19%)
20	PGV	P	1267	-	50,50,50	0.89	3 (6%)	51,56,56	1.50	9 (17%)
25	CDL	P	1270	-	99,99,99	1.37	13 (13%)	101,111,111	1.48	16 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	P	1271	-	29,32,32	0.82	0	48,51,51	5.30	30 (62%)
28	DMU	P	1272	-	34,34,34	1.28	4 (11%)	45,45,45	3.18	22 (48%)
22	CHD	P	1525	-	29,32,32	1.35	2 (6%)	48,51,51	5.67	37 (77%)
26	PSC	R	1230	-	51,51,51	1.17	3 (5%)	55,59,59	1.22	4 (7%)
24	PEK	T	1265	-	51,52,52	1.19	2 (3%)	52,57,57	1.42	7 (13%)
25	CDL	T	1269	-	99,99,99	1.34	12 (12%)	101,111,111	1.42	18 (17%)
24	PEK	T	263	-	51,52,52	1.18	3 (5%)	52,57,57	1.50	8 (15%)
22	CHD	W	1060	-	29,32,32	0.68	0	48,51,51	5.07	35 (72%)
19	TGL	Y	1522	-	62,62,62	1.49	6 (9%)	65,65,65	1.65	17 (26%)
28	DMU	Z	1526	-	34,34,34	1.08	3 (8%)	45,45,45	3.42	23 (51%)

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
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	A	520	18,14	-	0/0/0/0	0/0/0/0
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
20	PGV	A	522	-	-	0/55/55/55	0/0/0/0
20	PGV	A	524	-	-	0/55/55/55	0/0/0/0
22	CHD	B	1086	-	1/1/12/12	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
24	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
26	PSC	E	230	-	-	0/55/55/55	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
24	PEK	G	265	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
28	DMU	G	272	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	H	268	-	-	0/55/55/55	0/0/0/0
22	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
20	PGV	N	1268	-	-	0/55/55/55	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
18	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	N	520	18,14	-	0/0/0/0	0/0/0/0
19	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	O	1523	-	-	0/65/65/65	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
24	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	P	1272	-	4/4/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	PSC	R	1230	-	-	0/55/55/55	0/0/0/0
24	PEK	T	1265	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
24	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1060	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	Y	1522	-	-	0/65/65/65	0/0/0/0
28	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	1525	CHD	C13-C14	-4.26	1.48	1.55
22	C	525	CHD	C13-C12	-4.13	1.48	1.54
24	P	1264	PEK	O03-C01	-4.11	1.35	1.45
28	Z	1526	DMU	C3-C4	-3.81	1.42	1.52
19	L	522	TGL	C20-CA9	-3.73	1.30	1.51
25	T	1269	CDL	C59-C58	-3.49	1.31	1.51
25	G	269	CDL	C59-C58	-3.45	1.31	1.51
19	O	1521	TGL	C10-CB9	-3.39	1.32	1.51
25	T	1269	CDL	C62-C61	-3.30	1.32	1.51
19	Y	1522	TGL	C20-CA9	-3.29	1.32	1.51
25	C	270	CDL	C79-C78	-3.23	1.32	1.51
25	C	270	CDL	C59-C58	-3.22	1.32	1.51
19	Y	1522	TGL	C10-CB9	-3.22	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	522	TGL	C10-CB9	-3.22	1.32	1.51
25	P	1270	CDL	C59-C58	-3.18	1.33	1.51
22	C	525	CHD	C6-C7	-3.12	1.47	1.52
25	G	269	CDL	C19-C18	-3.09	1.33	1.51
25	T	1269	CDL	C42-C41	-3.08	1.33	1.51
25	C	270	CDL	C39-C38	-3.08	1.33	1.51
25	C	270	CDL	C62-C61	-3.07	1.33	1.51
25	C	270	CDL	C82-C81	-2.98	1.34	1.51
25	P	1270	CDL	C22-C21	-2.94	1.34	1.51
25	G	269	CDL	C22-C21	-2.94	1.34	1.51
19	O	1523	TGL	C10-CB9	-2.92	1.34	1.51
19	A	521	TGL	C10-CB9	-2.92	1.34	1.51
22	C	525	CHD	C13-C14	-2.91	1.50	1.55
25	P	1270	CDL	C19-C18	-2.91	1.34	1.51
25	P	1270	CDL	C79-C78	-2.89	1.34	1.51
25	G	269	CDL	C42-C41	-2.88	1.34	1.51
19	O	1521	TGL	C20-CA9	-2.87	1.35	1.51
25	G	269	CDL	C62-C61	-2.83	1.35	1.51
19	O	1523	TGL	C20-CA9	-2.83	1.35	1.51
19	O	1523	TGL	C15-CC9	-2.82	1.35	1.51
25	C	270	CDL	C22-C21	-2.81	1.35	1.51
25	C	270	CDL	C19-C18	-2.80	1.35	1.51
25	P	1270	CDL	C39-C38	-2.77	1.35	1.51
19	A	521	TGL	C20-CA9	-2.77	1.35	1.51
25	T	1269	CDL	C19-C18	-2.75	1.35	1.51
25	P	1270	CDL	C62-C61	-2.75	1.35	1.51
25	T	1269	CDL	C82-C81	-2.70	1.35	1.51
25	P	1270	CDL	C82-C81	-2.70	1.35	1.51
19	Y	1522	TGL	C15-CC9	-2.68	1.36	1.51
22	C	271	CHD	C10-C5	-2.67	1.50	1.55
18	N	515	HEA	C1A-NA	-2.66	1.33	1.36
25	C	270	CDL	C42-C41	-2.63	1.36	1.51
19	D	523	TGL	C10-CB9	-2.63	1.36	1.51
19	O	1521	TGL	C15-CC9	-2.61	1.36	1.51
25	G	269	CDL	C79-C78	-2.61	1.36	1.51
25	T	1269	CDL	C39-C38	-2.60	1.36	1.51
25	G	269	CDL	C39-C38	-2.60	1.36	1.51
25	T	1269	CDL	C79-C78	-2.60	1.36	1.51
19	D	523	TGL	C15-CC9	-2.59	1.36	1.51
19	D	523	TGL	C20-CA9	-2.58	1.36	1.51
22	O	229	CHD	C13-C12	-2.58	1.50	1.54
22	O	229	CHD	C18-C13	-2.57	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	269	CDL	C82-C81	-2.56	1.36	1.51
19	L	522	TGL	C15-CC9	-2.52	1.36	1.51
20	A	524	PGV	C2-C1	-2.51	1.43	1.50
25	T	1269	CDL	C22-C21	-2.49	1.37	1.51
22	O	229	CHD	C1-C10	-2.49	1.49	1.54
22	B	1086	CHD	C10-C5	-2.47	1.51	1.55
28	M	526	DMU	C3-C4	-2.47	1.46	1.52
19	A	521	TGL	C15-CC9	-2.46	1.37	1.51
22	B	1086	CHD	C11-C9	-2.46	1.49	1.53
18	A	516	HEA	C4A-NA	-2.44	1.33	1.36
20	A	522	PGV	P-O14	-2.42	1.44	1.54
22	C	525	CHD	C1-C10	-2.42	1.49	1.54
25	C	270	CDL	OB6-CB4	-2.40	1.40	1.46
25	P	1270	CDL	C42-C41	-2.39	1.37	1.51
22	P	1525	CHD	C10-C5	-2.38	1.51	1.55
22	C	525	CHD	C10-C5	-2.38	1.51	1.55
22	O	229	CHD	C1-C2	-2.30	1.48	1.53
19	A	521	TGL	OC1-CC1	-2.29	1.15	1.22
24	C	264	PEK	O03-C01	-2.24	1.40	1.45
22	O	229	CHD	C10-C5	-2.23	1.51	1.55
28	G	272	DMU	C3-C4	-2.21	1.46	1.52
28	P	1272	DMU	C3-C4	-2.21	1.46	1.52
22	B	1086	CHD	C13-C12	-2.10	1.51	1.54
20	P	1267	PGV	P-O14	-2.07	1.46	1.54
24	T	263	PEK	C01-C02	2.01	1.56	1.50
28	P	1272	DMU	O7-C10	2.01	1.47	1.41
25	G	269	CDL	C71-CB7	2.05	1.56	1.50
28	P	1272	DMU	O1-C10	2.07	1.47	1.41
22	C	271	CHD	C20-C17	2.09	1.58	1.54
18	A	515	HEA	CMB-C2B	2.10	1.56	1.51
28	Z	1526	DMU	O16-C6	2.11	1.44	1.40
18	A	515	HEA	C1B-CHB	2.16	1.45	1.39
18	A	515	HEA	C17-C18	2.18	1.56	1.50
25	P	1270	CDL	PB2-OB2	2.19	1.69	1.59
18	A	515	HEA	C13-C14	2.23	1.56	1.50
24	P	1264	PEK	C2-C1	2.25	1.57	1.50
18	N	515	HEA	O11-C11	2.25	1.48	1.42
28	G	272	DMU	O1-C10	2.28	1.47	1.41
18	N	516	HEA	C4D-CHA	2.29	1.46	1.39
24	P	1264	PEK	O03-C21	2.33	1.40	1.33
18	A	516	HEA	C3C-CAC	2.38	1.52	1.47
18	N	516	HEA	C17-C18	2.41	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z	1526	DMU	O1-C10	2.42	1.48	1.41
22	B	1086	CHD	C11-C12	2.45	1.57	1.53
18	N	515	HEA	C4A-NA	2.45	1.40	1.36
22	C	525	CHD	C18-C13	2.50	1.58	1.54
19	L	522	TGL	CG3-CG2	2.52	1.57	1.50
18	A	515	HEA	C4B-NB	2.59	1.40	1.36
18	A	516	HEA	CAD-C3D	2.61	1.56	1.52
20	P	1267	PGV	O01-C1	2.63	1.42	1.34
25	C	270	CDL	OB6-CB5	2.64	1.42	1.34
18	N	516	HEA	C1D-ND	2.67	1.40	1.36
18	A	515	HEA	C3C-C2C	2.70	1.43	1.40
20	C	267	PGV	O03-C19	2.75	1.41	1.33
18	A	516	HEA	O11-C11	2.76	1.49	1.42
20	N	1266	PGV	O03-C19	2.85	1.41	1.33
18	A	516	HEA	C1C-CHC	2.88	1.47	1.39
24	C	264	PEK	O03-C21	2.96	1.42	1.33
18	N	516	HEA	C4C-CHD	2.99	1.48	1.39
18	N	516	HEA	O11-C11	3.09	1.49	1.42
20	P	1267	PGV	O03-C19	3.09	1.42	1.33
18	N	515	HEA	C4B-NB	3.14	1.40	1.36
20	C	267	PGV	O01-C1	3.23	1.44	1.34
24	P	1264	PEK	O01-C1	3.27	1.44	1.34
18	A	515	HEA	C1C-CHC	3.29	1.48	1.39
19	A	521	TGL	OG3-CC1	3.37	1.43	1.33
18	N	516	HEA	C18-C19	3.41	1.39	1.33
18	N	515	HEA	C3A-C2A	3.47	1.44	1.40
18	N	515	HEA	CMD-C2D	3.48	1.59	1.51
20	N	1266	PGV	O01-C1	3.58	1.45	1.34
25	C	270	CDL	OB8-CB7	3.64	1.44	1.33
20	A	522	PGV	O01-C1	3.66	1.45	1.34
24	C	264	PEK	O01-C1	3.75	1.45	1.34
20	A	522	PGV	O03-C19	3.76	1.44	1.33
24	G	1263	PEK	O01-C1	3.77	1.45	1.34
26	R	1230	PSC	C13-C12	3.80	1.53	1.31
19	O	1521	TGL	OG3-CC1	3.88	1.45	1.33
18	A	516	HEA	C18-C19	3.89	1.40	1.33
20	N	1524	PGV	O01-C1	3.91	1.46	1.34
25	T	1269	CDL	OA8-CA7	3.91	1.45	1.33
26	R	1230	PSC	O03-C19	3.92	1.45	1.33
25	P	1270	CDL	OB6-CB5	3.93	1.46	1.34
26	E	230	PSC	C13-C12	3.94	1.54	1.31
19	A	521	TGL	OG2-CB1	3.97	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	1268	PGV	O03-C19	4.11	1.45	1.33
18	A	515	HEA	O11-C11	4.13	1.52	1.42
20	A	524	PGV	O01-C1	4.15	1.46	1.34
19	A	521	TGL	OG1-CA1	4.18	1.45	1.33
19	D	523	TGL	OG2-CB1	4.19	1.46	1.34
26	R	1230	PSC	O01-C1	4.24	1.47	1.34
25	C	270	CDL	OA6-CA5	4.25	1.47	1.34
25	P	1270	CDL	OA6-CA5	4.27	1.47	1.34
20	N	1524	PGV	O03-C19	4.40	1.46	1.33
25	G	269	CDL	OA8-CA7	4.40	1.46	1.33
19	D	523	TGL	OG3-CC1	4.43	1.46	1.33
24	G	265	PEK	C7-C8	4.44	1.75	1.51
25	T	1269	CDL	OB8-CB7	4.49	1.46	1.33
24	T	263	PEK	O01-C1	4.53	1.47	1.34
28	G	272	DMU	O16-C6	4.59	1.48	1.40
19	O	1523	TGL	OG3-CC1	4.59	1.47	1.33
18	A	516	HEA	CMD-C2D	4.60	1.61	1.51
25	T	1269	CDL	OA6-CA5	4.60	1.48	1.34
25	P	1270	CDL	OB8-CB7	4.62	1.47	1.33
25	G	269	CDL	OB8-CB7	4.64	1.47	1.33
25	T	1269	CDL	OB6-CB5	4.65	1.48	1.34
19	O	1521	TGL	OG1-CA1	4.66	1.47	1.33
24	T	1265	PEK	O03-C21	4.71	1.47	1.33
24	G	265	PEK	O03-C21	4.72	1.47	1.33
19	O	1521	TGL	OG2-CB1	4.72	1.48	1.34
26	E	230	PSC	O03-C19	4.81	1.47	1.33
19	D	523	TGL	OB1-CB1	4.82	1.37	1.22
20	H	268	PGV	O03-C19	4.83	1.47	1.33
24	G	265	PEK	O01-C1	4.86	1.48	1.34
19	Y	1522	TGL	OG1-CA1	4.88	1.48	1.33
19	Y	1522	TGL	OG3-CC1	4.88	1.48	1.33
20	A	524	PGV	O03-C19	4.91	1.48	1.33
26	E	230	PSC	O01-C1	4.94	1.49	1.34
18	A	516	HEA	C1D-ND	4.97	1.43	1.36
28	P	1272	DMU	O16-C6	4.97	1.49	1.40
19	L	522	TGL	OG3-CC1	5.00	1.48	1.33
19	L	522	TGL	OG1-CA1	5.05	1.48	1.33
19	O	1523	TGL	OG1-CA1	5.06	1.48	1.33
19	O	1523	TGL	OG2-CB1	5.07	1.49	1.34
20	N	1268	PGV	O01-C1	5.16	1.49	1.34
24	T	263	PEK	O03-C21	5.19	1.48	1.33
25	G	269	CDL	OA6-CA5	5.20	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1270	CDL	OA8-CA7	5.26	1.49	1.33
25	C	270	CDL	OA8-CA7	5.39	1.49	1.33
24	G	1263	PEK	O03-C21	5.42	1.49	1.33
24	T	1265	PEK	O01-C1	5.58	1.51	1.34
24	G	265	PEK	C10-C9	5.63	1.81	1.51
25	G	269	CDL	OB6-CB5	5.70	1.51	1.34
20	H	268	PGV	O01-C1	6.05	1.52	1.34
19	Y	1522	TGL	OG2-CB1	6.18	1.52	1.34
19	L	522	TGL	OG2-CB1	6.22	1.52	1.34
19	D	523	TGL	OG1-CA1	6.26	1.52	1.33
24	G	265	PEK	C9-C8	7.84	1.77	1.31

All (700) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C12	-15.83	93.65	109.09
22	P	1271	CHD	C18-C13-C12	-12.47	96.93	109.09
22	P	1525	CHD	C18-C13-C12	-12.30	97.09	109.09
22	C	525	CHD	C18-C13-C12	-11.88	97.51	109.09
22	C	271	CHD	C18-C13-C12	-9.88	99.46	109.09
22	O	229	CHD	C19-C10-C9	-9.57	96.84	111.18
22	C	525	CHD	C19-C10-C9	-9.42	97.06	111.18
22	B	1086	CHD	C19-C10-C9	-9.37	97.13	111.18
18	A	516	HEA	C13-C12-C11	-9.15	102.35	114.51
22	O	229	CHD	C18-C13-C12	-9.00	100.31	109.09
22	O	229	CHD	C6-C5-C4	-8.68	101.35	111.05
22	C	271	CHD	C21-C20-C22	-8.38	96.37	110.35
18	A	515	HEA	CAD-C3D-C4D	-8.05	118.27	127.01
22	C	271	CHD	C18-C13-C17	-8.02	98.56	111.22
22	O	229	CHD	C18-C13-C17	-8.01	98.58	111.22
22	P	1271	CHD	C19-C10-C9	-7.91	99.32	111.18
22	O	229	CHD	O12-C12-C13	-7.88	98.34	111.11
22	C	271	CHD	C19-C10-C9	-7.26	100.29	111.18
22	C	525	CHD	O12-C12-C13	-7.26	99.34	111.11
22	P	1271	CHD	O12-C12-C13	-6.86	99.99	111.11
22	C	271	CHD	O7-C7-C6	-6.61	93.87	110.06
22	C	525	CHD	C6-C5-C4	-6.53	103.75	111.05
22	P	1525	CHD	C19-C10-C9	-6.52	101.40	111.18
18	N	515	HEA	CAD-C3D-C4D	-6.46	120.00	127.01
18	N	516	HEA	OMA-CMA-C3A	-6.39	112.19	125.11
22	J	60	CHD	C18-C13-C12	-6.37	102.88	109.09
22	O	229	CHD	C18-C13-C14	-6.35	101.20	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C20-C21-C22	-6.11	95.69	111.69
18	N	515	HEA	C27-C19-C18	-6.11	111.51	123.50
22	P	1525	CHD	C18-C13-C17	-6.10	101.59	111.22
28	Z	1526	DMU	O7-C10-C5	-5.96	93.61	108.10
18	A	515	HEA	C27-C19-C18	-5.86	112.00	123.50
22	B	1086	CHD	C6-C5-C4	-5.80	104.57	111.05
18	N	515	HEA	OMA-CMA-C3A	-5.76	113.48	125.11
22	P	1271	CHD	O7-C7-C6	-5.75	95.98	110.06
22	W	1060	CHD	C18-C13-C12	-5.69	103.54	109.09
22	P	1271	CHD	C6-C5-C4	-5.62	104.76	111.05
25	C	270	CDL	CB4-OB6-CB5	-5.52	104.64	117.89
22	J	60	CHD	O12-C12-C11	-5.42	97.97	109.06
18	A	516	HEA	C1A-C2A-C3A	-5.41	101.66	107.07
28	M	526	DMU	O7-C10-C5	-5.40	94.97	108.10
22	W	1060	CHD	C1-C10-C9	-5.35	102.82	111.45
20	N	1266	PGV	O03-C19-O04	-5.29	109.85	123.49
22	B	1086	CHD	O12-C12-C11	-5.25	98.31	109.06
22	B	1086	CHD	C18-C13-C17	-5.25	102.94	111.22
22	J	60	CHD	C1-C10-C9	-5.21	103.04	111.45
22	C	271	CHD	O12-C12-C13	-5.14	102.78	111.11
22	P	1525	CHD	C23-C22-C20	-5.13	108.70	114.75
22	P	1525	CHD	O12-C12-C13	-5.04	102.94	111.11
22	P	1525	CHD	C6-C5-C4	-4.97	105.50	111.05
22	W	1060	CHD	O12-C12-C11	-4.87	99.09	109.06
22	P	1525	CHD	C18-C13-C14	-4.83	103.60	111.22
18	N	516	HEA	C13-C12-C11	-4.82	108.11	114.51
19	L	522	TGL	OG3-CC1-OC1	-4.62	111.58	123.49
25	G	269	CDL	CB6-CB4-CB3	-4.52	101.51	112.07
18	N	516	HEA	O11-C11-C3B	-4.46	98.65	111.82
22	W	1060	CHD	C19-C10-C5	-4.45	102.40	110.25
19	D	523	TGL	OG2-CB1-CB2	-4.40	101.96	111.53
25	C	270	CDL	OB8-CB7-OB9	-4.38	112.18	123.49
22	P	1525	CHD	O7-C7-C6	-4.35	99.39	110.06
22	P	1525	CHD	O12-C12-C11	-4.35	100.17	109.06
22	J	60	CHD	C19-C10-C5	-4.29	102.68	110.25
22	P	1525	CHD	C22-C20-C17	-4.28	101.25	110.24
18	N	516	HEA	CAA-CBA-CGA	-4.27	104.92	112.75
22	C	525	CHD	C18-C13-C14	-4.26	104.50	111.22
22	C	525	CHD	C1-C10-C9	-4.24	104.61	111.45
22	C	525	CHD	C4-C5-C10	-4.23	107.99	112.66
18	A	516	HEA	C20-C19-C18	-4.22	113.04	121.05
22	J	60	CHD	C18-C13-C14	-4.21	104.57	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1060	CHD	C6-C5-C4	-4.21	106.34	111.05
18	N	516	HEA	C1A-C2A-C3A	-4.20	102.87	107.07
22	B	1086	CHD	O7-C7-C6	-4.19	99.79	110.06
24	G	265	PEK	C8-C7-C6	-4.16	98.16	112.00
24	G	265	PEK	C10-C9-C8	-4.15	99.30	125.00
19	A	521	TGL	OG3-CC1-OC1	-4.15	112.77	123.49
20	P	1267	PGV	C8-C9-C10	-4.15	97.68	113.86
22	W	1060	CHD	C18-C13-C14	-4.09	104.76	111.22
24	P	1264	PEK	O03-C01-C02	-4.09	97.69	108.69
22	W	1060	CHD	C18-C13-C17	-4.01	104.89	111.22
24	C	264	PEK	O03-C01-C02	-4.00	97.93	108.69
20	N	1268	PGV	C03-C02-C01	-3.99	102.73	112.07
24	P	1264	PEK	O01-C1-O02	-3.96	113.03	123.67
22	W	1060	CHD	O7-C7-C6	-3.95	100.38	110.06
18	N	516	HEA	CMB-C2B-C1B	-3.93	121.86	128.36
22	P	1271	CHD	O12-C12-C11	-3.92	101.04	109.06
22	C	525	CHD	O7-C7-C6	-3.92	100.46	110.06
20	A	524	PGV	C4-C3-C2	-3.91	98.95	113.29
22	B	1086	CHD	O7-C7-C8	-3.85	100.76	109.26
19	A	521	TGL	CB7-CB6-CB5	-3.80	94.88	114.53
22	B	1086	CHD	O12-C12-C13	-3.80	104.95	111.11
22	P	1525	CHD	C1-C10-C9	-3.77	105.37	111.45
22	C	271	CHD	C6-C5-C4	-3.69	106.92	111.05
22	P	1525	CHD	O7-C7-C8	-3.65	101.20	109.26
22	O	229	CHD	O7-C7-C8	-3.63	101.24	109.26
22	J	60	CHD	C19-C10-C9	-3.63	105.73	111.18
20	A	522	PGV	O03-C19-O04	-3.63	114.13	123.49
22	P	1271	CHD	C18-C13-C17	-3.62	105.50	111.22
22	J	60	CHD	O7-C7-C6	-3.61	101.22	110.06
25	P	1270	CDL	C53-C52-C51	-3.59	100.14	113.29
22	P	1525	CHD	C4-C5-C10	-3.58	108.71	112.66
22	B	1086	CHD	C18-C13-C14	-3.57	105.58	111.22
24	G	265	PEK	O03-C21-O04	-3.56	114.30	123.49
24	C	264	PEK	C24-C23-C22	-3.55	100.27	113.29
20	A	524	PGV	C8-C9-C10	-3.53	100.09	113.86
18	A	516	HEA	C12-C13-C14	-3.45	102.73	112.40
24	G	1263	PEK	O01-C1-O02	-3.41	114.51	123.67
18	N	516	HEA	CAD-C3D-C2D	-3.40	119.28	129.00
22	J	60	CHD	C18-C13-C17	-3.40	105.85	111.22
18	N	515	HEA	C17-C18-C19	-3.36	120.45	127.76
19	A	521	TGL	OG1-CA1-OA1	-3.35	114.84	123.49
24	T	1265	PEK	O03-C21-O04	-3.34	114.87	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	524	PGV	O02-C1-C2	-3.32	110.43	123.72
25	C	270	CDL	C53-C52-C51	-3.28	101.27	113.29
25	G	269	CDL	OB8-CB7-OB9	-3.27	115.06	123.49
20	C	267	PGV	C27-C26-C25	-3.26	97.69	114.53
22	P	1525	CHD	C19-C10-C5	-3.26	104.49	110.25
19	O	1523	TGL	CG3-CG2-CG1	-3.22	104.55	112.07
20	C	267	PGV	O03-C19-O04	-3.21	115.20	123.49
20	P	1267	PGV	C27-C26-C25	-3.21	97.97	114.53
22	C	525	CHD	C18-C13-C17	-3.20	106.16	111.22
19	O	1523	TGL	OG3-CC1-OC1	-3.19	115.26	123.49
18	N	516	HEA	CAD-CBD-CGD	-3.19	106.90	112.75
20	N	1268	PGV	O03-C19-O04	-3.19	115.26	123.49
24	P	1264	PEK	C30-C29-C28	-3.19	98.08	114.53
20	N	1524	PGV	O01-C1-O02	-3.18	115.14	123.67
22	J	60	CHD	C6-C5-C4	-3.09	107.59	111.05
28	M	526	DMU	C25-C28-C31	-3.08	98.64	114.53
22	C	525	CHD	O12-C12-C11	-3.07	102.77	109.06
19	L	522	TGL	CB4-CB3-CB2	-3.07	102.03	113.29
18	A	515	HEA	OMA-CMA-C3A	-3.07	118.91	125.11
24	G	265	PEK	C7-C8-C9	-3.03	106.27	125.00
25	T	1269	CDL	CB2-C1-CA2	-3.02	103.14	112.92
20	P	1267	PGV	O03-C19-O04	-3.02	115.70	123.49
18	A	515	HEA	C17-C18-C19	-3.01	121.22	127.76
19	L	522	TGL	CA4-CA3-CA2	-2.99	102.32	113.29
19	Y	1522	TGL	OG3-CC1-OC1	-2.98	115.81	123.49
20	A	522	PGV	O01-C1-O02	-2.94	115.79	123.67
19	A	521	TGL	OB1-CB1-CB2	-2.90	112.11	123.72
24	T	263	PEK	O01-C1-O02	-2.89	115.90	123.67
22	C	271	CHD	O12-C12-C11	-2.88	103.17	109.06
22	O	229	CHD	O12-C12-C11	-2.86	103.21	109.06
20	P	1267	PGV	C4-C3-C2	-2.86	102.81	113.29
22	C	525	CHD	C19-C10-C5	-2.85	105.21	110.25
24	C	264	PEK	O11-P-O14	-2.84	98.58	109.62
20	N	1268	PGV	O04-C19-C20	-2.83	112.41	123.72
20	A	522	PGV	C01-O03-C19	-2.80	109.00	116.85
22	C	525	CHD	C23-C22-C20	-2.78	111.48	114.75
28	P	1272	DMU	O3-C5-C10	-2.77	103.95	110.02
19	L	522	TGL	C22-C21-C20	-2.76	100.27	114.53
19	L	522	TGL	C26-C25-C24	-2.75	100.33	114.53
25	C	270	CDL	C73-C72-C71	-2.75	103.22	113.29
20	H	268	PGV	O04-C19-C20	-2.74	112.78	123.72
28	G	272	DMU	O3-C5-C10	-2.73	104.04	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C1-C10-C9	-2.72	107.07	111.45
22	B	1086	CHD	C1-C10-C9	-2.70	107.09	111.45
20	C	267	PGV	O06-C06-C05	-2.68	97.17	110.18
28	Z	1526	DMU	C22-C19-C18	-2.68	101.50	113.47
19	A	521	TGL	CA3-CA2-CA1	-2.67	103.11	113.59
24	C	264	PEK	C25-C24-C23	-2.63	100.96	114.53
20	N	1266	PGV	C01-O03-C19	-2.63	109.50	116.85
25	P	1270	CDL	OB8-CB7-OB9	-2.62	116.72	123.49
22	C	525	CHD	C21-C20-C22	-2.61	106.00	110.35
25	C	270	CDL	OB6-CB5-OB7	-2.56	116.79	123.67
22	J	60	CHD	O12-C12-C13	-2.56	106.96	111.11
25	G	269	CDL	C58-C57-C56	-2.55	101.39	114.53
24	T	1265	PEK	C03-C02-C01	-2.54	106.12	112.07
22	C	271	CHD	C19-C10-C5	-2.54	105.76	110.25
24	C	264	PEK	O01-C1-O02	-2.54	116.85	123.67
19	L	522	TGL	CA5-CA4-CA3	-2.54	101.41	114.53
20	P	1267	PGV	O01-C02-C03	-2.52	99.48	108.36
26	R	1230	PSC	C29-C28-C27	-2.46	101.80	114.53
19	L	522	TGL	CA7-CA6-CA5	-2.45	101.86	114.53
24	P	1264	PEK	C24-C23-C22	-2.45	104.30	113.29
24	P	1264	PEK	C03-C02-C01	-2.43	106.38	112.07
20	N	1524	PGV	O03-C19-O04	-2.43	117.23	123.49
28	Z	1526	DMU	C22-C25-C28	-2.42	102.03	114.53
19	L	522	TGL	OB1-CB1-CB2	-2.42	114.05	123.72
18	A	515	HEA	O11-C11-C12	-2.39	103.90	109.73
19	O	1521	TGL	CB7-CB6-CB5	-2.35	102.38	114.53
20	A	524	PGV	O03-C19-O04	-2.35	117.43	123.49
25	T	1269	CDL	OA8-CA7-OA9	-2.35	117.44	123.49
18	N	516	HEA	C3C-CAC-CBC	-2.34	121.53	126.32
22	J	60	CHD	O7-C7-C8	-2.34	104.10	109.26
18	A	516	HEA	O11-C11-C3B	-2.32	104.97	111.82
22	C	525	CHD	O7-C7-C8	-2.32	104.15	109.26
18	A	516	HEA	C3C-C4C-NC	-2.31	106.22	109.21
25	T	1269	CDL	OA6-CA5-OA7	-2.31	117.47	123.67
18	A	515	HEA	C12-C13-C14	-2.31	105.93	112.40
19	O	1521	TGL	OG1-CA1-OA1	-2.31	117.54	123.49
28	M	526	DMU	O16-C18-C19	-2.30	100.71	109.88
18	N	516	HEA	CMC-C2C-C1C	-2.30	124.56	128.36
25	P	1270	CDL	OA6-CA5-OA7	-2.30	117.50	123.67
18	N	516	HEA	C26-C15-C14	-2.30	118.99	123.50
19	L	522	TGL	CA3-CA2-CA1	-2.29	104.59	113.59
20	H	268	PGV	O12-P-O13	-2.28	100.75	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1522	TGL	C26-C25-C24	-2.28	102.77	114.53
25	C	270	CDL	OB6-CB4-CB3	-2.27	100.36	108.36
19	Y	1522	TGL	C24-C23-C22	-2.26	102.88	114.53
25	T	1269	CDL	OB2-PB2-OB3	-2.26	100.86	109.62
24	C	264	PEK	C26-C25-C24	-2.25	102.92	114.53
18	N	515	HEA	C17-C16-C15	-2.23	105.43	112.71
24	C	264	PEK	C32-C31-C30	-2.19	103.21	114.53
19	Y	1522	TGL	CA9-CA8-CA7	-2.19	103.22	114.53
25	G	269	CDL	OB7-CB5-C51	-2.19	114.98	123.72
22	W	1060	CHD	C23-C22-C20	-2.18	112.19	114.75
24	T	1265	PEK	C33-C32-C31	-2.17	103.32	114.53
24	P	1264	PEK	C26-C25-C24	-2.17	103.33	114.53
19	O	1521	TGL	OB1-CB1-CB2	-2.17	115.05	123.72
18	A	515	HEA	CMB-C2B-C3B	-2.17	120.71	125.14
18	A	516	HEA	C26-C15-C16	-2.17	112.10	115.41
18	A	516	HEA	C3A-C4A-NA	-2.15	106.89	110.94
20	C	267	PGV	O01-C02-C03	-2.14	100.80	108.36
24	T	1265	PEK	C35-C34-C33	-2.14	103.47	114.53
25	T	1269	CDL	OB6-CB5-OB7	-2.14	117.92	123.67
19	O	1523	TGL	OG1-CA1-OA1	-2.13	118.00	123.49
25	T	1269	CDL	CA6-CA4-CA3	-2.12	107.10	112.07
20	H	268	PGV	O02-C1-C2	-2.10	115.32	123.72
25	P	1270	CDL	O1-C1-CA2	-2.10	101.37	109.35
22	B	1086	CHD	C5-C6-C7	-2.10	112.10	114.44
25	P	1270	CDL	CB6-CB4-CB3	-2.09	107.18	112.07
26	R	1230	PSC	C07-N-C06	-2.09	103.60	108.98
22	O	229	CHD	O7-C7-C6	-2.09	104.94	110.06
20	C	267	PGV	O11-P-O13	-2.08	101.56	109.62
26	E	230	PSC	C27-C26-C25	-2.06	103.89	114.53
28	Z	1526	DMU	C25-C28-C31	-2.06	103.89	114.53
18	A	515	HEA	C26-C15-C14	-2.05	119.47	123.50
19	Y	1522	TGL	OG1-CA1-OA1	-2.05	118.20	123.49
24	T	263	PEK	C13-C14-C15	-2.04	112.36	125.00
18	N	516	HEA	C12-C13-C14	-2.04	106.69	112.40
22	O	229	CHD	C4-C5-C10	-2.04	110.41	112.66
20	P	1267	PGV	O06-C06-C05	-2.04	100.31	110.18
25	C	270	CDL	O1-C1-CA2	-2.03	101.62	109.35
19	Y	1522	TGL	CB4-CB3-CB2	-2.03	105.85	113.29
19	D	523	TGL	CC3-CC2-CC1	-2.01	105.71	113.59
19	Y	1522	TGL	OB1-CB1-CB2	-2.00	115.71	123.72
28	P	1272	DMU	O7-C3-C4	2.02	114.62	109.32
22	P	1271	CHD	C16-C15-C14	2.02	109.19	105.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	CBD-CAD-C3D	2.02	116.15	112.53
25	G	269	CDL	C72-C71-CB7	2.03	121.56	113.59
20	H	268	PGV	C3-C2-C1	2.03	121.56	113.59
25	P	1270	CDL	OA8-CA6-CA4	2.03	114.15	108.69
25	G	269	CDL	C79-C78-C77	2.03	125.01	114.53
24	T	1265	PEK	O01-C02-C03	2.03	115.53	108.36
25	P	1270	CDL	C62-C61-C60	2.06	125.19	114.53
19	D	523	TGL	C15-CC9-CC8	2.07	125.21	114.53
20	H	268	PGV	O14-P-O13	2.07	123.73	112.53
19	O	1521	TGL	C16-C15-CC9	2.07	125.21	114.53
24	T	263	PEK	C2-C3-C4	2.07	117.42	113.30
20	N	1524	PGV	O01-C02-C03	2.07	115.65	108.36
25	T	1269	CDL	C80-C79-C78	2.07	125.23	114.53
25	T	1269	CDL	C20-C19-C18	2.07	125.23	114.53
24	C	264	PEK	O04-C21-C22	2.08	132.03	123.72
19	D	523	TGL	C20-CA9-CA8	2.08	125.28	114.53
25	G	269	CDL	OB8-CB7-C71	2.09	118.27	111.90
22	C	525	CHD	C19-C10-C1	2.09	111.72	108.20
28	M	526	DMU	O55-C2-C3	2.09	114.83	109.87
18	N	515	HEA	CAA-C2A-C1A	2.11	129.30	127.01
19	O	1521	TGL	C15-CC9-CC8	2.12	125.46	114.53
22	O	229	CHD	O3-C3-C2	2.14	116.11	110.05
22	P	1525	CHD	C21-C20-C22	2.15	113.93	110.35
19	L	522	TGL	C15-CC9-CC8	2.15	125.62	114.53
22	C	525	CHD	C6-C7-C8	2.16	113.76	111.47
22	C	271	CHD	C9-C10-C5	2.16	111.87	108.67
24	C	264	PEK	C2-C3-C4	2.16	117.60	113.30
28	G	272	DMU	C11-C9-C8	2.18	118.38	113.02
28	Z	1526	DMU	C10-C5-C7	2.18	114.27	109.97
24	C	264	PEK	O13-P-O14	2.18	124.36	112.53
19	D	523	TGL	C16-C15-CC9	2.19	125.83	114.53
28	G	272	DMU	O4-C7-C5	2.19	115.27	110.34
22	B	1086	CHD	C13-C17-C20	2.19	122.17	119.50
26	E	230	PSC	C08-N-C06	2.20	114.63	108.98
25	T	1269	CDL	C19-C18-C17	2.20	125.88	114.53
18	N	515	HEA	CMC-C2C-C3C	2.20	129.39	125.09
25	G	269	CDL	CB6-OB8-CB7	2.20	123.01	116.85
18	A	515	HEA	CAA-C2A-C1A	2.20	129.40	127.01
25	T	1269	CDL	OB4-PB2-OB3	2.21	124.52	112.53
25	T	1269	CDL	C82-C81-C80	2.21	125.96	114.53
19	O	1523	TGL	C21-C20-CA9	2.23	126.03	114.53
25	G	269	CDL	C80-C79-C78	2.23	126.07	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	O7-C3-C2	2.24	112.95	107.17
19	Y	1522	TGL	OG2-CG2-CG3	2.24	116.25	108.36
20	N	1266	PGV	O14-P-O11	2.24	119.76	108.46
19	A	521	TGL	C15-CC9-CC8	2.25	126.14	114.53
18	A	516	HEA	C16-C17-C18	2.25	117.58	111.69
19	Y	1522	TGL	C15-CC9-CC8	2.27	126.23	114.53
25	P	1270	CDL	C39-C38-C37	2.27	126.23	114.53
25	G	269	CDL	C43-C42-C41	2.28	126.28	114.53
25	P	1270	CDL	C79-C78-C77	2.28	126.31	114.53
28	G	272	DMU	O7-C10-O1	2.29	116.47	110.68
19	D	523	TGL	OG1-CG1-CG2	2.31	114.90	108.69
25	P	1270	CDL	C42-C41-C40	2.32	126.50	114.53
18	A	515	HEA	C3C-C4C-NC	2.32	112.21	109.21
25	C	270	CDL	OA8-CA7-C31	2.32	118.97	111.90
22	P	1525	CHD	O3-C3-C4	2.33	114.49	109.86
24	C	264	PEK	C11-C10-C9	2.33	119.74	112.00
18	A	515	HEA	CBA-CAA-C2A	2.33	116.70	112.53
28	M	526	DMU	O4-C7-C8	2.33	115.58	110.34
25	P	1270	CDL	OA8-CA7-C31	2.34	119.02	111.90
25	G	269	CDL	CB4-OB6-CB5	2.34	123.51	117.89
25	P	1270	CDL	OB2-PB2-OB3	2.35	118.74	109.62
22	O	229	CHD	C13-C14-C8	2.36	117.80	114.75
24	C	264	PEK	O01-C1-C2	2.37	116.68	111.53
20	N	1268	PGV	C02-O01-C1	2.37	123.58	117.89
19	O	1523	TGL	C24-C23-C22	2.37	126.78	114.53
20	H	268	PGV	O01-C02-C03	2.38	116.76	108.36
19	Y	1522	TGL	CC3-CC2-CC1	2.39	122.97	113.59
28	Z	1526	DMU	C18-O16-C6	2.40	118.14	113.94
25	C	270	CDL	C42-C41-C40	2.40	126.93	114.53
22	J	60	CHD	C9-C8-C7	2.41	114.77	111.92
19	A	521	TGL	OG2-CG2-CG1	2.42	116.87	108.36
20	P	1267	PGV	O01-C1-C2	2.42	116.78	111.53
22	O	229	CHD	C14-C8-C7	2.42	115.10	111.74
28	M	526	DMU	O55-C2-C1	2.42	115.79	110.34
25	G	269	CDL	C39-C38-C37	2.44	127.12	114.53
20	H	268	PGV	C01-O03-C19	2.45	123.71	116.85
18	N	515	HEA	C13-C12-C11	2.46	117.79	114.51
28	Z	1526	DMU	C6-C1-C2	2.47	114.84	109.97
24	P	1264	PEK	C02-O01-C1	2.47	123.83	117.89
28	P	1272	DMU	O7-C10-O1	2.49	116.99	110.68
22	B	1086	CHD	C2-C1-C10	2.49	117.29	112.84
25	T	1269	CDL	C40-C39-C38	2.51	127.47	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	O3-C3-C4	2.51	114.85	109.86
25	P	1270	CDL	OB6-CB4-CB6	2.51	117.20	108.36
20	N	1266	PGV	O01-C1-C2	2.53	117.03	111.53
18	A	515	HEA	CAD-C3D-C2D	2.53	136.24	129.00
18	N	516	HEA	CMB-C2B-C3B	2.54	130.34	125.14
24	T	263	PEK	O03-C21-C22	2.54	119.65	111.90
19	Y	1522	TGL	CB3-CB2-CB1	2.55	123.60	113.59
28	M	526	DMU	O5-C6-O16	2.56	116.21	110.05
25	G	269	CDL	C40-C39-C38	2.56	127.77	114.53
22	O	229	CHD	C11-C9-C10	2.57	116.47	113.79
18	A	515	HEA	C17-C16-C15	2.58	121.10	112.71
18	N	515	HEA	C4B-C3B-C11	2.59	129.82	127.01
28	G	272	DMU	O61-C57-C4	2.59	119.89	111.33
25	T	1269	CDL	OA8-CA7-C31	2.59	119.80	111.90
20	C	267	PGV	C01-O03-C19	2.59	124.10	116.85
19	D	523	TGL	OG2-CB1-OB1	2.61	130.69	123.67
19	O	1521	TGL	OG3-CG3-CG2	2.63	115.76	108.69
28	P	1272	DMU	O61-C57-C4	2.65	120.08	111.33
22	C	271	CHD	C14-C8-C7	2.65	115.42	111.74
20	N	1524	PGV	C02-O01-C1	2.68	124.31	117.89
28	Z	1526	DMU	O5-C6-O16	2.68	116.51	110.05
18	A	515	HEA	C20-C19-C18	2.69	126.14	121.05
19	L	522	TGL	OG2-CG2-CG3	2.69	117.83	108.36
18	A	516	HEA	C26-C15-C14	2.70	128.80	123.50
18	A	515	HEA	CMB-C2B-C1B	2.71	132.84	128.36
20	C	267	PGV	O14-P-O13	2.71	127.19	112.53
28	P	1272	DMU	C11-C9-C8	2.71	119.71	113.02
25	C	270	CDL	OA8-CA6-CA4	2.73	116.04	108.69
19	L	522	TGL	OG2-CB1-CB2	2.76	117.52	111.53
19	Y	1522	TGL	OG1-CG1-CG2	2.77	116.15	108.69
22	P	1271	CHD	C21-C20-C17	2.78	117.59	112.96
19	D	523	TGL	CB3-CB2-CB1	2.79	124.57	113.59
19	L	522	TGL	CC3-CC2-CC1	2.80	124.59	113.59
20	A	524	PGV	C01-O03-C19	2.81	124.70	116.85
18	A	515	HEA	C25-C23-C24	2.81	121.55	114.64
20	P	1267	PGV	O03-C19-C20	2.81	120.46	111.90
19	D	523	TGL	C21-C20-CA9	2.82	129.07	114.53
25	C	270	CDL	O1-C1-CB2	2.86	120.25	109.35
24	C	264	PEK	C02-O01-C1	2.88	124.79	117.89
20	N	1268	PGV	O01-C1-C2	2.89	117.81	111.53
20	A	524	PGV	O01-C1-O02	2.89	131.43	123.67
20	A	524	PGV	O01-C02-C03	2.90	118.58	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E	230	PSC	O03-C19-C20	2.90	120.74	111.90
24	P	1264	PEK	C01-O03-C21	2.91	124.98	116.85
18	A	516	HEA	C17-C18-C19	2.91	134.09	127.76
28	G	272	DMU	O7-C3-C4	2.91	116.97	109.32
19	D	523	TGL	CG2-OG2-CB1	2.91	124.88	117.89
18	A	515	HEA	C26-C15-C16	2.91	119.86	115.41
25	G	269	CDL	OA8-CA7-C31	2.92	120.79	111.90
28	M	526	DMU	C10-C5-C7	2.92	115.72	109.97
28	G	272	DMU	C10-O1-C9	2.92	119.41	113.75
25	C	270	CDL	CA6-OA8-CA7	2.93	125.03	116.85
20	A	524	PGV	O01-C1-C2	2.93	117.90	111.53
26	E	230	PSC	C02-O01-C1	2.94	124.95	117.89
25	T	1269	CDL	CB6-OB8-CB7	2.96	125.12	116.85
28	M	526	DMU	O49-C1-C2	2.96	116.99	110.34
19	O	1523	TGL	OG1-CA1-CA2	2.97	120.96	111.90
19	L	522	TGL	OG1-CG1-CG2	2.97	116.69	108.69
25	C	270	CDL	OB6-CB5-C51	2.98	117.99	111.53
22	C	525	CHD	C15-C16-C17	2.98	111.13	105.12
28	M	526	DMU	C18-O16-C6	2.98	119.16	113.94
19	D	523	TGL	C10-CB9-CB8	2.99	129.95	114.53
28	G	272	DMU	O5-C6-O16	2.99	117.26	110.05
24	T	263	PEK	O03-C01-C02	2.99	116.75	108.69
28	M	526	DMU	C57-C4-C3	3.00	121.96	113.25
22	P	1525	CHD	C9-C11-C12	3.01	118.16	114.36
28	G	272	DMU	C1-C2-C3	3.01	116.20	109.60
28	Z	1526	DMU	O3-C5-C7	3.01	117.11	110.34
22	P	1525	CHD	C5-C6-C7	3.03	117.81	114.44
22	O	229	CHD	C2-C1-C10	3.03	118.25	112.84
24	T	263	PEK	C01-O03-C21	3.04	125.34	116.85
28	M	526	DMU	C11-C9-C8	3.05	120.53	113.02
25	T	1269	CDL	C83-C82-C81	3.05	130.27	114.53
22	W	1060	CHD	C17-C13-C14	3.05	103.14	100.05
19	O	1523	TGL	OG1-CG1-CG2	3.05	116.90	108.69
25	T	1269	CDL	OB8-CB6-CB4	3.06	116.91	108.69
19	Y	1522	TGL	OG3-CC1-CC2	3.06	121.21	111.90
22	C	525	CHD	C13-C14-C8	3.07	118.71	114.75
22	P	1525	CHD	C15-C16-C17	3.08	111.33	105.12
22	B	1086	CHD	C16-C17-C20	3.09	117.56	112.05
28	M	526	DMU	C6-C1-C2	3.13	116.15	109.97
22	O	229	CHD	C5-C6-C7	3.14	117.94	114.44
20	P	1267	PGV	C02-O01-C1	3.17	125.50	117.89
19	A	521	TGL	CG3-OG3-CC1	3.18	125.74	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C9-C8-C7	3.19	115.69	111.92
19	A	521	TGL	OG3-CC1-CC2	3.19	121.63	111.90
22	C	525	CHD	C11-C9-C10	3.20	117.12	113.79
28	M	526	DMU	C1-C2-C3	3.22	116.66	109.60
22	W	1060	CHD	C14-C8-C9	3.24	114.07	109.62
22	B	1086	CHD	C23-C22-C20	3.26	118.59	114.75
25	G	269	CDL	CA6-OA8-CA7	3.26	125.97	116.85
24	G	1263	PEK	C01-O03-C21	3.27	125.98	116.85
19	L	522	TGL	OG1-CA1-CA2	3.27	121.87	111.90
24	G	1263	PEK	O03-C01-C02	3.27	117.50	108.69
22	C	525	CHD	O3-C3-C4	3.30	116.42	109.86
19	L	522	TGL	OG3-CG3-CG2	3.30	117.57	108.69
19	O	1521	TGL	OG3-CC1-CC2	3.30	121.97	111.90
28	Z	1526	DMU	C10-O1-C9	3.31	120.17	113.75
22	P	1271	CHD	C2-C1-C10	3.33	118.78	112.84
28	P	1272	DMU	C10-O1-C9	3.34	120.23	113.75
20	A	522	PGV	O01-C1-C2	3.36	118.84	111.53
18	A	516	HEA	C27-C19-C20	3.37	120.55	115.41
25	P	1270	CDL	CA6-OA8-CA7	3.38	126.31	116.85
28	P	1272	DMU	C7-C8-C9	3.40	116.12	110.20
22	P	1525	CHD	C13-C14-C8	3.40	119.13	114.75
18	N	516	HEA	C26-C15-C16	3.42	120.63	115.41
22	C	525	CHD	C2-C1-C10	3.42	118.94	112.84
22	W	1060	CHD	C9-C10-C5	3.42	113.73	108.67
22	B	1086	CHD	C11-C9-C8	3.43	115.61	110.73
26	R	1230	PSC	O03-C19-C20	3.43	122.36	111.90
20	N	1266	PGV	O03-C01-C02	3.45	117.97	108.69
28	Z	1526	DMU	C6-O5-C4	3.45	120.44	113.75
22	O	229	CHD	C6-C7-C8	3.46	115.14	111.47
28	G	272	DMU	C10-C5-C7	3.47	116.81	109.97
19	Y	1522	TGL	CG2-OG2-CB1	3.47	126.22	117.89
19	O	1521	TGL	CG1-OG1-CA1	3.48	126.57	116.85
20	N	1524	PGV	O03-C19-C20	3.48	122.52	111.90
22	C	271	CHD	C14-C8-C9	3.49	114.42	109.62
19	Y	1522	TGL	OG1-CA1-CA2	3.49	122.54	111.90
26	R	1230	PSC	O01-C1-C2	3.49	119.12	111.53
22	C	525	CHD	C11-C9-C8	3.50	115.70	110.73
24	P	1264	PEK	O01-C1-C2	3.52	119.17	111.53
22	P	1525	CHD	C14-C8-C9	3.52	114.47	109.62
18	A	515	HEA	C12-C11-C3B	3.53	119.90	112.59
22	P	1271	CHD	C17-C13-C14	3.56	103.65	100.05
28	Z	1526	DMU	C1-C2-C3	3.57	117.43	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C2-C1-C10	3.61	119.28	112.84
22	B	1086	CHD	C16-C17-C13	3.61	107.19	103.60
22	J	60	CHD	C17-C13-C14	3.65	103.74	100.05
19	O	1523	TGL	CG3-OG3-CC1	3.69	127.17	116.85
18	A	516	HEA	C4B-C3B-C11	3.71	131.03	127.01
28	G	272	DMU	C6-O5-C4	3.73	120.99	113.75
20	A	524	PGV	O03-C19-C20	3.76	123.35	111.90
22	O	229	CHD	C16-C17-C20	3.79	118.80	112.05
28	M	526	DMU	O1-C9-C11	3.79	115.93	106.36
28	P	1272	DMU	C10-C5-C7	3.83	117.52	109.97
19	O	1523	TGL	OG3-CC1-CC2	3.85	123.62	111.90
28	P	1272	DMU	C18-O16-C6	3.85	120.66	113.94
20	A	522	PGV	O03-C19-C20	3.85	123.63	111.90
25	T	1269	CDL	OA6-CA5-C11	3.88	119.95	111.53
28	Z	1526	DMU	O7-C3-C2	3.88	117.18	107.17
22	O	229	CHD	C13-C17-C20	3.88	124.23	119.50
28	P	1272	DMU	C2-C3-C4	3.89	119.64	110.84
22	P	1525	CHD	C6-C7-C8	3.90	115.61	111.47
24	G	1263	PEK	O03-C21-C22	3.91	123.82	111.90
22	O	229	CHD	C14-C8-C9	3.91	115.00	109.62
19	D	523	TGL	CG3-OG3-CC1	3.94	127.86	116.85
22	W	1060	CHD	C22-C20-C17	3.94	118.51	110.24
22	P	1525	CHD	C16-C17-C20	3.97	119.12	112.05
22	C	271	CHD	C23-C22-C20	3.97	119.44	114.75
22	C	525	CHD	C9-C11-C12	3.99	119.40	114.36
19	O	1521	TGL	OG2-CB1-CB2	3.99	120.21	111.53
28	P	1272	DMU	O1-C9-C11	4.00	116.45	106.36
24	T	263	PEK	C14-C13-C12	4.00	125.32	112.00
28	Z	1526	DMU	C7-C8-C9	4.01	117.19	110.20
19	O	1521	TGL	OG1-CA1-CA2	4.02	124.15	111.90
28	P	1272	DMU	C1-C2-C3	4.03	118.44	109.60
26	E	230	PSC	O01-C1-C2	4.07	120.38	111.53
28	M	526	DMU	O3-C5-C7	4.10	119.57	110.34
24	G	265	PEK	O01-C1-C2	4.13	120.51	111.53
28	P	1272	DMU	O5-C6-C1	4.14	118.78	110.28
20	A	522	PGV	O03-C01-C02	4.17	119.91	108.69
22	C	525	CHD	C14-C8-C9	4.18	115.37	109.62
22	C	271	CHD	C17-C13-C14	4.19	104.28	100.05
18	A	515	HEA	C27-C19-C20	4.19	121.81	115.41
28	P	1272	DMU	C6-O5-C4	4.19	121.89	113.75
22	J	60	CHD	C4-C5-C10	4.21	117.29	112.66
22	J	60	CHD	C9-C10-C5	4.22	114.91	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C15-C14-C13	4.23	107.81	103.60
22	B	1086	CHD	C14-C8-C9	4.24	115.45	109.62
28	M	526	DMU	C8-C7-C5	4.24	118.71	110.79
24	T	1265	PEK	O03-C21-C22	4.28	124.93	111.90
22	J	60	CHD	C22-C20-C17	4.29	119.26	110.24
22	C	271	CHD	C4-C5-C10	4.30	117.39	112.66
22	C	271	CHD	C9-C11-C12	4.31	119.81	114.36
22	P	1271	CHD	C9-C11-C12	4.31	119.81	114.36
19	Y	1522	TGL	CG3-OG3-CC1	4.34	128.97	116.85
22	W	1060	CHD	C16-C17-C20	4.34	119.79	112.05
28	G	272	DMU	C7-C8-C9	4.34	117.76	110.20
18	N	516	HEA	C4B-C3B-C11	4.35	131.73	127.01
22	P	1271	CHD	C13-C17-C20	4.36	124.81	119.50
19	D	523	TGL	OG1-CA1-CA2	4.38	125.25	111.90
18	N	515	HEA	C12-C11-C3B	4.38	121.65	112.59
19	O	1523	TGL	OG2-CB1-CB2	4.40	121.08	111.53
28	G	272	DMU	O7-C3-C2	4.41	118.55	107.17
22	C	271	CHD	C1-C2-C3	4.43	117.61	110.43
19	A	521	TGL	OG1-CA1-CA2	4.44	125.42	111.90
28	M	526	DMU	O5-C4-C57	4.44	117.57	106.36
28	M	526	DMU	C7-C8-C9	4.46	117.97	110.20
18	N	516	HEA	CBD-CAD-C3D	4.47	120.55	112.53
22	P	1525	CHD	C11-C12-C13	4.48	115.75	111.20
25	C	270	CDL	OB8-CB7-C71	4.49	125.57	111.90
24	G	265	PEK	O03-C21-C22	4.51	125.64	111.90
20	A	524	PGV	C02-O01-C1	4.54	128.79	117.89
18	N	515	HEA	C16-C17-C18	4.57	123.65	111.69
25	P	1270	CDL	OB8-CB7-C71	4.58	125.84	111.90
22	W	1060	CHD	C4-C5-C10	4.60	117.73	112.66
22	C	525	CHD	C5-C4-C3	4.62	119.79	112.91
28	P	1272	DMU	C6-C1-C2	4.65	119.14	109.97
22	W	1060	CHD	C11-C9-C8	4.67	117.36	110.73
22	C	525	CHD	C5-C6-C7	4.69	119.66	114.44
25	C	270	CDL	OA6-CA5-C11	4.73	121.81	111.53
18	A	515	HEA	C4B-C3B-C11	4.74	132.16	127.01
28	G	272	DMU	O5-C6-C1	4.79	120.11	110.28
28	G	272	DMU	C8-C7-C5	4.80	119.74	110.79
28	G	272	DMU	C6-C1-C2	4.87	119.56	109.97
28	G	272	DMU	C2-C3-C4	4.88	121.88	110.84
22	J	60	CHD	C11-C12-C13	4.88	116.16	111.20
22	J	60	CHD	C9-C11-C12	4.91	120.56	114.36
22	O	229	CHD	C1-C2-C3	4.92	118.42	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C1-C2-C3	4.96	118.49	110.43
22	W	1060	CHD	C13-C14-C8	4.97	121.15	114.75
22	C	271	CHD	C16-C17-C13	4.99	108.56	103.60
22	W	1060	CHD	C2-C1-C10	5.00	121.77	112.84
20	H	268	PGV	O01-C1-C2	5.02	122.44	111.53
20	H	268	PGV	O03-C19-C20	5.04	127.25	111.90
22	W	1060	CHD	C14-C8-C7	5.05	118.74	111.74
28	M	526	DMU	O5-C4-C3	5.05	120.42	109.75
28	Z	1526	DMU	C2-C3-C4	5.07	122.30	110.84
22	P	1525	CHD	C13-C17-C20	5.07	125.68	119.50
22	J	60	CHD	C15-C14-C8	5.08	125.69	118.32
22	O	229	CHD	C15-C14-C8	5.08	125.70	118.32
19	Y	1522	TGL	OG2-CB1-CB2	5.09	122.59	111.53
28	P	1272	DMU	C8-C7-C5	5.09	120.30	110.79
28	Z	1526	DMU	O5-C4-C3	5.10	120.52	109.75
19	O	1521	TGL	CG2-OG2-CB1	5.11	130.15	117.89
19	O	1521	TGL	CG3-OG3-CC1	5.15	131.25	116.85
28	G	272	DMU	O1-C9-C11	5.15	119.38	106.36
22	W	1060	CHD	C15-C14-C8	5.17	125.82	118.32
24	G	1263	PEK	O01-C1-C2	5.18	122.78	111.53
22	B	1086	CHD	C4-C3-C2	5.18	117.13	110.52
22	J	60	CHD	C2-C1-C10	5.19	122.10	112.84
22	C	271	CHD	C2-C1-C10	5.19	122.11	112.84
22	P	1271	CHD	C5-C4-C3	5.21	120.66	112.91
22	O	229	CHD	C11-C12-C13	5.22	116.50	111.20
22	P	1271	CHD	C15-C14-C13	5.27	108.84	103.60
24	T	1265	PEK	O01-C1-C2	5.27	122.99	111.53
28	P	1272	DMU	O5-C4-C57	5.28	119.69	106.36
22	W	1060	CHD	C15-C14-C13	5.28	108.85	103.60
22	C	525	CHD	C17-C13-C14	5.33	105.44	100.05
22	J	60	CHD	C16-C17-C20	5.36	121.62	112.05
22	J	60	CHD	C14-C8-C7	5.37	119.19	111.74
22	W	1060	CHD	C1-C2-C3	5.39	119.18	110.43
28	G	272	DMU	O5-C4-C3	5.39	121.13	109.75
22	J	60	CHD	C15-C14-C13	5.43	109.00	103.60
25	G	269	CDL	OA6-CA5-C11	5.43	123.33	111.53
28	M	526	DMU	C2-C3-C4	5.44	123.14	110.84
22	P	1525	CHD	C17-C13-C14	5.50	105.61	100.05
22	P	1271	CHD	C16-C17-C20	5.50	121.86	112.05
25	T	1269	CDL	OB6-CB5-C51	5.54	123.56	111.53
22	C	271	CHD	C5-C4-C3	5.54	121.16	112.91
25	P	1270	CDL	OA6-CA5-C11	5.57	123.64	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	OG3-CC1-CC2	5.58	128.90	111.90
22	O	229	CHD	C11-C9-C8	5.59	118.67	110.73
25	G	269	CDL	OB6-CB5-C51	5.60	123.70	111.53
19	D	523	TGL	CG1-OG1-CA1	5.63	132.59	116.85
28	P	1272	DMU	O1-C10-C5	5.67	121.91	110.28
22	P	1271	CHD	C14-C13-C12	5.72	112.51	107.39
22	O	229	CHD	C9-C11-C12	5.75	121.63	114.36
24	P	1264	PEK	C2-C3-C4	5.81	124.87	113.30
19	L	522	TGL	CG2-OG2-CB1	5.82	131.86	117.89
28	P	1272	DMU	O5-C4-C3	5.82	122.05	109.75
22	C	271	CHD	C11-C12-C13	5.87	117.16	111.20
22	W	1060	CHD	C16-C17-C13	5.87	109.44	103.60
22	C	271	CHD	C5-C6-C7	5.90	121.02	114.44
22	O	229	CHD	C4-C3-C2	5.96	118.12	110.52
28	Z	1526	DMU	O1-C9-C11	5.97	121.44	106.36
22	P	1525	CHD	C9-C8-C7	5.99	119.00	111.92
22	J	60	CHD	C5-C4-C3	6.05	121.92	112.91
24	T	263	PEK	O01-C1-C2	6.06	124.70	111.53
20	N	1266	PGV	O03-C19-C20	6.06	130.37	111.90
22	J	60	CHD	C16-C17-C13	6.08	109.65	103.60
22	W	1060	CHD	C6-C5-C10	6.09	119.36	112.66
22	P	1271	CHD	C4-C5-C10	6.09	119.36	112.66
22	C	525	CHD	C11-C12-C13	6.10	117.39	111.20
28	Z	1526	DMU	C8-C7-C5	6.12	122.22	110.79
22	B	1086	CHD	C5-C4-C3	6.18	122.10	112.91
22	J	60	CHD	C6-C5-C10	6.18	119.47	112.66
22	P	1271	CHD	C11-C12-C13	6.19	117.49	111.20
22	P	1271	CHD	C5-C6-C7	6.24	121.40	114.44
28	Z	1526	DMU	O1-C9-C8	6.29	121.48	109.68
22	J	60	CHD	C11-C9-C8	6.29	119.67	110.73
22	B	1086	CHD	C11-C9-C10	6.29	120.33	113.79
22	P	1271	CHD	C4-C3-C2	6.32	118.57	110.52
22	O	229	CHD	C5-C4-C3	6.34	122.34	112.91
22	P	1271	CHD	C15-C14-C8	6.35	127.53	118.32
22	C	525	CHD	C9-C8-C7	6.36	119.43	111.92
22	W	1060	CHD	C5-C4-C3	6.37	122.40	112.91
28	Z	1526	DMU	O5-C4-C57	6.39	122.50	106.36
22	B	1086	CHD	C1-C2-C3	6.40	120.81	110.43
22	C	271	CHD	C11-C9-C8	6.40	119.83	110.73
22	W	1060	CHD	C9-C11-C12	6.47	122.53	114.36
22	P	1525	CHD	C11-C9-C8	6.48	119.95	110.73
22	C	271	CHD	C15-C14-C13	6.49	110.06	103.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C11-C9-C8	6.53	120.01	110.73
22	B	1086	CHD	C17-C13-C14	6.55	106.67	100.05
22	C	525	CHD	C15-C14-C13	6.56	110.13	103.60
28	G	272	DMU	O1-C10-C5	6.60	123.81	110.28
28	G	272	DMU	O5-C4-C57	6.63	123.11	106.36
22	W	1060	CHD	C4-C3-C2	6.63	118.97	110.52
22	W	1060	CHD	C11-C12-C13	6.66	117.96	111.20
22	C	525	CHD	C13-C17-C20	6.66	127.61	119.50
19	A	521	TGL	OG2-CB1-CB2	6.67	126.02	111.53
28	Z	1526	DMU	O1-C10-C5	6.68	123.98	110.28
28	G	272	DMU	O1-C9-C8	6.68	122.22	109.68
22	O	229	CHD	C9-C8-C7	6.68	119.81	111.92
22	P	1271	CHD	C16-C17-C13	6.70	110.26	103.60
20	N	1268	PGV	O03-C19-C20	6.70	132.32	111.90
18	A	515	HEA	C16-C17-C18	6.71	129.25	111.69
22	C	271	CHD	C15-C14-C8	6.72	128.08	118.32
22	P	1271	CHD	C1-C2-C3	6.74	121.37	110.43
22	W	1060	CHD	C14-C13-C12	6.79	113.47	107.39
22	J	60	CHD	C5-C6-C7	6.82	122.04	114.44
22	C	525	CHD	C14-C13-C12	6.83	113.51	107.39
28	Z	1526	DMU	O5-C6-C1	6.87	124.38	110.28
22	J	60	CHD	C13-C17-C20	6.90	127.91	119.50
22	C	271	CHD	C4-C3-C2	6.92	119.34	110.52
22	P	1525	CHD	C5-C4-C3	6.95	123.25	112.91
22	C	271	CHD	C1-C10-C5	6.98	119.28	107.81
22	W	1060	CHD	C5-C6-C7	7.03	122.28	114.44
22	J	60	CHD	C17-C13-C12	7.08	123.95	117.68
22	P	1271	CHD	C1-C10-C5	7.11	119.49	107.81
22	C	271	CHD	C16-C17-C20	7.14	124.79	112.05
28	G	272	DMU	C18-O16-C6	7.17	126.48	113.94
28	M	526	DMU	O1-C9-C8	7.24	123.27	109.68
22	W	1060	CHD	C1-C10-C5	7.34	119.87	107.81
22	J	60	CHD	C4-C3-C2	7.35	119.89	110.52
28	M	526	DMU	O5-C6-C1	7.36	125.38	110.28
22	C	271	CHD	C6-C7-C8	7.36	119.28	111.47
22	P	1271	CHD	C6-C7-C8	7.36	119.28	111.47
22	J	60	CHD	C6-C7-C8	7.39	119.32	111.47
20	N	1524	PGV	O01-C1-C2	7.44	127.69	111.53
22	J	60	CHD	C14-C13-C12	7.47	114.08	107.39
28	M	526	DMU	O1-C10-C5	7.51	125.69	110.28
28	P	1272	DMU	O1-C9-C8	7.54	123.83	109.68
22	J	60	CHD	C1-C10-C5	7.60	120.30	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Z	1526	DMU	O16-C6-C1	7.62	117.66	108.04
22	C	271	CHD	C6-C5-C10	7.85	121.30	112.66
18	N	515	HEA	C27-C19-C20	7.88	127.44	115.41
22	W	1060	CHD	C6-C7-C8	7.94	119.89	111.47
28	P	1272	DMU	O16-C6-C1	8.03	118.18	108.04
22	W	1060	CHD	C13-C17-C20	8.17	129.44	119.50
19	A	521	TGL	CG2-OG2-CB1	8.38	137.99	117.89
22	W	1060	CHD	C17-C13-C12	8.43	125.15	117.68
18	N	516	HEA	CAD-C3D-C4D	8.56	136.30	127.01
22	C	271	CHD	C17-C13-C12	8.60	125.30	117.68
22	P	1271	CHD	C6-C5-C10	8.63	122.17	112.66
22	B	1086	CHD	C9-C11-C12	8.68	125.33	114.36
22	P	1271	CHD	C17-C13-C12	8.94	125.60	117.68
22	P	1525	CHD	C15-C14-C13	8.95	112.50	103.60
22	O	229	CHD	C17-C13-C12	9.04	125.69	117.68
22	B	1086	CHD	C14-C13-C12	9.10	115.54	107.39
22	C	271	CHD	C14-C13-C12	9.12	115.56	107.39
22	P	1525	CHD	C4-C3-C2	9.14	122.17	110.52
22	O	229	CHD	C17-C13-C14	9.25	109.40	100.05
22	B	1086	CHD	C1-C10-C5	9.51	123.44	107.81
22	O	229	CHD	C14-C13-C12	9.56	115.95	107.39
22	P	1525	CHD	C10-C9-C8	9.64	122.46	111.88
22	B	1086	CHD	C6-C7-C8	9.74	121.81	111.47
22	B	1086	CHD	C10-C9-C8	9.76	122.59	111.88
28	G	272	DMU	O16-C6-C1	9.91	120.55	108.04
22	C	525	CHD	C4-C3-C2	10.23	123.56	110.52
22	O	229	CHD	C1-C10-C5	10.25	124.66	107.81
22	C	525	CHD	C10-C9-C8	10.26	123.14	111.88
22	O	229	CHD	C10-C9-C8	10.31	123.20	111.88
22	P	1525	CHD	C17-C13-C12	10.32	126.82	117.68
22	C	525	CHD	C17-C13-C12	10.54	127.02	117.68
22	P	1525	CHD	C14-C13-C12	11.36	117.56	107.39
22	P	1525	CHD	C1-C10-C5	11.49	126.71	107.81
22	B	1086	CHD	C17-C13-C12	11.81	128.15	117.68
22	C	525	CHD	C6-C5-C10	12.00	125.87	112.66
22	C	271	CHD	C10-C9-C8	12.02	125.07	111.88
22	C	525	CHD	C1-C10-C5	12.05	127.62	107.81
22	J	60	CHD	C10-C9-C8	12.17	125.24	111.88
22	P	1525	CHD	C6-C5-C10	12.55	126.48	112.66
22	B	1086	CHD	C6-C5-C10	13.40	127.42	112.66
22	O	229	CHD	C6-C5-C10	13.67	127.72	112.66
22	W	1060	CHD	C10-C9-C8	13.74	126.96	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C10-C9-C8	13.84	127.07	111.88

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C2
28	P	1272	DMU	C4
28	P	1272	DMU	C9
28	P	1272	DMU	C5
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
28	Z	1526	DMU	C2
28	Z	1526	DMU	C4
28	Z	1526	DMU	C6
28	Z	1526	DMU	C9
28	Z	1526	DMU	C5
22	W	1060	CHD	C17
22	W	1060	CHD	C9
22	B	1086	CHD	C9
28	M	526	DMU	C2
28	M	526	DMU	C4
28	M	526	DMU	C9
28	M	526	DMU	C5
22	J	60	CHD	C17
22	J	60	CHD	C9
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
22	C	271	CHD	C9
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
22	P	1271	CHD	C9
28	G	272	DMU	C2
28	G	272	DMU	C4
28	G	272	DMU	C9
28	G	272	DMU	C6
28	G	272	DMU	C5

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C02-O01-C1-O02
20	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

40 monomers are involved in 344 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	9	0
18	A	516	HEA	2	0
15	A	520	PER	1	0
19	A	521	TGL	13	0
20	A	522	PGV	2	0
20	A	524	PGV	6	0
22	B	1086	CHD	2	0
24	C	264	PEK	7	0
20	C	267	PGV	4	0
25	C	270	CDL	19	0
22	C	271	CHD	2	0
22	C	525	CHD	3	0
19	D	523	TGL	9	0
26	E	230	PSC	22	0
24	G	1263	PEK	15	0
24	G	265	PEK	16	0
25	G	269	CDL	27	0
28	G	272	DMU	5	0
20	H	268	PGV	3	0
22	J	60	CHD	1	0
19	L	522	TGL	15	0
20	N	1268	PGV	1	0
20	N	1524	PGV	11	0
18	N	515	HEA	12	0
18	N	516	HEA	2	0
15	N	520	PER	1	0
19	O	1521	TGL	14	0
19	O	1523	TGL	9	0
24	P	1264	PEK	7	0
20	P	1267	PGV	11	0
25	P	1270	CDL	24	0
22	P	1271	CHD	1	0
28	P	1272	DMU	1	0
26	R	1230	PSC	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	T	1265	PEK	8	0
25	T	1269	CDL	19	0
24	T	263	PEK	22	0
22	W	1060	CHD	4	0
19	Y	1522	TGL	18	0
28	Z	1526	DMU	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.75	56 (10%) 7 12	23, 29, 37, 63	0
1	N	513/514 (99%)	0.53	42 (8%) 14 23	27, 34, 43, 64	0
2	B	226/227 (99%)	-0.09	2 (0%) 85 90	24, 34, 56, 82	0
2	O	226/227 (99%)	0.03	7 (3%) 52 62	30, 40, 63, 82	0
3	C	259/261 (99%)	-0.14	4 (1%) 76 84	25, 32, 44, 61	0
3	P	259/261 (99%)	-0.02	7 (2%) 58 68	28, 35, 47, 64	0
4	D	144/147 (97%)	-0.24	2 (1%) 78 85	29, 35, 50, 65	0
4	Q	144/147 (97%)	1.20	26 (18%) 2 2	36, 50, 70, 109	0
5	E	104/109 (95%)	0.21	6 (5%) 26 37	29, 35, 54, 70	0
5	R	104/109 (95%)	0.77	11 (10%) 8 13	32, 41, 57, 75	0
6	F	93/98 (94%)	0.28	4 (4%) 39 50	29, 38, 56, 93	0
6	S	93/98 (94%)	0.27	4 (4%) 39 50	32, 40, 62, 87	0
7	G	83/85 (97%)	0.92	15 (18%) 2 2	29, 38, 93, 99	0
7	T	83/85 (97%)	1.16	16 (19%) 2 2	30, 42, 90, 104	0
8	H	75/85 (88%)	0.64	12 (16%) 3 4	30, 41, 77, 83	0
8	U	75/85 (88%)	0.84	14 (18%) 2 2	36, 46, 80, 86	0
9	I	71/73 (97%)	0.71	10 (14%) 4 6	31, 41, 65, 71	0
9	V	71/73 (97%)	1.24	14 (19%) 1 2	36, 51, 66, 75	0
10	J	57/59 (96%)	0.49	8 (14%) 4 6	32, 41, 58, 73	0
10	W	57/59 (96%)	0.86	11 (19%) 2 2	36, 45, 62, 78	0
11	K	49/56 (87%)	0.01	0 100 100	32, 38, 49, 58	0
11	X	49/56 (87%)	1.61	17 (34%) 0 0	42, 47, 62, 69	0
12	L	46/47 (97%)	-0.04	2 (4%) 39 50	30, 35, 54, 79	0
12	Y	46/47 (97%)	0.04	2 (4%) 39 50	34, 42, 62, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.50	6 (13%) 4 6	29, 35, 87, 107	0
13	Z	43/46 (93%)	1.03	9 (20%) 1 1	37, 44, 96, 112	0
All	All	3526/3614 (97%)	0.44	307 (8%) 13 20	23, 36, 61, 112	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	19.8
4	Q	4	SER	12.7
4	Q	5	VAL	12.5
6	F	96	LEU	12.4
13	Z	43	SER	10.1
6	F	95	GLN	8.7
13	Z	40	TYR	8.3
13	M	43	SER	8.2
8	H	45	ALA	8.1
4	Q	8	SER	7.8
7	T	36	TRP	7.5
7	G	2	SER	7.1
13	Z	42	LYS	7.1
7	G	1	ALA	6.8
6	S	96	LEU	6.6
9	I	37	PHE	6.6
9	V	37	PHE	6.2
10	W	52	TRP	5.9
13	M	42	LYS	5.9
7	T	1	ALA	5.7
7	T	42	ARG	5.7
2	O	113	TYR	5.5
6	F	94	HIS	5.5
6	S	94	HIS	5.4
8	U	44	THR	5.2
9	V	36	LYS	5.1
11	X	13	TYR	5.1
7	T	40	GLY	5.1
13	Z	39	ASN	5.0
8	H	43	MET	5.0
8	U	49	ASP	5.0
7	T	3	ALA	5.0
5	R	109	VAL	5.0
13	M	40	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
8	H	47	GLY	4.9
4	Q	147	LYS	4.9
4	Q	48	TRP	4.9
7	T	8	HIS	4.9
8	U	45	ALA	4.8
10	W	57	HIS	4.8
7	G	5	LYS	4.7
7	T	4	ALA	4.6
8	U	42	ALA	4.6
6	S	93	PRO	4.6
8	H	44	THR	4.5
7	G	42	ARG	4.5
7	T	5	LYS	4.5
7	T	39	SER	4.5
8	H	50	VAL	4.4
8	U	48	GLY	4.4
4	Q	53	ILE	4.3
9	I	25	PHE	4.3
8	H	46	LYS	4.3
7	T	2	SER	4.2
11	X	19	ALA	4.2
7	G	3	ALA	4.2
13	Z	37	LEU	4.2
7	G	40	GLY	4.1
11	X	7	PRO	4.1
9	I	29	LEU	4.1
9	V	53	ASN	4.1
9	I	26	MET	4.1
7	G	36	TRP	4.1
7	G	84	LYS	4.1
7	T	84	LYS	4.0
10	J	1	PHE	3.9
9	V	34	PHE	3.9
11	X	23	THR	3.9
7	G	4	ALA	3.9
7	G	41	HIS	3.8
4	Q	7	LYS	3.8
8	U	50	VAL	3.8
9	I	33	THR	3.7
5	R	96	LEU	3.7
1	N	282	PHE	3.7
1	A	389	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
8	U	52	VAL	3.6
11	X	16	ALA	3.6
8	H	48	GLY	3.6
7	T	41	HIS	3.6
9	V	33	THR	3.6
1	A	202	LEU	3.6
4	Q	51	LEU	3.6
12	Y	45	LEU	3.6
13	Z	35	TYR	3.6
8	U	47	GLY	3.6
10	J	52	TRP	3.6
2	O	91	ASN	3.6
1	N	246	LEU	3.5
4	Q	138	TRP	3.5
12	Y	47	LYS	3.5
5	E	11	PHE	3.5
11	X	6	ALA	3.5
1	A	75	ILE	3.5
9	I	36	LYS	3.5
12	L	47	LYS	3.5
5	E	109	VAL	3.4
10	W	1	PHE	3.4
13	Z	32	TRP	3.4
1	N	193	VAL	3.4
8	U	46	LYS	3.4
1	A	66	ILE	3.4
11	X	27	ALA	3.4
6	S	95	GLN	3.3
7	G	9	GLY	3.3
1	N	126	TRP	3.3
7	T	9	GLY	3.3
1	N	66	ILE	3.3
1	A	385	ALA	3.3
4	Q	140	TYR	3.3
10	W	55	PHE	3.2
5	R	89	LEU	3.2
13	M	41	LYS	3.2
9	V	30	GLY	3.2
1	A	126	TRP	3.2
4	Q	46	ALA	3.2
1	N	78	PHE	3.2
4	Q	58	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	73	ILE	3.2
1	A	201	VAL	3.2
1	A	195	LEU	3.2
10	W	26	ALA	3.1
4	Q	43	LYS	3.1
1	A	246	LEU	3.1
8	U	11	TYR	3.1
3	P	3	HIS	3.1
1	A	247	ILE	3.0
1	A	193	VAL	3.0
4	Q	30	VAL	3.0
1	N	197	LEU	3.0
1	N	389	ILE	3.0
11	X	18	LEU	3.0
10	W	4	ARG	3.0
1	A	235	PHE	3.0
11	X	36	ILE	3.0
8	H	49	ASP	3.0
1	A	188	VAL	3.0
1	A	380	VAL	3.0
1	N	70	VAL	2.9
1	N	285	PHE	2.9
10	W	48	TYR	2.9
10	W	56	PRO	2.9
1	A	243	VAL	2.9
1	N	201	VAL	2.9
1	N	283	LEU	2.9
5	R	93	LEU	2.9
9	V	29	LEU	2.9
1	A	73	ILE	2.9
10	J	30	ILE	2.9
1	N	238	PHE	2.9
4	Q	102	TYR	2.9
1	A	197	LEU	2.9
1	A	248	LEU	2.9
9	V	3	ALA	2.9
11	X	17	VAL	2.9
3	C	38	ASN	2.8
1	N	388	ALA	2.8
1	A	396	TRP	2.8
11	X	47	ARG	2.8
2	O	90	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	195	LEU	2.8
13	M	39	ASN	2.8
1	N	247	ILE	2.7
7	T	12	GLY	2.7
9	I	34	PHE	2.7
11	X	24	PHE	2.7
1	A	60	ALA	2.7
1	A	203	ALA	2.7
7	T	43	GLU	2.7
7	G	8	HIS	2.7
9	V	25	PHE	2.7
13	Z	41	LYS	2.7
1	A	250	GLY	2.7
4	Q	107	ILE	2.7
1	N	128	VAL	2.6
8	H	42	ALA	2.6
1	N	202	LEU	2.6
5	R	52	LEU	2.6
1	A	67	PHE	2.6
1	N	251	PHE	2.6
3	C	92	LEU	2.6
9	V	19	PHE	2.6
2	B	59	GLN	2.6
1	N	245	ILE	2.6
5	R	24	ILE	2.6
10	J	48	TYR	2.6
4	D	4	SER	2.6
1	A	199	LEU	2.6
8	U	43	MET	2.5
1	A	20	LEU	2.5
1	A	161	ALA	2.5
10	W	18	LEU	2.5
1	A	237	PHE	2.5
1	N	83	VAL	2.5
3	P	38	ASN	2.5
1	N	184	PHE	2.5
3	P	91	VAL	2.5
12	L	2	HIS	2.5
2	O	217	LYS	2.4
1	A	245	ILE	2.4
11	X	12	LYS	2.4
3	P	182	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	2.4
1	A	192	ALA	2.4
9	I	53	ASN	2.4
1	A	377	PHE	2.4
8	H	53	CYS	2.4
10	W	30	ILE	2.4
1	N	196	LEU	2.4
4	Q	33	LEU	2.4
4	D	147	LYS	2.4
1	A	70	VAL	2.4
4	Q	111	PHE	2.4
9	V	26	MET	2.4
2	O	59	GLN	2.3
5	E	9	GLU	2.3
1	N	381	LEU	2.3
5	E	7	THR	2.3
5	E	19	PHE	2.3
1	N	190	ILE	2.3
11	X	52	GLU	2.3
5	R	51	ALA	2.3
5	R	97	GLY	2.3
7	G	6	GLY	2.3
1	A	63	PHE	2.3
1	N	248	LEU	2.3
1	A	284	GLY	2.3
2	B	91	ASN	2.3
1	N	75	ILE	2.3
4	Q	9	GLU	2.3
13	M	38	ASP	2.3
1	A	150	LEU	2.3
1	A	498	CYS	2.3
10	J	5	VAL	2.3
1	A	249	PRO	2.3
6	F	43	LYS	2.3
1	N	74	MET	2.3
7	G	37	LEU	2.2
9	V	15	ARG	2.2
1	N	373	VAL	2.2
3	C	91	VAL	2.2
8	H	52	VAL	2.2
3	P	37	PHE	2.2
1	A	74	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	158	ILE	2.2
4	Q	39	ALA	2.2
2	O	227	LEU	2.2
1	N	288	TRP	2.2
4	Q	128	VAL	2.2
11	X	48	VAL	2.2
1	N	377	PHE	2.2
4	Q	35	ALA	2.2
4	Q	97	ILE	2.2
2	O	130	PRO	2.2
1	N	194	LEU	2.2
1	A	350	VAL	2.2
1	N	243	VAL	2.2
4	Q	145	TRP	2.2
11	X	34	THR	2.2
11	X	49	THR	2.2
8	U	53	CYS	2.2
1	A	78	PHE	2.2
1	N	312	ILE	2.2
1	A	384	GLY	2.2
1	A	391	GLY	2.2
10	J	10	LYS	2.2
10	J	57	HIS	2.2
1	A	373	VAL	2.2
1	A	65	MET	2.2
1	N	189	MET	2.2
1	A	153	ALA	2.2
8	U	51	SER	2.2
9	I	18	ARG	2.2
10	J	55	PHE	2.2
4	Q	139	ASP	2.2
5	R	68	LEU	2.2
7	G	43	GLU	2.1
13	Z	36	HIS	2.1
1	A	194	LEU	2.1
8	H	79	GLY	2.1
7	T	38	HIS	2.1
1	A	285	PHE	2.1
10	W	27	THR	2.1
3	P	33	MET	2.1
1	A	381	LEU	2.1
1	A	64	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	6	GLU	2.1
1	A	281	GLY	2.1
9	I	4	LEU	2.1
3	P	95	THR	2.1
3	C	37	PHE	2.1
1	N	280	ILE	2.1
1	A	388	ALA	2.1
5	R	11	PHE	2.0
1	A	236	TRP	2.0
5	R	18	TYR	2.0
8	U	56	TYR	2.0
9	V	4	LEU	2.0
1	A	124	THR	2.0
1	A	191	THR	2.0
1	N	79	GLY	2.0
1	N	391	GLY	2.0
1	A	184	PHE	2.0
1	A	282	PHE	2.0
1	N	287	VAL	2.0
9	V	39	VAL	2.0
1	N	311	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	O	1	10/11	0.96	0.11	-	39,40,48,52	0
1	FME	N	1	10/11	0.94	0.16	-	47,49,70,71	0
2	FME	B	1	10/11	0.96	0.12	-	32,33,40,58	0
7	TPO	G	11	11/12	0.61	0.26	-	71,78,96,97	0
1	FME	A	1	10/11	0.93	0.12	-	48,51,72,78	0
7	TPO	T	11	11/12	0.55	0.25	-	71,78,95,96	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
28	DMU	P	1272	33/33	0.54	0.36	10.21	80,103,111,112	0
28	DMU	G	272	33/33	0.48	0.34	9.97	65,94,105,105	0
20	PGV	A	524	51/51	0.81	0.26	9.28	33,74,105,108	0
22	CHD	W	1060	29/29	0.72	0.37	9.20	87,91,96,97	0
19	TGL	Y	1522	63/63	0.67	0.29	5.41	45,72,86,88	0
17	NA	N	1519	1/1	0.92	0.21	5.30	45,45,45,45	0
22	CHD	J	60	29/29	0.79	0.30	5.17	77,83,93,94	0
26	PSC	R	1230	52/52	0.65	0.31	5.05	43,96,122,124	0
25	CDL	P	1270	100/100	0.75	0.30	4.96	41,85,115,120	0
25	CDL	C	270	100/100	0.82	0.31	4.80	41,84,118,119	0
20	PGV	N	1524	51/51	0.80	0.29	4.18	41,75,113,114	0
26	PSC	E	230	52/52	0.64	0.36	4.10	58,99,125,127	0
19	TGL	D	523	63/63	0.80	0.19	3.45	44,63,81,82	0
19	TGL	L	522	63/63	0.79	0.25	3.42	38,59,77,79	0
19	TGL	O	1521	63/63	0.82	0.21	2.97	53,77,88,89	0
25	CDL	G	269	100/100	0.61	0.30	2.75	64,87,115,118	0
19	TGL	O	1523	63/63	0.77	0.20	2.60	54,76,89,94	0
20	PGV	H	268	51/51	0.70	0.34	2.47	59,84,110,112	0
20	PGV	N	1268	51/51	0.72	0.33	2.04	67,91,112,114	0
25	CDL	T	1269	100/100	0.69	0.26	1.93	61,84,108,111	0
24	PEK	T	263	53/53	0.59	0.37	1.92	55,95,117,119	0
19	TGL	A	521	63/63	0.87	0.18	1.72	48,69,84,89	0
24	PEK	G	265	53/53	0.62	0.28	1.67	45,82,114,116	0
24	PEK	T	1265	53/53	0.67	0.29	1.63	44,79,110,112	0
24	PEK	G	1263	53/53	0.59	0.34	1.48	60,95,118,119	0
28	DMU	Z	1526	33/33	0.85	0.22	1.34	39,54,67,69	0
20	PGV	P	1267	51/51	0.96	0.12	1.06	28,40,72,79	0
20	PGV	C	267	51/51	0.96	0.12	1.01	25,36,67,70	0
28	DMU	M	526	33/33	0.90	0.13	0.88	39,47,65,67	0
22	CHD	C	525	29/29	0.96	0.15	0.80	28,33,40,45	0
16	MG	A	518	1/1	0.98	0.15	0.77	27,27,27,27	0
27	ZN	S	99	1/1	0.99	0.09	0.75	38,38,38,38	0
20	PGV	A	522	51/51	0.97	0.14	0.61	25,39,65,66	0
18	HEA	N	516	60/60	0.98	0.18	0.55	26,32,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CHD	P	1525	29/29	0.96	0.16	0.47	29,36,42,44	0
21	CUA	B	228	2/2	0.99	0.13	0.39	27,27,27,30	0
24	PEK	P	1264	53/53	0.95	0.13	0.37	29,48,75,78	0
22	CHD	C	271	29/29	0.94	0.14	0.33	46,51,53,55	0
20	PGV	N	1266	51/51	0.97	0.12	0.33	31,42,67,71	0
18	HEA	N	515	60/60	0.98	0.16	0.30	23,32,51,54	0
24	PEK	C	264	53/53	0.96	0.12	0.30	29,47,73,75	0
16	MG	N	1518	1/1	0.97	0.12	0.11	34,34,34,34	0
21	CUA	O	228	2/2	0.97	0.11	0.08	36,36,36,37	0
27	ZN	F	99	1/1	1.00	0.09	-0.04	34,34,34,34	0
18	HEA	A	515	60/60	0.99	0.17	-0.10	19,26,50,53	0
22	CHD	P	1271	29/29	0.94	0.15	-0.12	48,53,56,58	0
15	PER	A	520	2/2	0.97	0.17	-0.24	25,25,25,32	0
18	HEA	A	516	60/60	0.99	0.15	-0.33	20,26,33,36	0
22	CHD	O	229	29/29	0.96	0.09	-0.38	23,31,37,37	0
22	CHD	B	1086	29/29	0.97	0.08	-0.53	26,30,37,47	0
17	NA	A	519	1/1	0.92	0.11	-0.77	42,42,42,42	0
15	PER	N	520	2/2	0.97	0.16	-0.99	31,31,31,34	0
23	UNX	P	1262	1/1	0.87	0.47	-	22,22,22,22	0
14	CU	N	517	1/1	0.99	0.16	-	32,32,32,32	0
14	CU	A	517	1/1	1.00	0.15	-	29,29,29,29	0
23	UNX	C	262	1/1	0.71	0.47	-	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.