



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:33 am GMT

PDB ID : 3ABL
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (15-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 : 2.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

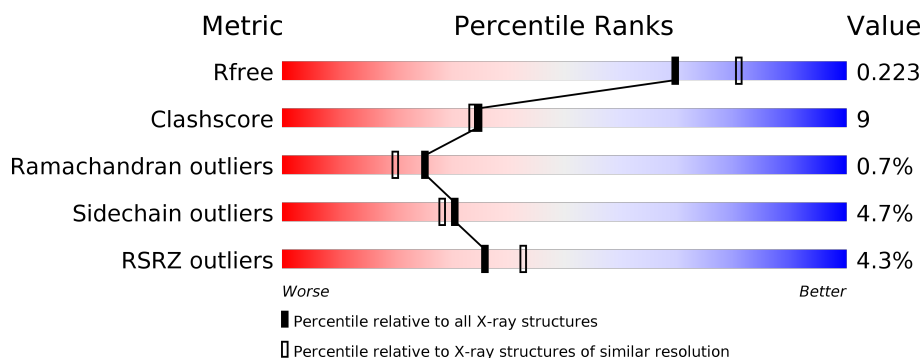
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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>76%</div> <div>21%</div> <div>.</div> </div>
1	N	514	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	B	227	<div> <div>75%</div> <div>21%</div> <div>..</div> </div>
2	O	227	<div> <div>2%</div> <div>71%</div> <div>23%</div> <div>5%</div> </div>
3	C	261	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>
3	P	261	<div> <div>%</div> <div>80%</div> <div>17%</div> <div>...</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PER	A	520	-	-	-	X
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	A	521	-	-	-	X
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1521	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	Q	1523	-	-	-	X
20	PGV	A	522	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	C	267	-	-	-	X
20	PGV	N	1266	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1267	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	PSC	B	230	-	-	-	X
22	PSC	O	1230	-	-	-	X
23	CHD	C	271	X	-	-	X
23	CHD	J	60	X	-	-	X
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	X
24	DMU	C	272	X	-	-	X
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	X
24	DMU	Z	1526	X	-	-	-
26	CDL	C	270	-	-	-	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	-	X
26	CDL	T	1269	-	-	X	-
28	PEK	G	264	-	-	-	X
28	PEK	P	1265	-	-	-	X
28	PEK	T	263	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32244 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 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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			

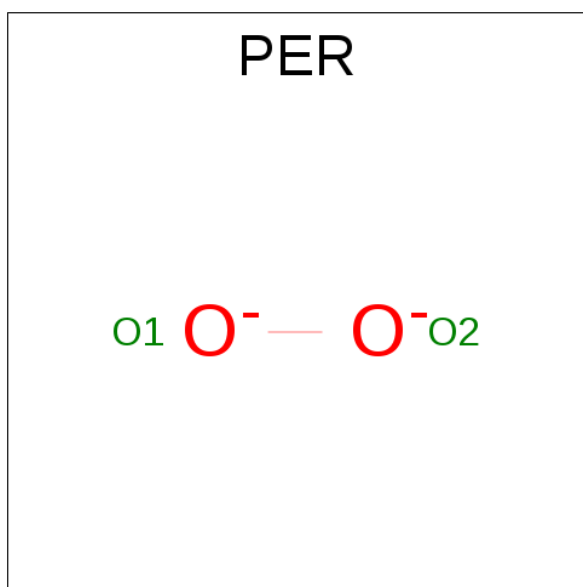
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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

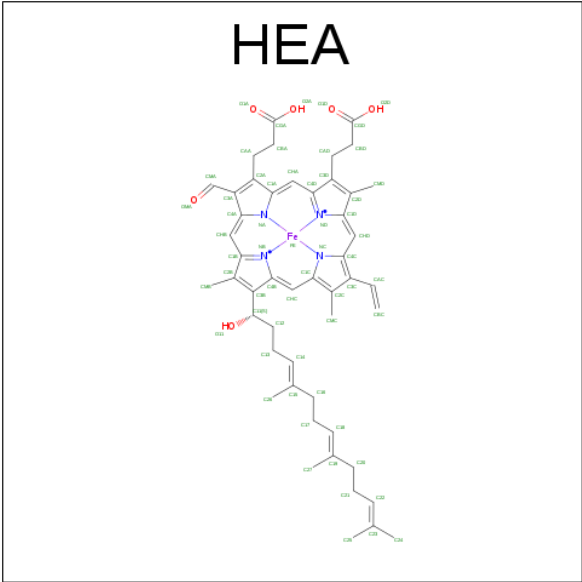
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

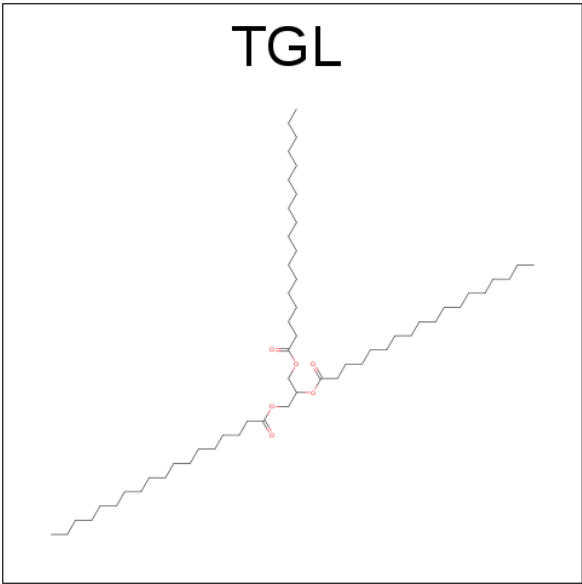
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



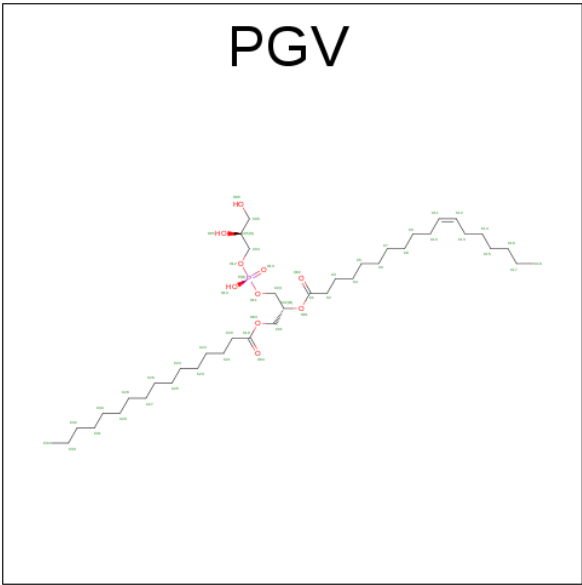
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- 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	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

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



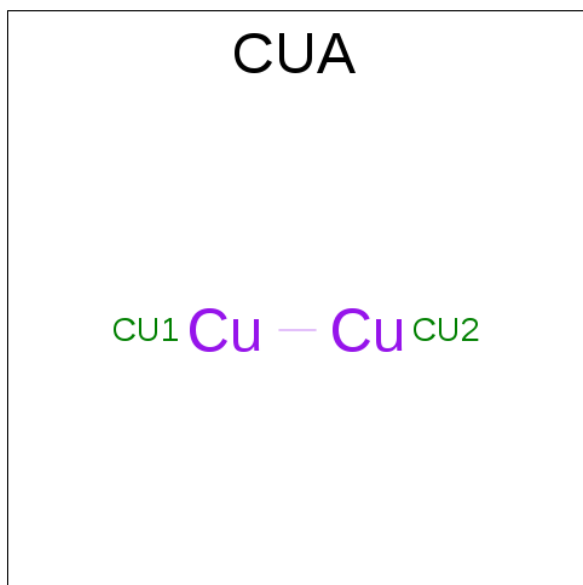
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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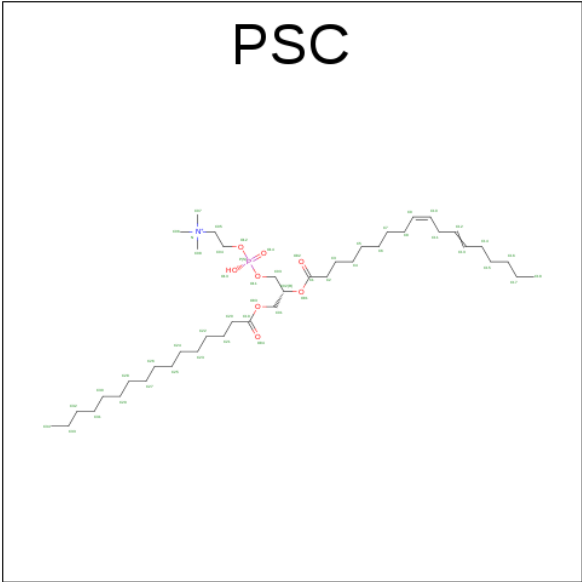
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



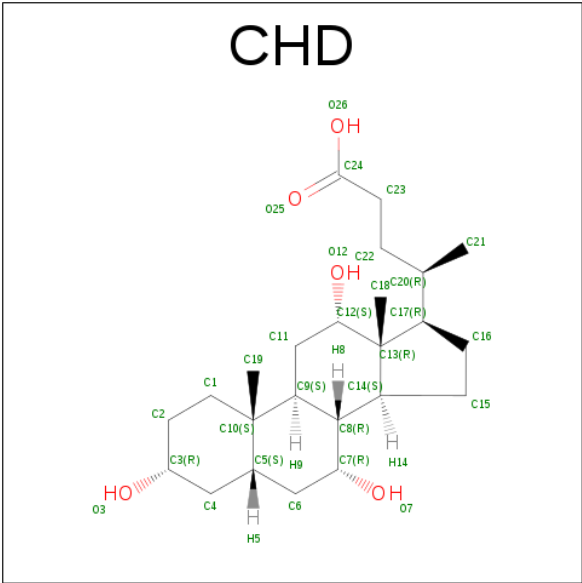
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is (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
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



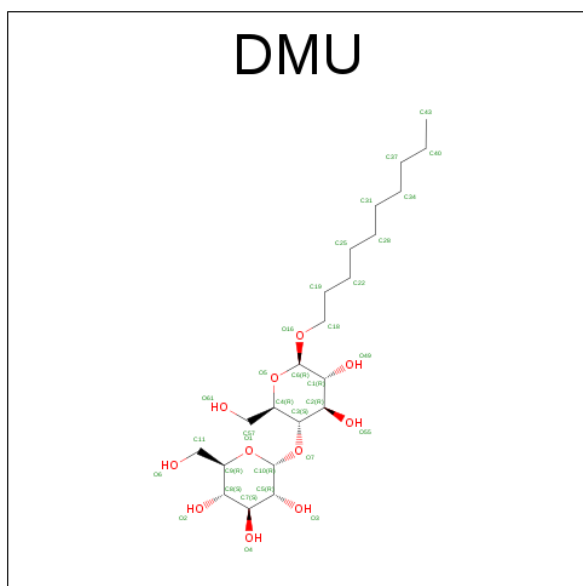
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

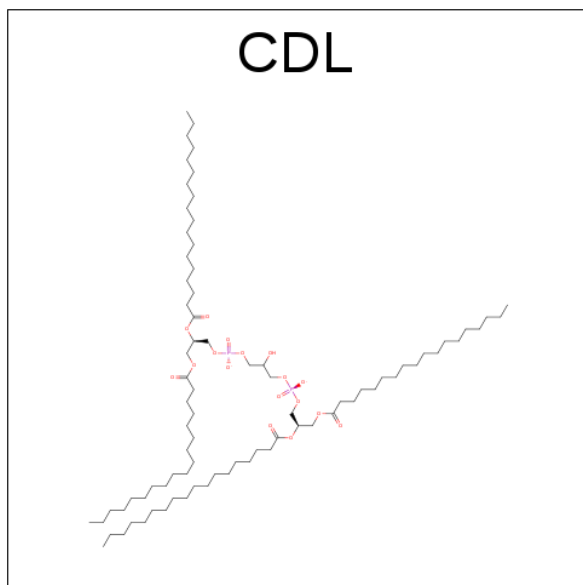


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



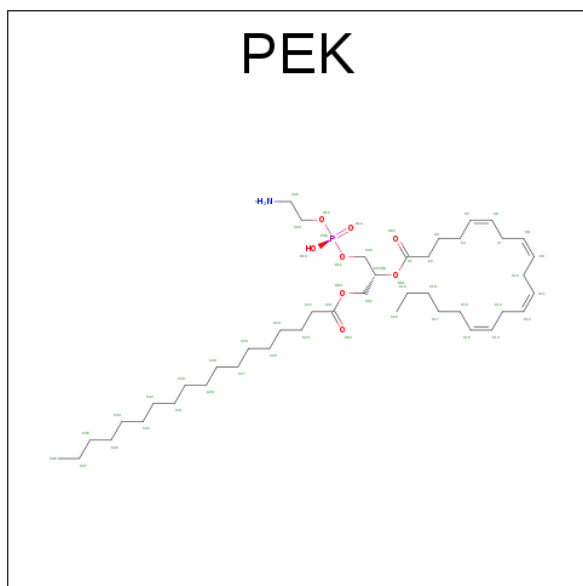
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O P 100 81 17 2	0	0
26	G	1	Total C O P 100 81 17 2	0	0
26	P	1	Total C O P 100 81 17 2	0	0
26	T	1	Total C O P 100 81 17 2	0	0

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

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

- Molecule 28 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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	219	Total	O	0	0
			219	219		
29	B	139	Total	O	0	0
			139	139		
29	C	105	Total	O	0	0
			105	105		
29	D	110	Total	O	0	0
			110	110		
29	E	68	Total	O	0	0
			68	68		

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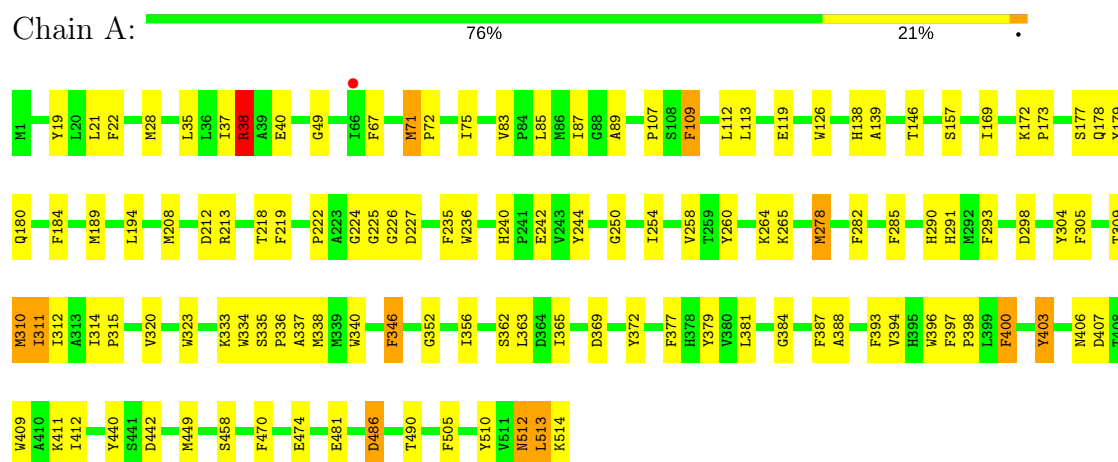
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	76	Total 76	O 76	0	0
29	G	45	Total 45	O 45	0	0
29	H	48	Total 48	O 48	0	0
29	I	35	Total 35	O 35	0	0
29	J	21	Total 21	O 21	0	0
29	K	22	Total 22	O 22	0	0
29	L	27	Total 27	O 27	0	0
29	M	18	Total 18	O 18	0	0
29	N	204	Total 204	O 204	0	0
29	O	109	Total 109	O 109	0	0
29	P	106	Total 106	O 106	0	0
29	Q	67	Total 67	O 67	0	0
29	R	52	Total 52	O 52	0	0
29	S	69	Total 69	O 69	0	0
29	T	48	Total 48	O 48	0	0
29	U	38	Total 38	O 38	0	0
29	V	19	Total 19	O 19	0	0
29	W	16	Total 16	O 16	0	0
29	X	16	Total 16	O 16	0	0
29	Y	17	Total 17	O 17	0	0
29	Z	14	Total 14	O 14	0	0

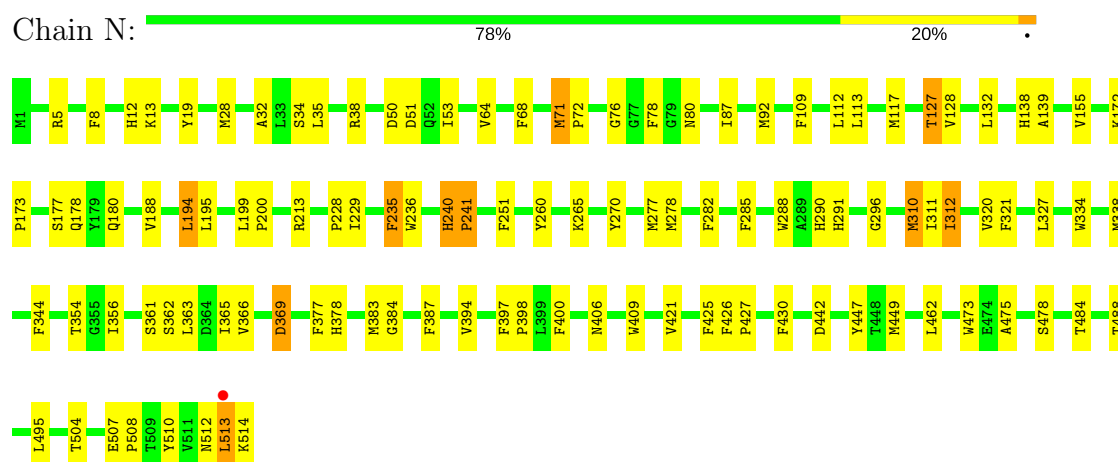
3 Residue-property plots

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

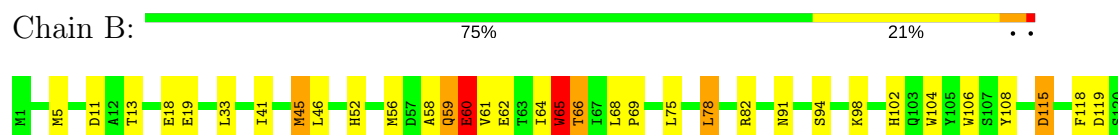
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

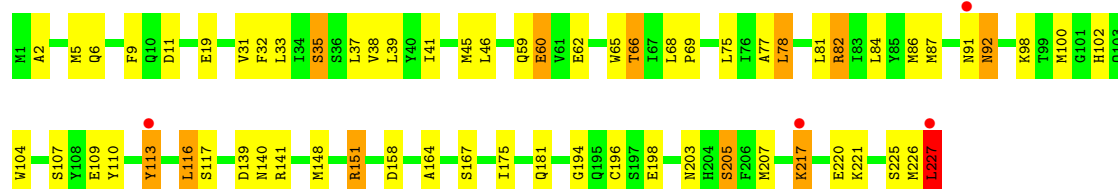


• Molecule 2: Cytochrome c oxidase subunit 2

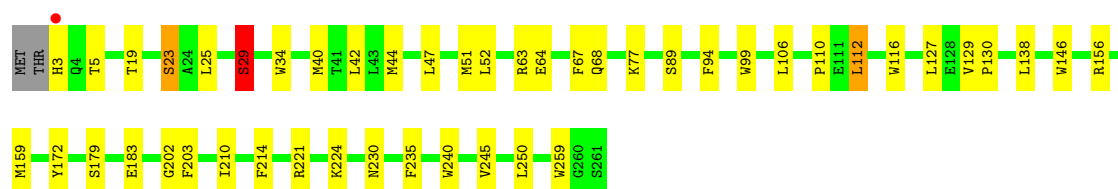
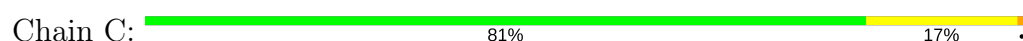




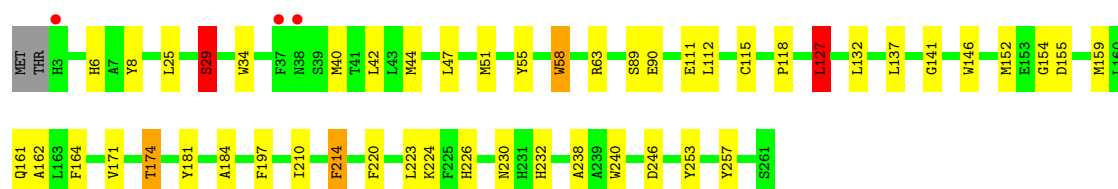
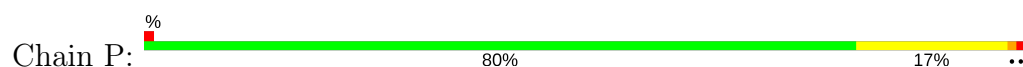
• Molecule 2: Cytochrome c oxidase subunit 2



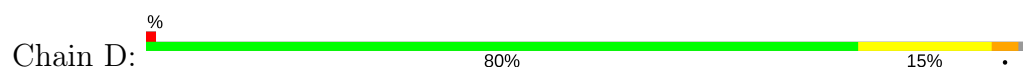
• Molecule 3: Cytochrome c oxidase subunit 3



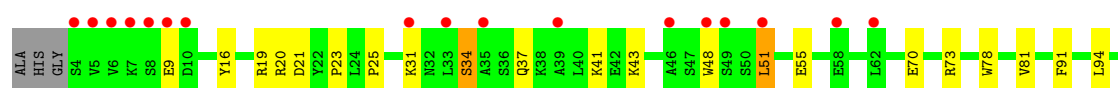
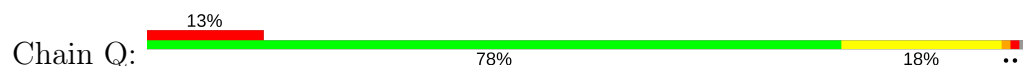
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

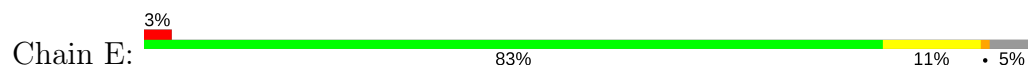


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

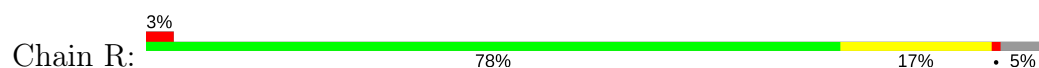




- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A



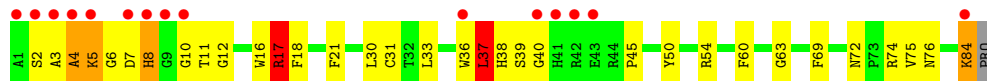
- Molecule 6: Cytochrome c oxidase subunit 5B



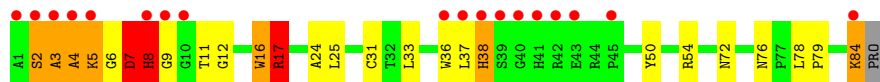
- Molecule 6: Cytochrome c oxidase subunit 5B



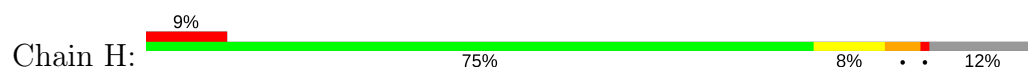
- Molecule 7: Cytochrome c oxidase subunit 6A2

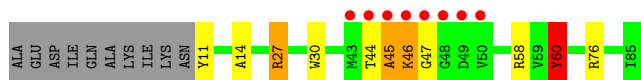


- Molecule 7: Cytochrome c oxidase subunit 6A2

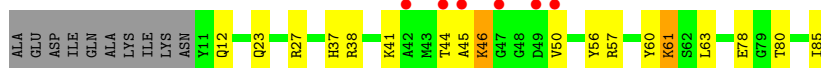


- Molecule 8: Cytochrome c oxidase subunit 6B1





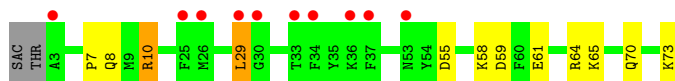
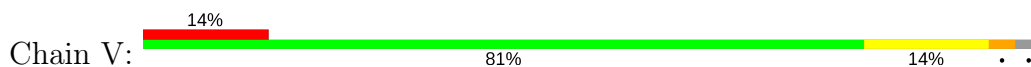
- Molecule 8: Cytochrome c oxidase subunit 6B1



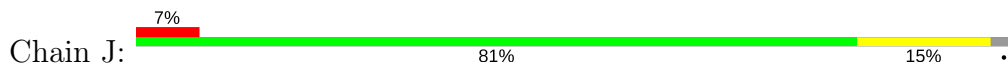
- Molecule 9: Cytochrome c oxidase subunit 6C



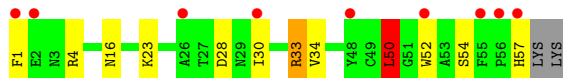
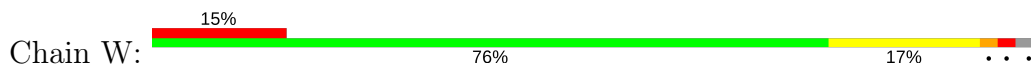
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



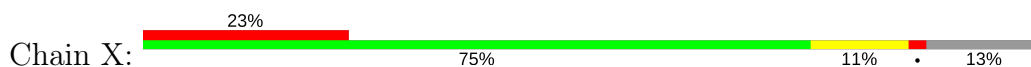
- Molecule 10: Cytochrome c oxidase polypeptide 7A1

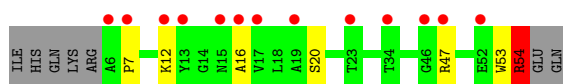


- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B

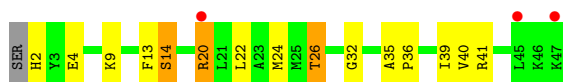




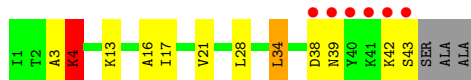
• Molecule 12: Cytochrome c oxidase subunit 7C



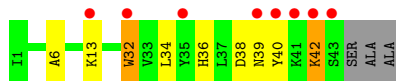
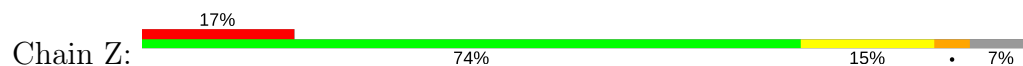
• Molecule 12: Cytochrome c oxidase subunit 7C



• Molecule 13: Cytochrome c oxidase subunit 8B



• Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.14Å 207.51Å 178.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 38.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.10) 98.6 (38.32-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.176 , 0.210 0.193 , 0.223	Depositor DCC
R_{free} test set	13838 reflections (3.68%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32244	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

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	1.72	46/4156 (1.1%)	1.25	23/5678 (0.4%)
1	N	1.55	27/4156 (0.6%)	1.16	20/5678 (0.4%)
2	B	1.61	18/1860 (1.0%)	1.29	13/2534 (0.5%)
2	O	1.36	7/1860 (0.4%)	1.11	5/2534 (0.2%)
3	C	1.52	12/2197 (0.5%)	1.04	3/3005 (0.1%)
3	P	1.53	18/2197 (0.8%)	1.07	6/3005 (0.2%)
4	D	1.67	20/1229 (1.6%)	1.24	8/1658 (0.5%)
4	Q	1.27	3/1229 (0.2%)	1.06	3/1658 (0.2%)
5	E	1.51	6/860 (0.7%)	1.17	4/1167 (0.3%)
5	R	1.27	3/860 (0.3%)	0.99	0/1167
6	F	1.57	9/733 (1.2%)	1.23	4/996 (0.4%)
6	S	1.34	2/733 (0.3%)	1.17	3/996 (0.3%)
7	G	1.44	5/690 (0.7%)	1.23	2/937 (0.2%)
7	T	1.48	5/690 (0.7%)	1.29	6/937 (0.6%)
8	H	1.51	5/648 (0.8%)	1.09	2/877 (0.2%)
8	U	1.28	2/648 (0.3%)	1.03	1/877 (0.1%)
9	I	1.53	6/598 (1.0%)	1.20	5/792 (0.6%)
9	V	1.24	0/598	1.04	2/792 (0.3%)
10	J	1.33	1/462 (0.2%)	0.99	1/625 (0.2%)
10	W	1.26	1/462 (0.2%)	1.09	3/625 (0.5%)
11	K	1.48	2/398 (0.5%)	1.06	1/546 (0.2%)
11	X	1.15	0/398	0.98	1/546 (0.2%)
12	L	1.57	4/393 (1.0%)	1.16	2/526 (0.4%)
12	Y	1.40	3/393 (0.8%)	0.98	0/526
13	M	1.54	3/345 (0.9%)	1.12	2/470 (0.4%)
13	Z	1.20	1/345 (0.3%)	0.98	0/470
All	All	1.51	209/29138 (0.7%)	1.15	120/39622 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	S	0	1
All	All	0	2

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	60	CYS	CB-SG	10.42	2.00	1.82
3	P	29	SER	CB-OG	-9.66	1.29	1.42
4	D	39	ALA	CA-CB	8.57	1.70	1.52
1	N	139	ALA	CA-CB	8.38	1.70	1.52
7	G	36	TRP	CB-CG	8.16	1.65	1.50
9	I	66	ALA	CA-CB	8.16	1.69	1.52
1	A	379	TYR	CD1-CE1	7.91	1.51	1.39
3	P	58	TRP	CG-CD1	7.85	1.47	1.36
2	B	19	GLU	CB-CG	-7.77	1.37	1.52
13	M	16	ALA	CA-CB	7.66	1.68	1.52
1	N	394	VAL	CB-CG2	-7.63	1.36	1.52
8	H	60	TYR	CD2-CE2	7.63	1.50	1.39
1	A	372	TYR	CD1-CE1	7.51	1.50	1.39
3	P	161	GLN	CB-CG	-7.48	1.32	1.52
7	T	24	ALA	CA-CB	7.44	1.68	1.52
4	Q	81	VAL	CB-CG1	7.29	1.68	1.52
1	A	346	PHE	CD1-CE1	7.27	1.53	1.39
1	A	157	SER	CB-OG	7.22	1.51	1.42
6	F	4	GLY	N-CA	7.03	1.56	1.46
4	D	60	TYR	CD1-CE1	6.98	1.49	1.39
2	B	118	PHE	CE2-CZ	6.96	1.50	1.37
2	B	106	TRP	CE3-CZ3	6.96	1.50	1.38
12	L	35	ALA	CA-CB	6.95	1.67	1.52
1	N	288	TRP	CB-CG	6.95	1.62	1.50
6	S	54	ASN	CB-CG	-6.94	1.35	1.51
1	A	119	GLU	CG-CD	6.92	1.62	1.51
3	P	197	PHE	CE1-CZ	6.89	1.50	1.37
4	D	58	GLU	CD-OE2	6.85	1.33	1.25
3	P	174	THR	CB-CG2	6.84	1.75	1.52
1	A	379	TYR	CE2-CZ	6.80	1.47	1.38
4	D	19	ARG	CZ-NH2	6.77	1.41	1.33
9	I	46	ALA	CA-CB	6.77	1.66	1.52
1	N	473	TRP	CE3-CZ3	6.73	1.49	1.38
1	N	270	TYR	CD1-CE1	6.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	LYS	CE-NZ	6.62	1.65	1.49
1	N	235	PHE	CD2-CE2	6.58	1.52	1.39
1	A	83	VAL	CB-CG1	6.54	1.66	1.52
1	A	352	GLY	N-CA	6.54	1.55	1.46
3	P	240	TRP	CE3-CZ3	6.53	1.49	1.38
1	N	251	PHE	CE2-CZ	6.44	1.49	1.37
4	D	65	LYS	CE-NZ	6.42	1.65	1.49
4	D	30	VAL	CB-CG1	6.40	1.66	1.52
3	P	257	TYR	CD1-CE1	6.39	1.49	1.39
4	D	58	GLU	CG-CD	6.39	1.61	1.51
1	A	244	TYR	CD1-CE1	6.35	1.48	1.39
2	B	206	PHE	CE2-CZ	6.34	1.49	1.37
2	B	108	TYR	CG-CD1	6.33	1.47	1.39
1	N	475	ALA	CA-CB	6.33	1.65	1.52
3	P	184	ALA	CA-CB	6.32	1.65	1.52
7	T	5	LYS	CB-CG	6.30	1.69	1.52
3	P	181	TYR	CD2-CE2	6.29	1.48	1.39
1	N	320	VAL	CB-CG1	6.28	1.66	1.52
3	P	214	PHE	CD1-CE1	6.27	1.51	1.39
2	O	113	TYR	CD2-CE2	6.25	1.48	1.39
13	M	3	ALA	CA-CB	6.24	1.65	1.52
1	A	242	GLU	CG-CD	6.23	1.61	1.51
8	H	11	TYR	N-CA	6.19	1.58	1.46
1	N	188	VAL	CB-CG1	6.18	1.65	1.52
1	A	126	TRP	CZ3-CH2	6.15	1.49	1.40
5	E	14	ARG	CG-CD	6.12	1.67	1.51
1	N	507	GLU	CB-CG	6.12	1.63	1.52
1	A	440	TYR	CE1-CZ	6.12	1.46	1.38
4	D	12	ALA	CA-CB	6.11	1.65	1.52
1	A	219	PHE	CD2-CE2	6.08	1.51	1.39
4	D	70	GLU	CD-OE2	6.06	1.32	1.25
3	C	172	TYR	CD2-CE2	6.03	1.48	1.39
4	D	60	TYR	CE1-CZ	6.02	1.46	1.38
1	A	40	GLU	CB-CG	6.02	1.63	1.52
1	N	8	PHE	CD1-CE1	6.02	1.51	1.39
4	D	138	TRP	CE3-CZ3	6.01	1.48	1.38
9	I	47	TYR	CD1-CE1	6.01	1.48	1.39
2	B	18	GLU	CG-CD	6.00	1.60	1.51
1	A	244	TYR	CD2-CE2	6.00	1.48	1.39
1	A	258	VAL	CB-CG2	5.97	1.65	1.52
1	A	474	GLU	CD-OE1	5.96	1.32	1.25
2	B	115	ASP	CB-CG	5.93	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	11	TYR	CB-CG	5.92	1.60	1.51
2	O	60	GLU	CB-CG	5.92	1.63	1.52
3	C	240	TRP	CZ3-CH2	5.92	1.49	1.40
2	O	198	GLU	C-O	5.92	1.34	1.23
2	B	198	GLU	C-O	5.90	1.34	1.23
3	C	235	PHE	CE2-CZ	5.88	1.48	1.37
12	Y	32	GLY	N-CA	5.87	1.54	1.46
12	L	33	PHE	CE1-CZ	5.85	1.48	1.37
3	P	8	TYR	CD1-CE1	5.84	1.48	1.39
10	W	1	PHE	CE1-CZ	5.83	1.48	1.37
1	A	388	ALA	CA-CB	5.83	1.64	1.52
4	Q	121	LYS	CE-NZ	5.81	1.63	1.49
3	P	115	CYS	CB-SG	5.81	1.92	1.82
5	R	80	GLU	CG-CD	5.80	1.60	1.51
1	A	323	TRP	CG-CD1	5.78	1.44	1.36
5	E	27	TRP	CE3-CZ3	5.76	1.48	1.38
5	R	9	GLU	CG-CD	5.74	1.60	1.51
1	A	236	TRP	CB-CG	5.73	1.60	1.50
5	E	84	TYR	CE2-CZ	5.70	1.46	1.38
7	T	36	TRP	CB-CG	5.69	1.60	1.50
1	N	387	PHE	CE1-CZ	5.69	1.48	1.37
1	N	64	VAL	CA-CB	5.68	1.66	1.54
1	N	19	TYR	CD2-CE2	5.68	1.47	1.39
4	D	60	TYR	CD2-CE2	5.68	1.47	1.39
12	L	37	PHE	CD1-CE1	5.67	1.50	1.39
1	A	293	PHE	CE2-CZ	5.65	1.48	1.37
1	A	470	PHE	CD1-CE1	5.65	1.50	1.39
1	A	146	THR	CB-CG2	5.64	1.71	1.52
1	A	184	PHE	CE2-CZ	5.64	1.48	1.37
1	A	486	ASP	CB-CG	5.64	1.63	1.51
3	P	90	GLU	CB-CG	5.64	1.62	1.52
7	G	75	VAL	CB-CG1	5.62	1.64	1.52
1	A	474	GLU	CB-CG	5.62	1.62	1.52
12	Y	4	GLU	CG-CD	5.62	1.60	1.51
1	A	260	TYR	CD2-CE2	5.62	1.47	1.39
8	U	56	TYR	CD1-CE1	5.61	1.47	1.39
3	P	141	GLY	N-CA	5.61	1.54	1.46
1	A	403	TYR	CG-CD1	5.59	1.46	1.39
3	P	181	TYR	CD1-CE1	5.58	1.47	1.39
3	C	29	SER	CB-OG	-5.58	1.35	1.42
4	D	57	VAL	CB-CG1	5.57	1.64	1.52
1	A	387	PHE	CD2-CE2	5.56	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	LYS	CB-CG	5.56	1.67	1.52
3	P	253	TYR	CD1-CE1	5.55	1.47	1.39
9	I	47	TYR	CG-CD1	5.55	1.46	1.39
5	E	28	GLU	CG-CD	5.54	1.60	1.51
1	A	67	PHE	CD2-CE2	5.53	1.50	1.39
4	Q	104	TYR	CD2-CE2	5.53	1.47	1.39
2	B	192	TYR	CG-CD1	5.52	1.46	1.39
2	B	98	LYS	CD-CE	5.51	1.65	1.51
3	C	94	PHE	CG-CD2	5.51	1.47	1.38
1	A	320	VAL	CB-CG2	5.49	1.64	1.52
1	A	340	TRP	CE3-CZ3	5.47	1.47	1.38
2	B	193	TYR	CB-CG	5.47	1.59	1.51
1	A	235	PHE	N-CA	-5.46	1.35	1.46
1	A	505	PHE	CE1-CZ	5.46	1.47	1.37
2	B	138	VAL	CB-CG1	5.45	1.64	1.52
8	H	58	ARG	CZ-NH1	5.44	1.40	1.33
3	C	203	PHE	CB-CG	5.44	1.60	1.51
6	F	69	VAL	CB-CG1	5.42	1.64	1.52
3	C	116	TRP	CE3-CZ3	5.42	1.47	1.38
1	A	109	PHE	CD2-CE2	5.42	1.50	1.39
1	N	387	PHE	CB-CG	5.40	1.60	1.51
2	O	38	VAL	CB-CG2	5.40	1.64	1.52
2	O	151	ARG	CZ-NH1	5.40	1.40	1.33
1	A	224	GLY	N-CA	5.39	1.54	1.46
2	O	9	PHE	CD2-CE2	5.39	1.50	1.39
1	N	507	GLU	CG-CD	5.39	1.60	1.51
7	T	50	TYR	CD2-CE2	5.38	1.47	1.39
3	C	94	PHE	CD1-CE1	5.38	1.50	1.39
5	R	102	GLU	CG-CD	5.37	1.60	1.51
1	A	38	ARG	CD-NE	5.37	1.55	1.46
2	B	60	GLU	CB-CG	5.36	1.62	1.52
7	G	60	PHE	CE1-CZ	5.35	1.47	1.37
1	A	235	PHE	CD2-CE2	5.35	1.50	1.39
1	A	403	TYR	CE2-CZ	5.35	1.45	1.38
2	B	59	GLN	CG-CD	5.35	1.63	1.51
6	F	44	GLU	CG-CD	5.34	1.59	1.51
6	F	58	VAL	CB-CG2	5.32	1.64	1.52
7	T	16	TRP	CZ3-CH2	5.32	1.48	1.40
4	D	11	TYR	CD2-CE2	-5.32	1.31	1.39
8	H	14	ALA	CA-CB	5.32	1.63	1.52
1	N	78	PHE	CB-CG	-5.32	1.42	1.51
5	E	70	VAL	CB-CG2	5.31	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	104	TYR	CG-CD1	5.30	1.46	1.39
11	K	31	TYR	CD2-CE2	5.30	1.47	1.39
12	Y	9	LYS	CD-CE	5.30	1.64	1.51
1	A	393	PHE	CE1-CZ	5.28	1.47	1.37
2	B	108	TYR	CE1-CZ	5.27	1.45	1.38
13	M	4	LYS	CB-CG	-5.27	1.38	1.52
3	P	89	SER	CB-OG	5.27	1.49	1.42
6	F	73	TRP	CE3-CZ3	5.22	1.47	1.38
5	E	27	TRP	CB-CG	5.22	1.59	1.50
1	A	305	PHE	CD1-CE1	5.22	1.49	1.39
3	C	250	LEU	N-CA	5.22	1.56	1.46
1	A	304	TYR	CE1-CZ	5.21	1.45	1.38
2	O	19	GLU	CB-CG	-5.20	1.42	1.52
1	N	387	PHE	CD2-CE2	5.19	1.49	1.39
4	D	9	GLU	CG-CD	5.19	1.59	1.51
7	G	50	TYR	CG-CD1	5.18	1.45	1.39
3	C	89	SER	CB-OG	5.17	1.49	1.42
1	N	92	MET	CB-CG	5.17	1.67	1.51
13	Z	32	TRP	CB-CG	5.17	1.59	1.50
9	I	69	PHE	CB-CG	-5.16	1.42	1.51
12	L	4	GLU	CG-CD	5.14	1.59	1.51
1	A	458	SER	CA-CB	5.13	1.60	1.52
3	C	245	VAL	CB-CG2	5.13	1.63	1.52
1	A	400	PHE	CB-CG	5.13	1.60	1.51
1	N	473	TRP	CB-CG	5.12	1.59	1.50
1	N	128	VAL	CB-CG1	5.12	1.63	1.52
6	F	56	ARG	CG-CD	5.12	1.64	1.51
6	S	65	ASP	CB-CG	5.12	1.62	1.51
2	B	143	VAL	CB-CG2	5.11	1.63	1.52
6	F	89	TYR	CD2-CE2	5.11	1.47	1.39
8	U	56	TYR	CE1-CZ	5.11	1.45	1.38
10	J	20	VAL	CB-CG1	5.10	1.63	1.52
4	D	142	LYS	CD-CE	5.08	1.64	1.51
4	D	60	TYR	CG-CD1	5.06	1.45	1.39
4	D	81	VAL	CB-CG2	5.06	1.63	1.52
6	F	31	TYR	CE1-CZ	5.06	1.45	1.38
1	A	139	ALA	CA-CB	5.05	1.63	1.52
1	N	447	TYR	CD2-CE2	5.05	1.47	1.39
1	A	179	TYR	CE2-CZ	5.05	1.45	1.38
2	B	214	VAL	CB-CG1	5.04	1.63	1.52
1	N	354	THR	CB-CG2	5.03	1.69	1.52
3	P	238	ALA	CA-CB	5.02	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	99	TRP	CE3-CZ3	5.02	1.47	1.38
11	K	39	GLU	CB-CG	5.02	1.61	1.52
4	D	87	PHE	CD1-CE1	5.02	1.49	1.39
1	N	344	PHE	CD2-CE2	5.01	1.49	1.39
9	I	40	ALA	CA-CB	5.00	1.62	1.52
1	N	513	LEU	C-O	5.00	1.32	1.23
1	N	260	TYR	CE2-CZ	5.00	1.45	1.38

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	17	ARG	NE-CZ-NH2	-15.09	112.76	120.30
7	T	17	ARG	NE-CZ-NH2	-14.08	113.26	120.30
4	D	19	ARG	NE-CZ-NH1	-12.84	113.88	120.30
4	Q	20	ARG	NE-CZ-NH2	-12.82	113.89	120.30
5	E	90	ARG	NE-CZ-NH2	-12.63	113.99	120.30
5	E	90	ARG	NE-CZ-NH1	11.22	125.91	120.30
4	Q	20	ARG	NE-CZ-NH1	10.93	125.76	120.30
7	G	17	ARG	NE-CZ-NH1	10.44	125.52	120.30
4	D	20	ARG	NE-CZ-NH2	-10.38	115.11	120.30
4	Q	137	LYS	CD-CE-NZ	-10.32	87.96	111.70
1	A	208	MET	CG-SD-CE	9.93	116.09	100.20
2	B	188	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	486	ASP	CB-CG-OD1	9.38	126.75	118.30
1	N	213	ARG	NE-CZ-NH2	-9.31	115.64	120.30
7	T	17	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	N	5	ARG	NE-CZ-NH2	-8.61	116.00	120.30
4	D	21	ASP	CB-CG-OD2	8.55	125.99	118.30
1	N	369	ASP	CB-CG-OD2	8.54	125.98	118.30
1	N	312	ILE	CG1-CB-CG2	-8.34	93.05	111.40
7	T	33	LEU	CA-CB-CG	8.33	134.45	115.30
1	N	71	MET	CG-SD-CE	-8.16	87.14	100.20
2	B	158	ASP	CB-CG-OD1	8.14	125.63	118.30
2	B	82	ARG	NE-CZ-NH2	-7.71	116.44	120.30
11	X	54	ARG	NE-CZ-NH2	7.71	124.16	120.30
9	I	59	ASP	CB-CG-OD1	-7.67	111.39	118.30
2	B	188	ARG	NE-CZ-NH1	7.61	124.11	120.30
6	F	81	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	N	194	LEU	CB-CG-CD2	7.23	123.29	111.00
3	P	152	MET	CG-SD-CE	7.19	111.71	100.20
12	L	41	ARG	NE-CZ-NH1	7.19	123.89	120.30
5	E	66	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	310	MET	CG-SD-CE	-6.97	89.05	100.20
1	A	35	LEU	CA-CB-CG	-6.92	99.38	115.30
1	A	213	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	71	MET	CG-SD-CE	-6.77	89.36	100.20
1	A	298	ASP	CB-CG-OD1	-6.76	112.22	118.30
4	D	19	ARG	NE-CZ-NH2	6.71	123.66	120.30
6	S	54	ASN	CB-CA-C	-6.71	96.98	110.40
3	C	221	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A	212	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	486	ASP	CB-CG-OD2	-6.55	112.40	118.30
3	P	137	LEU	CB-CG-CD1	-6.53	99.91	111.00
2	O	227	LEU	CA-CB-CG	-6.52	100.31	115.30
6	F	18	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	65	TRP	CB-CA-C	6.45	123.29	110.40
9	V	10	ARG	NE-CZ-NH2	-6.41	117.09	120.30
11	K	54	ARG	NE-CZ-NH1	-6.41	117.09	120.30
2	O	82	ARG	NE-CZ-NH2	-6.41	117.10	120.30
2	B	45	MET	CG-SD-CE	6.40	110.44	100.20
1	N	384	GLY	N-CA-C	-6.38	97.15	113.10
10	W	50	LEU	CA-CB-CG	6.36	129.92	115.30
1	N	310	MET	CG-SD-CE	-6.35	90.04	100.20
6	S	94	HIS	N-CA-C	6.20	127.73	111.00
1	N	195	LEU	CB-CG-CD1	-6.16	100.54	111.00
1	A	19	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
7	T	8	HIS	N-CA-C	6.05	127.33	111.00
1	N	240	HIS	N-CA-CB	6.00	121.40	110.60
9	I	10	ARG	NE-CZ-NH1	5.99	123.30	120.30
3	P	223	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	N	117	MET	CG-SD-CE	5.94	109.70	100.20
1	N	369	ASP	CB-CG-OD1	-5.91	112.98	118.30
6	S	53	THR	CA-CB-CG2	5.88	120.63	112.40
2	B	173	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	N	50	ASP	CB-CG-OD2	5.77	123.49	118.30
10	J	28	ASP	CB-CG-OD1	5.76	123.48	118.30
10	W	28	ASP	CB-CG-OD1	5.74	123.47	118.30
2	O	11	ASP	CB-CG-OD2	5.72	123.45	118.30
8	H	76	ARG	NE-CZ-NH1	5.71	123.16	120.30
4	D	51	LEU	CA-CB-CG	5.71	128.43	115.30
1	N	113	LEU	CB-CG-CD1	5.68	120.67	111.00
2	B	11	ASP	CB-CG-OD2	5.67	123.40	118.30
1	N	278	MET	CA-CB-CG	-5.67	103.67	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	127	LEU	CB-CG-CD1	5.66	120.63	111.00
4	D	20	ARG	NE-CZ-NH1	5.63	123.11	120.30
4	D	59	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	N	277	MET	CA-CB-CG	-5.61	103.77	113.30
5	E	56	ARG	NE-CZ-NH1	-5.59	117.50	120.30
8	H	27	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	N	366	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	A	49	GLY	N-CA-C	-5.55	99.21	113.10
1	A	512	ASN	CB-CA-C	-5.55	99.30	110.40
9	I	10	ARG	NE-CZ-NH2	-5.55	117.53	120.30
4	D	19	ARG	CB-CA-C	-5.54	99.31	110.40
1	A	312	ILE	CA-CB-CG1	-5.51	100.52	111.00
7	T	7	ASP	N-CA-C	5.50	125.86	111.00
3	C	44	MET	CG-SD-CE	5.49	108.98	100.20
1	N	442	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	122	MET	CG-SD-CE	5.45	108.92	100.20
8	U	63	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	311	ILE	CG1-CB-CG2	-5.41	99.50	111.40
2	B	102	HIS	CB-CA-C	-5.41	99.59	110.40
6	F	93	PRO	C-N-CA	5.40	135.21	121.70
7	T	17	ARG	CB-CG-CD	-5.38	97.60	111.60
9	I	43	ARG	NE-CZ-NH1	-5.34	117.63	120.30
13	M	34	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	442	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	85	LEU	CB-CG-CD1	-5.32	101.96	111.00
9	V	59	ASP	CB-CG-OD2	5.31	123.08	118.30
9	I	59	ASP	CB-CG-OD2	5.25	123.02	118.30
13	M	28	LEU	CB-CG-CD2	5.23	119.89	111.00
3	P	132	LEU	CB-CG-CD1	-5.20	102.16	111.00
10	W	33	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	244	TYR	CA-CB-CG	-5.19	103.53	113.40
3	P	214	PHE	CB-CG-CD2	-5.19	117.16	120.80
3	C	112	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	A	189	MET	CA-CB-CG	-5.16	104.53	113.30
1	N	327	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	312	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	A	113	LEU	CB-CG-CD2	5.10	119.67	111.00
1	N	132	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	384	GLY	N-CA-C	-5.08	100.40	113.10
2	O	92	ASN	N-CA-C	5.07	124.68	111.00
2	B	119	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	227	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	65	ASP	CB-CG-OD2	5.04	122.84	118.30
12	L	21	LEU	CB-CG-CD1	5.04	119.57	111.00
2	B	198	GLU	OE1-CD-OE2	-5.01	117.28	123.30
2	O	158	ASP	CB-CG-OD1	5.00	122.81	118.30
1	A	278	MET	CA-CB-CG	-5.00	104.80	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	S	93	PRO	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	61	0
1	N	4027	0	4001	54	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	41	0
3	C	2110	0	2027	29	0
3	P	2110	0	2027	28	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	17	0
5	E	842	0	838	4	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	20	0
7	G	675	0	643	34	0
7	T	675	0	643	43	0
8	H	628	0	580	5	0
8	U	628	0	580	5	0
9	I	585	0	597	10	0
9	V	585	0	597	12	0
10	J	451	0	446	5	0
10	W	451	0	446	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	11	0
12	Y	380	0	380	13	0
13	M	335	0	352	2	0
13	Z	335	0	352	5	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	0	0
17	N	1	0	0	0	0
18	A	120	0	108	12	0
18	N	120	0	108	9	0
19	A	63	0	110	6	0
19	D	63	0	110	15	0
19	L	63	0	110	16	0
19	N	126	0	220	20	0
19	Q	63	0	110	5	0
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	8	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	18	0
22	O	52	0	80	12	0
23	B	29	0	37	1	0
23	C	58	0	71	5	0
23	J	29	0	36	3	0
23	O	29	0	36	2	0
23	P	58	0	71	6	0
23	W	29	0	36	4	0
24	C	33	0	37	5	0
24	M	33	0	39	1	0
24	P	33	0	40	2	0
24	Z	33	0	39	1	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	G	100	0	156	24	0
26	P	100	0	156	16	0
26	T	100	0	156	23	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	20	0
28	P	106	0	154	14	0
28	T	53	0	77	21	0
29	A	219	0	0	6	0
29	B	139	0	0	3	0
29	C	105	0	0	2	0
29	D	110	0	0	0	0
29	E	68	0	0	0	0
29	F	76	0	0	3	0
29	G	45	0	0	7	0
29	H	48	0	0	1	0
29	I	35	0	0	1	0
29	J	21	0	0	1	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	18	0	0	0	0
29	N	204	0	0	2	0
29	O	109	0	0	0	0
29	P	106	0	0	2	0
29	Q	67	0	0	3	0
29	R	52	0	0	0	0
29	S	69	0	0	4	0
29	T	48	0	0	4	0
29	U	38	0	0	3	0
29	V	19	0	0	0	0
29	W	16	0	0	0	0
29	X	16	0	0	0	0
29	Y	17	0	0	1	0
29	Z	14	0	0	0	0
All	All	32244	0	31064	577	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 9.

All (577) 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)
1:A:75:ILE:CG1	1:A:75:ILE:CD1	1.74	1.62
3:P:174:THR:CB	3:P:174:THR:CG2	1.74	1.60
28:G:265:PEK:H383	26:G:269:CDL:C27	1.62	1.29
28:P:1265:PEK:H383	26:T:1269:CDL:C27	1.64	1.25
7:T:2:SER:OG	28:T:263:PEK:H302	1.33	1.23
28:G:265:PEK:H383	26:G:269:CDL:H272	1.18	1.15
26:G:269:CDL:HA21	26:G:269:CDL:H112	1.26	1.10
15:A:520:PER:O1	15:A:520:PER:O2	1.70	1.10
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.07	1.09
7:T:84:LYS:H	7:T:84:LYS:HD2	1.13	1.07
15:N:520:PER:O2	15:N:520:PER:O1	1.70	1.07
28:P:1265:PEK:H383	26:T:1269:CDL:H271	1.22	1.06
7:G:84:LYS:HD2	7:G:84:LYS:H	1.19	1.06
22:B:230:PSC:C07	9:I:10:ARG:HH21	1.68	1.05
7:G:5:LYS:HG3	28:G:1263:PEK:H382	1.07	1.04
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.41	1.02
22:O:1230:PSC:H212	22:O:1230:PSC:O01	1.59	1.02
6:S:95:GLN:HB2	29:S:4411:HOH:O	1.60	1.01
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.40	1.00
6:F:85:CYS:SG	6:F:87:THR:HG23	2.00	1.00
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.25	0.99
9:V:65:LYS:O	11:X:54:ARG:NH1	1.94	0.98
19:N:1522:TGL:H231	19:N:1522:TGL:HA92	1.45	0.97
7:T:2:SER:OG	28:T:263:PEK:C30	2.10	0.97
28:P:1265:PEK:C38	26:T:1269:CDL:C27	2.42	0.96
7:T:5:LYS:CG	28:T:263:PEK:H383	1.94	0.96
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.81	0.95
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.48	0.95
1:A:486:ASP:OD2	4:D:19:ARG:HD3	1.66	0.95
7:T:5:LYS:HD2	28:T:263:PEK:H381	1.48	0.95
7:G:5:LYS:HB2	28:G:1263:PEK:H361	1.49	0.95
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.31	0.93
20:C:267:PGV:H182	26:C:270:CDL:H671	1.50	0.93
7:G:5:LYS:CG	28:G:1263:PEK:H382	1.97	0.92
7:T:5:LYS:HG3	28:T:263:PEK:H383	1.51	0.91
28:G:265:PEK:C38	26:G:269:CDL:C27	2.49	0.90
7:T:31:CYS:SG	26:T:1269:CDL:H551	2.12	0.90
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.54	0.90
20:A:524:PGV:H152	20:A:524:PGV:H321	1.52	0.89
6:S:52:ILE:O	6:S:94:HIS:CE1	2.26	0.89
7:T:2:SER:HG	28:T:263:PEK:H302	1.36	0.89
26:G:269:CDL:H241	26:G:269:CDL:H541	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:H	7:G:84:LYS:CD	1.82	0.88
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.09	0.88
22:O:1230:PSC:C07	9:V:10:ARG:HH21	1.86	0.87
4:D:34:SER:H	4:D:37:GLN:HE21	1.20	0.87
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.41	0.86
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.40	0.86
7:T:84:LYS:H	7:T:84:LYS:CD	1.89	0.86
7:G:84:LYS:N	7:G:84:LYS:HD2	1.91	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.83
7:G:76:ASN:HD21	28:G:264:PEK:HN2	1.23	0.81
22:B:230:PSC:H072	9:I:10:ARG:NH2	1.93	0.80
7:G:5:LYS:HG3	28:G:1263:PEK:C38	2.02	0.80
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.17	0.80
4:Q:109:HIS:HD2	29:Q:3152:HOH:O	1.62	0.80
3:P:25:LEU:O	3:P:29:SER:HB2	1.81	0.80
1:A:365:ILE:HD11	29:A:4260:HOH:O	1.80	0.80
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.17	0.80
18:N:516:HEA:HBC1	18:N:516:HEA:HMC1	1.65	0.79
7:T:5:LYS:HD2	28:T:263:PEK:C38	2.13	0.79
3:P:111:GLU:HG3	29:U:4543:HOH:O	1.83	0.79
2:B:41:ILE:HD13	22:B:230:PSC:C34	2.12	0.78
12:L:24:MET:HG3	29:L:4843:HOH:O	1.82	0.78
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.47	0.78
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.64	0.78
6:S:95:GLN:HE21	6:S:95:GLN:HA	1.50	0.77
20:P:1267:PGV:H182	26:P:1270:CDL:H671	1.65	0.76
19:N:1521:TGL:H142	2:O:39:LEU:CD2	2.15	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
22:B:230:PSC:C07	9:I:10:ARG:NH2	2.47	0.75
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.65	0.75
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.68	0.75
7:G:72:ASN:H	7:G:76:ASN:HD22	1.32	0.74
19:N:1521:TGL:H142	2:O:39:LEU:HD22	1.68	0.74
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.51	0.74
22:O:1230:PSC:H072	9:V:10:ARG:HH21	1.50	0.74
28:G:265:PEK:H383	26:G:269:CDL:H273	1.66	0.74
9:I:33:THR:HG22	29:I:4648:HOH:O	1.86	0.74
3:P:55:TYR:HE1	26:P:1270:CDL:H521	1.53	0.73
20:A:524:PGV:H152	20:A:524:PGV:C32	2.17	0.73
7:T:84:LYS:N	7:T:84:LYS:HD2	1.97	0.73
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CD	28:T:263:PEK:C38	2.67	0.72
2:O:226:MET:O	2:O:227:LEU:C	2.25	0.72
3:C:25:LEU:O	3:C:29:SER:HB2	1.90	0.72
10:W:33:ARG:HG2	23:W:1060:CHD:C15	2.18	0.72
3:P:55:TYR:CE1	26:P:1270:CDL:H521	2.25	0.72
6:F:94:HIS:CE1	29:F:4660:HOH:O	2.42	0.71
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.55	0.71
6:S:94:HIS:CD2	6:S:95:GLN:H	2.07	0.71
2:B:41:ILE:HD13	22:B:230:PSC:H341	1.71	0.71
7:G:45:PRO:HD2	29:G:4665:HOH:O	1.90	0.71
6:S:52:ILE:O	6:S:94:HIS:HE1	1.70	0.71
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.31	0.71
26:T:1269:CDL:H571	26:T:1269:CDL:H782	1.72	0.71
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.73	0.70
26:P:1270:CDL:OB9	26:P:1270:CDL:H522	1.92	0.70
19:N:1522:TGL:H231	19:N:1522:TGL:CA9	2.11	0.70
7:T:5:LYS:HB2	28:T:263:PEK:H362	1.74	0.70
28:G:265:PEK:C38	26:G:269:CDL:H272	2.11	0.70
28:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.38	0.69
19:Q:1523:TGL:CC2	19:Q:1523:TGL:HG11	2.22	0.69
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.75	0.69
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.57	0.69
6:S:22:LEU:O	6:S:25:ARG:HB3	1.92	0.68
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.75	0.68
28:G:264:PEK:H161	28:G:264:PEK:H101	1.76	0.68
28:G:265:PEK:C38	26:G:269:CDL:H273	2.22	0.68
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.75	0.68
2:B:164:ALA:O	2:B:194:GLY:HA3	1.94	0.68
28:P:1265:PEK:C38	26:T:1269:CDL:H273	2.24	0.68
1:N:365:ILE:HD11	29:N:4837:HOH:O	1.94	0.68
4:D:34:SER:H	4:D:37:GLN:NE2	1.92	0.67
2:B:58:ALA:O	2:B:62:GLU:HG3	1.94	0.67
6:S:85:CYS:SG	6:S:87:THR:HG23	2.35	0.67
3:C:224:LYS:HE3	26:C:270:CDL:HB31	1.76	0.67
13:Z:42:LYS:HE3	13:Z:42:LYS:HA	1.76	0.67
9:V:61:GLU:HG3	9:V:64:ARG:HH21	1.60	0.66
7:T:5:LYS:CD	28:T:263:PEK:H381	2.25	0.66
6:F:94:HIS:HE1	29:F:4660:HOH:O	1.76	0.65
1:N:172:LYS:NZ	1:N:178:GLN:HE22	1.95	0.65
3:P:246:ASP:HB2	29:P:4199:HOH:O	1.96	0.65
4:D:78:TRP:HB3	19:D:523:TGL:CB2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:72:ASN:H	7:T:76:ASN:ND2	1.94	0.65
26:G:269:CDL:C54	26:G:269:CDL:H241	2.27	0.64
7:T:5:LYS:CG	28:T:263:PEK:C38	2.75	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.97	0.64
26:T:1269:CDL:C11	26:T:1269:CDL:HA21	2.27	0.64
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.78	0.64
29:B:2351:HOH:O	19:D:523:TGL:HC61	1.98	0.64
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.27	0.64
2:O:141:ARG:H	9:V:70:GLN:HE22	1.46	0.64
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.30	0.64
7:T:17:ARG:HD3	29:T:3300:HOH:O	1.98	0.64
26:G:269:CDL:C11	26:G:269:CDL:HA21	2.15	0.64
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.79	0.63
3:P:174:THR:CG2	3:P:174:THR:CA	2.70	0.63
4:Q:70:GLU:O	4:Q:73:ARG:HG2	1.98	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.97	0.63
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.62	0.63
7:G:37:LEU:HD21	26:G:269:CDL:H352	1.81	0.63
26:G:269:CDL:C24	26:G:269:CDL:H541	2.29	0.62
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.64	0.62
1:N:362:SER:HA	2:O:87:MET:HE1	1.82	0.62
2:O:116:LEU:HD12	2:O:117:SER:N	2.15	0.62
20:C:267:PGV:H172	26:C:270:CDL:H652	1.81	0.62
7:G:17:ARG:HD2	29:G:2300:HOH:O	1.98	0.62
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.88	0.62
2:B:68:LEU:HG	29:B:4723:HOH:O	1.99	0.61
7:T:17:ARG:CD	29:T:3300:HOH:O	2.47	0.61
7:G:3:ALA:O	7:G:4:ALA:CB	2.48	0.61
24:C:272:DMU:O1	24:C:272:DMU:H29	2.01	0.61
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.81	0.61
1:N:177:SER:H	1:N:180:GLN:NE2	1.98	0.61
3:C:3:HIS:HE1	6:F:96:LEU:CD2	2.14	0.61
20:N:1524:PGV:H011	20:N:1524:PGV:H22	1.83	0.60
2:B:62:GLU:O	2:B:66:THR:HB	2.01	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.83	0.60
19:Q:1523:TGL:HA91	19:Q:1523:TGL:H242	1.84	0.60
1:A:278:MET:SD	7:T:5:LYS:HB3	2.42	0.60
1:A:21:LEU:HD23	19:L:522:TGL:H211	1.83	0.60
18:N:515:HEA:H272	18:N:515:HEA:C16	2.32	0.60
6:S:94:HIS:CD2	6:S:95:GLN:N	2.70	0.60
20:N:1524:PGV:H011	20:N:1524:PGV:C2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HB2	28:T:263:PEK:C36	2.32	0.59
1:N:177:SER:H	1:N:180:GLN:HE21	1.50	0.59
7:G:31:CYS:SG	26:G:269:CDL:H532	2.42	0.59
2:B:59:GLN:O	2:B:60:GLU:HG3	2.03	0.59
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.17	0.59
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.50	0.59
20:A:524:PGV:H31	20:A:524:PGV:H232	1.83	0.59
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.01	0.59
26:G:269:CDL:H201	1:N:311:ILE:CD1	2.32	0.59
1:A:75:ILE:CD1	1:A:75:ILE:CB	2.76	0.59
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.83	0.59
9:V:55:ASP:OD2	9:V:58:LYS:HB2	2.03	0.59
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.85	0.58
23:C:525:CHD:H42	3:P:127:LEU:HD21	1.84	0.58
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.01	0.58
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.58
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.04	0.58
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.85	0.57
26:G:269:CDL:H473	29:G:4638:HOH:O	2.03	0.57
22:O:1230:PSC:C02	22:O:1230:PSC:H212	2.34	0.57
7:T:31:CYS:SG	26:T:1269:CDL:C55	2.90	0.57
4:D:107:ILE:HB	4:D:108:PRO:CD	2.35	0.57
7:T:38:HIS:HE2	26:T:1269:CDL:H111	1.69	0.57
2:B:59:GLN:C	2:B:60:GLU:HG3	2.26	0.57
3:P:226:HIS:HE1	26:P:1270:CDL:HB32	1.70	0.56
28:P:1265:PEK:C38	26:T:1269:CDL:H271	2.15	0.56
22:O:1230:PSC:H071	9:V:10:ARG:HH21	1.69	0.56
10:W:52:TRP:O	10:W:57:HIS:HE1	1.88	0.56
1:A:28:MET:CE	18:A:515:HEA:H271	2.36	0.56
6:S:19:GLU:HG2	29:S:4904:HOH:O	2.06	0.56
7:T:84:LYS:N	7:T:84:LYS:CD	2.64	0.56
19:D:523:TGL:H242	19:D:523:TGL:HA91	1.87	0.55
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.71	0.55
2:B:56:MET:HA	22:B:230:PSC:H202	1.87	0.55
18:N:515:HEA:H122	18:N:515:HEA:HHC	1.87	0.55
3:C:67:PHE:CE1	26:C:270:CDL:H1	2.31	0.55
4:D:78:TRP:N	19:D:523:TGL:HB21	2.21	0.55
24:C:272:DMU:H40	7:G:63:GLY:H	1.70	0.55
22:B:230:PSC:O01	22:B:230:PSC:H212	2.06	0.55
12:Y:35:ALA:O	12:Y:39:ILE:HG13	2.07	0.55
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HE3	29:A:2385:HOH:O	2.06	0.55
8:H:45:ALA:O	8:H:47:GLY:N	2.34	0.55
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.42	0.54
7:G:21:PHE:CD2	28:G:265:PEK:H222	2.42	0.54
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.20	0.54
6:F:64:GLU:O	6:F:65:ASP:HB2	2.07	0.54
4:D:118:LYS:HB3	11:K:53:TRP:HB3	1.90	0.54
19:N:1522:TGL:HC62	19:N:1522:TGL:HC22	1.89	0.54
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.73	0.54
1:N:488:THR:HB	1:N:495:LEU:HD13	1.90	0.54
19:A:521:TGL:C36	29:A:4497:HOH:O	2.56	0.54
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.90	0.53
26:G:269:CDL:OA7	26:G:269:CDL:H342	2.08	0.53
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.06	0.53
4:D:78:TRP:CA	19:D:523:TGL:HB21	2.38	0.53
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.73	0.53
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.39	0.53
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.90	0.53
3:C:3:HIS:HB2	29:C:4631:HOH:O	2.09	0.53
20:A:522:PGV:H171	28:G:264:PEK:H352	1.89	0.53
3:P:34:TRP:HE1	24:P:1272:DMU:H29	1.74	0.53
7:T:2:SER:O	28:T:263:PEK:H332	2.09	0.53
2:O:82:ARG:HH11	2:O:86:MET:CE	2.22	0.52
1:A:407:ASP:O	1:A:411:LYS:HG3	2.10	0.52
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.52
5:R:7:THR:OG1	5:R:10:GLU:HG3	2.08	0.52
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.43	0.52
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.92	0.52
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.73	0.52
3:P:226:HIS:CE1	26:P:1270:CDL:HB32	2.45	0.52
7:T:5:LYS:HB2	28:T:263:PEK:C37	2.39	0.52
19:N:1522:TGL:HC62	19:N:1522:TGL:CC2	2.40	0.52
18:N:515:HEA:C27	18:N:515:HEA:C16	2.88	0.51
26:P:1270:CDL:H262	26:P:1270:CDL:H672	1.91	0.51
26:G:269:CDL:H201	1:N:311:ILE:HD12	1.92	0.51
12:L:14:SER:H	19:L:522:TGL:HC31	1.74	0.51
19:A:521:TGL:H361	29:A:4497:HOH:O	2.10	0.51
26:C:270:CDL:H711	26:C:270:CDL:H121	1.91	0.51
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.91	0.51
18:N:515:HEA:CB	18:N:515:HEA:HMC1	2.33	0.51
1:N:76:GLY:O	1:N:80:ASN:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LEU:HB2	2:B:69:PRO:HD3	1.92	0.51
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.51
1:A:290:HIS:HD2	1:A:291:HIS:CD2	2.28	0.51
1:A:449:MET:SD	2:B:5:MET:HG2	2.50	0.51
10:J:7:GLU:HG3	29:J:4578:HOH:O	2.11	0.51
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.75	0.51
2:O:82:ARG:HG2	2:O:86:MET:CE	2.39	0.51
29:B:2351:HOH:O	19:D:523:TGL:CC6	2.55	0.51
1:N:449:MET:SD	2:O:5:MET:HG2	2.50	0.51
11:X:7:PRO:O	11:X:12:LYS:HE3	2.10	0.50
19:N:1522:TGL:HA22	12:Y:13:PHE:HB3	1.93	0.50
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.93	0.50
10:W:30:ILE:O	10:W:34:VAL:HG23	2.11	0.50
22:B:230:PSC:C13	22:B:230:PSC:H343	2.41	0.50
2:O:84:LEU:HA	2:O:87:MET:HE2	1.93	0.50
19:N:1521:TGL:H142	2:O:39:LEU:HD23	1.94	0.50
8:U:78:GLU:HG2	8:U:80:THR:HG23	1.93	0.50
12:Y:2:HIS:N	29:Y:4284:HOH:O	2.45	0.50
19:N:1521:TGL:HA52	2:O:32:PHE:CE2	2.46	0.50
10:W:16:ASN:OD1	10:W:23:LYS:HE3	2.11	0.50
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.47	0.50
1:N:513:LEU:O	1:N:514:LYS:HB2	2.12	0.50
20:N:1524:PGV:O11	20:N:1524:PGV:H061	2.12	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.59	0.49
12:Y:14:SER:O	12:Y:20:ARG:NH2	2.44	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.13	0.49
2:O:41:ILE:O	2:O:45:MET:HG2	2.12	0.49
20:A:524:PGV:H141	20:A:524:PGV:H301	1.94	0.49
19:N:1521:TGL:HC72	29:Q:4417:HOH:O	2.11	0.49
7:T:7:ASP:O	7:T:9:GLY:N	2.46	0.49
19:L:522:TGL:C23	19:L:522:TGL:HA92	2.43	0.49
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.94	0.49
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.21	0.49
10:J:37:THR:OG1	23:J:60:CHD:H7	2.12	0.49
19:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.95	0.49
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.48	0.49
19:D:523:TGL:H351	9:I:16:ARG:HH21	1.77	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.12	0.49
3:P:47:LEU:O	3:P:51:MET:HG2	2.13	0.49
23:O:229:CHD:H212	23:O:229:CHD:H12	1.94	0.49
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	2.13	0.49
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.94	0.48
24:C:272:DMU:H1	7:G:69:PHE:HZ	1.78	0.48
7:G:30:LEU:HB3	26:G:269:CDL:H531	1.94	0.48
7:T:17:ARG:HD2	29:T:3300:HOH:O	2.12	0.48
12:L:24:MET:SD	19:L:522:TGL:H161	2.54	0.48
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.14	0.48
10:W:33:ARG:HG2	23:W:1060:CHD:H151	1.95	0.48
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.48
26:G:269:CDL:H401	2:O:77:ALA:CB	2.44	0.48
26:C:270:CDL:H861	26:C:270:CDL:H831	1.50	0.48
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.46	0.48
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.45	0.48
18:A:516:HEA:HMC1	18:A:516:HEA:HBC1	1.96	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.48
26:G:269:CDL:H371	2:O:81:LEU:HD12	1.96	0.48
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.13	0.48
22:B:230:PSC:H071	5:E:8:ASP:HA	1.96	0.48
18:N:515:HEA:H122	18:N:515:HEA:H262	1.94	0.48
2:O:59:GLN:O	2:O:59:GLN:HG3	2.13	0.48
1:A:311:ILE:HD12	26:T:1269:CDL:H191	1.95	0.48
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.96	0.47
1:N:514:LYS:HE2	29:S:3330:HOH:O	2.13	0.47
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.49	0.47
7:G:10:GLY:HA3	29:G:4761:HOH:O	2.14	0.47
28:G:264:PEK:C10	28:G:264:PEK:H161	2.43	0.47
6:S:53:THR:HG22	6:S:54:ASN:H	1.78	0.47
23:W:1060:CHD:H12A	23:W:1060:CHD:H112	1.63	0.47
1:A:346:PHE:HZ	19:A:521:TGL:H122	1.79	0.47
6:F:55:LYS:HA	6:F:74:LEU:O	2.14	0.47
1:N:377:PHE:CE2	1:N:378:HIS:CE1	3.02	0.47
22:B:230:PSC:H073	5:E:11:PHE:CG	2.50	0.47
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.96	0.47
24:P:1272:DMU:H25	28:P:1264:PEK:H341	1.97	0.47
8:H:46:LYS:CE	29:H:4804:HOH:O	2.62	0.47
3:C:47:LEU:O	3:C:51:MET:HG2	2.15	0.47
2:O:62:GLU:O	2:O:66:THR:HB	2.15	0.47
7:T:5:LYS:CD	28:T:263:PEK:H383	2.35	0.47
19:N:1522:TGL:H251	19:N:1522:TGL:H282	1.54	0.47
2:O:100:MET:HB2	2:O:107:SER:OG	2.15	0.47
26:P:1270:CDL:H532	26:P:1270:CDL:H561	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.42	0.47
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.97	0.47
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.44	0.47
20:A:524:PGV:H262	20:A:524:PGV:H71	1.97	0.47
20:C:268:PGV:H062	29:C:4909:HOH:O	2.15	0.47
4:D:12:ALA:CB	6:F:55:LYS:HE3	2.45	0.47
28:G:1263:PEK:H331	28:G:1263:PEK:H372	1.96	0.47
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.38	0.47
26:T:1269:CDL:H761	26:T:1269:CDL:H242	1.97	0.47
3:C:3:HIS:CE1	6:F:96:LEU:CD2	2.97	0.46
20:N:1266:PGV:H181	28:P:1264:PEK:H321	1.96	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.14	0.46
2:O:82:ARG:NH1	2:O:86:MET:HE3	2.30	0.46
7:T:5:LYS:CB	28:T:263:PEK:H383	2.44	0.46
26:G:269:CDL:H332	2:O:78:LEU:HD12	1.97	0.46
2:O:37:LEU:O	2:O:41:ILE:HG13	2.15	0.46
5:R:80:GLU:CD	5:R:80:GLU:H	2.18	0.46
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.29	0.46
23:B:1086:CHD:H12A	23:B:1086:CHD:H112	1.59	0.46
3:C:52:LEU:HD23	26:C:270:CDL:H362	1.97	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.46
19:D:523:TGL:H122	19:D:523:TGL:HB81	1.97	0.46
26:G:269:CDL:H511	26:G:269:CDL:H181	1.97	0.46
18:N:515:HEA:CMC	18:N:515:HEA:HBC1	2.29	0.46
20:P:1268:PGV:H21	20:P:1268:PGV:H51	1.71	0.46
1:A:264:LYS:NZ	29:A:4192:HOH:O	2.48	0.46
26:C:270:CDL:H412	26:C:270:CDL:H382	1.60	0.46
4:D:78:TRP:CA	19:D:523:TGL:CB2	2.93	0.46
3:C:202:GLY:HA3	28:G:264:PEK:H21	1.98	0.46
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.96	0.46
1:N:28:MET:CE	18:N:515:HEA:H271	2.45	0.46
12:L:45:LEU:HA	12:L:45:LEU:HD23	1.77	0.46
3:P:155:ASP:OD1	3:P:155:ASP:C	2.54	0.46
2:B:68:LEU:CB	2:B:69:PRO:HD3	2.46	0.46
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.45	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.97	0.46
28:P:1264:PEK:H383	28:P:1264:PEK:H352	1.37	0.46
26:P:1270:CDL:H822	26:P:1270:CDL:H852	1.64	0.46
7:T:8:HIS:CD2	28:T:263:PEK:H232	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:HE2	18:A:515:HEA:H271	1.98	0.46
28:G:264:PEK:C7	28:G:264:PEK:H32	2.46	0.46
1:N:87:ILE:O	1:N:173:PRO:HD3	2.16	0.46
6:S:94:HIS:HD2	6:S:95:GLN:H	1.58	0.46
7:G:8:HIS:ND1	28:G:1263:PEK:H312	2.30	0.46
23:J:60:CHD:H12A	23:J:60:CHD:H112	1.61	0.46
6:S:94:HIS:HA	29:S:4898:HOH:O	2.16	0.46
28:T:263:PEK:H361	28:T:263:PEK:H332	1.68	0.46
10:J:27:THR:O	10:J:27:THR:HG22	2.16	0.45
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.46	0.45
1:A:218:THR:O	1:A:226:GLY:HA3	2.16	0.45
22:B:230:PSC:H073	5:E:11:PHE:CB	2.46	0.45
20:P:1268:PGV:H062	29:P:4599:HOH:O	2.15	0.45
2:B:41:ILE:CD1	22:B:230:PSC:H341	2.43	0.45
3:C:224:LYS:CD	26:C:270:CDL:HB32	2.46	0.45
4:D:98:TRP:CE2	24:M:526:DMU:H9	2.51	0.45
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.52	0.45
22:O:1230:PSC:C07	9:V:10:ARG:NH2	2.68	0.45
22:O:1230:PSC:C21	22:O:1230:PSC:O01	2.47	0.45
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.44	0.45
12:Y:22:LEU:O	12:Y:26:THR:HB	2.16	0.45
8:H:44:THR:O	8:H:45:ALA:O	2.35	0.45
1:A:172:LYS:NZ	1:A:178:GLN:NE2	2.64	0.45
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.52	0.45
1:A:177:SER:H	1:A:180:GLN:HE21	1.63	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.32	0.45
19:L:522:TGL:H252	19:L:522:TGL:H283	1.62	0.45
1:N:378:HIS:CG	1:N:425:PHE:CE2	3.05	0.45
5:R:63:SER:O	5:R:67:ILE:HG13	2.17	0.45
26:P:1270:CDL:H791	26:P:1270:CDL:H231	1.99	0.45
9:V:61:GLU:CG	9:V:64:ARG:HH21	2.26	0.45
19:N:1521:TGL:HA52	2:O:32:PHE:HE2	1.82	0.45
13:Z:32:TRP:N	24:Z:1526:DMU:H1	2.32	0.45
22:B:230:PSC:H212	22:B:230:PSC:C1	2.47	0.45
3:C:34:TRP:CD1	3:C:40:MET:HG3	2.52	0.45
7:G:8:HIS:CE1	28:G:1263:PEK:H342	2.52	0.45
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.97	0.45
2:O:31:VAL:O	2:O:35:SER:OG	2.34	0.45
6:S:94:HIS:CG	6:S:95:GLN:H	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:271:CHD:H212	23:C:271:CHD:H12	1.99	0.44
7:G:17:ARG:CD	29:G:2300:HOH:O	2.63	0.44
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.44
2:B:52:HIS:CE1	22:B:230:PSC:H211	2.52	0.44
7:G:12:GLY:HA3	29:G:2267:HOH:O	2.16	0.44
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.41	0.44
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.00	0.44
20:P:1267:PGV:H12	20:P:1267:PGV:H152	1.44	0.44
8:U:37:HIS:HD2	29:U:3142:HOH:O	2.00	0.44
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.52	0.44
20:A:522:PGV:H261	20:C:267:PGV:H292	1.98	0.44
1:A:71:MET:N	1:A:72:PRO:CD	2.81	0.44
4:D:78:TRP:HA	19:D:523:TGL:HB21	2.00	0.44
22:B:230:PSC:H071	9:I:10:ARG:NH2	2.31	0.44
10:J:52:TRP:O	10:J:57:HIS:HE1	2.01	0.44
1:N:312:ILE:HG21	1:N:312:ILE:HD13	1.61	0.44
2:O:82:ARG:HH11	2:O:86:MET:HE3	1.82	0.44
19:A:521:TGL:HA82	19:A:521:TGL:H222	2.00	0.44
13:M:17:ILE:O	13:M:21:VAL:HG23	2.16	0.44
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.98	0.44
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.18	0.44
2:B:65:TRP:CZ3	22:B:230:PSC:H322	2.53	0.44
19:N:1522:TGL:HC62	19:N:1522:TGL:HC32	1.79	0.44
2:O:59:GLN:O	2:O:59:GLN:CG	2.65	0.44
7:T:12:GLY:HA3	29:T:3267:HOH:O	2.17	0.44
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.82	0.44
19:D:523:TGL:HB42	19:D:523:TGL:HA32	2.00	0.44
1:A:87:ILE:HG13	1:A:89:ALA:HB2	1.99	0.44
3:C:179:SER:O	3:C:183:GLU:HG2	2.17	0.44
12:L:25:MET:HG2	19:L:522:TGL:HA62	2.00	0.44
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.82	0.44
4:Q:109:HIS:CD2	29:Q:3152:HOH:O	2.49	0.44
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.52	0.44
20:A:524:PGV:H232	20:A:524:PGV:H202	1.79	0.43
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.57	0.43
2:O:102:HIS:O	2:O:104:TRP:HA	2.17	0.43
6:S:94:HIS:HD2	6:S:95:GLN:N	2.12	0.43
6:F:55:LYS:HG3	6:F:73:TRP:CZ3	2.53	0.43
9:I:73:LYS:HD2	9:I:73:LYS:HA	1.73	0.43
28:P:1264:PEK:H262	28:P:1264:PEK:H231	1.80	0.43
23:P:1525:CHD:H12	23:P:1525:CHD:H212	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:H562	26:T:1269:CDL:H762	1.99	0.43
26:T:1269:CDL:H561	26:T:1269:CDL:H591	1.75	0.43
3:C:210:ILE:HD13	20:C:267:PGV:H301	2.00	0.43
3:C:210:ILE:HG12	20:C:267:PGV:H12	2.00	0.43
1:N:508:PRO:HG3	3:P:6:HIS:HB3	2.00	0.43
7:T:8:HIS:ND1	28:T:263:PEK:H321	2.33	0.43
12:Y:41:ARG:HH11	12:Y:41:ARG:HG2	1.82	0.43
13:Z:36:HIS:O	13:Z:39:ASN:HB2	2.18	0.43
19:A:521:TGL:HA91	19:A:521:TGL:H241	1.99	0.43
23:P:1525:CHD:H152	20:P:1268:PGV:H92	2.01	0.43
9:V:29:LEU:HD12	9:V:29:LEU:HA	1.54	0.43
24:C:272:DMU:C10	24:C:272:DMU:H29	2.49	0.43
1:N:155:VAL:CG2	28:P:1264:PEK:H381	2.48	0.43
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.18	0.43
8:U:57:ARG:O	8:U:61:LYS:HG3	2.18	0.43
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
1:N:199:LEU:N	1:N:200:PRO:CD	2.82	0.43
28:P:1265:PEK:H383	26:T:1269:CDL:H272	1.80	0.43
2:B:13:THR:HG22	2:B:13:THR:O	2.19	0.43
3:P:224:LYS:HD3	26:P:1270:CDL:HB31	2.01	0.43
2:B:200:CYS:SG	2:B:204:HIS:HA	2.59	0.43
22:O:1230:PSC:H201	22:O:1230:PSC:H231	1.70	0.43
23:P:1525:CHD:H12A	23:P:1525:CHD:H112	1.74	0.43
28:T:263:PEK:H271	28:T:263:PEK:H241	1.84	0.43
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.72	0.43
19:N:1521:TGL:C28	19:N:1521:TGL:H101	2.49	0.43
26:T:1269:CDL:H252	26:T:1269:CDL:H221	1.48	0.43
26:T:1269:CDL:OA7	26:T:1269:CDL:H342	2.19	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.43
1:A:309:THR:HG22	18:A:516:HEA:HMB2	2.01	0.42
3:P:29:SER:HB3	3:P:42:LEU:HD13	2.01	0.42
7:T:8:HIS:HB2	28:T:263:PEK:H282	2.01	0.42
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.18	0.42
1:A:112:LEU:HG	29:A:4496:HOH:O	2.19	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
1:A:169:ILE:HG23	7:T:9:GLY:HA3	2.01	0.42
26:G:269:CDL:H661	26:G:269:CDL:H631	1.64	0.42
1:N:240:HIS:O	1:N:241:PRO:C	2.58	0.42
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.01	0.42
28:P:1265:PEK:H311	28:P:1265:PEK:H282	1.91	0.42
10:J:40:LEU:HD12	23:J:60:CHD:H183	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1521:TGL:H241	19:N:1521:TGL:H211	1.78	0.42
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.63	0.42
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.19	0.42
1:N:430:PHE:HE1	19:N:1521:TGL:HB21	1.83	0.42
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.19	0.42
1:A:250:GLY:O	1:A:254:ILE:HG12	2.20	0.42
1:A:486:ASP:OD2	4:D:19:ARG:CD	2.51	0.42
1:A:22:PHE:HA	19:L:522:TGL:HB71	2.02	0.42
3:C:19:THR:O	3:C:23:SER:HB3	2.20	0.42
1:N:426:PHE:HB3	1:N:427:PRO:HD3	2.02	0.42
19:A:521:TGL:H121	19:A:521:TGL:H292	1.26	0.42
4:Q:43:LYS:NZ	4:Q:55:GLU:OE1	2.42	0.42
12:Y:41:ARG:HG2	12:Y:41:ARG:NH1	2.34	0.42
1:A:381:LEU:CD2	18:A:516:HEA:HBC2	2.50	0.41
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.02	0.41
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.02	0.41
19:N:1522:TGL:H352	29:N:4536:HOH:O	2.19	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.41
10:W:50:LEU:HD22	10:W:54:SER:HG	1.84	0.41
18:A:515:HEA:H172	18:A:515:HEA:H261	1.78	0.41
1:N:236:TRP:CE3	1:N:236:TRP:HA	2.55	0.41
3:P:171:VAL:HG22	26:P:1270:CDL:H841	2.02	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.20	0.41
11:X:16:ALA:O	11:X:20:SER:HB2	2.20	0.41
2:B:64:ILE:HA	2:B:64:ILE:HD13	1.95	0.41
26:C:270:CDL:H231	26:C:270:CDL:H642	2.02	0.41
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.82	0.41
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.68	0.41
5:R:26:ALA:O	5:R:30:ARG:HG3	2.21	0.41
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.03	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.55	0.41
6:F:87:THR:HG21	29:F:4882:HOH:O	2.19	0.41
3:P:220:PHE:CB	26:P:1270:CDL:H712	2.51	0.41
1:A:311:ILE:CD1	26:T:1269:CDL:H191	2.51	0.41
1:A:314:ILE:HB	1:A:315:PRO:CD	2.51	0.41
1:A:396:TRP:O	1:A:397:PHE:C	2.58	0.41
1:A:513:LEU:O	1:A:513:LEU:HD13	2.21	0.41
2:B:121:TYR:O	2:B:138:VAL:HA	2.20	0.41
3:C:156:ARG:HE	23:C:271:CHD:C24	2.34	0.41
5:E:72:LYS:HB2	5:E:82:TYR:CD2	2.56	0.41
1:N:51:ASP:OD2	2:O:205:SER:OG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:H071	9:V:10:ARG:NH2	2.33	0.41
1:A:381:LEU:HD13	18:A:515:HEA:HAC	2.03	0.41
18:A:516:HEA:HMB1	18:A:516:HEA:H11	1.88	0.41
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.84	0.41
3:C:3:HIS:HE1	6:F:96:LEU:HD21	1.85	0.41
19:D:523:TGL:HC21	19:D:523:TGL:HG12	2.03	0.41
7:G:12:GLY:CA	29:G:2267:HOH:O	2.69	0.41
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.86	0.41
1:A:400:PHE:HB3	19:L:522:TGL:H283	2.03	0.41
1:A:409:TRP:HA	1:A:412:ILE:HD12	2.03	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.41
2:B:146:MET:HA	2:B:213:LEU:HD12	2.03	0.41
1:N:365:ILE:HD11	29:U:4796:HOH:O	2.19	0.41
5:R:105:GLY:O	5:R:108:LYS:HG2	2.20	0.41
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.95	0.40
2:O:139:ASP:OD2	2:O:140:ASN:N	2.53	0.40
23:P:1271:CHD:H162	23:P:1271:CHD:H232	2.03	0.40
3:P:224:LYS:CD	26:P:1270:CDL:HB31	2.51	0.40
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.88	0.40
3:P:127:LEU:HG	26:T:1269:CDL:OB3	2.20	0.40
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.03	0.40
4:D:19:ARG:NH1	4:D:21:ASP:OD2	2.54	0.40
24:C:272:DMU:C11	7:G:63:GLY:H	2.34	0.40
4:Q:37:GLN:O	4:Q:41:LYS:HG2	2.22	0.40
28:P:1265:PEK:C37	26:T:1269:CDL:C27	2.99	0.40
8:U:38:ARG:HG2	8:U:85:ILE:HA	2.04	0.40
1:A:398:PRO:HA	1:A:403:TYR:O	2.20	0.40
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.03	0.40
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.03	0.40
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.40
3:C:106:LEU:HD21	3:C:259:TRP:CZ2	2.57	0.40
1:N:12:HIS:CE1	1:N:13:LYS:HG3	2.56	0.40
20:N:1524:PGV:H41	20:N:1524:PGV:H221	2.03	0.40
1:N:478:SER:O	13:Z:6:ALA:HB1	2.22	0.40
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.03	0.40
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.51	0.40
1:A:310:MET:CE	1:A:356:ILE:HG23	2.52	0.40
1:A:38:ARG:HD2	1:A:38:ARG:HH11	1.74	0.40
20:A:524:PGV:H151	4:D:87:PHE:CZ	2.57	0.40
9:I:43:ARG:HD3	9:I:43:ARG:HH11	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.57	0.40
3:P:164:PHE:CD1	23:P:1271:CHD:H192	2.57	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%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	484 (94%)	28 (6%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	38	35
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	38	35
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	38	35
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	25	20
5	E	102/109 (94%)	99 (97%)	3 (3%)	0	100	100
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	88 (97%)	1 (1%)	2 (2%)	8	3
6	S	91/98 (93%)	86 (94%)	3 (3%)	2 (2%)	8	3
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	0
8	H	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	6	2
8	U	73/85 (86%)	66 (90%)	4 (6%)	3 (4%)	3	1
9	I	69/73 (94%)	68 (99%)	1 (1%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3478/3614 (96%)	3316 (95%)	136 (4%)	26 (1%)	25	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
7	G	40	GLY
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	8	HIS
8	U	50	VAL
7	G	37	LEU
7	T	7	ASP
7	G	6	GLY
8	U	45	ALA
4	Q	34	SER
6	S	95	GLN
7	T	3	ALA
7	T	37	LEU
6	F	94	HIS
2	O	92	ASN
3	P	232	HIS
7	T	6	GLY
8	U	46	LYS

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%)	416 (98%)	10 (2%)	56	60
1	N	426/426 (100%)	412 (97%)	14 (3%)	43	45
2	B	210/210 (100%)	199 (95%)	11 (5%)	27	24
2	O	210/210 (100%)	192 (91%)	18 (9%)	12	8
3	C	224/226 (99%)	217 (97%)	7 (3%)	45	48
3	P	224/226 (99%)	219 (98%)	5 (2%)	57	62
4	D	128/129 (99%)	127 (99%)	1 (1%)	85	89
4	Q	128/129 (99%)	121 (94%)	7 (6%)	25	22
5	E	91/95 (96%)	89 (98%)	2 (2%)	57	62
5	R	91/95 (96%)	89 (98%)	2 (2%)	57	62
6	F	79/81 (98%)	72 (91%)	7 (9%)	11	7
6	S	79/81 (98%)	72 (91%)	7 (9%)	11	7
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	3
7	T	67/68 (98%)	61 (91%)	6 (9%)	11	7
8	H	67/75 (89%)	65 (97%)	2 (3%)	46	49
8	U	67/75 (89%)	60 (90%)	7 (10%)	8	5
9	I	56/57 (98%)	53 (95%)	3 (5%)	26	23
9	V	56/57 (98%)	53 (95%)	3 (5%)	26	23
10	J	48/50 (96%)	47 (98%)	1 (2%)	59	64
10	W	48/50 (96%)	46 (96%)	2 (4%)	34	33
11	K	39/46 (85%)	38 (97%)	1 (3%)	51	55
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	25
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	55
12	Y	39/40 (98%)	36 (92%)	3 (8%)	15	11
13	M	37/38 (97%)	30 (81%)	7 (19%)	2	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3022/3082 (98%)	2881 (95%)	141 (5%)	30	28

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	222	PRO
1	A	333	LYS
1	A	338	MET
1	A	362	SER
1	A	363	LEU
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	61	VAL
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	115	ASP
2	B	171	LYS
3	C	23	SER
3	C	29	SER
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	51	LEU
5	E	90	ARG
5	E	108	LYS
6	F	37	LYS
6	F	48	LEU
6	F	50	PRO
6	F	78	GLU
6	F	84	SER
6	F	87	THR

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Mol	Chain	Res	Type
6	F	95	GLN
7	G	2	SER
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	37	LEU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	27	ARG
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	61	GLU
10	J	50	LEU
11	K	20	SER
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
13	M	43	SER
1	N	34	SER
1	N	38	ARG
1	N	109	PHE
1	N	127	THR
1	N	138	HIS
1	N	228	PRO
1	N	241	PRO
1	N	265	LYS
1	N	338	MET
1	N	361	SER
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	504	THR
2	O	33	LEU
2	O	35	SER
2	O	60	GLU
2	O	65	TRP

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Mol	Chain	Res	Type
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	110	TYR
2	O	113	TYR
2	O	116	LEU
2	O	148	MET
2	O	167	SER
2	O	205	SER
2	O	217	LYS
2	O	221	LYS
2	O	225	SER
2	O	227	LEU
3	P	29	SER
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	9	GLU
4	Q	31	LYS
4	Q	51	LEU
4	Q	121	LYS
4	Q	127	LYS
4	Q	143	ASN
4	Q	147	LYS
5	R	31	LYS
5	R	80	GLU
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	78	GLU
6	S	84	SER
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	8	HIS
7	T	17	ARG
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	12	GLN

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Mol	Chain	Res	Type
8	U	27	ARG
8	U	41	LYS
8	U	44	THR
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	73	LYS
10	W	4	ARG
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	14	SER
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	178	GLN
1	A	180	GLN
1	A	360	ASN
1	A	503	HIS
1	A	512	ASN
2	B	10	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	149	HIS
4	D	29	HIS
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	76	ASN
10	J	29	ASN
10	J	57	HIS

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Mol	Chain	Res	Type
1	N	99	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
8	U	31	GLN
9	V	8	GLN
9	V	70	GLN
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	9,9,10	1.85	3 (33%)	7,9,11	5.32	5 (71%)
2	FME	B	1	2	9,9,10	2.04	3 (33%)	7,9,11	6.08	4 (57%)
7	TPO	G	11	7	9,10,11	2.32	5 (55%)	10,14,16	2.29	3 (30%)
1	FME	N	1	1	9,9,10	1.54	1 (11%)	7,9,11	5.18	4 (57%)
2	FME	O	1	2	9,9,10	1.15	1 (11%)	7,9,11	6.43	5 (71%)
7	TPO	T	11	7	9,10,11	2.26	5 (55%)	10,14,16	1.72	4 (40%)

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
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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.91	1.10	1.22
2	O	1	FME	O1-CN	-2.50	1.15	1.22
1	A	1	FME	CB-CA	-2.50	1.48	1.53
1	A	1	FME	O1-CN	-2.44	1.15	1.22
7	G	11	TPO	P-O2P	2.09	1.63	1.54
2	B	1	FME	O-C	2.10	1.28	1.19
7	T	11	TPO	O-C	2.29	1.29	1.19
7	T	11	TPO	P-O3P	2.39	1.64	1.54
7	G	11	TPO	O-C	2.40	1.30	1.19
7	G	11	TPO	P-OG1	2.44	1.63	1.59
7	T	11	TPO	CA-C	2.83	1.54	1.50
7	T	11	TPO	P-O1P	3.18	1.61	1.50
2	B	1	FME	CA-N	3.29	1.51	1.46
7	T	11	TPO	P-OG1	3.41	1.65	1.59
7	G	11	TPO	P-O1P	3.45	1.62	1.50
7	G	11	TPO	CA-C	3.72	1.55	1.50
1	A	1	FME	CA-C	3.93	1.55	1.50
1	N	1	FME	CA-C	4.01	1.55	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-15.94	98.31	122.82
2	B	1	FME	CA-N-CN	-14.83	100.01	122.82
1	A	1	FME	CA-N-CN	-13.10	102.67	122.82
1	N	1	FME	CA-N-CN	-12.51	103.58	122.82
2	B	1	FME	CG-CB-CA	-5.06	98.30	112.97
2	O	1	FME	CG-CB-CA	-2.82	104.82	112.97
1	A	1	FME	CB-CA-C	-2.82	107.01	111.65
7	T	11	TPO	C-CA-N	-2.58	104.65	109.86
7	T	11	TPO	O-C-CA	-2.53	119.24	125.15
2	B	1	FME	O-C-CA	-2.50	119.32	125.15
1	A	1	FME	CG-CB-CA	-2.38	106.09	112.97
1	A	1	FME	O-C-CA	-2.32	119.73	125.15
1	N	1	FME	O-C-CA	-2.27	119.86	125.15
7	G	11	TPO	OG1-P-O1P	-2.26	100.39	109.26
2	O	1	FME	O1-CN-N	-2.10	119.34	125.20
7	T	11	TPO	O3P-P-OG1	2.06	115.36	106.00
1	A	1	FME	CE-SD-CG	2.29	108.58	100.35
2	B	1	FME	O1-CN-N	2.51	132.20	125.20
1	N	1	FME	CE-SD-CG	2.62	109.75	100.35
2	O	1	FME	CB-CA-C	2.91	116.45	111.65
7	T	11	TPO	CG2-CB-CA	3.18	119.11	113.22
7	G	11	TPO	O2P-P-OG1	3.26	120.81	106.00
2	O	1	FME	CE-SD-CG	3.43	112.66	100.35
1	N	1	FME	CB-CA-C	3.90	118.08	111.65
7	G	11	TPO	CG2-CB-CA	5.17	122.81	113.22

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	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, 8 are monoatomic and 2 are unknown - 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	44,67,67	1.58	8 (18%)	37,103,103	2.55	14 (37%)
18	HEA	A	516	1,15	44,67,67	1.41	7 (15%)	37,103,103	2.55	12 (32%)
15	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.43	7 (11%)	65,65,65	2.44	14 (21%)
20	PGV	A	522	-	50,50,50	1.11	1 (2%)	51,56,56	1.46	8 (15%)
20	PGV	A	524	-	50,50,50	1.19	2 (4%)	51,56,56	1.53	8 (15%)
23	CHD	B	1086	-	29,32,32	1.83	7 (24%)	47,51,51	5.31	35 (74%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.39	3 (5%)	56,59,59	1.29	5 (8%)
20	PGV	C	267	-	50,50,50	0.96	3 (6%)	51,56,56	1.51	9 (17%)
20	PGV	C	268	-	50,50,50	1.23	2 (4%)	51,56,56	1.47	4 (7%)
26	CDL	C	270	-	99,99,99	1.41	12 (12%)	101,111,111	1.68	17 (16%)
23	CHD	C	271	-	29,32,32	0.79	1 (3%)	47,51,51	5.15	32 (68%)
24	DMU	C	272	-	34,34,34	1.22	2 (5%)	45,45,45	3.46	24 (53%)
23	CHD	C	525	-	29,32,32	1.67	7 (24%)	47,51,51	5.23	37 (78%)
19	TGL	D	523	-	62,62,62	1.59	7 (11%)	65,65,65	1.79	13 (20%)
28	PEK	G	1263	-	52,52,52	1.18	2 (3%)	54,57,57	1.36	7 (12%)
28	PEK	G	264	-	52,52,52	0.93	2 (3%)	54,57,57	2.30	12 (22%)
28	PEK	G	265	-	52,52,52	1.17	3 (5%)	54,57,57	1.16	4 (7%)
26	CDL	G	269	-	99,99,99	1.39	12 (12%)	101,111,111	1.35	12 (11%)
23	CHD	J	60	-	29,32,32	0.71	0	47,51,51	4.98	36 (76%)
19	TGL	L	522	-	62,62,62	1.46	7 (11%)	65,65,65	1.91	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	M	526	-	34,34,34	0.91	2 (5%)	45,45,45	3.34	26 (57%)
20	PGV	N	1266	-	50,50,50	0.87	2 (4%)	51,56,56	1.70	11 (21%)
19	TGL	N	1521	-	62,62,62	1.33	6 (9%)	65,65,65	1.68	12 (18%)
19	TGL	N	1522	-	62,62,62	1.49	7 (11%)	65,65,65	1.59	10 (15%)
20	PGV	N	1524	-	50,50,50	1.17	2 (4%)	51,56,56	1.33	7 (13%)
18	HEA	N	515	1	44,67,67	1.34	6 (13%)	37,103,103	2.70	16 (43%)
18	HEA	N	516	1,15	44,67,67	1.34	6 (13%)	37,103,103	1.99	10 (27%)
15	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	O	1230	-	51,51,51	1.25	3 (5%)	56,59,59	1.32	6 (10%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.62	6 (20%)	47,51,51	5.95	31 (65%)
28	PEK	P	1264	-	52,52,52	1.05	4 (7%)	54,57,57	1.74	8 (14%)
28	PEK	P	1265	-	52,52,52	1.21	2 (3%)	54,57,57	1.35	5 (9%)
20	PGV	P	1267	-	50,50,50	0.90	3 (6%)	51,56,56	1.56	11 (21%)
20	PGV	P	1268	-	50,50,50	1.20	2 (4%)	51,56,56	1.49	6 (11%)
26	CDL	P	1270	-	99,99,99	1.35	13 (13%)	101,111,111	1.47	15 (14%)
23	CHD	P	1271	-	29,32,32	0.84	1 (3%)	47,51,51	5.31	35 (74%)
24	DMU	P	1272	-	34,34,34	1.25	4 (11%)	45,45,45	3.23	23 (51%)
23	CHD	P	1525	-	29,32,32	1.31	5 (17%)	47,51,51	5.60	38 (80%)
19	TGL	Q	1523	-	62,62,62	1.40	6 (9%)	65,65,65	1.44	10 (15%)
26	CDL	T	1269	-	99,99,99	1.33	12 (12%)	101,111,111	1.55	16 (15%)
28	PEK	T	263	-	52,52,52	1.32	3 (5%)	54,57,57	1.42	6 (11%)
23	CHD	W	1060	-	29,32,32	0.85	1 (3%)	47,51,51	5.05	36 (76%)
24	DMU	Z	1526	-	34,34,34	1.03	2 (5%)	45,45,45	3.38	25 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	230	-	-	0/55/55/55	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
24	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
28	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
28	PEK	G	264	-	-	0/56/56/56	0/0/0/0
28	PEK	G	265	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	1/110/110/110	0/0/0/0
23	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
24	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
18	HEA	N	515	1	2/2/7/16	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
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	1/1/12/12	0/7/74/74	0/4/4/4
28	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
28	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	5/5/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
28	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	2/2/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C1D-ND	-5.24	1.30	1.36
18	N	515	HEA	C1A-NA	-4.18	1.31	1.36
23	B	1086	CHD	C8-C7	-3.91	1.46	1.53
23	C	525	CHD	C13-C12	-3.58	1.48	1.54
28	P	1264	PEK	O03-C01	-3.58	1.37	1.45
26	G	269	CDL	C59-C58	-3.47	1.31	1.51
18	N	516	HEA	C3C-C2C	-3.43	1.35	1.40
19	A	521	TGL	C10-CB9	-3.43	1.32	1.51
23	B	1086	CHD	C13-C12	-3.42	1.49	1.54
19	N	1521	TGL	C10-CB9	-3.39	1.32	1.51
19	L	522	TGL	C20-CA9	-3.39	1.32	1.51
19	L	522	TGL	C10-CB9	-3.37	1.32	1.51
18	A	515	HEA	C1A-NA	-3.32	1.32	1.36
26	C	270	CDL	C79-C78	-3.31	1.32	1.51
26	P	1270	CDL	C59-C58	-3.30	1.32	1.51
26	T	1269	CDL	C59-C58	-3.28	1.32	1.51
19	N	1522	TGL	C20-CA9	-3.26	1.33	1.51
26	T	1269	CDL	C42-C41	-3.22	1.33	1.51
24	Z	1526	DMU	C3-C4	-3.20	1.44	1.52
26	C	270	CDL	C59-C58	-3.17	1.33	1.51
26	G	269	CDL	C39-C38	-3.16	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.13	1.33	1.51
26	G	269	CDL	C62-C61	-3.09	1.33	1.51
24	M	526	DMU	C3-C4	-3.08	1.44	1.52
26	T	1269	CDL	C62-C61	-3.06	1.34	1.51
26	G	269	CDL	C42-C41	-3.02	1.34	1.51
26	P	1270	CDL	C22-C21	-2.99	1.34	1.51
26	T	1269	CDL	C19-C18	-2.97	1.34	1.51
26	P	1270	CDL	C79-C78	-2.96	1.34	1.51
26	C	270	CDL	C39-C38	-2.91	1.35	1.51
23	B	1086	CHD	C10-C5	-2.91	1.50	1.55
19	D	523	TGL	C15-CC9	-2.91	1.35	1.51
26	P	1270	CDL	C19-C18	-2.90	1.35	1.51
26	C	270	CDL	C62-C61	-2.90	1.35	1.51
26	C	270	CDL	C22-C21	-2.89	1.35	1.51
26	G	269	CDL	C19-C18	-2.87	1.35	1.51
26	P	1270	CDL	C39-C38	-2.85	1.35	1.51
26	C	270	CDL	C82-C81	-2.84	1.35	1.51
19	N	1522	TGL	C15-CC9	-2.83	1.35	1.51
26	G	269	CDL	C22-C21	-2.81	1.35	1.51
19	Q	1523	TGL	C10-CB9	-2.81	1.35	1.51
26	C	270	CDL	C19-C18	-2.81	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	1270	CDL	C62-C61	-2.81	1.35	1.51
19	Q	1523	TGL	C15-CC9	-2.79	1.35	1.51
19	A	521	TGL	OC1-CC1	-2.76	1.14	1.22
19	A	521	TGL	C20-CA9	-2.74	1.35	1.51
23	B	1086	CHD	C13-C14	-2.74	1.50	1.55
19	N	1521	TGL	C15-CC9	-2.72	1.36	1.51
26	T	1269	CDL	C39-C38	-2.71	1.36	1.51
26	P	1270	CDL	C82-C81	-2.71	1.36	1.51
26	P	1270	CDL	C42-C41	-2.71	1.36	1.51
26	T	1269	CDL	C79-C78	-2.70	1.36	1.51
26	C	270	CDL	C42-C41	-2.68	1.36	1.51
26	T	1269	CDL	C22-C21	-2.67	1.36	1.51
26	T	1269	CDL	C82-C81	-2.64	1.36	1.51
23	B	1086	CHD	C15-C14	-2.63	1.48	1.54
19	L	522	TGL	C15-CC9	-2.62	1.36	1.51
23	P	1525	CHD	C13-C12	-2.61	1.50	1.54
19	Q	1523	TGL	C20-CA9	-2.61	1.36	1.51
23	O	229	CHD	C15-C14	-2.59	1.48	1.54
26	G	269	CDL	C79-C78	-2.59	1.36	1.51
26	G	269	CDL	C82-C81	-2.57	1.36	1.51
19	D	523	TGL	C10-CB9	-2.53	1.37	1.51
19	A	521	TGL	C15-CC9	-2.49	1.37	1.51
19	D	523	TGL	C20-CA9	-2.48	1.37	1.51
18	A	516	HEA	C4A-NA	-2.39	1.34	1.36
18	N	516	HEA	C27-C19	-2.34	1.44	1.50
19	N	1521	TGL	C20-CA9	-2.30	1.38	1.51
23	O	229	CHD	C10-C5	-2.22	1.51	1.55
23	C	525	CHD	C6-C7	-2.21	1.49	1.52
23	P	1525	CHD	C1-C10	-2.17	1.50	1.54
23	P	1525	CHD	C13-C14	-2.14	1.51	1.55
24	P	1272	DMU	C3-C4	-2.03	1.47	1.52
18	N	516	HEA	C16-C15	2.00	1.55	1.51
18	N	516	HEA	C4C-CHD	2.00	1.45	1.40
24	C	272	DMU	O5-C6	2.04	1.46	1.41
18	N	516	HEA	C1C-CHC	2.05	1.45	1.40
24	M	526	DMU	O7-C10	2.05	1.47	1.41
18	A	516	HEA	C26-C15	2.06	1.56	1.50
20	N	1266	PGV	C01-C02	2.06	1.56	1.50
28	G	265	PEK	P-O12	2.06	1.67	1.59
23	C	525	CHD	C4-C3	2.08	1.55	1.51
18	N	515	HEA	C1B-CHB	2.10	1.45	1.40
18	N	515	HEA	C4D-CHA	2.11	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	O7-C10	2.11	1.47	1.41
23	P	1525	CHD	C16-C15	2.11	1.59	1.54
18	A	516	HEA	C3C-CAC	2.19	1.52	1.47
28	P	1264	PEK	C3-C2	2.21	1.60	1.52
19	N	1522	TGL	CG3-CG2	2.23	1.57	1.50
26	P	1270	CDL	PB2-OB2	2.24	1.68	1.59
18	A	515	HEA	C1B-CHB	2.26	1.46	1.40
23	O	229	CHD	C4-C3	2.26	1.56	1.51
23	C	525	CHD	C11-C12	2.26	1.57	1.53
20	C	267	PGV	O01-C1	2.27	1.40	1.34
18	N	515	HEA	C4C-NC	2.29	1.41	1.36
18	A	515	HEA	CMB-C2B	2.31	1.56	1.51
23	P	1525	CHD	C16-C17	2.34	1.59	1.54
18	A	515	HEA	C16-C15	2.36	1.56	1.51
18	A	516	HEA	C1C-CHC	2.37	1.46	1.40
28	T	263	PEK	C01-C02	2.38	1.57	1.50
23	O	229	CHD	C18-C13	2.40	1.58	1.54
23	P	1271	CHD	C20-C17	2.41	1.58	1.54
20	P	1267	PGV	O02-C1	2.41	1.29	1.22
24	Z	1526	DMU	O1-C10	2.42	1.47	1.41
24	P	1272	DMU	O1-C10	2.44	1.47	1.41
23	W	1060	CHD	C11-C9	2.47	1.57	1.53
19	L	522	TGL	CG1-CG2	2.48	1.57	1.50
23	C	525	CHD	C18-C13	2.51	1.58	1.54
23	C	271	CHD	C20-C17	2.59	1.59	1.54
18	A	516	HEA	C13-C14	2.64	1.59	1.50
18	N	516	HEA	C1D-ND	2.65	1.39	1.36
20	C	267	PGV	C03-C02	2.66	1.58	1.50
20	P	1267	PGV	O03-C19	2.74	1.41	1.33
18	A	516	HEA	C18-C19	2.74	1.39	1.33
28	P	1264	PEK	C2-C1	2.74	1.58	1.50
18	A	515	HEA	C3C-C2C	2.75	1.44	1.40
18	N	515	HEA	CMB-C2B	2.75	1.57	1.51
28	G	264	PEK	C2-C1	2.84	1.58	1.50
18	A	515	HEA	O11-C11	2.96	1.49	1.42
23	O	229	CHD	C11-C9	2.98	1.58	1.53
20	C	267	PGV	O03-C19	3.07	1.42	1.33
18	A	515	HEA	C3C-CAC	3.13	1.54	1.47
20	P	1267	PGV	C03-C02	3.24	1.59	1.50
28	P	1264	PEK	O01-C1	3.29	1.43	1.34
28	G	264	PEK	O01-C1	3.34	1.44	1.34
23	B	1086	CHD	C18-C13	3.36	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	1266	PGV	O03-C19	3.39	1.43	1.33
18	N	515	HEA	C1C-CHC	3.40	1.49	1.40
18	A	516	HEA	C16-C15	3.61	1.59	1.51
19	A	521	TGL	OG3-CC1	3.71	1.44	1.33
19	L	522	TGL	OG3-CC1	3.82	1.44	1.33
23	C	525	CHD	C11-C9	3.86	1.60	1.53
23	B	1086	CHD	C4-C3	3.88	1.59	1.51
23	C	525	CHD	O12-C12	3.93	1.50	1.43
22	O	1230	PSC	O03-C19	3.96	1.45	1.33
20	A	524	PGV	O01-C1	4.00	1.45	1.34
22	O	1230	PSC	C13-C12	4.06	1.54	1.31
26	P	1270	CDL	OB6-CB5	4.09	1.46	1.34
26	T	1269	CDL	OA8-CA7	4.10	1.45	1.33
19	N	1521	TGL	OG3-CC1	4.16	1.45	1.33
20	P	1268	PGV	O03-C19	4.21	1.45	1.33
22	B	230	PSC	C13-C12	4.22	1.55	1.31
23	O	229	CHD	C4-C5	4.26	1.61	1.53
26	T	1269	CDL	OB6-CB5	4.34	1.46	1.34
20	N	1524	PGV	O01-C1	4.36	1.46	1.34
24	C	272	DMU	O16-C6	4.40	1.47	1.40
26	C	270	CDL	OB6-CB5	4.42	1.47	1.34
26	T	1269	CDL	OA6-CA5	4.46	1.47	1.34
26	T	1269	CDL	OB8-CB7	4.48	1.46	1.33
26	P	1270	CDL	OB8-CB7	4.50	1.46	1.33
26	P	1270	CDL	OA6-CA5	4.54	1.47	1.34
19	Q	1523	TGL	OG1-CA1	4.54	1.46	1.33
28	G	1263	PEK	O01-C1	4.54	1.47	1.34
26	G	269	CDL	OB6-CB5	4.57	1.47	1.34
24	P	1272	DMU	O16-C6	4.57	1.48	1.40
19	D	523	TGL	OB1-CB1	4.59	1.36	1.22
20	C	268	PGV	O03-C19	4.59	1.46	1.33
28	G	265	PEK	O03-C21	4.61	1.46	1.33
26	G	269	CDL	OA6-CA5	4.63	1.47	1.34
26	G	269	CDL	OB8-CB7	4.65	1.47	1.33
26	C	270	CDL	OB8-CB7	4.67	1.47	1.33
26	G	269	CDL	OA8-CA7	4.74	1.47	1.33
22	O	1230	PSC	O01-C1	4.78	1.48	1.34
19	N	1521	TGL	OG1-CA1	4.80	1.47	1.33
26	C	270	CDL	OA6-CA5	4.83	1.48	1.34
19	N	1522	TGL	OG3-CC1	4.93	1.47	1.33
26	P	1270	CDL	OA8-CA7	4.94	1.47	1.33
28	P	1265	PEK	O01-C1	4.95	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1522	TGL	OG1-CA1	4.96	1.47	1.33
28	G	265	PEK	O01-C1	4.96	1.48	1.34
19	D	523	TGL	OG3-CC1	5.04	1.48	1.33
22	B	230	PSC	O01-C1	5.07	1.49	1.34
28	P	1265	PEK	O03-C21	5.11	1.48	1.33
28	G	1263	PEK	O03-C21	5.13	1.48	1.33
19	L	522	TGL	OG1-CA1	5.15	1.48	1.33
19	Q	1523	TGL	OG2-CB1	5.15	1.49	1.34
20	A	524	PGV	O03-C19	5.20	1.48	1.33
19	D	523	TGL	OG2-CB1	5.22	1.49	1.34
20	P	1268	PGV	O01-C1	5.22	1.49	1.34
19	A	521	TGL	OG2-CB1	5.23	1.49	1.34
26	C	270	CDL	OA8-CA7	5.24	1.48	1.33
19	Q	1523	TGL	OG3-CC1	5.27	1.48	1.33
28	T	263	PEK	O01-C1	5.33	1.49	1.34
20	C	268	PGV	O01-C1	5.36	1.49	1.34
20	N	1524	PGV	O03-C19	5.36	1.49	1.33
19	N	1521	TGL	OG2-CB1	5.40	1.50	1.34
22	B	230	PSC	O03-C19	5.41	1.49	1.33
19	A	521	TGL	OG1-CA1	5.44	1.49	1.33
20	A	522	PGV	O03-C19	5.48	1.49	1.33
19	D	523	TGL	OG1-CA1	5.70	1.50	1.33
19	L	522	TGL	OG2-CB1	5.82	1.51	1.34
19	N	1522	TGL	OG2-CB1	5.83	1.51	1.34
28	T	263	PEK	O03-C21	6.05	1.51	1.33

All (679) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C19-C10-C9	-12.24	93.64	111.16
23	O	229	CHD	C19-C10-C9	-11.36	94.91	111.16
23	B	1086	CHD	C18-C13-C12	-10.66	98.23	109.08
23	O	229	CHD	C18-C13-C12	-10.45	98.45	109.08
23	P	1525	CHD	C19-C10-C9	-10.00	96.85	111.16
23	O	229	CHD	C6-C5-C4	-9.67	100.15	111.13
23	P	1271	CHD	C18-C13-C12	-9.46	99.46	109.08
23	P	1525	CHD	C18-C13-C17	-8.94	97.09	111.23
18	A	516	HEA	C13-C12-C11	-8.58	101.47	114.46
23	C	271	CHD	C18-C13-C12	-8.43	100.51	109.08
19	L	522	TGL	OG3-CC1-OC1	-6.88	106.47	123.55
23	C	525	CHD	O12-C12-C13	-6.87	99.65	111.12
23	B	1086	CHD	C19-C10-C5	-6.76	98.65	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C18-C13-C17	-6.45	101.04	111.23
23	P	1525	CHD	O12-C12-C13	-6.44	100.36	111.12
23	P	1271	CHD	C19-C10-C9	-6.37	102.04	111.16
23	O	229	CHD	O12-C12-C13	-6.37	100.50	111.12
23	O	229	CHD	C18-C13-C14	-6.33	101.23	111.23
23	C	525	CHD	C18-C13-C12	-6.24	102.73	109.08
18	N	515	HEA	C1B-C2B-C3B	-6.21	102.68	107.00
23	C	525	CHD	C23-C22-C20	-6.12	106.48	114.72
23	P	1525	CHD	C18-C13-C14	-5.99	101.77	111.23
23	J	60	CHD	C18-C13-C12	-5.92	103.05	109.08
26	C	270	CDL	CB4-OB6-CB5	-5.88	103.99	117.88
19	A	521	TGL	OG3-CC1-OC1	-5.82	109.09	123.55
28	P	1264	PEK	O03-C01-C02	-5.80	94.08	108.66
23	C	525	CHD	C18-C13-C14	-5.76	102.12	111.23
28	G	264	PEK	O01-C1-O02	-5.73	109.38	123.68
18	A	515	HEA	C1B-C2B-C3B	-5.53	103.15	107.00
23	P	1271	CHD	C23-C22-C20	-5.40	107.44	114.72
23	B	1086	CHD	C19-C10-C9	-5.38	103.47	111.16
18	N	515	HEA	C27-C19-C18	-5.37	109.37	123.69
23	P	1271	CHD	O7-C7-C6	-5.31	97.17	110.02
28	P	1264	PEK	O01-C1-O02	-5.24	110.60	123.68
19	D	523	TGL	OG2-CB1-CB2	-5.23	100.69	111.55
23	C	525	CHD	O12-C12-C11	-5.22	98.40	109.11
18	A	515	HEA	C20-C21-C22	-5.17	94.24	111.97
23	P	1525	CHD	C6-C5-C4	-5.11	105.33	111.13
23	W	1060	CHD	C1-C10-C9	-5.07	103.30	111.39
23	J	60	CHD	C6-C5-C4	-5.06	105.38	111.13
23	P	1525	CHD	C1-C10-C9	-4.98	103.44	111.39
23	B	1086	CHD	C1-C10-C9	-4.96	103.48	111.39
20	N	1266	PGV	O03-C19-O04	-4.93	111.31	123.55
23	W	1060	CHD	C19-C10-C5	-4.92	101.82	110.30
23	W	1060	CHD	C6-C5-C4	-4.92	105.54	111.13
23	C	271	CHD	C18-C13-C17	-4.90	103.49	111.23
23	B	1086	CHD	C18-C13-C14	-4.89	103.51	111.23
23	J	60	CHD	C1-C10-C9	-4.86	103.63	111.39
18	N	516	HEA	C4B-C3B-C2B	-4.85	103.48	106.87
20	A	524	PGV	C8-C9-C10	-4.83	95.19	113.74
23	P	1271	CHD	C18-C13-C17	-4.79	103.66	111.23
20	C	267	PGV	C27-C26-C25	-4.79	89.79	114.45
24	Z	1526	DMU	O7-C10-C5	-4.77	97.37	108.11
23	P	1525	CHD	O12-C12-C11	-4.76	99.33	109.11
23	C	271	CHD	C6-C5-C4	-4.73	105.76	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	C20-C19-C18	-4.70	111.49	121.10
18	N	516	HEA	C13-C12-C11	-4.68	107.38	114.46
23	C	525	CHD	C18-C13-C17	-4.66	103.86	111.23
23	C	271	CHD	O7-C7-C6	-4.65	98.77	110.02
23	P	1525	CHD	C19-C10-C5	-4.59	102.39	110.30
23	C	271	CHD	C23-C22-C20	-4.57	108.56	114.72
23	P	1525	CHD	C22-C20-C17	-4.52	100.76	110.26
23	B	1086	CHD	O12-C12-C11	-4.49	99.90	109.11
23	B	1086	CHD	C18-C13-C17	-4.48	104.15	111.23
23	W	1060	CHD	C18-C13-C12	-4.43	104.57	109.08
23	C	525	CHD	C6-C5-C4	-4.38	106.15	111.13
23	O	229	CHD	O12-C12-C11	-4.38	100.12	109.11
23	C	271	CHD	C19-C10-C9	-4.33	104.96	111.16
20	P	1267	PGV	C8-C9-C10	-4.30	97.23	113.74
23	W	1060	CHD	O7-C7-C6	-4.28	99.67	110.02
23	P	1525	CHD	C4-C5-C10	-4.24	108.03	112.66
23	B	1086	CHD	O12-C12-C13	-4.16	104.19	111.12
23	O	229	CHD	C1-C10-C9	-4.09	104.86	111.39
19	A	521	TGL	OB1-CB1-CB2	-4.09	107.52	123.68
18	N	515	HEA	C16-C15-C14	-4.06	112.78	121.10
23	P	1271	CHD	C11-C9-C10	-4.06	109.45	113.74
23	P	1525	CHD	C23-C22-C20	-4.00	109.33	114.72
18	A	516	HEA	C4B-C3B-C2B	-3.98	104.09	106.87
18	A	516	HEA	CAD-CBD-CGD	-3.91	105.98	112.66
23	J	60	CHD	C19-C10-C5	-3.89	103.60	110.30
18	N	515	HEA	CAA-CBA-CGA	-3.87	106.04	112.66
23	J	60	CHD	C18-C13-C14	-3.87	105.11	111.23
23	P	1271	CHD	O12-C12-C13	-3.86	104.67	111.12
23	O	229	CHD	C4-C5-C10	-3.84	108.46	112.66
23	P	1525	CHD	O7-C7-C6	-3.81	100.80	110.02
23	P	1271	CHD	O12-C12-C11	-3.65	101.61	109.11
28	G	264	PEK	C24-C23-C22	-3.64	99.91	113.24
20	N	1266	PGV	O01-C1-O02	-3.62	114.63	123.68
28	G	264	PEK	C25-C24-C23	-3.61	95.83	114.45
20	A	522	PGV	C8-C9-C10	-3.60	99.90	113.74
23	C	271	CHD	O12-C12-C11	-3.60	101.72	109.11
28	G	265	PEK	O03-C21-O04	-3.57	114.69	123.55
23	W	1060	CHD	O12-C12-C11	-3.56	101.79	109.11
26	C	270	CDL	OB8-CB7-OB9	-3.56	114.70	123.55
24	M	526	DMU	O7-C10-C5	-3.55	100.12	108.11
20	C	267	PGV	C8-C9-C10	-3.52	100.23	113.74
28	P	1265	PEK	O03-C21-O04	-3.51	114.83	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	270	CDL	C52-C51-CB5	-3.51	100.77	113.58
18	A	515	HEA	CAA-CBA-CGA	-3.50	106.68	112.66
23	W	1060	CHD	C18-C13-C17	-3.49	105.71	111.23
18	A	516	HEA	CAA-CBA-CGA	-3.49	106.70	112.66
24	M	526	DMU	O7-C10-O1	-3.49	102.23	110.70
23	W	1060	CHD	C18-C13-C14	-3.42	105.82	111.23
20	N	1266	PGV	C01-O03-C19	-3.37	107.00	117.13
23	J	60	CHD	O12-C12-C11	-3.36	102.21	109.11
23	B	1086	CHD	C6-C5-C4	-3.30	107.38	111.13
26	T	1269	CDL	OA6-CA5-OA7	-3.30	115.45	123.68
28	P	1264	PEK	C03-C02-C01	-3.26	104.50	111.86
24	Z	1526	DMU	O49-C1-C6	-3.26	103.20	110.03
23	J	60	CHD	C18-C13-C17	-3.25	106.09	111.23
19	Q	1523	TGL	OG1-CA1-OA1	-3.22	115.54	123.55
18	A	516	HEA	CMC-C2C-C1C	-3.16	123.60	128.46
23	B	1086	CHD	O7-C7-C6	-3.16	102.37	110.02
23	J	60	CHD	O7-C7-C6	-3.12	102.48	110.02
20	P	1267	PGV	C27-C26-C25	-3.10	98.48	114.45
26	T	1269	CDL	OB6-CB5-OB7	-3.09	115.97	123.68
18	N	516	HEA	OMA-CMA-C3A	-3.07	118.01	125.08
20	P	1268	PGV	O04-C19-C20	-3.04	111.66	123.68
26	P	1270	CDL	OB8-CB7-OB9	-3.04	116.01	123.55
23	P	1271	CHD	O3-C3-C4	-3.01	103.86	109.87
26	P	1270	CDL	O1-C1-CA2	-2.99	98.30	109.34
23	C	271	CHD	C19-C10-C1	-2.96	103.38	108.24
20	P	1268	PGV	C03-C02-C01	-2.93	105.24	111.86
23	B	1086	CHD	O7-C7-C8	-2.90	102.84	109.33
26	P	1270	CDL	OA8-CA7-OA9	-2.87	116.42	123.55
26	G	269	CDL	OB6-CB5-OB7	-2.86	116.54	123.68
23	C	525	CHD	C1-C10-C9	-2.83	106.87	111.39
26	P	1270	CDL	CB4-OB6-CB5	-2.83	111.19	117.88
26	C	270	CDL	OB8-CB6-CB4	-2.83	101.56	108.66
20	P	1267	PGV	C3-C2-C1	-2.81	103.33	113.58
18	N	516	HEA	O11-C11-C3B	-2.81	103.75	111.83
23	C	525	CHD	O7-C7-C6	-2.80	103.25	110.02
19	Q	1523	TGL	OG3-CC1-OC1	-2.78	116.64	123.55
20	P	1267	PGV	C03-C02-C01	-2.78	105.58	111.86
28	G	264	PEK	O03-C01-C02	-2.78	101.68	108.66
20	C	268	PGV	O04-C19-C20	-2.75	112.82	123.68
20	C	267	PGV	C3-C2-C1	-2.75	103.55	113.58
20	C	267	PGV	C4-C3-C2	-2.74	103.20	113.24
22	B	230	PSC	C29-C28-C27	-2.70	100.52	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	OA6-CA5-OA7	-2.69	116.97	123.68
28	P	1264	PEK	C24-C23-C22	-2.68	103.43	113.24
19	N	1522	TGL	OG3-CC1-OC1	-2.67	116.91	123.55
23	C	525	CHD	C4-C5-C10	-2.67	109.74	112.66
20	A	524	PGV	C4-C3-C2	-2.64	103.55	113.24
18	A	516	HEA	CAA-C2A-C3A	-2.63	121.07	128.59
22	O	1230	PSC	C31-C30-C29	-2.61	101.02	114.45
26	T	1269	CDL	OB8-CB7-OB9	-2.60	117.09	123.55
28	G	264	PEK	C26-C25-C24	-2.60	101.06	114.45
26	G	269	CDL	OB8-CB7-OB9	-2.59	117.13	123.55
20	C	267	PGV	O01-C02-C03	-2.58	99.05	108.44
28	G	264	PEK	C31-C30-C29	-2.55	101.30	114.45
23	B	1086	CHD	C4-C5-C10	-2.54	109.89	112.66
23	C	271	CHD	O12-C12-C13	-2.53	106.90	111.12
20	A	522	PGV	O03-C19-O04	-2.53	117.28	123.55
26	C	270	CDL	OA8-CA7-OA9	-2.52	117.29	123.55
23	P	1525	CHD	O7-C7-C8	-2.52	103.70	109.33
24	Z	1526	DMU	O2-C8-C7	-2.50	104.92	110.36
18	N	515	HEA	C17-C18-C19	-2.49	121.41	127.68
26	P	1270	CDL	CA6-CA4-CA3	-2.48	106.26	111.86
20	C	267	PGV	O12-P-O13	-2.45	99.36	109.25
19	N	1521	TGL	OG3-CC1-OC1	-2.44	117.48	123.55
28	G	1263	PEK	C18-C17-C16	-2.44	104.36	113.74
18	N	516	HEA	CMC-C2C-C1C	-2.44	124.72	128.46
26	P	1270	CDL	CB6-CB4-CB3	-2.44	106.36	111.86
20	N	1266	PGV	C03-C02-C01	-2.43	106.37	111.86
20	P	1268	PGV	O03-C19-O04	-2.42	117.53	123.55
22	O	1230	PSC	O03-C19-O04	-2.42	117.53	123.55
23	C	525	CHD	O7-C7-C8	-2.41	103.95	109.33
18	N	516	HEA	CAD-CBD-CGD	-2.41	108.55	112.66
23	P	1525	CHD	C18-C13-C12	-2.39	106.64	109.08
23	J	60	CHD	C19-C10-C9	-2.37	107.77	111.16
20	P	1267	PGV	O01-C1-O02	-2.37	117.77	123.68
19	A	521	TGL	CB7-CB6-CB5	-2.37	102.26	114.45
19	L	522	TGL	CA5-CA4-CA3	-2.35	102.33	114.45
20	C	267	PGV	O01-C1-O02	-2.35	117.81	123.68
18	N	516	HEA	CAA-CBA-CGA	-2.35	108.65	112.66
26	C	270	CDL	CA6-CA4-CA3	-2.34	106.58	111.86
19	D	523	TGL	OG3-CC1-OC1	-2.33	117.76	123.55
20	N	1266	PGV	C8-C7-C6	-2.33	102.47	114.45
18	N	515	HEA	C20-C21-C22	-2.32	103.99	111.97
20	P	1267	PGV	O12-P-O13	-2.30	99.98	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	TGL	OG1-CA1-OA1	-2.30	117.85	123.55
18	A	515	HEA	C16-C15-C14	-2.29	116.41	121.10
19	L	522	TGL	CA9-CA8-CA7	-2.27	102.76	114.45
20	C	267	PGV	C22-C21-C20	-2.26	104.97	113.24
23	P	1525	CHD	C21-C20-C22	-2.25	106.81	110.35
23	B	1086	CHD	C21-C20-C22	-2.24	106.82	110.35
19	L	522	TGL	CB9-CB8-CB7	-2.23	102.94	114.45
26	T	1269	CDL	OA8-CA7-OA9	-2.23	118.00	123.55
28	G	264	PEK	C32-C31-C30	-2.23	102.97	114.45
23	P	1271	CHD	C19-C10-C5	-2.23	106.46	110.30
24	Z	1526	DMU	C25-C28-C31	-2.23	102.99	114.45
23	P	1271	CHD	C6-C5-C4	-2.22	108.61	111.13
20	P	1267	PGV	O06-C06-C05	-2.21	98.95	110.07
26	P	1270	CDL	OB6-CB4-CB3	-2.20	100.42	108.44
20	A	522	PGV	C03-C02-C01	-2.20	106.89	111.86
20	C	267	PGV	O03-C19-O04	-2.20	118.09	123.55
24	M	526	DMU	C28-C31-C34	-2.17	103.26	114.45
28	T	263	PEK	O04-C21-C22	-2.16	115.15	123.68
20	P	1267	PGV	C10-C11-C12	-2.16	109.04	124.81
18	A	516	HEA	CMB-C2B-C3B	-2.16	120.77	124.92
20	P	1267	PGV	C9-C8-C7	-2.15	103.35	114.45
26	T	1269	CDL	OB5-PB2-OB3	-2.15	100.57	109.25
28	G	1263	PEK	O01-C1-O02	-2.15	118.33	123.68
26	T	1269	CDL	CA4-OA6-CA5	-2.14	112.83	117.88
18	A	515	HEA	C12-C13-C14	-2.13	106.72	112.33
22	O	1230	PSC	O01-C1-O02	-2.13	118.37	123.68
26	P	1270	CDL	OA6-CA5-OA7	-2.10	118.44	123.68
19	N	1521	TGL	OG1-CA1-OA1	-2.09	118.36	123.55
20	P	1268	PGV	C21-C20-C19	-2.09	105.96	113.58
26	C	270	CDL	C53-C52-C51	-2.08	105.61	113.24
26	C	270	CDL	C57-C56-C55	-2.08	103.74	114.45
20	N	1524	PGV	O03-C19-O04	-2.07	118.41	123.55
20	A	522	PGV	C3-C2-C1	-2.07	106.03	113.58
20	N	1266	PGV	O14-P-O12	-2.07	98.39	108.14
28	P	1265	PEK	C33-C32-C31	-2.05	103.87	114.45
18	N	515	HEA	O11-C11-C12	-2.05	102.67	110.21
19	L	522	TGL	C24-C23-C22	-2.05	103.87	114.45
20	N	1524	PGV	O01-C1-O02	-2.05	118.56	123.68
24	Z	1526	DMU	C22-C25-C28	-2.05	103.90	114.45
18	A	516	HEA	C3A-C4A-NA	-2.04	107.08	110.94
28	G	264	PEK	C3-C2-C1	-2.04	106.12	113.58
20	A	524	PGV	O03-C19-O04	-2.04	118.49	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C26-C15-C14	-2.03	118.28	123.69
22	O	1230	PSC	C27-C26-C25	-2.03	104.01	114.45
26	T	1269	CDL	CB4-OB6-CB5	-2.01	113.13	117.88
23	W	1060	CHD	C16-C15-C14	2.00	109.12	105.12
19	D	523	TGL	OG3-CG3-CG2	2.01	113.71	108.66
28	G	264	PEK	O12-P-O14	2.02	117.39	109.25
19	A	521	TGL	C20-CA9-CA8	2.03	124.92	114.45
19	N	1521	TGL	OG2-CG2-CG3	2.05	115.89	108.44
24	C	272	DMU	O55-C2-C3	2.05	114.54	109.87
23	P	1271	CHD	C16-C15-C14	2.06	109.23	105.12
19	N	1521	TGL	C15-CC9-CC8	2.07	125.12	114.45
28	G	1263	PEK	C02-O01-C1	2.07	122.77	117.88
18	A	515	HEA	CAD-C3D-C2D	2.08	134.93	129.00
23	O	229	CHD	C19-C10-C5	2.09	113.89	110.30
23	B	1086	CHD	C16-C17-C20	2.09	115.48	112.14
23	C	271	CHD	C14-C8-C9	2.10	112.49	109.64
19	L	522	TGL	CG1-OG1-CA1	2.10	123.45	117.13
19	Q	1523	TGL	C16-C15-CC9	2.10	125.30	114.45
18	N	515	HEA	CMB-C2B-C3B	2.12	128.99	124.92
18	A	515	HEA	CMB-C2B-C3B	2.13	129.00	124.92
24	M	526	DMU	O49-C1-C6	2.13	114.49	110.03
19	Q	1523	TGL	C21-C20-CA9	2.14	125.48	114.45
23	P	1271	CHD	C13-C14-C8	2.14	117.53	114.77
23	J	60	CHD	C11-C9-C10	2.15	116.02	113.74
26	P	1270	CDL	OA8-CA6-CA4	2.15	114.06	108.66
24	P	1272	DMU	O16-C18-C19	2.15	117.36	109.68
28	P	1264	PEK	O02-C1-C2	2.15	132.20	123.68
24	C	272	DMU	C57-C4-C3	2.16	119.11	113.24
18	N	515	HEA	CMD-C2D-C3D	2.17	129.03	124.94
18	A	515	HEA	CMD-C2D-C3D	2.17	129.03	124.94
26	G	269	CDL	CA6-CA4-CA3	2.19	116.80	111.86
24	M	526	DMU	O7-C3-C2	2.20	112.49	107.19
26	T	1269	CDL	C23-C22-C21	2.20	125.80	114.45
23	C	271	CHD	C21-C20-C17	2.21	116.41	112.95
23	B	1086	CHD	C13-C14-C8	2.22	117.64	114.77
20	A	522	PGV	C28-C27-C26	2.23	125.92	114.45
19	N	1521	TGL	CB3-CB2-CB1	2.25	121.78	113.58
19	Q	1523	TGL	OG3-CG3-CG2	2.25	114.32	108.66
26	G	269	CDL	OB8-CB7-C71	2.26	118.46	111.90
24	P	1272	DMU	C18-O16-C6	2.26	117.74	113.87
20	N	1266	PGV	O14-P-O11	2.27	118.85	108.14
20	A	524	PGV	C3-C2-C1	2.27	121.86	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C20-C19-C18	2.28	125.76	121.10
26	C	270	CDL	C39-C38-C37	2.29	126.23	114.45
24	Z	1526	DMU	C11-C9-C8	2.29	118.36	113.00
28	G	1263	PEK	C01-O03-C21	2.30	124.05	117.13
26	G	269	CDL	C80-C79-C78	2.31	126.33	114.45
23	J	60	CHD	C13-C14-C8	2.31	117.75	114.77
23	C	525	CHD	C15-C16-C17	2.32	109.76	105.12
26	G	269	CDL	C83-C82-C81	2.34	126.51	114.45
19	A	521	TGL	CG1-OG1-CA1	2.34	124.17	117.13
20	A	522	PGV	C24-C23-C22	2.36	126.61	114.45
26	C	270	CDL	C63-C62-C61	2.38	126.71	114.45
24	Z	1526	DMU	C57-C4-C3	2.39	119.75	113.24
22	B	230	PSC	C01-O03-C19	2.40	124.35	117.13
19	N	1522	TGL	CB3-CB2-CB1	2.41	122.38	113.58
19	A	521	TGL	C15-CC9-CC8	2.43	126.96	114.45
28	P	1264	PEK	O01-C1-C2	2.43	116.60	111.55
28	G	264	PEK	O02-C1-C2	2.43	133.30	123.68
28	P	1264	PEK	O04-C21-C22	2.43	133.31	123.68
19	Q	1523	TGL	OG2-CG2-CG3	2.43	117.29	108.44
19	L	522	TGL	OG2-CB1-CB2	2.44	116.61	111.55
20	P	1267	PGV	O14-P-O13	2.44	124.89	112.28
22	B	230	PSC	C02-O01-C1	2.44	123.64	117.88
26	P	1270	CDL	C42-C41-C40	2.46	127.15	114.45
24	M	526	DMU	O49-C1-C2	2.47	115.73	110.36
28	G	265	PEK	C01-O03-C21	2.48	124.58	117.13
26	T	1269	CDL	C80-C79-C78	2.48	127.24	114.45
26	G	269	CDL	C82-C81-C80	2.49	127.28	114.45
26	P	1270	CDL	C39-C38-C37	2.49	127.29	114.45
26	T	1269	CDL	C83-C82-C81	2.51	127.40	114.45
23	W	1060	CHD	C11-C9-C10	2.53	116.42	113.74
19	N	1522	TGL	OG3-CC1-CC2	2.53	119.25	111.90
20	N	1266	PGV	O01-C1-C2	2.53	116.80	111.55
23	C	271	CHD	C14-C8-C7	2.54	115.25	111.80
26	T	1269	CDL	OB8-CB7-C71	2.55	119.32	111.90
20	N	1266	PGV	C02-O01-C1	2.58	123.97	117.88
20	N	1524	PGV	O01-C02-C01	2.58	117.83	108.44
24	P	1272	DMU	O7-C3-C2	2.59	113.42	107.19
28	T	263	PEK	C02-O01-C1	2.59	124.00	117.88
26	C	270	CDL	C42-C41-C40	2.60	127.83	114.45
23	C	525	CHD	C19-C10-C1	2.60	112.51	108.24
24	M	526	DMU	C6-O5-C4	2.60	118.61	113.72
26	P	1270	CDL	OB6-CB4-CB6	2.60	117.90	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	O5-C6-O16	2.61	116.22	110.02
20	N	1266	PGV	O03-C01-C02	2.63	115.27	108.66
20	C	268	PGV	O03-C01-C02	2.65	115.32	108.66
28	G	264	PEK	O01-C1-C2	2.66	117.07	111.55
22	B	230	PSC	O03-C19-C20	2.66	119.64	111.90
23	W	1060	CHD	C17-C13-C14	2.66	102.80	100.08
26	T	1269	CDL	OB8-CB6-CB4	2.67	115.37	108.66
19	D	523	TGL	C11-C10-CB9	2.67	128.24	114.45
26	C	270	CDL	O1-C1-CB2	2.69	119.27	109.34
24	P	1272	DMU	C57-C4-C3	2.70	120.60	113.24
24	P	1272	DMU	O7-C3-C4	2.71	116.02	109.34
24	C	272	DMU	O5-C6-O16	2.72	116.47	110.02
24	M	526	DMU	O3-C5-C7	2.72	116.28	110.36
26	C	270	CDL	OB6-CB5-C51	2.74	117.23	111.55
23	J	60	CHD	C9-C8-C7	2.74	115.14	111.92
23	O	229	CHD	C11-C9-C10	2.74	116.65	113.74
19	L	522	TGL	OG2-CG2-CG1	2.75	118.43	108.44
19	D	523	TGL	C10-CB9-CB8	2.76	128.68	114.45
28	P	1265	PEK	O03-C01-C02	2.77	115.61	108.66
19	N	1522	TGL	CG2-OG2-CB1	2.77	124.42	117.88
20	A	524	PGV	C01-O03-C19	2.78	125.50	117.13
23	C	525	CHD	C16-C17-C20	2.79	116.60	112.14
19	N	1522	TGL	CG3-OG3-CC1	2.80	125.54	117.13
18	A	516	HEA	CMC-C2C-C3C	2.82	130.13	124.89
24	Z	1526	DMU	O3-C5-C7	2.84	116.54	110.36
23	P	1525	CHD	C1-C2-C3	2.89	114.10	110.42
24	M	526	DMU	O4-C7-C8	2.90	116.66	110.36
23	W	1060	CHD	C9-C8-C7	2.90	115.33	111.92
20	A	524	PGV	O01-C02-C01	2.92	119.04	108.44
23	B	1086	CHD	C13-C17-C20	2.93	123.05	119.49
24	P	1272	DMU	O5-C6-O16	2.94	117.00	110.02
23	C	525	CHD	O3-C3-C4	2.94	115.74	109.87
18	A	516	HEA	CMB-C2B-C1B	2.96	133.01	128.46
24	M	526	DMU	C10-O1-C9	2.97	119.31	113.72
18	N	516	HEA	CBD-CAD-C3D	2.99	118.20	112.48
24	C	272	DMU	C10-C5-C7	3.00	115.56	109.98
19	N	1521	TGL	OG3-CG3-CG2	3.00	116.20	108.66
19	N	1522	TGL	CC3-CC2-CC1	3.01	124.59	113.58
20	N	1524	PGV	C01-O03-C19	3.02	126.21	117.13
19	Q	1523	TGL	OG1-CA1-CA2	3.02	120.69	111.90
26	T	1269	CDL	CB6-OB8-CB7	3.03	126.24	117.13
24	Z	1526	DMU	C6-C1-C2	3.03	115.62	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	523	TGL	C21-C20-CA9	3.04	130.14	114.45
26	G	269	CDL	OA8-CA7-C31	3.05	120.77	111.90
19	A	521	TGL	OG2-CG2-CG1	3.05	119.53	108.44
19	D	523	TGL	CB3-CB2-CB1	3.06	124.76	113.58
28	T	263	PEK	O03-C21-C22	3.07	120.82	111.90
24	M	526	DMU	C7-C8-C9	3.07	115.62	110.22
26	T	1269	CDL	OA8-CA7-C31	3.07	120.83	111.90
23	C	525	CHD	C13-C14-C8	3.09	118.75	114.77
24	C	272	DMU	O4-C7-C5	3.09	117.07	110.36
23	B	1086	CHD	O3-C3-C4	3.11	116.08	109.87
19	N	1521	TGL	CG1-OG1-CA1	3.12	126.51	117.13
24	P	1272	DMU	O7-C10-C5	3.13	115.16	108.11
19	D	523	TGL	OG3-CC1-CC2	3.15	121.07	111.90
24	P	1272	DMU	O7-C10-O1	3.16	118.37	110.70
24	C	272	DMU	C1-C2-C3	3.16	116.16	109.61
26	G	269	CDL	CA6-OA8-CA7	3.17	126.66	117.13
18	N	516	HEA	C1B-C2B-C3B	3.20	109.22	107.00
23	C	525	CHD	C15-C14-C8	3.20	122.84	118.32
23	J	60	CHD	C17-C13-C14	3.20	103.34	100.08
24	Z	1526	DMU	C10-C5-C7	3.22	115.97	109.98
24	Z	1526	DMU	C10-O1-C9	3.22	119.79	113.72
23	O	229	CHD	C9-C11-C12	3.24	118.59	114.32
20	N	1524	PGV	O03-C19-C20	3.26	121.38	111.90
19	Q	1523	TGL	OG2-CB1-CB2	3.29	118.38	111.55
23	O	229	CHD	O3-C3-C4	3.30	116.45	109.87
24	M	526	DMU	O16-C6-C1	3.30	113.62	108.23
28	G	265	PEK	O01-C1-C2	3.31	118.42	111.55
24	P	1272	DMU	C10-C5-C7	3.31	116.12	109.98
23	P	1271	CHD	C21-C20-C17	3.34	118.18	112.95
19	N	1521	TGL	OG3-CC1-CC2	3.34	121.63	111.90
23	W	1060	CHD	C13-C14-C8	3.36	119.09	114.77
24	Z	1526	DMU	C6-O5-C4	3.36	120.05	113.72
28	G	1263	PEK	O03-C21-C22	3.37	121.72	111.90
24	M	526	DMU	O5-C6-O16	3.39	118.06	110.02
23	C	525	CHD	C14-C8-C9	3.39	114.25	109.64
19	N	1522	TGL	OG1-CA1-CA2	3.39	121.77	111.90
28	T	263	PEK	C01-O03-C21	3.40	127.36	117.13
19	N	1521	TGL	OG1-CA1-CA2	3.42	121.86	111.90
24	M	526	DMU	O1-C9-C11	3.42	114.61	106.41
19	D	523	TGL	CG3-OG3-CC1	3.43	127.45	117.13
23	O	229	CHD	C15-C14-C8	3.43	123.18	118.32
24	C	272	DMU	C6-O5-C4	3.46	120.23	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	1524	PGV	C02-O01-C1	3.46	126.05	117.88
20	A	522	PGV	O03-C01-C02	3.46	117.35	108.66
24	Z	1526	DMU	C1-C2-C3	3.47	116.79	109.61
20	P	1267	PGV	O03-C01-C02	3.47	117.37	108.66
28	G	1263	PEK	O03-C01-C02	3.48	117.41	108.66
19	N	1522	TGL	OG1-CG1-CG2	3.49	117.43	108.66
24	M	526	DMU	C57-C4-C3	3.50	122.77	113.24
24	M	526	DMU	C10-C5-C7	3.52	116.51	109.98
24	M	526	DMU	C1-C2-C3	3.53	116.93	109.61
23	O	229	CHD	C2-C1-C10	3.55	118.98	112.80
23	B	1086	CHD	C14-C8-C7	3.56	116.62	111.80
24	C	272	DMU	C10-O1-C9	3.56	120.42	113.72
24	C	272	DMU	C11-C9-C8	3.56	121.34	113.00
23	P	1525	CHD	C14-C8-C9	3.57	114.49	109.64
22	O	1230	PSC	O03-C19-C20	3.57	122.29	111.90
23	C	525	CHD	C11-C9-C8	3.58	116.01	110.82
26	P	1270	CDL	OA8-CA7-C31	3.60	122.38	111.90
23	P	1525	CHD	C13-C14-C8	3.60	119.41	114.77
23	W	1060	CHD	C22-C20-C17	3.64	117.90	110.26
24	P	1272	DMU	C10-O1-C9	3.64	120.58	113.72
18	N	515	HEA	C4B-C3B-C2B	3.65	109.42	106.87
23	P	1525	CHD	C11-C9-C8	3.67	116.15	110.82
19	N	1522	TGL	OG3-CG3-CG2	3.69	117.94	108.66
28	P	1265	PEK	O01-C1-C2	3.70	119.23	111.55
24	M	526	DMU	C11-C9-C8	3.72	121.71	113.00
20	A	524	PGV	O03-C19-C20	3.74	122.79	111.90
23	P	1525	CHD	C2-C1-C10	3.81	119.43	112.80
24	C	272	DMU	O7-C10-C5	3.87	116.82	108.11
23	O	229	CHD	C14-C8-C9	3.90	114.94	109.64
19	D	523	TGL	CG2-OG2-CB1	3.90	127.09	117.88
26	C	270	CDL	OA8-CA6-CA4	3.92	118.50	108.66
18	N	516	HEA	C17-C18-C19	3.95	137.60	127.68
24	C	272	DMU	C7-C8-C9	3.98	117.22	110.22
24	P	1272	DMU	C2-C3-C4	4.00	119.35	110.88
20	A	522	PGV	O03-C19-C20	4.01	123.58	111.90
19	D	523	TGL	OG1-CA1-CA2	4.02	123.58	111.90
18	N	515	HEA	C16-C17-C18	4.02	125.75	111.97
24	C	272	DMU	O1-C9-C11	4.03	116.06	106.41
23	P	1525	CHD	C13-C17-C20	4.03	124.38	119.49
24	Z	1526	DMU	O7-C3-C2	4.04	116.92	107.19
23	P	1271	CHD	C17-C13-C12	4.05	121.40	117.67
24	Z	1526	DMU	C7-C8-C9	4.05	117.36	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	C6-O5-C4	4.06	121.36	113.72
23	W	1060	CHD	C9-C10-C5	4.07	114.51	108.63
19	Q	1523	TGL	CG3-OG3-CC1	4.10	129.45	117.13
23	C	525	CHD	C6-C7-C8	4.14	115.90	111.50
23	B	1086	CHD	C15-C14-C13	4.14	107.69	103.57
22	O	1230	PSC	O01-C1-C2	4.14	120.16	111.55
23	W	1060	CHD	C16-C17-C20	4.17	118.81	112.14
20	N	1524	PGV	O01-C1-C2	4.18	120.24	111.55
19	L	522	TGL	CG2-OG2-CB1	4.19	127.77	117.88
24	M	526	DMU	C18-O16-C6	4.19	121.06	113.87
23	P	1271	CHD	C4-C5-C10	4.21	117.26	112.66
24	P	1272	DMU	C7-C8-C9	4.22	117.66	110.22
23	B	1086	CHD	C11-C9-C8	4.24	116.96	110.82
28	T	263	PEK	O03-C01-C02	4.24	119.32	108.66
24	C	272	DMU	O7-C3-C2	4.26	117.45	107.19
23	W	1060	CHD	C4-C5-C10	4.28	117.34	112.66
23	P	1271	CHD	C15-C14-C13	4.29	107.84	103.57
18	A	515	HEA	C12-C11-C3B	4.32	123.21	112.65
24	C	272	DMU	O7-C3-C4	4.33	119.99	109.34
28	G	265	PEK	O03-C21-C22	4.33	124.51	111.90
18	A	515	HEA	C16-C17-C18	4.34	126.85	111.97
23	P	1271	CHD	C11-C12-C13	4.36	115.74	111.22
23	C	525	CHD	C15-C14-C13	4.37	107.92	103.57
22	B	230	PSC	O01-C1-C2	4.39	120.66	111.55
19	L	522	TGL	OG1-CA1-CA2	4.39	124.69	111.90
23	B	1086	CHD	C14-C8-C9	4.40	115.62	109.64
19	L	522	TGL	CC3-CC2-CC1	4.42	129.70	113.58
19	D	523	TGL	OG2-CB1-OB1	4.43	134.72	123.68
23	B	1086	CHD	C9-C8-C7	4.45	117.15	111.92
24	M	526	DMU	O5-C4-C57	4.46	117.09	106.41
23	J	60	CHD	C9-C10-C5	4.46	115.06	108.63
24	P	1272	DMU	C6-C1-C2	4.48	118.31	109.98
26	P	1270	CDL	OB8-CB7-C71	4.49	124.96	111.90
23	O	229	CHD	C15-C14-C13	4.50	108.05	103.57
24	P	1272	DMU	C1-C2-C3	4.54	119.02	109.61
18	A	515	HEA	C13-C12-C11	4.54	121.34	114.46
26	C	270	CDL	OA8-CA7-C31	4.55	125.13	111.90
23	B	1086	CHD	C17-C13-C12	4.58	121.88	117.67
28	P	1264	PEK	C2-C3-C4	4.60	121.49	113.29
19	N	1521	TGL	OG2-CB1-CB2	4.60	121.10	111.55
23	W	1060	CHD	C11-C9-C8	4.61	117.50	110.82
19	A	521	TGL	OG1-CA1-CA2	4.61	125.30	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C3C-C4C-NC	4.61	115.17	109.21
23	P	1525	CHD	C19-C10-C1	4.61	115.81	108.24
23	W	1060	CHD	C15-C14-C13	4.63	108.18	103.57
26	C	270	CDL	OB8-CB7-C71	4.63	125.37	111.90
24	P	1272	DMU	O5-C4-C57	4.63	117.51	106.41
23	B	1086	CHD	C5-C4-C3	4.64	119.68	112.87
19	Q	1523	TGL	OG3-CC1-CC2	4.66	125.45	111.90
18	N	515	HEA	C26-C15-C16	4.68	123.41	115.29
20	P	1268	PGV	O01-C1-C2	4.69	121.29	111.55
26	G	269	CDL	OA6-CA5-C11	4.70	121.30	111.55
23	C	271	CHD	C9-C11-C12	4.71	120.53	114.32
18	N	515	HEA	C12-C11-C3B	4.73	124.21	112.65
23	P	1525	CHD	C6-C7-C8	4.76	116.56	111.50
24	C	272	DMU	C6-C1-C2	4.77	118.85	109.98
20	A	524	PGV	C02-O01-C1	4.79	129.18	117.88
19	L	522	TGL	OG1-CG1-CG2	4.79	120.68	108.66
23	P	1271	CHD	C9-C11-C12	4.80	120.65	114.32
23	J	60	CHD	C22-C20-C17	4.83	120.40	110.26
23	P	1525	CHD	C15-C14-C13	4.84	108.39	103.57
23	P	1525	CHD	C9-C11-C12	4.85	120.71	114.32
23	C	525	CHD	C11-C9-C10	4.86	118.88	113.74
26	P	1270	CDL	OA6-CA5-C11	4.86	121.64	111.55
28	T	263	PEK	O01-C1-C2	4.89	121.70	111.55
23	C	271	CHD	C11-C12-C13	4.89	116.28	111.22
23	C	525	CHD	C9-C11-C12	4.95	120.84	114.32
23	O	229	CHD	C4-C3-C2	4.95	116.70	110.55
23	B	1086	CHD	C15-C14-C8	5.03	125.44	118.32
24	P	1272	DMU	O5-C6-C1	5.04	120.02	110.30
28	G	1263	PEK	O01-C1-C2	5.07	122.07	111.55
24	Z	1526	DMU	C2-C3-C4	5.07	121.63	110.88
24	M	526	DMU	O5-C4-C3	5.08	120.14	109.75
23	C	271	CHD	C4-C3-C2	5.09	116.88	110.55
19	A	521	TGL	OG3-CG3-CG2	5.10	121.46	108.66
23	C	525	CHD	C5-C6-C7	5.12	120.10	114.44
26	C	270	CDL	OA6-CA5-C11	5.14	122.23	111.55
23	J	60	CHD	C4-C5-C10	5.16	118.29	112.66
23	O	229	CHD	C13-C14-C8	5.17	121.44	114.77
23	C	271	CHD	C16-C17-C13	5.19	108.73	103.57
19	L	522	TGL	OG3-CC1-CC2	5.19	127.01	111.90
23	P	1271	CHD	C14-C8-C7	5.20	118.85	111.80
23	C	271	CHD	C4-C5-C10	5.20	118.34	112.66
20	N	1266	PGV	O03-C19-C20	5.21	127.06	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C9-C11-C12	5.22	121.20	114.32
19	N	1521	TGL	CG3-OG3-CC1	5.22	132.83	117.13
23	P	1525	CHD	C14-C13-C12	5.23	112.35	107.39
24	Z	1526	DMU	O1-C9-C11	5.24	118.96	106.41
28	P	1265	PEK	O03-C21-C22	5.24	127.14	111.90
24	M	526	DMU	C8-C7-C5	5.24	120.08	110.84
23	W	1060	CHD	C11-C12-C13	5.25	116.66	111.22
23	C	525	CHD	C9-C8-C7	5.26	118.10	111.92
23	B	1086	CHD	C11-C9-C10	5.27	119.32	113.74
23	J	60	CHD	C16-C17-C20	5.27	120.58	112.14
23	P	1525	CHD	O3-C3-C4	5.30	120.44	109.87
23	C	271	CHD	C17-C13-C14	5.32	105.50	100.08
23	J	60	CHD	C11-C9-C8	5.32	118.53	110.82
18	A	516	HEA	C27-C19-C20	5.32	124.52	115.29
24	C	272	DMU	C8-C7-C5	5.34	120.25	110.84
23	P	1271	CHD	C16-C17-C13	5.34	108.89	103.57
19	D	523	TGL	CG1-OG1-CA1	5.34	133.20	117.13
24	Z	1526	DMU	O5-C4-C3	5.36	120.71	109.75
23	C	525	CHD	C11-C12-C13	5.36	116.77	111.22
24	C	272	DMU	O5-C4-C3	5.39	120.79	109.75
23	C	525	CHD	C2-C1-C10	5.40	122.21	112.80
24	Z	1526	DMU	C8-C7-C5	5.41	120.37	110.84
24	C	272	DMU	C2-C3-C4	5.41	122.36	110.88
20	C	268	PGV	O01-C1-C2	5.42	122.80	111.55
18	N	515	HEA	C27-C19-C20	5.42	124.69	115.29
23	O	229	CHD	C16-C17-C20	5.44	120.84	112.14
24	Z	1526	DMU	O5-C4-C57	5.45	119.47	106.41
23	P	1525	CHD	C5-C4-C3	5.47	120.89	112.87
23	J	60	CHD	C2-C1-C10	5.49	122.36	112.80
23	J	60	CHD	C11-C12-C13	5.49	116.91	111.22
23	C	271	CHD	C2-C1-C10	5.52	122.42	112.80
23	J	60	CHD	C15-C14-C8	5.53	126.14	118.32
24	P	1272	DMU	C8-C7-C5	5.53	120.60	110.84
23	C	525	CHD	C17-C13-C14	5.55	105.73	100.08
23	P	1271	CHD	C2-C1-C10	5.60	122.56	112.80
19	N	1522	TGL	OG2-CB1-CB2	5.64	123.27	111.55
20	C	268	PGV	O03-C19-C20	5.65	128.33	111.90
23	W	1060	CHD	C2-C1-C10	5.65	122.65	112.80
23	C	271	CHD	C15-C14-C13	5.69	109.23	103.57
19	A	521	TGL	OG3-CC1-CC2	5.70	128.48	111.90
18	A	515	HEA	C3C-C4C-NC	5.70	116.58	109.21
24	C	272	DMU	O5-C4-C57	5.71	120.08	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C26-C15-C16	5.71	125.20	115.29
23	P	1271	CHD	C17-C13-C14	5.73	105.91	100.08
24	C	272	DMU	O5-C6-C1	5.82	121.52	110.30
19	N	1521	TGL	CG2-OG2-CB1	5.84	131.67	117.88
23	C	525	CHD	C13-C17-C20	5.84	126.58	119.49
23	C	271	CHD	C17-C13-C12	5.89	123.09	117.67
26	G	269	CDL	OB6-CB5-C51	5.91	123.82	111.55
23	C	271	CHD	C11-C9-C8	5.91	119.40	110.82
24	C	272	DMU	C18-O16-C6	5.92	124.02	113.87
24	P	1272	DMU	O1-C9-C11	5.92	120.59	106.41
24	P	1272	DMU	O5-C4-C3	5.93	121.89	109.75
23	J	60	CHD	C15-C14-C13	5.94	109.48	103.57
23	W	1060	CHD	C14-C13-C12	5.94	113.03	107.39
23	P	1525	CHD	C16-C17-C20	5.95	121.66	112.14
23	O	229	CHD	C1-C2-C3	5.97	118.03	110.42
23	J	60	CHD	C16-C17-C13	6.00	109.55	103.57
23	O	229	CHD	C11-C12-C13	6.02	117.45	111.22
23	P	1525	CHD	C11-C12-C13	6.06	117.49	111.22
23	J	60	CHD	C14-C8-C7	6.06	120.02	111.80
24	M	526	DMU	C2-C3-C4	6.08	123.78	110.88
26	T	1269	CDL	OA6-CA5-C11	6.14	124.30	111.55
23	W	1060	CHD	C15-C14-C8	6.17	127.05	118.32
24	Z	1526	DMU	O16-C6-C1	6.17	118.30	108.23
19	A	521	TGL	CG3-OG3-CC1	6.19	135.76	117.13
23	W	1060	CHD	C1-C2-C3	6.26	118.40	110.42
23	P	1271	CHD	C4-C3-C2	6.33	118.41	110.55
23	J	60	CHD	C17-C13-C12	6.33	123.50	117.67
23	P	1271	CHD	C1-C2-C3	6.34	118.50	110.42
23	J	60	CHD	C4-C3-C2	6.37	118.46	110.55
23	C	271	CHD	C5-C6-C7	6.37	121.49	114.44
23	W	1060	CHD	C17-C13-C12	6.42	123.58	117.67
23	B	1086	CHD	C1-C2-C3	6.42	118.61	110.42
23	W	1060	CHD	C9-C11-C12	6.46	122.84	114.32
20	P	1268	PGV	O03-C19-C20	6.48	130.77	111.90
24	P	1272	DMU	O16-C6-C1	6.51	118.86	108.23
23	W	1060	CHD	C5-C4-C3	6.54	122.47	112.87
24	C	272	DMU	O16-C6-C1	6.55	118.92	108.23
23	C	271	CHD	C1-C10-C5	6.57	117.97	107.79
23	P	1271	CHD	C5-C6-C7	6.57	121.71	114.44
23	P	1525	CHD	C10-C9-C8	6.58	118.97	111.87
23	J	60	CHD	C5-C4-C3	6.63	122.60	112.87
24	P	1272	DMU	O1-C9-C8	6.63	121.88	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O1-C10-C5	6.64	123.10	110.30
23	J	60	CHD	C5-C6-C7	6.65	121.80	114.44
23	B	1086	CHD	C9-C11-C12	6.71	123.17	114.32
23	C	271	CHD	C5-C4-C3	6.72	122.74	112.87
23	C	271	CHD	C14-C13-C12	6.79	113.83	107.39
23	P	1271	CHD	C16-C17-C20	6.79	123.02	112.14
24	Z	1526	DMU	O1-C10-C5	6.81	123.43	110.30
23	C	525	CHD	C5-C4-C3	6.86	122.94	112.87
26	T	1269	CDL	OB6-CB5-C51	6.90	125.87	111.55
23	J	60	CHD	C6-C5-C10	6.91	120.21	112.66
23	W	1060	CHD	C6-C7-C8	6.92	118.85	111.50
24	C	272	DMU	O1-C10-C5	6.93	123.66	110.30
23	O	229	CHD	C11-C9-C8	6.95	120.90	110.82
23	J	60	CHD	C1-C10-C5	6.98	118.61	107.79
23	W	1060	CHD	C6-C5-C10	6.99	120.30	112.66
23	P	1271	CHD	C14-C13-C12	6.99	114.03	107.39
24	C	272	DMU	O1-C9-C8	7.02	122.59	109.66
24	M	526	DMU	O1-C10-C5	7.04	123.87	110.30
24	Z	1526	DMU	O1-C9-C8	7.06	122.67	109.66
23	P	1271	CHD	C1-C10-C5	7.08	118.76	107.79
23	J	60	CHD	C14-C13-C12	7.19	114.21	107.39
23	J	60	CHD	C13-C17-C20	7.21	128.23	119.49
23	C	525	CHD	C14-C13-C12	7.21	114.23	107.39
23	J	60	CHD	C1-C2-C3	7.25	119.66	110.42
23	O	229	CHD	C17-C13-C14	7.25	107.47	100.08
23	W	1060	CHD	C4-C3-C2	7.30	119.61	110.55
23	B	1086	CHD	C17-C13-C14	7.31	107.52	100.08
24	M	526	DMU	O1-C9-C8	7.32	123.14	109.66
23	B	1086	CHD	C6-C7-C8	7.38	119.34	111.50
23	W	1060	CHD	C16-C17-C13	7.46	111.00	103.57
23	W	1060	CHD	C1-C10-C5	7.54	119.47	107.79
23	J	60	CHD	C6-C7-C8	7.54	119.52	111.50
23	P	1271	CHD	C5-C4-C3	7.60	124.02	112.87
23	W	1060	CHD	C13-C17-C20	7.60	128.71	119.49
24	Z	1526	DMU	O5-C6-C1	7.61	124.97	110.30
23	W	1060	CHD	C14-C8-C7	7.61	122.12	111.80
23	P	1271	CHD	C11-C9-C8	7.66	121.92	110.82
23	O	229	CHD	C5-C4-C3	7.70	124.17	112.87
23	W	1060	CHD	C5-C6-C7	7.72	122.98	114.44
23	P	1525	CHD	C9-C8-C7	7.75	121.03	111.92
23	P	1271	CHD	C15-C14-C8	7.82	129.38	118.32
23	P	1271	CHD	C6-C7-C8	7.83	119.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C6-C7-C8	7.88	119.88	111.50
23	B	1086	CHD	C4-C3-C2	7.92	120.38	110.55
23	C	271	CHD	C1-C2-C3	7.94	120.54	110.42
23	C	271	CHD	C15-C14-C8	7.95	129.56	118.32
23	P	1271	CHD	C6-C5-C10	7.99	121.39	112.66
23	C	525	CHD	C17-C13-C12	8.15	125.17	117.67
23	C	271	CHD	C6-C5-C10	8.33	121.75	112.66
19	A	521	TGL	OG2-CB1-CB2	8.33	128.85	111.55
23	C	525	CHD	C4-C3-C2	8.35	120.92	110.55
23	O	229	CHD	C10-C9-C8	8.48	121.01	111.87
23	P	1525	CHD	C11-C9-C10	8.52	122.77	113.74
23	P	1525	CHD	C17-C13-C14	8.59	108.83	100.08
24	M	526	DMU	O5-C6-C1	8.61	126.91	110.30
23	O	229	CHD	C14-C13-C12	8.67	115.61	107.39
19	A	521	TGL	CG2-OG2-CB1	8.68	138.39	117.88
23	C	271	CHD	C16-C17-C20	8.72	126.10	112.14
23	B	1086	CHD	C10-C9-C8	9.02	121.59	111.87
23	P	1525	CHD	C4-C3-C2	9.02	121.75	110.55
23	P	1525	CHD	C17-C13-C12	9.24	126.16	117.67
23	C	525	CHD	C10-C9-C8	9.84	122.47	111.87
23	C	525	CHD	C1-C10-C5	9.88	123.11	107.79
23	O	229	CHD	C9-C8-C7	9.99	123.66	111.92
23	C	525	CHD	C6-C5-C10	10.21	123.81	112.66
23	B	1086	CHD	C6-C5-C10	10.48	124.11	112.66
23	O	229	CHD	C17-C13-C12	10.81	127.61	117.67
23	O	229	CHD	C1-C10-C5	10.88	124.65	107.79
23	P	1525	CHD	C1-C10-C5	11.19	125.13	107.79
28	G	264	PEK	C2-C3-C4	11.24	133.35	113.29
23	B	1086	CHD	C14-C13-C12	11.41	118.22	107.39
23	J	60	CHD	C10-C9-C8	11.81	124.59	111.87
23	W	1060	CHD	C10-C9-C8	12.27	125.10	111.87
23	P	1525	CHD	C6-C5-C10	12.73	126.57	112.66
23	B	1086	CHD	C1-C10-C5	13.55	128.80	107.79
23	C	271	CHD	C10-C9-C8	14.55	127.55	111.87
23	P	1271	CHD	C10-C9-C8	15.34	128.40	111.87
23	O	229	CHD	C6-C5-C10	15.75	129.86	112.66

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	W	1060	CHD	C17
23	W	1060	CHD	C9

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Mol	Chain	Res	Type	Atom
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C9
24	M	526	DMU	C5
18	N	515	HEA	ND
18	N	515	HEA	NB
23	C	271	CHD	C9
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2
24	C	272	DMU	C3
23	O	229	CHD	C9
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
23	J	60	CHD	C17
23	J	60	CHD	C9
24	P	1272	DMU	C2
24	P	1272	DMU	C4
24	P	1272	DMU	C9
24	P	1272	DMU	C6
24	P	1272	DMU	C5
23	P	1271	CHD	C9

All (3) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C02-O01-C1-C2
26	G	269	CDL	PB2-OB2-CB2-C1

There are no ring outliers.

44 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	7	0
18	A	516	HEA	5	0
15	A	520	PER	1	0
19	A	521	TGL	6	0
20	A	522	PGV	2	0
20	A	524	PGV	8	0
23	B	1086	CHD	1	0
22	B	230	PSC	18	0
20	C	267	PGV	5	0
20	C	268	PGV	1	0
26	C	270	CDL	13	0
23	C	271	CHD	3	0
24	C	272	DMU	5	0
23	C	525	CHD	2	0
19	D	523	TGL	15	0
28	G	1263	PEK	7	0
28	G	264	PEK	6	0
28	G	265	PEK	7	0
26	G	269	CDL	24	0
23	J	60	CHD	3	0
19	L	522	TGL	16	0
24	M	526	DMU	1	0
20	N	1266	PGV	1	0
19	N	1521	TGL	9	0
19	N	1522	TGL	11	0
20	N	1524	PGV	6	0
18	N	515	HEA	8	0
18	N	516	HEA	1	0
15	N	520	PER	1	0
22	O	1230	PSC	12	0
23	O	229	CHD	2	0
28	P	1264	PEK	6	0
28	P	1265	PEK	8	0
20	P	1267	PGV	5	0
20	P	1268	PGV	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	1270	CDL	16	0
23	P	1271	CHD	3	0
24	P	1272	DMU	2	0
23	P	1525	CHD	3	0
19	Q	1523	TGL	5	0
26	T	1269	CDL	23	0
28	T	263	PEK	21	0
23	W	1060	CHD	4	0
24	Z	1526	DMU	1	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%)	-0.14	1 (0%) 94 95	20, 25, 32, 63	0
1	N	513/514 (99%)	-0.21	1 (0%) 94 95	24, 31, 38, 63	0
2	B	226/227 (99%)	-0.54	0 100 100	21, 29, 49, 77	0
2	O	226/227 (99%)	-0.26	4 (1%) 69 73	28, 37, 56, 77	0
3	C	259/261 (99%)	-0.66	1 (0%) 92 93	22, 28, 40, 63	0
3	P	259/261 (99%)	-0.53	3 (1%) 79 82	25, 32, 43, 63	0
4	D	144/147 (97%)	-0.55	1 (0%) 87 89	25, 31, 48, 64	0
4	Q	144/147 (97%)	0.72	19 (13%) 4 5	33, 44, 67, 108	0
5	E	104/109 (95%)	-0.57	3 (2%) 52 59	26, 31, 51, 65	0
5	R	104/109 (95%)	-0.14	3 (2%) 52 59	31, 38, 58, 74	0
6	F	93/98 (94%)	-0.18	3 (3%) 48 55	23, 34, 52, 94	0
6	S	93/98 (94%)	0.19	4 (4%) 36 43	29, 38, 59, 91	0
7	G	83/85 (97%)	0.33	15 (18%) 1 2	25, 35, 94, 102	0
7	T	83/85 (97%)	0.53	18 (21%) 1 1	27, 38, 93, 100	0
8	H	75/85 (88%)	-0.13	8 (10%) 7 8	28, 36, 69, 75	0
8	U	75/85 (88%)	0.14	6 (8%) 13 17	32, 41, 72, 76	0
9	I	71/73 (97%)	0.18	7 (9%) 8 10	28, 38, 65, 70	0
9	V	71/73 (97%)	0.61	10 (14%) 3 4	30, 48, 65, 75	0
10	J	57/59 (96%)	-0.17	4 (7%) 17 22	28, 37, 57, 70	0
10	W	57/59 (96%)	0.52	9 (15%) 2 3	33, 42, 62, 79	0
11	K	49/56 (87%)	-0.26	0 100 100	28, 35, 47, 55	0
11	X	49/56 (87%)	1.38	13 (26%) 1 1	38, 45, 60, 71	0
12	L	46/47 (97%)	-0.42	3 (6%) 20 25	26, 31, 51, 75	0
12	Y	46/47 (97%)	0.05	3 (6%) 20 25	33, 39, 60, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.09	6 (13%) 3 4	27, 30, 65, 89	0
13	Z	43/46 (93%)	0.57	8 (18%) 1 2	35, 39, 77, 95	0
All	All	3526/3614 (97%)	-0.15	153 (4%) 36 43	20, 33, 58, 108	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	17.2
4	Q	5	VAL	11.9
4	Q	4	SER	10.4
6	F	96	LEU	9.0
4	Q	8	SER	8.9
13	Z	43	SER	8.5
6	S	96	LEU	7.7
7	G	8	HIS	7.0
10	W	57	HIS	6.7
6	S	94	HIS	6.4
11	X	6	ALA	6.4
13	M	43	SER	6.2
10	W	52	TRP	6.2
6	F	95	GLN	5.9
12	Y	47	LYS	5.7
7	T	36	TRP	5.5
7	T	42	ARG	5.4
7	T	8	HIS	5.3
7	G	40	GLY	5.3
8	H	45	ALA	5.1
6	S	95	GLN	5.0
7	G	3	ALA	5.0
11	X	13	TYR	5.0
10	W	56	PRO	4.9
13	Z	42	LYS	4.8
11	X	7	PRO	4.8
4	Q	7	LYS	4.6
9	V	37	PHE	4.6
10	W	55	PHE	4.6
9	I	29	LEU	4.5
7	T	3	ALA	4.5
2	O	113	TYR	4.4
7	G	2	SER	4.4
7	T	40	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
9	I	37	PHE	4.3
6	F	94	HIS	4.3
6	S	93	PRO	4.3
13	Z	39	ASN	4.3
7	G	42	ARG	4.3
7	T	39	SER	4.2
13	M	42	LYS	4.1
7	T	84	LYS	4.0
7	G	5	LYS	4.0
13	Z	40	TYR	3.9
4	Q	147	LYS	3.9
7	T	41	HIS	3.9
9	I	34	PHE	3.9
2	O	227	LEU	3.8
8	H	47	GLY	3.8
7	T	2	SER	3.8
2	O	91	ASN	3.7
7	G	10	GLY	3.6
7	T	4	ALA	3.6
11	X	19	ALA	3.6
3	P	3	HIS	3.6
9	V	30	GLY	3.5
7	T	1	ALA	3.5
7	T	10	GLY	3.5
7	G	1	ALA	3.5
9	V	34	PHE	3.4
5	R	109	VAL	3.4
9	I	25	PHE	3.4
11	X	23	THR	3.4
7	G	36	TRP	3.3
10	W	48	TYR	3.3
12	L	2	HIS	3.3
4	Q	51	LEU	3.2
8	U	45	ALA	3.2
11	X	12	LYS	3.2
10	J	57	HIS	3.2
7	T	5	LYS	3.2
9	I	26	MET	3.2
9	I	33	THR	3.1
7	T	37	LEU	3.1
4	Q	9	GLU	3.1
10	J	52	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
7	G	84	LYS	3.0
7	G	41	HIS	3.0
11	X	47	ARG	3.0
10	J	56	PRO	3.0
4	Q	33	LEU	3.0
8	U	50	VAL	3.0
10	W	1	PHE	2.9
3	P	38	ASN	2.9
9	V	29	LEU	2.9
5	E	109	VAL	2.8
12	L	45	LEU	2.8
9	V	26	MET	2.8
5	R	108	LYS	2.8
4	Q	48	TRP	2.8
13	M	40	TYR	2.8
5	R	96	LEU	2.8
8	U	44	THR	2.7
8	U	49	ASP	2.7
4	Q	46	ALA	2.7
10	W	26	ALA	2.7
4	Q	58	GLU	2.7
4	Q	39	ALA	2.7
2	O	217	LYS	2.7
9	V	53	ASN	2.7
10	J	1	PHE	2.7
7	G	7	ASP	2.7
1	N	513	LEU	2.7
7	T	43	GLU	2.6
8	H	49	ASP	2.6
7	G	4	ALA	2.6
8	U	47	GLY	2.6
13	Z	35	TYR	2.5
5	E	7	THR	2.5
13	M	39	ASN	2.5
8	U	42	ALA	2.5
13	Z	32	TRP	2.5
13	Z	41	LYS	2.5
9	V	33	THR	2.5
9	V	36	LYS	2.5
4	Q	10	ASP	2.4
11	X	46	GLY	2.4
4	Q	35	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
11	X	34	THR	2.4
11	X	17	VAL	2.4
4	Q	142	LYS	2.3
3	P	37	PHE	2.3
7	G	43	GLU	2.3
12	L	47	LYS	2.3
7	G	9	GLY	2.3
9	V	3	ALA	2.3
10	W	30	ILE	2.3
9	V	25	PHE	2.3
4	D	147	LYS	2.3
10	W	2	GLU	2.3
13	Z	13	LYS	2.2
4	Q	62	LEU	2.2
11	X	16	ALA	2.2
13	M	38	ASP	2.2
8	H	46	LYS	2.2
8	H	48	GLY	2.2
8	H	44	THR	2.2
5	E	9	GLU	2.1
4	Q	31	LYS	2.1
4	Q	49	SER	2.1
12	Y	45	LEU	2.1
3	C	3	HIS	2.1
1	A	66	ILE	2.1
13	M	41	LYS	2.1
8	H	43	MET	2.1
11	X	15	ASN	2.1
9	I	30	GLY	2.1
12	Y	20	ARG	2.0
7	T	45	PRO	2.0
7	T	38	HIS	2.0
8	H	50	VAL	2.0
11	X	52	GLU	2.0
7	T	9	GLY	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
7	TPO	G	11	11/12	0.53	0.34	-	68,74,91,92	0
2	FME	O	1	10/11	0.96	0.11	-	36,37,46,55	0
1	FME	N	1	10/11	0.91	0.20	-	48,54,69,70	0
2	FME	B	1	10/11	0.97	0.14	-	27,29,39,57	0
1	FME	A	1	10/11	0.91	0.16	-	42,48,68,76	0
7	TPO	T	11	11/12	0.38	0.36	-	70,77,97,98	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CHD	W	1060	29/29	0.52	0.46	9.67	107,109,111,111	0
20	PGV	A	524	51/51	0.77	0.23	9.10	33,71,98,101	0
24	DMU	C	272	33/33	0.30	0.36	7.63	70,99,105,105	0
26	CDL	C	270	100/100	0.77	0.25	6.14	43,84,127,129	0
23	CHD	J	60	29/29	0.67	0.41	5.67	99,100,106,106	0
19	TGL	N	1522	63/63	0.59	0.31	5.60	45,73,89,92	0
26	CDL	P	1270	100/100	0.72	0.27	5.24	43,87,117,123	0
19	TGL	L	522	63/63	0.71	0.26	4.62	36,66,84,86	0
24	DMU	P	1272	33/33	0.47	0.40	4.43	89,103,109,111	0
15	PER	A	520	2/2	0.99	0.21	3.87	16,16,16,19	0
22	PSC	O	1230	52/52	0.66	0.30	3.84	41,93,121,122	0
19	TGL	A	521	63/63	0.81	0.21	3.48	47,71,92,98	0
19	TGL	D	523	63/63	0.76	0.19	3.48	41,69,96,98	0
19	TGL	N	1521	63/63	0.74	0.23	3.25	53,75,92,94	0
20	PGV	N	1266	51/51	0.96	0.21	3.21	28,41,63,64	0
22	PSC	B	230	52/52	0.68	0.28	2.94	39,96,121,123	0
20	PGV	A	522	51/51	0.97	0.18	2.58	25,37,63,68	0
20	PGV	C	267	51/51	0.96	0.17	2.58	20,31,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
19	TGL	Q	1523	63/63	0.67	0.20	2.48	53,78,92,94	0
28	PEK	G	264	53/53	0.96	0.18	2.48	23,43,71,73	0
26	CDL	G	269	100/100	0.66	0.26	2.46	62,86,114,116	0
20	PGV	N	1524	51/51	0.76	0.22	2.45	43,72,104,106	0
23	CHD	C	271	29/29	0.85	0.23	2.35	59,69,71,72	0
28	PEK	P	1265	53/53	0.59	0.30	2.30	42,86,105,108	0
20	PGV	P	1267	51/51	0.96	0.17	2.17	21,37,76,85	0
20	PGV	P	1268	51/51	0.73	0.23	2.04	64,97,112,113	0
28	PEK	G	265	53/53	0.49	0.27	1.89	45,91,106,111	0
15	PER	N	520	2/2	0.97	0.13	1.78	20,20,20,27	0
23	CHD	P	1271	29/29	0.88	0.21	1.68	68,74,77,78	0
20	PGV	C	268	51/51	0.72	0.19	1.60	59,88,104,105	0
24	DMU	Z	1526	33/33	0.77	0.20	1.51	42,51,63,65	0
28	PEK	P	1264	53/53	0.95	0.17	1.50	26,47,80,82	0
26	CDL	T	1269	100/100	0.69	0.22	1.45	52,85,111,116	0
28	PEK	T	263	53/53	0.54	0.30	1.28	48,93,126,127	0
28	PEK	G	1263	53/53	0.57	0.32	1.22	50,107,128,129	0
24	DMU	M	526	33/33	0.85	0.14	0.69	35,44,55,60	0
18	HEA	N	515	60/60	0.97	0.15	0.66	22,28,54,56	0
18	HEA	A	515	60/60	0.98	0.15	0.14	16,23,46,47	0
18	HEA	N	516	60/60	0.98	0.12	-0.02	23,28,35,38	0
21	CUA	B	228	2/2	1.00	0.10	-0.09	23,23,23,26	0
23	CHD	C	525	29/29	0.95	0.08	-0.28	24,32,36,43	0
23	CHD	B	1086	29/29	0.96	0.08	-0.35	23,28,35,44	0
16	MG	A	518	1/1	0.98	0.12	-0.45	21,21,21,21	0
18	HEA	A	516	60/60	0.99	0.11	-0.49	13,22,29,32	0
17	NA	A	519	1/1	0.98	0.07	-0.55	25,25,25,25	0
23	CHD	P	1525	29/29	0.94	0.09	-0.57	25,33,39,39	0
27	ZN	F	99	1/1	1.00	0.07	-0.58	30,30,30,30	0
23	CHD	O	229	29/29	0.96	0.07	-0.62	21,25,34,39	0
27	ZN	S	99	1/1	0.99	0.06	-1.14	34,34,34,34	0
16	MG	N	1518	1/1	0.91	0.09	-1.49	29,29,29,29	0
21	CUA	O	228	2/2	0.97	0.07	-1.52	31,31,31,32	0
17	NA	N	1519	1/1	0.95	0.06	-1.84	30,30,30,30	0
14	CU	N	517	1/1	1.00	0.13	-	30,30,30,30	0
14	CU	A	517	1/1	0.99	0.11	-	24,24,24,24	0
25	UNX	C	262	1/1	0.68	0.27	-	39,39,39,39	0
25	UNX	P	1262	1/1	0.76	0.33	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.