Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:55 AM GMT

PDB ID	:	2EIJ
Title	:	Bovine heart cytochrome C oxidase in the fully reduced state
Authors	:	Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2007-03-13
Resolution	:	1.90 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 (i) symbol.

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

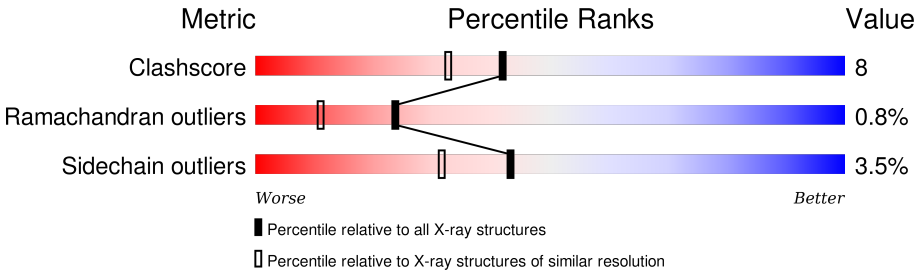
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	88% 11% •
1	N	514	82% 17% •
2	B	227	84% 15% •
2	O	227	73% 25% •
3	C	261	89% 11% •
3	P	261	87% 11% ••
4	D	147	89% 9% •

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Mol	Chain	Length	Quality of chain
4	Q	147	76% 21%
5	E	109	85% 11%
5	R	109	78% 18%
6	F	98	80% 17%
6	S	98	74% 18% 5%
7	G	85	74% 16% 8%
7	T	85	74% 20% 5%
8	H	85	80% 12% 7%
8	U	85	75% 15% 7%
9	I	73	90% 8%
9	V	73	86% 14%
10	J	59	90% 7%
10	W	59	90% 8%
11	K	56	77% 11% 13%
11	X	56	73% 13% 13%
12	L	47	81% 17%
12	Y	47	81% 15%
13	M	46	74% 17% 7%
13	Z	46	63% 28% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
22	CHD	C	271	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	DMU	C	272	X	-	-	-
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	-
23	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 32488 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 polypeptide Va.

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

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

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

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

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

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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

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

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

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 polypeptide VIIc.

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 polypeptide VIII-heart.

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		

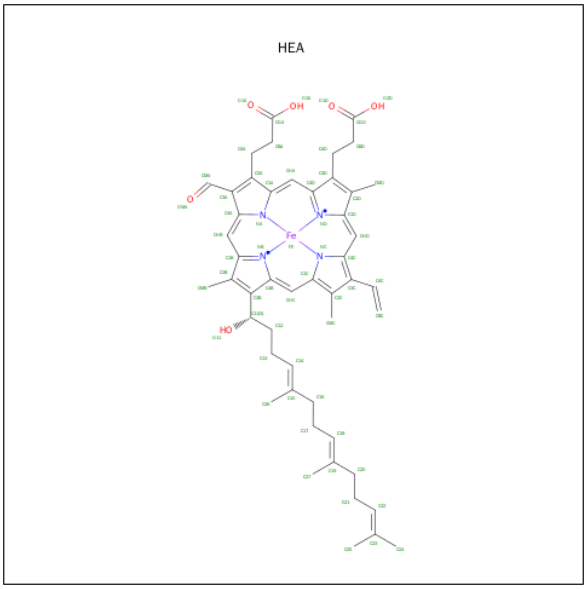
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

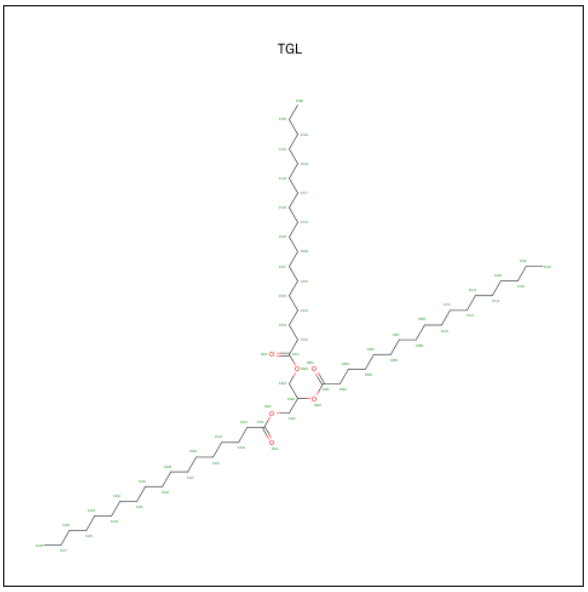
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



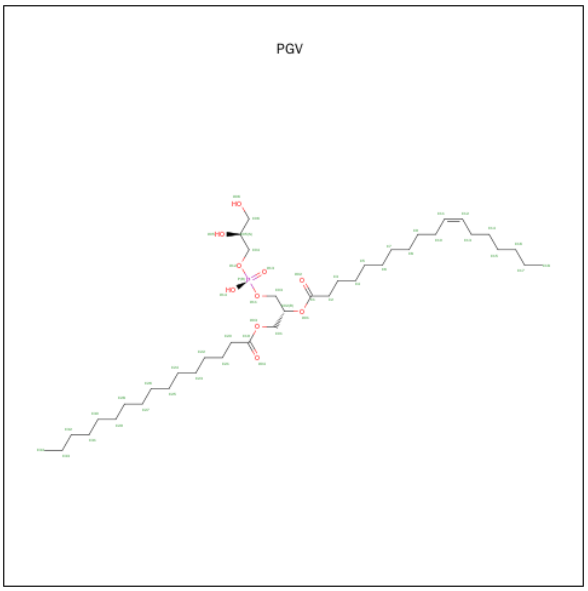
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



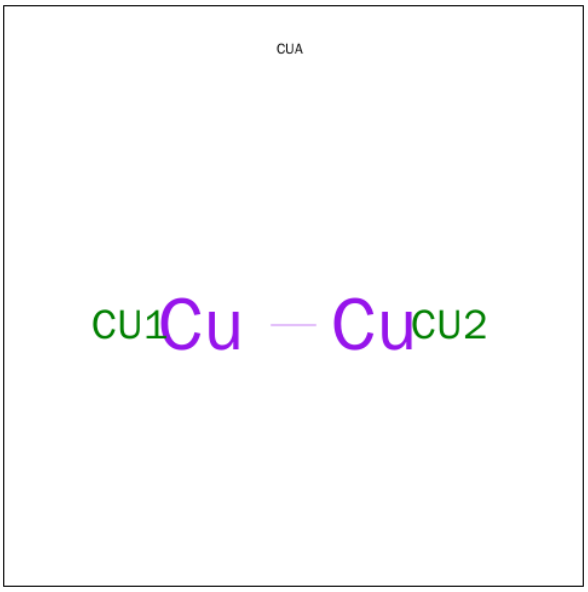
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	B	1	Total C O 63 57 6	0	0
18	L	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



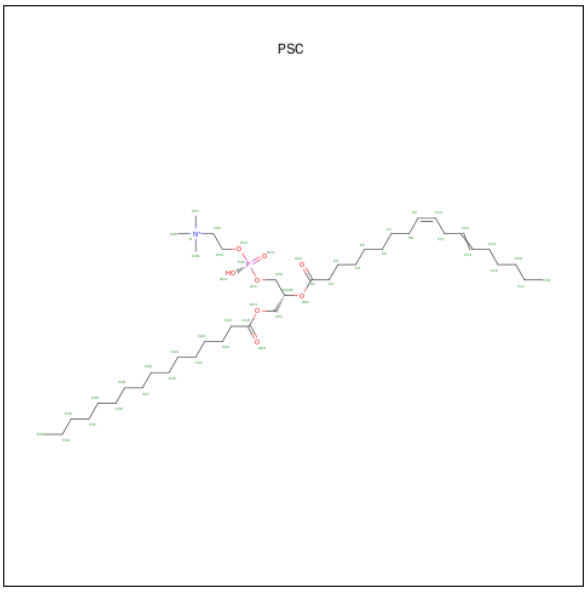
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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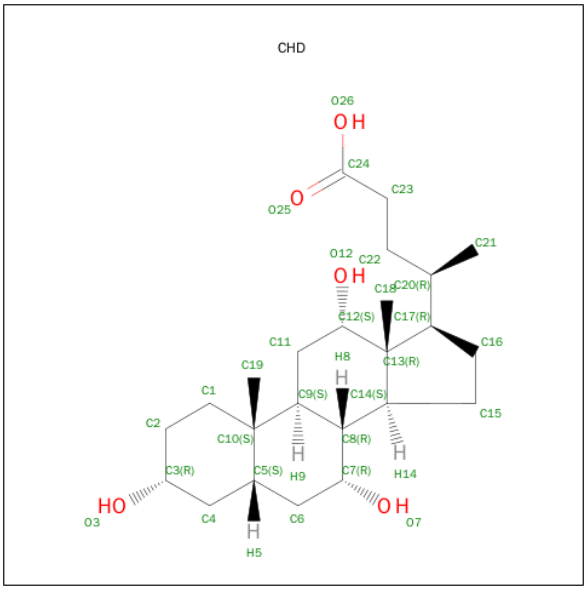
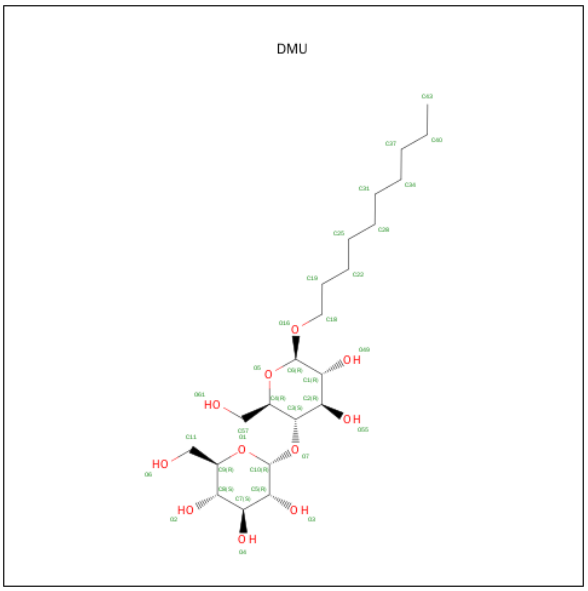
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 23 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

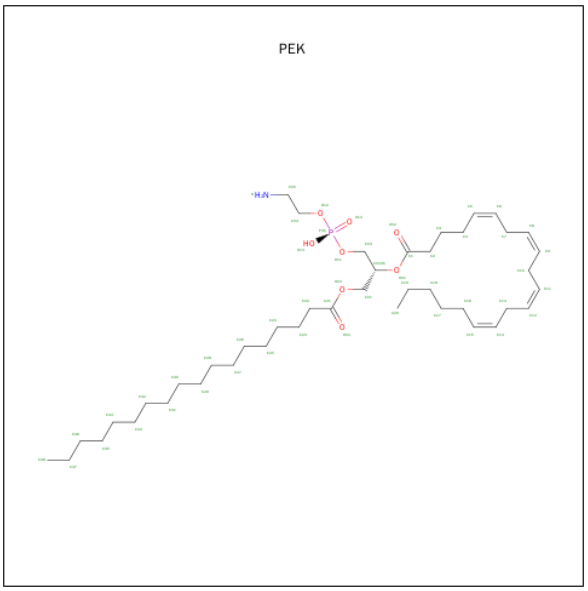


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 33 22 11	0	0
23	M	1	Total C O 33 22 11	0	0
23	P	1	Total C O 33 22 11	0	0
23	Z	1	Total C O 33 22 11	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

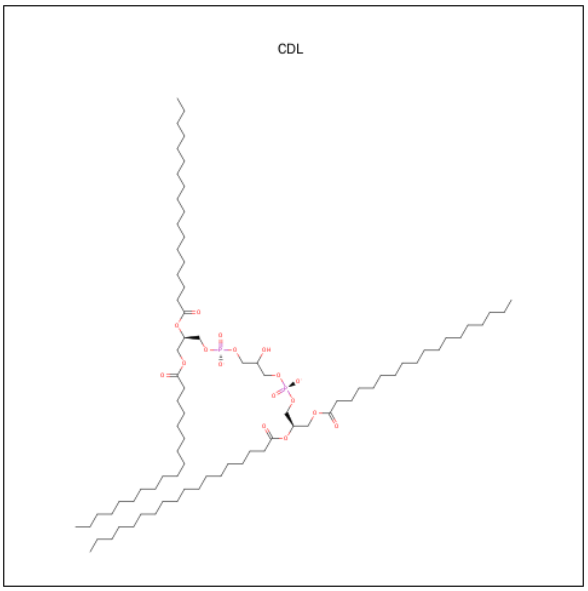
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total Zn 1 1	0	0
24	C	1	Total Zn 1 1	0	0
24	F	1	Total Zn 1 1	0	0
24	S	1	Total Zn 1 1	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- 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	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	237	Total	O	0	0
			237	237		
27	B	145	Total	O	0	0
			145	145		
27	C	110	Total	O	0	0
			110	110		
27	D	94	Total	O	0	0
			94	94		
27	E	60	Total	O	0	0
			60	60		
27	F	72	Total	O	0	0
			72	72		
27	G	44	Total	O	0	0
			44	44		
27	H	50	Total	O	0	0
			50	50		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	38	Total O 38 38	0	0
27	J	23	Total O 23 23	0	0
27	K	22	Total O 22 22	0	0
27	L	27	Total O 27 27	0	0
27	M	24	Total O 24 24	0	0
27	N	218	Total O 218 218	0	0
27	O	122	Total O 122 122	0	0
27	P	112	Total O 112 112	0	0
27	Q	53	Total O 53 53	0	0
27	R	45	Total O 45 45	0	0
27	S	76	Total O 76 76	0	0
27	T	42	Total O 42 42	0	0
27	U	46	Total O 46 46	0	0
27	V	25	Total O 25 25	0	0
27	W	18	Total O 18 18	0	0
27	X	21	Total O 21 21	0	0
27	Y	17	Total O 17 17	0	0
27	Z	15	Total O 15 15	0	0

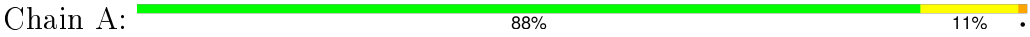
3 Residue-property plots (i)

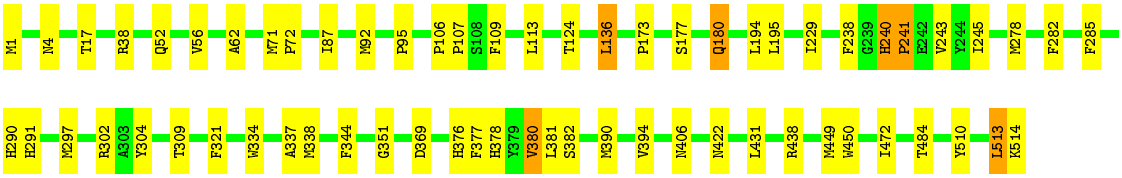
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1

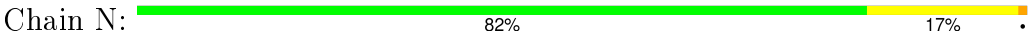
Chain A:

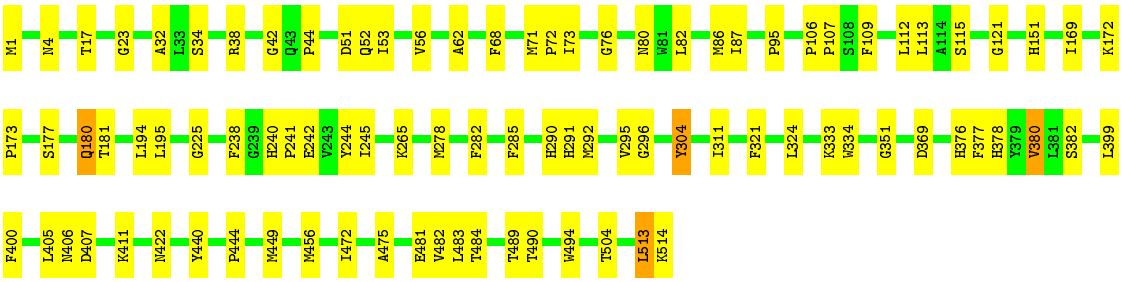




• Molecule 1: Cytochrome c oxidase subunit 1

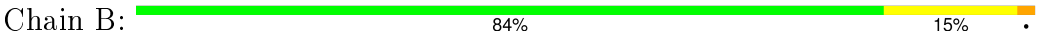
Chain N:

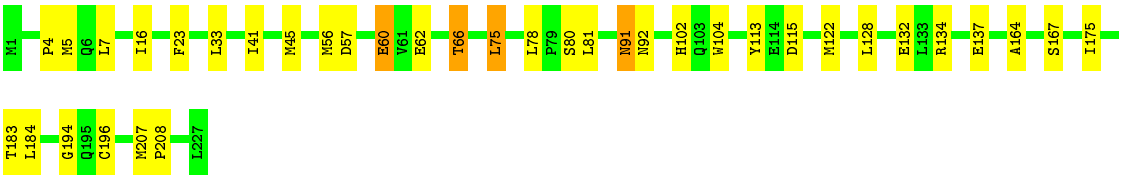




• Molecule 2: Cytochrome c oxidase subunit 2

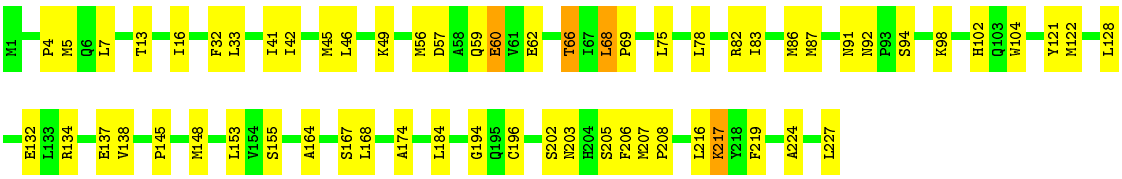
Chain B:





• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

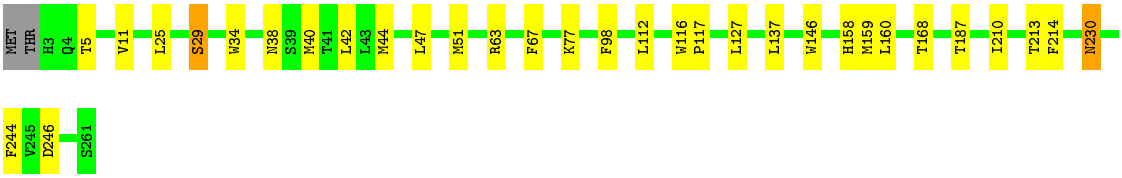


• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

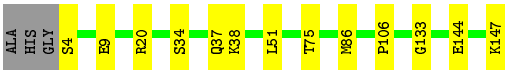
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



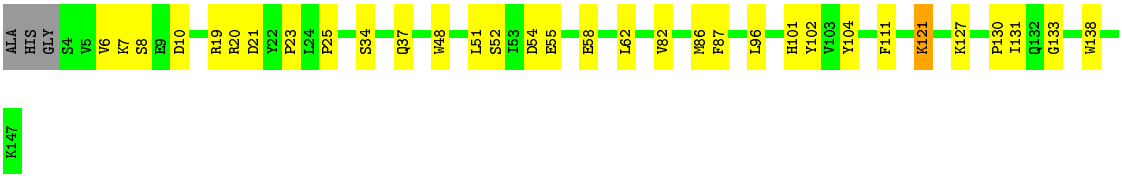
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



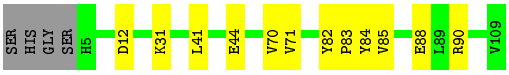
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



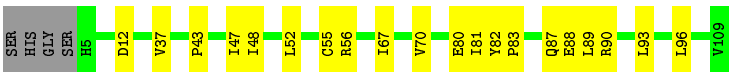
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



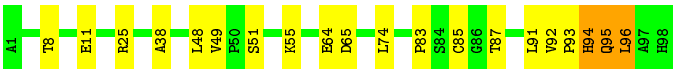
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



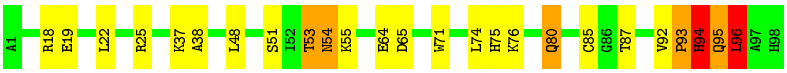
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:



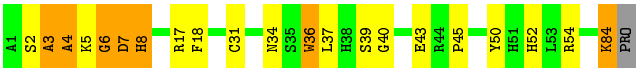
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:



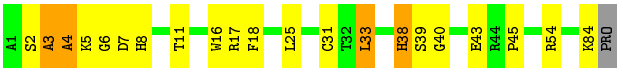
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



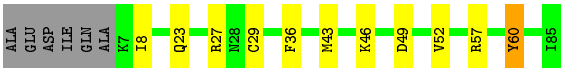
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:

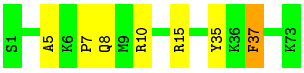


• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:

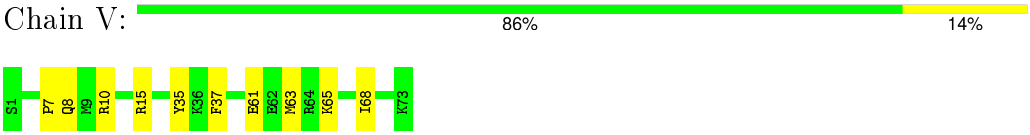
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



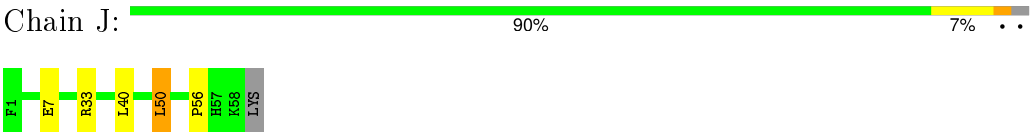
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



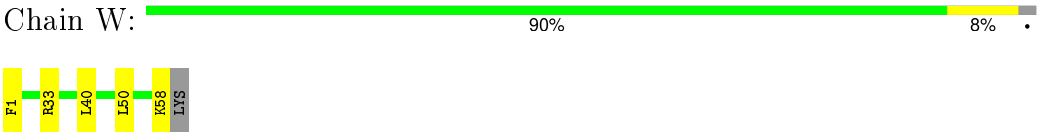
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:



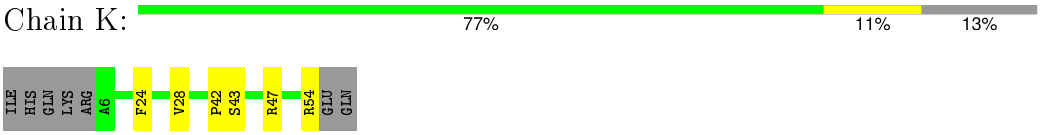
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



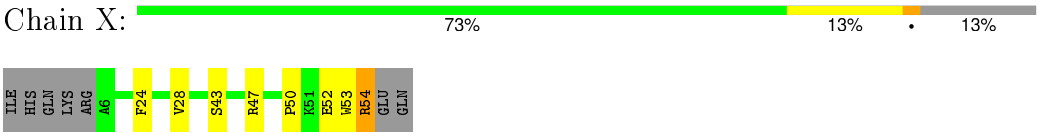
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



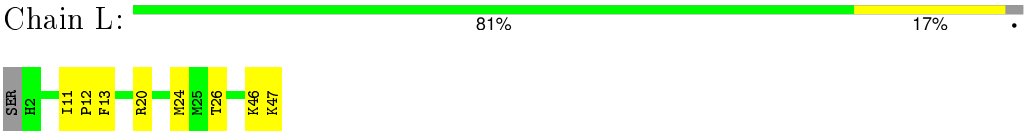
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



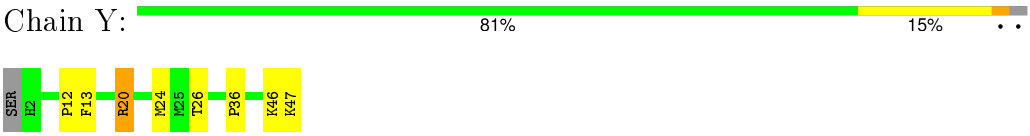
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



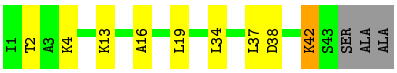
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.06Å 206.58Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32488	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

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, PGV, SAC, 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	0.52	0/4156	0.69	2/5678 (0.0%)
1	N	0.52	0/4156	0.66	0/5678
2	B	0.51	0/1860	0.77	1/2534 (0.0%)
2	O	0.52	0/1860	0.79	1/2534 (0.0%)
3	C	0.53	0/2197	0.59	0/3005
3	P	0.51	0/2197	0.62	1/3005 (0.0%)
4	D	0.51	0/1229	0.67	1/1658 (0.1%)
4	Q	0.54	0/1229	0.67	1/1658 (0.1%)
5	E	0.53	0/871	0.67	0/1182
5	R	0.54	0/871	0.70	0/1182
6	F	0.50	0/765	0.82	2/1038 (0.2%)
6	S	0.49	0/765	0.81	2/1038 (0.2%)
7	G	0.51	0/690	0.71	1/937 (0.1%)
7	T	0.55	0/690	0.72	1/937 (0.1%)
8	H	0.49	0/682	0.68	0/921
8	U	0.48	0/682	0.69	0/921
9	I	0.52	0/605	0.61	0/802
9	V	0.49	0/605	0.60	0/802
10	J	0.46	0/471	0.63	0/636
10	W	0.48	0/471	0.65	0/636
11	K	0.53	0/398	0.68	0/546
11	X	0.50	0/398	0.66	0/546
12	L	0.51	0/393	0.59	0/526
12	Y	0.54	0/393	0.60	0/526
13	M	0.50	0/345	0.65	0/470
13	Z	0.47	0/345	0.60	0/470
All	All	0.52	0/29324	0.68	13/39866 (0.0%)

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

of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	3
8	U	0	1
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	33	LEU	CA-CB-CG	6.53	130.31	115.30
6	S	94	HIS	N-CA-C	6.39	128.27	111.00
4	D	133	GLY	N-CA-C	6.33	128.93	113.10
6	F	94	HIS	N-CA-C	6.21	127.75	111.00
4	Q	133	GLY	N-CA-C	5.94	127.94	113.10
6	F	93	PRO	N-CA-C	5.58	126.60	112.10
3	P	127	LEU	CA-CB-CG	5.20	127.25	115.30
6	S	93	PRO	N-CA-C	5.19	125.59	112.10
2	B	184	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	136	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	438	ARG	CB-CA-C	-5.06	100.28	110.40
2	O	184	LEU	CA-CB-CG	5.02	126.86	115.30
7	G	6	GLY	N-CA-C	5.00	125.60	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
1	N	244	TYR	Sidechain
1	N	304	TYR	Sidechain
8	U	11	TYR	Sidechain

5.2 Too-close contacts (i)

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	57	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	20	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	21	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	23	0
5	E	852	0	845	7	0
5	R	852	0	845	12	0
6	F	748	0	728	12	0
6	S	748	0	728	21	0
7	G	675	0	644	26	0
7	T	675	0	644	20	0
8	H	662	0	623	6	0
8	U	662	0	623	9	0
9	I	601	0	613	4	0
9	V	601	0	613	7	0
10	J	460	0	459	5	0
10	W	460	0	459	5	0
11	K	384	0	366	3	0
11	X	384	0	366	10	0
12	L	380	0	380	12	0
12	Y	380	0	380	8	0
13	M	335	0	352	7	0
13	Z	335	0	352	8	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	6	0
17	N	120	0	108	5	0
18	A	63	0	110	4	0
18	B	63	0	110	7	0
18	L	63	0	110	20	0
18	N	189	0	330	27	0
19	A	51	0	76	7	0
19	C	153	0	228	6	0
19	N	102	0	152	8	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	2	0	0	0	0
21	B	52	0	80	11	0
21	O	52	0	80	15	0
22	B	29	0	39	1	0
22	C	58	0	78	3	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	1	0
22	W	29	0	39	4	0
23	C	33	0	36	3	0
23	M	33	0	36	0	0
23	P	33	0	36	8	0
23	Z	33	0	36	0	0
24	C	1	0	0	0	0
24	F	1	0	0	0	0
24	P	1	0	0	0	0
24	S	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	10	0
25	P	106	0	154	13	0
25	T	53	0	77	6	0
26	C	100	0	156	11	0
26	G	100	0	156	18	0
26	P	100	0	156	15	0
26	T	100	0	156	19	0
27	A	237	0	0	3	0
27	B	145	0	0	1	0
27	C	110	0	0	1	0
27	D	94	0	0	3	0
27	E	60	0	0	0	0
27	F	72	0	0	1	0
27	G	44	0	0	2	0
27	H	50	0	0	2	0
27	I	38	0	0	2	0
27	J	23	0	0	1	0
27	K	22	0	0	1	0
27	L	27	0	0	0	0
27	M	24	0	0	1	0
27	N	218	0	0	5	0
27	O	122	0	0	3	0
27	P	112	0	0	4	0
27	Q	53	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	R	45	0	0	0	0
27	S	76	0	0	6	0
27	T	42	0	0	1	0
27	U	46	0	0	2	0
27	V	25	0	0	1	0
27	W	18	0	0	0	0
27	X	21	0	0	2	0
27	Y	17	0	0	0	0
27	Z	15	0	0	1	0
All	All	32488	0	31294	523	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 8.

All (523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:HD2	7:G:84:LYS:H	1.18	1.05
7:T:84:LYS:H	7:T:84:LYS:HD2	1.20	1.02
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
10:W:33:ARG:HG2	22:W:1060:CHD:H152	1.40	1.00
21:B:230:PSC:H343	21:B:230:PSC:H142	1.44	0.99
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.47	0.96
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.29	0.96
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.30	0.95
4:D:34:SER:H	4:D:37:GLN:HE21	1.10	0.94
26:C:270:CDL:H642	26:C:270:CDL:H191	1.50	0.93
18:N:1522:TGL:HC62	18:N:1522:TGL:HC22	1.52	0.92
25:C:264:PEK:H102	25:C:264:PEK:H161	1.51	0.91
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.50	0.91
18:L:522:TGL:HC62	18:L:522:TGL:HC22	1.53	0.91
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.54	0.88
6:S:85:CYS:SG	6:S:87:THR:HG23	2.12	0.87
26:G:269:CDL:H541	26:G:269:CDL:H231	1.55	0.87
6:S:94:HIS:CD2	6:S:95:GLN:H	1.94	0.86
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.57	0.85
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.60	0.84
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.18	0.83
6:F:85:CYS:SG	6:F:87:THR:HG23	2.20	0.82
12:L:20:ARG:HH12	18:L:522:TGL:HC61	1.44	0.81
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.63	0.80
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.61	0.79
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.62	0.79
2:O:41:ILE:HD13	21:O:1230:PSC:H342	1.65	0.79
1:A:278:MET:SD	7:T:5:LYS:HB3	2.24	0.77
1:N:113:LEU:HB3	27:N:4646:HOH:O	1.82	0.77
18:L:522:TGL:H242	18:L:522:TGL:H202	1.68	0.76
18:B:521:TGL:H281	18:B:521:TGL:H102	1.67	0.76
6:S:75:HIS:H	6:S:80:GLN:HE22	1.35	0.74
18:N:1522:TGL:H202	18:N:1522:TGL:H242	1.68	0.74
18:N:1521:TGL:H102	18:N:1521:TGL:H281	1.68	0.74
2:O:224:ALA:O	2:O:227:LEU:HG	1.87	0.74
10:J:33:ARG:HG2	22:J:60:CHD:H152	1.68	0.73
1:N:1:FME:HCN	1:N:4:ASN:H	1.54	0.73
6:S:94:HIS:CG	6:S:95:GLN:H	2.04	0.73
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.89	0.72
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.70	0.72
18:N:1521:TGL:H102	18:N:1521:TGL:C28	2.20	0.72
18:B:521:TGL:C28	18:B:521:TGL:H102	2.20	0.71
7:G:31:CYS:SG	26:G:269:CDL:H532	2.29	0.71
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.73	0.71
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.71
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.06	0.71
1:N:472:ILE:HG21	18:N:1522:TGL:HA92	1.71	0.70
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.55	0.70
18:B:521:TGL:H241	18:B:521:TGL:H201	1.74	0.70
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.71	0.70
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.27	0.69
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.75	0.69
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.74	0.69
3:P:246:ASP:HB2	27:P:4318:HOH:O	1.93	0.69
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.58	0.69
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.68
8:H:23:GLN:HG3	27:H:4369:HOH:O	1.92	0.68
18:N:1521:TGL:H201	18:N:1521:TGL:H241	1.74	0.68
26:G:269:CDL:C23	26:G:269:CDL:H541	2.23	0.68
21:B:230:PSC:H072	9:I:10:ARG:HH21	1.59	0.68
6:S:94:HIS:CD2	6:S:95:GLN:N	2.62	0.67
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.59	0.67
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.25	0.67
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:267:PGV:H172	26:C:270:CDL:H662	1.77	0.67
7:T:84:LYS:N	7:T:84:LYS:HD2	2.04	0.66
2:B:41:ILE:HD13	21:B:230:PSC:H342	1.77	0.66
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.77	0.66
26:P:1270:CDL:H391	27:P:4876:HOH:O	1.95	0.66
5:R:89:LEU:O	5:R:93:LEU:HG	1.96	0.66
21:B:230:PSC:C07	9:I:10:ARG:HH21	2.08	0.66
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.09	0.66
19:P:1267:PGV:H12	19:P:1267:PGV:H161	1.77	0.66
4:D:34:SER:H	4:D:37:GLN:NE2	1.91	0.66
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.60	0.66
12:L:20:ARG:HH22	18:L:522:TGL:HC32	1.61	0.65
1:A:334:TRP:CZ3	18:A:523:TGL:HA51	2.31	0.65
1:N:378:HIS:O	1:N:382:SER:HB2	1.96	0.65
18:N:1521:TGL:H161	2:O:7:LEU:HD11	1.78	0.65
7:G:84:LYS:N	7:G:84:LYS:HD2	2.02	0.65
18:N:1523:TGL:HG11	18:N:1523:TGL:HC21	1.77	0.65
19:C:267:PGV:H12	19:C:267:PGV:H161	1.77	0.64
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.63	0.64
18:A:523:TGL:HG11	18:A:523:TGL:HC21	1.80	0.64
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.80	0.64
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.80	0.64
21:O:1230:PSC:H071	9:V:10:ARG:HE	1.62	0.63
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.81	0.63
7:G:84:LYS:H	7:G:84:LYS:CD	2.01	0.63
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.63
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.81	0.62
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.80	0.62
21:O:1230:PSC:H142	21:O:1230:PSC:C34	2.25	0.62
21:O:1230:PSC:C07	9:V:10:ARG:HE	2.12	0.62
12:L:24:MET:SD	18:L:522:TGL:H162	2.38	0.62
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.00	0.62
1:A:484:THR:HB	13:M:2:THR:OG1	1.99	0.62
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.81	0.62
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.82	0.62
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.82	0.62
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.82	0.62
18:A:523:TGL:HC51	27:B:4817:HOH:O	2.00	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.41	0.61
6:F:92:VAL:O	6:F:92:VAL:HG23	1.99	0.61
9:V:65:LYS:O	11:X:54:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.81	0.61
21:O:1230:PSC:H222	21:O:1230:PSC:H21	1.81	0.61
26:G:269:CDL:H172	26:G:269:CDL:H511	1.82	0.61
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.02	0.60
2:O:57:ASP:H	21:O:1230:PSC:H201	1.66	0.60
19:A:524:PGV:H302	13:M:19:LEU:HD23	1.82	0.59
1:A:282:PHE:HA	7:T:4:ALA:CB	2.32	0.59
3:C:51:MET:HB3	26:C:270:CDL:H622	1.84	0.59
21:B:230:PSC:C34	21:B:230:PSC:H142	2.27	0.59
21:B:230:PSC:H21	21:B:230:PSC:H222	1.84	0.59
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.37	0.59
19:A:524:PGV:H152	19:A:524:PGV:H321	1.84	0.59
2:B:62:GLU:O	2:B:66:THR:HB	2.03	0.59
10:J:7:GLU:HG3	27:J:4832:HOH:O	2.02	0.59
18:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.68	0.59
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.84	0.58
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.86	0.58
18:B:521:TGL:HA82	18:B:521:TGL:H222	1.85	0.58
3:P:34:TRP:CZ2	23:P:1272:DMU:H29	2.38	0.58
18:N:1521:TGL:H222	18:N:1521:TGL:HA82	1.85	0.58
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.85	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.85	0.58
1:N:113:LEU:CD1	18:N:1522:TGL:H292	2.34	0.58
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.17	0.58
3:C:213:THR:HG23	26:C:270:CDL:H762	1.86	0.58
12:L:20:ARG:NH1	18:L:522:TGL:HC61	2.14	0.58
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.85	0.57
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.34	0.57
18:B:521:TGL:HC22	27:I:2383:HOH:O	2.03	0.57
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.86	0.57
26:G:269:CDL:H522	26:G:269:CDL:H202	1.87	0.57
1:A:449:MET:SD	2:B:5:MET:HG2	2.45	0.57
25:C:264:PEK:H102	25:C:264:PEK:C16	2.31	0.57
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.68	0.57
1:A:377:PHE:O	1:A:381:LEU:HB3	2.05	0.57
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.86	0.57
27:P:4928:HOH:O	10:W:1:PHE:HE2	1.88	0.56
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.20	0.56
1:N:472:ILE:HD13	18:N:1522:TGL:HA91	1.88	0.56
1:A:321:PHE:CD2	21:B:230:PSC:H341	2.40	0.56
3:C:34:TRP:HZ2	23:C:272:DMU:H29	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.54	0.56
1:A:17:THR:OG1	18:L:522:TGL:H281	2.05	0.56
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.86	0.56
4:D:20:ARG:HG3	27:D:4319:HOH:O	2.04	0.56
1:N:333:LYS:HD2	27:N:4741:HOH:O	2.06	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.56
1:A:472:ILE:HG21	18:L:522:TGL:CA9	2.36	0.56
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.41	0.55
12:L:20:ARG:NH2	18:L:522:TGL:HC32	2.21	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.06	0.55
4:D:34:SER:N	4:D:37:GLN:HE21	1.93	0.55
12:L:20:ARG:HH22	18:L:522:TGL:HC61	1.71	0.55
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.72	0.55
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.07	0.55
1:A:136:LEU:HB2	27:A:4400:HOH:O	2.06	0.55
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.42	0.54
5:R:48:ILE:O	5:R:52:LEU:HG	2.06	0.54
19:A:524:PGV:H062	27:M:2160:HOH:O	2.06	0.54
7:T:45:PRO:HD2	27:T:3152:HOH:O	2.06	0.54
6:F:64:GLU:O	6:F:65:ASP:HB2	2.08	0.54
26:C:270:CDL:H661	26:C:270:CDL:H242	1.90	0.54
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.33	0.54
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.89	0.54
8:U:23:GLN:HG3	27:U:4331:HOH:O	2.08	0.54
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.73	0.54
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.90	0.54
4:D:34:SER:O	4:D:38:LYS:HG3	2.08	0.54
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.89	0.54
10:J:40:LEU:HD12	22:J:60:CHD:H183	1.89	0.54
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.90	0.54
18:N:1521:TGL:HB91	2:O:32:PHE:CE2	2.42	0.54
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.73	0.54
1:N:52:GLN:O	1:N:56:VAL:HG23	2.08	0.54
11:K:24:PHE:O	11:K:28:VAL:HG12	2.08	0.54
3:C:246:ASP:HB2	27:C:4168:HOH:O	2.07	0.53
1:A:1:FME:HCN	1:A:4:ASN:H	1.73	0.53
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.32	0.53
3:C:187:THR:HG22	25:C:264:PEK:H052	1.90	0.53
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.53
25:C:265:PEK:H031	27:O:4672:HOH:O	2.07	0.53
2:B:91:ASN:HD21	2:B:183:THR:HG21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:HIS:O	1:A:382:SER:HB2	2.08	0.53
12:Y:20:ARG:HB3	12:Y:20:ARG:NH1	2.22	0.53
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.44	0.53
3:C:34:TRP:CZ2	23:C:272:DMU:H29	2.44	0.53
5:E:31:LYS:HE3	6:F:83:PRO:O	2.09	0.53
26:P:1270:CDL:H242	26:P:1270:CDL:H661	1.91	0.53
25:C:264:PEK:H32	25:C:264:PEK:H71	1.91	0.53
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.91	0.53
3:P:47:LEU:O	3:P:51:MET:HG2	2.09	0.53
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.38	0.53
26:C:270:CDL:C19	26:C:270:CDL:H642	2.33	0.53
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.91	0.53
25:C:265:PEK:C38	26:G:269:CDL:H273	2.39	0.53
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.90	0.53
11:X:52:GLU:HB3	27:X:4935:HOH:O	2.08	0.52
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.91	0.52
13:M:42:LYS:HA	13:M:42:LYS:CE	2.38	0.52
4:D:86:MET:HE3	27:K:4869:HOH:O	2.09	0.52
1:N:87:ILE:O	1:N:173:PRO:HD3	2.08	0.52
2:B:56:MET:HG2	21:B:230:PSC:H211	1.91	0.52
19:C:267:PGV:H12	19:C:267:PGV:C16	2.40	0.52
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.91	0.52
8:U:7:LYS:O	8:U:8:ILE:HG22	2.10	0.52
7:T:3:ALA:O	7:T:4:ALA:HB2	2.09	0.52
1:N:514:LYS:HE3	27:N:3395:HOH:O	2.09	0.52
4:Q:86:MET:HE1	27:X:4838:HOH:O	2.08	0.52
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.39	0.52
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.91	0.52
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.91	0.52
2:O:59:GLN:HG3	2:O:59:GLN:O	2.10	0.52
18:N:1521:TGL:HC22	27:Q:3383:HOH:O	2.09	0.52
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.23	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.10	0.52
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.52
17:N:516:HEA:HMD1	17:N:516:HEA:HBD2	1.92	0.52
1:A:297:MET:HE2	1:A:302:ARG:HG2	1.92	0.51
25:P:1264:PEK:H32	25:P:1264:PEK:H71	1.92	0.51
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.10	0.51
7:G:17:ARG:HD2	27:G:2309:HOH:O	2.10	0.51
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.76	0.51
17:A:515:HEA:HMC1	17:A:515:HEA:HBC1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.99	0.51
25:C:265:PEK:H292	27:O:4536:HOH:O	2.11	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.93	0.50
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.93	0.50
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.24	0.50
6:S:76:LYS:HE3	6:S:93:PRO:HG3	1.92	0.50
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.93	0.50
1:N:177:SER:H	1:N:180:GLN:NE2	2.10	0.50
6:S:19:GLU:HG2	27:S:4579:HOH:O	2.10	0.50
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.12	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.12	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.50
3:C:168:THR:HG22	25:C:265:PEK:H14	1.92	0.49
25:C:265:PEK:H383	26:G:269:CDL:H273	1.92	0.49
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.77	0.49
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.11	0.49
2:O:203:ASN:HD22	2:O:203:ASN:N	2.10	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.13	0.49
17:A:516:HEA:HMD1	17:A:516:HEA:HBD2	1.93	0.49
18:L:522:TGL:C24	18:L:522:TGL:H202	2.41	0.49
2:O:41:ILE:CD1	21:O:1230:PSC:H342	2.39	0.49
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.93	0.49
2:B:7:LEU:HD11	18:B:521:TGL:H161	1.94	0.49
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.95	0.49
6:S:51:SER:O	6:S:94:HIS:N	2.46	0.49
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.95	0.49
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.77	0.49
1:A:113:LEU:HB3	27:A:4608:HOH:O	2.12	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.13	0.49
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.95	0.49
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.13	0.49
1:A:472:ILE:HD13	18:L:522:TGL:HA91	1.94	0.48
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.95	0.48
1:N:113:LEU:HD12	18:N:1522:TGL:H292	1.93	0.48
1:N:34:SER:HB2	17:N:515:HEA:C2B	2.44	0.48
2:O:62:GLU:O	2:O:66:THR:HB	2.13	0.48
1:A:1:FME:HA	1:A:1:FME:CE	2.43	0.48
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.48	0.48
6:S:22:LEU:HD12	27:S:4871:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:321:PHE:CD2	21:O:1230:PSC:H341	2.48	0.48
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.12	0.48
19:A:524:PGV:H311	13:M:16:ALA:HA	1.96	0.48
7:G:7:ASP:O	1:N:169:ILE:HD12	2.14	0.48
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.48
18:N:1523:TGL:H363	27:O:4849:HOH:O	2.13	0.47
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.47
2:O:56:MET:HG2	21:O:1230:PSC:H211	1.95	0.47
19:C:267:PGV:H182	26:C:270:CDL:H673	1.97	0.47
1:A:240:HIS:O	1:A:243:VAL:HG22	2.15	0.47
1:N:17:THR:OG1	18:N:1522:TGL:H281	2.14	0.47
5:E:84:TYR:CZ	5:E:88:GLU:HG3	2.49	0.47
2:O:56:MET:HA	21:O:1230:PSC:H202	1.96	0.47
10:W:40:LEU:HD12	22:W:1060:CHD:H183	1.97	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.11	0.47
1:N:76:GLY:O	1:N:80:ASN:HB2	2.14	0.47
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.96	0.47
3:P:168:THR:HG21	25:P:1265:PEK:H12	1.97	0.47
8:U:49:ASP:O	8:U:52:VAL:HG22	2.15	0.47
8:H:49:ASP:O	8:H:52:VAL:HG22	2.15	0.47
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.96	0.47
23:C:272:DMU:H30	23:C:272:DMU:O1	2.15	0.47
5:R:87:GLN:HG2	5:R:88:GLU:N	2.30	0.47
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.97	0.47
22:W:1060:CHD:H161	22:W:1060:CHD:H212	1.75	0.47
21:B:230:PSC:H12	21:B:230:PSC:H322	1.97	0.47
7:T:2:SER:O	7:T:3:ALA:HB3	2.15	0.47
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.50	0.47
9:I:5:ALA:O	9:I:7:PRO:HD3	2.15	0.47
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.96	0.47
3:C:244:PHE:HA	25:T:263:PEK:H9	1.98	0.46
18:L:522:TGL:H272	18:L:522:TGL:H231	1.97	0.46
21:O:1230:PSC:H322	21:O:1230:PSC:H12	1.98	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.34	0.46
26:P:1270:CDL:H532	26:P:1270:CDL:H561	1.63	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.50	0.46
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.44	0.46
6:S:92:VAL:HG23	6:S:92:VAL:O	2.16	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.14	0.46
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.51	0.46
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.81	0.46
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.50	0.46
19:P:1267:PGV:H12	19:P:1267:PGV:C16	2.40	0.46
18:N:1522:TGL:H202	18:N:1522:TGL:C24	2.41	0.46
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.98	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.16	0.46
1:A:422:ASN:HB3	18:B:521:TGL:H242	1.97	0.46
1:N:422:ASN:HB3	18:N:1521:TGL:H242	1.98	0.46
2:B:102:HIS:O	2:B:104:TRP:HA	2.16	0.46
4:D:75:THR:HB	27:D:2332:HOH:O	2.16	0.46
7:G:45:PRO:HD2	27:G:2152:HOH:O	2.15	0.46
6:F:25:ARG:HD2	27:F:4476:HOH:O	2.16	0.46
19:N:1524:PGV:H062	27:Z:3160:HOH:O	2.15	0.46
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.51	0.46
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.46	0.45
2:B:57:ASP:H	21:B:230:PSC:H201	1.81	0.45
1:A:513:LEU:HD22	1:A:513:LEU:HA	1.79	0.45
1:A:113:LEU:HD12	18:L:522:TGL:H292	1.97	0.45
2:O:216:LEU:O	2:O:219:PHE:HB3	2.17	0.45
6:S:87:THR:HG21	27:S:3339:HOH:O	2.16	0.45
18:N:1523:TGL:HG11	18:N:1523:TGL:CC2	2.45	0.45
4:D:106:PRO:HA	27:D:4808:HOH:O	2.16	0.45
6:S:22:LEU:O	6:S:25:ARG:HB3	2.16	0.45
1:N:377:PHE:CD1	17:N:516:HEA:HAD1	2.51	0.45
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.16	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.17	0.45
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.99	0.45
5:E:41:LEU:HA	27:I:2336:HOH:O	2.16	0.45
2:O:121:TYR:O	2:O:138:VAL:HA	2.16	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.16	0.45
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.45
26:C:270:CDL:H532	26:C:270:CDL:H561	1.66	0.45
26:P:1270:CDL:H112	27:P:4853:HOH:O	2.16	0.45
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.99	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.46	0.45
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.99	0.45
26:G:269:CDL:H571	26:G:269:CDL:H601	1.63	0.44
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.99	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.59	0.44
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.98	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.44
3:P:34:TRP:HE1	23:P:1272:DMU:H29	1.81	0.44
6:S:94:HIS:CG	6:S:95:GLN:N	2.80	0.44
3:P:40:MET:O	3:P:44:MET:HG2	2.18	0.44
1:N:82:LEU:O	1:N:86:MET:HG3	2.17	0.44
5:R:52:LEU:O	5:R:55:CYS:HB2	2.16	0.44
1:A:52:GLN:O	1:A:56:VAL:HG23	2.18	0.44
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.99	0.44
18:L:522:TGL:HC62	18:L:522:TGL:CC2	2.29	0.44
10:J:50:LEU:HD22	10:J:50:LEU:O	2.18	0.44
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.80	0.44
7:T:2:SER:O	25:T:263:PEK:H322	2.17	0.44
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.79	0.44
25:C:265:PEK:H383	26:G:269:CDL:C27	2.48	0.44
6:S:18:ARG:HG2	27:S:4871:HOH:O	2.18	0.44
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.83	0.44
1:N:292:MET:O	1:N:295:VAL:HG22	2.18	0.44
1:N:484:THR:HA	27:N:4470:HOH:O	2.18	0.44
1:N:321:PHE:CZ	21:O:1230:PSC:H171	2.53	0.44
3:P:34:TRP:HZ2	23:P:1272:DMU:H29	1.80	0.44
1:N:405:LEU:HD23	1:N:475:ALA:HB2	2.00	0.44
18:N:1522:TGL:H272	18:N:1522:TGL:H231	1.99	0.44
3:P:34:TRP:HE1	23:P:1272:DMU:C57	2.30	0.44
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.00	0.44
18:A:523:TGL:HG11	18:A:523:TGL:CC2	2.45	0.44
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.52	0.44
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.75	0.44
2:O:83:ILE:O	2:O:87:MET:HG3	2.18	0.44
7:T:84:LYS:H	7:T:84:LYS:CD	2.04	0.44
10:W:58:LYS:HE3	12:Y:47:LYS:HE3	2.00	0.44
11:X:24:PHE:O	11:X:28:VAL:HG12	2.18	0.44
6:S:75:HIS:H	6:S:80:GLN:NE2	2.10	0.43
19:A:524:PGV:H152	19:A:524:PGV:H301	2.00	0.43
1:A:297:MET:CE	1:A:302:ARG:HG2	2.48	0.43
1:A:390:MET:O	1:A:394:VAL:HG13	2.18	0.43
1:N:95:PRO:HG2	3:P:11:VAL:CG2	2.48	0.43
4:D:9:GLU:CD	4:D:9:GLU:H	2.21	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.43
8:U:50:VAL:HG23	27:U:4689:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:115:SER:O	1:N:121:GLY:HA2	2.18	0.43
12:L:12:PRO:HB2	18:L:522:TGL:HG2	2.00	0.43
19:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.53	0.43
7:G:36:TRP:HA	7:G:36:TRP:CE3	2.53	0.43
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.00	0.43
3:P:158:HIS:NE2	25:P:1265:PEK:H051	2.34	0.43
3:P:34:TRP:NE1	23:P:1272:DMU:H29	2.34	0.43
2:O:102:HIS:O	2:O:104:TRP:HA	2.18	0.43
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.00	0.43
22:B:1086:CHD:H212	22:B:1086:CHD:H12	2.00	0.43
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.00	0.43
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.84	0.43
3:C:47:LEU:O	3:C:51:MET:HG2	2.18	0.43
12:L:20:ARG:NH2	18:L:522:TGL:HC61	2.33	0.43
8:H:27:ARG:NH1	27:H:2303:HOH:O	2.51	0.43
9:V:35:TYR:C	9:V:37:PHE:H	2.22	0.43
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.84	0.43
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.54	0.43
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.18	0.43
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.54	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.19	0.43
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.01	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.63	0.43
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.53	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.19	0.43
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.48	0.43
3:C:210:ILE:HG23	19:C:267:PGV:H102	2.00	0.43
7:G:2:SER:O	7:G:3:ALA:HB3	2.19	0.43
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.43
8:H:43:MET:HE3	8:H:49:ASP:N	2.34	0.43
7:G:36:TRP:HA	7:G:36:TRP:HE3	1.84	0.43
6:S:53:THR:HB	6:S:54:ASN:H	1.65	0.43
22:O:229:CHD:H212	22:O:229:CHD:H12	1.99	0.43
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	2.01	0.42
9:I:35:TYR:C	9:I:37:PHE:H	2.22	0.42
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	0.42
1:A:87:ILE:O	1:A:173:PRO:HD3	2.19	0.42
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.01	0.42
1:A:92:MET:O	1:A:95:PRO:HD3	2.18	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.19	0.42
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:1272:DMU:H25	25:P:1264:PEK:H341	2.01	0.42
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.54	0.42
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.01	0.42
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.49	0.42
3:C:158:HIS:CE1	25:C:265:PEK:H051	2.54	0.42
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.55	0.42
7:T:25:LEU:HA	7:T:25:LEU:HD23	1.88	0.42
2:O:56:MET:HA	21:O:1230:PSC:C20	2.50	0.42
26:T:1269:CDL:H571	26:T:1269:CDL:H771	2.01	0.42
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.50	0.42
22:C:271:CHD:H222	22:C:271:CHD:H162	1.76	0.42
5:E:84:TYR:O	5:E:88:GLU:HG2	2.19	0.42
8:U:36:PHE:CE1	8:U:57:ARG:HB2	2.54	0.42
2:O:145:PRO:HB2	2:O:148:MET:HG3	2.01	0.42
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.49	0.42
1:A:513:LEU:O	1:A:514:LYS:HB2	2.20	0.42
1:N:53:ILE:HG12	27:N:3076:HOH:O	2.19	0.42
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.01	0.42
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.19	0.42
21:O:1230:PSC:H241	21:O:1230:PSC:H62	2.01	0.42
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.02	0.42
25:G:1263:PEK:H9	3:P:244:PHE:HA	2.02	0.42
13:M:42:LYS:HE3	13:M:42:LYS:CA	2.45	0.42
1:N:483:LEU:HA	1:N:483:LEU:HD23	1.85	0.42
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.19	0.42
9:V:15:ARG:HD2	27:V:4749:HOH:O	2.19	0.42
26:T:1269:CDL:H222	26:T:1269:CDL:H251	1.90	0.42
3:C:164:PHE:CE1	22:C:271:CHD:H192	2.55	0.42
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.02	0.42
26:C:270:CDL:H602	26:C:270:CDL:H632	1.59	0.42
1:N:400:PHE:HB3	18:N:1522:TGL:H283	2.02	0.42
2:O:98:LYS:HG2	2:O:153:LEU:HB2	2.01	0.42
2:B:75:LEU:HA	2:B:75:LEU:HD12	1.89	0.42
10:W:33:ARG:CG	22:W:1060:CHD:H152	2.29	0.42
1:A:376:HIS:O	1:A:380:VAL:HG22	2.19	0.42
2:B:4:PRO:HB2	11:K:43:SER:HA	2.02	0.42
2:O:42:ILE:O	2:O:46:LEU:HG	2.19	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.41
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.88	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.39	0.41
1:N:514:LYS:HE2	27:S:3339:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:H152	26:G:269:CDL:H181	1.85	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.55	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.20	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.01	0.41
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.55	0.41
26:T:1269:CDL:H181	26:T:1269:CDL:H152	1.87	0.41
1:A:351:GLY:HA3	1:A:380:VAL:HG13	2.02	0.41
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.41
21:B:230:PSC:H241	21:B:230:PSC:H62	2.01	0.41
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.03	0.41
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.41
1:N:376:HIS:O	1:N:380:VAL:HG22	2.21	0.41
1:N:351:GLY:C	1:N:380:VAL:HG13	2.41	0.41
1:N:440:TYR:CZ	2:O:205:SER:HA	2.56	0.41
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.08	0.41
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.19	0.41
19:N:1524:PGV:H152	19:N:1524:PGV:H301	2.02	0.41
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	2.02	0.41
3:P:230:ASN:HB2	27:S:3287:HOH:O	2.20	0.41
23:P:1272:DMU:O1	23:P:1272:DMU:H30	2.21	0.41
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.36	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.41
1:A:344:PHE:C	1:A:344:PHE:CD1	2.94	0.41
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	0.41
2:B:81:LEU:HD13	26:T:1269:CDL:H122	2.03	0.41
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	2.51	0.41
7:G:34:ASN:ND2	26:G:269:CDL:H151	2.35	0.41
1:A:378:HIS:CD2	1:A:382:SER:OG	2.74	0.41
1:A:124:THR:HB	27:A:4100:HOH:O	2.20	0.41
1:A:510:TYR:CD2	6:F:49:VAL:HG13	2.56	0.41
7:G:8:HIS:HD2	25:G:1263:PEK:H232	1.86	0.41
1:A:1:FME:HE2	1:A:1:FME:HA	2.02	0.41
1:N:95:PRO:HG2	3:P:11:VAL:HG23	2.02	0.41
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.72	0.41
5:R:82:TYR:N	5:R:83:PRO:CD	2.84	0.41
1:A:309:THR:HG22	17:A:516:HEA:HMB2	2.04	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.04	0.40
3:P:34:TRP:CE2	23:P:1272:DMU:H29	2.57	0.40
26:G:269:CDL:H222	26:G:269:CDL:H251	1.91	0.40
4:D:20:ARG:HG3	4:D:20:ARG:H	1.69	0.40
2:O:155:SER:O	2:O:174:ALA:HB1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.87	0.40
5:R:67:ILE:O	5:R:70:VAL:HG12	2.21	0.40
8:H:57:ARG:HA	8:H:60:TYR:CD2	2.56	0.40
4:Q:121:LYS:HG2	11:X:53:TRP:HD1	1.87	0.40
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.57	0.40
17:A:516:HEA:HMB1	17:A:516:HEA:H11	1.91	0.40
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.02	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%)	499 (98%)	13 (2%)	0	100 100
1	N	512/514 (100%)	501 (98%)	11 (2%)	0	100 100
2	B	225/227 (99%)	213 (95%)	10 (4%)	2 (1%)	21 9
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21 9
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100 100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	39 27
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100 100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100 100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100 100
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5 1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5 1
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1 0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7 1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7 1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100 100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100 100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
10	W	56/59 (95%)	56 (100%)	0	0	100 100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100 100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100
13	Z	41/46 (89%)	41 (100%)	0	0	100 100
All	All	3504/3614 (97%)	3359 (96%)	116 (3%)	29 (1%)	24 11

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
6	F	94	HIS
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
7	T	3	ALA
7	T	40	GLY
8	U	8	ILE
8	U	46	LYS
2	B	60	GLU

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Mol	Chain	Res	Type
2	O	60	GLU
6	F	96	LEU
3	P	38	ASN
6	S	96	LEU
7	G	6	GLY
7	T	6	GLY
2	B	92	ASN
2	O	92	ASN

5.3.2 Protein sidechains (i)

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%)	417 (98%)	9 (2%)	61	55
1	N	426/426 (100%)	416 (98%)	10 (2%)	58	51
2	B	210/210 (100%)	200 (95%)	10 (5%)	31	19
2	O	210/210 (100%)	199 (95%)	11 (5%)	29	17
3	C	224/226 (99%)	218 (97%)	6 (3%)	52	43
3	P	224/226 (99%)	220 (98%)	4 (2%)	66	61
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	66
4	Q	128/129 (99%)	124 (97%)	4 (3%)	47	37
5	E	92/95 (97%)	90 (98%)	2 (2%)	60	53
5	R	92/95 (97%)	90 (98%)	2 (2%)	60	53
6	F	81/81 (100%)	79 (98%)	2 (2%)	55	47
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	7
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	7
7	T	67/68 (98%)	62 (92%)	5 (8%)	17	7
8	H	71/75 (95%)	69 (97%)	2 (3%)	51	41
8	U	71/75 (95%)	68 (96%)	3 (4%)	36	24
9	I	57/57 (100%)	54 (95%)	3 (5%)	28	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	V	57/57 (100%)	55 (96%)	2 (4%)	43 31
10	J	49/50 (98%)	48 (98%)	1 (2%)	63 57
10	W	49/50 (98%)	48 (98%)	1 (2%)	63 57
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 45
11	X	39/46 (85%)	37 (95%)	2 (5%)	29 17
12	L	39/40 (98%)	38 (97%)	1 (3%)	54 45
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29 17
13	M	37/38 (97%)	32 (86%)	5 (14%)	5 1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 3
All	All	3040/3082 (99%)	2935 (96%)	105 (4%)	43 31

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	113	TYR
2	B	115	ASP
2	B	167	SER
3	C	17	PRO
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN

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Mol	Chain	Res	Type
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	96	LEU
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	369	ASP
1	N	380	VAL
1	N	444	PRO
1	N	504	THR
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN

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Mol	Chain	Res	Type
2	O	94	SER
2	O	167	SER
2	O	217	LYS
3	P	29	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	51	LEU
4	Q	54	ASP
4	Q	121	LYS
5	R	80	GLU
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
6	S	96	LEU
7	T	18	PHE
7	T	33	LEU
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
8	U	21	PRO
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	61	GLU
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
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 (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
9	I	8	GLN
9	I	53	ASN
10	J	29	ASN
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
9	V	8	GLN
10	W	57	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.58	0	6,9,11	1.47	2 (33%)
2	FME	B	1	2	8,9,10	0.77	0	6,9,11	1.72	1 (16%)
7	TPO	G	11	7	8,10,11	1.68	1 (12%)	7,14,16	0.97	0
9	SAC	I	1	9	7,8,9	2.36	2 (28%)	7,9,11	2.05	2 (28%)
1	FME	N	1	1	8,9,10	0.73	0	6,9,11	1.95	2 (33%)
2	FME	O	1	2	8,9,10	0.65	0	6,9,11	1.51	1 (16%)
7	TPO	T	11	7	8,10,11	1.24	1 (12%)	7,14,16	0.99	0
9	SAC	V	1	9	7,8,9	2.70	2 (28%)	7,9,11	2.19	4 (57%)

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
9	SAC	I	1	9	-	0/6/8/10	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
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.29	1.58	1.54
7	G	11	TPO	CB-CA	3.72	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	3.75	1.51	1.46
9	V	1	SAC	CA-N	4.67	1.53	1.46
9	I	1	SAC	OAC-C1A	4.82	1.34	1.23
9	V	1	SAC	OAC-C1A	5.00	1.34	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	CA-N-CN	-4.06	116.57	122.82
2	B	1	FME	CA-N-CN	-3.66	117.20	122.82
2	O	1	FME	CA-N-CN	-3.36	117.65	122.82
9	V	1	SAC	CA-N-C1A	-3.14	110.72	121.37
9	I	1	SAC	CA-N-C1A	-2.97	111.30	121.37
1	A	1	FME	CA-N-CN	-2.46	119.03	122.82
1	N	1	FME	O-C-CA	-2.33	119.28	125.44
9	V	1	SAC	OAC-C1A-C2A	-2.22	117.98	122.06
1	A	1	FME	O-C-CA	-2.10	119.91	125.44
9	V	1	SAC	C2A-C1A-N	2.55	120.98	116.11
9	V	1	SAC	CB-CA-N	2.90	116.96	110.60
9	I	1	SAC	CB-CA-N	3.32	117.88	110.60

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	N	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
1	N	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 10 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	HEA	A	515	1	40,67,67	1.28	5 (12%)	41,103,103	1.72	8 (19%)
17	HEA	A	516	1	40,67,67	1.59	6 (15%)	41,103,103	1.49	8 (19%)
18	TGL	A	523	-	62,62,62	0.71	0	65,65,65	1.28	7 (10%)
19	PGV	A	524	-	50,50,50	1.07	3 (6%)	51,56,56	0.92	4 (7%)
22	CHD	B	1086	-	29,32,32	0.68	0	48,51,51	1.76	14 (29%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	PSC	B	230	-	51,51,51	1.21	3 (5%)	55,59,59	0.99	1 (1%)
18	TGL	B	521	-	62,62,62	0.69	0	65,65,65	1.54	9 (13%)
25	PEK	C	264	-	51,52,52	1.40	4 (7%)	52,57,57	1.03	3 (5%)
25	PEK	C	265	-	51,52,52	1.63	9 (17%)	52,57,57	1.13	5 (9%)
19	PGV	C	266	-	50,50,50	0.88	2 (4%)	51,56,56	0.77	2 (3%)
19	PGV	C	267	-	50,50,50	0.81	1 (2%)	51,56,56	0.88	2 (3%)
19	PGV	C	268	-	50,50,50	1.14	3 (6%)	51,56,56	0.79	1 (1%)
26	CDL	C	270	-	99,99,99	0.80	2 (2%)	101,111,111	0.90	4 (3%)
22	CHD	C	271	-	29,32,32	0.85	0	48,51,51	3.65	22 (45%)
23	DMU	C	272	-	34,34,34	2.69	11 (32%)	45,45,45	4.33	19 (42%)
22	CHD	C	525	-	29,32,32	0.76	0	48,51,51	1.55	7 (14%)
25	PEK	G	1263	-	51,52,52	1.80	8 (15%)	52,57,57	1.14	4 (7%)
26	CDL	G	269	-	99,99,99	0.97	5 (5%)	101,111,111	0.94	7 (6%)
22	CHD	J	60	-	29,32,32	1.04	1 (3%)	48,51,51	3.48	30 (62%)
18	TGL	L	522	-	62,62,62	1.07	5 (8%)	65,65,65	1.66	12 (18%)
23	DMU	M	526	-	34,34,34	3.21	8 (23%)	45,45,45	4.36	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	N	1266	-	50,50,50	0.93	3 (6%)	51,56,56	0.85	3 (5%)
18	TGL	N	1521	-	62,62,62	0.74	1 (1%)	65,65,65	1.49	9 (13%)
18	TGL	N	1522	-	62,62,62	1.12	4 (6%)	65,65,65	1.63	11 (16%)
18	TGL	N	1523	-	62,62,62	0.76	2 (3%)	65,65,65	1.28	6 (9%)
19	PGV	N	1524	-	50,50,50	1.06	4 (8%)	51,56,56	0.91	5 (9%)
17	HEA	N	515	1	40,67,67	1.31	5 (12%)	41,103,103	1.79	10 (24%)
17	HEA	N	516	1	40,67,67	1.46	6 (15%)	41,103,103	1.49	9 (21%)
21	PSC	O	1230	-	51,51,51	1.20	3 (5%)	55,59,59	0.99	1 (1%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	0.68	1 (3%)	48,51,51	1.82	14 (29%)
25	PEK	P	1264	-	51,52,52	1.41	5 (9%)	52,57,57	1.05	3 (5%)
25	PEK	P	1265	-	51,52,52	1.64	10 (19%)	52,57,57	1.12	5 (9%)
19	PGV	P	1267	-	50,50,50	0.87	2 (4%)	51,56,56	0.83	2 (3%)
19	PGV	P	1268	-	50,50,50	1.14	2 (4%)	51,56,56	0.81	2 (3%)
26	CDL	P	1270	-	99,99,99	0.83	3 (3%)	101,111,111	0.87	4 (3%)
22	CHD	P	1271	-	29,32,32	0.79	0	48,51,51	3.65	23 (47%)
23	DMU	P	1272	-	34,34,34	2.81	11 (32%)	45,45,45	4.37	19 (42%)
22	CHD	P	1525	-	29,32,32	0.78	1 (3%)	48,51,51	1.49	9 (18%)
26	CDL	T	1269	-	99,99,99	0.96	5 (5%)	101,111,111	0.96	7 (6%)
25	PEK	T	263	-	51,52,52	1.84	10 (19%)	52,57,57	1.14	4 (7%)
22	CHD	W	1060	-	29,32,32	1.15	3 (10%)	48,51,51	3.49	29 (60%)
23	DMU	Z	1526	-	34,34,34	3.13	8 (23%)	45,45,45	4.31	20 (44%)

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
17	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
18	TGL	A	523	-	-	0/65/65/65	0/0/0/0
19	PGV	A	524	-	-	2/55/55/55	0/0/0/0
22	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	230	-	-	0/55/55/55	0/0/0/0
18	TGL	B	521	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	266	-	-	0/55/55/55	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
22	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
18	TGL	L	522	-	-	0/65/65/65	0/0/0/0
23	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
17	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
21	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	526	DMU	O7-C3	-8.55	1.22	1.43
23	Z	1526	DMU	O7-C3	-8.05	1.23	1.43
23	M	526	DMU	O16-C6	-6.96	1.27	1.40
23	Z	1526	DMU	O16-C6	-6.84	1.27	1.40
23	M	526	DMU	O16-C18	-6.80	1.23	1.42
23	Z	1526	DMU	O16-C18	-6.57	1.24	1.42
23	M	526	DMU	O7-C10	-6.49	1.24	1.41
23	P	1272	DMU	O1-C9	-6.46	1.28	1.44
23	Z	1526	DMU	O7-C10	-6.43	1.24	1.41
23	M	526	DMU	O1-C9	-6.40	1.28	1.44
23	P	1272	DMU	O7-C3	-6.35	1.28	1.43
23	Z	1526	DMU	O1-C9	-6.29	1.28	1.44
23	M	526	DMU	O5-C4	-6.26	1.28	1.44
23	C	272	DMU	O1-C9	-6.05	1.29	1.44
23	P	1272	DMU	O16-C18	-5.99	1.26	1.42
23	P	1272	DMU	O16-C6	-5.86	1.29	1.40
23	C	272	DMU	O7-C3	-5.83	1.29	1.43
23	Z	1526	DMU	O5-C4	-5.78	1.29	1.44
23	M	526	DMU	O1-C10	-5.66	1.27	1.41
23	Z	1526	DMU	O1-C10	-5.63	1.27	1.41
23	C	272	DMU	O16-C18	-5.55	1.27	1.42
23	C	272	DMU	O16-C6	-5.35	1.30	1.40
23	C	272	DMU	O5-C4	-4.75	1.32	1.44
23	P	1272	DMU	O5-C4	-4.73	1.32	1.44
23	P	1272	DMU	O7-C10	-4.72	1.28	1.41
23	C	272	DMU	O1-C10	-4.61	1.30	1.41
23	M	526	DMU	O5-C6	-4.60	1.30	1.41
23	P	1272	DMU	O1-C10	-4.59	1.30	1.41
23	Z	1526	DMU	O5-C6	-4.45	1.30	1.41
23	C	272	DMU	O7-C10	-4.44	1.29	1.41
23	P	1272	DMU	O5-C6	-4.14	1.31	1.41
23	C	272	DMU	O5-C6	-3.85	1.31	1.41
17	N	515	HEA	C3A-CMA	-3.38	1.38	1.46
17	N	516	HEA	C3A-CMA	-3.22	1.39	1.46
17	A	516	HEA	C3A-CMA	-3.17	1.39	1.46
17	A	516	HEA	C3A-C2A	-3.14	1.36	1.40
17	A	515	HEA	C3A-CMA	-3.10	1.39	1.46
17	N	516	HEA	C3A-C2A	-2.48	1.37	1.40
17	A	516	HEA	C3C-C2C	-2.38	1.37	1.40
17	N	515	HEA	C3A-C2A	-2.30	1.37	1.40
17	A	515	HEA	C3A-C2A	-2.03	1.37	1.40
25	P	1264	PEK	C2-C1	2.01	1.56	1.50
18	N	1523	TGL	CG3-CG2	2.03	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1524	PGV	C03-C02	2.04	1.56	1.50
19	C	268	PGV	C04-C05	2.06	1.59	1.51
25	P	1265	PEK	P-O12	2.09	1.68	1.59
25	C	265	PEK	P-O11	2.11	1.68	1.59
17	N	516	HEA	C18-C19	2.11	1.37	1.33
23	P	1272	DMU	C5-C7	2.13	1.58	1.52
19	N	1266	PGV	C20-C19	2.16	1.57	1.50
26	P	1270	CDL	C31-CA7	2.16	1.57	1.50
18	N	1523	TGL	OG2-CB1	2.16	1.40	1.34
22	W	1060	CHD	C20-C17	2.18	1.58	1.54
25	P	1265	PEK	P-O11	2.18	1.69	1.59
18	L	522	TGL	CC2-CC1	2.20	1.57	1.50
23	P	1272	DMU	C6-C1	2.20	1.59	1.52
26	T	1269	CDL	OA6-CA5	2.21	1.40	1.34
23	C	272	DMU	C6-C1	2.22	1.59	1.52
22	O	229	CHD	C8-C9	2.23	1.58	1.53
18	N	1522	TGL	CG3-CG2	2.23	1.57	1.50
23	C	272	DMU	C5-C7	2.24	1.58	1.52
19	A	524	PGV	C20-C19	2.24	1.57	1.50
19	P	1267	PGV	C01-C02	2.26	1.57	1.50
22	W	1060	CHD	C8-C7	2.27	1.57	1.53
18	L	522	TGL	CG3-CG2	2.29	1.57	1.50
26	T	1269	CDL	CA6-CA4	2.32	1.57	1.50
18	N	1521	TGL	OG2-CB1	2.34	1.41	1.34
22	P	1525	CHD	C8-C9	2.37	1.58	1.53
25	C	265	PEK	C22-C21	2.39	1.57	1.50
17	N	516	HEA	C3C-CAC	2.40	1.52	1.47
17	N	515	HEA	C4B-NB	2.41	1.39	1.36
23	P	1272	DMU	C3-C4	2.41	1.59	1.52
26	C	270	CDL	CA3-CA4	2.42	1.57	1.50
19	N	1524	PGV	C20-C19	2.43	1.57	1.50
25	T	263	PEK	O01-C1	2.44	1.41	1.34
25	T	263	PEK	C2-C1	2.46	1.58	1.50
25	P	1265	PEK	C22-C21	2.46	1.58	1.50
21	B	230	PSC	C2-C1	2.47	1.58	1.50
26	G	269	CDL	CA6-CA4	2.48	1.57	1.50
25	G	1263	PEK	P-O11	2.49	1.70	1.59
26	T	1269	CDL	C11-CA5	2.49	1.58	1.50
26	G	269	CDL	C11-CA5	2.49	1.58	1.50
19	C	266	PGV	C20-C19	2.50	1.58	1.50
17	A	515	HEA	C4B-NB	2.52	1.40	1.36
26	P	1270	CDL	CA3-CA4	2.54	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	1230	PSC	C2-C1	2.54	1.58	1.50
23	C	272	DMU	C3-C4	2.58	1.60	1.52
25	P	1265	PEK	C03-C02	2.58	1.58	1.50
26	C	270	CDL	CA6-CA4	2.61	1.58	1.50
17	A	515	HEA	C1A-NA	2.63	1.40	1.36
25	C	265	PEK	O03-C21	2.64	1.41	1.33
19	C	268	PGV	O01-C1	2.68	1.42	1.34
25	T	263	PEK	P-O11	2.68	1.71	1.59
17	A	516	HEA	C3C-CAC	2.69	1.53	1.47
25	C	265	PEK	C01-C02	2.70	1.58	1.50
18	L	522	TGL	OG1-CA1	2.73	1.41	1.33
26	G	269	CDL	OA6-CA5	2.75	1.42	1.34
25	P	1265	PEK	O03-C21	2.78	1.41	1.33
26	P	1270	CDL	CA6-CA4	2.79	1.58	1.50
25	P	1265	PEK	C01-C02	2.80	1.58	1.50
19	N	1524	PGV	O03-C19	2.83	1.41	1.33
25	C	265	PEK	C03-C02	2.84	1.58	1.50
26	G	269	CDL	CB3-CB4	2.85	1.58	1.50
19	P	1268	PGV	O01-C1	2.89	1.42	1.34
18	N	1522	TGL	CG1-CG2	2.97	1.59	1.50
19	N	1266	PGV	C01-C02	2.99	1.59	1.50
26	T	1269	CDL	CB3-CB4	3.00	1.59	1.50
18	L	522	TGL	CG1-CG2	3.02	1.59	1.50
22	J	60	CHD	C13-C17	3.02	1.60	1.55
17	N	515	HEA	C4A-NA	3.12	1.40	1.36
19	C	267	PGV	C12-C11	3.22	1.50	1.31
19	A	524	PGV	O03-C19	3.27	1.43	1.33
19	P	1267	PGV	C12-C11	3.30	1.50	1.31
17	N	515	HEA	C1D-ND	3.33	1.41	1.36
25	G	1263	PEK	O03-C21	3.43	1.43	1.33
26	G	269	CDL	CB6-CB4	3.56	1.60	1.50
17	A	515	HEA	C1D-ND	3.58	1.41	1.36
25	T	263	PEK	O03-C21	3.61	1.44	1.33
18	N	1522	TGL	OG1-CA1	3.63	1.44	1.33
22	W	1060	CHD	C13-C17	3.68	1.62	1.55
25	T	263	PEK	C01-C02	3.72	1.61	1.50
19	C	266	PGV	C12-C11	3.76	1.53	1.31
19	N	1266	PGV	C12-C11	3.88	1.54	1.31
19	A	524	PGV	C12-C11	3.88	1.54	1.31
21	B	230	PSC	C13-C12	3.91	1.54	1.31
26	T	1269	CDL	CB6-CB4	3.94	1.61	1.50
25	G	1263	PEK	C01-C02	3.94	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1264	PEK	C9-C8	3.95	1.54	1.31
25	C	264	PEK	C9-C8	3.96	1.54	1.31
17	N	516	HEA	C4B-NB	3.98	1.42	1.36
19	N	1524	PGV	C12-C11	4.04	1.55	1.31
25	C	265	PEK	C6-C5	4.04	1.55	1.31
25	C	264	PEK	C6-C5	4.07	1.55	1.31
25	P	1264	PEK	C6-C5	4.09	1.55	1.31
21	O	1230	PSC	C13-C12	4.14	1.55	1.31
25	G	1263	PEK	C15-C14	4.14	1.55	1.31
25	P	1265	PEK	C15-C14	4.14	1.55	1.31
25	P	1265	PEK	C9-C8	4.17	1.55	1.31
25	G	1263	PEK	C9-C8	4.22	1.56	1.31
21	B	230	PSC	C10-C9	4.23	1.56	1.31
25	T	263	PEK	C15-C14	4.24	1.56	1.31
25	P	1265	PEK	C6-C5	4.25	1.56	1.31
25	G	1263	PEK	C6-C5	4.26	1.56	1.31
25	P	1265	PEK	C12-C11	4.27	1.56	1.31
25	T	263	PEK	C9-C8	4.27	1.56	1.31
25	C	265	PEK	C12-C11	4.29	1.56	1.31
21	O	1230	PSC	C10-C9	4.29	1.56	1.31
25	C	265	PEK	C15-C14	4.30	1.56	1.31
25	T	263	PEK	C03-C02	4.33	1.63	1.50
25	T	263	PEK	C6-C5	4.37	1.56	1.31
25	C	265	PEK	C9-C8	4.37	1.57	1.31
18	L	522	TGL	OG2-CB1	4.40	1.47	1.34
19	P	1268	PGV	C12-C11	4.42	1.57	1.31
25	G	1263	PEK	C03-C02	4.43	1.63	1.50
19	C	268	PGV	C12-C11	4.43	1.57	1.31
25	C	264	PEK	C12-C11	4.51	1.57	1.31
25	P	1264	PEK	C15-C14	4.55	1.58	1.31
25	C	264	PEK	C15-C14	4.64	1.58	1.31
25	P	1264	PEK	C12-C11	4.65	1.58	1.31
18	N	1522	TGL	OG2-CB1	4.65	1.48	1.34
25	T	263	PEK	C12-C11	4.67	1.58	1.31
25	G	1263	PEK	C12-C11	4.79	1.59	1.31
17	N	516	HEA	C1D-ND	4.83	1.43	1.36
17	A	516	HEA	C4B-NB	4.86	1.43	1.36
17	A	516	HEA	C1D-ND	5.02	1.43	1.36

All (384) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1271	CHD	C17-C13-C12	-9.14	109.58	117.68
22	C	271	CHD	C17-C13-C12	-8.87	109.82	117.68
22	C	271	CHD	C19-C10-C9	-7.60	99.79	111.18
23	M	526	DMU	C8-C7-C5	-7.45	96.90	110.79
23	Z	1526	DMU	C8-C7-C5	-7.36	97.06	110.79
22	P	1271	CHD	C19-C10-C9	-7.12	100.50	111.18
17	N	515	HEA	C4B-C3B-C11	-6.89	119.53	127.01
17	A	515	HEA	C4B-C3B-C11	-5.80	120.71	127.01
22	C	271	CHD	C19-C10-C1	-5.76	98.52	108.20
22	P	1271	CHD	C19-C10-C1	-5.50	98.95	108.20
22	W	1060	CHD	C15-C14-C8	-5.28	110.65	118.32
22	J	60	CHD	C15-C14-C8	-5.18	110.80	118.32
18	B	521	TGL	CG1-OG1-CA1	-5.03	102.77	116.85
22	P	1271	CHD	C15-C14-C8	-4.83	111.30	118.32
18	L	522	TGL	C12-C11-C10	-4.80	89.74	114.53
18	N	1521	TGL	CG1-OG1-CA1	-4.73	103.63	116.85
18	N	1522	TGL	C12-C11-C10	-4.72	90.17	114.53
22	C	271	CHD	C15-C14-C8	-4.70	111.49	118.32
22	J	60	CHD	C18-C13-C14	-4.62	103.93	111.22
22	W	1060	CHD	C18-C13-C14	-4.62	103.94	111.22
17	A	515	HEA	CAD-C3D-C4D	-4.40	122.23	127.01
18	N	1522	TGL	CB9-CB8-CB7	-4.26	92.52	114.53
22	W	1060	CHD	C18-C13-C12	-4.15	105.05	109.09
18	N	1523	TGL	CG1-OG1-CA1	-4.08	105.45	116.85
18	L	522	TGL	CB9-CB8-CB7	-4.06	93.57	114.53
22	C	525	CHD	C14-C13-C12	-4.03	103.78	107.39
17	N	516	HEA	CAD-C3D-C4D	-3.88	122.79	127.01
17	A	516	HEA	CAD-C3D-C4D	-3.87	122.80	127.01
21	B	230	PSC	C01-O03-C19	-3.86	106.05	116.85
18	A	523	TGL	CG1-OG1-CA1	-3.80	106.23	116.85
21	O	1230	PSC	C01-O03-C19	-3.75	106.36	116.85
22	B	1086	CHD	C16-C17-C13	-3.71	99.91	103.60
22	B	1086	CHD	C15-C14-C8	-3.63	113.05	118.32
22	C	271	CHD	C18-C13-C12	-3.57	105.61	109.09
17	N	515	HEA	CAD-C3D-C4D	-3.56	123.15	127.01
22	W	1060	CHD	C17-C13-C12	-3.46	114.62	117.68
22	J	60	CHD	C17-C13-C12	-3.45	114.63	117.68
22	J	60	CHD	C18-C13-C12	-3.42	105.75	109.09
26	P	1270	CDL	CB6-OB8-CB7	-3.39	107.37	116.85
22	B	1086	CHD	C15-C14-C13	-3.35	100.26	103.60
22	O	229	CHD	C15-C14-C8	-3.35	113.46	118.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1525	CHD	C15-C14-C8	-3.30	113.53	118.32
26	C	270	CDL	CB6-OB8-CB7	-3.27	107.71	116.85
22	C	525	CHD	C15-C14-C8	-3.24	113.62	118.32
17	N	516	HEA	CAA-C2A-C1A	-3.22	123.51	127.01
22	O	229	CHD	C16-C17-C13	-3.22	100.40	103.60
17	A	516	HEA	CAA-C2A-C1A	-3.15	123.59	127.01
23	C	272	DMU	C2-C3-C4	-3.08	103.87	110.84
17	A	515	HEA	CAA-C2A-C1A	-3.08	123.67	127.01
25	C	264	PEK	O03-C21-C22	-3.06	102.58	111.90
26	C	270	CDL	OB6-CB5-C51	-3.04	104.92	111.53
23	P	1272	DMU	C2-C3-C4	-2.99	104.08	110.84
23	M	526	DMU	C2-C3-C4	-2.94	104.18	110.84
22	B	1086	CHD	C18-C13-C12	-2.93	106.23	109.09
25	P	1264	PEK	O03-C21-C22	-2.90	103.07	111.90
22	P	1271	CHD	C18-C13-C12	-2.88	106.28	109.09
22	O	229	CHD	C14-C13-C12	-2.85	104.84	107.39
23	Z	1526	DMU	C2-C3-C4	-2.85	104.40	110.84
22	C	525	CHD	C14-C8-C9	-2.81	105.75	109.62
22	P	1525	CHD	C14-C8-C9	-2.77	105.81	109.62
22	O	229	CHD	C15-C14-C13	-2.73	100.88	103.60
25	P	1264	PEK	C3-C2-C1	-2.68	103.06	113.59
26	P	1270	CDL	OB6-CB5-C51	-2.65	105.77	111.53
17	N	515	HEA	CMB-C2B-C1B	-2.64	124.00	128.36
19	C	267	PGV	O01-C1-C2	-2.56	105.95	111.53
17	A	516	HEA	C20-C19-C18	-2.56	116.19	121.05
25	C	264	PEK	C3-C2-C1	-2.53	103.64	113.59
22	J	60	CHD	C19-C10-C5	-2.51	105.82	110.25
22	P	1525	CHD	C14-C13-C12	-2.51	105.14	107.39
19	N	1266	PGV	C01-O03-C19	-2.50	109.84	116.85
22	W	1060	CHD	C19-C10-C5	-2.49	105.86	110.25
17	A	515	HEA	C26-C15-C14	-2.49	118.62	123.50
19	C	267	PGV	C9-C10-C11	-2.48	99.45	112.45
19	N	1266	PGV	O01-C1-C2	-2.47	106.15	111.53
17	A	515	HEA	CMC-C2C-C1C	-2.46	124.29	128.36
22	O	229	CHD	C18-C13-C12	-2.45	106.70	109.09
19	P	1267	PGV	C9-C10-C11	-2.43	99.68	112.45
22	J	60	CHD	C19-C10-C9	-2.43	107.54	111.18
17	N	516	HEA	C20-C19-C18	-2.40	116.50	121.05
22	P	1271	CHD	C18-C13-C14	-2.40	107.43	111.22
19	P	1268	PGV	C01-O03-C19	-2.37	110.22	116.85
22	B	1086	CHD	C14-C13-C12	-2.37	105.27	107.39
19	C	266	PGV	O01-C1-C2	-2.34	106.44	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T	1269	CDL	OB8-CB7-C71	-2.33	104.80	111.90
18	B	521	TGL	CA8-CA7-CA6	-2.33	102.52	114.53
19	N	1524	PGV	C3-C2-C1	-2.31	104.53	113.59
19	C	268	PGV	C01-O03-C19	-2.30	110.42	116.85
22	O	229	CHD	C19-C10-C1	-2.29	104.36	108.20
22	B	1086	CHD	C14-C8-C9	-2.26	106.52	109.62
18	N	1521	TGL	CA8-CA7-CA6	-2.25	102.91	114.53
22	W	1060	CHD	C19-C10-C1	-2.22	104.46	108.20
22	C	271	CHD	C18-C13-C14	-2.22	107.71	111.22
17	N	515	HEA	C26-C15-C14	-2.21	119.16	123.50
17	N	515	HEA	C17-C18-C19	-2.17	123.05	127.76
17	N	516	HEA	C16-C15-C14	-2.12	117.03	121.05
19	P	1268	PGV	C02-O01-C1	-2.12	112.80	117.89
22	B	1086	CHD	C19-C10-C1	-2.11	104.65	108.20
17	A	515	HEA	C17-C18-C19	-2.11	123.18	127.76
17	N	515	HEA	OMA-CMA-C3A	-2.10	120.87	125.11
22	O	229	CHD	C13-C17-C20	-2.09	116.95	119.50
19	A	524	PGV	C3-C2-C1	-2.09	105.38	113.59
26	G	269	CDL	OB8-CB7-C71	-2.09	105.55	111.90
18	N	1521	TGL	CA6-CA5-CA4	-2.08	103.78	114.53
22	J	60	CHD	C19-C10-C1	-2.05	104.76	108.20
19	P	1267	PGV	O01-C1-C2	-2.04	107.08	111.53
18	B	521	TGL	CA6-CA5-CA4	-2.03	104.02	114.53
19	C	266	PGV	C01-O03-C19	-2.02	111.19	116.85
22	W	1060	CHD	C19-C10-C9	-2.01	108.16	111.18
18	A	523	TGL	OG3-CG3-CG2	-2.01	103.28	108.69
17	N	515	HEA	CMD-C2D-C3D	2.00	129.42	125.24
18	L	522	TGL	C10-CB9-CB8	2.00	124.87	114.53
26	P	1270	CDL	OB6-CB5-OB7	2.01	129.08	123.67
18	N	1523	TGL	OG2-CG2-CG1	2.02	115.46	108.36
25	T	263	PEK	C14-C13-C12	2.02	118.72	112.00
26	T	1269	CDL	C79-C78-C77	2.04	125.07	114.53
22	J	60	CHD	O7-C7-C6	2.05	115.08	110.06
26	G	269	CDL	C79-C78-C77	2.05	125.11	114.53
22	P	1271	CHD	O12-C12-C13	2.05	114.44	111.11
17	A	516	HEA	C17-C18-C19	2.06	132.25	127.76
26	T	1269	CDL	C20-C19-C18	2.07	125.20	114.53
22	B	1086	CHD	C5-C4-C3	2.08	116.00	112.91
22	B	1086	CHD	C5-C6-C7	2.08	116.76	114.44
25	P	1265	PEK	C2-C3-C4	2.08	117.44	113.30
18	N	1521	TGL	OG1-CG1-CG2	2.08	114.30	108.69
25	C	265	PEK	P-O12-C04	2.09	133.44	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	1524	PGV	C04-C05-C06	2.09	119.54	111.08
19	A	524	PGV	C04-C05-C06	2.10	119.56	111.08
19	N	1524	PGV	C03-C02-C01	2.10	116.98	112.07
22	P	1525	CHD	C1-C2-C3	2.10	113.84	110.43
18	A	523	TGL	OG2-CG2-CG1	2.12	115.82	108.36
22	C	271	CHD	C1-C2-C3	2.13	113.88	110.43
17	N	516	HEA	C4B-C3B-C11	2.14	129.33	127.01
26	P	1270	CDL	OA8-CA6-CA4	2.14	114.44	108.69
17	A	516	HEA	CMC-C2C-C3C	2.14	129.28	125.09
22	P	1271	CHD	C1-C2-C3	2.15	113.92	110.43
17	N	515	HEA	CMC-C2C-C3C	2.15	129.30	125.09
19	A	524	PGV	O01-C02-C03	2.16	115.98	108.36
26	G	269	CDL	OB8-CB6-CB4	2.17	114.52	108.69
18	B	521	TGL	OG1-CG1-CG2	2.18	114.55	108.69
25	C	265	PEK	C2-C3-C4	2.19	117.66	113.30
26	G	269	CDL	C20-C19-C18	2.20	125.90	114.53
26	C	270	CDL	OB6-CB5-OB7	2.21	129.61	123.67
18	N	1523	TGL	OG1-CG1-CG2	2.21	114.65	108.69
22	P	1525	CHD	C10-C9-C8	2.21	114.31	111.88
22	J	60	CHD	C14-C8-C7	2.22	114.82	111.74
26	T	1269	CDL	C19-C18-C17	2.22	126.00	114.53
22	O	229	CHD	C1-C2-C3	2.23	114.05	110.43
25	P	1265	PEK	P-O12-C04	2.24	134.27	121.50
22	W	1060	CHD	C14-C8-C7	2.24	114.84	111.74
26	G	269	CDL	C19-C18-C17	2.24	126.11	114.53
18	B	521	TGL	C10-CB9-CB8	2.26	126.22	114.53
23	C	272	DMU	O1-C10-C5	2.27	114.93	110.28
22	P	1525	CHD	C9-C11-C12	2.27	117.23	114.36
19	N	1524	PGV	O01-C02-C03	2.27	116.37	108.36
25	G	1263	PEK	C14-C13-C12	2.28	119.58	112.00
23	P	1272	DMU	O1-C10-C5	2.29	114.97	110.28
26	C	270	CDL	OA8-CA6-CA4	2.30	114.88	108.69
23	P	1272	DMU	C10-O7-C3	2.31	124.04	118.01
17	A	516	HEA	C26-C15-C16	2.31	118.94	115.41
22	J	60	CHD	C14-C13-C12	2.32	109.47	107.39
22	O	229	CHD	C17-C13-C14	2.35	102.43	100.05
22	C	525	CHD	C5-C6-C7	2.36	117.07	114.44
25	C	264	PEK	O03-C21-O04	2.36	129.58	123.49
23	Z	1526	DMU	C10-O1-C9	2.36	118.33	113.75
26	T	1269	CDL	OB8-CB6-CB4	2.37	115.07	108.69
25	P	1264	PEK	O03-C21-O04	2.37	129.62	123.49
18	N	1521	TGL	C10-CB9-CB8	2.38	126.85	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	P	1265	PEK	O03-C01-C02	2.39	115.11	108.69
25	G	1263	PEK	C03-C02-C01	2.39	117.67	112.07
18	N	1522	TGL	CC4-CC3-CC2	2.40	122.09	113.29
18	B	521	TGL	OG2-CG2-CG3	2.41	116.84	108.36
25	C	265	PEK	O03-C01-C02	2.43	115.23	108.69
19	N	1266	PGV	O03-C01-C02	2.45	115.29	108.69
19	N	1524	PGV	C02-O01-C1	2.46	123.80	117.89
17	N	516	HEA	C26-C15-C16	2.47	119.18	115.41
19	A	524	PGV	C02-O01-C1	2.48	123.83	117.89
18	N	1521	TGL	CG3-CG2-CG1	2.49	117.89	112.07
22	O	229	CHD	C5-C4-C3	2.50	116.63	112.91
25	T	263	PEK	C03-C02-C01	2.51	117.95	112.07
18	N	1523	TGL	CB3-CB2-CB1	2.51	123.47	113.59
17	N	515	HEA	C26-C15-C16	2.51	119.25	115.41
18	N	1521	TGL	OG2-CG2-CG3	2.53	117.26	108.36
18	L	522	TGL	C13-C12-C11	2.55	127.70	114.53
18	N	1522	TGL	C20-CA9-CA8	2.55	127.71	114.53
22	B	1086	CHD	C1-C2-C3	2.56	114.59	110.43
25	P	1265	PEK	C24-C23-C22	2.58	122.76	113.29
18	A	523	TGL	OG1-CG1-CG2	2.59	115.65	108.69
22	P	1271	CHD	C9-C11-C12	2.60	117.64	114.36
22	C	271	CHD	C6-C5-C10	2.62	115.54	112.66
22	W	1060	CHD	C15-C16-C17	2.62	110.41	105.12
23	M	526	DMU	C10-O1-C9	2.64	118.86	113.75
18	B	521	TGL	CG3-CG2-CG1	2.65	118.26	112.07
17	N	516	HEA	C3C-C4C-NC	2.66	112.65	109.21
17	N	515	HEA	CMB-C2B-C3B	2.66	130.58	125.14
18	L	522	TGL	CC4-CC3-CC2	2.66	123.06	113.29
18	A	523	TGL	OG2-CG2-CG3	2.68	117.80	108.36
22	P	1525	CHD	C5-C6-C7	2.69	117.44	114.44
22	P	1271	CHD	C16-C15-C14	2.70	110.56	105.12
18	L	522	TGL	C20-CA9-CA8	2.70	128.48	114.53
17	N	516	HEA	C17-C18-C19	2.70	133.64	127.76
17	A	515	HEA	C26-C15-C16	2.72	119.56	115.41
22	C	271	CHD	C16-C15-C14	2.72	110.60	105.12
22	C	271	CHD	C9-C11-C12	2.73	117.80	114.36
22	C	271	CHD	C5-C4-C3	2.73	116.97	112.91
22	W	1060	CHD	C14-C13-C12	2.73	109.83	107.39
18	N	1522	TGL	OG1-CG1-CG2	2.74	116.07	108.69
18	N	1522	TGL	C13-C12-C11	2.75	128.73	114.53
22	J	60	CHD	C15-C16-C17	2.76	110.68	105.12
22	P	1271	CHD	C6-C5-C10	2.77	115.70	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	515	HEA	CMC-C2C-C3C	2.78	130.52	125.09
26	G	269	CDL	C23-C22-C21	2.79	128.91	114.53
22	C	271	CHD	C15-C16-C17	2.79	110.74	105.12
22	O	229	CHD	C1-C10-C5	2.79	112.40	107.81
26	G	269	CDL	C22-C21-C20	2.79	128.96	114.53
22	W	1060	CHD	C4-C5-C10	2.80	115.74	112.66
25	C	265	PEK	C24-C23-C22	2.80	123.56	113.29
22	P	1271	CHD	C15-C16-C17	2.81	110.79	105.12
26	T	1269	CDL	C22-C21-C20	2.82	129.08	114.53
23	Z	1526	DMU	C10-O7-C3	2.82	125.38	118.01
22	W	1060	CHD	C1-C2-C3	2.82	115.01	110.43
18	L	522	TGL	OG1-CG1-CG2	2.83	116.31	108.69
26	T	1269	CDL	C23-C22-C21	2.84	129.21	114.53
22	J	60	CHD	C1-C2-C3	2.88	115.10	110.43
22	B	1086	CHD	C17-C13-C14	2.88	102.96	100.05
23	M	526	DMU	O7-C10-O1	2.89	118.00	110.68
22	J	60	CHD	C16-C15-C14	2.91	110.98	105.12
18	A	523	TGL	CB3-CB2-CB1	2.93	125.11	113.59
22	C	525	CHD	C13-C17-C20	2.94	123.08	119.50
17	A	516	HEA	C4B-C3B-C11	2.95	130.21	127.01
23	P	1272	DMU	O5-C6-O16	2.96	117.18	110.05
22	J	60	CHD	C4-C5-C10	2.97	115.93	112.66
18	N	1523	TGL	OG2-CG2-CG3	3.02	119.02	108.36
18	L	522	TGL	CC3-CC2-CC1	3.04	125.53	113.59
18	N	1522	TGL	CC3-CC2-CC1	3.04	125.55	113.59
22	J	60	CHD	C9-C11-C12	3.05	118.21	114.36
22	W	1060	CHD	C16-C15-C14	3.09	111.34	105.12
25	T	263	PEK	C02-O01-C1	3.11	125.36	117.89
22	C	525	CHD	C1-C10-C5	3.12	112.94	107.81
22	P	1271	CHD	C14-C8-C7	3.16	116.12	111.74
22	J	60	CHD	C13-C14-C8	3.21	118.89	114.75
22	C	525	CHD	C10-C9-C8	3.22	115.42	111.88
22	O	229	CHD	C5-C6-C7	3.22	118.03	114.44
22	B	1086	CHD	C1-C10-C5	3.23	113.12	107.81
25	G	1263	PEK	C02-O01-C1	3.24	125.66	117.89
23	Z	1526	DMU	O7-C10-O1	3.26	118.92	110.68
22	O	229	CHD	C9-C11-C12	3.26	118.47	114.36
23	C	272	DMU	C10-O7-C3	3.26	126.52	118.01
22	W	1060	CHD	C9-C11-C12	3.26	118.48	114.36
22	W	1060	CHD	C13-C14-C8	3.27	118.96	114.75
22	P	1271	CHD	C5-C4-C3	3.28	117.79	112.91
22	B	1086	CHD	C9-C11-C12	3.29	118.52	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	1060	CHD	C14-C8-C9	3.30	114.16	109.62
22	C	271	CHD	C14-C8-C7	3.31	116.34	111.74
22	J	60	CHD	C14-C8-C9	3.32	114.18	109.62
17	N	516	HEA	C27-C19-C20	3.39	120.58	115.41
18	N	1522	TGL	C11-C10-CB9	3.39	132.05	114.53
23	C	272	DMU	O5-C6-O16	3.40	118.23	110.05
23	M	526	DMU	C10-O7-C3	3.40	126.90	118.01
22	P	1525	CHD	C13-C17-C20	3.44	123.69	119.50
18	L	522	TGL	C11-C10-CB9	3.44	132.32	114.53
18	N	1522	TGL	CG2-OG2-CB1	3.47	126.22	117.89
22	C	271	CHD	C1-C10-C9	3.53	117.14	111.45
17	A	516	HEA	C27-C19-C20	3.53	120.80	115.41
18	N	1522	TGL	C16-C15-CC9	3.61	133.16	114.53
18	L	522	TGL	C16-C15-CC9	3.62	133.24	114.53
22	J	60	CHD	C5-C4-C3	3.64	118.33	112.91
22	P	1525	CHD	C1-C10-C5	3.64	113.80	107.81
18	L	522	TGL	CG2-OG2-CB1	3.64	126.64	117.89
22	W	1060	CHD	C6-C5-C4	3.67	115.14	111.05
18	N	1522	TGL	C15-CC9-CC8	3.67	133.49	114.53
22	J	60	CHD	C6-C5-C4	3.69	115.16	111.05
18	L	522	TGL	C15-CC9-CC8	3.71	133.67	114.53
22	C	271	CHD	C5-C6-C7	3.72	118.58	114.44
22	P	1271	CHD	C1-C10-C9	3.73	117.47	111.45
22	W	1060	CHD	C5-C4-C3	3.73	118.47	112.91
22	P	1271	CHD	C5-C6-C7	3.74	118.61	114.44
25	C	265	PEK	C11-C10-C9	3.83	124.73	112.00
25	P	1265	PEK	C11-C10-C9	3.87	124.87	112.00
22	W	1060	CHD	C1-C10-C5	3.89	114.20	107.81
23	C	272	DMU	O7-C10-O1	3.94	120.66	110.68
22	J	60	CHD	C1-C10-C5	3.95	114.31	107.81
22	B	1086	CHD	C10-C9-C8	3.96	116.23	111.88
23	Z	1526	DMU	O7-C10-C5	3.96	117.74	108.10
23	C	272	DMU	C8-C7-C5	3.99	118.24	110.79
23	P	1272	DMU	O7-C10-O1	4.03	120.89	110.68
25	G	1263	PEK	O03-C01-C02	4.05	119.58	108.69
25	T	263	PEK	O03-C01-C02	4.05	119.60	108.69
18	A	523	TGL	CG3-OG3-CC1	4.14	128.43	116.85
18	N	1523	TGL	CG3-OG3-CC1	4.28	128.81	116.85
23	Z	1526	DMU	O16-C6-C1	4.30	113.47	108.04
23	M	526	DMU	O7-C10-C5	4.31	118.60	108.10
18	B	521	TGL	CG3-OG3-CC1	4.33	128.97	116.85
23	C	272	DMU	O5-C6-C1	4.36	119.23	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1271	CHD	C4-C3-C2	4.37	116.10	110.52
23	P	1272	DMU	O5-C6-C1	4.42	119.35	110.28
22	W	1060	CHD	C2-C1-C10	4.43	120.75	112.84
18	N	1521	TGL	CG3-OG3-CC1	4.46	129.31	116.85
23	M	526	DMU	O7-C3-C4	4.46	121.05	109.32
22	J	60	CHD	C2-C1-C10	4.48	120.84	112.84
23	Z	1526	DMU	O7-C3-C4	4.52	121.21	109.32
22	P	1271	CHD	C4-C5-C10	4.60	117.73	112.66
23	M	526	DMU	O5-C6-C1	4.74	120.00	110.28
22	W	1060	CHD	C9-C8-C7	4.75	117.53	111.92
22	P	1271	CHD	C9-C8-C7	4.78	117.56	111.92
22	J	60	CHD	C9-C8-C7	4.78	117.57	111.92
22	C	271	CHD	C4-C3-C2	4.82	116.66	110.52
23	Z	1526	DMU	O5-C6-C1	4.85	120.22	110.28
22	P	1271	CHD	C14-C13-C12	4.85	111.73	107.39
22	C	271	CHD	C9-C8-C7	4.86	117.66	111.92
18	N	1521	TGL	CG2-OG2-CB1	4.94	129.75	117.89
22	C	271	CHD	C4-C5-C10	4.95	118.11	112.66
22	C	271	CHD	C14-C13-C12	4.97	111.84	107.39
22	W	1060	CHD	C11-C9-C10	5.08	119.07	113.79
23	M	526	DMU	O16-C6-C1	5.16	114.55	108.04
22	O	229	CHD	C10-C9-C8	5.22	117.61	111.88
23	P	1272	DMU	C10-O1-C9	5.22	123.88	113.75
22	J	60	CHD	C11-C9-C10	5.24	119.23	113.79
18	B	521	TGL	CG2-OG2-CB1	5.33	130.68	117.89
23	C	272	DMU	O1-C9-C8	5.34	119.70	109.68
22	W	1060	CHD	C5-C6-C7	5.35	120.40	114.44
22	P	1271	CHD	C1-C10-C5	5.37	116.63	107.81
22	J	60	CHD	C5-C6-C7	5.40	120.46	114.44
22	J	60	CHD	C6-C5-C10	5.40	118.61	112.66
23	C	272	DMU	C10-O1-C9	5.47	124.36	113.75
22	C	271	CHD	C1-C10-C5	5.47	116.80	107.81
22	J	60	CHD	C11-C12-C13	5.53	116.81	111.20
23	P	1272	DMU	O7-C3-C2	5.53	121.44	107.17
22	W	1060	CHD	C11-C12-C13	5.64	116.93	111.20
23	Z	1526	DMU	C18-O16-C6	5.65	123.81	113.94
22	W	1060	CHD	C4-C3-C2	5.71	117.80	110.52
22	W	1060	CHD	C6-C5-C10	5.76	119.00	112.66
23	M	526	DMU	C18-O16-C6	5.92	124.29	113.94
23	P	1272	DMU	O5-C4-C57	5.94	121.37	106.36
22	J	60	CHD	C4-C3-C2	5.95	118.11	110.52
23	C	272	DMU	O7-C3-C2	5.99	122.63	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Z	1526	DMU	O7-C3-C2	6.01	122.67	107.17
23	M	526	DMU	O7-C3-C2	6.06	122.80	107.17
23	C	272	DMU	O5-C4-C57	6.21	122.04	106.36
23	P	1272	DMU	O7-C10-C5	6.25	123.32	108.10
23	C	272	DMU	O7-C10-C5	6.35	123.54	108.10
22	J	60	CHD	C10-C9-C8	6.35	118.85	111.88
23	M	526	DMU	O5-C4-C57	6.38	122.49	106.36
23	M	526	DMU	O5-C6-O16	6.38	125.43	110.05
23	P	1272	DMU	O1-C9-C8	6.42	121.72	109.68
22	W	1060	CHD	C10-C9-C8	6.42	118.93	111.88
22	J	60	CHD	C13-C17-C20	6.44	127.35	119.50
22	W	1060	CHD	C13-C17-C20	6.50	127.42	119.50
23	Z	1526	DMU	O5-C4-C57	6.65	123.15	106.36
23	Z	1526	DMU	O5-C6-O16	6.75	126.30	110.05
23	Z	1526	DMU	O1-C9-C8	6.75	122.36	109.68
23	P	1272	DMU	C8-C7-C5	6.91	123.69	110.79
23	C	272	DMU	O5-C4-C3	6.94	124.41	109.75
23	M	526	DMU	O1-C9-C8	7.08	122.98	109.68
23	P	1272	DMU	O5-C4-C3	7.30	125.16	109.75
23	P	1272	DMU	O1-C9-C11	7.36	124.94	106.36
23	M	526	DMU	O1-C9-C11	7.36	124.96	106.36
23	Z	1526	DMU	O1-C9-C11	7.50	125.32	106.36
23	P	1272	DMU	C18-O16-C6	7.57	127.17	113.94
23	Z	1526	DMU	O5-C4-C3	7.61	125.83	109.75
23	C	272	DMU	O7-C3-C4	7.70	129.55	109.32
23	M	526	DMU	O5-C4-C3	7.76	126.14	109.75
23	M	526	DMU	C7-C8-C9	7.93	124.02	110.20
23	Z	1526	DMU	C7-C8-C9	7.93	124.03	110.20
23	C	272	DMU	O1-C9-C11	8.12	126.87	106.36
23	Z	1526	DMU	C6-O5-C4	8.21	129.68	113.75
23	M	526	DMU	C6-O5-C4	8.23	129.73	113.75
23	C	272	DMU	C18-O16-C6	8.39	128.60	113.94
23	P	1272	DMU	O7-C3-C4	8.50	131.65	109.32
23	P	1272	DMU	C6-O5-C4	8.78	130.79	113.75
22	W	1060	CHD	C17-C13-C14	8.88	109.02	100.05
23	Z	1526	DMU	C1-C2-C3	9.16	129.73	109.60
23	M	526	DMU	C1-C2-C3	9.27	129.95	109.60
22	J	60	CHD	C17-C13-C14	9.30	109.45	100.05
23	C	272	DMU	C6-O5-C4	9.43	132.04	113.75
23	P	1272	DMU	C1-C2-C3	9.78	131.08	109.60
22	C	271	CHD	C10-C9-C8	9.84	122.68	111.88
23	C	272	DMU	C1-C2-C3	10.04	131.66	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1271	CHD	C10-C9-C8	10.27	123.15	111.88
22	C	271	CHD	C17-C13-C14	10.38	110.54	100.05
22	P	1271	CHD	C17-C13-C14	10.52	110.69	100.05
23	Z	1526	DMU	C10-C5-C7	10.95	131.55	109.97
23	M	526	DMU	C10-C5-C7	11.16	131.97	109.97
23	C	272	DMU	O16-C6-C1	11.27	122.28	108.04
23	P	1272	DMU	O16-C6-C1	11.92	123.09	108.04

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
22	W	1060	CHD	C12
22	W	1060	CHD	C8
22	W	1060	CHD	C9
22	W	1060	CHD	C14
22	W	1060	CHD	C17
23	M	526	DMU	C2
23	M	526	DMU	C4
23	M	526	DMU	C6
23	M	526	DMU	C5
23	M	526	DMU	C9
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
22	J	60	CHD	C12
22	J	60	CHD	C8
22	J	60	CHD	C9
22	J	60	CHD	C14
22	J	60	CHD	C17
23	P	1272	DMU	C5
23	P	1272	DMU	C6
23	P	1272	DMU	C9
23	P	1272	DMU	C4
23	P	1272	DMU	C2
23	P	1272	DMU	C10
22	P	1271	CHD	C12

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Mol	Chain	Res	Type	Atom
22	P	1271	CHD	C8
22	P	1271	CHD	C3
22	P	1271	CHD	C9
22	P	1271	CHD	C14
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
23	C	272	DMU	C5
23	C	272	DMU	C6
23	C	272	DMU	C9
23	C	272	DMU	C4
23	C	272	DMU	C2
23	C	272	DMU	C10
22	C	271	CHD	C12
22	C	271	CHD	C8
22	C	271	CHD	C3
22	C	271	CHD	C9
22	C	271	CHD	C14
23	Z	1526	DMU	C2
23	Z	1526	DMU	C4
23	Z	1526	DMU	C6
23	Z	1526	DMU	C5
23	Z	1526	DMU	C9

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C02-O01-C1-C2
19	N	1524	PGV	C02-O01-C1-C2
19	N	1524	PGV	P-O11-C03-C02
19	A	524	PGV	P-O11-C03-C02

There are no ring outliers.

36 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	515	HEA	2	0
17	A	516	HEA	4	0
18	A	523	TGL	4	0
19	A	524	PGV	7	0
22	B	1086	CHD	1	0
21	B	230	PSC	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	521	TGL	7	0
25	C	264	PEK	4	0
25	C	265	PEK	7	0
19	C	267	PGV	5	0
19	C	268	PGV	1	0
26	C	270	CDL	11	0
22	C	271	CHD	3	0
23	C	272	DMU	3	0
25	G	1263	PEK	10	0
26	G	269	CDL	18	0
22	J	60	CHD	2	0
18	L	522	TGL	20	0
18	N	1521	TGL	9	0
18	N	1522	TGL	14	0
18	N	1523	TGL	4	0
19	N	1524	PGV	8	0
17	N	515	HEA	3	0
17	N	516	HEA	2	0
21	O	1230	PSC	15	0
22	O	229	CHD	1	0
25	P	1264	PEK	6	0
25	P	1265	PEK	7	0
19	P	1267	PGV	5	0
19	P	1268	PGV	1	0
26	P	1270	CDL	15	0
22	P	1271	CHD	1	0
23	P	1272	DMU	8	0
26	T	1269	CDL	19	0
25	T	263	PEK	6	0
22	W	1060	CHD	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.