Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:54 AM GMT

PDB ID	:	2EIK
Title	:	Cadmium ion binding structure of 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	:	2.10 Å(reported)

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

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

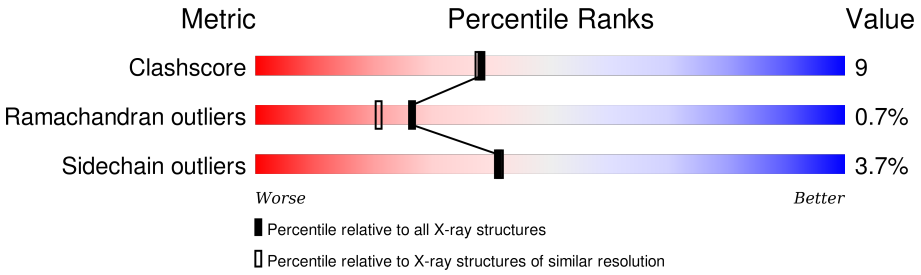
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	87% 12% •
1	N	514	82% 17% •
2	B	227	81% 18% •
2	O	227	75% 23% •
3	C	261	86% 13% •
3	P	261	84% 15% ••
4	D	147	85% 12% ••

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Mol	Chain	Length	Quality of chain
4	Q	147	74% 23%
5	E	109	86% 10%
5	R	109	68% 28%
6	F	98	83% 15%
6	S	98	87% 9%
7	G	85	74% 20% 5%
7	T	85	71% 21% 7%
8	H	85	85% 6% 7%
8	U	85	75% 15% 7%
9	I	73	88% 11%
9	V	73	84% 15%
10	J	59	88% 8%
10	W	59	86% 10%
11	K	56	73% 14% 13%
11	X	56	79% 7% 13%
12	L	47	74% 19%
12	Y	47	81% 17%
13	M	46	76% 15% 7%
13	Z	46	74% 20% 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
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	L	522	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32450 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		

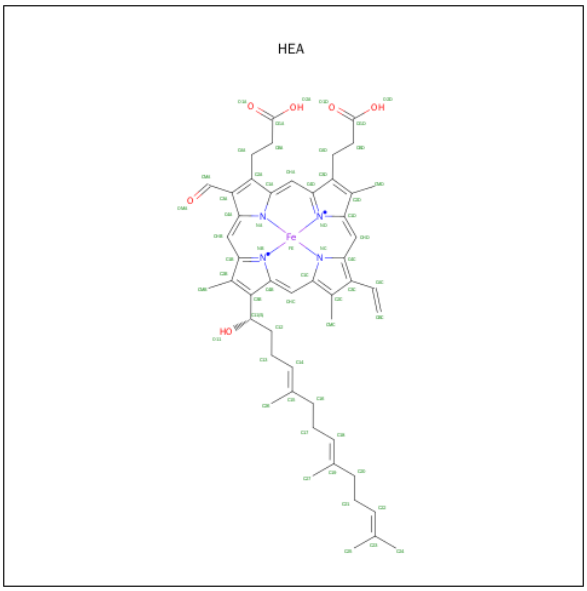
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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 CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	2	Total Cd 2 2	0	0
17	A	1	Total Cd 1 1	0	0
17	C	1	Total Cd 1 1	0	0
17	N	1	Total Cd 1 1	0	0
17	E	1	Total Cd 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

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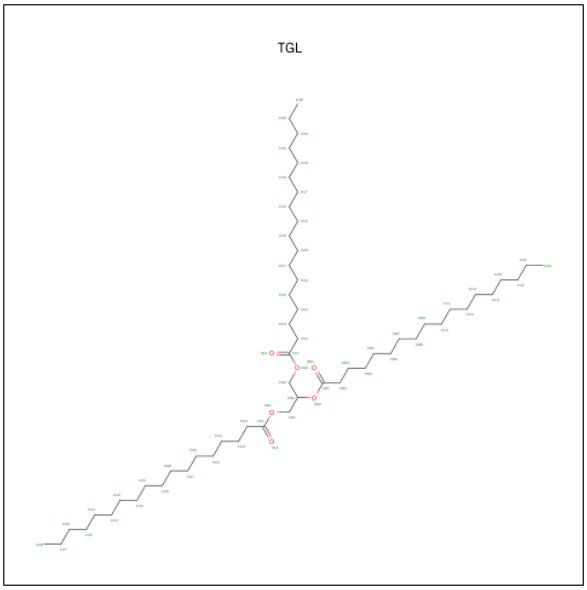
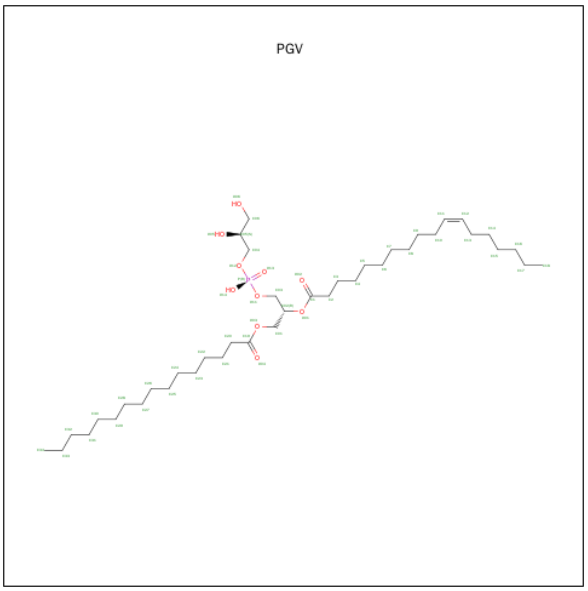
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



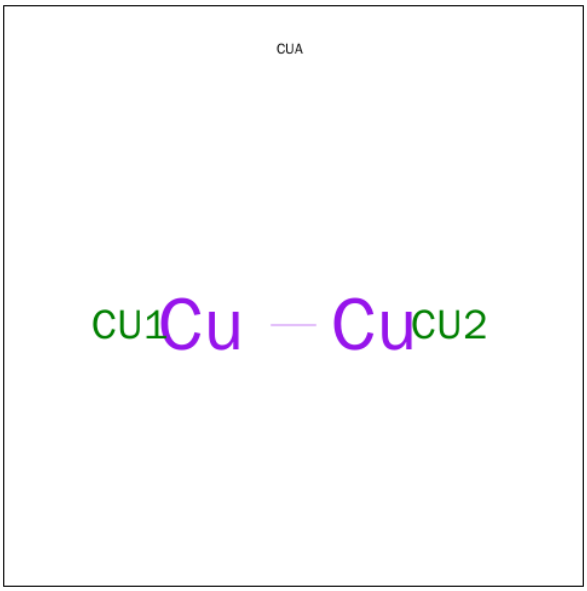
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	A	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



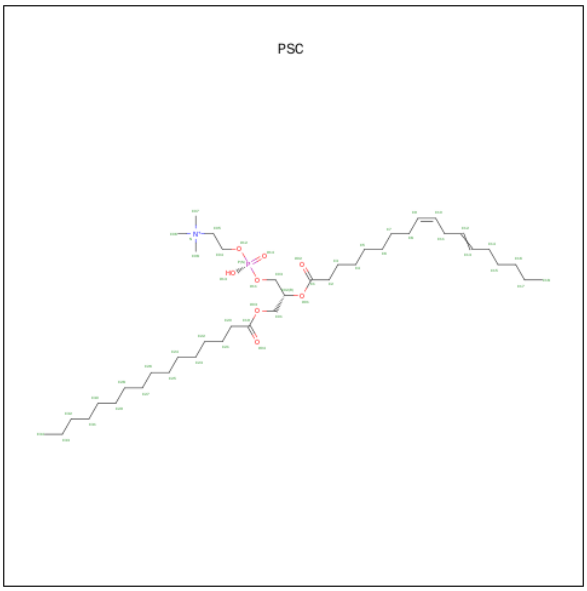
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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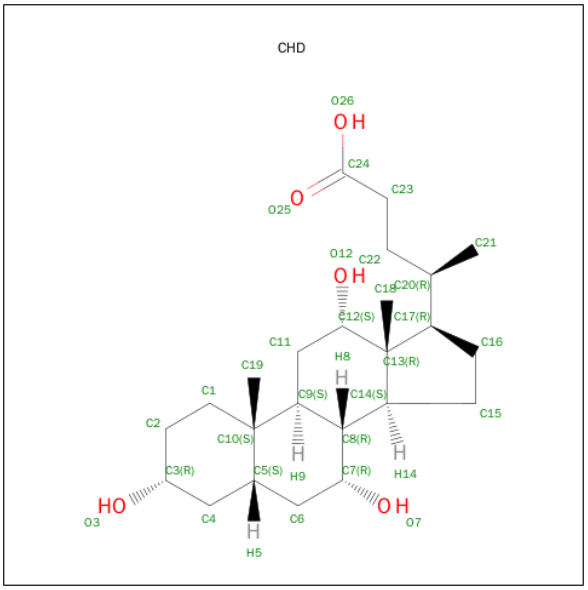
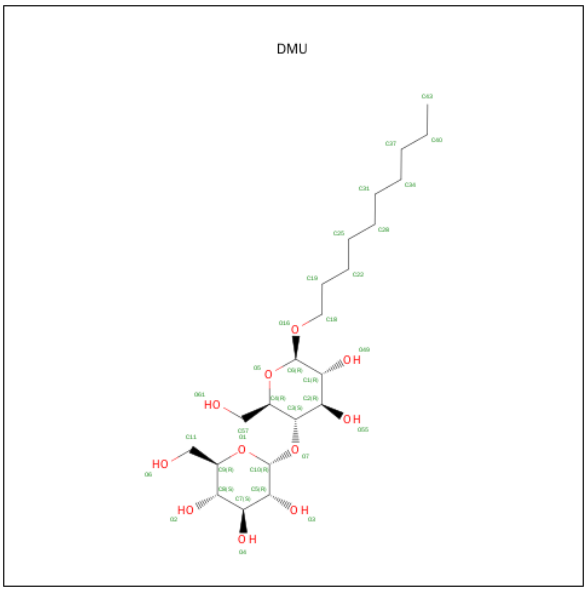
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



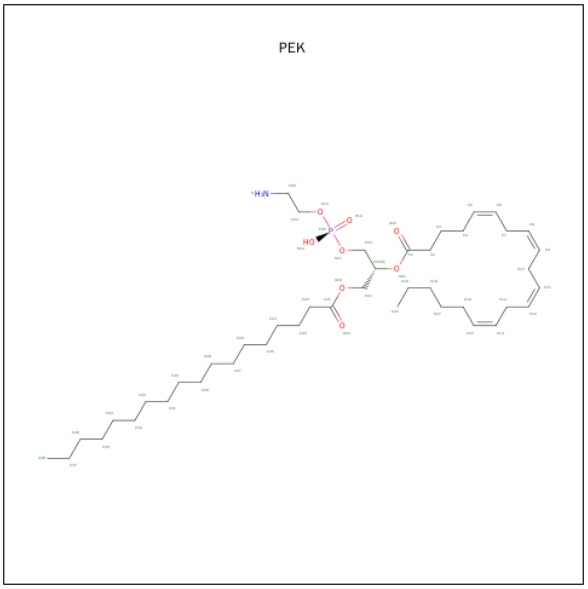
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	O			0	0
			29	24	5				
23	C	1	Total	C	O			0	0
			29	24	5				
23	C	1	Total	C	O			0	0
			29	24	5				
23	J	1	Total	C	O			0	0
			29	24	5				
23	O	1	Total	C	O			0	0
			29	24	5				
23	P	1	Total	C	O			0	0
			29	24	5				
23	P	1	Total	C	O			0	0
			29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

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



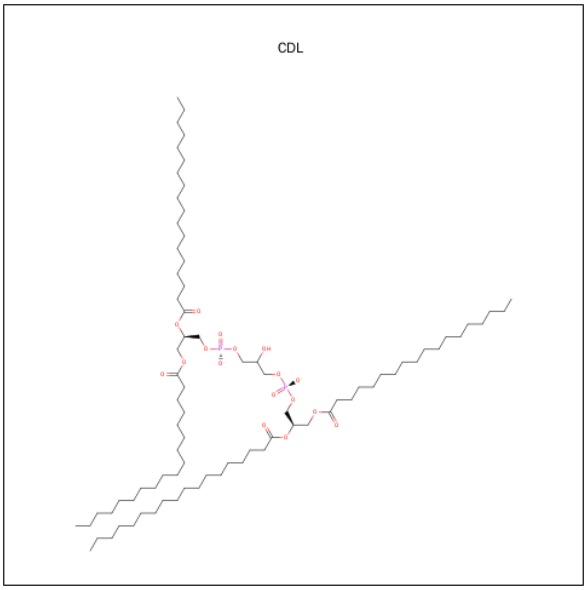
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 33 22 11	0	0
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	223	Total O 223 223	0	0
28	B	146	Total O 146 146	0	0
28	C	102	Total O 102 102	0	0
28	D	98	Total O 98 98	0	0
28	E	60	Total O 60 60	0	0
28	F	85	Total O 85 85	0	0
28	G	41	Total O 41 41	0	0
28	H	49	Total O 49 49	0	0
28	I	44	Total O 44 44	0	0
28	J	26	Total O 26 26	0	0
28	K	25	Total O 25 25	0	0
28	L	23	Total O 23 23	0	0
28	M	22	Total O 22 22	0	0
28	N	213	Total O 213 213	0	0
28	O	116	Total O 116 116	0	0
28	P	103	Total O 103 103	0	0
28	Q	52	Total O 52 52	0	0
28	R	41	Total O 41 41	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	S	69	Total O 69 69	0	0
28	T	47	Total O 47 47	0	0
28	U	43	Total O 43 43	0	0
28	V	25	Total O 25 25	0	0
28	W	15	Total O 15 15	0	0
28	X	17	Total O 17 17	0	0
28	Y	15	Total O 15 15	0	0
28	Z	14	Total O 14 14	0	0

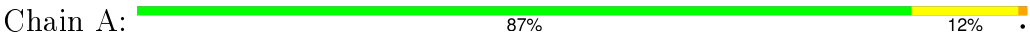
3 Residue-property plots (i)

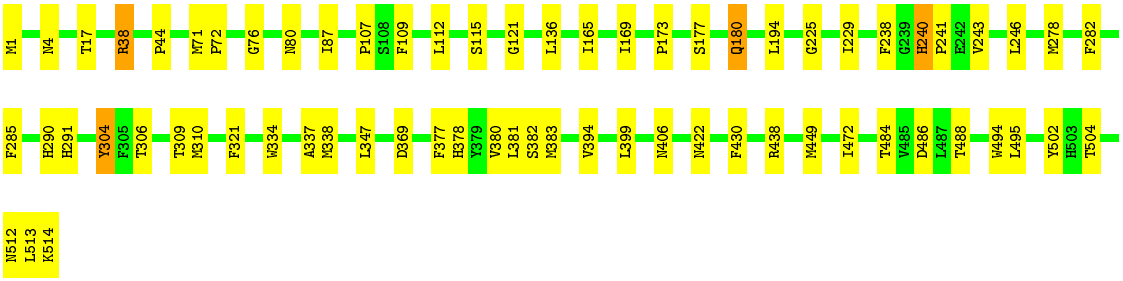
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

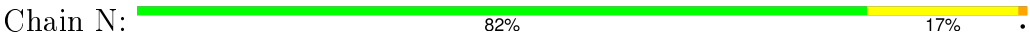
Chain A:

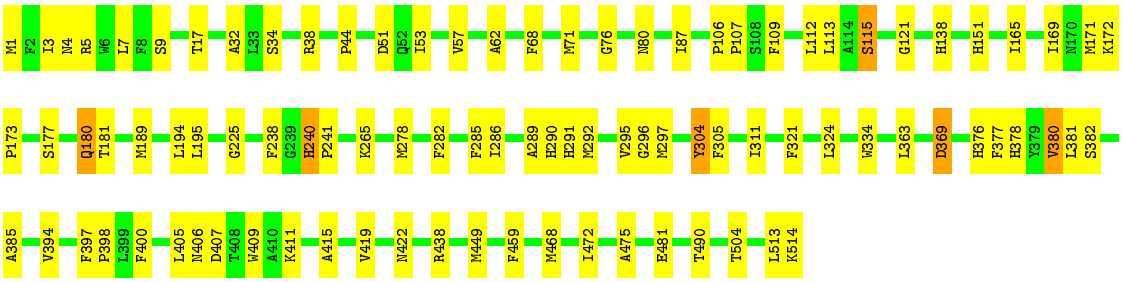




- Molecule 1: Cytochrome c oxidase subunit 1

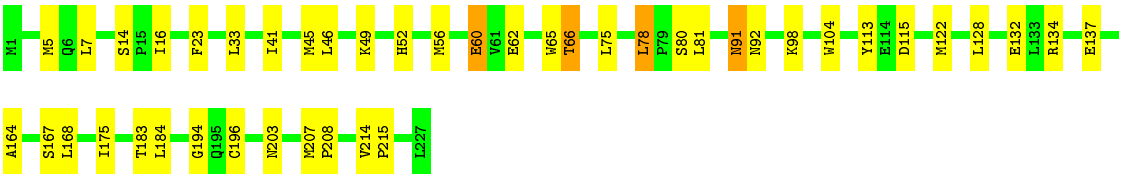
Chain N:





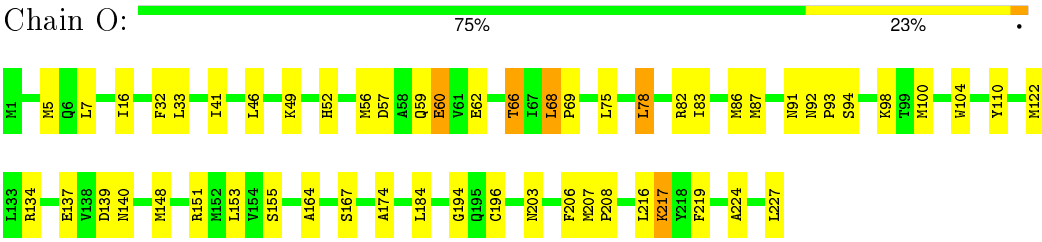
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



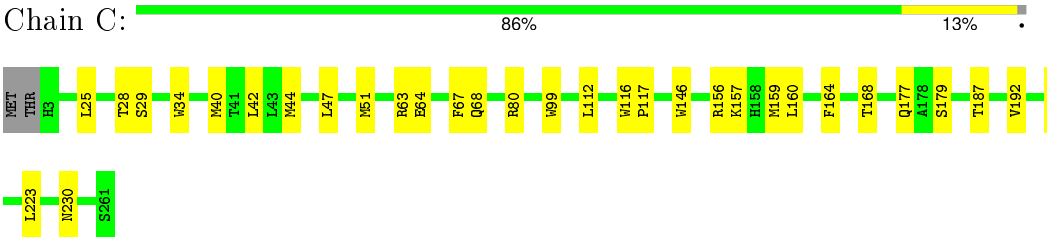
- Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



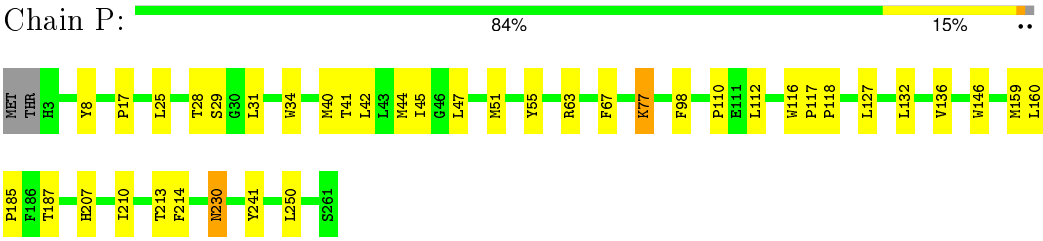
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



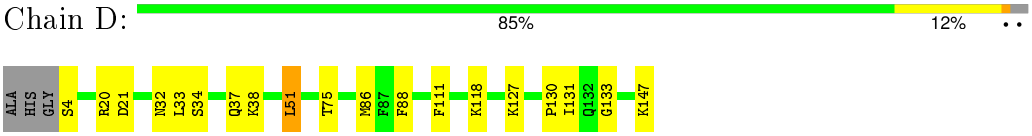
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



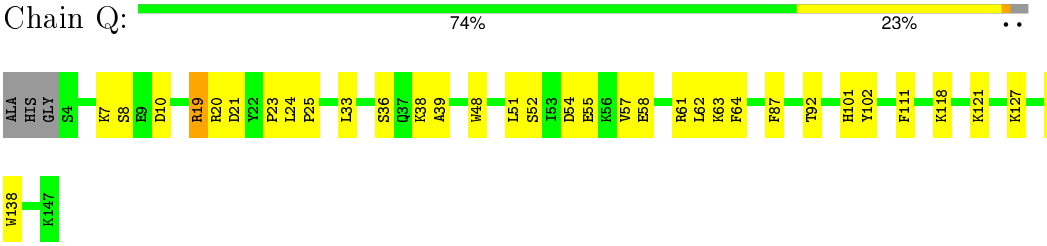
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



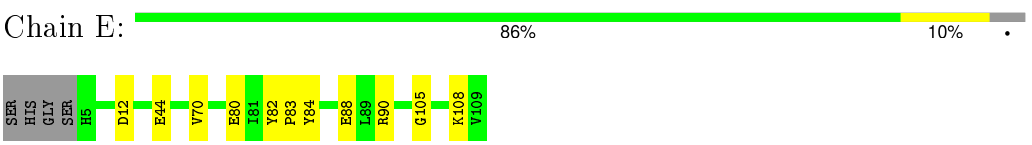
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



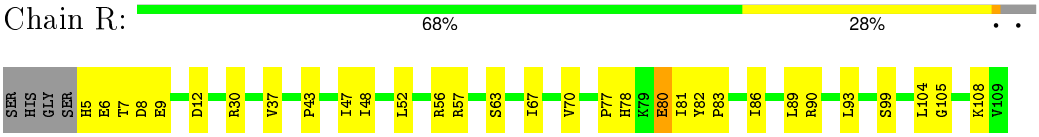
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



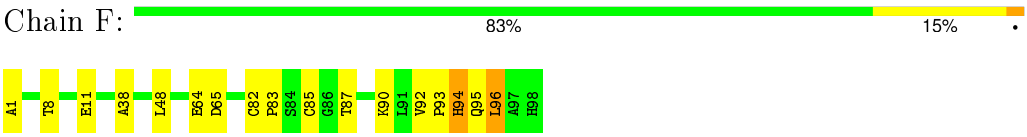
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



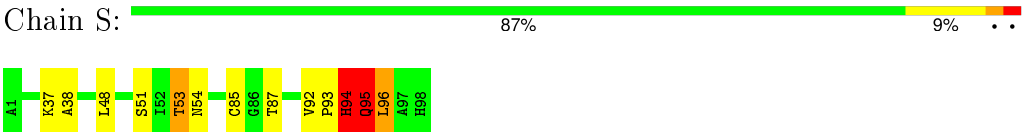
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:



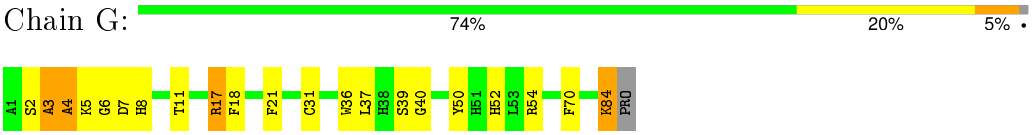
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:



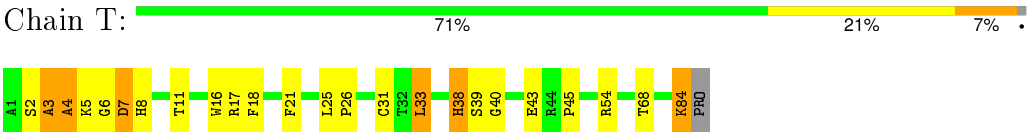
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



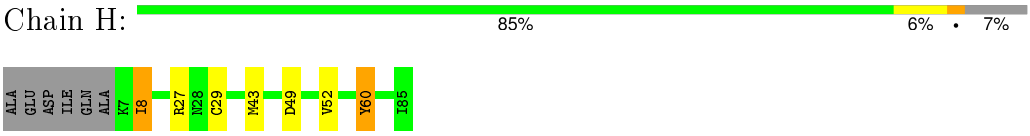
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



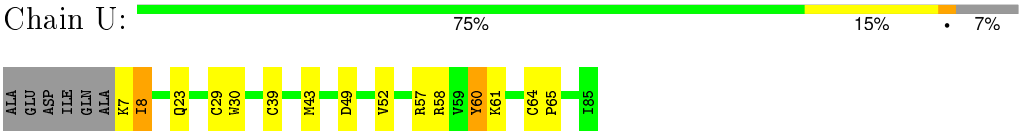
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:



• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:

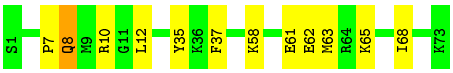


• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:

• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:

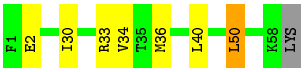


• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:

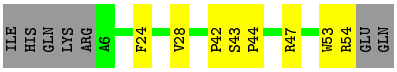
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



• Molecule 11: Cytochrome c oxidase polypeptide VIIb

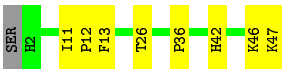
Chain X:

• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:

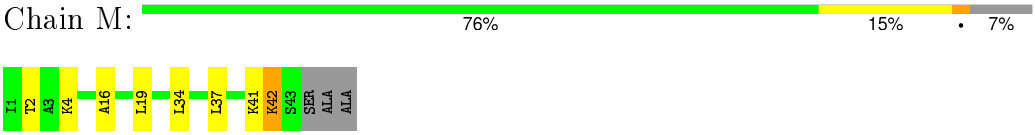
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



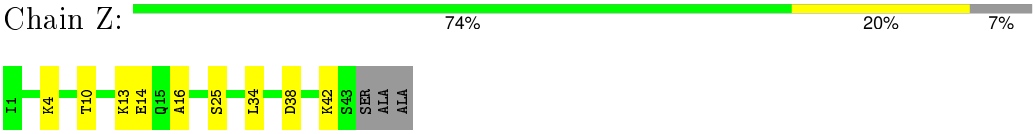
• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

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	183.32Å 206.53Å 178.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.199 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32450	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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, CD, 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	0.68	1/5678 (0.0%)
1	N	0.52	0/4156	0.67	0/5678
2	B	0.52	0/1860	0.77	0/2534
2	O	0.53	0/1860	0.78	1/2534 (0.0%)
3	C	0.52	0/2197	0.61	0/3005
3	P	0.50	0/2197	0.62	0/3005
4	D	0.52	0/1229	0.68	2/1658 (0.1%)
4	Q	0.56	0/1229	0.67	1/1658 (0.1%)
5	E	0.52	0/871	0.68	0/1182
5	R	0.56	1/871 (0.1%)	0.73	0/1182
6	F	0.49	0/765	0.81	2/1038 (0.2%)
6	S	0.50	0/765	0.80	2/1038 (0.2%)
7	G	0.53	0/690	0.70	0/937
7	T	0.55	0/690	0.71	1/937 (0.1%)
8	H	0.49	0/682	0.68	0/921
8	U	0.47	0/682	0.65	0/921
9	I	0.53	0/605	0.64	0/802
9	V	0.51	0/605	0.63	0/802
10	J	0.49	0/471	0.64	0/636
10	W	0.50	0/471	0.66	0/636
11	K	0.57	0/398	0.69	0/546
11	X	0.53	0/398	0.68	0/546
12	L	0.54	0/393	0.60	0/526
12	Y	0.57	0/393	0.63	0/526
13	M	0.48	0/345	0.63	0/470
13	Z	0.50	0/345	0.64	0/470
All	All	0.52	1/29324 (0.0%)	0.69	10/39866 (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	2
1	N	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CD-OE2	5.15	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	94	HIS	N-CA-C	6.57	128.74	111.00
6	F	94	HIS	N-CA-C	6.02	127.25	111.00
4	D	133	GLY	N-CA-C	5.85	127.72	113.10
4	Q	133	GLY	N-CA-C	5.48	126.80	113.10
6	F	93	PRO	N-CA-C	5.47	126.33	112.10
2	O	184	LEU	CA-CB-CG	5.35	127.61	115.30
7	T	33	LEU	CA-CB-CG	5.35	127.60	115.30
4	D	51	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	438	ARG	CB-CA-C	-5.15	100.10	110.40
6	S	93	PRO	N-CA-C	5.10	125.36	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	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	59	0
1	N	4027	0	4001	76	0
2	B	1824	0	1833	31	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	30	0
3	P	2110	0	2027	42	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	4	0
5	R	852	0	845	20	0
6	F	748	0	728	9	0
6	S	748	0	728	9	0
7	G	675	0	644	25	0
7	T	675	0	644	25	0
8	H	662	0	623	5	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	12	0
10	J	460	0	459	6	0
10	W	460	0	459	6	0
11	K	384	0	366	5	0
11	X	384	0	366	4	0
12	L	380	0	380	17	0
12	Y	380	0	380	8	0
13	M	335	0	352	8	0
13	Z	335	0	352	5	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	1	0	0	0	0
17	C	1	0	0	0	0
17	E	1	0	0	0	0
17	N	1	0	0	0	0
17	P	2	0	0	0	0
18	A	120	0	108	5	0
18	N	120	0	108	4	0
19	A	126	0	220	16	0
19	L	63	0	110	23	0
19	N	63	0	110	8	0
19	Q	63	0	110	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	63	0	110	17	0
20	A	102	0	152	9	0
20	C	102	0	152	7	0
20	N	102	0	152	10	0
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	14	0
22	O	52	0	80	15	0
23	B	29	0	39	1	0
23	C	58	0	78	7	0
23	J	29	0	39	3	0
23	O	29	0	39	1	0
23	P	58	0	78	1	0
23	W	29	0	39	5	0
24	C	33	0	36	2	0
24	M	33	0	38	0	0
24	P	33	0	36	8	0
24	Z	33	0	38	0	0
25	C	106	0	154	11	0
25	G	53	0	77	9	0
25	P	106	0	154	12	0
25	T	53	0	77	9	0
26	C	100	0	156	16	0
26	G	100	0	156	22	0
26	P	100	0	156	18	0
26	T	100	0	156	19	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	223	0	0	2	0
28	B	146	0	0	4	0
28	C	102	0	0	2	0
28	D	98	0	0	4	0
28	E	60	0	0	1	0
28	F	85	0	0	1	0
28	G	41	0	0	1	0
28	H	49	0	0	2	0
28	I	44	0	0	3	0
28	J	26	0	0	2	0
28	K	25	0	0	1	0
28	L	23	0	0	0	0
28	M	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	N	213	0	0	3	0
28	O	116	0	0	1	0
28	P	103	0	0	2	0
28	Q	52	0	0	1	0
28	R	41	0	0	0	0
28	S	69	0	0	3	0
28	T	47	0	0	4	0
28	U	43	0	0	1	0
28	V	25	0	0	1	0
28	W	15	0	0	2	0
28	X	17	0	0	0	0
28	Y	15	0	0	1	0
28	Z	14	0	0	1	0
All	All	32450	0	31298	566	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (566) 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)
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.31	1.11
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.39	1.02
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.42	1.00
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.40	0.99
22:B:230:PSC:H343	22:B:230:PSC:H142	1.40	0.99
7:G:84:LYS:HD2	7:G:84:LYS:H	1.24	0.99
7:T:84:LYS:H	7:T:84:LYS:HD2	1.25	0.96
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.30	0.95
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.94
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.33	0.91
25:C:264:PEK:H102	25:C:264:PEK:H161	1.52	0.91
26:G:269:CDL:H541	26:G:269:CDL:H231	1.52	0.90
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.89
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.55	0.89
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.56	0.88
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.55	0.88
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.54	0.88
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.39	0.87
26:C:270:CDL:H642	26:C:270:CDL:H191	1.56	0.86
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:CYS:SG	26:G:269:CDL:H532	2.16	0.86
28:C:4303:HOH:O	6:F:1:ALA:HB2	1.74	0.86
19:A:521:TGL:H102	19:A:521:TGL:H281	1.57	0.86
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.15	0.86
19:N:1521:TGL:H102	19:N:1521:TGL:H281	1.58	0.84
1:A:278:MET:SD	7:T:5:LYS:HB3	2.18	0.83
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.61	0.82
19:Y:1522:TGL:HC22	19:Y:1522:TGL:HC62	1.62	0.82
19:L:522:TGL:HC22	19:L:522:TGL:HC62	1.61	0.82
19:N:1521:TGL:H102	19:N:1521:TGL:C28	2.11	0.81
12:L:24:MET:SD	19:L:522:TGL:H162	2.22	0.80
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.46	0.80
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.47	0.80
19:A:521:TGL:H102	19:A:521:TGL:C28	2.12	0.80
4:D:147:LYS:HG2	28:D:4622:HOH:O	1.81	0.79
1:N:514:LYS:HE2	28:S:3395:HOH:O	1.82	0.79
7:G:5:LYS:HB3	1:N:278:MET:SD	2.24	0.78
1:N:1:FME:HCN	1:N:4:ASN:H	1.49	0.78
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.65	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.65	0.77
26:G:269:CDL:H622	20:P:1268:PGV:H152	1.65	0.77
1:N:472:ILE:HG21	19:Y:1522:TGL:HA92	1.65	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.69	0.75
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.67	0.75
19:A:521:TGL:H201	19:A:521:TGL:H241	1.70	0.74
26:G:269:CDL:H522	26:G:269:CDL:H202	1.69	0.74
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.67	0.74
19:N:1521:TGL:H201	19:N:1521:TGL:H241	1.69	0.73
19:Y:1522:TGL:HC41	28:Y:4411:HOH:O	1.88	0.73
6:F:8:THR:OG1	6:F:11:GLU:HG3	1.88	0.72
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.72	0.72
12:Y:13:PHE:HA	19:Y:1522:TGL:HC31	1.70	0.72
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.69	0.72
5:R:89:LEU:O	5:R:93:LEU:HG	1.90	0.72
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.72
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.54	0.72
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.71	0.71
12:L:13:PHE:HA	19:L:522:TGL:HC31	1.72	0.71
6:S:94:HIS:CG	6:S:95:GLN:H	2.09	0.70
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.73	0.70
12:L:20:ARG:NH2	19:L:522:TGL:HC61	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.74	0.70
26:G:269:CDL:C23	26:G:269:CDL:H541	2.23	0.69
28:B:4845:HOH:O	4:D:21:ASP:HB2	1.91	0.69
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.28	0.69
6:F:85:CYS:SG	6:F:87:THR:HG23	2.33	0.69
6:F:92:VAL:O	6:F:92:VAL:HG23	1.94	0.68
19:Y:1522:TGL:H242	19:Y:1522:TGL:H202	1.76	0.68
19:L:522:TGL:H202	19:L:522:TGL:H242	1.76	0.67
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.29	0.67
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.77	0.67
26:P:1270:CDL:H391	28:P:4551:HOH:O	1.95	0.67
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.77	0.67
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.10	0.66
20:C:267:PGV:H172	26:C:270:CDL:H662	1.76	0.66
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.78	0.65
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.96	0.65
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.26	0.65
20:C:268:PGV:H152	26:T:1269:CDL:H622	1.79	0.65
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.60	0.65
8:H:8:ILE:HG21	28:H:4749:HOH:O	1.97	0.65
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.79	0.64
11:K:24:PHE:O	11:K:28:VAL:HG12	1.96	0.64
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.64
26:G:269:CDL:H511	26:G:269:CDL:H172	1.78	0.64
3:C:168:THR:HG22	25:C:265:PEK:H14	1.80	0.64
3:C:40:MET:O	3:C:44:MET:HG2	1.98	0.64
1:N:53:ILE:O	1:N:57:VAL:HG23	1.98	0.64
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.27	0.64
1:A:177:SER:H	1:A:180:GLN:HE21	1.46	0.63
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.10	0.63
19:N:1521:TGL:H161	2:O:7:LEU:HD11	1.81	0.63
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.79	0.63
2:B:56:MET:HG2	22:B:230:PSC:H211	1.80	0.63
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.63	0.63
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.12	0.63
10:J:7:GLU:HG3	28:J:4635:HOH:O	1.98	0.63
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.80	0.62
1:N:378:HIS:O	1:N:382:SER:HB2	1.99	0.62
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.34	0.62
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.65	0.62
3:C:168:THR:CG2	25:C:265:PEK:H14	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.80	0.62
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.82	0.62
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.80	0.62
1:N:76:GLY:O	1:N:80:ASN:HB2	1.98	0.62
20:A:524:PGV:H152	20:A:524:PGV:H321	1.82	0.62
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.34	0.62
4:D:34:SER:H	4:D:37:GLN:NE2	1.93	0.61
20:P:1267:PGV:H12	20:P:1267:PGV:H161	1.82	0.61
6:S:53:THR:HG22	28:S:4719:HOH:O	1.99	0.61
19:A:523:TGL:HG11	19:A:523:TGL:HC21	1.83	0.61
6:F:64:GLU:O	6:F:65:ASP:HB2	2.00	0.61
1:N:169:ILE:HD11	1:N:189:MET:SD	2.40	0.61
20:C:267:PGV:H12	20:C:267:PGV:H161	1.81	0.61
1:N:472:ILE:HG21	19:Y:1522:TGL:CA9	2.31	0.60
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.60
22:B:230:PSC:H21	22:B:230:PSC:H222	1.83	0.60
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.36	0.60
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.36	0.60
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.83	0.60
20:P:1268:PGV:H062	28:U:4194:HOH:O	2.01	0.60
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.37	0.60
3:P:40:MET:O	3:P:44:MET:HG2	2.01	0.60
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.83	0.60
2:B:91:ASN:HD21	2:B:183:THR:HG21	1.65	0.59
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.85	0.59
20:A:604:PGV:H182	3:C:28:THR:HG22	1.85	0.59
1:A:484:THR:HB	13:M:2:THR:OG1	2.03	0.59
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.84	0.59
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.83	0.59
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.68	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.59
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.85	0.59
1:A:177:SER:H	1:A:180:GLN:NE2	2.01	0.58
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.38	0.58
5:R:48:ILE:O	5:R:52:LEU:HG	2.03	0.58
7:G:2:SER:O	25:G:1263:PEK:H322	2.03	0.58
19:A:521:TGL:HA82	19:A:521:TGL:H222	1.85	0.58
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.17	0.58
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.85	0.58
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.39	0.58
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.86	0.57
2:B:62:GLU:O	2:B:66:THR:HB	2.04	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.57
1:N:449:MET:SD	2:O:5:MET:HG2	2.44	0.57
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.85	0.57
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.31	0.57
19:A:521:TGL:HC22	28:I:2383:HOH:O	2.04	0.57
6:F:90:LYS:HD2	28:F:4237:HOH:O	2.05	0.57
4:D:34:SER:O	4:D:38:LYS:HG3	2.05	0.57
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.40	0.57
2:B:49:LYS:HE2	28:E:4310:HOH:O	2.03	0.57
1:N:71:MET:HE1	1:N:195:LEU:HD21	1.87	0.57
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.70	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.57
28:B:4901:HOH:O	25:P:1265:PEK:H031	2.04	0.56
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.56
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.88	0.56
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.87	0.56
12:Y:12:PRO:HB2	19:Y:1522:TGL:HG2	1.87	0.56
2:O:224:ALA:O	2:O:227:LEU:HG	2.05	0.56
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.69	0.56
26:C:270:CDL:C19	26:C:270:CDL:H642	2.31	0.56
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.40	0.56
19:N:1521:TGL:H222	19:N:1521:TGL:HA82	1.87	0.56
5:E:84:TYR:O	5:E:88:GLU:HG2	2.06	0.55
11:X:24:PHE:O	11:X:28:VAL:HG12	2.06	0.55
20:N:1524:PGV:H311	13:Z:16:ALA:HA	1.89	0.55
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.88	0.55
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.42	0.55
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.72	0.55
1:A:1:FME:HCN	1:A:4:ASN:H	1.71	0.55
10:W:40:LEU:HD12	23:W:1060:CHD:H183	1.87	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.55
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.40	0.55
1:A:378:HIS:O	1:A:382:SER:HB2	2.07	0.54
1:A:17:THR:OG1	19:L:522:TGL:H281	2.07	0.54
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.90	0.54
22:O:1230:PSC:C34	22:O:1230:PSC:H142	2.27	0.54
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.90	0.54
20:A:524:PGV:H062	28:M:2160:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:524:PGV:H311	13:M:16:ALA:HA	1.89	0.54
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.71	0.54
8:U:49:ASP:O	8:U:52:VAL:HG22	2.08	0.54
4:Q:33:LEU:HB2	4:Q:38:LYS:HG2	1.89	0.54
4:D:20:ARG:HG3	28:D:4203:HOH:O	2.06	0.53
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.73	0.53
1:A:240:HIS:O	1:A:243:VAL:HG22	2.08	0.53
19:Q:1523:TGL:H363	28:V:4756:HOH:O	2.09	0.53
4:D:86:MET:HE3	28:K:4855:HOH:O	2.08	0.53
8:U:7:LYS:O	8:U:8:ILE:HG22	2.08	0.53
1:N:165:ILE:O	1:N:169:ILE:HG12	2.08	0.53
9:V:65:LYS:O	11:X:54:ARG:NH1	2.41	0.53
22:B:230:PSC:C34	22:B:230:PSC:H142	2.28	0.53
2:O:83:ILE:O	2:O:87:MET:HG3	2.09	0.53
7:T:3:ALA:O	7:T:4:ALA:HB2	2.09	0.53
7:G:84:LYS:N	7:G:84:LYS:HD2	2.09	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.53
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.44	0.53
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.91	0.53
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.35	0.52
7:T:2:SER:O	25:T:263:PEK:H322	2.09	0.52
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.34	0.52
3:C:156:ARG:HE	23:C:271:CHD:H232	1.74	0.52
1:A:472:ILE:HG21	19:L:522:TGL:CA9	2.35	0.52
1:A:406:ASN:HD21	20:A:524:PGV:C2	2.23	0.52
1:A:502:TYR:CD1	12:L:2:HIS:HD2	2.28	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.90	0.52
2:O:56:MET:HA	22:O:1230:PSC:H202	1.91	0.52
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.44	0.52
10:W:2:GLU:HA	28:W:4707:HOH:O	2.08	0.52
12:L:20:ARG:NH1	19:L:522:TGL:HC61	2.24	0.52
19:A:521:TGL:H161	2:B:7:LEU:HD11	1.92	0.52
1:A:1:FME:HE2	1:A:1:FME:HA	1.93	0.51
7:T:84:LYS:H	7:T:84:LYS:CD	2.05	0.51
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.13	0.51
1:A:377:PHE:O	1:A:381:LEU:HB3	2.10	0.51
22:B:230:PSC:H12	22:B:230:PSC:H322	1.93	0.51
1:N:112:LEU:HG	28:N:3073:HOH:O	2.11	0.51
25:C:265:PEK:C38	26:G:269:CDL:H273	2.41	0.51
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.93	0.51
1:N:422:ASN:HB3	19:N:1521:TGL:H242	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.45	0.51
20:C:267:PGV:H182	26:C:270:CDL:H673	1.92	0.51
1:A:472:ILE:HD13	19:L:522:TGL:HA91	1.93	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.93	0.51
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.92	0.51
19:L:522:TGL:OA1	19:L:522:TGL:HC21	2.10	0.51
3:C:80:ARG:NH1	25:T:263:PEK:H032	2.25	0.51
1:N:472:ILE:HD13	19:Y:1522:TGL:HA91	1.93	0.51
1:N:406:ASN:HD21	20:N:1524:PGV:C2	2.24	0.50
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.46	0.50
22:O:1230:PSC:H322	22:O:1230:PSC:H12	1.94	0.50
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.94	0.50
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.50
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.92	0.50
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.47	0.50
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.94	0.50
5:R:78:HIS:HD2	9:V:12:LEU:HD13	1.76	0.50
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.99	0.50
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.12	0.50
1:N:369:ASP:C	1:N:438:ARG:HG3	2.33	0.49
19:N:1521:TGL:HC22	28:Q:3383:HOH:O	2.12	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.12	0.49
10:W:50:LEU:HD22	10:W:50:LEU:O	2.12	0.49
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.26	0.49
20:N:1524:PGV:H062	28:Z:3160:HOH:O	2.12	0.49
1:A:334:TRP:CZ3	19:A:523:TGL:HA51	2.47	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.95	0.49
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.35	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.11	0.49
2:B:91:ASN:ND2	2:B:183:THR:HG21	2.28	0.49
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.95	0.49
3:C:51:MET:HB3	26:C:270:CDL:H622	1.94	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.13	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.49
2:O:57:ASP:H	22:O:1230:PSC:H201	1.78	0.49
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.78	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.13	0.49
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.77	0.49
7:T:84:LYS:N	7:T:84:LYS:HD2	2.10	0.48
3:C:157:LYS:NZ	25:C:265:PEK:H052	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:271:CHD:H161	28:C:4708:HOH:O	2.12	0.48
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.93	0.48
20:N:1266:PGV:H182	3:P:28:THR:HG22	1.95	0.48
1:N:449:MET:SD	2:O:5:MET:CG	3.01	0.48
4:D:127:LYS:HD2	28:I:2391:HOH:O	2.14	0.48
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.43	0.48
19:L:522:TGL:H272	19:L:522:TGL:H231	1.96	0.48
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.44	0.48
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.95	0.48
1:A:76:GLY:O	1:A:80:ASN:HB2	2.13	0.48
4:D:33:LEU:HD22	4:D:37:GLN:HB3	1.94	0.48
3:P:34:TRP:CE2	24:P:1272:DMU:H29	2.49	0.48
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.45	0.48
6:S:51:SER:O	6:S:94:HIS:N	2.46	0.48
5:R:105:GLY:O	5:R:108:LYS:HG2	2.13	0.48
7:T:45:PRO:HD2	28:T:3152:HOH:O	2.13	0.48
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.43	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.14	0.48
26:C:270:CDL:H602	26:C:270:CDL:H632	1.59	0.48
3:P:34:TRP:NE1	24:P:1272:DMU:H29	2.29	0.48
19:Y:1522:TGL:C24	19:Y:1522:TGL:H202	2.43	0.48
2:O:203:ASN:HD22	2:O:203:ASN:N	2.12	0.48
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.14	0.48
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.96	0.48
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.96	0.48
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.78	0.48
1:A:422:ASN:HB3	19:A:521:TGL:H242	1.96	0.48
6:S:85:CYS:SG	6:S:87:THR:HG23	2.54	0.48
2:O:139:ASP:OD2	2:O:140:ASN:N	2.46	0.48
1:N:377:PHE:CD1	18:N:516:HEA:HAD1	2.49	0.48
7:G:17:ARG:HD2	28:G:2309:HOH:O	2.14	0.47
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.78	0.47
19:Y:1522:TGL:H231	19:Y:1522:TGL:H272	1.95	0.47
20:A:524:PGV:H302	13:M:19:LEU:HD23	1.95	0.47
1:A:87:ILE:O	1:A:173:PRO:HD3	2.14	0.47
1:A:321:PHE:CZ	22:B:230:PSC:H171	2.50	0.47
19:L:522:TGL:C24	19:L:522:TGL:H202	2.41	0.47
6:F:92:VAL:O	6:F:92:VAL:CG2	2.61	0.47
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.50	0.47
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.35	0.47
19:Y:1522:TGL:H361	19:Y:1522:TGL:HB91	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.78	0.47
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.80	0.47
28:O:4280:HOH:O	8:U:61:LYS:HD2	2.14	0.47
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.96	0.47
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.44	0.47
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.96	0.47
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.28	0.47
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.15	0.47
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.33	0.47
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.50	0.47
7:T:2:SER:O	7:T:3:ALA:HB3	2.15	0.47
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.97	0.47
3:C:156:ARG:HE	23:C:271:CHD:C23	2.28	0.47
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.96	0.47
2:B:214:VAL:HB	2:B:215:PRO:CD	2.44	0.47
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.15	0.47
2:O:98:LYS:HG2	2:O:153:LEU:HB2	1.97	0.47
1:A:306:THR:O	1:A:310:MET:HG3	2.15	0.47
1:N:321:PHE:CZ	22:O:1230:PSC:H171	2.50	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.14	0.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	2.30	0.47
22:O:1230:PSC:C07	9:V:10:ARG:HH21	2.28	0.46
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.97	0.46
3:P:132:LEU:O	3:P:136:VAL:HG23	2.16	0.46
7:T:33:LEU:HD12	28:T:4821:HOH:O	2.14	0.46
26:G:269:CDL:C54	26:G:269:CDL:H231	2.32	0.46
1:N:34:SER:HB2	18:N:515:HEA:C2B	2.46	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.46
8:H:27:ARG:NH1	28:H:2303:HOH:O	2.47	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.15	0.46
19:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.79	0.46
5:R:7:THR:HB	5:R:9:GLU:OE2	2.16	0.46
1:N:115:SER:O	1:N:121:GLY:HA2	2.16	0.46
3:P:34:TRP:HE1	24:P:1272:DMU:H29	1.80	0.46
6:S:92:VAL:HG23	6:S:92:VAL:O	2.16	0.46
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.97	0.46
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.97	0.46
19:A:521:TGL:HC92	28:B:4798:HOH:O	2.14	0.46
4:D:34:SER:N	4:D:37:GLN:HE21	1.96	0.46
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.97	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.46
26:P:1270:CDL:H672	26:P:1270:CDL:H641	1.84	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
2:O:62:GLU:O	2:O:66:THR:HB	2.16	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.16	0.46
20:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.51	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.46
2:O:155:SER:O	2:O:174:ALA:HB1	2.15	0.46
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.81	0.45
1:N:415:ALA:O	1:N:419:VAL:HG23	2.16	0.45
26:C:270:CDL:H202	26:C:270:CDL:H171	1.79	0.45
19:Y:1522:TGL:OA1	19:Y:1522:TGL:HC21	2.15	0.45
8:H:43:MET:HE3	8:H:49:ASP:N	2.30	0.45
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.98	0.45
23:O:229:CHD:H212	23:O:229:CHD:H12	1.98	0.45
4:D:32:ASN:ND2	28:D:4451:HOH:O	2.45	0.45
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.98	0.45
19:L:522:TGL:HB91	19:L:522:TGL:H361	1.98	0.45
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.97	0.45
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.80	0.45
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.17	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
12:L:22:LEU:O	12:L:26:THR:HB	2.17	0.45
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.98	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.17	0.45
1:N:400:PHE:HB3	19:Y:1522:TGL:H283	1.98	0.45
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.99	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.52	0.45
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.51	0.45
1:A:1:FME:HA	1:A:1:FME:CE	2.46	0.45
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.99	0.45
7:T:7:ASP:HB2	28:T:4278:HOH:O	2.16	0.45
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.98	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.98	0.45
3:P:168:THR:HG21	25:P:1265:PEK:H14	1.99	0.45
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.59	0.45
1:A:309:THR:HG22	18:A:516:HEA:HMB2	1.99	0.45
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.99	0.45
26:T:1269:CDL:H571	26:T:1269:CDL:H771	1.99	0.45
19:L:522:TGL:HC62	19:L:522:TGL:CC2	2.33	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:267:PGV:H12	20:C:267:PGV:C16	2.45	0.44
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.77	0.44
26:G:269:CDL:H571	26:G:269:CDL:H601	1.57	0.44
19:Y:1522:TGL:HB61	19:Y:1522:TGL:HB31	1.81	0.44
19:Q:1523:TGL:H242	19:Q:1523:TGL:H212	1.78	0.44
9:I:2:THR:HG22	9:I:3:ALA:N	2.32	0.44
3:P:34:TRP:HE1	24:P:1272:DMU:C57	2.30	0.44
3:C:213:THR:HG23	26:C:270:CDL:H762	1.98	0.44
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.17	0.44
12:L:20:ARG:CZ	19:L:522:TGL:HC61	2.47	0.44
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.98	0.44
2:O:100:MET:SD	2:O:155:SER:HB3	2.57	0.44
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.98	0.44
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.44
3:P:213:THR:HG23	26:P:1270:CDL:H762	2.00	0.44
19:A:523:TGL:HC51	19:A:523:TGL:HC22	1.89	0.44
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.33	0.44
2:O:56:MET:HA	22:O:1230:PSC:C20	2.47	0.44
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.99	0.44
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.17	0.44
1:N:407:ASP:O	1:N:411:LYS:HG3	2.18	0.44
7:G:5:LYS:HD3	1:N:278:MET:HB3	2.00	0.44
1:A:449:MET:SD	2:B:5:MET:HG2	2.57	0.44
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.52	0.44
1:A:347:LEU:HD13	1:A:383:MET:SD	2.57	0.44
3:P:67:PHE:HE1	26:P:1270:CDL:C1	2.25	0.44
20:A:524:PGV:C15	20:A:524:PGV:H321	2.48	0.44
28:N:3339:HOH:O	6:S:87:THR:HG21	2.17	0.44
5:R:5:HIS:HB3	5:R:6:GLU:H	1.58	0.44
1:A:165:ILE:O	1:A:169:ILE:HG12	2.17	0.44
7:G:2:SER:O	7:G:3:ALA:HB3	2.18	0.43
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.43
7:G:31:CYS:HG	26:G:269:CDL:H532	1.79	0.43
1:N:400:PHE:HB3	19:Y:1522:TGL:C28	2.48	0.43
4:D:75:THR:HB	28:D:2332:HOH:O	2.18	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.56	0.43
7:T:5:LYS:HD2	25:T:263:PEK:C37	2.44	0.43
5:R:63:SER:O	5:R:67:ILE:HG13	2.19	0.43
8:U:58:ARG:HA	8:U:58:ARG:HD2	1.80	0.43
2:B:52:HIS:HE1	22:B:230:PSC:H02	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:270:CDL:H672	26:C:270:CDL:H641	1.84	0.43
1:N:5:ARG:O	1:N:9:SER:HB2	2.18	0.43
2:O:52:HIS:HE1	22:O:1230:PSC:H212	1.83	0.43
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.43
1:N:376:HIS:O	1:N:380:VAL:HG22	2.19	0.43
5:R:57:ARG:HH11	5:R:57:ARG:HG3	1.84	0.43
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.53	0.43
9:I:35:TYR:C	9:I:37:PHE:H	2.22	0.43
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.76	0.43
10:W:36:MET:HB3	23:W:1060:CHD:H181	2.01	0.43
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.01	0.43
13:M:42:LYS:HA	13:M:42:LYS:CE	2.39	0.43
2:B:14:SER:HB3	2:B:168:LEU:HD23	2.01	0.43
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.79	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
3:P:41:THR:O	3:P:45:ILE:HG13	2.18	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.01	0.43
26:C:270:CDL:H661	26:C:270:CDL:H242	2.01	0.43
26:P:1270:CDL:H273	28:P:4551:HOH:O	2.17	0.43
3:P:187:THR:HB	7:T:68:THR:HG21	2.01	0.43
20:N:1524:PGV:C15	20:N:1524:PGV:H321	2.46	0.43
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.48	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.92	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	2.01	0.42
2:O:59:GLN:O	2:O:59:GLN:HG3	2.19	0.42
25:C:265:PEK:H371	26:G:269:CDL:H261	2.00	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.19	0.42
23:B:1086:CHD:H212	23:B:1086:CHD:H12	2.01	0.42
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.84	0.42
7:T:5:LYS:CB	25:T:263:PEK:H362	2.32	0.42
26:P:1270:CDL:H242	26:P:1270:CDL:H661	2.02	0.42
1:N:113:LEU:CD1	19:Y:1522:TGL:H292	2.49	0.42
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.84	0.42
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.07	0.42
3:C:187:THR:HG22	25:C:264:PEK:H052	2.01	0.42
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.72	0.42
9:V:35:TYR:C	9:V:37:PHE:H	2.23	0.42
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.01	0.42
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1265:PEK:H371	26:T:1269:CDL:H261	2.02	0.42
2:B:56:MET:HA	22:B:230:PSC:H202	2.02	0.42
26:G:269:CDL:H771	26:G:269:CDL:H571	2.02	0.42
19:Q:1523:TGL:CC2	19:Q:1523:TGL:HG11	2.48	0.42
1:N:292:MET:O	1:N:295:VAL:HG22	2.20	0.42
1:A:136:LEU:HD11	28:B:4860:HOH:O	2.20	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42
2:B:81:LEU:HD13	26:T:1269:CDL:H122	2.01	0.42
3:C:164:PHE:CD1	23:C:271:CHD:H192	2.54	0.42
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.53	0.42
1:N:3:ILE:HG23	1:N:7:LEU:HD22	2.02	0.42
28:A:4044:HOH:O	12:L:3:TYR:HB3	2.19	0.42
9:I:2:THR:CG2	9:I:3:ALA:N	2.82	0.42
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.02	0.42
5:E:105:GLY:O	5:E:108:LYS:HG2	2.19	0.42
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.42
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
19:Q:1523:TGL:HB81	19:Q:1523:TGL:H122	2.01	0.42
19:A:523:TGL:H242	19:A:523:TGL:H212	1.77	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.91	0.41
10:J:50:LEU:HD22	10:J:50:LEU:O	2.20	0.41
2:O:217:LYS:HA	2:O:217:LYS:HE2	2.01	0.41
12:L:11:ILE:CG2	19:L:522:TGL:H271	2.49	0.41
26:G:269:CDL:H152	26:G:269:CDL:H181	1.94	0.41
1:A:136:LEU:HD12	28:A:4243:HOH:O	2.19	0.41
25:C:265:PEK:H383	26:G:269:CDL:H273	2.01	0.41
26:G:269:CDL:H221	1:N:286:ILE:CD1	2.51	0.41
18:A:515:HEA:H11	18:A:515:HEA:HHC	1.87	0.41
1:N:297:MET:HB2	28:N:4474:HOH:O	2.21	0.41
9:I:1:SAC:OAC	9:I:1:SAC:HB2	2.20	0.41
1:A:304:TYR:CD1	26:T:1269:CDL:HB32	2.53	0.41
26:C:270:CDL:H532	26:C:270:CDL:H561	1.74	0.41
1:N:17:THR:OG1	19:Y:1522:TGL:H281	2.20	0.41
3:C:223:LEU:HD21	23:C:271:CHD:C18	2.50	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.97	0.41
10:J:40:LEU:HD12	23:J:60:CHD:H183	2.03	0.41
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.55	0.41
19:A:521:TGL:H201	19:A:521:TGL:C24	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:381:LEU:O	1:N:385:ALA:HB3	2.20	0.41
9:V:58:LYS:O	9:V:62:GLU:HG3	2.19	0.41
23:W:1060:CHD:H161	23:W:1060:CHD:H212	1.73	0.41
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.88	0.41
25:P:1265:PEK:H201	28:T:4510:HOH:O	2.19	0.41
1:N:468:MET:O	1:N:472:ILE:HG13	2.20	0.41
10:J:14:GLU:HG3	28:J:4760:HOH:O	2.21	0.41
8:U:57:ARG:HA	8:U:60:TYR:CE2	2.56	0.41
2:B:98:LYS:HB2	2:B:98:LYS:HE3	1.90	0.41
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.21	0.41
19:A:523:TGL:HB81	19:A:523:TGL:H122	2.03	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.84	0.41
12:L:2:HIS:HB3	12:L:3:TYR:H	1.55	0.41
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.35	0.41
23:J:60:CHD:H161	23:J:60:CHD:H212	1.74	0.41
20:P:1267:PGV:H182	26:P:1270:CDL:H673	2.01	0.41
26:P:1270:CDL:H352	26:P:1270:CDL:H162	2.03	0.41
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.41
25:C:264:PEK:H041	7:G:70:PHE:HB2	2.03	0.41
7:G:2:SER:OG	25:G:1263:PEK:H291	2.20	0.41
24:P:1272:DMU:O1	24:P:1272:DMU:H30	2.21	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
9:I:5:ALA:HB3	28:I:4611:HOH:O	2.21	0.41
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.41
7:T:21:PHE:HD2	7:T:25:LEU:HD12	1.85	0.41
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.87	0.41
23:W:1060:CHD:H211	28:W:4516:HOH:O	2.20	0.41
22:B:230:PSC:C07	9:I:10:ARG:HE	2.34	0.41
3:P:184:ALA:HA	3:P:185:PRO:HD2	1.94	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
11:K:43:SER:HA	11:K:44:PRO:HD3	1.97	0.41
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.86	0.40
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.22	0.40
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.56	0.40
2:O:46:LEU:HD12	19:Q:1523:TGL:H271	2.03	0.40
13:M:37:LEU:O	13:M:41:LYS:HG3	2.21	0.40
3:P:230:ASN:HB2	28:S:3287:HOH:O	2.21	0.40
26:C:270:CDL:H162	26:C:270:CDL:H352	2.02	0.40
19:A:523:TGL:HG11	19:A:523:TGL:CC2	2.49	0.40
1:A:246:LEU:HD13	1:A:381:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:122:MET:SD	2:O:206:PHE:HB3	2.62	0.40
3:P:42:LEU:HA	3:P:42:LEU:HD23	1.94	0.40
2:O:217:LYS:CA	2:O:217:LYS:HE2	2.52	0.40
6:F:82:CYS:HA	6:F:83:PRO:HD3	1.95	0.40
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.55	0.40
10:J:29:ASN:H	10:J:29:ASN:HD22	1.68	0.40
7:G:11:TPO:CG2	7:G:11:TPO:O	2.68	0.40
4:D:118:LYS:HB3	11:K:53:TRP:HB3	2.02	0.40
3:C:99:TRP:CE2	20:C:268:PGV:H232	2.57	0.40
5:R:81:ILE:HD11	9:V:8:GLN:O	2.21	0.40
20:N:1524:PGV:H011	20:N:1524:PGV:H202	1.94	0.40
8:H:49:ASP:O	8:H:52:VAL:HG22	2.21	0.40
3:P:31:LEU:HA	3:P:31:LEU:HD23	1.86	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%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	21	15
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	39	37
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	5 1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5 1
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1 0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1 0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15 9
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15 9
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100 100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100 100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
12	L	44/47 (94%)	43 (98%)	1 (2%)	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%)	3354 (96%)	125 (4%)	25 (1%)	26 21

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
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
2	B	60	GLU
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE

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Mol	Chain	Res	Type
2	O	60	GLU
7	T	3	ALA
7	T	40	GLY
8	U	8	ILE
6	F	94	HIS
6	S	96	LEU
6	F	96	LEU
7	G	6	GLY
7	T	6	GLY
2	B	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%)	414 (97%)	12 (3%)	51	55
1	N	426/426 (100%)	415 (97%)	11 (3%)	54	58
2	B	210/210 (100%)	200 (95%)	10 (5%)	31	29
2	O	210/210 (100%)	198 (94%)	12 (6%)	25	22
3	C	224/226 (99%)	219 (98%)	5 (2%)	60	64
3	P	224/226 (99%)	218 (97%)	6 (3%)	52	56
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	76
4	Q	128/129 (99%)	123 (96%)	5 (4%)	39	39
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	47
5	R	92/95 (97%)	89 (97%)	3 (3%)	45	47
6	F	81/81 (100%)	79 (98%)	2 (2%)	55	59
6	S	81/81 (100%)	74 (91%)	7 (9%)	13	9
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	13
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	8
8	H	71/75 (95%)	69 (97%)	2 (3%)	51	55
8	U	71/75 (95%)	69 (97%)	2 (3%)	51	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	57/57 (100%)	54 (95%)	3 (5%)	28 25
9	V	57/57 (100%)	55 (96%)	2 (4%)	43 44
10	J	49/50 (98%)	48 (98%)	1 (2%)	63 68
10	W	49/50 (98%)	48 (98%)	1 (2%)	63 68
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 58
11	X	39/46 (85%)	38 (97%)	1 (3%)	54 58
12	L	39/40 (98%)	37 (95%)	2 (5%)	29 26
12	Y	39/40 (98%)	39 (100%)	0	100 100
13	M	37/38 (97%)	34 (92%)	3 (8%)	15 10
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 4
All	All	3040/3082 (99%)	2929 (96%)	111 (4%)	41 41

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	112	LEU
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	486	ASP
1	A	504	THR
1	A	512	ASN
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	159	MET

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Mol	Chain	Res	Type
3	C	179	SER
3	C	192	VAL
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	80	GLU
5	E	90	ARG
6	F	48	LEU
6	F	96	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
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	2	HIS
12	L	26	THR
13	M	4	LYS
13	M	34	LEU
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	369	ASP
1	N	380	VAL
1	N	394	VAL
1	N	504	THR
1	N	513	LEU
2	O	33	LEU
2	O	60	GLU
2	O	66	THR

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Mol	Chain	Res	Type
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	148	MET
2	O	167	SER
2	O	217	LYS
3	P	17	PRO
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	19	ARG
4	Q	51	LEU
4	Q	54	ASP
4	Q	121	LYS
5	R	77	PRO
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	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	18	PHE
7	T	26	PRO
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	61	GLU
10	W	50	LEU
11	X	54	ARG

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Mol	Chain	Res	Type
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	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
9	I	8	GLN
10	J	29	ASN
11	K	35	GLN
11	K	41	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN

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Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
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

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	0.57	0	6,9,11	1.24	1 (16%)
2	FME	B	1	2	8,9,10	0.64	0	6,9,11	1.37	1 (16%)
7	TPO	G	11	7	8,10,11	1.63	1 (12%)	7,14,16	1.01	0
9	SAC	I	1	9	7,8,9	2.89	2 (28%)	7,9,11	2.03	3 (42%)
1	FME	N	1	1	8,9,10	0.69	0	6,9,11	1.74	2 (33%)
2	FME	O	1	2	8,9,10	0.62	0	6,9,11	1.74	1 (16%)
7	TPO	T	11	7	8,10,11	1.36	1 (12%)	7,14,16	0.93	0
9	SAC	V	1	9	7,8,9	2.87	2 (28%)	7,9,11	2.20	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/8/10	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	2.52	1.58	1.54
7	G	11	TPO	CB-CA	3.67	1.60	1.54
9	V	1	SAC	OAC-C1A	4.79	1.34	1.23
9	I	1	SAC	CA-N	5.16	1.53	1.46
9	V	1	SAC	CA-N	5.39	1.54	1.46
9	I	1	SAC	OAC-C1A	5.47	1.35	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1	FME	CA-N-CN	-3.98	116.71	122.82
1	N	1	FME	CA-N-CN	-3.51	117.42	122.82
9	V	1	SAC	CA-N-C1A	-2.94	111.38	121.37
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82
9	I	1	SAC	CA-N-C1A	-2.45	113.05	121.37
9	V	1	SAC	OAC-C1A-C2A	-2.32	117.80	122.06
9	I	1	SAC	O-C-CA	-2.19	119.67	125.44
1	N	1	FME	O-C-CA	-2.09	119.93	125.44
1	A	1	FME	O-C-CA	-2.04	120.04	125.44
9	V	1	SAC	CB-CA-N	2.83	116.80	110.60
9	V	1	SAC	C2A-C1A-N	2.86	121.59	116.11
9	I	1	SAC	CB-CA-N	3.55	118.38	110.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	OAC-C1A-N-CA
1	N	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA

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

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
7	G	11	TPO	1	0
9	I	1	SAC	1	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 58 ligands modelled in this entry, 14 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	$\#\|Z\| > 2$
18	HEA	A	515	1	40,67,67	1.10	6 (15%)	41,103,103	1.72	10 (24%)
18	HEA	A	516	1	40,67,67	1.48	5 (12%)	41,103,103	1.61	9 (21%)
19	TGL	A	521	-	62,62,62	0.70	1 (1%)	65,65,65	1.52	9 (13%)
19	TGL	A	523	-	62,62,62	0.75	1 (1%)	65,65,65	1.36	8 (12%)
20	PGV	A	524	-	50,50,50	1.05	4 (8%)	51,56,56	0.92	3 (5%)
20	PGV	A	604	-	50,50,50	0.86	1 (2%)	51,56,56	0.77	2 (3%)
23	CHD	B	1086	-	29,32,32	0.65	0	48,51,51	1.75	12 (25%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.22	4 (7%)	55,59,59	0.97	1 (1%)
25	PEK	C	264	-	51,52,52	1.41	5 (9%)	52,57,57	1.25	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	PEK	C	265	-	51,52,52	1.64	9 (17%)	52,57,57	1.16	6 (11%)
20	PGV	C	267	-	50,50,50	0.82	1 (2%)	51,56,56	0.97	2 (3%)
20	PGV	C	268	-	50,50,50	1.15	2 (4%)	51,56,56	0.78	0
26	CDL	C	270	-	99,99,99	0.84	3 (3%)	101,111,111	0.98	5 (4%)
23	CHD	C	271	-	29,32,32	0.93	1 (3%)	48,51,51	3.71	25 (52%)
24	DMU	C	272	-	34,34,34	2.77	11 (32%)	45,45,45	4.36	20 (44%)
23	CHD	C	525	-	29,32,32	0.84	1 (3%)	48,51,51	1.88	12 (25%)
25	PEK	G	1263	-	51,52,52	1.80	10 (19%)	52,57,57	1.12	5 (9%)
26	CDL	G	269	-	99,99,99	0.99	7 (7%)	101,111,111	0.94	6 (5%)
23	CHD	J	60	-	29,32,32	1.31	3 (10%)	48,51,51	3.56	27 (56%)
19	TGL	L	522	-	62,62,62	1.10	5 (8%)	65,65,65	1.69	13 (20%)
24	DMU	M	526	-	34,34,34	3.28	8 (23%)	45,45,45	4.09	20 (44%)
20	PGV	N	1266	-	50,50,50	0.90	2 (4%)	51,56,56	0.87	3 (5%)
19	TGL	N	1521	-	62,62,62	0.71	1 (1%)	65,65,65	1.50	9 (13%)
20	PGV	N	1524	-	50,50,50	1.05	4 (8%)	51,56,56	0.91	3 (5%)
18	HEA	N	515	1	40,67,67	1.35	5 (12%)	41,103,103	1.82	11 (26%)
18	HEA	N	516	1	40,67,67	1.34	5 (12%)	41,103,103	1.58	10 (24%)
22	PSC	O	1230	-	51,51,51	1.22	3 (5%)	55,59,59	0.99	1 (1%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	0.63	0	48,51,51	1.72	12 (25%)
25	PEK	P	1264	-	51,52,52	1.49	5 (9%)	52,57,57	1.24	8 (15%)
25	PEK	P	1265	-	51,52,52	1.65	9 (17%)	52,57,57	1.16	6 (11%)
20	PGV	P	1267	-	50,50,50	0.81	1 (2%)	51,56,56	0.89	1 (1%)
20	PGV	P	1268	-	50,50,50	1.13	2 (4%)	51,56,56	0.82	1 (1%)
26	CDL	P	1270	-	99,99,99	0.88	4 (4%)	101,111,111	0.97	5 (4%)
23	CHD	P	1271	-	29,32,32	0.87	1 (3%)	48,51,51	3.63	26 (54%)
24	DMU	P	1272	-	34,34,34	2.81	11 (32%)	45,45,45	4.18	19 (42%)
23	CHD	P	1525	-	29,32,32	0.82	1 (3%)	48,51,51	1.78	12 (25%)
19	TGL	Q	1523	-	62,62,62	0.79	1 (1%)	65,65,65	1.34	6 (9%)
26	CDL	T	1269	-	99,99,99	0.97	7 (7%)	101,111,111	0.95	6 (5%)
25	PEK	T	263	-	51,52,52	1.83	9 (17%)	52,57,57	1.11	5 (9%)
23	CHD	W	1060	-	29,32,32	1.37	3 (10%)	48,51,51	3.59	26 (54%)
19	TGL	Y	1522	-	62,62,62	1.14	5 (8%)	65,65,65	1.67	13 (20%)
24	DMU	Z	1526	-	34,34,34	3.19	9 (26%)	45,45,45	4.02	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
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
19	TGL	A	523	-	-	0/65/65/65	0/0/0/0
20	PGV	A	524	-	-	2/55/55/55	0/0/0/0
20	PGV	A	604	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	230	-	-	0/55/55/55	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
24	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
18	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	-	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
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	5/5/12/12	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
19	TGL	Y	1522	-	-	0/65/65/65	0/0/0/0
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.67	1.22	1.43
24	Z	1526	DMU	O7-C3	-8.21	1.23	1.43
24	M	526	DMU	O16-C6	-7.25	1.27	1.40
24	Z	1526	DMU	O16-C6	-7.09	1.27	1.40
24	M	526	DMU	O5-C4	-6.63	1.27	1.44
24	M	526	DMU	O7-C10	-6.56	1.23	1.41
24	M	526	DMU	O1-C9	-6.52	1.28	1.44
24	M	526	DMU	O16-C18	-6.47	1.24	1.42
24	Z	1526	DMU	O7-C10	-6.46	1.24	1.41
24	P	1272	DMU	O7-C3	-6.41	1.27	1.43
24	Z	1526	DMU	O5-C4	-6.32	1.28	1.44
24	Z	1526	DMU	O16-C18	-6.29	1.25	1.42
24	Z	1526	DMU	O1-C9	-6.26	1.28	1.44
24	P	1272	DMU	O1-C9	-6.24	1.28	1.44
24	C	272	DMU	O7-C3	-6.15	1.28	1.43
24	P	1272	DMU	O16-C18	-5.93	1.26	1.42
24	P	1272	DMU	O16-C6	-5.92	1.29	1.40
24	C	272	DMU	O1-C9	-5.91	1.29	1.44
24	C	272	DMU	O16-C18	-5.80	1.26	1.42
24	C	272	DMU	O16-C6	-5.69	1.29	1.40
24	M	526	DMU	O1-C10	-5.66	1.27	1.41
24	Z	1526	DMU	O1-C10	-5.22	1.28	1.41
24	C	272	DMU	O5-C4	-5.09	1.31	1.44
24	Z	1526	DMU	O5-C6	-4.97	1.29	1.41
24	M	526	DMU	O5-C6	-4.90	1.29	1.41
24	P	1272	DMU	O7-C10	-4.84	1.28	1.41
24	C	272	DMU	O7-C10	-4.61	1.29	1.41
24	P	1272	DMU	O5-C4	-4.58	1.32	1.44
24	P	1272	DMU	O1-C10	-4.55	1.30	1.41
24	C	272	DMU	O1-C10	-4.34	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	272	DMU	O5-C6	-4.11	1.31	1.41
24	P	1272	DMU	O5-C6	-3.93	1.31	1.41
18	A	516	HEA	C3A-C2A	-3.24	1.36	1.40
18	N	516	HEA	C3A-CMA	-3.02	1.39	1.46
18	N	515	HEA	C3A-C2A	-2.86	1.36	1.40
18	N	515	HEA	C3A-CMA	-2.86	1.39	1.46
18	A	516	HEA	C3A-CMA	-2.84	1.39	1.46
18	A	516	HEA	C3C-C2C	-2.58	1.36	1.40
18	A	515	HEA	C3A-CMA	-2.56	1.40	1.46
18	N	516	HEA	C3A-C2A	-2.44	1.37	1.40
23	C	525	CHD	C13-C12	-2.12	1.51	1.54
18	A	515	HEA	C3A-C2A	-2.00	1.37	1.40
20	A	524	PGV	C03-C02	2.00	1.56	1.50
26	T	1269	CDL	C71-CB7	2.00	1.56	1.50
23	P	1525	CHD	C8-C9	2.02	1.57	1.53
26	G	269	CDL	CA3-CA4	2.02	1.56	1.50
19	L	522	TGL	CC2-CC1	2.02	1.56	1.50
26	G	269	CDL	C71-CB7	2.02	1.56	1.50
25	C	264	PEK	C4-C5	2.03	1.59	1.50
24	P	1272	DMU	C8-C9	2.04	1.57	1.53
19	A	523	TGL	OG3-CC1	2.04	1.39	1.33
25	G	1263	PEK	C2-C1	2.05	1.56	1.50
25	G	1263	PEK	P-O12	2.05	1.68	1.59
25	P	1265	PEK	C22-C21	2.05	1.56	1.50
22	B	230	PSC	C01-C02	2.07	1.56	1.50
18	A	515	HEA	C1D-ND	2.08	1.39	1.36
19	A	521	TGL	OG2-CB1	2.10	1.40	1.34
19	Y	1522	TGL	CC2-CC1	2.11	1.56	1.50
25	C	265	PEK	P-O11	2.12	1.68	1.59
26	C	270	CDL	OA8-CA7	2.13	1.39	1.33
24	C	272	DMU	C5-C7	2.14	1.58	1.52
25	C	265	PEK	C22-C21	2.14	1.57	1.50
18	A	515	HEA	C4A-NA	2.15	1.39	1.36
26	T	1269	CDL	CB2-C1	2.16	1.59	1.51
23	P	1271	CHD	C13-C14	2.20	1.59	1.55
25	P	1265	PEK	P-O11	2.23	1.69	1.59
23	J	60	CHD	C20-C17	2.24	1.58	1.54
20	A	524	PGV	C20-C19	2.25	1.57	1.50
26	T	1269	CDL	OA6-CA5	2.27	1.41	1.34
20	N	1524	PGV	C20-C19	2.28	1.57	1.50
20	N	1524	PGV	C03-C02	2.31	1.57	1.50
23	W	1060	CHD	C20-C17	2.32	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C1A-NA	2.32	1.39	1.36
19	L	522	TGL	CG3-CG2	2.33	1.57	1.50
24	Z	1526	DMU	C8-C9	2.33	1.58	1.53
25	G	1263	PEK	P-O11	2.36	1.69	1.59
19	Q	1523	TGL	CG3-CG2	2.36	1.57	1.50
18	A	515	HEA	C4B-NB	2.37	1.39	1.36
19	Y	1522	TGL	CG3-CG2	2.39	1.57	1.50
26	P	1270	CDL	OA8-CA7	2.40	1.40	1.33
26	P	1270	CDL	C31-CA7	2.40	1.57	1.50
19	N	1521	TGL	OG2-CB1	2.43	1.41	1.34
23	C	271	CHD	C13-C14	2.44	1.59	1.55
26	T	1269	CDL	C11-CA5	2.46	1.58	1.50
26	G	269	CDL	OA6-CA5	2.46	1.41	1.34
22	B	230	PSC	C2-C1	2.50	1.58	1.50
23	J	60	CHD	C8-C7	2.51	1.57	1.53
22	O	1230	PSC	C2-C1	2.51	1.58	1.50
24	C	272	DMU	C6-C1	2.51	1.60	1.52
25	C	265	PEK	O03-C21	2.52	1.40	1.33
26	G	269	CDL	CB3-CB4	2.54	1.57	1.50
25	T	263	PEK	P-O11	2.55	1.70	1.59
24	P	1272	DMU	C3-C4	2.55	1.60	1.52
24	C	272	DMU	C3-C4	2.55	1.60	1.52
24	P	1272	DMU	C6-C1	2.55	1.60	1.52
26	T	1269	CDL	CB3-CB4	2.58	1.58	1.50
26	C	270	CDL	CA3-CA4	2.58	1.58	1.50
26	P	1270	CDL	CA3-CA4	2.59	1.58	1.50
26	G	269	CDL	CA6-CA4	2.61	1.58	1.50
20	N	1524	PGV	O03-C19	2.62	1.41	1.33
20	C	268	PGV	O01-C1	2.62	1.42	1.34
25	C	265	PEK	C01-C02	2.70	1.58	1.50
20	N	1266	PGV	C01-C02	2.70	1.58	1.50
25	P	1265	PEK	O03-C21	2.72	1.41	1.33
26	T	1269	CDL	CA6-CA4	2.73	1.58	1.50
25	P	1265	PEK	C03-C02	2.77	1.58	1.50
18	N	516	HEA	C4A-NA	2.77	1.40	1.36
26	G	269	CDL	C11-CA5	2.78	1.59	1.50
20	P	1268	PGV	O01-C1	2.79	1.42	1.34
25	T	263	PEK	C2-C1	2.81	1.59	1.50
26	C	270	CDL	CA6-CA4	2.86	1.58	1.50
20	A	524	PGV	O03-C19	2.86	1.41	1.33
25	P	1265	PEK	C01-C02	2.87	1.58	1.50
18	N	515	HEA	C1A-NA	2.90	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	1060	CHD	C8-C7	2.95	1.58	1.53
25	P	1264	PEK	C2-C1	2.99	1.59	1.50
26	P	1270	CDL	CA6-CA4	3.02	1.59	1.50
25	C	265	PEK	C03-C02	3.05	1.59	1.50
19	Y	1522	TGL	CG1-CG2	3.09	1.59	1.50
20	C	267	PGV	C12-C11	3.11	1.49	1.31
19	L	522	TGL	OG1-CA1	3.14	1.42	1.33
18	N	515	HEA	C4A-NA	3.18	1.41	1.36
19	L	522	TGL	CG1-CG2	3.18	1.59	1.50
18	N	516	HEA	C4B-NB	3.19	1.41	1.36
20	P	1267	PGV	C12-C11	3.25	1.50	1.31
18	N	515	HEA	C1D-ND	3.32	1.41	1.36
25	G	1263	PEK	O03-C21	3.46	1.43	1.33
26	G	269	CDL	CB6-CB4	3.52	1.60	1.50
25	T	263	PEK	C01-C02	3.60	1.60	1.50
25	G	1263	PEK	C01-C02	3.70	1.61	1.50
19	Y	1522	TGL	OG1-CA1	3.71	1.44	1.33
26	T	1269	CDL	CB6-CB4	3.71	1.61	1.50
25	T	263	PEK	O03-C21	3.74	1.44	1.33
25	P	1264	PEK	C6-C5	3.77	1.53	1.31
25	C	264	PEK	C9-C8	3.80	1.53	1.31
20	A	524	PGV	C12-C11	3.82	1.53	1.31
18	N	516	HEA	C1D-ND	3.92	1.42	1.36
20	A	604	PGV	C12-C11	3.95	1.54	1.31
25	G	1263	PEK	C03-C02	3.97	1.61	1.50
20	N	1524	PGV	C12-C11	3.98	1.54	1.31
22	B	230	PSC	C13-C12	4.00	1.54	1.31
25	C	264	PEK	C6-C5	4.01	1.54	1.31
25	T	263	PEK	C03-C02	4.04	1.62	1.50
25	G	1263	PEK	C15-C14	4.06	1.55	1.31
20	N	1266	PGV	C12-C11	4.07	1.55	1.31
25	T	263	PEK	C15-C14	4.08	1.55	1.31
25	P	1264	PEK	C9-C8	4.08	1.55	1.31
25	C	265	PEK	C6-C5	4.10	1.55	1.31
23	J	60	CHD	C13-C17	4.10	1.62	1.55
25	P	1265	PEK	C6-C5	4.11	1.55	1.31
25	T	263	PEK	C9-C8	4.17	1.55	1.31
25	P	1265	PEK	C15-C14	4.19	1.55	1.31
25	P	1265	PEK	C9-C8	4.21	1.56	1.31
18	A	516	HEA	C1D-ND	4.21	1.42	1.36
25	G	1263	PEK	C9-C8	4.23	1.56	1.31
22	O	1230	PSC	C13-C12	4.24	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C4B-NB	4.25	1.42	1.36
22	B	230	PSC	C10-C9	4.25	1.56	1.31
22	O	1230	PSC	C10-C9	4.27	1.56	1.31
25	C	265	PEK	C9-C8	4.30	1.56	1.31
25	C	265	PEK	C15-C14	4.35	1.56	1.31
25	C	265	PEK	C12-C11	4.37	1.56	1.31
19	L	522	TGL	OG2-CB1	4.39	1.47	1.34
25	P	1264	PEK	C12-C11	4.39	1.57	1.31
23	W	1060	CHD	C13-C17	4.39	1.63	1.55
25	P	1265	PEK	C12-C11	4.40	1.57	1.31
20	C	268	PGV	C12-C11	4.41	1.57	1.31
25	G	1263	PEK	C6-C5	4.44	1.57	1.31
25	C	264	PEK	C12-C11	4.46	1.57	1.31
20	P	1268	PGV	C12-C11	4.51	1.57	1.31
25	T	263	PEK	C6-C5	4.57	1.58	1.31
19	Y	1522	TGL	OG2-CB1	4.65	1.48	1.34
25	T	263	PEK	C12-C11	4.70	1.58	1.31
25	C	264	PEK	C15-C14	4.81	1.59	1.31
25	G	1263	PEK	C12-C11	4.85	1.59	1.31
25	P	1264	PEK	C15-C14	4.91	1.60	1.31

All (403) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1271	CHD	C17-C13-C12	-8.42	110.22	117.68
23	C	271	CHD	C17-C13-C12	-8.16	110.44	117.68
23	C	271	CHD	C19-C10-C9	-8.13	98.99	111.18
23	P	1271	CHD	C19-C10-C9	-7.47	99.98	111.18
24	M	526	DMU	C8-C7-C5	-7.32	97.13	110.79
24	Z	1526	DMU	C8-C7-C5	-7.21	97.33	110.79
18	N	515	HEA	C4B-C3B-C11	-6.49	119.97	127.01
23	W	1060	CHD	C18-C13-C14	-5.97	101.79	111.22
23	J	60	CHD	C18-C13-C14	-5.63	102.34	111.22
23	C	525	CHD	C14-C13-C12	-5.38	102.57	107.39
18	A	515	HEA	C4B-C3B-C11	-5.34	121.21	127.01
23	J	60	CHD	C15-C14-C8	-5.33	110.57	118.32
23	W	1060	CHD	C15-C14-C8	-5.33	110.58	118.32
19	A	521	TGL	CG1-OG1-CA1	-5.30	102.02	116.85
19	N	1521	TGL	CG1-OG1-CA1	-5.28	102.09	116.85
23	P	1271	CHD	C15-C14-C8	-4.96	111.11	118.32
23	C	271	CHD	C15-C14-C8	-4.84	111.29	118.32
19	L	522	TGL	C12-C11-C10	-4.71	90.22	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	1522	TGL	C12-C11-C10	-4.69	90.31	114.53
23	B	1086	CHD	C15-C14-C13	-4.64	98.99	103.60
19	Y	1522	TGL	CB9-CB8-CB7	-4.55	91.02	114.53
23	P	1525	CHD	C14-C13-C12	-4.51	103.35	107.39
19	L	522	TGL	CB9-CB8-CB7	-4.46	91.51	114.53
23	B	1086	CHD	C16-C17-C13	-4.44	99.18	103.60
23	O	229	CHD	C16-C17-C13	-4.38	99.24	103.60
18	N	515	HEA	CAD-C3D-C4D	-4.24	122.40	127.01
23	C	271	CHD	C18-C13-C12	-4.18	105.01	109.09
23	C	271	CHD	C19-C10-C1	-4.00	101.47	108.20
18	A	516	HEA	CAD-C3D-C4D	-3.96	122.70	127.01
22	O	1230	PSC	C01-O03-C19	-3.91	105.92	116.85
26	P	1270	CDL	CB6-OB8-CB7	-3.89	105.96	116.85
19	Q	1523	TGL	CG1-OG1-CA1	-3.83	106.13	116.85
23	C	525	CHD	C15-C14-C8	-3.82	112.78	118.32
26	C	270	CDL	CB6-OB8-CB7	-3.79	106.24	116.85
18	N	516	HEA	CAA-C2A-C1A	-3.75	122.94	127.01
22	B	230	PSC	C01-O03-C19	-3.69	106.52	116.85
23	P	1525	CHD	C15-C14-C8	-3.63	113.04	118.32
18	A	516	HEA	CAA-C2A-C1A	-3.61	123.08	127.01
19	A	523	TGL	CG1-OG1-CA1	-3.61	106.76	116.85
23	O	229	CHD	C15-C14-C13	-3.50	100.12	103.60
18	N	516	HEA	CAD-C3D-C4D	-3.47	123.24	127.01
24	C	272	DMU	C2-C3-C4	-3.42	103.10	110.84
23	B	1086	CHD	C15-C14-C8	-3.40	113.39	118.32
25	C	264	PEK	O03-C21-C22	-3.39	101.57	111.90
23	P	1271	CHD	C19-C10-C1	-3.37	102.54	108.20
23	P	1525	CHD	C11-C12-C13	-3.30	107.85	111.20
23	W	1060	CHD	C18-C13-C12	-3.29	105.88	109.09
23	P	1271	CHD	C18-C13-C12	-3.29	105.88	109.09
23	P	1525	CHD	C14-C8-C9	-3.28	105.10	109.62
18	A	515	HEA	CAD-C3D-C4D	-3.28	123.45	127.01
23	O	229	CHD	C15-C14-C8	-3.25	113.60	118.32
18	A	515	HEA	C26-C15-C14	-3.18	117.25	123.50
26	C	270	CDL	OB6-CB5-C51	-3.16	104.67	111.53
23	J	60	CHD	C18-C13-C12	-3.02	106.15	109.09
20	N	1266	PGV	C01-O03-C19	-3.02	108.41	116.85
18	A	516	HEA	CMC-C2C-C1C	-3.00	123.40	128.36
25	P	1264	PEK	O03-C01-C02	-2.98	100.66	108.69
23	C	525	CHD	C14-C8-C9	-2.97	105.54	109.62
20	C	267	PGV	O01-C1-C2	-2.87	105.29	111.53
26	P	1270	CDL	OB6-CB5-C51	-2.85	105.34	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	1267	PGV	C9-C10-C11	-2.73	98.10	112.45
25	P	1264	PEK	C3-C2-C1	-2.72	102.89	113.59
25	C	264	PEK	C3-C2-C1	-2.72	102.90	113.59
25	P	1264	PEK	O03-C21-C22	-2.63	103.88	111.90
18	N	515	HEA	C26-C15-C14	-2.61	118.38	123.50
18	N	515	HEA	CMB-C2B-C1B	-2.54	124.16	128.36
20	C	267	PGV	C9-C10-C11	-2.53	99.18	112.45
23	J	60	CHD	C19-C10-C1	-2.52	103.97	108.20
18	A	515	HEA	C20-C21-C22	-2.51	105.12	111.69
20	N	1266	PGV	O01-C1-C2	-2.50	106.09	111.53
18	N	516	HEA	CMC-C2C-C1C	-2.48	124.27	128.36
25	C	264	PEK	C23-C22-C21	-2.47	103.87	113.59
23	W	1060	CHD	C19-C10-C1	-2.47	104.05	108.20
19	A	521	TGL	CA8-CA7-CA6	-2.45	101.86	114.53
18	A	515	HEA	CMB-C2B-C1B	-2.45	124.32	128.36
19	N	1521	TGL	CA8-CA7-CA6	-2.44	101.92	114.53
23	B	1086	CHD	C14-C8-C9	-2.43	106.28	109.62
23	C	525	CHD	C11-C12-C13	-2.34	108.83	111.20
20	A	604	PGV	C01-O03-C19	-2.33	110.33	116.85
23	B	1086	CHD	C14-C13-C12	-2.33	105.31	107.39
23	O	229	CHD	C14-C8-C9	-2.32	106.44	109.62
25	P	1264	PEK	C23-C22-C21	-2.27	104.69	113.59
20	N	1524	PGV	C3-C2-C1	-2.27	104.69	113.59
23	O	229	CHD	C19-C10-C1	-2.24	104.43	108.20
25	C	264	PEK	O01-C1-C2	-2.24	106.66	111.53
24	P	1272	DMU	C2-C3-C4	-2.24	105.78	110.84
23	W	1060	CHD	C19-C10-C5	-2.19	106.39	110.25
20	A	604	PGV	O01-C1-C2	-2.18	106.79	111.53
26	C	270	CDL	C52-C51-CB5	-2.17	105.05	113.59
20	A	524	PGV	C3-C2-C1	-2.16	105.11	113.59
26	T	1269	CDL	OB8-CB7-C71	-2.15	105.34	111.90
23	J	60	CHD	C19-C10-C5	-2.15	106.46	110.25
18	A	516	HEA	C13-C14-C15	-2.14	123.11	127.76
26	G	269	CDL	OB8-CB7-C71	-2.13	105.41	111.90
23	P	1525	CHD	C19-C10-C9	-2.13	107.98	111.18
18	N	515	HEA	C20-C21-C22	-2.11	106.17	111.69
18	N	515	HEA	C17-C18-C19	-2.10	123.19	127.76
25	P	1264	PEK	C24-C23-C22	-2.10	105.58	113.29
26	P	1270	CDL	C52-C51-CB5	-2.09	105.39	113.59
19	N	1521	TGL	CA6-CA5-CA4	-2.09	103.76	114.53
18	N	516	HEA	C20-C19-C18	-2.07	117.12	121.05
19	A	521	TGL	CA6-CA5-CA4	-2.02	104.08	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1271	CHD	C18-C13-C14	-2.02	108.03	111.22
25	P	1264	PEK	C01-O03-C21	-2.01	111.23	116.85
19	A	523	TGL	CB4-CB3-CB2	2.00	120.63	113.29
23	C	525	CHD	C11-C9-C10	2.01	115.88	113.79
19	A	523	TGL	CG2-OG2-CB1	2.01	122.72	117.89
23	B	1086	CHD	C5-C6-C7	2.02	116.69	114.44
25	P	1264	PEK	C11-C10-C9	2.03	118.74	112.00
18	A	515	HEA	C1A-C2A-C3A	2.03	109.10	107.07
25	G	1263	PEK	C03-C02-C01	2.03	116.81	112.07
20	P	1268	PGV	O03-C01-C02	2.03	114.15	108.69
23	C	525	CHD	C6-C5-C10	2.05	114.91	112.66
18	N	515	HEA	C3C-C4C-NC	2.05	111.86	109.21
25	C	265	PEK	C2-C3-C4	2.05	117.38	113.30
19	Y	1522	TGL	CC7-CC6-CC5	2.06	125.16	114.53
23	P	1525	CHD	C9-C11-C12	2.07	116.97	114.36
25	T	263	PEK	C03-C02-C01	2.09	116.95	112.07
24	C	272	DMU	O55-C2-C3	2.10	114.85	109.87
18	N	515	HEA	CMB-C2B-C3B	2.12	129.47	125.14
23	C	271	CHD	C6-C5-C10	2.12	114.99	112.66
26	G	269	CDL	OB8-CB6-CB4	2.12	114.40	108.69
19	N	1521	TGL	OG1-CG1-CG2	2.13	114.42	108.69
19	A	521	TGL	OG1-CG1-CG2	2.14	114.46	108.69
25	P	1265	PEK	C2-C3-C4	2.15	117.57	113.30
18	N	516	HEA	C4B-C3B-C11	2.15	129.34	127.01
20	N	1266	PGV	O03-C01-C02	2.15	114.47	108.69
19	N	1521	TGL	CG3-CG2-CG1	2.15	117.11	112.07
24	C	272	DMU	O5-C6-O16	2.16	115.24	110.05
25	C	265	PEK	C03-C02-C01	2.16	117.14	112.07
19	A	521	TGL	C10-CB9-CB8	2.17	125.75	114.53
23	C	525	CHD	C18-C13-C12	2.18	111.22	109.09
25	P	1264	PEK	O03-C21-O04	2.18	129.12	123.49
18	A	515	HEA	CMB-C2B-C3B	2.18	129.60	125.14
25	P	1265	PEK	C24-C23-C22	2.19	121.31	113.29
23	J	60	CHD	C4-C5-C10	2.19	115.07	112.66
23	P	1525	CHD	C11-C9-C10	2.19	116.07	113.79
25	C	265	PEK	P-O12-C04	2.20	134.07	121.50
18	N	515	HEA	CMC-C2C-C3C	2.20	129.39	125.09
23	O	229	CHD	C1-C2-C3	2.20	114.01	110.43
26	G	269	CDL	C19-C18-C17	2.20	125.92	114.53
26	P	1270	CDL	OB6-CB5-OB7	2.21	129.60	123.67
26	T	1269	CDL	OB8-CB6-CB4	2.21	114.64	108.69
26	T	1269	CDL	C19-C18-C17	2.21	125.97	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	1272	DMU	O5-C6-O16	2.23	115.43	110.05
19	L	522	TGL	CC7-CC6-CC5	2.23	126.06	114.53
25	P	1265	PEK	P-O12-C04	2.24	134.28	121.50
18	A	516	HEA	C26-C15-C16	2.24	118.83	115.41
23	C	271	CHD	C9-C10-C5	2.26	112.02	108.67
19	N	1521	TGL	C10-CB9-CB8	2.26	126.22	114.53
23	P	1525	CHD	C1-C2-C3	2.26	114.11	110.43
25	P	1265	PEK	C03-C02-C01	2.27	117.37	112.07
23	C	271	CHD	C2-C1-C10	2.29	116.93	112.84
23	C	271	CHD	C11-C12-C13	2.31	113.54	111.20
18	N	516	HEA	C21-C20-C19	2.31	120.24	112.71
25	P	1265	PEK	O03-C01-C02	2.31	114.92	108.69
25	T	263	PEK	C11-C10-C9	2.33	119.74	112.00
20	N	1524	PGV	O01-C02-C03	2.33	116.56	108.36
18	N	516	HEA	C17-C18-C19	2.34	132.86	127.76
19	L	522	TGL	C10-CB9-CB8	2.34	126.63	114.53
25	C	265	PEK	O03-C01-C02	2.34	115.00	108.69
19	A	521	TGL	CG3-CG2-CG1	2.35	117.57	112.07
25	C	264	PEK	O03-C21-O04	2.36	129.57	123.49
19	Q	1523	TGL	OG2-CG2-CG1	2.36	116.68	108.36
25	G	1263	PEK	C11-C10-C9	2.37	119.88	112.00
23	C	271	CHD	C1-C2-C3	2.37	114.28	110.43
26	C	270	CDL	OB6-CB5-OB7	2.37	130.04	123.67
20	A	524	PGV	O01-C02-C03	2.38	116.75	108.36
23	P	1271	CHD	C1-C2-C3	2.38	114.30	110.43
19	A	523	TGL	OG2-CG2-CG1	2.39	116.80	108.36
23	P	1271	CHD	C1-C10-C9	2.40	115.31	111.45
25	C	265	PEK	C24-C23-C22	2.40	122.08	113.29
23	C	525	CHD	C9-C11-C12	2.41	117.40	114.36
26	P	1270	CDL	OA8-CA6-CA4	2.41	115.19	108.69
18	A	515	HEA	CMD-C2D-C3D	2.42	130.29	125.24
19	Q	1523	TGL	OG1-CG1-CG2	2.42	115.20	108.69
23	C	271	CHD	C11-C9-C10	2.42	116.31	113.79
19	A	521	TGL	OG2-CG2-CG3	2.42	116.90	108.36
19	Y	1522	TGL	C10-CB9-CB8	2.43	127.06	114.53
19	Y	1522	TGL	C20-CA9-CA8	2.43	127.06	114.53
26	T	1269	CDL	C20-C19-C18	2.44	127.13	114.53
24	Z	1526	DMU	C10-O1-C9	2.44	118.49	113.75
23	P	1271	CHD	C6-C5-C4	2.45	113.78	111.05
19	L	522	TGL	C13-C12-C11	2.46	127.24	114.53
19	Q	1523	TGL	CB3-CB2-CB1	2.47	123.30	113.59
23	P	1271	CHD	C9-C10-C5	2.47	112.33	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	269	CDL	C20-C19-C18	2.47	127.30	114.53
23	C	271	CHD	C5-C4-C3	2.48	116.59	112.91
23	J	60	CHD	C9-C11-C12	2.48	117.49	114.36
19	Y	1522	TGL	OG1-CG1-CG2	2.49	115.39	108.69
23	P	1271	CHD	C11-C9-C10	2.50	116.39	113.79
23	B	1086	CHD	C1-C2-C3	2.51	114.50	110.43
19	N	1521	TGL	OG2-CG2-CG3	2.51	117.22	108.36
23	C	525	CHD	C1-C10-C5	2.52	111.95	107.81
23	P	1271	CHD	C2-C1-C10	2.52	117.34	112.84
18	A	516	HEA	C27-C19-C20	2.53	119.27	115.41
23	O	229	CHD	C9-C11-C12	2.53	117.56	114.36
24	Z	1526	DMU	C1-C2-C3	2.53	115.16	109.60
26	C	270	CDL	OA8-CA6-CA4	2.54	115.54	108.69
23	O	229	CHD	C1-C10-C5	2.56	112.01	107.81
19	L	522	TGL	OG1-CG1-CG2	2.56	115.58	108.69
19	Y	1522	TGL	C13-C12-C11	2.56	127.77	114.53
18	A	515	HEA	CMC-C2C-C3C	2.57	130.11	125.09
18	A	516	HEA	C21-C20-C19	2.57	121.07	112.71
23	P	1271	CHD	C11-C12-C13	2.58	113.82	111.20
23	P	1271	CHD	C16-C15-C14	2.58	110.32	105.12
23	P	1525	CHD	C5-C6-C7	2.58	117.32	114.44
18	N	516	HEA	C3C-C4C-NC	2.59	112.56	109.21
23	C	271	CHD	C16-C15-C14	2.60	110.36	105.12
19	L	522	TGL	C20-CA9-CA8	2.61	128.01	114.53
23	O	229	CHD	C17-C13-C14	2.62	102.70	100.05
25	T	263	PEK	C14-C13-C12	2.62	120.73	112.00
23	W	1060	CHD	C1-C2-C3	2.65	114.72	110.43
24	P	1272	DMU	O1-C10-C5	2.65	115.72	110.28
23	B	1086	CHD	C1-C10-C5	2.66	112.18	107.81
18	N	516	HEA	CMC-C2C-C3C	2.67	130.30	125.09
23	P	1271	CHD	C15-C16-C17	2.68	110.53	105.12
24	M	526	DMU	C1-C2-C3	2.69	115.52	109.60
23	C	271	CHD	C1-C10-C9	2.70	115.81	111.45
25	T	263	PEK	C02-O01-C1	2.71	124.40	117.89
26	G	269	CDL	C23-C22-C21	2.72	128.56	114.53
24	C	272	DMU	O1-C10-C5	2.72	115.86	110.28
26	G	269	CDL	C22-C21-C20	2.72	128.60	114.53
19	A	523	TGL	CB3-CB2-CB1	2.73	124.31	113.59
23	J	60	CHD	C1-C2-C3	2.73	114.86	110.43
26	T	1269	CDL	C22-C21-C20	2.74	128.70	114.53
25	G	1263	PEK	C14-C13-C12	2.76	121.19	112.00
19	A	523	TGL	OG2-CG2-CG3	2.78	118.17	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	1263	PEK	C02-O01-C1	2.81	124.63	117.89
26	T	1269	CDL	C23-C22-C21	2.81	129.05	114.53
23	B	1086	CHD	C5-C4-C3	2.83	117.12	112.91
23	C	525	CHD	C5-C6-C7	2.84	117.61	114.44
24	Z	1526	DMU	O7-C10-C5	2.85	115.04	108.10
23	B	1086	CHD	C17-C13-C14	2.87	102.95	100.05
23	C	271	CHD	C5-C6-C7	2.87	117.64	114.44
23	B	1086	CHD	C9-C11-C12	2.89	118.01	114.36
18	N	515	HEA	CMD-C2D-C3D	2.90	131.30	125.24
23	C	271	CHD	C15-C16-C17	2.90	110.96	105.12
24	Z	1526	DMU	C10-O7-C3	2.90	125.59	118.01
23	W	1060	CHD	C9-C11-C12	2.91	118.03	114.36
19	A	523	TGL	OG1-CG1-CG2	2.94	116.61	108.69
23	W	1060	CHD	C15-C16-C17	2.94	111.05	105.12
19	Y	1522	TGL	CC4-CC3-CC2	2.95	124.09	113.29
24	M	526	DMU	C10-O1-C9	2.97	119.52	113.75
18	A	516	HEA	C4B-C3B-C11	2.98	130.25	127.01
24	P	1272	DMU	C10-O7-C3	2.99	125.81	118.01
23	J	60	CHD	C15-C16-C17	2.99	111.15	105.12
19	Q	1523	TGL	OG2-CG2-CG3	3.01	118.96	108.36
19	L	522	TGL	CC4-CC3-CC2	3.01	124.34	113.29
24	C	272	DMU	C10-O7-C3	3.04	125.95	118.01
23	P	1271	CHD	C5-C4-C3	3.06	117.47	112.91
23	P	1525	CHD	C10-C9-C8	3.07	115.25	111.88
23	J	60	CHD	C16-C15-C14	3.09	111.35	105.12
23	O	229	CHD	C5-C4-C3	3.13	117.57	112.91
23	B	1086	CHD	C10-C9-C8	3.13	115.32	111.88
23	W	1060	CHD	C14-C8-C9	3.14	113.95	109.62
19	Y	1522	TGL	CC3-CC2-CC1	3.19	126.13	113.59
20	N	1524	PGV	C02-O01-C1	3.23	125.63	117.89
18	N	515	HEA	C26-C15-C16	3.24	120.36	115.41
19	Y	1522	TGL	CG2-OG2-CB1	3.26	125.71	117.89
24	M	526	DMU	O7-C3-C4	3.26	117.89	109.32
23	C	271	CHD	C14-C8-C7	3.26	116.26	111.74
23	W	1060	CHD	C11-C12-C13	3.26	114.51	111.20
23	P	1271	CHD	C5-C6-C7	3.27	118.08	114.44
23	W	1060	CHD	C16-C15-C14	3.28	111.72	105.12
23	J	60	CHD	C14-C8-C9	3.28	114.13	109.62
23	P	1525	CHD	C1-C10-C5	3.30	113.23	107.81
23	C	525	CHD	C10-C9-C8	3.30	115.50	111.88
19	Y	1522	TGL	C11-C10-CB9	3.33	131.74	114.53
20	A	524	PGV	C02-O01-C1	3.36	125.94	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	515	HEA	C26-C15-C16	3.37	120.56	115.41
23	P	1271	CHD	C14-C8-C7	3.39	116.44	111.74
19	L	522	TGL	C11-C10-CB9	3.39	132.06	114.53
19	L	522	TGL	CC3-CC2-CC1	3.40	126.97	113.59
18	N	516	HEA	C27-C19-C20	3.40	120.61	115.41
24	M	526	DMU	O7-C10-O1	3.41	119.33	110.68
24	Z	1526	DMU	O5-C6-C1	3.42	117.29	110.28
24	M	526	DMU	C10-O7-C3	3.44	127.00	118.01
23	O	229	CHD	C5-C6-C7	3.46	118.29	114.44
18	A	516	HEA	CMC-C2C-C3C	3.47	131.87	125.09
19	L	522	TGL	CG2-OG2-CB1	3.47	126.21	117.89
23	W	1060	CHD	C6-C5-C4	3.47	114.92	111.05
24	M	526	DMU	O5-C6-C1	3.50	117.45	110.28
23	P	1271	CHD	C9-C11-C12	3.61	118.92	114.36
23	J	60	CHD	C11-C12-C13	3.63	114.88	111.20
24	Z	1526	DMU	O7-C3-C4	3.64	118.89	109.32
19	L	522	TGL	C16-C15-CC9	3.69	133.59	114.53
19	Y	1522	TGL	C16-C15-CC9	3.71	133.67	114.53
25	T	263	PEK	O03-C01-C02	3.71	118.68	108.69
23	J	60	CHD	C6-C5-C4	3.76	115.24	111.05
25	G	1263	PEK	O03-C01-C02	3.77	118.84	108.69
24	P	1272	DMU	C8-C7-C5	3.79	117.87	110.79
23	W	1060	CHD	C5-C4-C3	3.85	118.64	112.91
23	W	1060	CHD	C14-C8-C7	3.86	117.10	111.74
23	J	60	CHD	C5-C4-C3	3.86	118.66	112.91
24	M	526	DMU	O7-C10-C5	3.87	117.53	108.10
23	C	271	CHD	C9-C11-C12	3.89	119.28	114.36
19	L	522	TGL	C15-CC9-CC8	3.91	134.73	114.53
19	N	1521	TGL	CG3-OG3-CC1	3.91	127.79	116.85
23	O	229	CHD	C10-C9-C8	3.94	116.20	111.88
19	Y	1522	TGL	C15-CC9-CC8	3.95	134.94	114.53
23	J	60	CHD	C14-C8-C7	3.99	117.27	111.74
23	J	60	CHD	C1-C10-C5	4.02	114.41	107.81
23	W	1060	CHD	C13-C14-C8	4.03	119.94	114.75
23	J	60	CHD	C13-C14-C8	4.04	119.95	114.75
19	A	521	TGL	CG3-OG3-CC1	4.06	128.19	116.85
23	W	1060	CHD	C2-C1-C10	4.07	120.10	112.84
24	C	272	DMU	O5-C6-C1	4.11	118.72	110.28
25	C	265	PEK	C11-C10-C9	4.12	125.72	112.00
24	C	272	DMU	O7-C10-O1	4.21	121.33	110.68
25	P	1265	PEK	C11-C10-C9	4.21	126.00	112.00
24	P	1272	DMU	O7-C10-O1	4.22	121.37	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	60	CHD	C2-C1-C10	4.25	120.42	112.84
24	Z	1526	DMU	O7-C10-O1	4.26	121.45	110.68
23	J	60	CHD	C9-C8-C7	4.26	116.96	111.92
23	W	1060	CHD	C1-C10-C5	4.31	114.89	107.81
23	W	1060	CHD	C5-C6-C7	4.35	119.29	114.44
23	W	1060	CHD	C9-C8-C7	4.41	117.13	111.92
23	W	1060	CHD	O12-C12-C13	4.43	118.30	111.11
23	J	60	CHD	O12-C12-C13	4.47	118.36	111.11
24	M	526	DMU	C6-C1-C2	4.59	119.03	109.97
19	Q	1523	TGL	CG3-OG3-CC1	4.77	130.20	116.85
24	C	272	DMU	O1-C9-C8	4.83	118.74	109.68
24	Z	1526	DMU	C6-C1-C2	4.83	119.49	109.97
19	N	1521	TGL	CG2-OG2-CB1	4.86	129.56	117.89
23	J	60	CHD	C5-C6-C7	4.87	119.87	114.44
19	A	523	TGL	CG3-OG3-CC1	4.91	130.58	116.85
24	Z	1526	DMU	C18-O16-C6	5.01	122.70	113.94
19	A	521	TGL	CG2-OG2-CB1	5.05	130.00	117.89
24	C	272	DMU	C8-C7-C5	5.07	120.25	110.79
23	P	1525	CHD	C13-C17-C20	5.14	125.76	119.50
23	C	525	CHD	C13-C17-C20	5.27	125.92	119.50
23	J	60	CHD	C11-C9-C10	5.30	119.30	113.79
23	P	1271	CHD	C1-C10-C5	5.34	116.58	107.81
24	P	1272	DMU	C10-O1-C9	5.34	124.11	113.75
24	P	1272	DMU	O7-C10-C5	5.37	121.17	108.10
24	P	1272	DMU	O1-C9-C8	5.39	119.79	109.68
24	P	1272	DMU	O5-C6-C1	5.41	121.39	110.28
24	M	526	DMU	C18-O16-C6	5.42	123.41	113.94
23	P	1271	CHD	C4-C3-C2	5.45	117.47	110.52
23	P	1271	CHD	C9-C8-C7	5.47	118.38	111.92
24	Z	1526	DMU	O7-C3-C2	5.49	121.35	107.17
23	C	271	CHD	C9-C8-C7	5.55	118.47	111.92
24	C	272	DMU	C10-O1-C9	5.58	124.57	113.75
23	C	271	CHD	C1-C10-C5	5.61	117.02	107.81
23	P	1271	CHD	C4-C5-C10	5.62	118.84	112.66
24	C	272	DMU	O5-C4-C57	5.64	120.61	106.36
23	J	60	CHD	C6-C5-C10	5.66	118.89	112.66
23	W	1060	CHD	C11-C9-C10	5.69	119.71	113.79
24	P	1272	DMU	O7-C3-C2	5.74	121.97	107.17
24	C	272	DMU	O7-C10-C5	5.77	122.16	108.10
23	W	1060	CHD	C4-C3-C2	5.86	118.00	110.52
23	J	60	CHD	C4-C3-C2	5.87	118.00	110.52
23	C	271	CHD	C4-C5-C10	5.88	119.14	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	M	526	DMU	O7-C3-C2	5.94	122.50	107.17
23	P	1271	CHD	C14-C13-C12	5.98	112.75	107.39
23	C	271	CHD	C4-C3-C2	5.99	118.16	110.52
24	C	272	DMU	O7-C3-C2	6.01	122.69	107.17
24	C	272	DMU	C18-O16-C6	6.04	124.49	113.94
23	C	271	CHD	C14-C13-C12	6.10	112.86	107.39
23	W	1060	CHD	C10-C9-C8	6.21	118.69	111.88
24	Z	1526	DMU	O16-C6-C1	6.29	115.99	108.04
23	J	60	CHD	C10-C9-C8	6.40	118.90	111.88
23	W	1060	CHD	C6-C5-C10	6.46	119.77	112.66
24	P	1272	DMU	O5-C4-C57	6.47	122.72	106.36
24	M	526	DMU	O5-C4-C3	6.48	123.44	109.75
24	P	1272	DMU	O5-C4-C3	6.52	123.52	109.75
24	M	526	DMU	O5-C6-O16	6.58	125.91	110.05
24	M	526	DMU	O16-C6-C1	6.60	116.37	108.04
24	Z	1526	DMU	O5-C4-C3	6.61	123.71	109.75
24	C	272	DMU	O7-C3-C4	6.62	126.71	109.32
24	P	1272	DMU	C18-O16-C6	6.78	125.80	113.94
24	Z	1526	DMU	O5-C6-O16	6.84	126.52	110.05
24	Z	1526	DMU	C6-O5-C4	7.01	127.35	113.75
24	Z	1526	DMU	O1-C9-C11	7.12	124.35	106.36
24	Z	1526	DMU	O1-C9-C8	7.13	123.06	109.68
24	M	526	DMU	O1-C9-C11	7.13	124.38	106.36
24	Z	1526	DMU	O5-C4-C57	7.27	124.73	106.36
24	M	526	DMU	C6-O5-C4	7.29	127.89	113.75
24	M	526	DMU	O5-C4-C57	7.32	124.86	106.36
24	M	526	DMU	O1-C9-C8	7.39	123.54	109.68
24	C	272	DMU	O5-C4-C3	7.39	125.35	109.75
24	P	1272	DMU	O7-C3-C4	7.39	128.75	109.32
24	Z	1526	DMU	C7-C8-C9	7.41	123.11	110.20
24	M	526	DMU	C7-C8-C9	7.44	123.17	110.20
23	J	60	CHD	C13-C17-C20	7.76	128.95	119.50
23	W	1060	CHD	C13-C17-C20	7.88	129.09	119.50
24	P	1272	DMU	O1-C9-C11	7.96	126.48	106.36
24	P	1272	DMU	C6-O5-C4	8.43	130.11	113.75
24	C	272	DMU	O1-C9-C11	8.57	128.01	106.36
24	C	272	DMU	C6-O5-C4	8.83	130.89	113.75
23	P	1271	CHD	C17-C13-C14	9.49	109.64	100.05
24	P	1272	DMU	C1-C2-C3	9.54	130.54	109.60
23	C	271	CHD	C10-C9-C8	9.58	122.40	111.88
24	C	272	DMU	C1-C2-C3	9.65	130.78	109.60
23	J	60	CHD	C17-C13-C14	9.81	109.97	100.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C17-C13-C14	9.83	109.98	100.05
23	C	271	CHD	C17-C13-C14	9.84	110.00	100.05
23	P	1271	CHD	C10-C9-C8	9.87	122.71	111.88
24	Z	1526	DMU	C10-C5-C7	10.80	131.26	109.97
24	M	526	DMU	C10-C5-C7	10.95	131.56	109.97
24	P	1272	DMU	O16-C6-C1	11.98	123.17	108.04
24	C	272	DMU	O16-C6-C1	14.25	126.04	108.04

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
23	J	60	CHD	C12
23	J	60	CHD	C8
23	J	60	CHD	C9
23	J	60	CHD	C14
23	J	60	CHD	C17
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C5
24	Z	1526	DMU	C9
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2
24	C	272	DMU	C10
23	P	1271	CHD	C12
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C9
23	P	1271	CHD	C14
18	N	516	HEA	ND

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Mol	Chain	Res	Type	Atom
18	N	516	HEA	NA
18	N	516	HEA	NB
23	C	271	CHD	C12
23	C	271	CHD	C8
23	C	271	CHD	C3
23	C	271	CHD	C9
23	C	271	CHD	C14
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C5
24	M	526	DMU	C9
23	W	1060	CHD	C12
23	W	1060	CHD	C8
23	W	1060	CHD	C9
23	W	1060	CHD	C14
23	W	1060	CHD	C17
24	P	1272	DMU	C5
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C2
24	P	1272	DMU	C10

All (4) torsion outliers are listed below:

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

There are no ring outliers.

38 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	3	0
18	A	516	HEA	2	0
19	A	521	TGL	10	0
19	A	523	TGL	6	0
20	A	524	PGV	8	0
20	A	604	PGV	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1086	CHD	1	0
22	B	230	PSC	14	0
25	C	264	PEK	4	0
25	C	265	PEK	7	0
20	C	267	PGV	5	0
20	C	268	PGV	2	0
26	C	270	CDL	16	0
23	C	271	CHD	7	0
24	C	272	DMU	2	0
25	G	1263	PEK	9	0
26	G	269	CDL	22	0
23	J	60	CHD	3	0
19	L	522	TGL	23	0
20	N	1266	PGV	1	0
19	N	1521	TGL	8	0
20	N	1524	PGV	9	0
18	N	515	HEA	3	0
18	N	516	HEA	1	0
22	O	1230	PSC	15	0
23	O	229	CHD	1	0
25	P	1264	PEK	5	0
25	P	1265	PEK	7	0
20	P	1267	PGV	4	0
20	P	1268	PGV	2	0
26	P	1270	CDL	18	0
23	P	1271	CHD	1	0
24	P	1272	DMU	8	0
19	Q	1523	TGL	7	0
26	T	1269	CDL	19	0
25	T	263	PEK	9	0
23	W	1060	CHD	5	0
19	Y	1522	TGL	17	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.