Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:54 AM GMT

PDB ID	:	2EIL
Title	:	Cadmium ion binding structure of bovine heart cytochrome C oxidase in the fully oxidized 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:

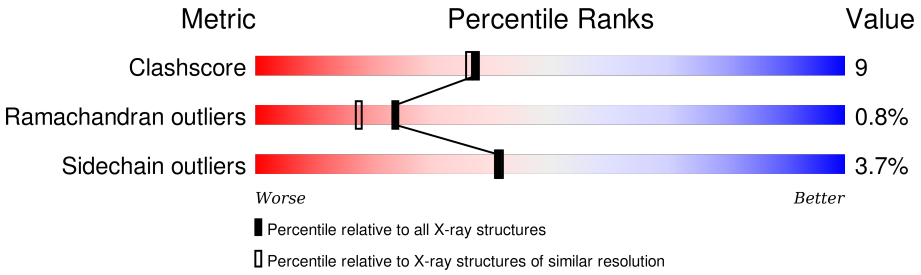
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	86% 13% •
1	N	514	82% 16% •
2	B	227	78% 19% •
2	O	227	73% 24% •
3	C	261	85% 15% •
3	P	261	84% 15% •
4	D	147	88% 10% •

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Mol	Chain	Length	Quality of chain
4	Q	147	73% 24%
5	E	109	83% 13%
5	R	109	72% 25%
6	F	98	82% 15%
6	S	98	81% 16%
7	G	85	73% 18% 8%
7	T	85	68% 20% 11%
8	H	85	84% 7% 7%
8	U	85	69% 20% 7%
9	I	73	90% 8%
9	V	73	82% 18%
10	J	59	90% 7%
10	W	59	85% 12%
11	K	56	79% 9% 13%
11	X	56	75% 11% 13%
12	L	47	77% 21%
12	Y	47	74% 21%
13	M	46	74% 15% 7%
13	Z	46	57% 37% 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	T	1269	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32357 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		

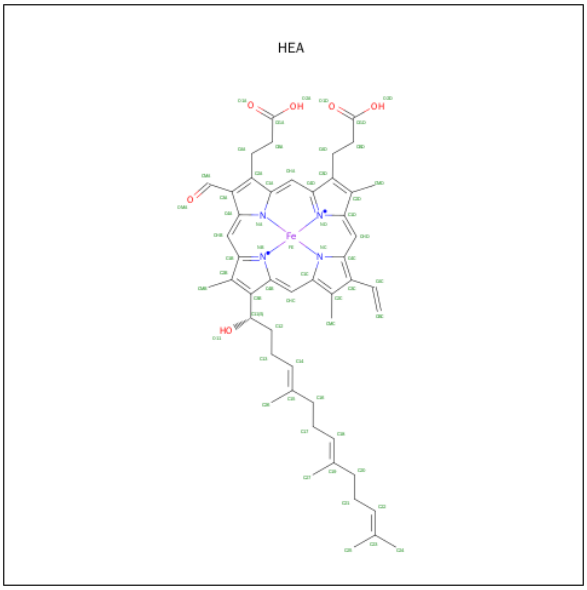
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

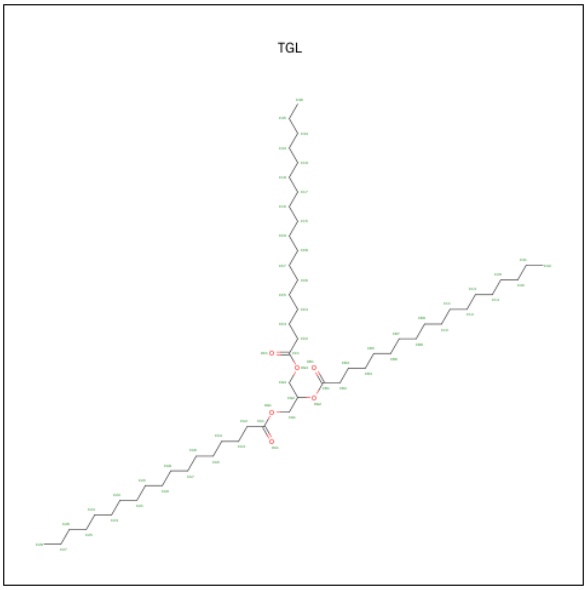
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Cd 1 1	0	0
17	A	1	Total Cd 1 1	0	0
17	C	1	Total Cd 1 1	0	0

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



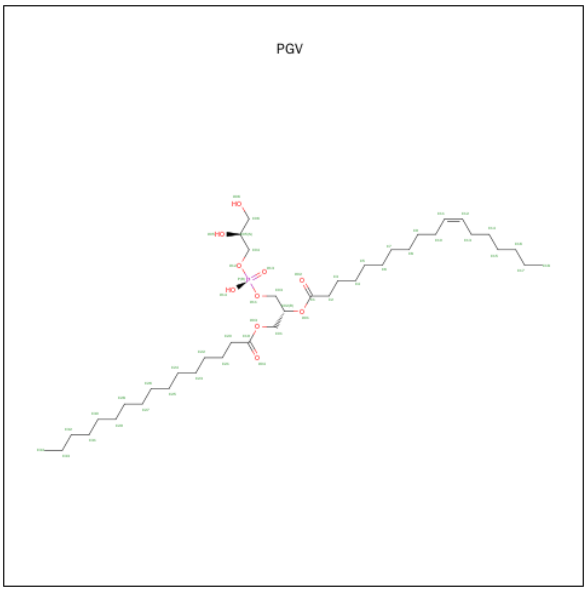
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C Fe N O 60 49 1 4 6	0	0
18	A	1	Total C Fe N O 60 49 1 4 6	0	0
18	N	1	Total C Fe N O 60 49 1 4 6	0	0
18	N	1	Total C Fe N O 60 49 1 4 6	0	0

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



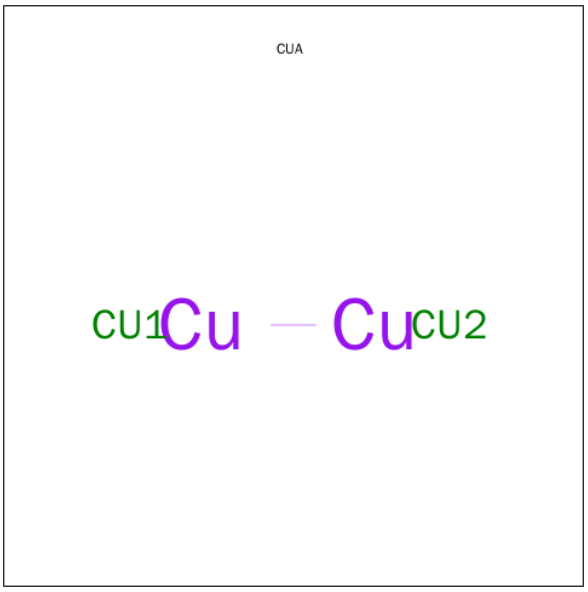
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0

- 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: $C_{40}H_{77}O_{10}P$).



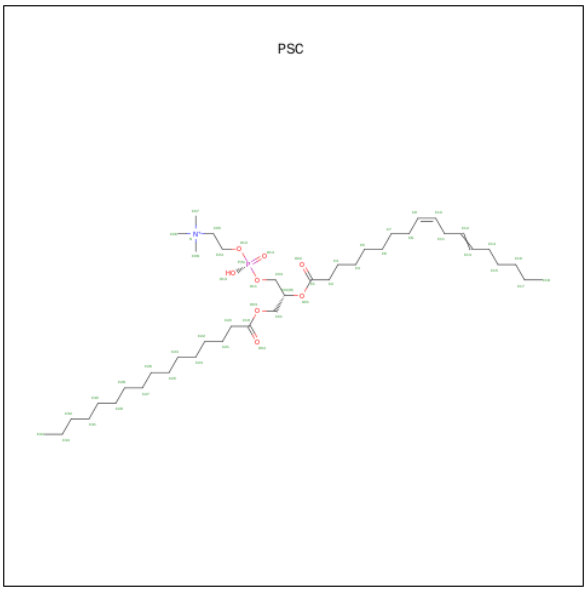
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	Z	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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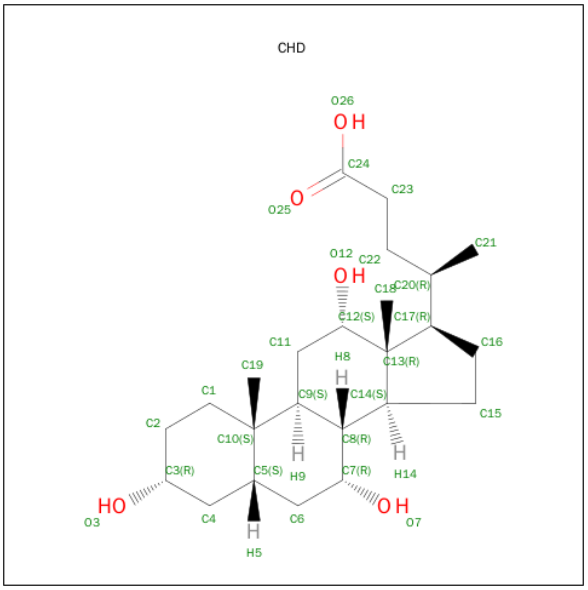
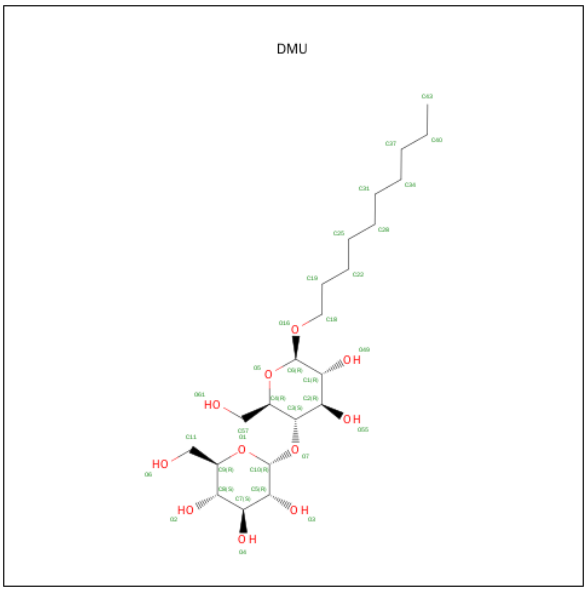
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



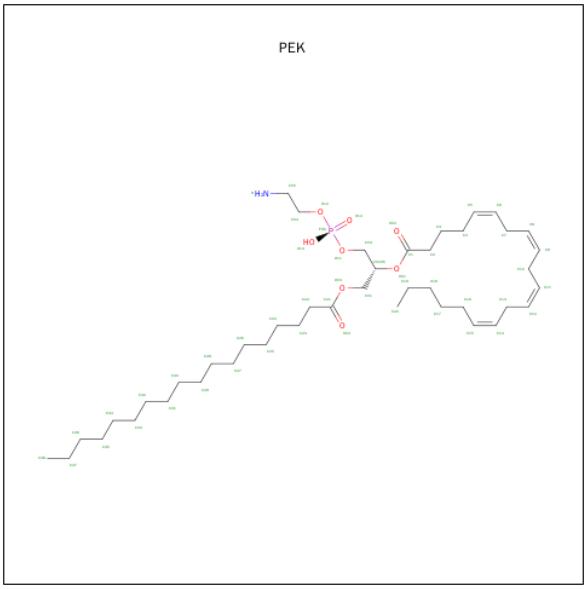
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	O			0	0
			29	24	5				
23	C	1	Total	C	O			0	0
			29	24	5				
23	C	1	Total	C	O			0	0
			29	24	5				
23	J	1	Total	C	O			0	0
			29	24	5				
23	O	1	Total	C	O			0	0
			29	24	5				
23	P	1	Total	C	O			0	0
			29	24	5				
23	P	1	Total	C	O			0	0
			29	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: $C_{22}H_{42}O_{11}$).



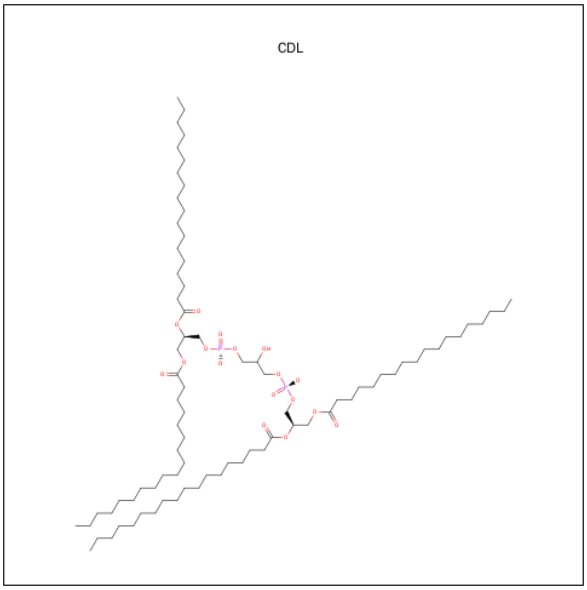
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 33 22 11	0	0
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

- 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	220	Total O 220 220	0	0
28	B	128	Total O 128 128	0	0
28	C	103	Total O 103 103	0	0
28	D	90	Total O 90 90	0	0
28	E	58	Total O 58 58	0	0
28	F	75	Total O 75 75	0	0
28	G	42	Total O 42 42	0	0
28	H	44	Total O 44 44	0	0
28	I	45	Total O 45 45	0	0
28	J	21	Total O 21 21	0	0
28	K	24	Total O 24 24	0	0
28	L	20	Total O 20 20	0	0
28	M	21	Total O 21 21	0	0
28	N	198	Total O 198 198	0	0
28	O	118	Total O 118 118	0	0
28	P	94	Total O 94 94	0	0
28	Q	53	Total O 53 53	0	0
28	R	43	Total O 43 43	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	S	62	Total O 62 62	0	0
28	T	44	Total O 44 44	0	0
28	U	38	Total O 38 38	0	0
28	V	23	Total O 23 23	0	0
28	W	16	Total O 16 16	0	0
28	X	16	Total O 16 16	0	0
28	Y	15	Total O 15 15	0	0
28	Z	13	Total O 13 13	0	0

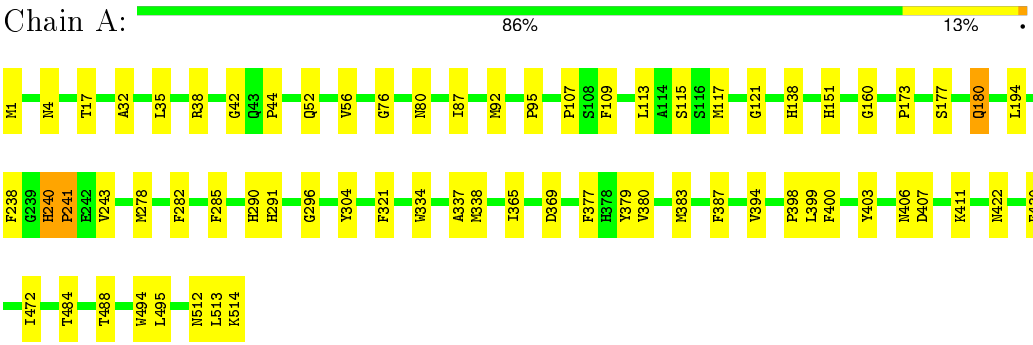
3 Residue-property plots (i)

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.

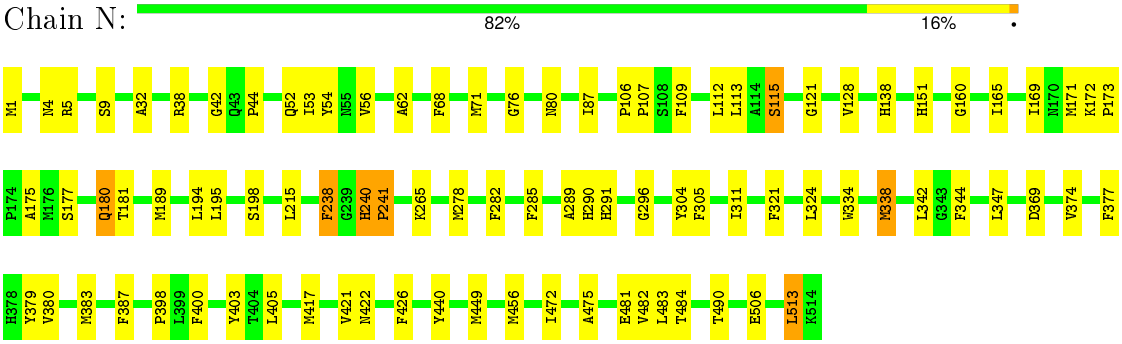
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



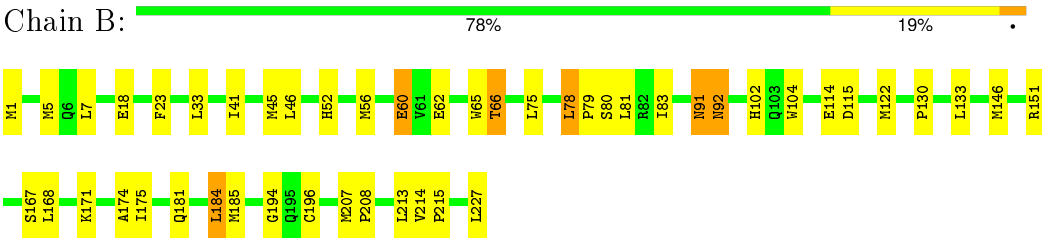
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



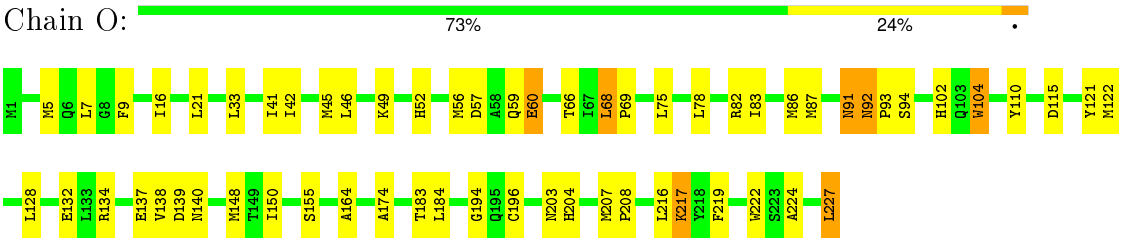
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



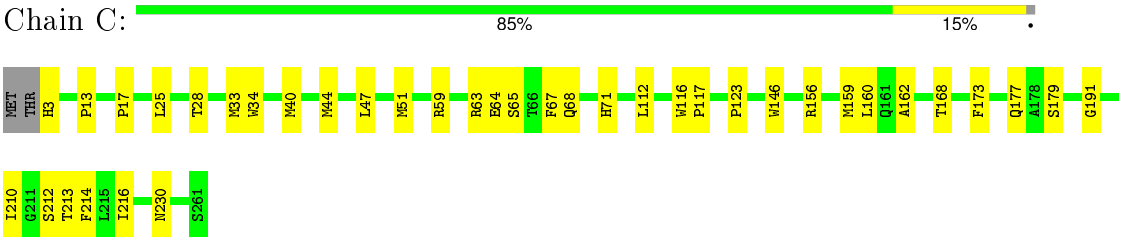
- Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



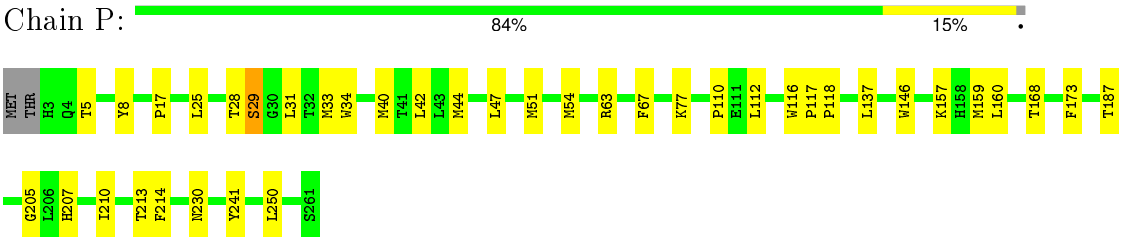
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



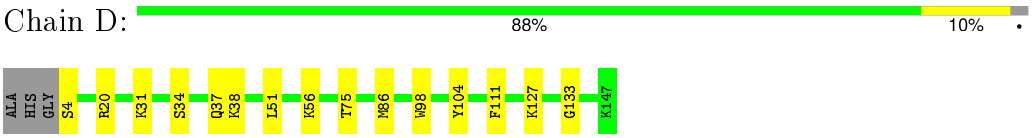
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



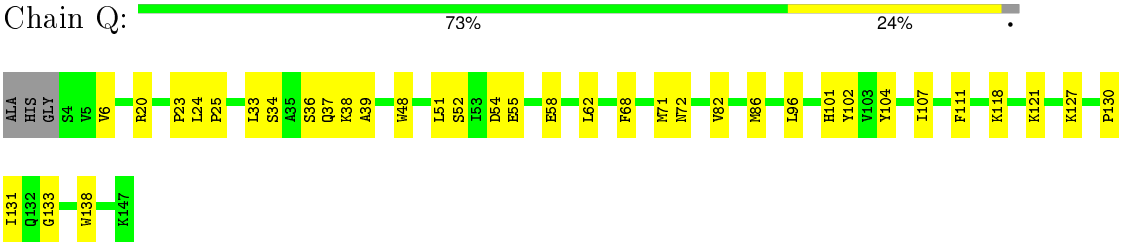
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



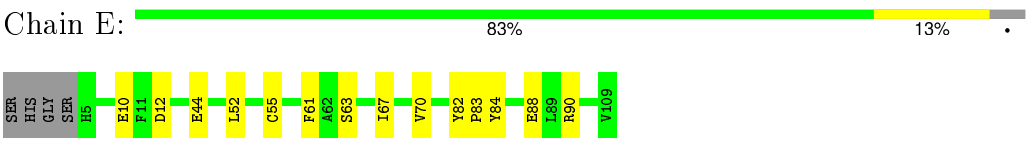
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



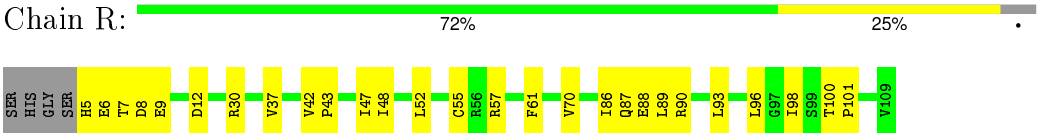
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



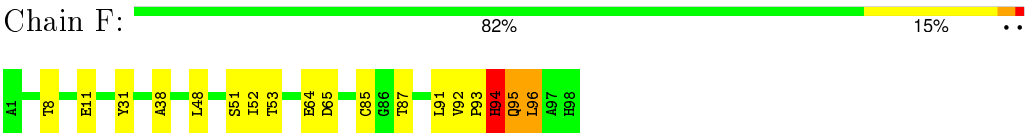
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



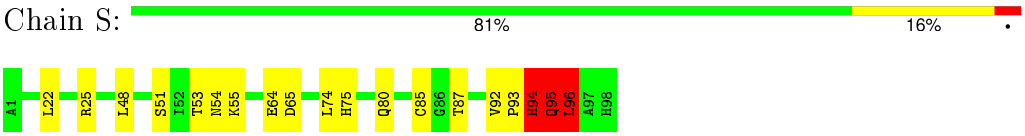
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:



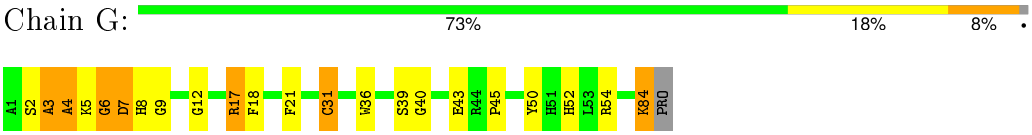
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:



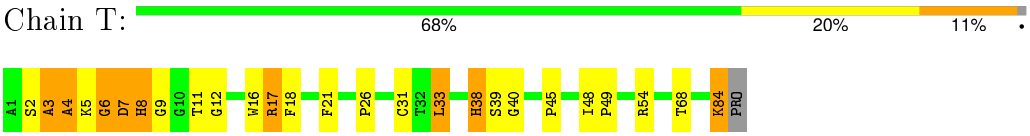
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



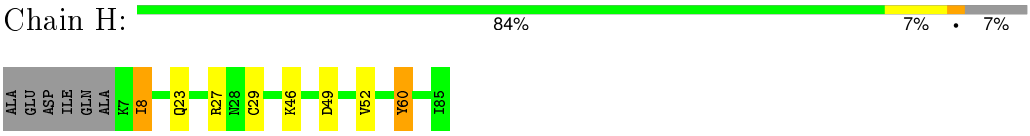
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



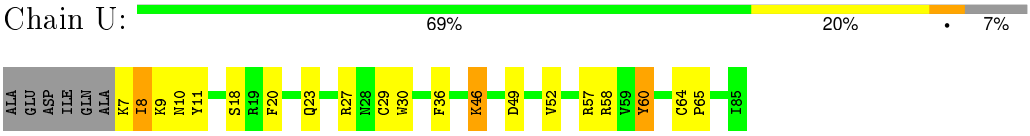
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

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

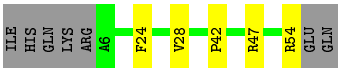
Chain J:

• 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

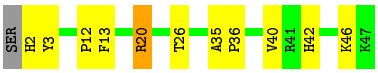
Chain X:

• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:

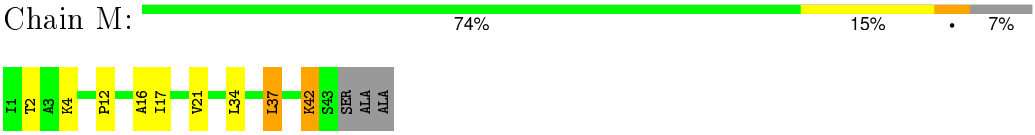
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



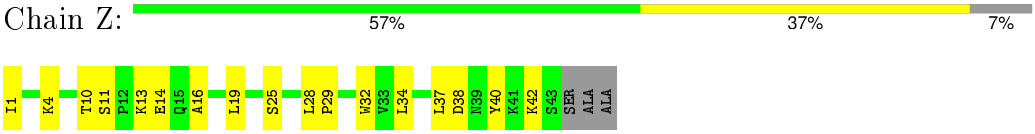
• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

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	183.38Å 205.90Å 178.18Å 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 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32357	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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	0.55	0/4156	0.70	0/5678
1	N	0.55	2/4156 (0.0%)	0.67	0/5678
2	B	0.53	0/1860	0.78	1/2534 (0.0%)
2	O	0.55	0/1860	0.81	2/2534 (0.1%)
3	C	0.57	0/2197	0.62	0/3005
3	P	0.53	0/2197	0.63	0/3005
4	D	0.54	0/1229	0.69	1/1658 (0.1%)
4	Q	0.57	0/1229	0.67	1/1658 (0.1%)
5	E	0.56	0/871	0.70	0/1182
5	R	0.54	0/871	0.72	1/1182 (0.1%)
6	F	0.52	0/765	0.83	2/1038 (0.2%)
6	S	0.53	0/765	0.83	2/1038 (0.2%)
7	G	0.58	1/690 (0.1%)	0.74	1/937 (0.1%)
7	T	0.59	0/690	0.76	2/937 (0.2%)
8	H	0.52	0/682	0.68	0/921
8	U	0.50	0/682	0.67	0/921
9	I	0.54	0/605	0.63	0/802
9	V	0.54	0/605	0.61	0/802
10	J	0.51	0/471	0.65	0/636
10	W	0.51	0/471	0.66	0/636
11	K	0.56	0/398	0.69	0/546
11	X	0.53	0/398	0.66	0/546
12	L	0.53	0/393	0.57	0/526
12	Y	0.54	0/393	0.63	0/526
13	M	0.55	0/345	0.65	0/470
13	Z	0.52	0/345	0.64	0/470
All	All	0.54	3/29324 (0.0%)	0.70	13/39866 (0.0%)

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

of a sidechain that are expected to be planar.

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	506	GLU	CB-CG	5.12	1.61	1.52
1	N	506	GLU	CG-CD	5.09	1.59	1.51
7	G	31	CYS	CB-SG	-5.02	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	33	LEU	CA-CB-CG	6.75	130.82	115.30
6	F	94	HIS	N-CA-C	6.51	128.58	111.00
6	S	94	HIS	N-CA-C	6.27	127.93	111.00
2	O	227	LEU	CA-CB-CG	6.11	129.35	115.30
4	D	133	GLY	N-CA-C	5.72	127.40	113.10
4	Q	133	GLY	N-CA-C	5.58	127.06	113.10
6	F	93	PRO	N-CA-C	5.39	126.13	112.10
5	R	42	VAL	N-CA-C	-5.38	96.49	111.00
2	B	184	LEU	CA-CB-CG	5.34	127.58	115.30
7	G	6	GLY	N-CA-C	5.24	126.19	113.10
2	O	104	TRP	N-CA-CB	-5.22	101.20	110.60
6	S	93	PRO	N-CA-C	5.15	125.48	112.10
7	T	6	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	60	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	32	0
2	O	1824	0	1833	41	0
3	C	2110	0	2027	32	0
3	P	2110	0	2027	36	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	27	0
5	E	852	0	845	7	0
5	R	852	0	845	16	0
6	F	748	0	728	9	0
6	S	748	0	728	14	0
7	G	675	0	644	25	0
7	T	675	0	644	31	0
8	H	662	0	623	6	0
8	U	662	0	623	12	0
9	I	601	0	613	5	0
9	V	601	0	613	10	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	2	0
11	X	384	0	366	5	0
12	L	380	0	380	15	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	10	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	P	1	0	0	0	0
18	A	120	0	108	4	0
18	N	120	0	108	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	63	0	110	9	0
19	D	63	0	110	4	0
19	L	63	0	110	24	0
19	N	126	0	220	24	0
19	Q	63	0	110	5	0
20	A	102	0	152	10	0
20	C	102	0	152	7	0
20	N	51	0	76	1	0
20	P	102	0	152	6	0
20	Z	51	0	76	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	15	0
22	O	52	0	80	15	0
23	B	29	0	39	0	0
23	C	58	0	78	4	0
23	J	29	0	39	2	0
23	O	29	0	39	0	0
23	P	58	0	78	2	0
23	W	29	0	39	3	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	37	5	0
24	Z	33	0	38	0	0
25	C	106	0	154	12	0
25	G	53	0	77	7	0
25	P	106	0	154	16	0
25	T	53	0	77	9	0
26	C	100	0	156	18	0
26	G	100	0	156	18	0
26	P	100	0	156	16	0
26	T	100	0	156	22	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	220	0	0	4	0
28	B	128	0	0	2	0
28	C	103	0	0	1	0
28	D	90	0	0	2	0
28	E	58	0	0	1	0
28	F	75	0	0	0	0
28	G	42	0	0	6	0
28	H	44	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	I	45	0	0	3	0
28	J	21	0	0	2	0
28	K	24	0	0	1	0
28	L	20	0	0	1	0
28	M	21	0	0	1	0
28	N	198	0	0	3	0
28	O	118	0	0	2	0
28	P	94	0	0	1	0
28	Q	53	0	0	1	0
28	R	43	0	0	0	0
28	S	62	0	0	2	0
28	T	44	0	0	3	0
28	U	38	0	0	0	0
28	V	23	0	0	1	0
28	W	16	0	0	0	0
28	X	16	0	0	0	0
28	Y	15	0	0	1	0
28	Z	13	0	0	1	0
All	All	32357	0	31299	579	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 (579) 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)
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.29	1.09
22:B:230:PSC:H343	22:B:230:PSC:H142	1.31	1.05
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.31	1.05
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.23	1.04
7:T:84:LYS:H	7:T:84:LYS:HD2	1.23	0.99
4:D:34:SER:H	4:D:37:GLN:HE21	1.07	0.98
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.43	0.97
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.27	0.97
19:N:1521:TGL:H281	19:N:1521:TGL:H102	1.48	0.95
7:G:84:LYS:HD2	7:G:84:LYS:H	1.30	0.95
19:A:521:TGL:H281	19:A:521:TGL:H102	1.50	0.93
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.52	0.92
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.52	0.91
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.53	0.91
26:G:269:CDL:H541	26:G:269:CDL:H231	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1522:TGL:HC62	19:N:1522:TGL:HC22	1.55	0.89
25:C:264:PEK:H102	25:C:264:PEK:H161	1.55	0.88
26:C:270:CDL:H642	26:C:270:CDL:H191	1.54	0.88
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.57	0.87
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.14	0.86
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.57	0.86
19:N:1521:TGL:C28	19:N:1521:TGL:H102	2.08	0.83
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.59	0.83
6:S:94:HIS:CD2	6:S:95:GLN:H	1.97	0.83
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.62	0.82
1:N:472:ILE:HG21	19:N:1522:TGL:HA92	1.61	0.81
19:A:521:TGL:C28	19:A:521:TGL:H102	2.11	0.80
1:A:278:MET:SD	7:T:5:LYS:HB3	2.21	0.79
9:I:1:SAC:HA	28:I:4751:HOH:O	1.82	0.79
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.66	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.66	0.78
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.50	0.77
1:N:112:LEU:HG	28:N:3073:HOH:O	1.84	0.77
26:G:269:CDL:H622	20:P:1268:PGV:H152	1.65	0.76
19:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.65	0.76
6:S:94:HIS:CG	6:S:95:GLN:H	2.03	0.76
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.69	0.75
12:L:13:PHE:HA	19:L:522:TGL:HC31	1.67	0.75
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.51	0.75
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.22	0.74
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.70	0.74
19:L:522:TGL:H242	19:L:522:TGL:H202	1.69	0.74
7:G:31:CYS:SG	26:G:269:CDL:H532	2.27	0.74
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.36	0.74
19:N:1521:TGL:H201	19:N:1521:TGL:H241	1.69	0.73
2:O:224:ALA:O	2:O:227:LEU:HG	1.88	0.73
19:N:1522:TGL:H202	19:N:1522:TGL:H242	1.70	0.73
12:L:24:MET:SD	19:L:522:TGL:H162	2.29	0.73
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.73
19:A:521:TGL:H201	19:A:521:TGL:H241	1.72	0.71
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.25	0.71
7:T:84:LYS:H	7:T:84:LYS:CD	2.02	0.71
5:R:89:LEU:O	5:R:93:LEU:HG	1.91	0.70
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.56	0.70
26:G:269:CDL:C23	26:G:269:CDL:H541	2.22	0.70
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:268:PGV:H152	26:T:1269:CDL:H622	1.75	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.74	0.69
4:D:34:SER:H	4:D:37:GLN:NE2	1.87	0.69
26:G:269:CDL:H522	26:G:269:CDL:H202	1.75	0.69
7:G:84:LYS:H	7:G:84:LYS:CD	2.00	0.68
22:B:230:PSC:C34	22:B:230:PSC:H142	2.17	0.68
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.74	0.68
19:N:1521:TGL:H161	2:O:7:LEU:HD11	1.76	0.68
20:Z:1524:PGV:H321	20:Z:1524:PGV:H152	1.75	0.68
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.29	0.67
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.76	0.67
20:P:1267:PGV:H12	20:P:1267:PGV:H161	1.75	0.67
1:N:449:MET:SD	2:O:5:MET:HG2	2.34	0.67
7:T:45:PRO:HD2	28:T:3152:HOH:O	1.95	0.67
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.66
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.76	0.66
1:N:1:FME:HCN	1:N:4:ASN:H	1.60	0.66
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.76	0.66
20:C:267:PGV:H172	26:C:270:CDL:H662	1.77	0.66
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.08	0.65
7:G:5:LYS:HB3	1:N:278:MET:SD	2.36	0.65
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.79	0.65
20:C:267:PGV:H12	20:C:267:PGV:H161	1.76	0.65
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.26	0.64
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.32	0.64
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.78	0.64
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.61	0.64
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.32	0.64
6:F:92:VAL:O	6:F:92:VAL:HG23	1.97	0.64
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.28	0.64
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.33	0.64
1:N:54:TYR:HB2	28:N:3113:HOH:O	1.97	0.64
19:N:1521:TGL:HC92	28:Q:4513:HOH:O	1.98	0.64
1:N:347:LEU:HD13	1:N:383:MET:SD	2.38	0.64
22:B:230:PSC:H21	22:B:230:PSC:H222	1.80	0.64
1:N:472:ILE:HG21	19:N:1522:TGL:CA9	2.27	0.64
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.62	0.63
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.81	0.63
5:E:84:TYR:O	5:E:88:GLU:HG2	1.98	0.63
12:L:9:LYS:HG3	28:L:4708:HOH:O	1.97	0.63
20:A:524:PGV:H152	20:A:524:PGV:H321	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:C34	22:O:1230:PSC:H142	2.16	0.63
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.81	0.63
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.81	0.63
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.29	0.62
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.82	0.62
12:L:20:ARG:NH2	19:L:522:TGL:HC61	2.14	0.62
8:H:23:GLN:HG3	28:H:4576:HOH:O	2.00	0.61
26:G:269:CDL:H172	26:G:269:CDL:H511	1.82	0.61
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.01	0.61
2:B:56:MET:HG2	22:B:230:PSC:H211	1.82	0.61
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.64	0.61
1:A:379:TYR:O	1:A:383:MET:HB2	2.00	0.61
20:A:524:PGV:H062	28:M:2160:HOH:O	2.01	0.61
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.83	0.60
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.19	0.60
7:G:2:SER:O	25:G:1263:PEK:H322	2.01	0.60
10:J:7:GLU:HG3	28:J:4786:HOH:O	2.00	0.60
20:C:267:PGV:H182	26:C:270:CDL:H673	1.83	0.60
26:C:270:CDL:C19	26:C:270:CDL:H642	2.29	0.60
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.81	0.60
26:C:270:CDL:H431	28:J:4770:HOH:O	2.01	0.60
1:A:484:THR:HB	13:M:2:THR:OG1	2.02	0.60
1:A:334:TRP:CZ3	19:D:523:TGL:HA51	2.37	0.60
1:A:472:ILE:HG21	19:L:522:TGL:CA9	2.32	0.60
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.83	0.60
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.00	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.59
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.83	0.59
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.84	0.59
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.64	0.59
4:D:34:SER:N	4:D:37:GLN:HE21	1.90	0.59
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.83	0.59
1:N:87:ILE:O	1:N:173:PRO:HD3	2.02	0.59
1:N:472:ILE:HD13	19:N:1522:TGL:HA91	1.83	0.59
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.85	0.59
25:C:265:PEK:C38	26:G:269:CDL:H273	2.34	0.58
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.33	0.58
12:L:20:ARG:NH1	19:L:522:TGL:HC61	2.19	0.58
26:P:1270:CDL:H112	28:P:4729:HOH:O	2.04	0.57
1:A:177:SER:H	1:A:180:GLN:HE21	1.51	0.57
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:MET:HA	22:O:1230:PSC:H202	1.87	0.57
3:C:33:MET:HG2	28:C:4095:HOH:O	2.05	0.57
1:A:17:THR:OG1	19:L:522:TGL:H281	2.04	0.57
8:H:49:ASP:O	8:H:52:VAL:HG22	2.05	0.57
6:S:22:LEU:HD12	28:S:4738:HOH:O	2.03	0.57
1:A:87:ILE:O	1:A:173:PRO:HD3	2.05	0.57
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.87	0.57
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.39	0.57
1:N:449:MET:SD	2:O:5:MET:CG	2.92	0.56
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.20	0.56
6:S:75:HIS:H	6:S:80:GLN:HE22	1.53	0.56
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.86	0.56
7:T:2:SER:O	25:T:263:PEK:H322	2.05	0.56
1:A:472:ILE:HD13	19:L:522:TGL:HA91	1.88	0.56
7:G:45:PRO:HD2	28:G:2152:HOH:O	2.04	0.56
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.56
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.88	0.56
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.34	0.56
28:B:4533:HOH:O	25:P:1265:PEK:H031	2.05	0.56
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.88	0.56
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.56
25:C:265:PEK:H383	26:G:269:CDL:H273	1.87	0.55
1:N:1:FME:HE3	28:Y:4681:HOH:O	2.06	0.55
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.89	0.55
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.42	0.55
3:P:47:LEU:O	3:P:51:MET:HG2	2.07	0.55
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.18	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.55
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.41	0.55
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.87	0.55
3:C:168:THR:HG22	25:C:265:PEK:H14	1.88	0.55
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.88	0.55
1:A:282:PHE:HA	7:T:4:ALA:CB	2.37	0.55
19:D:523:TGL:HC21	19:D:523:TGL:HG11	1.89	0.55
6:S:92:VAL:HG23	6:S:92:VAL:O	2.07	0.55
22:B:230:PSC:H12	22:B:230:PSC:H322	1.89	0.54
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.89	0.54
20:Z:1524:PGV:H062	28:Z:3160:HOH:O	2.05	0.54
3:C:168:THR:CG2	25:C:265:PEK:H14	2.38	0.54
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.88	0.54
2:O:59:GLN:O	2:O:59:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:321:PHE:CZ	22:O:1230:PSC:H171	2.43	0.54
12:L:20:ARG:NH2	19:L:522:TGL:HC32	2.23	0.54
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.71	0.54
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.54
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.90	0.54
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.71	0.54
1:N:115:SER:O	1:N:121:GLY:HA2	2.08	0.54
1:A:449:MET:SD	2:B:5:MET:HG2	2.47	0.54
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.90	0.54
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.73	0.53
2:O:57:ASP:H	22:O:1230:PSC:H201	1.72	0.53
1:N:165:ILE:O	1:N:169:ILE:HG12	2.07	0.53
19:L:522:TGL:OA1	19:L:522:TGL:HC21	2.08	0.53
6:S:85:CYS:SG	6:S:87:THR:HG23	2.48	0.53
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.09	0.53
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.07	0.53
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.89	0.53
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.53
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.44	0.53
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.90	0.53
1:N:379:TYR:O	1:N:383:MET:HB2	2.08	0.53
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.91	0.53
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.91	0.52
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.39	0.52
11:X:24:PHE:O	11:X:28:VAL:HG12	2.09	0.52
19:L:522:TGL:C24	19:L:522:TGL:H202	2.37	0.52
1:A:383:MET:O	1:A:387:PHE:HB2	2.09	0.52
1:A:406:ASN:HD21	20:A:524:PGV:C2	2.23	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.91	0.52
2:O:56:MET:HA	22:O:1230:PSC:C20	2.39	0.52
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.10	0.52
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.10	0.52
22:O:1230:PSC:H322	22:O:1230:PSC:H12	1.92	0.52
19:A:521:TGL:H161	2:B:7:LEU:HD11	1.91	0.52
19:A:521:TGL:HA82	19:A:521:TGL:H222	1.92	0.52
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.25	0.52
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.91	0.51
19:N:1522:TGL:H202	19:N:1522:TGL:C24	2.39	0.51
6:S:87:THR:HG21	28:S:3339:HOH:O	2.09	0.51
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.41	0.51
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.92	0.51
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.10	0.51
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.51
19:N:1521:TGL:H222	19:N:1521:TGL:HA82	1.92	0.51
1:N:169:ILE:HD11	1:N:189:MET:SD	2.49	0.51
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.75	0.51
1:N:177:SER:H	1:N:180:GLN:NE2	2.09	0.51
8:U:57:ARG:HA	8:U:60:TYR:CE2	2.45	0.51
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.10	0.51
28:A:4493:HOH:O	19:D:523:TGL:HG2	2.09	0.51
5:R:48:ILE:O	5:R:52:LEU:HG	2.10	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.93	0.51
2:O:46:LEU:HD12	19:Q:1523:TGL:H271	1.92	0.51
2:O:91:ASN:HD21	2:O:183:THR:HG21	1.76	0.51
8:H:27:ARG:NH1	28:H:2303:HOH:O	2.43	0.51
7:T:84:LYS:N	7:T:84:LYS:HD2	2.07	0.50
1:A:321:PHE:CZ	22:B:230:PSC:H171	2.47	0.50
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.46	0.50
1:N:76:GLY:O	1:N:80:ASN:HB2	2.11	0.50
13:Z:16:ALA:HA	20:Z:1524:PGV:H311	1.94	0.50
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.45	0.50
20:P:1267:PGV:H182	26:P:1270:CDL:H673	1.93	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.12	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.12	0.50
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.41	0.50
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.94	0.50
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.50
2:B:1:FME:SD	2:B:133:LEU:HD11	2.52	0.49
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.95	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.99	0.49
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.11	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.94	0.49
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.48	0.49
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.28	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.58	0.49
19:N:1522:TGL:HC21	19:N:1522:TGL:OA1	2.12	0.49
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.46	0.49
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.47	0.49
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:SER:O	1:A:121:GLY:HA2	2.13	0.49
3:C:40:MET:O	3:C:44:MET:HG2	2.11	0.49
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.95	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.13	0.49
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.78	0.48
4:D:127:LYS:HD2	28:I:2391:HOH:O	2.12	0.48
8:U:7:LYS:O	8:U:8:ILE:HG22	2.13	0.48
2:B:102:HIS:O	2:B:104:TRP:HA	2.13	0.48
9:I:22:VAL:O	9:I:26:MET:HG2	2.13	0.48
6:F:85:CYS:SG	6:F:87:THR:HG23	2.53	0.48
5:E:10:GLU:HB3	28:E:4759:HOH:O	2.13	0.48
20:A:524:PGV:H311	13:M:16:ALA:HA	1.94	0.48
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.47	0.48
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.48	0.48
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.48	0.48
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.00	0.48
8:H:8:ILE:HB	28:H:4704:HOH:O	2.14	0.48
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.12	0.48
1:A:160:GLY:HA3	28:A:2064:HOH:O	2.14	0.48
1:N:417:MET:O	1:N:421:VAL:HG22	2.13	0.48
18:A:515:HEA:H122	18:A:515:HEA:HHC	1.94	0.48
20:A:604:PGV:H182	3:C:28:THR:HG22	1.95	0.48
1:N:383:MET:O	1:N:387:PHE:HB2	2.13	0.48
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.48	0.48
3:P:205:GLY:HA3	25:P:1264:PEK:H181	1.96	0.48
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.95	0.48
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.94	0.48
2:B:1:FME:SD	2:B:133:LEU:CD1	3.01	0.48
2:O:68:LEU:HD23	22:O:1230:PSC:H182	1.94	0.48
10:W:40:LEU:HD12	23:W:1060:CHD:H183	1.96	0.48
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.44	0.48
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.73	0.48
4:D:34:SER:O	4:D:38:LYS:HG3	2.14	0.47
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.96	0.47
7:G:2:SER:OG	25:G:1263:PEK:H301	2.14	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.13	0.47
7:T:12:GLY:HA3	28:T:3274:HOH:O	2.14	0.47
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.47
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.96	0.47
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.96	0.47
2:B:56:MET:HA	22:B:230:PSC:H202	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:8:HIS:ND1	25:T:263:PEK:H312	2.29	0.47
10:W:50:LEU:HD22	10:W:50:LEU:O	2.15	0.47
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.44	0.47
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.28	0.47
3:C:51:MET:SD	26:C:270:CDL:H622	2.53	0.47
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.96	0.47
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.79	0.47
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.29	0.47
20:P:1267:PGV:H12	20:P:1267:PGV:C16	2.42	0.47
25:P:1265:PEK:H231	7:T:21:PHE:CD2	2.50	0.47
1:N:426:PHE:CZ	19:N:1521:TGL:HA62	2.50	0.47
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.96	0.47
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.15	0.47
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.97	0.47
2:O:82:ARG:HG2	2:O:86:MET:HE1	1.95	0.47
1:N:422:ASN:HB3	19:N:1521:TGL:H242	1.97	0.47
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.97	0.47
5:E:52:LEU:O	5:E:55:CYS:HB2	2.15	0.47
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.15	0.47
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.50	0.47
9:V:65:LYS:O	11:X:54:ARG:NH1	2.44	0.47
1:A:113:LEU:CD1	19:L:522:TGL:H292	2.45	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.46
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.50	0.46
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.62	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.15	0.46
1:N:215:LEU:HD11	25:P:1264:PEK:H271	1.97	0.46
18:N:515:HEA:H122	18:N:515:HEA:HHC	1.98	0.46
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.72	0.46
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.15	0.46
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.14	0.46
1:A:488:THR:HB	1:A:495:LEU:HD13	1.98	0.46
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.81	0.46
23:P:1271:CHD:H12A	23:P:1271:CHD:H112	1.66	0.46
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.96	0.46
28:A:4241:HOH:O	4:D:20:ARG:HG3	2.15	0.46
19:N:1522:TGL:H361	19:N:1522:TGL:HB91	1.97	0.46
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.37	0.46
20:Z:1524:PGV:C15	20:Z:1524:PGV:H321	2.44	0.46
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.81	0.46
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.81	0.46
2:B:52:HIS:HE1	22:B:230:PSC:H02	1.81	0.46
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.97	0.46
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.98	0.46
10:J:29:ASN:HD22	10:J:29:ASN:H	1.63	0.46
3:P:187:THR:HB	7:T:68:THR:HG21	1.97	0.46
2:B:56:MET:HA	22:B:230:PSC:C20	2.46	0.45
1:N:160:GLY:HA3	28:N:3064:HOH:O	2.15	0.45
7:G:12:GLY:HA3	28:G:2274:HOH:O	2.14	0.45
1:A:113:LEU:O	1:A:117:MET:HG2	2.15	0.45
7:T:5:LYS:CB	25:T:263:PEK:H362	2.31	0.45
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.60	0.45
26:G:269:CDL:H571	26:G:269:CDL:H601	1.55	0.45
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.99	0.45
4:D:86:MET:HE3	28:K:4516:HOH:O	2.15	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
28:H:4673:HOH:O	8:U:46:LYS:HD3	2.16	0.45
2:B:41:ILE:O	2:B:45:MET:HG2	2.16	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.16	0.45
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.76	0.45
6:S:94:HIS:CG	6:S:95:GLN:N	2.79	0.45
7:T:2:SER:O	7:T:3:ALA:HB3	2.17	0.45
19:A:521:TGL:HC22	28:I:2383:HOH:O	2.16	0.45
19:L:522:TGL:H272	19:L:522:TGL:H231	1.99	0.45
25:C:265:PEK:H383	26:G:269:CDL:C27	2.47	0.45
19:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.98	0.45
24:P:1272:DMU:O1	24:P:1272:DMU:H30	2.16	0.45
13:M:42:LYS:HA	13:M:42:LYS:CE	2.38	0.45
12:L:2:HIS:HE1	12:L:5:GLU:OE1	2.00	0.45
5:R:87:GLN:HG2	5:R:88:GLU:N	2.31	0.45
26:C:270:CDL:H202	26:C:270:CDL:H171	1.76	0.45
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.48	0.45
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.99	0.45
4:D:31:LYS:HE3	28:D:4485:HOH:O	2.16	0.45
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.99	0.45
1:N:400:PHE:HB3	19:N:1522:TGL:C28	2.47	0.45
5:R:52:LEU:O	5:R:55:CYS:HB2	2.16	0.45
1:A:365:ILE:HD11	28:A:4177:HOH:O	2.15	0.45
1:N:128:VAL:HG12	1:N:128:VAL:O	2.17	0.45
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.55	0.45
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.84	0.45
10:W:30:ILE:O	10:W:34:VAL:HG23	2.17	0.45
25:C:265:PEK:H031	28:O:4625:HOH:O	2.17	0.45
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.99	0.45
2:B:91:ASN:HD22	2:B:92:ASN:N	2.15	0.45
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.47	0.44
23:C:271:CHD:H222	23:C:271:CHD:H162	1.72	0.44
19:D:523:TGL:H242	19:D:523:TGL:H212	1.74	0.44
2:O:52:HIS:HE1	22:O:1230:PSC:H212	1.82	0.44
2:B:146:MET:HA	2:B:213:LEU:HD12	1.99	0.44
2:B:214:VAL:HB	2:B:215:PRO:CD	2.46	0.44
1:A:240:HIS:O	1:A:243:VAL:HG22	2.17	0.44
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.82	0.44
19:N:1522:TGL:H272	19:N:1522:TGL:H231	1.98	0.44
23:J:60:CHD:H212	23:J:60:CHD:H161	1.74	0.44
19:Q:1523:TGL:H361	28:V:4566:HOH:O	2.17	0.44
4:D:56:LYS:HB3	5:E:61:PHE:CE2	2.52	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.16	0.44
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.44
5:E:63:SER:O	5:E:67:ILE:HG13	2.18	0.44
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.99	0.44
6:S:51:SER:O	6:S:94:HIS:N	2.50	0.44
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.53	0.44
3:P:63:ARG:NE	26:P:1270:CDL:HA22	2.11	0.44
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.99	0.44
3:P:34:TRP:CE2	24:P:1272:DMU:H29	2.52	0.44
2:B:62:GLU:O	2:B:66:THR:HB	2.18	0.44
3:C:3:HIS:HE1	6:F:31:TYR:OH	2.00	0.44
26:G:269:CDL:C54	26:G:269:CDL:H231	2.35	0.44
7:G:4:ALA:CB	1:N:282:PHE:HA	2.48	0.44
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.32	0.44
1:N:5:ARG:O	1:N:9:SER:HB2	2.17	0.44
10:W:9:GLN:O	10:W:13:GLN:HG3	2.17	0.44
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.84	0.44
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.83	0.44
20:A:524:PGV:C15	20:A:524:PGV:H321	2.47	0.44
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.99	0.44
10:J:50:LEU:HD22	10:J:50:LEU:O	2.17	0.44
3:C:213:THR:HG23	26:C:270:CDL:H762	1.99	0.43
7:G:84:LYS:N	7:G:84:LYS:HD2	2.13	0.43
19:Q:1523:TGL:H212	19:Q:1523:TGL:H242	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.17	0.43
6:S:22:LEU:O	6:S:25:ARG:HB3	2.18	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.00	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H771	2.00	0.43
7:T:17:ARG:HD2	28:T:3309:HOH:O	2.19	0.43
3:C:116:TRP:HA	3:C:117:PRO:C	2.38	0.43
2:O:216:LEU:O	2:O:219:PHE:HB3	2.19	0.43
4:D:75:THR:HB	28:D:2332:HOH:O	2.19	0.43
1:N:52:GLN:O	1:N:56:VAL:HG23	2.18	0.43
6:F:52:ILE:HA	6:F:94:HIS:HA	2.01	0.43
1:N:240:HIS:HB3	1:N:241:PRO:HD3	2.01	0.43
7:G:5:LYS:HD3	1:N:278:MET:HB3	2.00	0.43
3:P:54:MET:HE3	26:P:1270:CDL:H612	2.01	0.43
2:O:42:ILE:O	2:O:46:LEU:HG	2.18	0.43
7:G:17:ARG:HD2	28:G:2309:HOH:O	2.17	0.43
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.01	0.43
1:N:398:PRO:HA	1:N:403:TYR:O	2.19	0.43
1:N:175:ALA:CB	1:N:513:LEU:HD23	2.49	0.43
4:Q:24:LEU:HD12	5:R:30:ARG:HA	2.01	0.43
26:T:1269:CDL:H152	26:T:1269:CDL:H181	1.93	0.43
26:T:1269:CDL:H222	26:T:1269:CDL:H251	1.93	0.43
1:N:113:LEU:HD12	19:N:1522:TGL:H292	1.99	0.43
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.36	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.43
3:C:51:MET:HB3	26:C:270:CDL:H622	2.01	0.43
4:Q:131:ILE:H	4:Q:131:ILE:HD12	1.84	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.01	0.43
26:C:270:CDL:H532	26:C:270:CDL:H561	1.77	0.42
24:C:272:DMU:H41	28:G:4668:HOH:O	2.19	0.42
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.01	0.42
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.00	0.42
2:O:155:SER:O	2:O:174:ALA:HB1	2.19	0.42
6:S:64:GLU:O	6:S:65:ASP:HB2	2.18	0.42
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.54	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.38	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
26:C:270:CDL:H602	26:C:270:CDL:H632	1.57	0.42
12:L:20:ARG:CZ	19:L:522:TGL:HC61	2.49	0.42
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.01	0.42
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.71	0.42
1:A:422:ASN:HB3	19:A:521:TGL:H242	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:19:LEU:HD23	20:Z:1524:PGV:H322	2.01	0.42
9:V:36:LYS:HA	9:V:40:ALA:HB3	2.01	0.42
8:U:9:LYS:HB3	8:U:10:ASN:H	1.64	0.42
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.02	0.42
26:C:270:CDL:H672	26:C:270:CDL:H641	1.83	0.42
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.48	0.42
5:R:100:THR:HB	5:R:101:PRO:HD2	2.00	0.42
1:A:1:FME:HCN	1:A:4:ASN:HB2	2.02	0.42
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.50	0.42
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.54	0.42
3:C:156:ARG:HE	23:C:271:CHD:C23	2.33	0.42
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.61	0.42
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.49	0.42
1:A:377:PHE:HA	1:A:380:VAL:HG22	2.01	0.42
5:R:5:HIS:HB3	5:R:6:GLU:H	1.67	0.42
9:V:58:LYS:O	9:V:62:GLU:HG3	2.19	0.42
20:C:267:PGV:H182	26:C:270:CDL:C67	2.49	0.42
7:G:7:ASP:O	7:G:9:GLY:N	2.52	0.42
2:B:18:GLU:HB3	28:B:4772:HOH:O	2.19	0.42
25:C:265:PEK:H292	28:O:4283:HOH:O	2.19	0.42
18:A:516:HEA:HMB1	18:A:516:HEA:H11	1.87	0.42
8:U:49:ASP:O	8:U:52:VAL:HG22	2.20	0.42
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.84	0.42
3:C:212:SER:O	3:C:216:ILE:HG13	2.20	0.42
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.35	0.42
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.84	0.42
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.02	0.42
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.42
2:O:222:TRP:HB2	9:V:71:SER:HB2	2.01	0.42
22:B:230:PSC:H251	22:B:230:PSC:H221	1.79	0.42
23:W:1060:CHD:H161	23:W:1060:CHD:H212	1.77	0.42
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	2.50	0.42
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.90	0.42
19:L:522:TGL:HB91	19:L:522:TGL:H361	2.02	0.42
2:O:128:LEU:HD22	2:O:132:GLU:HB3	2.02	0.42
1:N:344:PHE:C	1:N:344:PHE:CD1	2.93	0.42
3:P:213:THR:HG23	26:P:1270:CDL:H762	2.02	0.41
12:L:12:PRO:HB2	19:L:522:TGL:HG2	2.02	0.41
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.54	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.92	0.41
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.35	0.41
3:C:117:PRO:HG3	3:C:123:PRO:HG2	2.02	0.41
3:C:191:GLY:HA3	28:G:2163:HOH:O	2.20	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.20	0.41
1:N:198:SER:HB2	1:N:238:PHE:HA	2.02	0.41
5:R:57:ARG:HH11	5:R:57:ARG:HG3	1.85	0.41
1:A:407:ASP:O	1:A:411:LYS:HG3	2.21	0.41
3:C:59:ARG:HG3	26:C:270:CDL:H512	2.01	0.41
20:A:524:PGV:H011	20:A:524:PGV:H202	1.92	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.55	0.41
1:A:398:PRO:HA	1:A:403:TYR:O	2.21	0.41
2:B:79:PRO:O	2:B:83:ILE:HG13	2.20	0.41
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.53	0.41
19:N:1522:TGL:HB61	19:N:1522:TGL:HB31	1.85	0.41
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.41
1:A:1:FME:HA	1:A:1:FME:CE	2.51	0.41
3:P:173:PHE:CD2	3:P:173:PHE:C	2.94	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
19:L:522:TGL:HB31	19:L:522:TGL:HB61	1.85	0.41
20:N:1266:PGV:H182	3:P:28:THR:HG22	2.03	0.41
3:P:31:LEU:HD23	3:P:31:LEU:HA	1.77	0.41
26:P:1270:CDL:H651	26:P:1270:CDL:C77	2.51	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.21	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.55	0.41
7:T:48:ILE:HA	7:T:49:PRO:HD3	1.82	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.89	0.41
13:M:17:ILE:O	13:M:21:VAL:HG23	2.20	0.41
7:T:31:CYS:HG	26:T:1269:CDL:H532	1.85	0.41
26:G:269:CDL:H732	26:G:269:CDL:H762	1.97	0.41
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.20	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.93	0.41
10:J:31:LEU:HA	10:J:31:LEU:HD12	1.84	0.41
1:A:92:MET:O	1:A:95:PRO:HD3	2.20	0.41
2:O:121:TYR:O	2:O:138:VAL:HA	2.20	0.41
3:C:210:ILE:HD13	20:C:267:PGV:H301	2.02	0.41
26:C:270:CDL:CB3	26:C:270:CDL:HB21	2.50	0.41
4:Q:33:LEU:HB2	4:Q:38:LYS:CG	2.51	0.41
20:A:524:PGV:H061	20:A:524:PGV:P	2.61	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.03	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.24	0.41
9:V:73:LYS:HE3	9:V:73:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:15:ARG:HD3	9:I:15:ARG:C	2.41	0.41
2:O:139:ASP:OD2	2:O:140:ASN:N	2.54	0.41
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.08	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.94	0.41
7:T:7:ASP:O	7:T:9:GLY:N	2.54	0.41
2:O:102:HIS:O	2:O:104:TRP:HA	2.21	0.40
1:N:338:MET:O	1:N:342:LEU:HG	2.21	0.40
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.02	0.40
7:T:3:ALA:HB1	25:T:263:PEK:C38	2.48	0.40
20:Z:1524:PGV:P	20:Z:1524:PGV:H061	2.61	0.40
7:G:12:GLY:CA	28:G:2274:HOH:O	2.69	0.40
5:R:7:THR:HB	5:R:9:GLU:OE2	2.21	0.40
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.74	0.40
7:T:3:ALA:O	7:T:4:ALA:CB	2.69	0.40
26:G:269:CDL:H222	26:G:269:CDL:H251	1.94	0.40
7:G:7:ASP:O	1:N:169:ILE:HD12	2.21	0.40
3:P:187:THR:CB	7:T:68:THR:HG21	2.52	0.40
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.86	0.40
7:G:2:SER:O	7:G:3:ALA:HB3	2.21	0.40
5:R:61:PHE:HE1	5:R:98:ILE:HA	1.86	0.40
4:D:98:TRP:CD2	24:M:526:DMU:H10	2.56	0.40
1:A:52:GLN:O	1:A:56:VAL:HG23	2.21	0.40
19:A:521:TGL:H201	19:A:521:TGL:C24	2.48	0.40
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.85	0.40
1:A:400:PHE:HB3	19:L:522:TGL:H283	2.04	0.40
25:C:264:PEK:H32	25:C:264:PEK:H71	2.04	0.40
25:P:1264:PEK:H71	25:P:1264:PEK:H32	2.03	0.40
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	2.04	0.40
8:U:58:ARG:HA	8:U:58:ARG:HD2	1.86	0.40
3:C:173:PHE:CD2	3:C:173:PHE:C	2.94	0.40
3:P:40:MET:O	3:P:44:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21	15
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	21	15
3	C	257/261 (98%)	252 (98%)	5 (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%)	139 (98%)	3 (2%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	5	1
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	5	1
7	G	81/85 (95%)	64 (79%)	10 (12%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	2
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	2
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	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%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3504/3614 (97%)	3343 (95%)	133 (4%)	28 (1%)	24	17

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	60	GLU
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
2	O	60	GLU
7	T	3	ALA
7	T	40	GLY
8	U	46	LYS
6	F	94	HIS
6	F	96	LEU
8	U	8	ILE
6	S	96	LEU
2	B	92	ASN
7	G	6	GLY
7	T	6	GLY
2	O	92	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/426 (100%)	416 (98%)	10 (2%)	58 62
1	N	426/426 (100%)	415 (97%)	11 (3%)	54 58
2	B	210/210 (100%)	199 (95%)	11 (5%)	29 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	O	210/210 (100%)	198 (94%)	12 (6%)	25 22
3	C	224/226 (99%)	218 (97%)	6 (3%)	52 56
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%)	125 (98%)	3 (2%)	58 62
5	E	92/95 (97%)	90 (98%)	2 (2%)	60 64
5	R	92/95 (97%)	91 (99%)	1 (1%)	80 85
6	F	81/81 (100%)	78 (96%)	3 (4%)	41 41
6	S	81/81 (100%)	76 (94%)	5 (6%)	23 19
7	G	67/68 (98%)	61 (91%)	6 (9%)	12 8
7	T	67/68 (98%)	60 (90%)	7 (10%)	9 5
8	H	71/75 (95%)	69 (97%)	2 (3%)	51 55
8	U	71/75 (95%)	68 (96%)	3 (4%)	36 35
9	I	57/57 (100%)	54 (95%)	3 (5%)	28 25
9	V	57/57 (100%)	56 (98%)	1 (2%)	66 72
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%)	37 (95%)	2 (5%)	29 26
12	L	39/40 (98%)	38 (97%)	1 (3%)	54 58
12	Y	39/40 (98%)	38 (97%)	1 (3%)	54 58
13	M	37/38 (97%)	32 (86%)	5 (14%)	5 2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	5 2
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	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO

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Mol	Chain	Res	Type
1	A	338	MET
1	A	369	ASP
1	A	512	ASN
1	A	513	LEU
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	115	ASP
2	B	130	PRO
2	B	167	SER
2	B	171	LYS
2	B	185	MET
3	C	13	PRO
3	C	17	PRO
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	53	THR
6	F	96	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
12	L	26	THR

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Mol	Chain	Res	Type
13	M	4	LYS
13	M	12	PRO
13	M	34	LEU
13	M	37	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	241	PRO
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	513	LEU
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	148	MET
2	O	217	LYS
3	P	17	PRO
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	51	LEU
4	Q	54	ASP
4	Q	121	LYS
5	R	90	ARG
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	95	GLN

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Mol	Chain	Res	Type
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	26	PRO
7	T	33	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	18	SER
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
13	Z	13	LYS
13	Z	34	LEU
13	Z	37	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
9	I	8	GLN
9	I	53	ASN
10	J	29	ASN

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Mol	Chain	Res	Type
1	N	99	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS

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	0.70	0	6,9,11	1.59	2 (33%)
2	FME	B	1	2	8,9,10	0.87	0	6,9,11	1.59	1 (16%)
7	TPO	G	11	7	8,10,11	1.73	1 (12%)	7,14,16	1.02	1 (14%)
9	SAC	I	1	9	7,8,9	2.46	2 (28%)	7,9,11	2.14	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	FME	N	1	1	8,9,10	0.65	0	6,9,11	1.55	2 (33%)
2	FME	O	1	2	8,9,10	0.71	0	6,9,11	1.21	1 (16%)
7	TPO	T	11	7	8,10,11	1.38	1 (12%)	7,14,16	1.03	1 (14%)
9	SAC	V	1	9	7,8,9	2.79	2 (28%)	7,9,11	2.17	4 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.53	1.58	1.54
9	I	1	SAC	CA-N	3.55	1.51	1.46
7	G	11	TPO	CB-CA	3.79	1.60	1.54
9	V	1	SAC	CA-N	4.63	1.53	1.46
9	I	1	SAC	OAC-C1A	5.21	1.35	1.23
9	V	1	SAC	OAC-C1A	5.23	1.35	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	SAC	CA-N-C1A	-3.38	109.88	121.37
2	B	1	FME	CA-N-CN	-3.30	117.75	122.82
1	A	1	FME	CA-N-CN	-3.03	118.17	122.82
1	N	1	FME	CA-N-CN	-2.97	118.25	122.82
9	V	1	SAC	CA-N-C1A	-2.97	111.29	121.37
2	O	1	FME	CA-N-CN	-2.53	118.94	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.42	117.63	122.06
1	N	1	FME	O-C-CA	-2.16	119.72	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	11	TPO	O-C-CA	-2.08	119.94	125.44
7	T	11	TPO	O-C-CA	-2.02	120.11	125.44
1	A	1	FME	O-C-CA	-2.01	120.13	125.44
9	V	1	SAC	C2A-C1A-N	2.69	121.25	116.11
9	V	1	SAC	CB-CA-N	2.74	116.61	110.60
9	I	1	SAC	CB-CA-N	3.45	118.16	110.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
2	B	1	FME	2	0
9	I	1	SAC	1	0
1	N	1	FME	2	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 11 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	1.37	6 (15%)	41,103,103	1.81	14 (34%)
18	HEA	A	516	1	40,67,67	1.58	7 (17%)	41,103,103	1.46	7 (17%)
19	TGL	A	521	-	62,62,62	0.72	0	65,65,65	1.60	12 (18%)
20	PGV	A	524	-	50,50,50	1.22	4 (8%)	51,56,56	1.00	4 (7%)
20	PGV	A	604	-	50,50,50	0.81	1 (2%)	51,56,56	0.81	3 (5%)
23	CHD	B	1086	-	29,32,32	0.64	0	48,51,51	1.79	12 (25%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.24	5 (9%)	55,59,59	0.99	1 (1%)
25	PEK	C	264	-	51,52,52	1.43	4 (7%)	52,57,57	1.15	4 (7%)
25	PEK	C	265	-	51,52,52	1.70	11 (21%)	52,57,57	1.15	5 (9%)
20	PGV	C	267	-	50,50,50	0.82	1 (2%)	51,56,56	0.96	2 (3%)
20	PGV	C	268	-	50,50,50	1.29	5 (10%)	51,56,56	0.85	2 (3%)
26	CDL	C	270	-	99,99,99	0.85	4 (4%)	101,111,111	0.93	4 (3%)
23	CHD	C	271	-	29,32,32	0.93	1 (3%)	48,51,51	3.59	24 (50%)
24	DMU	C	272	-	34,34,34	2.71	14 (41%)	45,45,45	4.32	18 (40%)
23	CHD	C	525	-	29,32,32	0.86	1 (3%)	48,51,51	1.90	13 (27%)
19	TGL	D	523	-	62,62,62	0.87	3 (4%)	65,65,65	1.51	8 (12%)
25	PEK	G	1263	-	51,52,52	1.87	11 (21%)	52,57,57	1.18	5 (9%)
26	CDL	G	269	-	99,99,99	1.09	9 (9%)	101,111,111	0.95	7 (6%)
23	CHD	J	60	-	29,32,32	1.20	2 (6%)	48,51,51	3.53	26 (54%)
19	TGL	L	522	-	62,62,62	1.14	6 (9%)	65,65,65	1.71	14 (21%)
24	DMU	M	526	-	34,34,34	3.30	8 (23%)	45,45,45	3.85	19 (42%)
20	PGV	N	1266	-	50,50,50	0.94	4 (8%)	51,56,56	0.82	2 (3%)
19	TGL	N	1521	-	62,62,62	0.72	1 (1%)	65,65,65	1.56	11 (16%)
19	TGL	N	1522	-	62,62,62	1.26	6 (9%)	65,65,65	1.67	13 (20%)
18	HEA	N	515	1	40,67,67	1.36	6 (15%)	41,103,103	1.68	14 (34%)
18	HEA	N	516	1	40,67,67	1.59	6 (15%)	41,103,103	1.51	8 (19%)
22	PSC	O	1230	-	51,51,51	1.23	4 (7%)	55,59,59	1.00	2 (3%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	0.68	0	48,51,51	1.94	14 (29%)
25	PEK	P	1264	-	51,52,52	1.49	6 (11%)	52,57,57	1.21	5 (9%)
25	PEK	P	1265	-	51,52,52	1.66	10 (19%)	52,57,57	1.13	5 (9%)
20	PGV	P	1267	-	50,50,50	0.81	1 (2%)	51,56,56	0.91	2 (3%)
20	PGV	P	1268	-	50,50,50	1.27	4 (8%)	51,56,56	0.86	3 (5%)
26	CDL	P	1270	-	99,99,99	0.90	5 (5%)	101,111,111	0.96	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CHD	P	1271	-	29,32,32	0.80	0	48,51,51	3.61	23 (47%)
24	DMU	P	1272	-	34,34,34	2.73	15 (44%)	45,45,45	4.13	18 (40%)
23	CHD	P	1525	-	29,32,32	0.80	1 (3%)	48,51,51	1.90	11 (22%)
19	TGL	Q	1523	-	62,62,62	0.83	4 (6%)	65,65,65	1.50	8 (12%)
26	CDL	T	1269	-	99,99,99	1.08	7 (7%)	101,111,111	0.98	7 (6%)
25	PEK	T	263	-	51,52,52	1.97	12 (23%)	52,57,57	1.15	5 (9%)
23	CHD	W	1060	-	29,32,32	1.34	3 (10%)	48,51,51	3.60	26 (54%)
20	PGV	Z	1524	-	50,50,50	1.24	4 (8%)	51,56,56	0.96	3 (5%)
24	DMU	Z	1526	-	34,34,34	3.19	9 (26%)	45,45,45	3.78	18 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
20	PGV	A	524	-	-	1/55/55/55	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
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	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
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
20	PGV	Z	1524	-	-	1/55/55/55	0/0/0/0
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.44	1.22	1.43
24	Z	1526	DMU	O7-C3	-8.09	1.23	1.43
24	M	526	DMU	O16-C6	-7.20	1.27	1.40
24	M	526	DMU	O1-C9	-7.06	1.26	1.44
24	Z	1526	DMU	O16-C6	-7.03	1.27	1.40
24	M	526	DMU	O5-C4	-6.76	1.27	1.44
24	Z	1526	DMU	O1-C9	-6.67	1.27	1.44
24	M	526	DMU	O16-C18	-6.56	1.24	1.42
24	Z	1526	DMU	O5-C4	-6.49	1.28	1.44
24	Z	1526	DMU	O16-C18	-6.38	1.25	1.42
24	M	526	DMU	O7-C10	-6.25	1.24	1.41
24	P	1272	DMU	O16-C18	-6.09	1.25	1.42
24	P	1272	DMU	O7-C3	-6.05	1.28	1.43
24	C	272	DMU	O16-C18	-6.01	1.26	1.42
24	Z	1526	DMU	O7-C10	-5.96	1.25	1.41
24	M	526	DMU	O1-C10	-5.81	1.26	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	O1-C9	-5.53	1.30	1.44
24	C	272	DMU	O16-C6	-5.46	1.30	1.40
24	C	272	DMU	O7-C3	-5.43	1.30	1.43
24	Z	1526	DMU	O1-C10	-5.27	1.28	1.41
24	C	272	DMU	O5-C4	-5.17	1.31	1.44
24	C	272	DMU	O1-C9	-5.14	1.31	1.44
24	P	1272	DMU	O16-C6	-5.11	1.30	1.40
24	M	526	DMU	O5-C6	-4.93	1.29	1.41
18	A	516	HEA	C3A-C2A	-4.86	1.33	1.40
24	Z	1526	DMU	O5-C6	-4.79	1.29	1.41
24	P	1272	DMU	O7-C10	-4.76	1.28	1.41
24	C	272	DMU	O5-C6	-4.30	1.30	1.41
24	C	272	DMU	O1-C10	-4.24	1.30	1.41
24	C	272	DMU	O7-C10	-4.21	1.30	1.41
24	P	1272	DMU	O5-C4	-4.03	1.34	1.44
18	N	516	HEA	C3A-CMA	-3.94	1.37	1.46
18	A	516	HEA	C3A-CMA	-3.84	1.37	1.46
24	P	1272	DMU	O1-C10	-3.65	1.32	1.41
18	N	516	HEA	C3A-C2A	-3.27	1.36	1.40
18	N	515	HEA	C3A-CMA	-3.17	1.39	1.46
18	N	515	HEA	C3A-C2A	-3.01	1.36	1.40
24	P	1272	DMU	O5-C6	-2.90	1.34	1.41
18	A	515	HEA	C3A-CMA	-2.72	1.40	1.46
25	P	1264	PEK	O03-C01	-2.16	1.40	1.45
18	A	515	HEA	C3B-C2B	-2.12	1.33	1.41
23	C	525	CHD	C10-C9	-2.11	1.52	1.56
23	C	271	CHD	C19-C10	-2.01	1.50	1.54
26	C	270	CDL	OA8-CA7	2.01	1.39	1.33
20	N	1266	PGV	O03-C19	2.02	1.39	1.33
20	C	268	PGV	P-O11	2.02	1.68	1.59
26	G	269	CDL	C31-CA7	2.02	1.56	1.50
22	O	1230	PSC	P-O12	2.02	1.68	1.59
23	J	60	CHD	C20-C17	2.02	1.58	1.54
19	Q	1523	TGL	CA2-CA1	2.03	1.56	1.50
22	B	230	PSC	P-O12	2.04	1.68	1.59
24	C	272	DMU	C10-C5	2.05	1.58	1.52
26	P	1270	CDL	OA8-CA7	2.05	1.39	1.33
20	P	1268	PGV	P-O12	2.05	1.68	1.59
25	G	1263	PEK	C22-C21	2.06	1.56	1.50
19	N	1522	TGL	CB2-CB1	2.06	1.56	1.50
19	L	522	TGL	CB2-CB1	2.06	1.56	1.50
24	C	272	DMU	C8-C7	2.07	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	C71-CB7	2.07	1.56	1.50
24	C	272	DMU	C8-C9	2.08	1.57	1.53
26	G	269	CDL	OB8-CB7	2.08	1.39	1.33
26	T	1269	CDL	CB2-C1	2.09	1.59	1.51
26	G	269	CDL	CA6-CA4	2.10	1.56	1.50
25	C	265	PEK	O01-C1	2.10	1.40	1.34
19	Q	1523	TGL	OG3-CC1	2.10	1.39	1.33
26	G	269	CDL	PB2-OB2	2.10	1.68	1.59
20	C	268	PGV	C2-C1	2.12	1.57	1.50
26	T	1269	CDL	CA6-CA4	2.12	1.56	1.50
20	N	1266	PGV	C20-C19	2.13	1.57	1.50
24	Z	1526	DMU	C8-C9	2.15	1.57	1.53
18	A	516	HEA	C21-C22	2.16	1.56	1.50
20	C	268	PGV	P-O12	2.16	1.68	1.59
26	P	1270	CDL	PB2-OB2	2.16	1.68	1.59
18	A	515	HEA	C1A-NA	2.19	1.39	1.36
20	P	1268	PGV	C2-C1	2.19	1.57	1.50
25	G	1263	PEK	O03-C01	2.19	1.50	1.45
18	A	516	HEA	C20-C19	2.19	1.56	1.51
23	P	1525	CHD	C8-C9	2.20	1.58	1.53
22	B	230	PSC	C01-C02	2.21	1.57	1.50
24	P	1272	DMU	C2-C1	2.25	1.58	1.52
25	P	1265	PEK	P-O12	2.26	1.69	1.59
25	P	1265	PEK	P-O11	2.28	1.69	1.59
24	P	1272	DMU	C10-C5	2.28	1.59	1.52
20	A	524	PGV	C03-C02	2.28	1.57	1.50
22	B	230	PSC	C2-C1	2.29	1.57	1.50
18	A	515	HEA	C4A-NA	2.29	1.39	1.36
23	W	1060	CHD	C8-C7	2.30	1.57	1.53
25	T	263	PEK	P-O12	2.30	1.69	1.59
26	T	1269	CDL	OA6-CA5	2.30	1.41	1.34
19	Q	1523	TGL	CB2-CB1	2.32	1.57	1.50
18	N	516	HEA	C18-C19	2.33	1.37	1.33
25	T	263	PEK	C22-C21	2.36	1.57	1.50
26	T	1269	CDL	C71-CB7	2.36	1.57	1.50
19	D	523	TGL	OG1-CA1	2.37	1.40	1.33
20	N	1266	PGV	C01-C02	2.37	1.57	1.50
18	A	516	HEA	C4B-NB	2.38	1.39	1.36
26	G	269	CDL	C71-CB7	2.40	1.57	1.50
19	L	522	TGL	OG1-CA1	2.40	1.40	1.33
25	P	1265	PEK	C22-C21	2.42	1.57	1.50
25	G	1263	PEK	P-O12	2.43	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1521	TGL	OG2-CB1	2.45	1.41	1.34
25	C	265	PEK	P-O11	2.46	1.70	1.59
25	C	265	PEK	P-O12	2.46	1.70	1.59
19	N	1522	TGL	CA2-CA1	2.47	1.58	1.50
19	L	522	TGL	CC2-CC1	2.48	1.58	1.50
26	C	270	CDL	CA3-CA4	2.48	1.57	1.50
25	C	265	PEK	C22-C21	2.50	1.58	1.50
24	P	1272	DMU	C5-C7	2.50	1.59	1.52
25	T	263	PEK	O01-C1	2.53	1.41	1.34
19	N	1522	TGL	CG3-CG2	2.55	1.57	1.50
19	L	522	TGL	CG3-CG2	2.56	1.57	1.50
19	D	523	TGL	CB2-CB1	2.57	1.58	1.50
26	G	269	CDL	CB3-CB4	2.57	1.58	1.50
24	C	272	DMU	C5-C7	2.59	1.59	1.52
25	C	265	PEK	O03-C21	2.62	1.41	1.33
26	P	1270	CDL	CA3-CA4	2.62	1.58	1.50
18	N	515	HEA	C4A-NA	2.64	1.40	1.36
23	W	1060	CHD	C20-C17	2.65	1.59	1.54
25	G	1263	PEK	P-O11	2.65	1.71	1.59
26	P	1270	CDL	C31-CA7	2.66	1.58	1.50
25	T	263	PEK	C2-C1	2.71	1.58	1.50
26	C	270	CDL	CA6-CA4	2.71	1.58	1.50
20	A	524	PGV	C20-C19	2.72	1.58	1.50
26	T	1269	CDL	CB3-CB4	2.74	1.58	1.50
25	P	1265	PEK	C03-C02	2.74	1.58	1.50
25	T	263	PEK	P-O11	2.75	1.71	1.59
19	D	523	TGL	OG3-CC1	2.79	1.41	1.33
25	P	1264	PEK	C2-C1	2.80	1.59	1.50
20	Z	1524	PGV	C20-C19	2.80	1.59	1.50
19	Q	1523	TGL	OG1-CA1	2.81	1.41	1.33
18	A	516	HEA	C3C-CAC	2.82	1.53	1.47
22	O	1230	PSC	C2-C1	2.82	1.59	1.50
24	C	272	DMU	C3-C4	2.89	1.61	1.52
24	P	1272	DMU	C8-C7	2.90	1.60	1.52
20	C	267	PGV	C12-C11	2.92	1.48	1.31
24	P	1272	DMU	C3-C4	2.92	1.61	1.52
25	P	1265	PEK	O03-C21	2.94	1.42	1.33
18	N	515	HEA	C1D-ND	2.97	1.40	1.36
25	P	1265	PEK	C01-C02	2.97	1.59	1.50
24	P	1272	DMU	C8-C9	2.98	1.59	1.53
25	C	265	PEK	C01-C02	2.98	1.59	1.50
26	P	1270	CDL	CA6-CA4	2.98	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	272	DMU	C6-C1	3.02	1.61	1.52
26	T	1269	CDL	C11-CA5	3.02	1.59	1.50
26	G	269	CDL	OA6-CA5	3.03	1.43	1.34
18	A	515	HEA	C1D-ND	3.08	1.40	1.36
20	P	1267	PGV	C12-C11	3.08	1.49	1.31
18	N	516	HEA	C4B-NB	3.09	1.40	1.36
20	Z	1524	PGV	C03-C02	3.10	1.59	1.50
26	G	269	CDL	C11-CA5	3.11	1.59	1.50
20	Z	1524	PGV	O03-C19	3.12	1.42	1.33
18	N	515	HEA	C1A-NA	3.17	1.41	1.36
25	C	265	PEK	C03-C02	3.18	1.59	1.50
18	N	515	HEA	C4B-NB	3.19	1.41	1.36
26	G	269	CDL	CB6-CB4	3.20	1.59	1.50
19	N	1522	TGL	CG1-CG2	3.20	1.59	1.50
19	L	522	TGL	CG1-CG2	3.26	1.59	1.50
25	G	1263	PEK	O03-C21	3.40	1.43	1.33
24	P	1272	DMU	C6-C1	3.49	1.63	1.52
20	C	268	PGV	O01-C1	3.49	1.44	1.34
20	P	1268	PGV	O01-C1	3.51	1.44	1.34
18	N	516	HEA	C4A-NA	3.52	1.41	1.36
20	A	604	PGV	C12-C11	3.61	1.52	1.31
25	P	1264	PEK	C9-C8	3.76	1.53	1.31
20	A	524	PGV	O03-C19	3.80	1.44	1.33
25	C	264	PEK	C9-C8	3.85	1.53	1.31
26	T	1269	CDL	CB6-CB4	3.87	1.61	1.50
18	A	516	HEA	C1D-ND	3.88	1.41	1.36
25	C	265	PEK	C6-C5	3.94	1.54	1.31
22	B	230	PSC	C13-C12	3.95	1.54	1.31
20	N	1266	PGV	C12-C11	3.96	1.54	1.31
19	N	1522	TGL	OG1-CA1	4.02	1.45	1.33
20	A	524	PGV	C12-C11	4.03	1.55	1.31
22	O	1230	PSC	C13-C12	4.03	1.55	1.31
25	P	1265	PEK	C6-C5	4.04	1.55	1.31
25	C	264	PEK	C6-C5	4.12	1.55	1.31
25	P	1265	PEK	C15-C14	4.13	1.55	1.31
22	B	230	PSC	C10-C9	4.14	1.55	1.31
25	P	1264	PEK	C6-C5	4.14	1.55	1.31
25	P	1265	PEK	C9-C8	4.17	1.55	1.31
25	G	1263	PEK	C03-C02	4.18	1.62	1.50
22	O	1230	PSC	C10-C9	4.18	1.55	1.31
20	Z	1524	PGV	C12-C11	4.19	1.55	1.31
25	T	263	PEK	C9-C8	4.23	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	1263	PEK	C15-C14	4.24	1.56	1.31
23	J	60	CHD	C13-C17	4.24	1.63	1.55
25	C	265	PEK	C9-C8	4.25	1.56	1.31
25	T	263	PEK	C15-C14	4.26	1.56	1.31
25	G	1263	PEK	C01-C02	4.31	1.62	1.50
25	G	1263	PEK	C9-C8	4.31	1.56	1.31
25	T	263	PEK	O03-C21	4.32	1.46	1.33
25	T	263	PEK	C01-C02	4.33	1.63	1.50
25	C	265	PEK	C15-C14	4.35	1.56	1.31
25	C	265	PEK	C12-C11	4.36	1.56	1.31
25	P	1265	PEK	C12-C11	4.37	1.57	1.31
18	N	516	HEA	C1D-ND	4.39	1.42	1.36
25	T	263	PEK	C03-C02	4.47	1.63	1.50
25	C	264	PEK	C12-C11	4.53	1.57	1.31
25	T	263	PEK	C6-C5	4.54	1.57	1.31
25	G	1263	PEK	C6-C5	4.56	1.58	1.31
19	L	522	TGL	OG2-CB1	4.63	1.48	1.34
18	A	515	HEA	C4B-NB	4.68	1.43	1.36
25	P	1264	PEK	C12-C11	4.70	1.58	1.31
20	P	1268	PGV	C12-C11	4.73	1.59	1.31
20	C	268	PGV	C12-C11	4.73	1.59	1.31
25	G	1263	PEK	C12-C11	4.80	1.59	1.31
25	T	263	PEK	C12-C11	4.81	1.59	1.31
25	C	264	PEK	C15-C14	4.84	1.59	1.31
23	W	1060	CHD	C13-C17	4.89	1.64	1.55
25	P	1264	PEK	C15-C14	4.97	1.60	1.31
19	N	1522	TGL	OG2-CB1	5.44	1.50	1.34

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1271	CHD	C17-C13-C12	-9.60	109.17	117.68
23	C	271	CHD	C17-C13-C12	-9.13	109.59	117.68
23	C	271	CHD	C19-C10-C9	-7.82	99.45	111.18
23	P	1271	CHD	C19-C10-C9	-7.67	99.68	111.18
23	C	525	CHD	C14-C13-C12	-5.81	102.19	107.39
19	A	521	TGL	CG1-OG1-CA1	-5.76	100.75	116.85
19	N	1521	TGL	CG1-OG1-CA1	-5.63	101.09	116.85
23	W	1060	CHD	C15-C14-C8	-5.32	110.59	118.32
23	J	60	CHD	C15-C14-C8	-5.25	110.69	118.32
23	P	1271	CHD	C15-C14-C8	-5.06	110.97	118.32
23	C	271	CHD	C15-C14-C8	-4.88	111.22	118.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	1522	TGL	CB9-CB8-CB7	-4.81	89.71	114.53
19	L	522	TGL	C12-C11-C10	-4.70	90.24	114.53
19	N	1522	TGL	C12-C11-C10	-4.68	90.38	114.53
23	C	271	CHD	C19-C10-C1	-4.63	100.42	108.20
23	W	1060	CHD	C18-C13-C14	-4.54	104.05	111.22
19	L	522	TGL	CB9-CB8-CB7	-4.53	91.15	114.53
23	O	229	CHD	C16-C17-C13	-4.45	99.17	103.60
23	P	1525	CHD	C14-C13-C12	-4.41	103.44	107.39
23	J	60	CHD	C18-C13-C14	-4.30	104.44	111.22
23	P	1271	CHD	C19-C10-C1	-4.22	101.10	108.20
19	Q	1523	TGL	CG1-OG1-CA1	-4.14	105.28	116.85
24	Z	1526	DMU	C8-C7-C5	-4.13	103.09	110.79
24	C	272	DMU	C2-C3-C4	-4.06	101.65	110.84
23	O	229	CHD	C19-C10-C1	-4.03	101.43	108.20
19	D	523	TGL	CG1-OG1-CA1	-4.03	105.59	116.85
18	A	515	HEA	C27-C19-C18	-3.98	115.68	123.50
26	P	1270	CDL	CB6-OB8-CB7	-3.98	105.72	116.85
24	M	526	DMU	C8-C7-C5	-3.89	103.53	110.79
23	B	1086	CHD	C16-C17-C13	-3.89	99.73	103.60
18	A	515	HEA	CAD-C3D-C4D	-3.88	122.79	127.01
22	O	1230	PSC	C01-O03-C19	-3.76	106.32	116.85
22	B	230	PSC	C01-O03-C19	-3.73	106.42	116.85
18	N	515	HEA	C27-C19-C18	-3.71	116.22	123.50
26	C	270	CDL	CB6-OB8-CB7	-3.61	106.75	116.85
23	B	1086	CHD	C15-C14-C13	-3.60	100.02	103.60
23	O	229	CHD	C15-C14-C13	-3.54	100.08	103.60
23	B	1086	CHD	C15-C14-C8	-3.53	113.19	118.32
18	N	516	HEA	CAA-C2A-C1A	-3.52	123.19	127.01
23	W	1060	CHD	C18-C13-C12	-3.43	105.74	109.09
23	O	229	CHD	C15-C14-C8	-3.43	113.33	118.32
18	N	515	HEA	CAD-C3D-C4D	-3.38	123.34	127.01
23	P	1525	CHD	C15-C14-C8	-3.35	113.45	118.32
18	A	515	HEA	CMB-C2B-C1B	-3.35	122.82	128.36
23	C	525	CHD	C15-C14-C8	-3.25	113.59	118.32
18	N	515	HEA	CMB-C2B-C1B	-3.21	123.06	128.36
23	B	1086	CHD	C19-C10-C1	-3.19	102.83	108.20
18	A	516	HEA	CMC-C2C-C1C	-3.18	123.10	128.36
20	N	1266	PGV	C01-O03-C19	-3.06	108.30	116.85
26	P	1270	CDL	OB6-CB5-C51	-2.98	105.05	111.53
18	N	515	HEA	C17-C18-C19	-2.92	121.42	127.76
25	C	264	PEK	O03-C21-C22	-2.81	103.32	111.90
20	C	267	PGV	C9-C10-C11	-2.81	97.69	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	P	1264	PEK	C3-C2-C1	-2.80	102.59	113.59
23	O	229	CHD	C14-C13-C12	-2.79	104.89	107.39
25	C	264	PEK	C3-C2-C1	-2.78	102.67	113.59
20	P	1267	PGV	C9-C10-C11	-2.77	97.93	112.45
18	A	515	HEA	CMC-C2C-C1C	-2.76	123.79	128.36
26	C	270	CDL	OB6-CB5-C51	-2.70	105.66	111.53
23	P	1525	CHD	C6-C5-C4	-2.69	108.04	111.05
23	C	525	CHD	C14-C8-C9	-2.68	105.94	109.62
23	O	229	CHD	O3-C3-C4	-2.67	104.56	109.86
20	C	267	PGV	O01-C1-C2	-2.66	105.75	111.53
25	P	1264	PEK	C01-O03-C21	-2.65	109.44	116.85
18	A	515	HEA	C17-C18-C19	-2.63	122.03	127.76
20	C	268	PGV	C02-O01-C1	-2.62	111.61	117.89
18	N	516	HEA	CMC-C2C-C1C	-2.61	124.05	128.36
23	P	1525	CHD	C19-C10-C9	-2.58	107.31	111.18
20	P	1268	PGV	C02-O01-C1	-2.55	111.77	117.89
23	J	60	CHD	C18-C13-C12	-2.48	106.67	109.09
19	A	521	TGL	CA3-CA2-CA1	-2.46	103.92	113.59
23	C	525	CHD	C19-C10-C9	-2.44	107.53	111.18
18	N	515	HEA	C13-C14-C15	-2.43	122.48	127.76
19	A	521	TGL	CA8-CA7-CA6	-2.42	102.03	114.53
25	C	264	PEK	O01-C1-C2	-2.41	106.29	111.53
23	B	1086	CHD	C14-C13-C12	-2.39	105.25	107.39
19	N	1521	TGL	CB7-CB6-CB5	-2.38	102.23	114.53
25	P	1264	PEK	O03-C21-C22	-2.37	104.69	111.90
19	A	521	TGL	CB7-CB6-CB5	-2.34	102.44	114.53
26	T	1269	CDL	OB8-CB7-C71	-2.32	104.84	111.90
19	N	1521	TGL	CA8-CA7-CA6	-2.28	102.75	114.53
24	P	1272	DMU	C2-C3-C4	-2.27	105.71	110.84
20	A	524	PGV	C3-C2-C1	-2.26	104.72	113.59
20	P	1268	PGV	C01-O03-C19	-2.24	110.58	116.85
19	A	521	TGL	CA6-CA5-CA4	-2.23	102.99	114.53
19	N	1521	TGL	CA6-CA5-CA4	-2.23	103.03	114.53
19	N	1521	TGL	CA3-CA2-CA1	-2.23	104.85	113.59
23	W	1060	CHD	C19-C10-C1	-2.22	104.46	108.20
20	Z	1524	PGV	C3-C2-C1	-2.22	104.85	113.59
26	C	270	CDL	C52-C51-CB5	-2.22	104.86	113.59
18	N	515	HEA	CMC-C2C-C1C	-2.21	124.70	128.36
23	P	1525	CHD	C14-C8-C9	-2.19	106.60	109.62
23	J	60	CHD	C19-C10-C9	-2.19	107.90	111.18
23	B	1086	CHD	O3-C3-C4	-2.18	105.52	109.86
23	C	271	CHD	C18-C13-C12	-2.17	106.97	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C17-C13-C12	-2.16	115.76	117.68
18	A	515	HEA	C13-C14-C15	-2.16	123.06	127.76
18	N	515	HEA	C21-C20-C19	-2.16	105.69	112.71
25	P	1264	PEK	O01-C1-C2	-2.13	106.89	111.53
20	A	604	PGV	O01-C1-C2	-2.13	106.90	111.53
23	J	60	CHD	C19-C10-C1	-2.13	104.62	108.20
26	G	269	CDL	OB8-CB7-C71	-2.13	105.42	111.90
23	C	271	CHD	C18-C13-C14	-2.12	107.87	111.22
18	A	515	HEA	C26-C15-C14	-2.12	119.35	123.50
19	A	521	TGL	CB9-CB8-CB7	-2.11	103.62	114.53
20	P	1267	PGV	O01-C1-C2	-2.11	106.94	111.53
19	Q	1523	TGL	CA3-CA2-CA1	-2.11	105.31	113.59
23	C	525	CHD	C9-C10-C5	-2.10	105.57	108.67
18	N	516	HEA	CAD-C3D-C4D	-2.09	124.74	127.01
20	C	268	PGV	C01-O03-C19	-2.08	111.03	116.85
23	O	229	CHD	C14-C8-C9	-2.08	106.76	109.62
18	A	515	HEA	C21-C20-C19	-2.08	105.95	112.71
19	D	523	TGL	CC3-CC2-CC1	-2.06	105.48	113.59
20	A	524	PGV	O01-C1-C2	-2.06	107.04	111.53
22	O	1230	PSC	O01-C1-C2	-2.06	107.05	111.53
20	A	604	PGV	C01-O03-C19	-2.06	111.09	116.85
19	N	1521	TGL	C12-C11-C10	-2.05	103.93	114.53
18	A	516	HEA	CAA-C2A-C1A	-2.04	124.79	127.01
23	P	1271	CHD	C18-C13-C14	-2.04	108.00	111.22
19	A	521	TGL	C12-C11-C10	-2.04	104.02	114.53
19	N	1522	TGL	CA8-CA7-CA6	-2.02	104.11	114.53
23	W	1060	CHD	C19-C10-C5	-2.02	106.69	110.25
24	P	1272	DMU	O55-C2-C1	2.00	114.84	110.34
23	C	525	CHD	C6-C5-C10	2.00	114.86	112.66
26	P	1270	CDL	OA8-CA6-CA4	2.01	114.09	108.69
23	P	1271	CHD	C9-C10-C5	2.01	111.65	108.67
18	N	515	HEA	C3C-C4C-NC	2.02	111.82	109.21
23	C	525	CHD	C9-C11-C12	2.03	116.92	114.36
26	C	270	CDL	OA8-CA6-CA4	2.04	114.18	108.69
18	A	516	HEA	C3C-C4C-NC	2.04	111.85	109.21
19	Q	1523	TGL	OG2-CG2-CG1	2.05	115.59	108.36
19	L	522	TGL	C10-CB9-CB8	2.05	125.12	114.53
18	N	515	HEA	C20-C19-C18	2.06	124.95	121.05
19	N	1522	TGL	OG1-CG1-CG2	2.06	114.24	108.69
19	L	522	TGL	OG2-CG2-CG3	2.06	115.63	108.36
23	P	1525	CHD	C5-C4-C3	2.07	115.99	112.91
25	P	1265	PEK	C2-C3-C4	2.07	117.43	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	269	CDL	C80-C79-C78	2.09	125.31	114.53
26	G	269	CDL	C83-C82-C81	2.10	125.36	114.53
25	C	265	PEK	C2-C3-C4	2.10	117.49	113.30
19	N	1522	TGL	C10-CB9-CB8	2.13	125.53	114.53
25	G	1263	PEK	P-O12-C04	2.13	133.67	121.50
26	T	1269	CDL	OB8-CB6-CB4	2.14	114.44	108.69
20	A	604	PGV	O03-C01-C02	2.14	114.45	108.69
25	T	263	PEK	P-O12-C04	2.14	133.72	121.50
18	N	515	HEA	C16-C17-C18	2.14	117.30	111.69
18	N	515	HEA	CMD-C2D-C3D	2.15	129.72	125.24
23	C	525	CHD	C18-C13-C12	2.15	111.19	109.09
23	P	1525	CHD	C6-C5-C10	2.16	115.03	112.66
19	L	522	TGL	CC7-CC6-CC5	2.17	125.71	114.53
20	P	1268	PGV	O03-C01-C02	2.18	114.55	108.69
26	T	1269	CDL	C20-C19-C18	2.19	125.85	114.53
26	G	269	CDL	C19-C18-C17	2.20	125.91	114.53
18	A	515	HEA	C20-C19-C18	2.21	125.23	121.05
25	P	1265	PEK	O03-C01-C02	2.21	114.64	108.69
18	N	516	HEA	C20-C21-C22	2.22	117.49	111.69
19	L	522	TGL	CC4-CC3-CC2	2.23	121.45	113.29
18	N	515	HEA	C27-C19-C20	2.23	118.82	115.41
26	T	1269	CDL	C83-C82-C81	2.24	126.11	114.53
26	T	1269	CDL	C19-C18-C17	2.25	126.16	114.53
23	J	60	CHD	C9-C11-C12	2.25	117.21	114.36
26	P	1270	CDL	OB6-CB5-OB7	2.26	129.74	123.67
19	N	1521	TGL	OG1-CG1-CG2	2.28	114.83	108.69
25	P	1265	PEK	C24-C23-C22	2.29	121.68	113.29
25	T	263	PEK	C14-C13-C12	2.30	119.66	112.00
23	P	1271	CHD	C1-C2-C3	2.31	114.17	110.43
19	N	1521	TGL	OG2-CG2-CG3	2.31	116.50	108.36
25	P	1264	PEK	O03-C21-O04	2.33	129.50	123.49
25	C	264	PEK	O03-C21-O04	2.35	129.55	123.49
23	O	229	CHD	C1-C2-C3	2.36	114.27	110.43
23	C	525	CHD	C5-C4-C3	2.37	116.44	112.91
23	C	271	CHD	C9-C10-C5	2.38	112.19	108.67
23	C	271	CHD	C9-C11-C12	2.38	117.36	114.36
24	M	526	DMU	C10-O1-C9	2.38	118.37	113.75
19	N	1522	TGL	C20-CA9-CA8	2.39	126.88	114.53
19	N	1522	TGL	CC4-CC3-CC2	2.39	122.06	113.29
19	A	521	TGL	OG2-CG2-CG3	2.39	116.79	108.36
25	C	265	PEK	O03-C01-C02	2.40	115.14	108.69
23	W	1060	CHD	C1-C2-C3	2.40	114.33	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	515	HEA	C27-C19-C20	2.40	119.07	115.41
23	P	1271	CHD	C9-C11-C12	2.41	117.40	114.36
18	A	515	HEA	C16-C15-C14	2.42	125.64	121.05
26	G	269	CDL	C20-C19-C18	2.42	127.04	114.53
18	A	516	HEA	CBD-CAD-C3D	2.45	116.91	112.53
23	C	525	CHD	C1-C10-C5	2.45	111.83	107.81
19	L	522	TGL	OG1-CG1-CG2	2.46	115.31	108.69
20	Z	1524	PGV	C02-O01-C1	2.46	123.80	117.89
20	N	1266	PGV	O03-C01-C02	2.47	115.33	108.69
23	B	1086	CHD	C10-C9-C8	2.48	114.60	111.88
23	C	271	CHD	C2-C1-C10	2.48	117.27	112.84
23	O	229	CHD	C1-C10-C5	2.49	111.89	107.81
18	A	515	HEA	C16-C17-C18	2.49	118.20	111.69
25	C	265	PEK	P-O12-C04	2.50	135.75	121.50
25	P	1265	PEK	P-O12-C04	2.50	135.77	121.50
25	T	263	PEK	C11-C10-C9	2.50	120.33	112.00
18	N	515	HEA	C16-C15-C14	2.51	125.82	121.05
19	L	522	TGL	C20-CA9-CA8	2.52	127.54	114.53
25	C	265	PEK	C24-C23-C22	2.52	122.53	113.29
25	G	1263	PEK	C11-C10-C9	2.52	120.40	112.00
23	J	60	CHD	C4-C5-C10	2.53	115.44	112.66
23	P	1271	CHD	C6-C5-C10	2.54	115.46	112.66
23	C	271	CHD	C1-C2-C3	2.56	114.59	110.43
19	L	522	TGL	C13-C12-C11	2.57	127.81	114.53
26	G	269	CDL	C22-C21-C20	2.60	127.95	114.53
25	G	1263	PEK	C14-C13-C12	2.61	120.67	112.00
18	A	515	HEA	CMC-C2C-C3C	2.61	130.19	125.09
26	T	1269	CDL	C22-C21-C20	2.62	128.04	114.53
23	C	271	CHD	C5-C4-C3	2.62	116.81	112.91
19	D	523	TGL	OG2-CG2-CG1	2.63	117.63	108.36
26	G	269	CDL	C23-C22-C21	2.63	128.13	114.53
19	A	521	TGL	OG1-CG1-CG2	2.63	115.78	108.69
23	P	1271	CHD	C16-C15-C14	2.64	110.44	105.12
19	N	1522	TGL	C13-C12-C11	2.65	128.23	114.53
23	C	271	CHD	C16-C15-C14	2.67	110.50	105.12
20	A	524	PGV	O01-C02-C03	2.67	117.78	108.36
23	B	1086	CHD	C1-C10-C5	2.70	112.24	107.81
23	O	229	CHD	C17-C13-C14	2.71	102.79	100.05
18	N	516	HEA	C26-C15-C16	2.72	119.55	115.41
18	N	516	HEA	C4B-C3B-C11	2.73	129.97	127.01
23	B	1086	CHD	C17-C13-C14	2.74	102.82	100.05
23	J	60	CHD	C1-C2-C3	2.75	114.90	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	1521	TGL	CG3-CG2-CG1	2.76	118.52	112.07
23	P	1271	CHD	C2-C1-C10	2.77	117.78	112.84
19	Q	1523	TGL	CB3-CB2-CB1	2.79	124.55	113.59
18	N	516	HEA	C3C-C4C-NC	2.79	112.82	109.21
26	T	1269	CDL	C23-C22-C21	2.81	129.05	114.53
24	C	272	DMU	C7-C8-C9	2.81	115.10	110.20
18	N	515	HEA	C4B-C3B-C11	2.82	130.07	127.01
18	A	516	HEA	CMC-C2C-C3C	2.82	130.60	125.09
23	C	271	CHD	C6-C5-C10	2.83	115.78	112.66
24	Z	1526	DMU	C10-O7-C3	2.83	125.41	118.01
24	C	272	DMU	O1-C10-C5	2.83	116.09	110.28
23	W	1060	CHD	C15-C16-C17	2.84	110.84	105.12
23	C	271	CHD	C15-C16-C17	2.85	110.87	105.12
23	O	229	CHD	C9-C11-C12	2.85	117.97	114.36
23	B	1086	CHD	C1-C2-C3	2.87	115.10	110.43
19	Q	1523	TGL	OG1-CG1-CG2	2.88	116.44	108.69
23	C	271	CHD	C1-C10-C9	2.89	116.10	111.45
19	A	521	TGL	CG3-CG2-CG1	2.90	118.85	112.07
23	P	1271	CHD	C15-C16-C17	2.91	110.98	105.12
23	W	1060	CHD	C6-C5-C4	2.91	114.30	111.05
24	C	272	DMU	C8-C7-C5	2.92	116.23	110.79
20	Z	1524	PGV	O01-C02-C03	2.92	118.66	108.36
23	J	60	CHD	C15-C16-C17	2.95	111.06	105.12
23	W	1060	CHD	C9-C11-C12	2.99	118.14	114.36
23	C	271	CHD	C5-C6-C7	3.00	117.78	114.44
25	T	263	PEK	C02-O01-C1	3.03	125.17	117.89
19	D	523	TGL	OG2-CG2-CG3	3.04	119.06	108.36
23	J	60	CHD	C16-C15-C14	3.06	111.28	105.12
20	A	524	PGV	C02-O01-C1	3.07	125.26	117.89
19	D	523	TGL	CB3-CB2-CB1	3.10	125.78	113.59
18	A	516	HEA	C27-C19-C20	3.10	120.15	115.41
24	M	526	DMU	O7-C10-O1	3.11	118.56	110.68
23	O	229	CHD	C5-C6-C7	3.14	117.94	114.44
19	N	1522	TGL	CC3-CC2-CC1	3.19	126.13	113.59
23	P	1271	CHD	C5-C4-C3	3.19	117.66	112.91
18	A	515	HEA	C4B-C3B-C11	3.19	130.47	127.01
23	P	1525	CHD	C1-C10-C5	3.19	113.06	107.81
25	G	1263	PEK	C02-O01-C1	3.20	125.57	117.89
23	W	1060	CHD	C14-C8-C9	3.21	114.03	109.62
23	C	271	CHD	C14-C8-C7	3.25	116.24	111.74
23	P	1271	CHD	C1-C10-C9	3.26	116.71	111.45
23	J	60	CHD	C14-C8-C7	3.29	116.31	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	60	CHD	C5-C4-C3	3.32	117.85	112.91
19	D	523	TGL	OG1-CG1-CG2	3.33	117.65	108.69
23	J	60	CHD	C14-C8-C9	3.33	114.20	109.62
23	W	1060	CHD	C16-C15-C14	3.34	111.85	105.12
19	N	1522	TGL	C11-C10-CB9	3.38	132.00	114.53
23	O	229	CHD	C5-C4-C3	3.39	117.95	112.91
19	Q	1523	TGL	OG2-CG2-CG3	3.39	120.31	108.36
24	P	1272	DMU	O7-C10-O1	3.39	119.27	110.68
18	N	516	HEA	C27-C19-C20	3.40	120.60	115.41
23	P	1525	CHD	C10-C9-C8	3.40	115.62	111.88
23	B	1086	CHD	C9-C11-C12	3.40	118.66	114.36
23	B	1086	CHD	C5-C4-C3	3.43	118.01	112.91
23	P	1271	CHD	C5-C6-C7	3.45	118.29	114.44
19	N	1522	TGL	CG2-OG2-CB1	3.46	126.19	117.89
19	L	522	TGL	C11-C10-CB9	3.47	132.47	114.53
23	P	1271	CHD	C14-C8-C7	3.49	116.58	111.74
19	A	521	TGL	CG3-OG3-CC1	3.49	126.61	116.85
23	W	1060	CHD	C5-C4-C3	3.55	118.19	112.91
23	J	60	CHD	C6-C5-C4	3.55	115.01	111.05
19	L	522	TGL	CC3-CC2-CC1	3.58	127.65	113.59
23	W	1060	CHD	C14-C8-C7	3.58	116.71	111.74
24	Z	1526	DMU	O7-C10-C5	3.61	116.89	108.10
24	Z	1526	DMU	O7-C10-O1	3.67	119.97	110.68
24	M	526	DMU	C10-O7-C3	3.73	127.75	118.01
19	L	522	TGL	CG2-OG2-CB1	3.74	126.87	117.89
19	N	1521	TGL	CG3-OG3-CC1	3.77	127.39	116.85
25	C	265	PEK	C11-C10-C9	3.78	124.57	112.00
24	M	526	DMU	O7-C3-C4	3.78	119.25	109.32
19	L	522	TGL	C16-C15-CC9	3.79	134.11	114.53
23	O	229	CHD	C10-C9-C8	3.81	116.06	111.88
19	N	1522	TGL	C16-C15-CC9	3.82	134.23	114.53
18	A	516	HEA	C4B-C3B-C11	3.84	131.18	127.01
25	P	1265	PEK	C11-C10-C9	3.85	124.82	112.00
23	J	60	CHD	C1-C10-C5	3.89	114.20	107.81
24	C	272	DMU	O7-C10-O1	3.90	120.56	110.68
19	N	1522	TGL	C15-CC9-CC8	3.93	134.84	114.53
19	L	522	TGL	C15-CC9-CC8	3.94	134.87	114.53
23	C	525	CHD	C5-C6-C7	3.97	118.86	114.44
23	J	60	CHD	C2-C1-C10	4.00	119.98	112.84
25	T	263	PEK	O03-C01-C02	4.04	119.56	108.69
23	W	1060	CHD	C2-C1-C10	4.07	120.11	112.84
23	C	525	CHD	C10-C9-C8	4.09	116.37	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Z	1526	DMU	O7-C3-C4	4.13	120.18	109.32
24	C	272	DMU	C10-O1-C9	4.17	121.84	113.75
23	J	60	CHD	C13-C14-C8	4.17	120.12	114.75
23	W	1060	CHD	C1-C10-C5	4.18	114.68	107.81
23	P	1271	CHD	C14-C13-C12	4.22	111.17	107.39
24	M	526	DMU	O7-C10-C5	4.23	118.39	108.10
24	P	1272	DMU	C10-O1-C9	4.23	121.95	113.75
23	C	271	CHD	C14-C13-C12	4.26	111.21	107.39
23	W	1060	CHD	C13-C14-C8	4.32	120.33	114.75
23	C	525	CHD	C13-C17-C20	4.36	124.81	119.50
25	G	1263	PEK	O03-C01-C02	4.38	120.47	108.69
24	P	1272	DMU	O1-C10-C5	4.40	119.31	110.28
24	C	272	DMU	O5-C6-C1	4.42	119.35	110.28
23	P	1525	CHD	C5-C6-C7	4.48	119.43	114.44
24	C	272	DMU	O5-C4-C57	4.50	117.72	106.36
23	W	1060	CHD	C11-C9-C10	4.51	118.48	113.79
19	D	523	TGL	CG2-OG2-CB1	4.52	128.72	117.89
23	W	1060	CHD	C9-C8-C7	4.53	117.27	111.92
19	Q	1523	TGL	CG3-OG3-CC1	4.53	129.52	116.85
19	D	523	TGL	CG3-OG3-CC1	4.58	129.65	116.85
23	J	60	CHD	C11-C9-C10	4.58	118.55	113.79
19	N	1521	TGL	CG2-OG2-CB1	4.62	128.97	117.89
24	Z	1526	DMU	O5-C6-C1	4.63	119.77	110.28
23	J	60	CHD	C9-C8-C7	4.65	117.41	111.92
23	P	1271	CHD	C4-C3-C2	4.74	116.56	110.52
24	M	526	DMU	O5-C6-C1	4.78	120.08	110.28
24	P	1272	DMU	O7-C3-C2	4.84	119.67	107.17
23	P	1525	CHD	C13-C17-C20	4.89	125.46	119.50
24	P	1272	DMU	C8-C7-C5	4.90	119.94	110.79
19	A	521	TGL	CG2-OG2-CB1	4.92	129.69	117.89
19	Q	1523	TGL	CG2-OG2-CB1	4.97	129.82	117.89
24	P	1272	DMU	O7-C10-C5	4.99	120.26	108.10
23	W	1060	CHD	C5-C6-C7	5.05	120.06	114.44
23	P	1271	CHD	C4-C5-C10	5.06	118.23	112.66
23	P	1271	CHD	C1-C10-C5	5.08	116.16	107.81
23	J	60	CHD	C5-C6-C7	5.09	120.11	114.44
23	C	271	CHD	C4-C3-C2	5.17	117.12	110.52
24	P	1272	DMU	O5-C6-C1	5.27	121.08	110.28
24	M	526	DMU	O5-C6-O16	5.27	122.75	110.05
23	C	271	CHD	C1-C10-C5	5.30	116.52	107.81
23	J	60	CHD	C4-C3-C2	5.31	117.30	110.52
24	C	272	DMU	O1-C9-C8	5.33	119.69	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	1060	CHD	C4-C3-C2	5.37	117.37	110.52
23	J	60	CHD	C6-C5-C10	5.39	118.59	112.66
24	P	1272	DMU	C18-O16-C6	5.50	123.56	113.94
24	C	272	DMU	C18-O16-C6	5.66	123.83	113.94
23	C	271	CHD	C4-C5-C10	5.67	118.90	112.66
24	M	526	DMU	C7-C8-C9	5.70	120.13	110.20
24	Z	1526	DMU	O5-C6-O16	5.72	123.82	110.05
23	P	1271	CHD	C9-C8-C7	5.89	118.88	111.92
24	P	1272	DMU	O5-C4-C57	5.90	121.27	106.36
24	Z	1526	DMU	C1-C2-C3	5.92	122.61	109.60
24	Z	1526	DMU	C7-C8-C9	5.96	120.58	110.20
24	P	1272	DMU	O1-C9-C8	5.97	120.89	109.68
24	C	272	DMU	O7-C10-C5	5.98	122.65	108.10
23	C	271	CHD	C9-C8-C7	6.02	119.03	111.92
24	M	526	DMU	C1-C2-C3	6.20	123.22	109.60
24	Z	1526	DMU	O16-C6-C1	6.24	115.92	108.04
24	Z	1526	DMU	O7-C3-C2	6.28	123.39	107.17
23	W	1060	CHD	C6-C5-C10	6.31	119.60	112.66
24	Z	1526	DMU	C18-O16-C6	6.47	125.25	113.94
24	M	526	DMU	C18-O16-C6	6.49	125.28	113.94
23	W	1060	CHD	C11-C12-C13	6.56	117.86	111.20
24	C	272	DMU	O7-C3-C2	6.72	124.51	107.17
24	M	526	DMU	O16-C6-C1	6.75	116.56	108.04
24	M	526	DMU	O7-C3-C2	6.75	124.60	107.17
24	Z	1526	DMU	O5-C4-C57	6.82	123.60	106.36
24	M	526	DMU	O5-C4-C3	6.83	124.17	109.75
24	Z	1526	DMU	O1-C9-C8	6.88	122.60	109.68
23	J	60	CHD	C10-C9-C8	6.92	119.47	111.88
24	C	272	DMU	O7-C3-C4	6.92	127.51	109.32
24	Z	1526	DMU	C10-C5-C7	7.07	123.90	109.97
24	M	526	DMU	O5-C4-C57	7.09	124.28	106.36
24	M	526	DMU	O1-C9-C8	7.12	123.05	109.68
23	J	60	CHD	C11-C12-C13	7.14	118.45	111.20
23	W	1060	CHD	C10-C9-C8	7.20	119.78	111.88
24	C	272	DMU	C6-O5-C4	7.20	127.72	113.75
24	M	526	DMU	O1-C9-C11	7.20	124.56	106.36
24	M	526	DMU	C10-C5-C7	7.21	124.17	109.97
24	Z	1526	DMU	O5-C4-C3	7.26	125.08	109.75
24	Z	1526	DMU	O1-C9-C11	7.26	124.71	106.36
24	P	1272	DMU	O5-C4-C3	7.36	125.30	109.75
24	Z	1526	DMU	C6-O5-C4	7.47	128.24	113.75
24	P	1272	DMU	C6-O5-C4	7.49	128.29	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	1272	DMU	O1-C9-C11	7.52	125.36	106.36
24	M	526	DMU	C6-O5-C4	7.75	128.79	113.75
24	P	1272	DMU	O7-C3-C4	7.78	129.77	109.32
24	C	272	DMU	O1-C9-C11	8.41	127.61	106.36
23	J	60	CHD	C13-C17-C20	8.64	130.02	119.50
23	C	271	CHD	C10-C9-C8	8.94	121.69	111.88
23	W	1060	CHD	C13-C17-C20	9.02	130.49	119.50
24	C	272	DMU	O5-C4-C3	9.16	129.09	109.75
23	J	60	CHD	C17-C13-C14	9.30	109.45	100.05
23	W	1060	CHD	C17-C13-C14	9.43	109.58	100.05
23	P	1271	CHD	C10-C9-C8	9.49	122.29	111.88
24	P	1272	DMU	C1-C2-C3	9.59	130.65	109.60
24	C	272	DMU	C1-C2-C3	9.75	131.01	109.60
23	C	271	CHD	C17-C13-C14	10.27	110.43	100.05
23	P	1271	CHD	C17-C13-C14	10.34	110.50	100.05
24	P	1272	DMU	O16-C6-C1	12.73	124.12	108.04
24	C	272	DMU	O16-C6-C1	14.23	126.01	108.04

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
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	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
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
23	P	1271	CHD	C12
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C9

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Mol	Chain	Res	Type	Atom
23	P	1271	CHD	C14
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	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	C9
24	M	526	DMU	C5
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
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	Z	1524	PGV	P-O11-C03-C02
20	A	524	PGV	P-O11-C03-C02

There are no ring outliers.

36 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	2	0
18	A	516	HEA	2	0
19	A	521	TGL	9	0
20	A	524	PGV	9	0
20	A	604	PGV	1	0
22	B	230	PSC	15	0
25	C	264	PEK	4	0
25	C	265	PEK	8	0
20	C	267	PGV	6	0
20	C	268	PGV	1	0
26	C	270	CDL	18	0
23	C	271	CHD	4	0
24	C	272	DMU	3	0
19	D	523	TGL	4	0
25	G	1263	PEK	7	0
26	G	269	CDL	18	0
23	J	60	CHD	2	0
19	L	522	TGL	24	0
24	M	526	DMU	1	0
20	N	1266	PGV	1	0
19	N	1521	TGL	8	0
19	N	1522	TGL	16	0
18	N	515	HEA	3	0
22	O	1230	PSC	15	0
25	P	1264	PEK	7	0
25	P	1265	PEK	9	0
20	P	1267	PGV	5	0
20	P	1268	PGV	1	0
26	P	1270	CDL	16	0
23	P	1271	CHD	2	0
24	P	1272	DMU	5	0
19	Q	1523	TGL	5	0
26	T	1269	CDL	22	0
25	T	263	PEK	9	0
23	W	1060	CHD	3	0
20	Z	1524	PGV	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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