Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:25 AM GMT

PDB ID	:	3AG4
Title	:	Bovine Heart Cytochrome c Oxidase in the Cyanide Ion-bound Fully Reduced State at 100 K
Authors	:	Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2010-03-19
Resolution	:	2.05 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 (1)) were used in the production of this report:

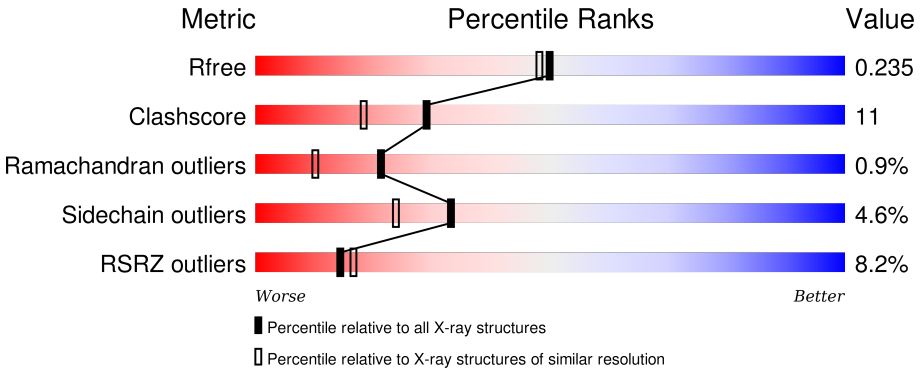
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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.

Mol	Chain	Length	Quality of chain
1	A	514	11% 76% 20%
1	N	514	6% 77% 20%
2	B	227	2% 74% 22%
2	O	227	3% 71% 26%
3	C	261	80% 16%

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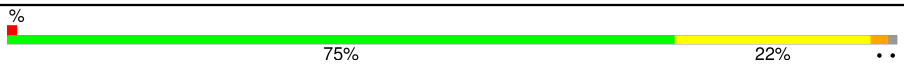
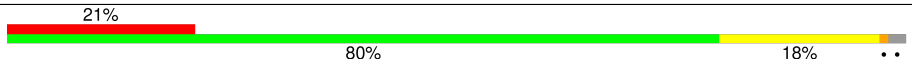
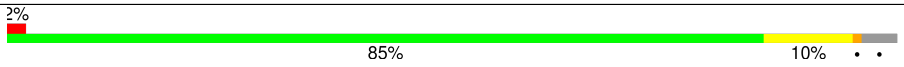
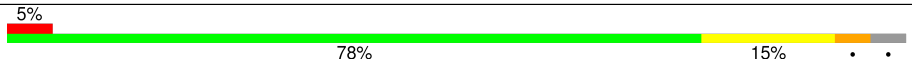
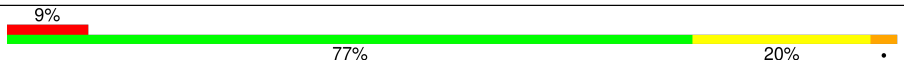
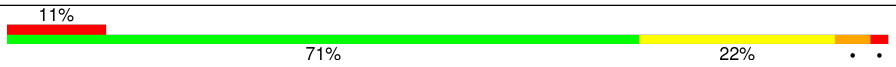
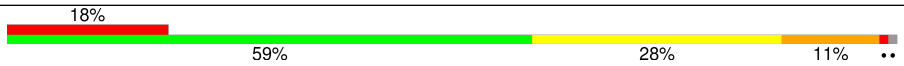
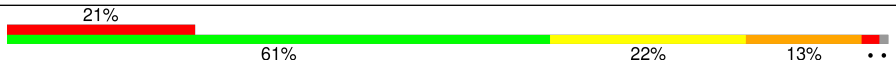
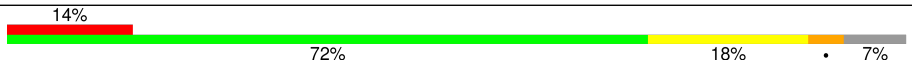
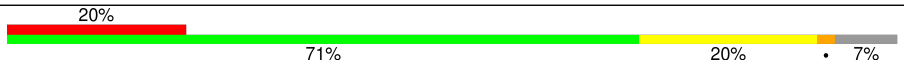
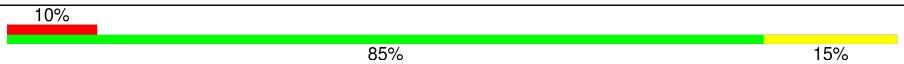
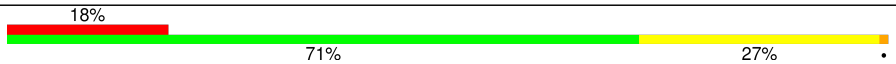
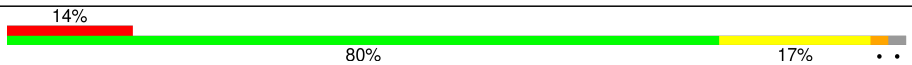
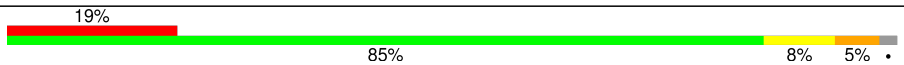
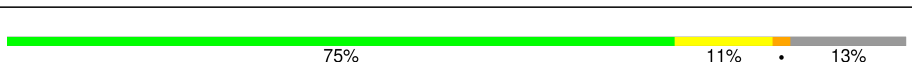
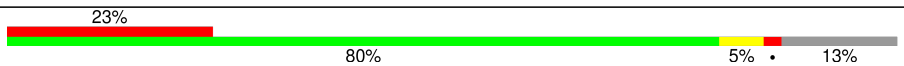
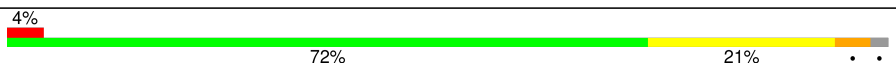
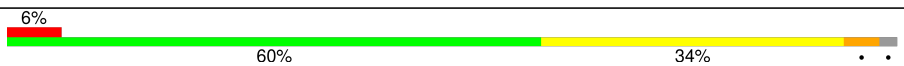
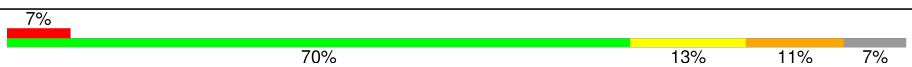
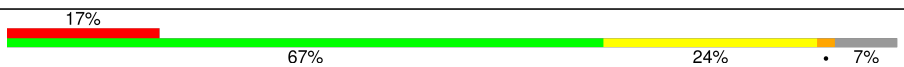
Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	515	X	-	-	-
14	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	-
14	HEA	N	516	X	-	-	-
15	CYN	N	520	-	-	X	-
19	TGL	A	521	-	-	-	X
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1521	-	-	-	X
19	TGL	N	1522	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	X
22	CHD	P	1271	X	-	-	-
22	CHD	W	1059	X	-	-	X
25	CDL	C	270	-	-	X	X
25	CDL	G	269	-	-	X	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
26	PSC	E	229	-	-	-	X
26	PSC	R	1229	-	-	-	X
28	DMU	G	272	X	-	-	X
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	X
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	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 subunit 5B.

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 subunit 6A2.

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 6B1.

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 subunit 6C.

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 7A1.

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 subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

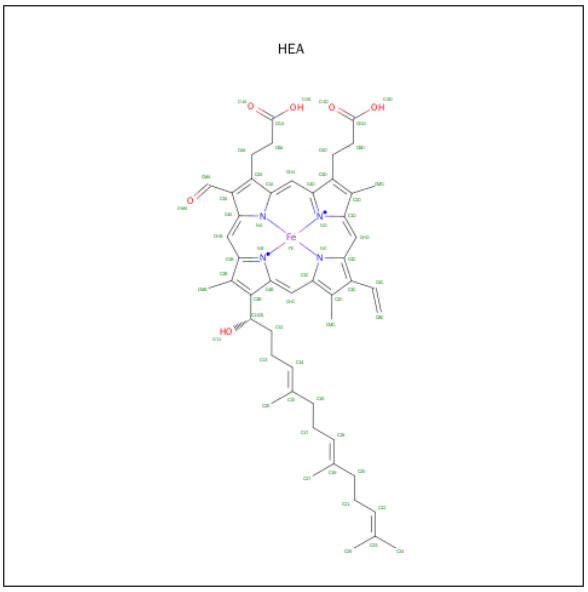
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

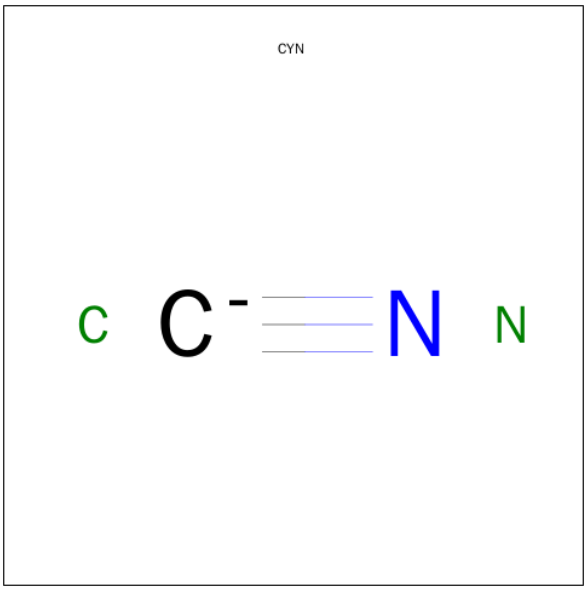
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 15 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

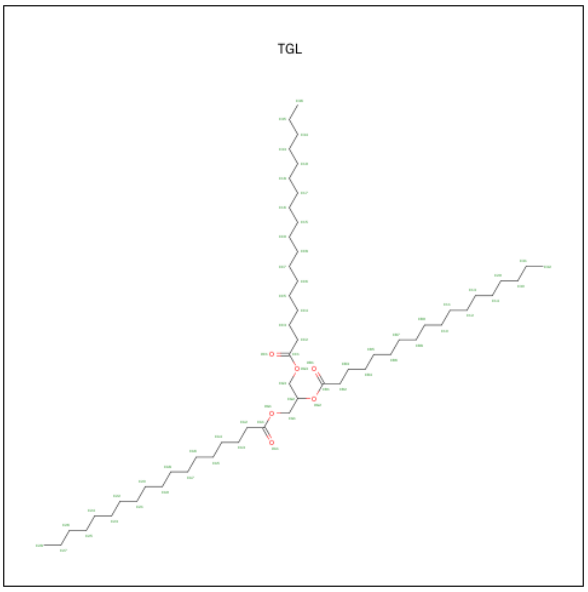
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

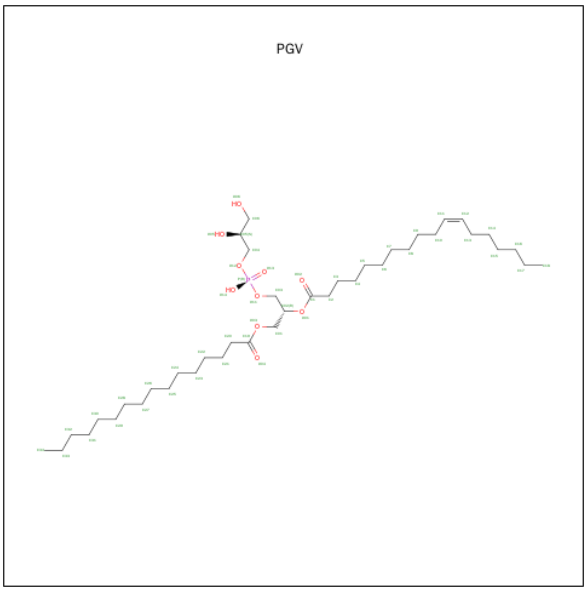
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



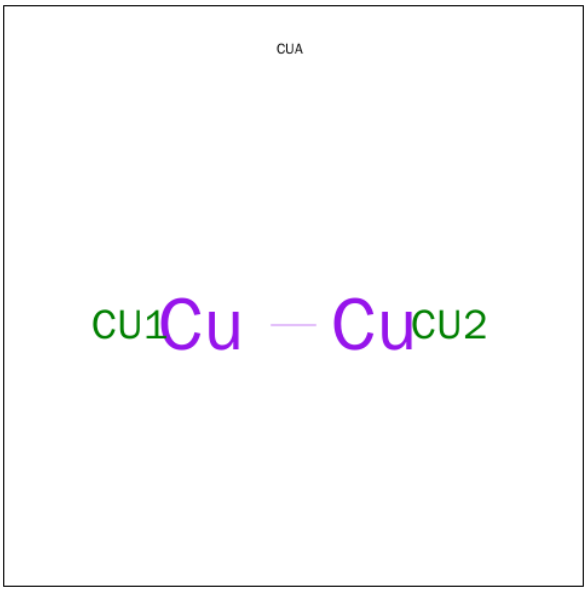
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0

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



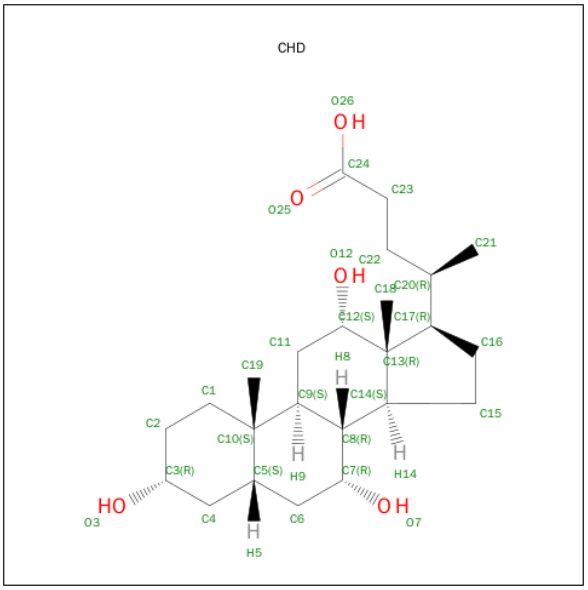
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

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



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

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



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

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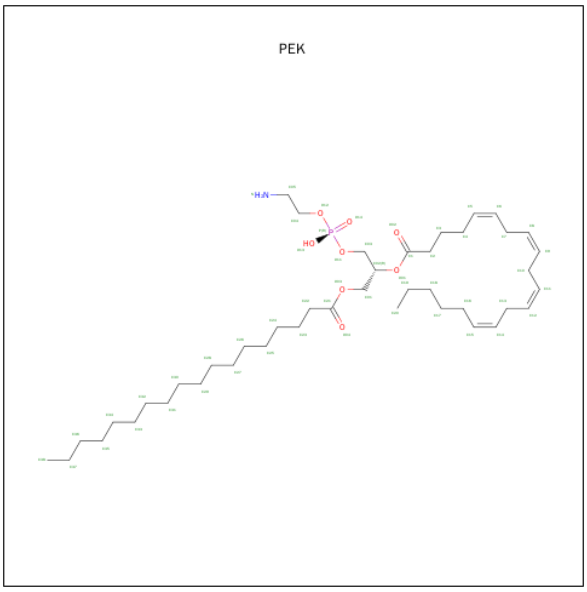
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

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

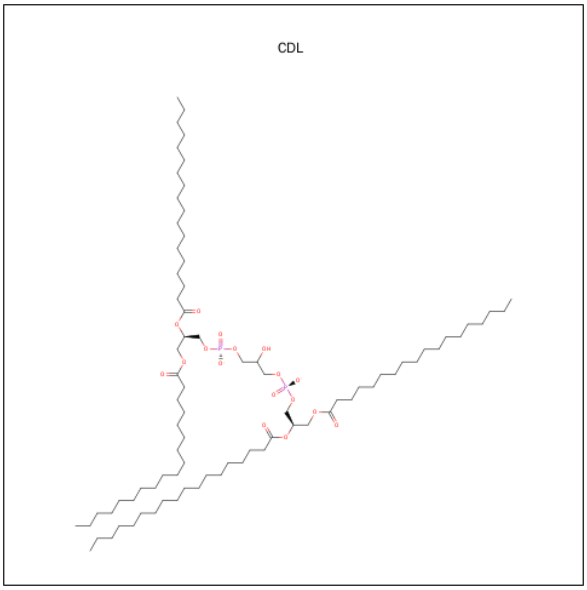
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



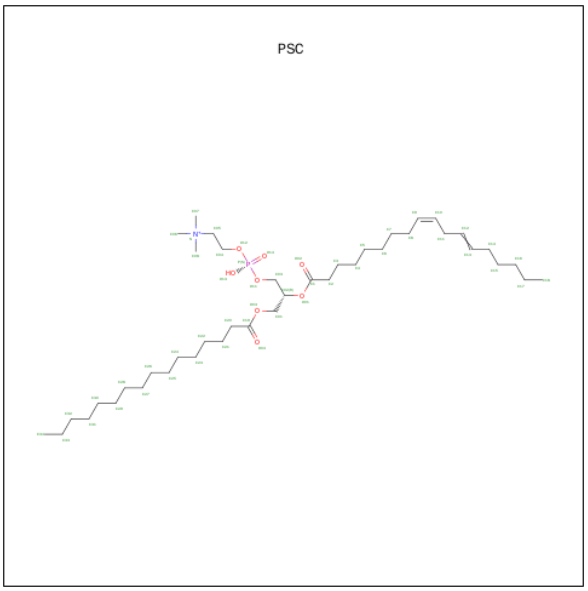
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

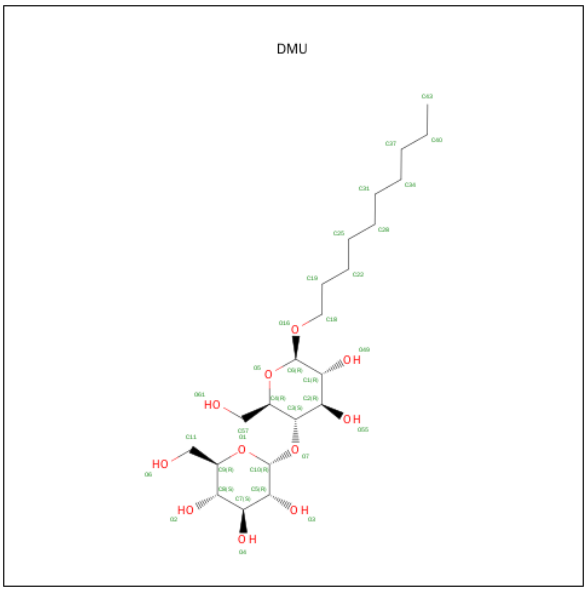


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	225	Total O 225 225	0	0
29	B	125	Total O 125 125	0	0
29	C	106	Total O 106 106	0	0
29	D	91	Total O 91 91	0	0
29	E	62	Total O 62 62	0	0
29	F	75	Total O 75 75	0	0
29	G	41	Total O 41 41	0	0
29	H	47	Total O 47 47	0	0

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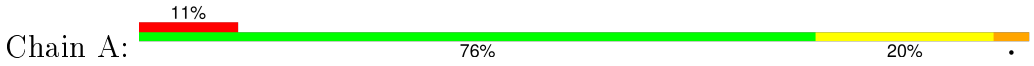
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	38	Total O 38 38	0	0
29	J	20	Total O 20 20	0	0
29	K	20	Total O 20 20	0	0
29	L	22	Total O 22 22	0	0
29	M	15	Total O 15 15	0	0
29	N	199	Total O 199 199	0	0
29	O	107	Total O 107 107	0	0
29	P	100	Total O 100 100	0	0
29	Q	55	Total O 55 55	0	0
29	R	40	Total O 40 40	0	0
29	S	56	Total O 56 56	0	0
29	T	36	Total O 36 36	0	0
29	U	41	Total O 41 41	0	0
29	V	18	Total O 18 18	0	0
29	W	12	Total O 12 12	0	0
29	X	14	Total O 14 14	0	0
29	Y	12	Total O 12 12	0	0
29	Z	11	Total O 11 11	0	0

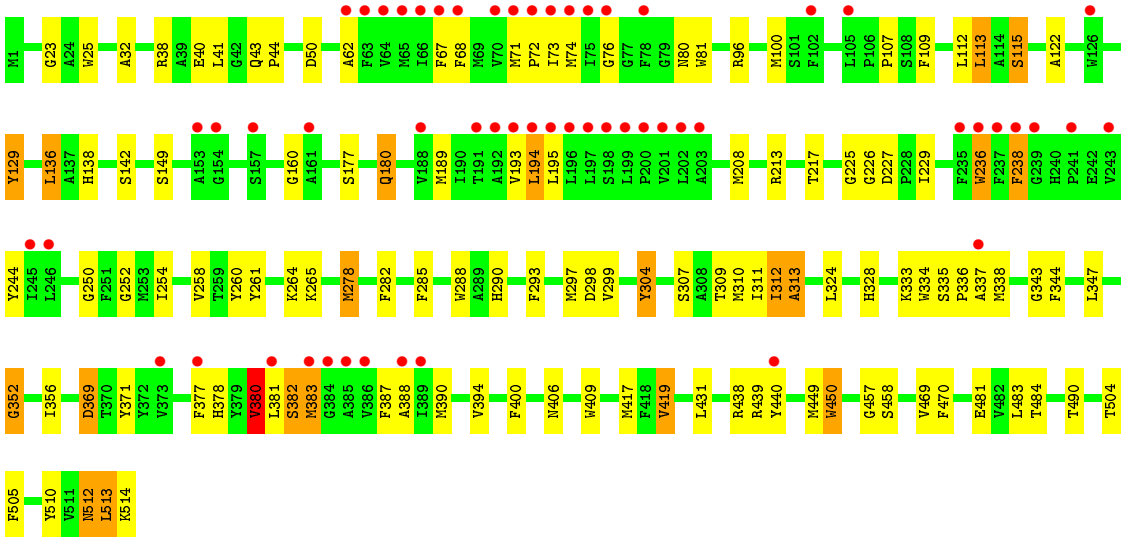
3 Residue-property plots (i)

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

- Molecule 1: Cytochrome c oxidase subunit 1

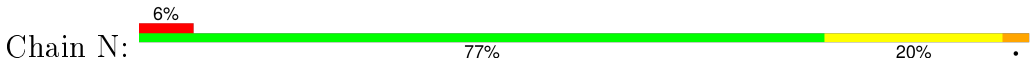
Chain A:

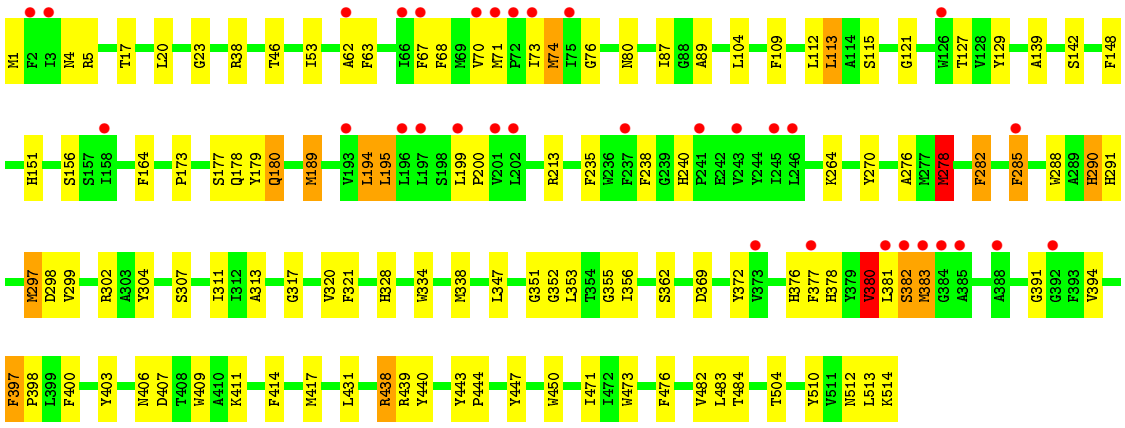




- Molecule 1: Cytochrome c oxidase subunit 1

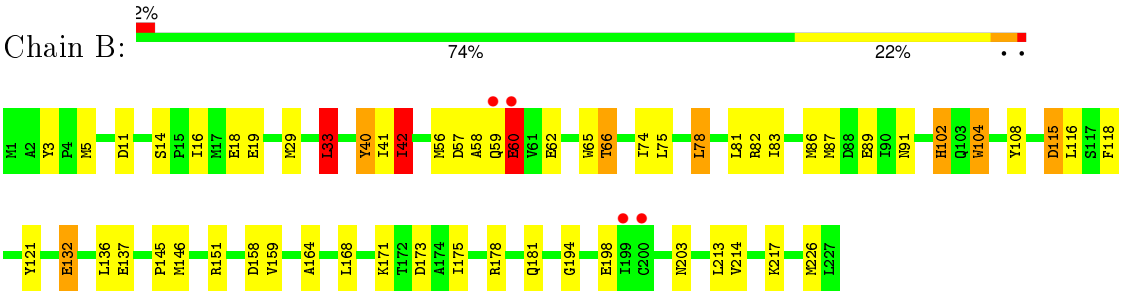
Chain N:





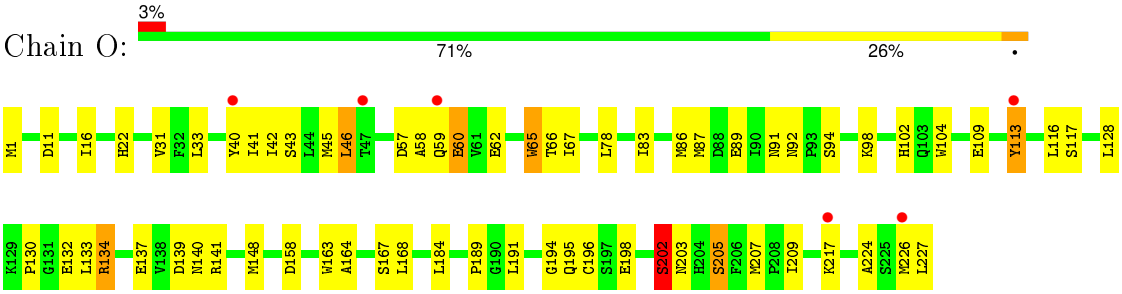
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



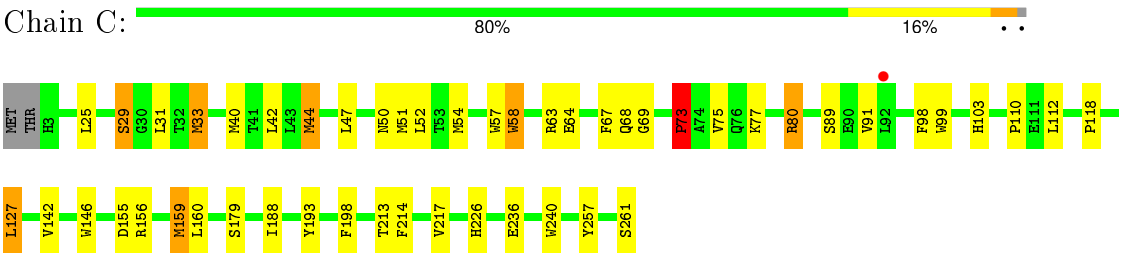
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



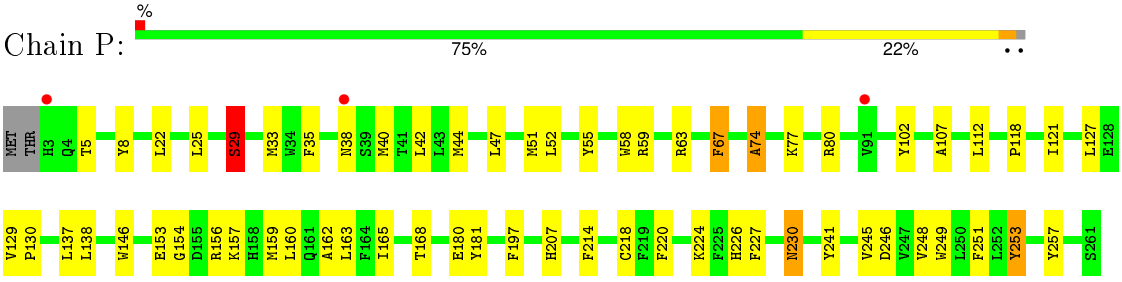
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



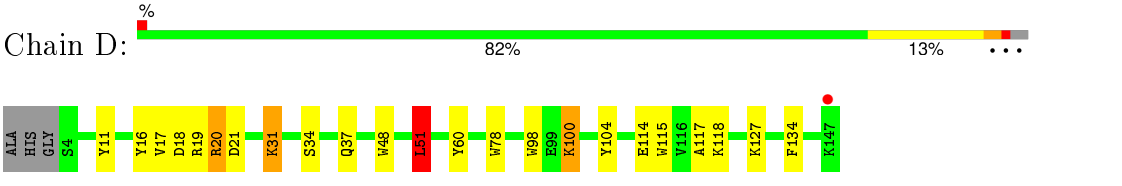
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



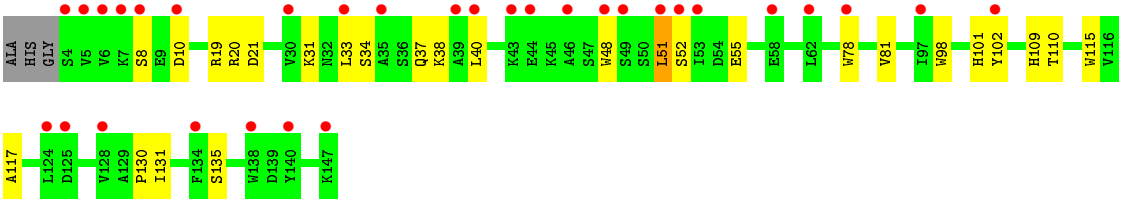
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:

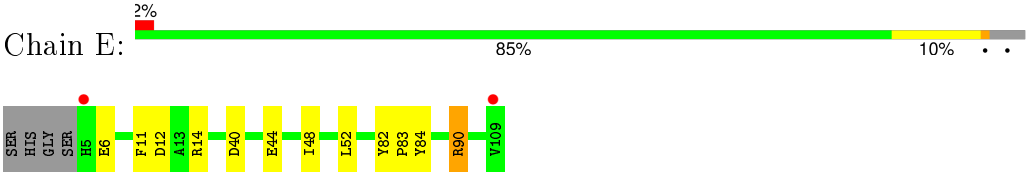


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

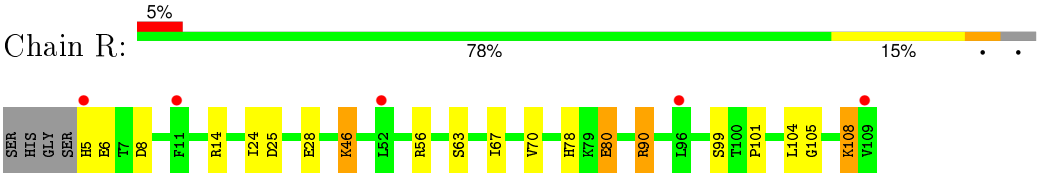
Chain Q:



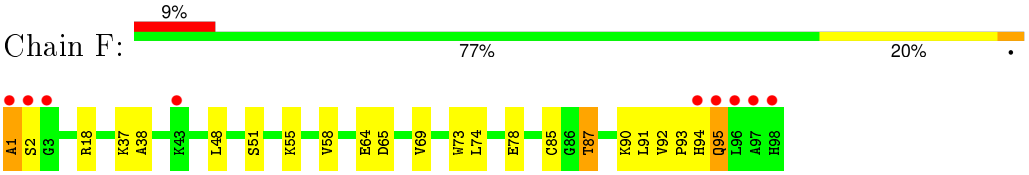
• Molecule 5: Cytochrome c oxidase subunit 5A



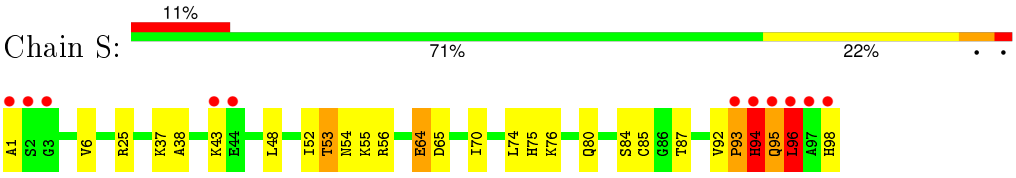
• Molecule 5: Cytochrome c oxidase subunit 5A



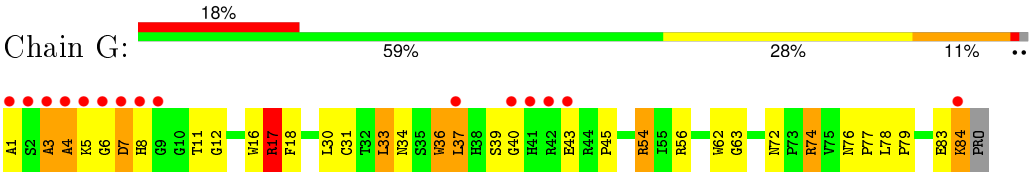
• Molecule 6: Cytochrome c oxidase subunit 5B



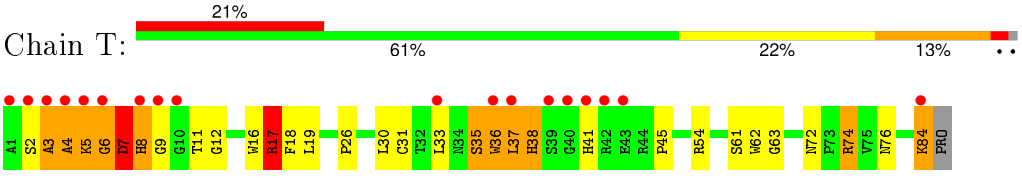
• Molecule 6: Cytochrome c oxidase subunit 5B



• Molecule 7: Cytochrome c oxidase subunit 6A2

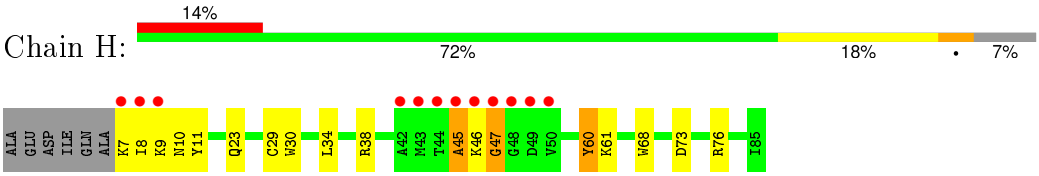


• Molecule 7: Cytochrome c oxidase subunit 6A2



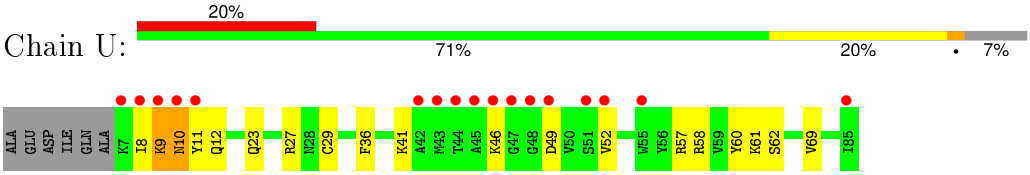
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



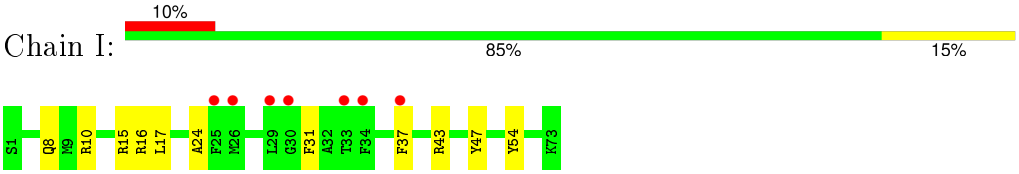
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



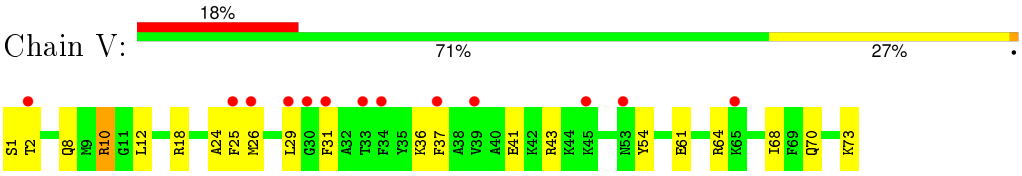
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



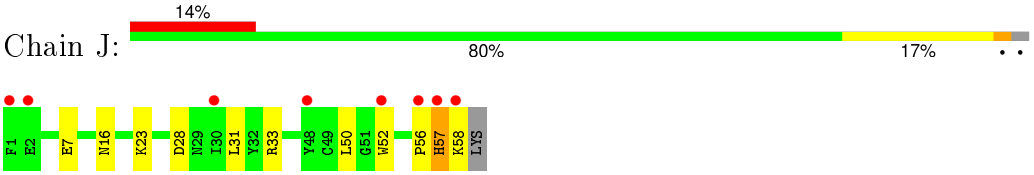
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



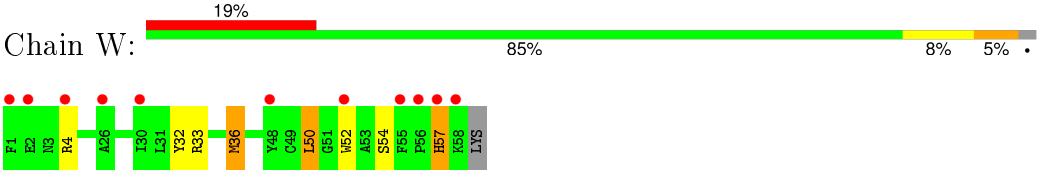
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain J:



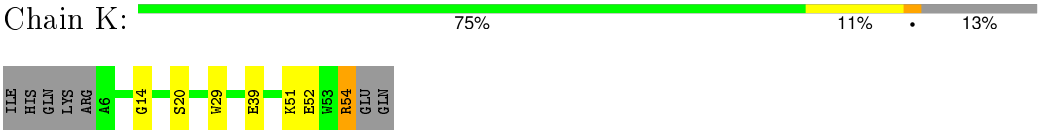
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain W:



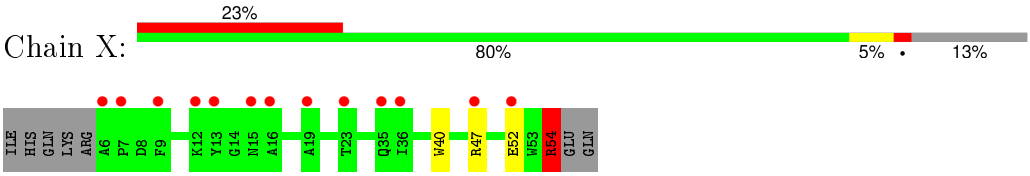
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



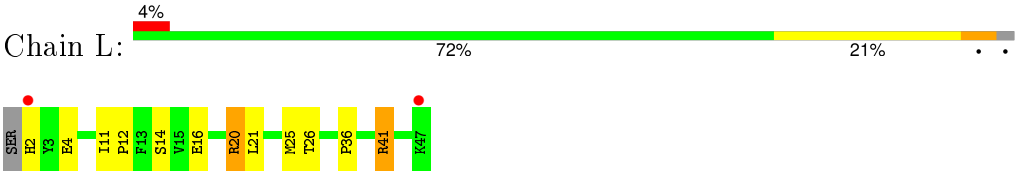
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:



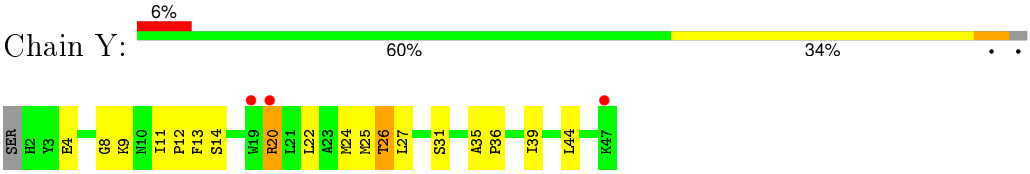
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:



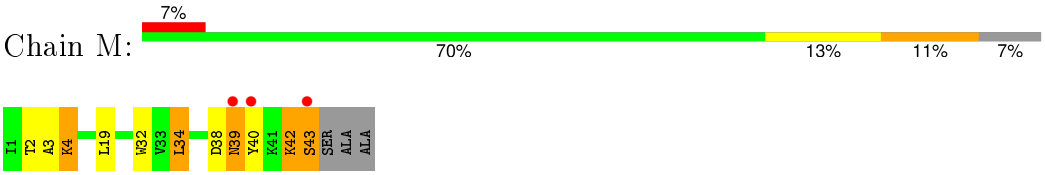
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:



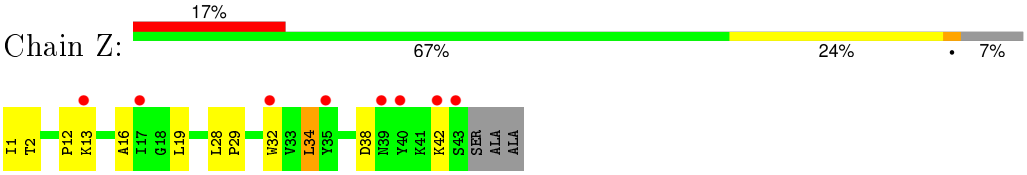
• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.36Å 206.65Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 52.61 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.05) 99.8 (52.61-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.186 , 0.219 0.204 , 0.235	Depositor DCC
R_{free} test set	21000 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.1	EDS
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 419430 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32324	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.69	52/4156 (1.3%)	1.27	32/5678 (0.6%)
1	N	1.51	31/4156 (0.7%)	1.11	14/5678 (0.2%)
2	B	1.53	13/1860 (0.7%)	1.21	11/2534 (0.4%)
2	O	1.24	3/1860 (0.2%)	1.08	5/2534 (0.2%)
3	C	1.52	14/2197 (0.6%)	1.07	6/3005 (0.2%)
3	P	1.51	16/2197 (0.7%)	1.05	3/3005 (0.1%)
4	D	1.55	12/1229 (1.0%)	1.22	7/1658 (0.4%)
4	Q	1.12	2/1229 (0.2%)	0.95	3/1658 (0.2%)
5	E	1.45	1/871 (0.1%)	1.04	2/1182 (0.2%)
5	R	1.20	2/871 (0.2%)	0.96	1/1182 (0.1%)
6	F	1.46	4/765 (0.5%)	1.17	2/1038 (0.2%)
6	S	1.28	1/765 (0.1%)	1.16	4/1038 (0.4%)
7	G	1.35	1/690 (0.1%)	1.10	5/937 (0.5%)
7	T	1.36	3/690 (0.4%)	1.23	5/937 (0.5%)
8	H	1.35	1/682 (0.1%)	1.12	5/921 (0.5%)
8	U	1.13	1/682 (0.1%)	0.95	0/921
9	I	1.34	3/605 (0.5%)	1.03	0/802
9	V	1.18	0/605	0.95	1/802 (0.1%)
10	J	1.25	0/471	1.04	1/636 (0.2%)
10	W	1.16	0/471	1.00	0/636
11	K	1.44	3/398 (0.8%)	1.08	1/546 (0.2%)
11	X	1.18	2/398 (0.5%)	0.96	2/546 (0.4%)
12	L	1.64	4/393 (1.0%)	1.11	2/526 (0.4%)
12	Y	1.42	0/393	1.04	0/526
13	M	1.49	1/345 (0.3%)	1.18	1/470 (0.2%)
13	Z	1.22	0/345	0.97	1/470 (0.2%)
All	All	1.45	170/29324 (0.6%)	1.12	114/39866 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
12	L	0	1
All	All	0	5

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	181	TYR	CD1-CE1	9.79	1.54	1.39
1	A	438	ARG	CB-CG	-9.36	1.27	1.52
1	A	388	ALA	CA-CB	8.80	1.71	1.52
3	P	29	SER	CB-OG	-8.78	1.30	1.42
1	N	139	ALA	CA-CB	8.50	1.70	1.52
1	A	81	TRP	CE3-CZ3	8.43	1.52	1.38
7	T	36	TRP	CB-CG	8.38	1.65	1.50
1	N	270	TYR	CD2-CE2	8.23	1.51	1.39
1	A	288	TRP	CE3-CZ3	8.19	1.52	1.38
4	D	100	LYS	CE-NZ	7.99	1.69	1.49
1	N	74	MET	CB-CG	7.90	1.76	1.51
1	A	469	VAL	CB-CG2	7.73	1.69	1.52
1	A	68	PHE	CD2-CE2	7.69	1.54	1.39
2	O	198	GLU	C-O	7.62	1.37	1.23
4	D	11	TYR	CB-CG	7.41	1.62	1.51
1	A	470	PHE	CE2-CZ	7.40	1.51	1.37
3	P	180	GLU	CD-OE1	7.21	1.33	1.25
2	B	198	GLU	C-O	7.18	1.37	1.23
4	D	104	TYR	CD2-CE2	6.99	1.49	1.39
1	A	74	MET	CB-CG	6.90	1.73	1.51
3	C	57	TRP	CB-CG	6.88	1.62	1.50
1	A	244	TYR	CD2-CE2	6.81	1.49	1.39
1	N	414	PHE	CE1-CZ	6.80	1.50	1.37
1	A	261	TYR	CE2-CZ	6.78	1.47	1.38
7	G	36	TRP	CB-CG	6.71	1.62	1.50
11	K	29	TRP	CB-CG	6.69	1.62	1.50
4	D	100	LYS	CD-CE	6.65	1.67	1.51
1	A	238	PHE	CE2-CZ	6.64	1.50	1.37
12	L	16	GLU	CG-CD	6.57	1.61	1.51
11	K	20	SER	CB-OG	-6.53	1.33	1.42
1	N	63	PHE	CG-CD1	6.50	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	253	TYR	CD2-CE2	6.48	1.49	1.39
9	I	47	TYR	CE2-CZ	6.46	1.47	1.38
12	L	4	GLU	CG-CD	6.46	1.61	1.51
3	P	74	ALA	CA-CB	6.37	1.65	1.52
1	A	371	TYR	CD1-CE1	6.33	1.48	1.39
1	A	193	VAL	CB-CG2	6.29	1.66	1.52
1	A	352	GLY	N-CA	6.28	1.55	1.46
1	N	299	VAL	CB-CG1	6.22	1.66	1.52
1	N	372	TYR	CD1-CE1	6.21	1.48	1.39
1	A	236	TRP	CB-CG	6.14	1.61	1.50
1	A	244	TYR	CE1-CZ	6.14	1.46	1.38
2	B	18	GLU	CG-CD	6.14	1.61	1.51
3	C	29	SER	CB-OG	-6.13	1.34	1.42
4	D	127	LYS	CB-CG	6.11	1.69	1.52
1	N	288	TRP	CB-CG	6.09	1.61	1.50
3	C	193	TYR	CD1-CE1	6.08	1.48	1.39
1	A	261	TYR	CZ-OH	6.06	1.48	1.37
7	T	5	LYS	CB-CG	6.04	1.68	1.52
3	P	227	PHE	CE2-CZ	6.03	1.48	1.37
12	L	16	GLU	CB-CG	6.02	1.63	1.52
1	N	195	LEU	C-O	6.01	1.34	1.23
1	A	458	SER	CB-OG	6.01	1.50	1.42
1	N	397	PHE	CE2-CZ	6.00	1.48	1.37
1	A	129	TYR	CD2-CE2	5.98	1.48	1.39
2	B	132	GLU	CD-OE1	-5.97	1.19	1.25
9	I	54	TYR	CD2-CE2	5.96	1.48	1.39
1	N	473	TRP	CB-CG	5.96	1.60	1.50
3	C	240	TRP	CG-CD1	5.94	1.45	1.36
1	A	112	LEU	CG-CD1	5.92	1.73	1.51
1	A	244	TYR	CD1-CE1	5.91	1.48	1.39
5	E	84	TYR	CE2-CZ	5.90	1.46	1.38
5	R	70	VAL	CB-CG2	5.90	1.65	1.52
3	C	58	TRP	CB-CG	5.89	1.60	1.50
1	N	164	PHE	CD1-CE1	5.88	1.51	1.39
3	C	75	VAL	CB-CG2	5.88	1.65	1.52
1	N	447	TYR	CD1-CE1	5.85	1.48	1.39
1	N	476	PHE	CD1-CE1	5.84	1.50	1.39
2	B	115	ASP	CB-CG	5.82	1.64	1.51
3	P	257	TYR	CD1-CE1	5.82	1.48	1.39
1	A	304	TYR	CD1-CE1	5.79	1.48	1.39
2	B	159	VAL	CB-CG2	5.78	1.65	1.52
6	F	58	VAL	CB-CG2	5.77	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	TYR	CD1-CE1	5.77	1.48	1.39
2	O	198	GLU	CG-CD	5.77	1.60	1.51
3	C	198	PHE	CE2-CZ	5.75	1.48	1.37
1	A	113	LEU	CG-CD1	5.74	1.73	1.51
1	N	89	ALA	C-O	5.74	1.34	1.23
3	C	142	VAL	CB-CG1	5.74	1.65	1.52
1	A	457	GLY	N-CA	5.74	1.54	1.46
4	D	134	PHE	CG-CD2	5.73	1.47	1.38
6	S	54	ASN	CB-CG	-5.71	1.38	1.51
1	N	320	VAL	CB-CG2	5.69	1.64	1.52
1	A	113	LEU	CB-CG	5.69	1.69	1.52
1	N	473	TRP	CE3-CZ3	5.69	1.48	1.38
3	C	99	TRP	CE3-CZ3	5.68	1.48	1.38
3	P	35	PHE	CG-CD2	5.66	1.47	1.38
1	A	40	GLU	CB-CG	5.66	1.62	1.52
1	A	419	VAL	CB-CG1	5.64	1.64	1.52
3	P	153	GLU	CG-CD	5.63	1.60	1.51
2	B	121	TYR	CG-CD1	5.62	1.46	1.39
1	A	149	SER	CA-CB	5.62	1.61	1.52
8	U	69	VAL	CB-CG1	5.61	1.64	1.52
2	B	40	TYR	N-CA	-5.58	1.35	1.46
1	A	122	ALA	CA-CB	5.55	1.64	1.52
1	A	409	TRP	CB-CG	5.54	1.60	1.50
4	D	19	ARG	CZ-NH2	5.52	1.40	1.33
3	P	245	VAL	CB-CG2	5.52	1.64	1.52
3	C	80	ARG	CZ-NH1	5.50	1.40	1.33
2	B	121	TYR	CE2-CZ	5.50	1.45	1.38
2	B	104	TRP	CZ3-CH2	5.49	1.48	1.40
1	N	179	TYR	CB-CG	5.49	1.59	1.51
1	A	67	PHE	CE2-CZ	5.49	1.47	1.37
1	N	113	LEU	CG-CD1	5.48	1.72	1.51
11	K	39	GLU	CB-CG	5.45	1.62	1.52
1	N	297	MET	CG-SD	5.45	1.95	1.81
4	D	60	TYR	CE1-CZ	5.44	1.45	1.38
1	A	505	PHE	CE1-CZ	5.43	1.47	1.37
1	A	264	LYS	CG-CD	-5.41	1.34	1.52
4	D	117	ALA	CA-CB	5.39	1.63	1.52
1	A	313	ALA	CA-CB	5.39	1.63	1.52
1	A	293	PHE	CG-CD1	5.38	1.46	1.38
2	B	60	GLU	CB-CG	5.38	1.62	1.52
1	A	258	VAL	CB-CG2	5.37	1.64	1.52
3	C	89	SER	CB-OG	5.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	235	PHE	CD2-CE2	5.37	1.50	1.39
6	F	69	VAL	CB-CG1	5.36	1.64	1.52
4	Q	117	ALA	CA-CB	5.33	1.63	1.52
1	A	469	VAL	CB-CG1	5.33	1.64	1.52
9	I	54	TYR	CD1-CE1	5.33	1.47	1.39
1	N	447	TYR	CD2-CE2	5.31	1.47	1.39
1	A	260	TYR	CD1-CE1	5.30	1.47	1.39
1	A	419	VAL	CA-CB	5.27	1.65	1.54
1	N	70	VAL	CB-CG1	5.27	1.64	1.52
2	B	118	PHE	CE2-CZ	5.26	1.47	1.37
1	A	252	GLY	N-CA	5.26	1.53	1.46
3	P	218	CYS	CB-SG	5.25	1.91	1.82
8	H	68	TRP	CB-CG	5.25	1.59	1.50
1	A	382	SER	CB-OG	5.24	1.49	1.42
4	D	118	LYS	CD-CE	5.23	1.64	1.51
2	O	198	GLU	CD-OE1	-5.23	1.19	1.25
1	A	115	SER	CB-OG	-5.23	1.35	1.42
3	P	251	PHE	CE2-CZ	5.22	1.47	1.37
1	N	276	ALA	CA-CB	5.22	1.63	1.52
3	P	257	TYR	CE2-CZ	5.20	1.45	1.38
4	D	60	TYR	CD2-CE2	5.20	1.47	1.39
1	A	297	MET	CG-SD	5.19	1.94	1.81
3	C	58	TRP	CE3-CZ3	5.19	1.47	1.38
13	M	3	ALA	CA-CB	5.18	1.63	1.52
3	C	73	PRO	CB-CG	5.17	1.75	1.50
1	N	394	VAL	CB-CG2	-5.17	1.42	1.52
1	A	438	ARG	CG-CD	5.17	1.64	1.51
1	A	450	TRP	CB-CG	5.15	1.59	1.50
1	N	282	PHE	CB-CG	-5.14	1.42	1.51
3	P	102	TYR	CD1-CE1	5.14	1.47	1.39
1	A	299	VAL	CB-CG2	-5.13	1.42	1.52
4	D	115	TRP	CZ3-CH2	5.13	1.48	1.40
3	P	197	PHE	CE1-CZ	5.13	1.47	1.37
1	N	391	GLY	N-CA	5.13	1.53	1.46
2	B	108	TYR	CE2-CZ	5.12	1.45	1.38
1	N	148	PHE	CD1-CE1	5.12	1.49	1.39
6	F	73	TRP	CE3-CZ3	5.12	1.47	1.38
4	Q	81	VAL	CB-CG1	5.10	1.63	1.52
1	N	285	PHE	CD2-CE2	5.10	1.49	1.39
1	A	67	PHE	CD2-CE2	5.07	1.49	1.39
5	R	70	VAL	CB-CG1	-5.06	1.42	1.52
6	F	1	ALA	C-O	5.06	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	TRP	CE2-CZ2	5.05	1.48	1.39
3	P	67	PHE	CE1-CZ	5.05	1.47	1.37
1	A	226	GLY	N-CA	5.05	1.53	1.46
3	C	69	GLY	CA-C	5.04	1.59	1.51
1	A	38	ARG	CD-NE	5.04	1.55	1.46
1	N	67	PHE	CE2-CZ	5.03	1.47	1.37
1	A	40	GLU	CD-OE2	-5.03	1.20	1.25
12	L	21	LEU	CG-CD1	5.03	1.70	1.51
7	T	26	PRO	CG-CD	5.03	1.67	1.50
11	X	52	GLU	CG-CD	5.03	1.59	1.51
11	X	40	TRP	CG-CD1	5.02	1.43	1.36
1	A	387	PHE	CD2-CE2	5.01	1.49	1.39
1	N	443	TYR	CD1-CE1	5.01	1.46	1.39

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	20	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	A	310	MET	CG-SD-CE	-14.80	76.53	100.20
1	A	278	MET	CG-SD-CE	-14.00	77.80	100.20
1	N	278	MET	CG-SD-CE	-12.95	79.47	100.20
4	D	20	ARG	NE-CZ-NH1	12.84	126.72	120.30
7	T	17	ARG	NE-CZ-NH1	10.76	125.68	120.30
7	T	17	ARG	NE-CZ-NH2	-10.38	115.11	120.30
3	C	80	ARG	NE-CZ-NH2	-10.14	115.23	120.30
6	F	18	ARG	NE-CZ-NH2	-9.52	115.54	120.30
4	Q	20	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	297	MET	CG-SD-CE	-8.89	85.98	100.20
6	F	18	ARG	NE-CZ-NH1	8.66	124.63	120.30
13	M	34	LEU	CB-CG-CD1	8.47	125.39	111.00
1	A	227	ASP	CB-CG-OD2	8.34	125.81	118.30
2	O	11	ASP	CB-CG-OD2	8.34	125.81	118.30
3	C	80	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	96	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	189	MET	CG-SD-CE	-8.12	87.22	100.20
4	Q	20	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	449	MET	CA-CB-CG	-7.50	100.54	113.30
11	K	54	ARG	NE-CZ-NH1	-7.49	116.55	120.30
1	A	194	LEU	CB-CG-CD2	7.43	123.63	111.00
8	H	38	ARG	NE-CZ-NH1	-7.37	116.61	120.30
7	T	33	LEU	CA-CB-CG	7.25	131.98	115.30
1	A	380	VAL	CG1-CB-CG2	7.13	122.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	54	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	438	ARG	CB-CA-C	-6.98	96.44	110.40
1	A	380	VAL	CB-CA-C	-6.90	98.28	111.40
6	S	56	ARG	NE-CZ-NH1	-6.82	116.89	120.30
11	X	54	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	N	113	LEU	CB-CG-CD1	6.70	122.38	111.00
1	A	383	MET	CB-CA-C	-6.67	97.06	110.40
1	A	113	LEU	CB-CG-CD2	6.65	122.31	111.00
5	E	40	ASP	CB-CG-OD2	6.54	124.19	118.30
1	N	383	MET	CA-CB-CG	6.50	124.35	113.30
2	B	29	MET	CG-SD-CE	6.47	110.55	100.20
1	A	213	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	P	80	ARG	CG-CD-NE	-6.37	98.43	111.80
3	P	80	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	136	LEU	CA-CB-CG	6.25	129.69	115.30
8	H	38	ARG	NE-CZ-NH2	6.25	123.43	120.30
3	P	163	LEU	CB-CG-CD1	6.25	121.63	111.00
1	A	298	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	278	MET	CA-CB-CG	-6.22	102.73	113.30
2	B	42	ILE	CG1-CB-CG2	-6.16	97.85	111.40
1	A	512	ASN	CB-CA-C	-6.15	98.10	110.40
1	A	213	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	C	31	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	N	240	HIS	N-CA-CB	6.10	121.58	110.60
3	C	44	MET	CG-SD-CE	6.05	109.89	100.20
4	Q	10	ASP	CB-CG-OD1	6.01	123.71	118.30
6	S	94	HIS	N-CA-C	6.01	127.22	111.00
2	B	158	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	74	MET	CB-CG-SD	-5.97	94.50	112.40
3	C	33	MET	CG-SD-CE	5.96	109.74	100.20
6	S	54	ASN	CB-CA-C	-5.94	98.52	110.40
1	A	380	VAL	CA-CB-CG2	5.93	119.80	110.90
1	N	298	ASP	CB-CG-OD2	5.92	123.63	118.30
1	N	438	ARG	NE-CZ-NH1	5.90	123.25	120.30
5	E	90	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	96	ARG	NE-CZ-NH1	5.89	123.24	120.30
7	G	33	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	417	MET	CG-SD-CE	-5.88	90.78	100.20
2	O	202	SER	CB-CA-C	-5.85	98.99	110.10
2	B	178	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	208	MET	CG-SD-CE	5.76	109.42	100.20
5	R	90	ARG	NE-CZ-NH2	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	LEU	CA-CB-CG	-5.74	102.10	115.30
8	H	34	LEU	CB-CG-CD1	-5.74	101.25	111.00
2	B	11	ASP	CB-CG-OD2	5.69	123.42	118.30
8	H	61	LYS	CB-CG-CD	-5.68	96.84	111.60
2	O	46	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	A	439	ARG	NE-CZ-NH1	-5.64	117.48	120.30
11	X	54	ARG	NE-CZ-NH1	-5.61	117.50	120.30
2	B	178	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	438	ARG	CA-CB-CG	5.59	125.70	113.40
12	L	41	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	369	ASP	CB-CG-OD2	5.55	123.30	118.30
2	O	158	ASP	CB-CG-OD1	5.54	123.29	118.30
4	D	31	LYS	CD-CE-NZ	-5.54	98.96	111.70
1	N	380	VAL	CB-CA-C	-5.53	100.89	111.40
7	T	19	LEU	CB-CG-CD2	-5.50	101.66	111.00
3	C	236	GLU	CA-CB-CG	-5.49	101.33	113.40
2	B	173	ASP	CB-CG-OD1	5.48	123.23	118.30
1	N	302	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	50	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	5	MET	CG-SD-CE	-5.44	91.49	100.20
8	H	73	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	N	5	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	B	136	LEU	CB-CG-CD1	-5.39	101.84	111.00
7	T	7	ASP	N-CA-C	5.38	125.52	111.00
1	N	383	MET	CB-CA-C	-5.36	99.68	110.40
6	S	53	THR	C-N-CA	5.34	135.04	121.70
1	A	194	LEU	CB-CG-CD1	5.33	120.07	111.00
2	B	102	HIS	CB-CA-C	-5.32	99.76	110.40
7	G	17	ARG	CB-CG-CD	-5.32	97.78	111.60
1	N	194	LEU	CB-CG-CD2	5.31	120.02	111.00
12	L	20	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	100	MET	CG-SD-CE	5.29	108.66	100.20
1	N	213	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	N	74	MET	CB-CG-SD	-5.24	96.69	112.40
1	N	189	MET	CA-CB-CG	-5.21	104.45	113.30
7	G	54	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	113	LEU	CB-CG-CD1	5.19	119.83	111.00
4	D	21	ASP	CB-CG-OD2	5.18	122.97	118.30
10	J	28	ASP	CB-CG-OD1	5.17	122.95	118.30
4	D	19	ARG	NE-CZ-NH1	-5.17	117.72	120.30
2	O	134	ARG	NE-CZ-NH2	-5.15	117.72	120.30
9	V	10	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	82	ARG	NE-CZ-NH2	-5.14	117.73	120.30
4	D	51	LEU	CA-CB-CG	5.05	126.91	115.30
4	D	20	ARG	CG-CD-NE	-5.04	101.21	111.80
7	G	56	ARG	NE-CZ-NH2	-5.04	117.78	120.30
13	Z	34	LEU	CB-CG-CD1	5.04	119.56	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
12	L	2	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	74	0
1	N	4027	0	4001	84	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	11	0
6	F	748	0	728	16	0
6	S	748	0	728	25	0
7	G	675	0	643	37	0
7	T	675	0	643	49	0
8	H	662	0	623	6	0
8	U	662	0	623	11	0
9	I	601	0	613	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	601	0	613	17	0
10	J	460	0	459	7	0
10	W	460	0	459	9	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	11	0
12	Y	380	0	380	15	0
13	M	335	0	352	9	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	13	0
15	A	2	0	0	0	0
15	N	2	0	0	2	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	7	0
19	D	63	0	110	13	0
19	L	63	0	110	15	0
19	N	126	0	220	22	0
19	Q	63	0	110	10	0
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	3	0
22	C	58	0	70	4	0
22	J	29	0	36	2	0
22	O	29	0	36	1	0
22	P	58	0	73	5	0
22	W	29	0	35	6	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	3	0
24	G	106	0	154	24	0
24	S	53	0	77	16	0
24	T	106	0	154	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	100	0	156	21	0
25	G	100	0	156	28	0
25	P	100	0	156	19	0
25	T	100	0	156	34	0
26	E	52	0	80	16	0
26	R	52	0	80	14	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	3	0
28	M	33	0	38	1	0
28	P	33	0	38	5	0
28	Z	33	0	39	2	0
29	A	225	0	0	8	0
29	B	125	0	0	4	0
29	C	106	0	0	2	0
29	D	91	0	0	1	0
29	E	62	0	0	0	0
29	F	75	0	0	2	0
29	G	41	0	0	3	0
29	H	47	0	0	2	0
29	I	38	0	0	1	0
29	J	20	0	0	1	0
29	K	20	0	0	1	0
29	L	22	0	0	1	0
29	M	15	0	0	1	0
29	N	199	0	0	4	0
29	O	107	0	0	4	0
29	P	100	0	0	3	0
29	Q	55	0	0	2	0
29	R	40	0	0	1	0
29	S	56	0	0	5	0
29	T	36	0	0	4	0
29	U	41	0	0	4	0
29	V	18	0	0	1	0
29	W	12	0	0	0	0
29	X	14	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	0	0
All	All	32324	0	31275	705	0

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

All (705) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:MET:CB	1:N:74:MET:CG	1.76	1.56
1:A:312:ILE:CG1	1:A:312:ILE:CD1	1.78	1.54
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.69	1.51
3:C:73:PRO:CB	3:C:73:PRO:CG	1.75	1.48
14:A:516:HEA:O11	14:A:516:HEA:C11	1.64	1.45
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.58	1.17
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.07	1.16
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.11	1.15
10:W:33:ARG:HG2	22:W:1059:CHD:H152	1.24	1.14
25:G:269:CDL:H241	25:G:269:CDL:H541	1.29	1.13
26:E:229:PSC:H072	9:I:10:ARG:HH21	1.13	1.09
6:S:52:ILE:O	6:S:94:HIS:CE1	2.07	1.08
2:B:41:ILE:HD13	26:E:229:PSC:H342	1.36	1.07
7:T:5:LYS:HD2	24:T:263:PEK:H383	1.37	1.07
6:F:1:ALA:HB2	29:G:4415:HOH:O	1.54	1.06
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.19	1.06
26:E:229:PSC:C07	9:I:10:ARG:HH21	1.67	1.06
7:T:84:LYS:H	7:T:84:LYS:HD2	0.94	1.05
6:S:94:HIS:CD2	6:S:95:GLN:H	1.75	1.05
24:S:1265:PEK:C38	25:T:1269:CDL:H272	1.86	1.04
25:T:1269:CDL:C11	25:T:1269:CDL:HA21	1.87	1.04
6:F:85:CYS:SG	6:F:87:THR:HG23	1.97	1.03
25:G:269:CDL:C24	25:G:269:CDL:H541	1.89	1.02
25:G:269:CDL:C11	25:G:269:CDL:HA21	1.92	0.99
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.84	0.98
7:T:84:LYS:H	7:T:84:LYS:CD	1.76	0.98
6:F:1:ALA:N	24:G:265:PEK:H041	1.77	0.98
25:G:269:CDL:HA21	25:G:269:CDL:H112	1.45	0.97
7:T:5:LYS:CD	24:T:263:PEK:H383	1.94	0.96
7:T:84:LYS:N	7:T:84:LYS:HD2	1.79	0.96
20:C:267:PGV:H181	29:C:4710:HOH:O	1.62	0.96
20:N:1524:PGV:H22	20:N:1524:PGV:H011	1.46	0.96
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.49	0.95
7:G:84:LYS:HD2	7:G:84:LYS:H	1.30	0.95
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.49	0.95
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.82	0.94
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.32	0.93
7:G:5:LYS:HB3	1:N:278:MET:SD	2.07	0.93
14:N:516:HEA:HMD1	14:N:516:HEA:HBD2	1.47	0.93
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CG	24:T:263:PEK:H383	2.01	0.91
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.10	0.91
24:C:264:PEK:H32	24:C:264:PEK:H71	1.54	0.89
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.55	0.88
1:A:311:ILE:HD12	25:T:1269:CDL:H212	1.56	0.88
7:G:72:ASN:H	7:G:76:ASN:HD22	1.13	0.88
24:S:1265:PEK:H383	25:T:1269:CDL:H272	1.56	0.87
25:T:1269:CDL:H112	25:T:1269:CDL:HA21	1.53	0.87
1:N:74:MET:CB	1:N:74:MET:SD	2.62	0.87
7:G:84:LYS:H	7:G:84:LYS:CD	1.88	0.86
12:L:20:ARG:HH22	19:L:522:TGL:CC3	1.81	0.86
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.40	0.85
4:D:34:SER:H	4:D:37:GLN:HE21	1.25	0.85
3:P:157:LYS:NZ	24:S:1265:PEK:H051	1.91	0.85
25:G:269:CDL:H601	25:G:269:CDL:H751	1.59	0.84
9:V:1:SAC:HB3	9:V:1:SAC:OAC	1.77	0.84
6:S:94:HIS:HD2	6:S:95:GLN:H	1.22	0.84
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.43	0.84
7:G:5:LYS:HG3	24:G:1263:PEK:H383	1.59	0.84
28:P:1272:DMU:O1	28:P:1272:DMU:H30	1.78	0.83
1:N:347:LEU:HD13	1:N:383:MET:SD	2.18	0.83
2:O:227:LEU:CB	29:O:4762:HOH:O	2.27	0.82
6:S:75:HIS:H	6:S:80:GLN:HE22	1.27	0.82
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.61	0.82
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.62	0.81
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.43	0.81
2:O:227:LEU:HB3	29:O:4762:HOH:O	1.78	0.81
14:A:516:HEA:HMD1	14:A:516:HEA:HBD2	1.62	0.81
8:U:9:LYS:O	8:U:10:ASN:HB2	1.79	0.81
3:C:80:ARG:NH1	24:T:263:PEK:H032	1.97	0.80
7:T:76:ASN:HD21	24:T:1264:PEK:HN2	1.26	0.80
6:F:1:ALA:H2	24:G:265:PEK:H041	1.44	0.80
24:S:1265:PEK:H381	25:T:1269:CDL:H272	1.62	0.80
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.22	0.80
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.64	0.79
7:T:37:LEU:HD23	25:T:1269:CDL:H352	1.63	0.79
6:F:1:ALA:H1	24:G:265:PEK:H041	1.47	0.79
25:G:269:CDL:C54	25:G:269:CDL:H241	2.12	0.79
24:T:1264:PEK:H71	24:T:1264:PEK:H31	1.65	0.79
8:H:23:GLN:HG3	29:H:4165:HOH:O	1.83	0.79
26:E:229:PSC:C07	9:I:10:ARG:NH2	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.12	0.79
3:C:63:ARG:HE	25:C:270:CDL:CA2	1.97	0.77
7:G:84:LYS:HD2	7:G:84:LYS:N	2.00	0.77
6:S:52:ILE:O	6:S:94:HIS:HE1	1.65	0.77
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.20	0.76
28:P:1272:DMU:H34	7:T:63:GLY:H	1.49	0.76
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.49	0.76
1:A:312:ILE:CD1	1:A:312:ILE:CG2	2.64	0.76
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.67	0.76
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.69	0.75
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.75
7:T:72:ASN:H	7:T:76:ASN:HD22	1.35	0.74
6:S:1:ALA:H1	24:S:1265:PEK:C04	2.00	0.74
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.23	0.74
7:G:72:ASN:H	7:G:76:ASN:ND2	1.84	0.74
6:S:85:CYS:SG	6:S:87:THR:HG23	2.28	0.74
1:A:484:THR:HB	13:M:2:THR:OG1	1.88	0.74
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.69	0.73
24:S:1265:PEK:H381	25:T:1269:CDL:C27	2.18	0.73
3:C:80:ARG:HH11	24:T:263:PEK:H032	1.52	0.73
11:K:52:GLU:HG3	29:K:4738:HOH:O	1.87	0.73
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.71	0.73
10:W:36:MET:HB3	22:W:1059:CHD:C18	2.19	0.73
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.71	0.73
2:B:41:ILE:HD13	26:E:229:PSC:C34	2.17	0.72
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG12	1.70	0.72
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.47	0.72
1:N:381:LEU:HB2	14:N:516:HEA:CAC	2.20	0.72
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.70	0.72
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.02	0.72
26:E:229:PSC:O01	26:E:229:PSC:H212	1.88	0.72
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.72	0.72
24:G:265:PEK:H383	25:G:269:CDL:H272	1.72	0.72
19:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.70	0.72
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.20	0.71
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.20	0.71
1:A:347:LEU:HD13	1:A:383:MET:HB3	1.72	0.71
7:T:5:LYS:HD2	24:T:263:PEK:C38	2.15	0.71
10:J:52:TRP:O	10:J:57:HIS:HE1	1.72	0.71
11:X:54:ARG:NH2	11:X:54:ARG:HG3	1.84	0.71
1:A:278:MET:SD	7:T:5:LYS:HB3	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.72	0.71
6:S:1:ALA:N	24:S:1265:PEK:C04	2.53	0.71
20:C:268:PGV:H31	29:C:4316:HOH:O	1.91	0.71
26:E:229:PSC:H32	26:E:229:PSC:H011	1.72	0.71
7:T:31:CYS:SG	25:T:1269:CDL:C55	2.79	0.71
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.36	0.71
25:T:1269:CDL:H522	25:T:1269:CDL:H222	1.73	0.70
6:F:1:ALA:N	24:G:265:PEK:C04	2.55	0.70
1:N:317:GLY:HA3	14:N:516:HEA:H202	1.72	0.70
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	1.92	0.69
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.74	0.69
1:A:312:ILE:CD1	1:A:312:ILE:CB	2.69	0.69
14:N:516:HEA:NB	15:N:520:CYN:C	2.55	0.69
24:G:265:PEK:C38	25:G:269:CDL:H272	2.23	0.69
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.75	0.69
25:G:269:CDL:H181	25:G:269:CDL:H511	1.75	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.75	0.69
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.56	0.68
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.27	0.68
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.76	0.68
6:S:1:ALA:N	24:S:1265:PEK:H041	2.09	0.68
25:T:1269:CDL:H541	25:T:1269:CDL:H241	1.76	0.68
26:E:229:PSC:H072	9:I:10:ARG:NH2	1.99	0.68
3:P:157:LYS:HZ1	24:S:1265:PEK:H051	1.59	0.68
2:O:67:ILE:HD11	29:O:4812:HOH:O	1.92	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.67
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.77	0.67
25:G:269:CDL:H201	1:N:311:ILE:HD12	1.77	0.66
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.77	0.66
8:H:45:ALA:O	8:H:47:GLY:N	2.28	0.66
7:T:5:LYS:HB2	24:T:263:PEK:C36	2.24	0.66
3:P:246:ASP:HB2	29:P:4260:HOH:O	1.95	0.66
1:N:151:HIS:CD2	24:T:1264:PEK:H382	2.30	0.66
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.76	0.66
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.66
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.25	0.66
8:U:49:ASP:O	8:U:52:VAL:HG22	1.95	0.66
3:P:224:LYS:HD3	25:P:1270:CDL:HB31	1.76	0.66
3:P:157:LYS:HZ2	24:S:1265:PEK:H051	1.57	0.66
4:Q:52:SER:OG	4:Q:55:GLU:HG3	1.96	0.65
25:C:270:CDL:H661	25:C:270:CDL:H242	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:227:LEU:HB2	29:O:4762:HOH:O	1.94	0.65
25:C:270:CDL:H661	25:C:270:CDL:C24	2.26	0.65
25:T:1269:CDL:H562	25:T:1269:CDL:H762	1.77	0.65
1:N:113:LEU:HD12	19:N:1522:TGL:H292	1.79	0.64
26:E:229:PSC:H241	26:E:229:PSC:H62	1.79	0.64
7:T:38:HIS:HD1	7:T:38:HIS:N	1.95	0.64
7:T:3:ALA:HB3	24:T:263:PEK:H382	1.78	0.64
24:S:1265:PEK:C38	25:T:1269:CDL:C27	2.69	0.64
10:W:33:ARG:CG	22:W:1059:CHD:H152	2.14	0.64
19:A:521:TGL:H281	19:A:521:TGL:H102	1.80	0.64
6:S:64:GLU:O	6:S:65:ASP:HB2	1.96	0.64
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.80	0.64
6:S:1:ALA:H2	24:S:1265:PEK:H041	1.62	0.64
2:O:42:ILE:HG22	19:Q:1523:TGL:H251	1.80	0.64
6:S:94:HIS:CD2	6:S:95:GLN:N	2.59	0.63
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.81	0.63
20:N:1524:PGV:H22	20:N:1524:PGV:C01	2.24	0.63
2:B:81:LEU:HD12	25:T:1269:CDL:H362	1.81	0.63
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.64	0.63
1:N:514:LYS:HE2	29:S:3514:HOH:O	1.99	0.63
7:G:5:LYS:CG	24:G:1263:PEK:H383	2.27	0.63
2:O:141:ARG:H	9:V:70:GLN:HE22	1.47	0.63
9:I:31:PHE:CD1	9:I:31:PHE:C	2.72	0.63
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.80	0.63
3:P:55:TYR:CE1	25:P:1270:CDL:H521	2.34	0.63
19:N:1522:TGL:HA22	12:Y:13:PHE:HB3	1.81	0.63
2:B:83:ILE:O	2:B:87:MET:HG3	1.99	0.63
1:A:400:PHE:HB3	19:L:522:TGL:H283	1.81	0.62
25:G:269:CDL:HA21	25:G:269:CDL:H111	1.81	0.62
24:G:265:PEK:H381	25:G:269:CDL:C27	2.28	0.62
26:R:1229:PSC:C07	9:V:10:ARG:HH21	2.13	0.62
1:N:20:LEU:HB3	19:N:1522:TGL:H221	1.80	0.62
2:O:42:ILE:HG21	19:Q:1523:TGL:H232	1.82	0.62
24:G:265:PEK:C38	25:G:269:CDL:C27	2.78	0.61
4:D:78:TRP:HA	19:D:523:TGL:HB22	1.79	0.61
1:N:177:SER:H	1:N:180:GLN:NE2	1.99	0.61
1:N:53:ILE:HG12	29:N:3704:HOH:O	1.99	0.61
6:S:95:GLN:HB2	29:S:4526:HOH:O	2.01	0.61
7:T:8:HIS:ND1	24:T:263:PEK:H312	2.14	0.61
2:O:57:ASP:H	26:R:1229:PSC:H202	1.65	0.61
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB2	1:A:356:ILE:HD11	1.81	0.61
6:F:1:ALA:H1	24:G:265:PEK:C04	2.13	0.61
2:O:41:ILE:HD13	26:R:1229:PSC:H342	1.81	0.61
22:P:1271:CHD:H151	29:P:4657:HOH:O	2.00	0.61
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.32	0.61
1:A:513:LEU:O	1:A:514:LYS:HB2	2.01	0.60
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	1.84	0.60
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.34	0.60
14:A:516:HEA:HO1	14:A:516:HEA:C11	2.07	0.60
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.48	0.60
1:A:265:LYS:HE3	29:F:4709:HOH:O	2.01	0.60
1:A:136:LEU:HB2	29:A:4376:HOH:O	2.02	0.60
10:W:36:MET:HG3	22:W:1059:CHD:H183	1.84	0.60
7:T:30:LEU:HD12	25:T:1269:CDL:H261	1.84	0.60
13:M:42:LYS:HA	13:M:42:LYS:CE	2.27	0.60
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.20	0.60
7:T:12:GLY:HA3	29:T:3372:HOH:O	2.02	0.60
1:N:87:ILE:O	1:N:173:PRO:HD3	2.02	0.59
1:N:74:MET:CA	1:N:74:MET:CG	2.75	0.59
7:T:3:ALA:CB	24:T:263:PEK:H382	2.33	0.59
1:A:312:ILE:CD1	1:A:312:ILE:HG23	2.31	0.59
7:T:37:LEU:CD2	25:T:1269:CDL:H352	2.31	0.59
20:A:524:PGV:H062	29:M:2126:HOH:O	2.02	0.59
24:G:265:PEK:H381	25:G:269:CDL:H273	1.84	0.59
3:P:226:HIS:CE1	25:P:1270:CDL:HB32	2.38	0.59
20:N:1524:PGV:H312	13:Z:16:ALA:HA	1.84	0.59
29:B:2562:HOH:O	19:D:523:TGL:HC72	2.02	0.59
26:E:229:PSC:H071	9:I:10:ARG:NH2	2.17	0.58
1:A:378:HIS:HA	1:A:382:SER:HB2	1.85	0.58
29:A:4410:HOH:O	4:D:100:LYS:HD3	2.01	0.58
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.42	0.58
1:N:381:LEU:HB2	14:N:516:HEA:HAC	1.83	0.58
20:A:522:PGV:H183	24:C:264:PEK:H332	1.85	0.58
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	1.86	0.58
3:P:226:HIS:HE1	25:P:1270:CDL:HB32	1.69	0.58
20:A:522:PGV:H343	29:A:4723:HOH:O	2.03	0.58
6:F:90:LYS:HD2	29:F:4397:HOH:O	2.03	0.58
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.04	0.58
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.39	0.58
10:W:36:MET:HB3	22:W:1059:CHD:H183	1.86	0.58
7:G:31:CYS:SG	25:G:269:CDL:H532	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:3:ALA:O	7:G:4:ALA:HB2	2.04	0.58
7:G:7:ASP:HA	1:N:178:GLN:HG2	1.86	0.58
2:O:224:ALA:O	2:O:227:LEU:HG	2.03	0.57
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.85	0.57
26:R:1229:PSC:H212	26:R:1229:PSC:C02	2.34	0.57
3:C:127:LEU:HG	25:G:269:CDL:OB3	2.04	0.57
2:B:86:MET:O	2:B:89:GLU:HB2	2.04	0.57
25:G:269:CDL:CA2	25:G:269:CDL:H112	2.28	0.57
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.87	0.57
6:S:94:HIS:HD2	6:S:95:GLN:N	1.98	0.57
19:A:521:TGL:H201	19:A:521:TGL:H241	1.86	0.57
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.86	0.57
10:J:7:GLU:HG3	29:J:4595:HOH:O	2.04	0.57
12:L:14:SER:H	19:L:522:TGL:HC31	1.69	0.56
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.71	0.56
8:U:61:LYS:HD3	29:U:4240:HOH:O	2.05	0.56
20:A:524:PGV:H02	20:A:524:PGV:O14	2.04	0.56
19:N:1521:TGL:C28	19:N:1521:TGL:H111	2.36	0.56
3:P:40:MET:O	3:P:44:MET:HG2	2.05	0.56
2:O:116:LEU:HD12	2:O:117:SER:N	2.20	0.56
3:C:217:VAL:HG22	25:C:270:CDL:H732	1.86	0.56
25:G:269:CDL:H201	1:N:311:ILE:CD1	2.36	0.56
12:L:25:MET:HG2	19:L:522:TGL:HA62	1.87	0.56
19:N:1522:TGL:H362	29:Y:4623:HOH:O	2.06	0.55
7:G:45:PRO:HD2	29:G:2099:HOH:O	2.05	0.55
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.71	0.55
20:C:267:PGV:H182	25:C:270:CDL:H662	1.86	0.55
7:G:5:LYS:CD	24:G:1263:PEK:H383	2.36	0.55
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.88	0.55
26:R:1229:PSC:H142	26:R:1229:PSC:H343	1.87	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.88	0.55
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.35	0.55
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.37	0.55
1:A:311:ILE:CD1	25:T:1269:CDL:H212	2.35	0.55
10:J:56:PRO:HB2	10:J:58:LYS:HD3	1.89	0.55
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.88	0.55
19:N:1521:TGL:H102	19:N:1521:TGL:H281	1.89	0.55
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.89	0.54
7:G:30:LEU:CD2	25:G:269:CDL:H471	2.37	0.54
24:T:1264:PEK:H242	24:T:1264:PEK:H12	1.88	0.54
25:P:1270:CDL:H781	25:P:1270:CDL:H231	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:VAL:HG13	24:T:263:PEK:H15	1.90	0.54
7:T:3:ALA:O	7:T:4:ALA:HB2	2.08	0.54
7:G:62:TRP:HB3	28:G:272:DMU:H29	1.90	0.54
9:V:61:GLU:HG3	9:V:64:ARG:HH21	1.72	0.54
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.43	0.54
3:C:47:LEU:O	3:C:51:MET:HG2	2.07	0.54
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.90	0.54
1:A:312:ILE:HD12	1:A:312:ILE:CG2	2.39	0.53
2:B:217:LYS:HG2	29:B:4225:HOH:O	2.06	0.53
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.41	0.53
13:M:39:ASN:O	13:M:43:SER:HB2	2.07	0.53
1:N:362:SER:HA	2:O:87:MET:HE1	1.91	0.53
7:G:30:LEU:HD23	25:G:269:CDL:H471	1.90	0.53
1:A:343:GLY:O	1:A:347:LEU:HG	2.08	0.53
7:T:6:GLY:O	24:T:263:PEK:H311	2.08	0.53
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.90	0.53
26:R:1229:PSC:O01	26:R:1229:PSC:H212	2.09	0.53
1:A:347:LEU:HD22	1:A:383:MET:SD	2.48	0.53
1:N:76:GLY:O	1:N:80:ASN:HB2	2.08	0.53
2:O:164:ALA:O	2:O:194:GLY:HA3	2.08	0.53
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.91	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.90	0.53
19:D:523:TGL:H363	9:I:16:ARG:HH21	1.74	0.53
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.24	0.53
2:B:164:ALA:O	2:B:194:GLY:HA3	2.07	0.53
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.91	0.53
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.90	0.53
14:N:516:HEA:HMD1	14:N:516:HEA:CBD	2.27	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.52
1:A:73:ILE:CD1	14:A:515:HEA:H22	2.39	0.52
13:Z:28:LEU:N	13:Z:29:PRO:CD	2.73	0.52
2:B:59:GLN:C	2:B:60:GLU:HG3	2.30	0.52
2:O:191:LEU:HG	9:V:68:ILE:HD12	1.91	0.52
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.09	0.52
4:D:78:TRP:HA	19:D:523:TGL:CB2	2.39	0.52
9:V:18:ARG:HG3	29:V:3588:HOH:O	2.09	0.52
1:N:317:GLY:CA	14:N:516:HEA:H202	2.39	0.52
24:T:1264:PEK:H42	24:T:1264:PEK:H222	1.90	0.52
12:Y:22:LEU:O	12:Y:26:THR:HB	2.09	0.52
7:T:38:HIS:ND1	7:T:38:HIS:N	2.55	0.52
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:33:LEU:O	4:Q:38:LYS:HE2	2.09	0.52
7:G:12:GLY:HA3	29:G:4330:HOH:O	2.08	0.52
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.92	0.52
5:E:48:ILE:O	5:E:52:LEU:HG	2.10	0.52
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.90	0.51
1:A:304:TYR:HD1	25:T:1269:CDL:HB32	1.74	0.51
1:N:151:HIS:HD2	24:T:1264:PEK:H382	1.72	0.51
3:C:226:HIS:CE1	25:C:270:CDL:HB31	2.45	0.51
1:N:378:HIS:HA	1:N:382:SER:HB2	1.93	0.51
2:B:58:ALA:O	2:B:62:GLU:HG3	2.11	0.51
2:O:83:ILE:O	2:O:87:MET:HG3	2.10	0.51
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.51
25:C:270:CDL:H311	25:C:270:CDL:H151	1.93	0.51
25:T:1269:CDL:H171	29:T:4401:HOH:O	2.10	0.51
7:T:12:GLY:CA	29:T:3372:HOH:O	2.58	0.51
12:Y:35:ALA:O	12:Y:39:ILE:HG13	2.11	0.51
7:T:30:LEU:CD1	25:T:1269:CDL:H261	2.40	0.50
20:A:524:PGV:H212	29:A:4691:HOH:O	2.12	0.50
7:T:37:LEU:HB3	7:T:38:HIS:HD1	1.75	0.50
4:D:98:TRP:CE3	28:M:526:DMU:H12	2.46	0.50
7:T:5:LYS:HG3	24:T:263:PEK:C38	2.39	0.50
20:N:1524:PGV:H252	13:Z:12:PRO:HG3	1.93	0.50
2:O:134:ARG:HB2	4:Q:110:THR:HG21	1.92	0.50
1:N:406:ASN:ND2	20:N:1524:PGV:H032	2.26	0.50
20:P:1267:PGV:H172	25:P:1270:CDL:H662	1.94	0.50
3:P:59:ARG:HB2	25:P:1270:CDL:H512	1.93	0.50
7:G:5:LYS:HD2	24:G:1263:PEK:H383	1.94	0.50
1:A:309:THR:HG22	14:A:516:HEA:HMB2	1.93	0.50
1:N:307:SER:O	1:N:311:ILE:HG13	2.12	0.50
3:C:213:THR:HG23	25:C:270:CDL:H771	1.94	0.50
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.92	0.50
1:A:25:TRP:CE3	19:L:522:TGL:HB91	2.47	0.49
1:N:417:MET:HE3	29:N:3166:HOH:O	2.12	0.49
2:O:89:GLU:O	2:O:91:ASN:ND2	2.46	0.49
3:P:168:THR:HG22	24:S:1265:PEK:H14	1.94	0.49
7:T:38:HIS:NE2	25:T:1269:CDL:H131	2.28	0.49
4:D:78:TRP:CA	19:D:523:TGL:CB2	2.89	0.49
2:B:19:GLU:HA	2:B:19:GLU:OE2	2.12	0.49
2:B:57:ASP:H	26:E:229:PSC:H201	1.78	0.49
28:P:1272:DMU:C10	28:P:1272:DMU:H30	2.42	0.49
19:A:521:TGL:H281	19:A:521:TGL:C10	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:40:TYR:CE2	9:V:24:ALA:HB2	2.48	0.49
7:T:2:SER:O	24:T:263:PEK:H331	2.12	0.49
1:A:347:LEU:HD13	1:A:383:MET:SD	2.52	0.49
10:J:52:TRP:O	10:J:57:HIS:CE1	2.61	0.49
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.43	0.49
3:P:107:ALA:HB2	20:P:1268:PGV:H031	1.94	0.49
7:G:63:GLY:H	28:G:272:DMU:H40	1.77	0.49
2:O:168:LEU:HD13	2:O:184:LEU:HG	1.95	0.49
1:N:351:GLY:C	1:N:380:VAL:HG13	2.33	0.49
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.44	0.49
2:B:66:THR:HG21	22:B:1085:CHD:H42	1.95	0.49
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.11	0.49
10:W:50:LEU:HD22	10:W:54:SER:HG	1.77	0.49
2:O:57:ASP:N	26:R:1229:PSC:H202	2.27	0.48
13:Z:32:TRP:N	28:Z:1526:DMU:H1	2.28	0.48
3:P:165:ILE:HG12	24:S:1265:PEK:H102	1.96	0.48
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.79	0.48
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.11	0.48
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.49	0.48
19:A:521:TGL:H122	19:A:521:TGL:H283	1.95	0.48
4:Q:101:HIS:CD2	4:Q:102:TYR:CD2	3.02	0.48
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.97	0.48
1:N:189:MET:O	1:N:189:MET:HG3	2.13	0.48
1:N:377:PHE:CD1	14:N:516:HEA:HAD1	2.49	0.48
3:C:103:HIS:HA	20:C:268:PGV:H012	1.95	0.48
5:R:63:SER:O	5:R:67:ILE:HG13	2.13	0.48
1:N:113:LEU:HD13	19:N:1522:TGL:H292	1.95	0.48
14:N:516:HEA:NA	15:N:520:CYN:C	2.76	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.07	0.48
22:O:229:CHD:H212	22:O:229:CHD:H12	1.95	0.48
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.79	0.48
3:C:52:LEU:HD23	25:C:270:CDL:H362	1.96	0.48
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.66	0.48
1:N:1:FME:HCN	1:N:4:ASN:H	1.79	0.48
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.79	0.48
6:S:87:THR:HG22	29:S:4655:HOH:O	2.14	0.47
3:P:129:VAL:N	3:P:130:PRO:CD	2.76	0.47
1:N:353:LEU:HB3	2:O:31:VAL:HG13	1.96	0.47
26:E:229:PSC:C02	26:E:229:PSC:H212	2.43	0.47
24:T:1264:PEK:H11	24:T:1264:PEK:C15	2.44	0.47
1:N:334:TRP:HB2	19:Q:1523:TGL:HG11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:HD13	1:A:383:MET:CB	2.42	0.47
1:N:438:ARG:O	1:N:439:ARG:HB2	2.14	0.47
26:E:229:PSC:H21	29:I:4186:HOH:O	2.15	0.47
19:Q:1523:TGL:HG12	19:Q:1523:TGL:CC2	2.43	0.47
4:Q:40:LEU:HD11	4:Q:55:GLU:HB3	1.95	0.47
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.97	0.47
7:T:30:LEU:HD12	25:T:1269:CDL:C26	2.45	0.47
26:R:1229:PSC:H222	26:R:1229:PSC:H32	1.97	0.47
1:N:53:ILE:CD1	12:Y:44:LEU:HD23	2.45	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
6:S:55:LYS:HA	6:S:74:LEU:O	2.13	0.47
12:Y:8:GLY:HA2	12:Y:11:ILE:HD11	1.95	0.47
2:B:57:ASP:H	26:E:229:PSC:C20	2.28	0.47
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.49	0.47
1:A:328:HIS:CE1	9:I:17:LEU:HD22	2.49	0.47
25:G:269:CDL:H242	25:G:269:CDL:H541	1.87	0.47
3:C:63:ARG:NE	25:C:270:CDL:HA22	2.21	0.47
2:B:74:ILE:HG13	25:T:1269:CDL:H441	1.97	0.47
7:G:3:ALA:O	7:G:4:ALA:CB	2.61	0.47
24:G:1263:PEK:H042	3:P:77:LYS:NZ	2.29	0.47
8:U:9:LYS:HE2	8:U:9:LYS:HB2	1.68	0.47
2:O:40:TYR:HE2	9:V:24:ALA:HB2	1.79	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.47
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.77	0.47
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.30	0.47
8:U:27:ARG:NH1	29:U:3431:HOH:O	2.46	0.47
19:N:1521:TGL:H281	19:N:1521:TGL:H111	1.96	0.47
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.29	0.47
28:P:1272:DMU:H29	7:T:62:TRP:HB3	1.97	0.47
2:O:163:TRP:NE1	2:O:209:ILE:HG12	2.30	0.47
1:A:73:ILE:HD11	14:A:515:HEA:H22	1.97	0.46
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.64	0.46
25:C:270:CDL:H652	25:C:270:CDL:H621	1.33	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.46
14:A:516:HEA:HMC1	14:A:516:HEA:CBC	2.46	0.46
28:P:1272:DMU:H34	7:T:63:GLY:N	2.24	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.46
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.98	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.15	0.46
26:R:1229:PSC:H343	26:R:1229:PSC:C13	2.45	0.46
4:Q:98:TRP:CD2	28:Z:1526:DMU:H10	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD21	1:A:440:TYR:O	2.15	0.46
2:O:42:ILE:HG21	19:Q:1523:TGL:C23	2.45	0.46
19:A:521:TGL:C30	19:A:521:TGL:H122	2.45	0.46
1:N:407:ASP:O	1:N:411:LYS:HG3	2.16	0.46
3:P:25:LEU:O	3:P:29:SER:HB2	2.15	0.46
3:P:230:ASN:HB2	29:S:3400:HOH:O	2.16	0.46
3:C:257:TYR:O	3:C:261:SER:HB3	2.16	0.46
7:G:83:GLU:HG2	7:G:84:LYS:HZ2	1.79	0.46
20:A:524:PGV:H41	20:A:524:PGV:H232	1.98	0.46
1:N:115:SER:HB2	1:N:142:SER:O	2.14	0.46
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.98	0.46
7:T:8:HIS:O	7:T:9:GLY:C	2.54	0.46
28:G:272:DMU:O1	28:G:272:DMU:H30	2.16	0.46
7:T:45:PRO:HD2	29:T:3099:HOH:O	2.16	0.46
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.98	0.46
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.97	0.46
4:D:114:GLU:OE1	11:K:51:LYS:NZ	2.40	0.46
5:R:46:LYS:HG2	29:R:4450:HOH:O	2.15	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.46
1:N:178:GLN:HB2	29:N:3430:HOH:O	2.16	0.45
19:N:1522:TGL:HG11	12:Y:12:PRO:HG2	1.97	0.45
7:T:7:ASP:O	7:T:9:GLY:N	2.47	0.45
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.51	0.45
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.97	0.45
1:A:307:SER:O	1:A:311:ILE:HG13	2.17	0.45
1:A:177:SER:H	1:A:180:GLN:HE21	1.65	0.45
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.81	0.45
1:N:112:LEU:HD23	1:N:112:LEU:C	2.36	0.45
29:A:4735:HOH:O	4:D:17:VAL:CG1	2.65	0.45
24:T:1264:PEK:H71	24:T:1264:PEK:C3	2.40	0.45
2:O:116:LEU:CD1	2:O:226:MET:HG3	2.46	0.45
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.45
8:U:23:GLN:HG3	29:U:4336:HOH:O	2.15	0.45
22:C:525:CHD:H112	22:C:525:CHD:H12A	1.69	0.45
26:R:1229:PSC:H251	26:R:1229:PSC:H221	1.72	0.45
1:N:53:ILE:HD12	12:Y:44:LEU:CD2	2.46	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.16	0.45
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.98	0.45
12:Y:27:LEU:O	12:Y:31:SER:HB3	2.17	0.45
29:B:3446:HOH:O	7:T:17:ARG:HD2	2.16	0.45
9:V:25:PHE:CE2	9:V:29:LEU:HD22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:523:TGL:H332	19:D:523:TGL:H172	1.76	0.45
1:A:514:LYS:HE3	29:A:2645:HOH:O	2.17	0.45
7:G:1:ALA:HB2	20:P:1268:PGV:H321	1.98	0.45
1:N:127:THR:HB	1:N:129:TYR:CE2	2.51	0.45
1:N:352:GLY:N	1:N:380:VAL:HG13	2.32	0.45
22:P:1525:CHD:H112	22:P:1525:CHD:H12A	1.55	0.45
6:F:1:ALA:H2	24:G:265:PEK:C04	2.20	0.44
2:B:56:MET:HG2	26:E:229:PSC:H211	1.99	0.44
25:G:269:CDL:H152	25:G:269:CDL:H182	1.33	0.44
1:N:355:GLY:C	14:N:516:HEA:HMB3	2.38	0.44
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.99	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.44
25:P:1270:CDL:H262	25:P:1270:CDL:H232	1.79	0.44
1:N:17:THR:OG1	19:N:1522:TGL:H281	2.18	0.44
1:A:390:MET:O	1:A:394:VAL:HG22	2.17	0.44
2:B:102:HIS:O	2:B:104:TRP:HA	2.17	0.44
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.98	0.44
20:P:1267:PGV:H12	20:P:1267:PGV:H152	1.20	0.44
25:G:269:CDL:H181	25:G:269:CDL:C51	2.46	0.44
29:B:3446:HOH:O	7:T:17:ARG:CD	2.66	0.44
3:P:253:TYR:CE2	25:T:1269:CDL:H641	2.52	0.44
1:N:113:LEU:HD12	19:N:1522:TGL:C29	2.46	0.44
19:D:523:TGL:H132	19:D:523:TGL:H302	1.69	0.44
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.52	0.44
9:V:36:LYS:O	9:V:41:GLU:CG	2.65	0.44
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.17	0.44
7:G:34:ASN:HB2	25:G:269:CDL:H162	2.00	0.44
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.45	0.44
3:C:63:ARG:HE	25:C:270:CDL:HA21	1.81	0.44
2:O:1:FME:SD	2:O:133:LEU:HD11	2.57	0.44
1:A:250:GLY:O	1:A:254:ILE:HG12	2.17	0.44
6:S:92:VAL:O	6:S:92:VAL:HG23	2.18	0.44
3:P:224:LYS:CD	25:P:1270:CDL:HB31	2.44	0.44
19:N:1522:TGL:HC62	19:N:1522:TGL:HC32	1.43	0.44
2:O:41:ILE:O	2:O:42:ILE:C	2.56	0.44
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.44
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.71	0.44
1:N:199:LEU:N	1:N:200:PRO:CD	2.81	0.44
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.90	0.44
5:E:11:PHE:CG	26:E:229:PSC:H073	2.53	0.43
25:C:270:CDL:H241	25:C:270:CDL:H661	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:1523:TGL:H122	19:Q:1523:TGL:HB92	1.76	0.43
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.00	0.43
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.53	0.43
14:A:516:HEA:CBD	14:A:516:HEA:HMD1	2.41	0.43
2:O:139:ASP:OD2	2:O:140:ASN:N	2.50	0.43
6:S:70:ILE:HG13	6:S:84:SER:HB3	2.00	0.43
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.99	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
7:G:72:ASN:OD1	7:G:74:ARG:HB2	2.18	0.43
3:P:156:ARG:HE	22:P:1271:CHD:C24	2.31	0.43
22:J:60:CHD:H12A	22:J:60:CHD:H112	1.81	0.43
3:P:118:PRO:HD2	3:P:121:ILE:HG13	2.01	0.43
6:F:64:GLU:O	6:F:65:ASP:HB2	2.18	0.43
1:A:309:THR:CG2	14:A:516:HEA:HMB2	2.48	0.43
1:A:113:LEU:CD1	19:L:522:TGL:H292	2.49	0.43
1:A:113:LEU:HD12	19:L:522:TGL:H292	2.00	0.43
19:N:1522:TGL:HC22	19:N:1522:TGL:HC82	2.00	0.43
1:N:484:THR:HB	13:Z:2:THR:OG1	2.18	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
1:A:115:SER:HB2	1:A:142:SER:O	2.18	0.43
25:C:270:CDL:PA1	25:C:270:CDL:CB2	3.07	0.43
7:G:76:ASN:HA	7:G:77:PRO:HD2	1.93	0.43
1:A:347:LEU:CD1	1:A:383:MET:HB3	2.45	0.43
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.67	0.43
1:N:104:LEU:HB2	1:N:156:SER:HB2	2.00	0.43
5:R:105:GLY:O	5:R:108:LYS:HG3	2.18	0.43
26:R:1229:PSC:H201	26:R:1229:PSC:H232	1.28	0.43
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.00	0.43
29:A:4735:HOH:O	4:D:17:VAL:HG11	2.19	0.43
12:L:41:ARG:HG3	13:M:40:TYR:CE1	2.54	0.43
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	2.01	0.43
1:N:46:THR:O	1:N:46:THR:HG23	2.18	0.43
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.48	0.43
1:A:307:SER:CB	25:T:1269:CDL:H182	2.49	0.43
24:G:1263:PEK:H042	3:P:77:LYS:HZ1	1.82	0.43
19:N:1522:TGL:H251	19:N:1522:TGL:H282	1.41	0.43
19:N:1521:TGL:H283	19:N:1521:TGL:H111	2.00	0.43
1:N:440:TYR:CZ	2:O:205:SER:HA	2.53	0.43
3:C:50:ASN:ND2	3:C:54:MET:CE	2.82	0.43
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:MET:O	2:O:226:MET:HG3	2.19	0.43
13:Z:1:ILE:HG23	13:Z:1:ILE:O	2.19	0.43
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.54	0.43
8:H:60:TYR:CD1	8:H:60:TYR:C	2.92	0.43
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.84	0.43
4:Q:101:HIS:CD2	4:Q:102:TYR:CE2	3.07	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.43
25:T:1269:CDL:H252	25:T:1269:CDL:H221	1.65	0.42
19:D:523:TGL:HB62	19:D:523:TGL:HA52	2.01	0.42
3:C:159:MET:C	3:C:159:MET:SD	2.97	0.42
1:A:352:GLY:N	1:A:380:VAL:HG13	2.33	0.42
1:N:71:MET:CE	1:N:195:LEU:HD21	2.49	0.42
3:C:156:ARG:HE	22:C:271:CHD:C24	2.33	0.42
1:N:328:HIS:HB2	2:O:45:MET:SD	2.58	0.42
8:H:45:ALA:C	8:H:47:GLY:H	2.21	0.42
6:S:25:ARG:HD3	29:S:4617:HOH:O	2.19	0.42
10:W:50:LEU:HD22	10:W:54:SER:OG	2.19	0.42
20:C:267:PGV:H152	20:C:267:PGV:H12	1.12	0.42
4:D:20:ARG:HG3	29:D:4124:HOH:O	2.19	0.42
1:A:129:TYR:HH	1:A:236:TRP:HE1	1.66	0.42
2:O:59:GLN:CG	2:O:59:GLN:O	2.67	0.42
14:A:516:HEA:HHA	14:A:516:HEA:HAD2	1.72	0.42
19:Q:1523:TGL:H302	19:Q:1523:TGL:H132	1.85	0.42
1:N:177:SER:H	1:N:180:GLN:HE21	1.67	0.42
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.83	0.42
2:B:33:LEU:HA	2:B:33:LEU:HD12	1.36	0.42
24:G:265:PEK:H312	2:O:66:THR:HG23	2.01	0.42
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.42
2:O:202:SER:HB2	2:O:203:ASN:ND2	2.15	0.42
29:L:4496:HOH:O	13:M:32:TRP:HH2	2.02	0.42
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.74	0.42
2:B:62:GLU:O	2:B:66:THR:HB	2.20	0.42
14:N:515:HEA:HHC	14:N:515:HEA:H11	1.77	0.42
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.55	0.42
22:B:1085:CHD:H11	24:S:1265:PEK:H271	2.01	0.42
25:T:1269:CDL:H161	25:T:1269:CDL:H391	2.02	0.42
29:N:3132:HOH:O	3:P:112:LEU:CD2	2.67	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.42
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.02	0.42
10:J:31:LEU:HA	10:J:31:LEU:HD12	1.89	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:112:LEU:O	1:N:112:LEU:HD23	2.20	0.42
1:N:409:TRP:HB3	1:N:471:ILE:HG12	2.01	0.42
2:B:116:LEU:HD11	2:B:226:MET:HB3	2.00	0.42
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.56	0.41
10:W:32:TYR:OH	22:W:1059:CHD:H213	2.20	0.41
24:G:265:PEK:C38	25:G:269:CDL:H273	2.49	0.41
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.20	0.41
2:O:202:SER:CB	2:O:203:ASN:HD22	2.18	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.85	0.41
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.01	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.01	0.41
3:P:220:PHE:HB2	25:P:1270:CDL:H712	2.00	0.41
24:T:263:PEK:H312	24:T:263:PEK:H282	1.93	0.41
3:P:138:LEU:HD12	25:T:1269:CDL:H591	2.02	0.41
1:A:419:VAL:HG23	19:D:523:TGL:H121	2.01	0.41
2:O:40:TYR:O	2:O:43:SER:N	2.54	0.41
4:D:16:TYR:OH	4:D:18:ASP:OD2	2.32	0.41
3:C:58:TRP:HB2	25:C:270:CDL:H552	2.02	0.41
22:B:1085:CHD:H12A	22:B:1085:CHD:H112	1.64	0.41
7:G:3:ALA:CB	24:G:1263:PEK:H382	2.50	0.41
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.41
2:B:146:MET:HA	2:B:213:LEU:HD12	2.01	0.41
10:W:52:TRP:CE2	10:W:57:HIS:CE1	3.08	0.41
25:P:1270:CDL:HB21	25:P:1270:CDL:OB6	2.21	0.41
2:O:227:LEU:HA	2:O:227:LEU:HD23	1.93	0.41
24:T:1264:PEK:C11	24:T:1264:PEK:C15	2.98	0.41
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.03	0.41
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.55	0.41
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.01	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.21	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.75	0.41
2:B:145:PRO:HA	2:B:214:VAL:O	2.19	0.41
3:P:157:LYS:HZ2	24:S:1265:PEK:C05	2.28	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.03	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
1:A:217:THR:HG22	3:C:188:ILE:HG12	2.02	0.41
6:F:92:VAL:HG23	6:F:92:VAL:O	2.20	0.41
5:R:24:ILE:HG23	5:R:24:ILE:O	2.20	0.41
6:F:1:ALA:HB3	6:S:65:ASP:OD1	2.21	0.41
24:G:1263:PEK:H15	3:P:248:VAL:HG22	2.03	0.41
5:R:8:ASP:HA	26:R:1229:PSC:H071	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:11:TYR:HH	8:U:62:SER:CB	2.30	0.41
1:N:321:PHE:CD1	2:O:65:TRP:HB2	2.55	0.41
19:A:521:TGL:H102	19:A:521:TGL:C28	2.48	0.41
1:A:378:HIS:HA	1:A:382:SER:CB	2.50	0.41
1:N:376:HIS:O	1:N:380:VAL:HG22	2.20	0.41
6:S:94:HIS:CG	6:S:95:GLN:N	2.86	0.41
25:C:270:CDL:H532	25:C:270:CDL:H561	1.41	0.41
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.78	0.41
1:N:115:SER:O	1:N:121:GLY:HA2	2.21	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.02	0.41
25:G:269:CDL:HB32	1:N:304:TYR:CD1	2.56	0.41
7:T:31:CYS:SG	25:T:1269:CDL:C53	2.95	0.41
1:A:406:ASN:ND2	20:A:524:PGV:H032	2.36	0.41
19:N:1521:TGL:C11	19:N:1521:TGL:H281	2.51	0.41
19:N:1521:TGL:HC22	29:Q:3606:HOH:O	2.21	0.41
8:U:46:LYS:HD2	29:U:4404:HOH:O	2.20	0.41
9:V:31:PHE:C	9:V:31:PHE:CD1	2.94	0.41
1:A:377:PHE:O	1:A:381:LEU:HB3	2.21	0.41
3:C:112:LEU:HD13	3:C:118:PRO:HG3	2.02	0.41
3:C:155:ASP:OD2	6:F:2:SER:HA	2.20	0.41
5:R:80:GLU:CD	5:R:80:GLU:H	2.24	0.41
25:C:270:CDL:H201	25:C:270:CDL:C64	2.50	0.40
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.56	0.40
3:C:25:LEU:O	3:C:29:SER:HB2	2.21	0.40
19:A:521:TGL:HB91	19:A:521:TGL:HB61	1.46	0.40
14:A:515:HEA:H11	14:A:515:HEA:HHC	1.86	0.40
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.34	0.40
1:N:444:PRO:HD3	2:O:195:GLN:HE22	1.86	0.40
1:A:43:GLN:HB2	1:A:44:PRO:HD2	2.03	0.40
3:P:249:TRP:HD1	29:P:3165:HOH:O	2.04	0.40
3:C:40:MET:O	3:C:44:MET:HG2	2.21	0.40
8:H:76:ARG:HD2	29:H:4210:HOH:O	2.20	0.40
26:R:1229:PSC:H212	26:R:1229:PSC:C01	2.51	0.40
20:A:524:PGV:H152	20:A:524:PGV:C32	2.51	0.40
10:J:16:ASN:OD1	10:J:23:LYS:HE3	2.21	0.40
3:C:98:PHE:CD2	24:T:263:PEK:H182	2.56	0.40
7:T:35:SER:C	7:T:37:LEU:H	2.25	0.40
26:R:1229:PSC:C14	26:R:1229:PSC:H343	2.51	0.40
20:C:268:PGV:H11	20:C:268:PGV:H241	2.03	0.40
1:N:398:PRO:HA	1:N:403:TYR:O	2.21	0.40
3:P:8:TYR:CE1	3:P:74:ALA:HB1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:263:PEK:H271	24:T:263:PEK:H241	1.96	0.40
7:G:5:LYS:HD2	24:G:1263:PEK:C38	2.52	0.40
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.66	0.40
1:A:344:PHE:C	1:A:344:PHE:CD1	2.95	0.40
1:A:304:TYR:C	1:A:304:TYR:CD2	2.94	0.40
19:N:1521:TGL:H131	19:N:1521:TGL:H302	1.78	0.40
1:A:160:GLY:HA3	29:A:2648:HOH:O	2.22	0.40
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.85	0.40
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100 100
1	N	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	52 43
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	21 10
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21 10
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100 100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	39 28
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100 100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100 100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100 100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	9 2
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5 0
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2 0
8	H	77/85 (91%)	67 (87%)	4 (5%)	6 (8%)	1 0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7 1
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100 100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100 100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
11	K	47/56 (84%)	46 (98%)	0	1 (2%)	9 2
11	X	47/56 (84%)	44 (94%)	3 (6%)	0	100 100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100 100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100 100
All	All	3504/3614 (97%)	3336 (95%)	135 (4%)	33 (1%)	21 10

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
3	P	38	ASN
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	8	ILE
8	U	10	ASN
7	G	39	SER
8	H	10	ASN
8	H	11	TYR

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Mol	Chain	Res	Type
8	H	45	ALA
7	T	3	ALA
6	F	94	HIS
7	G	6	GLY
2	O	60	GLU
6	S	96	LEU
2	B	33	LEU
7	G	3	ALA
7	G	37	LEU
2	O	92	ASN
1	N	382	SER
11	K	14	GLY
7	T	6	GLY
8	H	47	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/426 (100%)	414 (97%)	12 (3%)	51 44
1	N	426/426 (100%)	414 (97%)	12 (3%)	51 44
2	B	210/210 (100%)	200 (95%)	10 (5%)	31 22
2	O	210/210 (100%)	197 (94%)	13 (6%)	23 13
3	C	224/226 (99%)	217 (97%)	7 (3%)	47 39
3	P	224/226 (99%)	218 (97%)	6 (3%)	52 45
4	D	128/129 (99%)	126 (98%)	2 (2%)	70 67
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58 51
5	E	92/95 (97%)	91 (99%)	1 (1%)	80 79
5	R	92/95 (97%)	86 (94%)	6 (6%)	21 11
6	F	81/81 (100%)	76 (94%)	5 (6%)	23 13
6	S	81/81 (100%)	73 (90%)	8 (10%)	10 3
7	G	67/68 (98%)	59 (88%)	8 (12%)	6 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	T	67/68 (98%)	57 (85%)	10 (15%)	4 1
8	H	71/75 (95%)	67 (94%)	4 (6%)	26 16
8	U	71/75 (95%)	66 (93%)	5 (7%)	19 10
9	I	57/57 (100%)	53 (93%)	4 (7%)	19 10
9	V	57/57 (100%)	53 (93%)	4 (7%)	19 10
10	J	49/50 (98%)	48 (98%)	1 (2%)	63 58
10	W	49/50 (98%)	46 (94%)	3 (6%)	23 13
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 47
11	X	39/46 (85%)	37 (95%)	2 (5%)	29 19
12	L	39/40 (98%)	38 (97%)	1 (3%)	54 47
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29 19
13	M	37/38 (97%)	31 (84%)	6 (16%)	3 0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 2
All	All	3040/3082 (99%)	2900 (95%)	140 (5%)	33 24

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	290	HIS
1	A	312	ILE
1	A	333	LYS
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	504	THR
1	A	513	LEU
2	B	33	LEU
2	B	42	ILE
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	33	MET
3	C	73	PRO
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	214	PHE
4	D	31	LYS
4	D	51	LEU
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	78	GLU
6	F	87	THR
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	43	ARG
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS

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Mol	Chain	Res	Type
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	238	PHE
1	N	264	LYS
1	N	278	MET
1	N	290	HIS
1	N	297	MET
1	N	338	MET
1	N	369	ASP
1	N	380	VAL
1	N	504	THR
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	78	LEU
2	O	86	MET
2	O	94	SER
2	O	113	TYR
2	O	148	MET
2	O	167	SER
2	O	202	SER
2	O	205	SER
2	O	217	LYS
3	P	29	SER
3	P	33	MET
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	31	LYS
4	Q	51	LEU
5	R	5	HIS
5	R	46	LYS
5	R	80	GLU
5	R	90	ARG
5	R	101	PRO
5	R	108	LYS
6	S	37	LYS

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Mol	Chain	Res	Type
6	S	43	LYS
6	S	48	LEU
6	S	53	THR
6	S	64	GLU
6	S	94	HIS
6	S	96	LEU
6	S	98	HIS
7	T	17	ARG
7	T	18	PHE
7	T	35	SER
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	61	SER
7	T	74	ARG
7	T	84	LYS
8	U	9	LYS
8	U	12	GLN
8	U	29	CYS
8	U	41	LYS
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	26	MET
9	V	37	PHE
10	W	4	ARG
10	W	36	MET
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	512	ASN
2	B	22	HIS
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	23	GLN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	99	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
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
2	O	203	ASN
3	P	68	GLN
3	P	149	HIS
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	5	HIS
5	R	78	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
9	V	8	GLN
9	V	70	GLN
10	W	57	HIS
13	Z	39	ASN

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	1.01	1 (12%)	6,9,11	6.38	4 (66%)
2	FME	B	1	2	8,9,10	1.97	2 (25%)	6,9,11	7.04	4 (66%)
7	TPO	G	11	7	8,10,11	2.04	4 (50%)	7,14,16	1.84	2 (28%)
9	SAC	I	1	9	7,8,9	2.32	2 (28%)	7,9,11	1.11	1 (14%)
1	FME	N	1	1	8,9,10	1.33	1 (12%)	6,9,11	6.11	4 (66%)
2	FME	O	1	2	8,9,10	1.09	1 (12%)	6,9,11	6.52	2 (33%)
7	TPO	T	11	7	8,10,11	2.07	4 (50%)	7,14,16	2.43	2 (28%)
9	SAC	V	1	9	7,8,9	3.08	2 (28%)	7,9,11	1.71	3 (42%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.18	1.09	1.22
2	O	1	FME	O1-CN	-2.48	1.15	1.22
1	A	1	FME	O1-CN	-2.39	1.15	1.22
2	B	1	FME	CB-CA	-2.01	1.49	1.53
7	T	11	TPO	CB-CA	2.14	1.57	1.54
7	G	11	TPO	P-O3P	2.15	1.62	1.54
7	T	11	TPO	P-O2P	2.18	1.62	1.54
7	G	11	TPO	P-OG1	2.32	1.67	1.60
7	G	11	TPO	P-O2P	2.51	1.63	1.54
7	T	11	TPO	P-O3P	2.66	1.64	1.54
1	N	1	FME	CA-N	3.00	1.50	1.46
7	T	11	TPO	P-O1P	3.20	1.61	1.51
7	G	11	TPO	P-O1P	3.61	1.63	1.51
9	I	1	SAC	OAC-C1A	4.17	1.32	1.23
9	I	1	SAC	CA-N	4.24	1.52	1.46
9	V	1	SAC	OAC-C1A	5.40	1.35	1.23
9	V	1	SAC	CA-N	5.67	1.54	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-16.27	97.80	122.82
2	O	1	FME	CA-N-CN	-15.72	98.64	122.82
1	A	1	FME	CA-N-CN	-14.12	101.11	122.82
1	N	1	FME	CA-N-CN	-13.38	102.24	122.82
2	B	1	FME	CG-CB-CA	-4.47	99.92	113.06
1	A	1	FME	CG-CB-CA	-3.86	101.71	113.06
1	A	1	FME	O-C-CA	-2.51	118.82	125.44
2	B	1	FME	O1-CN-N	-2.42	121.27	124.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	11	TPO	O-C-CA	-2.42	119.05	125.44
2	B	1	FME	O-C-CA	-2.41	119.07	125.44
7	G	11	TPO	O-C-CA	-2.28	119.42	125.44
9	I	1	SAC	CB-CA-N	-2.28	105.61	110.60
1	N	1	FME	O-C-CA	-2.25	119.51	125.44
9	V	1	SAC	OAC-C1A-C2A	-2.12	118.18	122.06
2	O	1	FME	O-C-CA	-2.09	119.93	125.44
9	V	1	SAC	O-C-CA	-2.06	119.99	125.44
9	V	1	SAC	CA-N-C1A	2.45	129.69	121.37
7	G	11	TPO	CG2-CB-CA	2.46	118.17	113.17
1	N	1	FME	CE-SD-CG	2.64	109.39	100.37
1	A	1	FME	CE-SD-CG	4.71	116.44	100.37
7	T	11	TPO	CG2-CB-CA	5.62	124.59	113.17
1	N	1	FME	O1-CN-N	5.67	132.93	124.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
1	N	1	FME	1	0
2	O	1	FME	1	0
7	T	11	TPO	1	0
9	V	1	SAC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	HEA	A	515	1	40,67,67	1.48	9 (22%)	41,103,103	2.58	17 (41%)
14	HEA	A	516	1,15	40,67,67	2.21	10 (25%)	41,103,103	3.37	23 (56%)
15	CYN	A	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.41	7 (11%)	65,65,65	2.41	16 (24%)
20	PGV	A	522	-	50,50,50	0.97	2 (4%)	51,56,56	1.30	5 (9%)
20	PGV	A	524	-	50,50,50	1.15	2 (4%)	51,56,56	1.39	7 (13%)
22	CHD	B	1085	-	29,32,32	1.50	5 (17%)	48,51,51	5.70	35 (72%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
24	PEK	C	264	-	51,52,52	0.89	2 (3%)	52,57,57	1.80	12 (23%)
20	PGV	C	267	-	50,50,50	0.87	3 (6%)	51,56,56	1.42	6 (11%)
20	PGV	C	268	-	50,50,50	1.25	2 (4%)	51,56,56	1.51	7 (13%)
25	CDL	C	270	-	99,99,99	1.33	12 (12%)	101,111,111	1.44	15 (14%)
22	CHD	C	271	-	29,32,32	0.82	1 (3%)	48,51,51	5.09	34 (70%)
22	CHD	C	525	-	29,32,32	1.80	6 (20%)	48,51,51	5.50	34 (70%)
19	TGL	D	523	-	62,62,62	1.57	7 (11%)	65,65,65	1.56	11 (16%)
26	PSC	E	229	-	51,51,51	1.25	3 (5%)	55,59,59	1.39	6 (10%)
24	PEK	G	1263	-	51,52,52	1.15	3 (5%)	52,57,57	1.22	6 (11%)
24	PEK	G	265	-	51,52,52	1.18	3 (5%)	52,57,57	1.26	3 (5%)
25	CDL	G	269	-	99,99,99	1.45	14 (14%)	101,111,111	1.54	17 (16%)
28	DMU	G	272	-	34,34,34	1.24	4 (11%)	45,45,45	3.36	23 (51%)
22	CHD	J	60	-	29,32,32	0.69	0	48,51,51	4.93	40 (83%)
19	TGL	L	522	-	62,62,62	1.53	8 (12%)	65,65,65	1.84	17 (26%)
28	DMU	M	526	-	34,34,34	0.83	1 (2%)	45,45,45	3.46	26 (57%)
20	PGV	N	1266	-	50,50,50	0.92	1 (2%)	51,56,56	1.37	6 (11%)
19	TGL	N	1521	-	62,62,62	1.30	6 (9%)	65,65,65	1.55	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	TGL	N	1522	-	62,62,62	1.54	7 (11%)	65,65,65	1.65	15 (23%)
20	PGV	N	1524	-	50,50,50	1.18	2 (4%)	51,56,56	1.35	6 (11%)
14	HEA	N	515	1	40,67,67	1.08	3 (7%)	41,103,103	2.41	9 (21%)
14	HEA	N	516	1,15	40,67,67	1.74	7 (17%)	41,103,103	3.28	19 (46%)
15	CYN	N	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	1.26	3 (10%)	48,51,51	5.62	33 (68%)
20	PGV	P	1267	-	50,50,50	0.84	2 (4%)	51,56,56	1.46	7 (13%)
20	PGV	P	1268	-	50,50,50	1.22	2 (4%)	51,56,56	1.54	7 (13%)
25	CDL	P	1270	-	99,99,99	1.33	12 (12%)	101,111,111	1.40	13 (12%)
22	CHD	P	1271	-	29,32,32	0.72	0	48,51,51	4.91	37 (77%)
28	DMU	P	1272	-	34,34,34	1.20	1 (2%)	45,45,45	3.30	24 (53%)
22	CHD	P	1525	-	29,32,32	1.39	4 (13%)	48,51,51	5.20	38 (79%)
19	TGL	Q	1523	-	62,62,62	1.32	6 (9%)	65,65,65	1.29	10 (15%)
26	PSC	R	1229	-	51,51,51	1.20	3 (5%)	55,59,59	1.05	4 (7%)
24	PEK	S	1265	-	51,52,52	1.32	4 (7%)	52,57,57	1.32	4 (7%)
24	PEK	T	1264	-	51,52,52	0.93	2 (3%)	52,57,57	1.91	8 (15%)
25	CDL	T	1269	-	99,99,99	1.34	12 (12%)	101,111,111	1.45	17 (16%)
24	PEK	T	263	-	51,52,52	1.19	2 (3%)	52,57,57	1.22	5 (9%)
22	CHD	W	1059	-	29,32,32	1.07	2 (6%)	48,51,51	5.17	33 (68%)
28	DMU	Z	1526	-	34,34,34	0.94	2 (5%)	45,45,45	3.23	21 (46%)

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
14	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	CYN	A	520	14,16	-	0/0/0/0	0/0/0/0
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
20	PGV	A	522	-	-	0/55/55/55	0/0/0/0
20	PGV	A	524	-	-	1/55/55/55	0/0/0/0
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
24	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
26	PSC	E	229	-	-	0/55/55/55	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
24	PEK	G	265	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
28	DMU	G	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
28	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	3/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	CYN	N	520	14,16	-	0/0/0/0	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
24	PEK	S	1265	-	-	0/56/56/56	0/0/0/0
24	PEK	T	1264	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
24	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1059	-	2/2/12/12	0/7/74/74	0/4/4/4
28	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (187) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	C3C-C2C	-5.25	1.33	1.40
22	C	525	CHD	C13-C12	-4.86	1.46	1.54
22	C	525	CHD	C1-C10	-4.41	1.45	1.54
14	N	516	HEA	C3C-C2C	-3.62	1.35	1.40
19	A	521	TGL	OC1-CC1	-3.61	1.11	1.22
25	T	1269	CDL	C59-C58	-3.54	1.31	1.51
25	P	1270	CDL	C59-C58	-3.37	1.32	1.51
19	L	522	TGL	C20-CA9	-3.33	1.32	1.51
19	L	522	TGL	C10-CB9	-3.32	1.32	1.51
25	G	269	CDL	C59-C58	-3.32	1.32	1.51
22	B	1085	CHD	C13-C14	-3.30	1.49	1.55
25	T	1269	CDL	C42-C41	-3.20	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.20	1.33	1.51
25	C	270	CDL	C62-C61	-3.18	1.33	1.51
22	B	1085	CHD	C10-C5	-3.18	1.50	1.55
25	T	1269	CDL	C62-C61	-3.12	1.33	1.51
25	C	270	CDL	C59-C58	-3.11	1.33	1.51
25	P	1270	CDL	C62-C61	-3.10	1.33	1.51
14	A	516	HEA	C4A-NA	-3.09	1.32	1.36
19	N	1522	TGL	C20-CA9	-3.08	1.33	1.51
25	G	269	CDL	C42-C41	-3.01	1.34	1.51
25	P	1270	CDL	C19-C18	-2.97	1.34	1.51
19	A	521	TGL	C10-CB9	-2.97	1.34	1.51
19	N	1521	TGL	C10-CB9	-2.96	1.34	1.51
19	D	523	TGL	C15-CC9	-2.94	1.34	1.51
19	A	521	TGL	C20-CA9	-2.94	1.34	1.51
25	C	270	CDL	C19-C18	-2.93	1.34	1.51
19	Q	1523	TGL	C20-CA9	-2.93	1.34	1.51
25	G	269	CDL	C22-C21	-2.92	1.34	1.51
25	G	269	CDL	C62-C61	-2.91	1.34	1.51
25	C	270	CDL	C79-C78	-2.90	1.34	1.51
28	Z	1526	DMU	C3-C4	-2.88	1.44	1.52
25	P	1270	CDL	C79-C78	-2.87	1.35	1.51
25	T	1269	CDL	C22-C21	-2.86	1.35	1.51
25	T	1269	CDL	C79-C78	-2.85	1.35	1.51
24	T	1264	PEK	O03-C01	-2.83	1.38	1.45
25	P	1270	CDL	C22-C21	-2.82	1.35	1.51
25	C	270	CDL	C22-C21	-2.82	1.35	1.51
25	C	270	CDL	C39-C38	-2.82	1.35	1.51
25	C	270	CDL	C82-C81	-2.81	1.35	1.51
25	T	1269	CDL	C19-C18	-2.80	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	269	CDL	C39-C38	-2.79	1.35	1.51
25	P	1270	CDL	C82-C81	-2.78	1.35	1.51
19	Q	1523	TGL	C15-CC9	-2.78	1.35	1.51
19	Q	1523	TGL	C10-CB9	-2.78	1.35	1.51
25	T	1269	CDL	C39-C38	-2.76	1.35	1.51
19	N	1521	TGL	C20-CA9	-2.74	1.35	1.51
25	G	269	CDL	C19-C18	-2.66	1.36	1.51
25	P	1270	CDL	C39-C38	-2.65	1.36	1.51
19	L	522	TGL	C15-CC9	-2.65	1.36	1.51
19	D	523	TGL	C20-CA9	-2.60	1.36	1.51
25	C	270	CDL	C42-C41	-2.59	1.36	1.51
25	T	1269	CDL	C82-C81	-2.58	1.36	1.51
19	N	1521	TGL	C15-CC9	-2.58	1.36	1.51
19	N	1522	TGL	C15-CC9	-2.58	1.36	1.51
22	O	229	CHD	C10-C5	-2.57	1.51	1.55
25	P	1270	CDL	C42-C41	-2.52	1.37	1.51
25	G	269	CDL	C79-C78	-2.51	1.37	1.51
25	G	269	CDL	C82-C81	-2.50	1.37	1.51
19	D	523	TGL	C10-CB9	-2.45	1.37	1.51
28	M	526	DMU	C3-C4	-2.42	1.46	1.52
19	A	521	TGL	C15-CC9	-2.40	1.37	1.51
14	A	515	HEA	C1D-ND	-2.35	1.33	1.36
22	P	1525	CHD	C10-C5	-2.22	1.51	1.55
14	N	515	HEA	C3C-C2C	-2.20	1.37	1.40
28	G	272	DMU	C3-C4	-2.10	1.47	1.52
14	N	515	HEA	C1A-NA	-2.06	1.33	1.36
22	O	229	CHD	C6-C7	-2.04	1.49	1.52
14	N	516	HEA	CMB-C2B	2.01	1.55	1.51
24	G	265	PEK	P-O12	2.01	1.68	1.59
24	G	1263	PEK	C03-C02	2.01	1.56	1.50
14	N	516	HEA	CMD-C2D	2.02	1.56	1.51
28	G	272	DMU	O1-C10	2.03	1.47	1.41
14	A	516	HEA	CMB-C2B	2.03	1.55	1.51
25	G	269	CDL	C16-C15	2.05	1.63	1.51
20	P	1267	PGV	O01-C1	2.08	1.40	1.34
28	G	272	DMU	O5-C6	2.09	1.47	1.41
22	P	1525	CHD	C21-C20	2.10	1.58	1.53
22	C	525	CHD	C11-C12	2.11	1.57	1.53
14	A	516	HEA	CMD-C2D	2.12	1.56	1.51
14	A	515	HEA	C22-C23	2.15	1.38	1.32
24	S	1265	PEK	C03-C02	2.16	1.56	1.50
14	A	515	HEA	C4B-NB	2.17	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	CMC-C2C	2.17	1.56	1.51
22	C	525	CHD	C21-C20	2.20	1.58	1.53
20	A	522	PGV	O06-C06	2.21	1.51	1.42
28	Z	1526	DMU	O16-C6	2.21	1.44	1.40
14	N	515	HEA	CMB-C2B	2.25	1.56	1.51
19	L	522	TGL	CG1-CG2	2.26	1.57	1.50
22	B	1085	CHD	C18-C13	2.27	1.58	1.54
19	L	522	TGL	CG3-CG2	2.27	1.57	1.50
24	S	1265	PEK	P-O11	2.28	1.69	1.59
22	C	525	CHD	C19-C10	2.31	1.58	1.54
14	A	516	HEA	CAA-C2A	2.32	1.56	1.52
20	C	267	PGV	C03-C02	2.36	1.57	1.50
14	A	515	HEA	C1B-CHB	2.37	1.46	1.39
22	P	1525	CHD	O12-C12	2.38	1.47	1.43
19	N	1522	TGL	CG3-CG2	2.39	1.57	1.50
24	C	264	PEK	O03-C21	2.44	1.40	1.33
14	A	515	HEA	CMB-C2B	2.46	1.56	1.51
22	B	1085	CHD	C19-C10	2.49	1.59	1.54
24	C	264	PEK	O01-C1	2.53	1.41	1.34
14	A	516	HEA	C1D-ND	2.60	1.40	1.36
25	G	269	CDL	C17-C16	2.62	1.66	1.51
20	C	267	PGV	O01-C1	2.63	1.42	1.34
14	N	516	HEA	C18-C19	2.64	1.38	1.33
14	A	516	HEA	C4B-NB	2.67	1.40	1.36
14	A	515	HEA	C1C-CHC	2.71	1.47	1.39
22	W	1059	CHD	C20-C17	2.71	1.59	1.54
22	B	1085	CHD	C4-C3	2.72	1.57	1.51
22	C	271	CHD	C20-C17	2.76	1.59	1.54
14	A	516	HEA	C18-C19	2.86	1.38	1.33
20	P	1267	PGV	O03-C19	2.87	1.42	1.33
14	N	516	HEA	C1D-ND	2.88	1.40	1.36
22	P	1525	CHD	C16-C17	2.90	1.61	1.54
20	C	267	PGV	O03-C19	2.97	1.42	1.33
14	A	515	HEA	C12-C13	3.05	1.63	1.53
14	N	516	HEA	C4B-NB	3.06	1.40	1.36
22	C	525	CHD	O12-C12	3.13	1.49	1.43
24	T	1264	PEK	O01-C1	3.15	1.43	1.34
14	A	515	HEA	O11-C11	3.17	1.50	1.42
22	W	1059	CHD	C11-C9	3.26	1.59	1.53
14	A	516	HEA	C1B-CHB	3.62	1.49	1.39
25	C	270	CDL	OB6-CB5	3.63	1.45	1.34
22	O	229	CHD	C11-C9	3.63	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1269	CDL	OA8-CA7	3.64	1.44	1.33
20	A	522	PGV	O03-C19	3.83	1.44	1.33
26	E	229	PSC	C13-C12	3.89	1.54	1.31
25	P	1270	CDL	OA6-CA5	3.89	1.46	1.34
26	R	1229	PSC	C13-C12	3.94	1.54	1.31
20	A	524	PGV	O01-C1	4.04	1.46	1.34
26	R	1229	PSC	O03-C19	4.08	1.45	1.33
25	P	1270	CDL	OB8-CB7	4.12	1.45	1.33
19	D	523	TGL	OG3-CC1	4.16	1.45	1.33
25	C	270	CDL	OB8-CB7	4.18	1.45	1.33
19	N	1521	TGL	OG3-CC1	4.20	1.46	1.33
25	C	270	CDL	OA6-CA5	4.21	1.46	1.34
20	N	1524	PGV	O01-C1	4.23	1.47	1.34
19	A	521	TGL	OG2-CB1	4.26	1.47	1.34
26	R	1229	PSC	O01-C1	4.35	1.47	1.34
24	G	1263	PEK	O01-C1	4.36	1.47	1.34
25	P	1270	CDL	OB6-CB5	4.43	1.47	1.34
20	P	1268	PGV	O03-C19	4.43	1.46	1.33
19	L	522	TGL	OG3-CC1	4.43	1.46	1.33
25	T	1269	CDL	OB8-CB7	4.44	1.46	1.33
19	Q	1523	TGL	OG2-CB1	4.48	1.47	1.34
20	N	1266	PGV	O03-C19	4.51	1.46	1.33
28	G	272	DMU	O16-C6	4.52	1.48	1.40
25	T	1269	CDL	OA6-CA5	4.55	1.47	1.34
19	N	1521	TGL	OG1-CA1	4.55	1.47	1.33
25	G	269	CDL	OB8-CB7	4.56	1.47	1.33
28	P	1272	DMU	O16-C6	4.58	1.48	1.40
19	A	521	TGL	OG3-CC1	4.62	1.47	1.33
26	E	229	PSC	O03-C19	4.65	1.47	1.33
26	E	229	PSC	O01-C1	4.66	1.48	1.34
24	T	263	PEK	O01-C1	4.66	1.48	1.34
24	G	265	PEK	O01-C1	4.66	1.48	1.34
24	S	1265	PEK	O01-C1	4.68	1.48	1.34
19	Q	1523	TGL	OG3-CC1	4.70	1.47	1.33
20	C	268	PGV	O03-C19	4.76	1.47	1.33
25	T	1269	CDL	OB6-CB5	4.82	1.48	1.34
19	Q	1523	TGL	OG1-CA1	4.90	1.48	1.33
24	G	1263	PEK	O03-C21	4.91	1.48	1.33
19	N	1521	TGL	OG2-CB1	4.91	1.49	1.34
25	G	269	CDL	OA6-CA5	4.91	1.49	1.34
24	G	265	PEK	O03-C21	5.02	1.48	1.33
19	D	523	TGL	OG2-CB1	5.03	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1522	TGL	OG1-CA1	5.07	1.48	1.33
19	N	1522	TGL	OG3-CC1	5.09	1.48	1.33
25	G	269	CDL	OB6-CB5	5.15	1.49	1.34
25	C	270	CDL	OA8-CA7	5.15	1.48	1.33
25	P	1270	CDL	OA8-CA7	5.16	1.48	1.33
25	G	269	CDL	OA8-CA7	5.17	1.48	1.33
19	D	523	TGL	OB1-CB1	5.23	1.38	1.22
20	N	1524	PGV	O03-C19	5.25	1.49	1.33
19	L	522	TGL	OG1-CA1	5.26	1.49	1.33
20	A	524	PGV	O03-C19	5.31	1.49	1.33
19	A	521	TGL	OG1-CA1	5.34	1.49	1.33
24	T	263	PEK	O03-C21	5.48	1.49	1.33
19	D	523	TGL	OG1-CA1	5.55	1.50	1.33
24	S	1265	PEK	O03-C21	5.64	1.50	1.33
20	C	268	PGV	O01-C1	5.74	1.51	1.34
20	P	1268	PGV	O01-C1	5.90	1.52	1.34
19	L	522	TGL	OG2-CB1	6.03	1.52	1.34
19	N	1522	TGL	OG2-CB1	6.44	1.53	1.34
14	N	516	HEA	O11-C11	6.96	1.59	1.42
14	A	516	HEA	O11-C11	9.17	1.64	1.42

All (687) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	1085	CHD	C18-C13-C12	-17.19	92.32	109.09
22	O	229	CHD	C18-C13-C12	-12.62	96.78	109.09
22	C	525	CHD	C19-C10-C9	-9.83	96.45	111.18
22	P	1525	CHD	C18-C13-C12	-8.93	100.38	109.09
22	C	271	CHD	C18-C13-C12	-8.70	100.61	109.09
14	N	516	HEA	CMC-C2C-C1C	-8.69	113.99	128.36
22	O	229	CHD	C19-C10-C9	-8.63	98.24	111.18
22	O	229	CHD	O12-C12-C13	-8.53	97.28	111.11
22	C	525	CHD	C23-C22-C20	-7.98	105.35	114.75
14	N	515	HEA	C13-C12-C11	-7.77	104.19	114.51
22	C	525	CHD	C18-C13-C12	-7.68	101.60	109.09
14	A	515	HEA	C13-C12-C11	-7.58	104.44	114.51
22	J	60	CHD	C18-C13-C12	-7.52	101.75	109.09
22	W	1059	CHD	C6-C5-C4	-7.39	102.80	111.05
22	B	1085	CHD	C18-C13-C17	-7.18	99.89	111.22
22	B	1085	CHD	C19-C10-C9	-7.12	100.50	111.18
22	P	1525	CHD	C18-C13-C14	-7.12	99.98	111.22
22	C	525	CHD	O12-C12-C13	-7.03	99.71	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1525	CHD	C19-C10-C9	-6.81	100.97	111.18
22	P	1271	CHD	C18-C13-C12	-6.73	102.53	109.09
14	N	515	HEA	C4B-C3B-C11	-6.73	119.71	127.01
14	N	516	HEA	C3C-CAC-CBC	-6.63	112.76	126.32
22	P	1525	CHD	O7-C7-C6	-6.38	94.43	110.06
22	O	229	CHD	C18-C13-C17	-6.30	101.29	111.22
14	A	516	HEA	C20-C19-C18	-6.07	109.55	121.05
22	C	525	CHD	C6-C5-C4	-6.04	104.30	111.05
19	A	521	TGL	OG3-CC1-OC1	-6.03	107.92	123.49
14	A	516	HEA	CAA-CBA-CGA	-5.97	101.81	112.75
22	O	229	CHD	C1-C10-C9	-5.90	101.94	111.45
14	A	515	HEA	CAA-C2A-C1A	-5.70	120.81	127.01
19	D	523	TGL	OG2-CB1-CB2	-5.63	99.29	111.53
22	W	1059	CHD	C1-C10-C9	-5.61	102.40	111.45
22	B	1085	CHD	O12-C12-C13	-5.59	102.05	111.11
22	O	229	CHD	C6-C5-C4	-5.57	104.82	111.05
24	T	1264	PEK	O03-C01-C02	-5.56	93.73	108.69
22	P	1525	CHD	C18-C13-C17	-5.45	102.62	111.22
22	C	525	CHD	C18-C13-C14	-5.37	102.75	111.22
22	C	525	CHD	C18-C13-C17	-5.29	102.88	111.22
22	W	1059	CHD	C18-C13-C12	-5.20	104.02	109.09
22	P	1525	CHD	O12-C12-C13	-5.17	102.72	111.11
14	A	516	HEA	CMB-C2B-C1B	-5.12	119.89	128.36
14	A	515	HEA	CAA-CBA-CGA	-5.10	103.39	112.75
22	P	1525	CHD	O12-C12-C11	-5.09	98.64	109.06
22	C	525	CHD	C4-C5-C10	-5.01	107.14	112.66
22	O	229	CHD	C18-C13-C14	-4.96	103.40	111.22
28	Z	1526	DMU	O7-C10-C5	-4.86	96.27	108.10
22	C	271	CHD	C6-C5-C4	-4.85	105.63	111.05
22	P	1271	CHD	C23-C22-C20	-4.85	109.04	114.75
22	C	271	CHD	C18-C13-C17	-4.84	103.58	111.22
19	L	522	TGL	OG3-CC1-OC1	-4.76	111.22	123.49
14	N	515	HEA	C17-C18-C19	-4.60	117.76	127.76
22	C	525	CHD	O7-C7-C6	-4.59	98.82	110.06
14	N	516	HEA	C26-C15-C14	-4.49	114.69	123.50
22	P	1271	CHD	O7-C7-C6	-4.45	99.17	110.06
22	W	1059	CHD	C18-C13-C14	-4.43	104.22	111.22
22	P	1271	CHD	O12-C12-C11	-4.37	100.11	109.06
20	C	267	PGV	C27-C26-C25	-4.32	92.25	114.53
14	A	516	HEA	C26-C15-C14	-4.31	115.05	123.50
20	C	267	PGV	C8-C9-C10	-4.28	97.15	113.86
22	C	271	CHD	C19-C10-C1	-4.27	101.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	1085	CHD	O12-C12-C11	-4.26	100.34	109.06
22	P	1271	CHD	C19-C10-C9	-4.26	104.80	111.18
22	J	60	CHD	C19-C10-C5	-4.26	102.74	110.25
22	P	1525	CHD	C1-C10-C9	-4.25	104.60	111.45
22	J	60	CHD	C18-C13-C17	-4.23	104.55	111.22
20	P	1267	PGV	C8-C9-C10	-4.23	97.36	113.86
22	O	229	CHD	C4-C5-C10	-4.18	108.05	112.66
22	P	1525	CHD	C22-C20-C17	-4.17	101.48	110.24
22	C	525	CHD	C22-C20-C17	-4.15	101.52	110.24
25	C	270	CDL	CB4-OB6-CB5	-4.07	108.13	117.89
24	C	264	PEK	C24-C23-C22	-4.02	98.54	113.29
22	W	1059	CHD	C19-C10-C5	-4.00	103.18	110.25
22	C	271	CHD	C23-C22-C20	-3.98	110.06	114.75
14	N	516	HEA	OMA-CMA-C3A	-3.97	117.08	125.11
22	B	1085	CHD	O7-C7-C6	-3.95	100.39	110.06
22	B	1085	CHD	C6-C5-C4	-3.94	106.65	111.05
14	A	516	HEA	CAD-C3D-C4D	-3.88	122.80	127.01
22	C	525	CHD	C1-C10-C9	-3.83	105.27	111.45
22	P	1525	CHD	C19-C10-C5	-3.80	103.55	110.25
28	M	526	DMU	O7-C10-C5	-3.71	99.07	108.10
14	A	515	HEA	CMC-C2C-C1C	-3.69	122.25	128.36
14	A	516	HEA	C1A-C2A-C3A	-3.69	103.38	107.07
20	P	1267	PGV	O03-C19-O04	-3.66	114.05	123.49
20	N	1266	PGV	O01-C1-O02	-3.64	113.90	123.67
22	J	60	CHD	C6-C5-C4	-3.63	107.00	111.05
22	J	60	CHD	C18-C13-C14	-3.62	105.50	111.22
25	P	1270	CDL	OB8-CB7-OB9	-3.62	114.15	123.49
22	P	1271	CHD	C18-C13-C17	-3.61	105.52	111.22
22	W	1059	CHD	C23-C22-C20	-3.61	110.50	114.75
22	J	60	CHD	C19-C10-C9	-3.59	105.79	111.18
25	C	270	CDL	OB8-CB7-OB9	-3.54	114.36	123.49
22	B	1085	CHD	C1-C10-C9	-3.51	105.78	111.45
22	P	1271	CHD	O12-C12-C13	-3.49	105.45	111.11
28	M	526	DMU	O7-C10-O1	-3.46	101.93	110.68
19	A	521	TGL	CB3-CB2-CB1	-3.45	100.03	113.59
22	C	271	CHD	O12-C12-C11	-3.41	102.09	109.06
22	J	60	CHD	C23-C22-C20	-3.36	110.79	114.75
22	J	60	CHD	O7-C7-C6	-3.35	101.86	110.06
14	A	515	HEA	C3C-CAC-CBC	-3.31	119.55	126.32
14	A	515	HEA	C27-C19-C18	-3.20	117.22	123.50
14	A	516	HEA	CBA-CAA-C2A	-3.20	106.80	112.53
24	C	264	PEK	O01-C1-O02	-3.18	115.12	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	265	PEK	O03-C21-O04	-3.17	115.30	123.49
22	P	1271	CHD	C6-C5-C4	-3.17	107.51	111.05
14	A	515	HEA	C26-C15-C14	-3.10	117.42	123.50
14	N	516	HEA	CAA-CBA-CGA	-3.09	107.08	112.75
20	P	1268	PGV	C03-C02-C01	-3.07	104.88	112.07
20	C	268	PGV	O04-C19-C20	-3.05	111.53	123.72
14	N	515	HEA	C27-C19-C18	-3.02	117.57	123.50
22	W	1059	CHD	O7-C7-C6	-2.97	102.79	110.06
22	B	1085	CHD	C19-C10-C5	-2.91	105.11	110.25
22	C	525	CHD	O12-C12-C11	-2.90	103.12	109.06
28	M	526	DMU	C25-C28-C31	-2.86	99.75	114.53
20	P	1267	PGV	C27-C26-C25	-2.86	99.77	114.53
26	E	229	PSC	O01-C1-O02	-2.84	116.04	123.67
24	C	264	PEK	O03-C21-C22	-2.83	103.28	111.90
14	N	516	HEA	C25-C23-C24	-2.82	107.70	114.64
20	P	1268	PGV	O04-C19-C20	-2.81	112.47	123.72
25	T	1269	CDL	CA4-OA6-CA5	-2.79	111.19	117.89
14	A	516	HEA	C13-C14-C15	-2.76	121.77	127.76
22	B	1085	CHD	C4-C5-C10	-2.75	109.62	112.66
20	A	522	PGV	O03-C19-O04	-2.75	116.39	123.49
24	T	1264	PEK	C24-C23-C22	-2.74	103.24	113.29
19	A	521	TGL	CG3-CG2-CG1	-2.73	105.68	112.07
19	L	522	TGL	CB4-CB3-CB2	-2.72	103.32	113.29
22	O	229	CHD	O12-C12-C11	-2.71	103.51	109.06
22	P	1525	CHD	C23-C22-C20	-2.71	111.56	114.75
20	A	524	PGV	C3-C2-C1	-2.69	103.02	113.59
25	C	270	CDL	C52-C51-CB5	-2.68	103.04	113.59
14	A	516	HEA	C17-C16-C15	-2.65	104.09	112.71
25	T	1269	CDL	CB6-CB4-CB3	-2.64	105.91	112.07
14	A	516	HEA	C3C-CAC-CBC	-2.64	120.93	126.32
22	P	1525	CHD	C4-C5-C10	-2.63	109.76	112.66
19	N	1522	TGL	OG3-CC1-OC1	-2.63	116.71	123.49
14	A	515	HEA	C4B-C3B-C11	-2.63	124.16	127.01
24	C	264	PEK	O03-C01-C02	-2.62	101.63	108.69
25	G	269	CDL	CB6-CB4-CB3	-2.61	105.98	112.07
14	N	516	HEA	CAD-C3D-C4D	-2.59	124.19	127.01
24	G	1263	PEK	O03-C21-O04	-2.59	116.81	123.49
22	P	1271	CHD	C19-C10-C1	-2.58	103.86	108.20
24	C	264	PEK	O01-C02-C01	-2.56	99.34	108.36
26	E	229	PSC	C32-C31-C30	-2.56	101.33	114.53
24	T	1264	PEK	O01-C1-O02	-2.55	116.83	123.67
19	N	1522	TGL	OB1-CB1-CB2	-2.54	113.58	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	1265	PEK	O03-C21-O04	-2.53	116.97	123.49
24	C	264	PEK	C30-C29-C28	-2.50	101.60	114.53
22	P	1525	CHD	C21-C20-C22	-2.50	106.19	110.35
20	P	1268	PGV	O02-C1-C2	-2.49	113.78	123.72
14	A	515	HEA	CAD-C3D-C4D	-2.48	124.32	127.01
20	N	1266	PGV	C23-C22-C21	-2.47	101.77	114.53
24	T	1264	PEK	C03-C02-C01	-2.47	106.30	112.07
19	L	522	TGL	CA5-CA4-CA3	-2.46	101.80	114.53
25	C	270	CDL	C53-C52-C51	-2.45	104.30	113.29
14	A	515	HEA	OMA-CMA-C3A	-2.44	120.19	125.11
19	L	522	TGL	OB1-CB1-CB2	-2.44	113.98	123.72
14	N	516	HEA	CAA-C2A-C1A	-2.43	124.37	127.01
22	C	271	CHD	C19-C10-C9	-2.42	107.55	111.18
25	G	269	CDL	OB8-CB7-OB9	-2.42	117.25	123.49
20	C	268	PGV	O02-C1-C2	-2.41	114.08	123.72
14	A	515	HEA	C20-C21-C22	-2.40	105.41	111.69
25	G	269	CDL	C17-C16-C15	-2.40	102.16	114.53
25	T	1269	CDL	OB8-CB7-OB9	-2.39	117.32	123.49
25	G	269	CDL	OB7-CB5-C51	-2.38	114.19	123.72
20	N	1266	PGV	O03-C19-O04	-2.37	117.37	123.49
22	P	1271	CHD	C22-C23-C24	-2.37	103.34	113.02
20	C	267	PGV	C14-C13-C12	-2.37	100.01	112.45
22	C	271	CHD	C19-C10-C5	-2.36	106.08	110.25
22	J	60	CHD	C1-C10-C9	-2.33	107.69	111.45
24	C	264	PEK	C32-C31-C30	-2.33	102.50	114.53
20	P	1268	PGV	O12-P-O13	-2.31	100.63	109.62
20	A	524	PGV	C8-C9-C10	-2.29	104.91	113.86
19	Q	1523	TGL	OG3-CC1-OC1	-2.27	117.63	123.49
22	P	1271	CHD	C11-C9-C10	-2.27	111.43	113.79
28	M	526	DMU	C19-C22-C25	-2.27	102.81	114.53
22	P	1271	CHD	C19-C10-C5	-2.27	106.24	110.25
25	P	1270	CDL	CB4-OB6-CB5	-2.26	112.46	117.89
19	N	1522	TGL	CA5-CA4-CA3	-2.26	102.87	114.53
19	N	1521	TGL	OG1-CA1-OA1	-2.26	117.67	123.49
22	C	271	CHD	C22-C23-C24	-2.25	103.82	113.02
22	P	1525	CHD	O7-C7-C8	-2.24	104.32	109.26
22	O	229	CHD	O7-C7-C6	-2.24	104.57	110.06
14	A	515	HEA	CMB-C2B-C1B	-2.24	124.66	128.36
19	L	522	TGL	C26-C25-C24	-2.24	102.98	114.53
26	R	1229	PSC	O03-C19-O04	-2.23	117.75	123.49
25	G	269	CDL	OA8-CA7-OA9	-2.22	117.76	123.49
25	P	1270	CDL	OA6-CA5-OA7	-2.22	117.72	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	522	PGV	C7-C6-C5	-2.21	103.11	114.53
22	O	229	CHD	C19-C10-C5	-2.21	106.35	110.25
24	C	264	PEK	C26-C25-C24	-2.20	103.16	114.53
14	N	516	HEA	CMD-C2D-C3D	-2.19	120.67	125.24
22	J	60	CHD	O12-C12-C11	-2.18	104.60	109.06
19	N	1521	TGL	CC4-CC3-CC2	-2.18	105.30	113.29
25	T	1269	CDL	CB2-C1-CA2	-2.17	105.90	112.92
22	J	60	CHD	O12-C12-C13	-2.16	107.61	111.11
22	W	1059	CHD	C19-C10-C1	-2.15	104.58	108.20
14	N	516	HEA	C1A-C2A-C3A	-2.15	104.92	107.07
24	T	1264	PEK	C30-C29-C28	-2.15	103.43	114.53
19	A	521	TGL	OB1-CB1-CB2	-2.14	115.15	123.72
19	L	522	TGL	C24-C23-C22	-2.12	103.56	114.53
25	C	270	CDL	C57-C56-C55	-2.12	103.61	114.53
20	N	1524	PGV	O01-C1-O02	-2.11	117.99	123.67
25	T	1269	CDL	OA8-CA7-OA9	-2.11	118.06	123.49
20	P	1267	PGV	O01-C1-O02	-2.10	118.03	123.67
20	C	268	PGV	O12-P-O13	-2.10	101.48	109.62
22	J	60	CHD	O7-C7-C8	-2.09	104.64	109.26
25	C	270	CDL	C61-C60-C59	-2.08	103.77	114.53
22	C	525	CHD	C21-C20-C17	-2.08	109.49	112.96
19	L	522	TGL	CA3-CA2-CA1	-2.07	105.45	113.59
19	Q	1523	TGL	CG3-CG2-CG1	-2.07	107.23	112.07
19	L	522	TGL	CB9-CB8-CB7	-2.07	103.84	114.53
24	C	264	PEK	C27-C26-C25	-2.07	103.85	114.53
25	T	1269	CDL	OA8-CA6-CA4	-2.06	103.14	108.69
22	B	1085	CHD	C23-C22-C20	-2.06	112.33	114.75
19	D	523	TGL	OG1-CA1-OA1	-2.06	118.19	123.49
14	N	516	HEA	CBA-CAA-C2A	-2.05	108.85	112.53
19	Q	1523	TGL	OG1-CA1-OA1	-2.05	118.20	123.49
25	C	270	CDL	CA6-CA4-CA3	-2.05	107.28	112.07
20	C	267	PGV	O12-P-O13	-2.04	101.68	109.62
24	G	1263	PEK	C18-C17-C16	-2.04	105.89	113.86
20	C	267	PGV	C9-C10-C11	-2.04	101.75	112.45
25	P	1270	CDL	C55-C54-C53	-2.03	104.03	114.53
25	G	269	CDL	C18-C17-C16	-2.02	104.12	114.53
25	G	269	CDL	OA6-CA5-OA7	-2.01	118.26	123.67
19	A	521	TGL	OA1-CA1-CA2	-2.01	115.69	123.72
14	A	515	HEA	C17-C18-C19	-2.00	123.41	127.76
24	T	1264	PEK	C28-C27-C26	-2.00	104.19	114.53
20	N	1524	PGV	O01-C02-C03	2.01	115.43	108.36
19	N	1522	TGL	C16-C15-CC9	2.01	124.92	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1271	CHD	C13-C14-C8	2.02	117.35	114.75
22	W	1059	CHD	C21-C20-C17	2.02	116.32	112.96
26	E	229	PSC	O03-C19-C20	2.03	118.08	111.90
19	N	1521	TGL	C16-C15-CC9	2.04	125.05	114.53
25	T	1269	CDL	CA6-OA8-CA7	2.06	122.61	116.85
28	P	1272	DMU	O7-C10-O1	2.08	115.95	110.68
22	O	229	CHD	C19-C10-C1	2.09	111.72	108.20
25	G	269	CDL	C43-C42-C41	2.11	125.41	114.53
14	N	516	HEA	CMB-C2B-C3B	2.11	129.46	125.14
22	B	1085	CHD	C16-C17-C13	2.11	105.70	103.60
25	P	1270	CDL	C42-C41-C40	2.11	125.45	114.53
22	P	1525	CHD	C15-C14-C8	2.13	121.41	118.32
19	A	521	TGL	C16-C15-CC9	2.14	125.56	114.53
22	P	1271	CHD	C21-C20-C17	2.14	116.52	112.96
19	D	523	TGL	OG3-CC1-CC2	2.14	118.44	111.90
14	A	516	HEA	C27-C19-C18	2.15	127.72	123.50
25	P	1270	CDL	C40-C39-C38	2.15	125.62	114.53
19	L	522	TGL	OG3-CG3-CG2	2.15	114.47	108.69
19	D	523	TGL	C13-C12-C11	2.15	125.65	114.53
20	N	1266	PGV	O02-C1-C2	2.15	132.34	123.72
26	R	1229	PSC	O01-C02-C03	2.16	115.98	108.36
26	E	229	PSC	O01-C02-C03	2.17	116.00	108.36
25	P	1270	CDL	OA8-CA6-CA4	2.17	114.54	108.69
28	M	526	DMU	O49-C1-C2	2.18	115.24	110.34
25	T	1269	CDL	C43-C42-C41	2.18	125.81	114.53
20	P	1267	PGV	O02-C1-C2	2.20	132.51	123.72
22	P	1271	CHD	C9-C10-C5	2.20	111.92	108.67
20	P	1267	PGV	O14-P-O13	2.20	124.44	112.53
19	L	522	TGL	C15-CC9-CC8	2.20	125.89	114.53
24	T	263	PEK	C02-O01-C1	2.21	123.19	117.89
28	Z	1526	DMU	C11-C9-C8	2.21	118.47	113.02
25	P	1270	CDL	C39-C38-C37	2.21	125.95	114.53
19	N	1522	TGL	CC3-CC2-CC1	2.21	122.29	113.59
22	O	229	CHD	C16-C17-C13	2.22	105.81	103.60
25	C	270	CDL	C42-C41-C40	2.24	126.09	114.53
19	D	523	TGL	CB3-CB2-CB1	2.24	122.39	113.59
19	N	1522	TGL	C10-CB9-CB8	2.24	126.10	114.53
28	P	1272	DMU	O61-C57-C4	2.24	118.73	111.33
20	P	1268	PGV	O01-C02-C03	2.24	116.26	108.36
25	C	270	CDL	OA8-CA6-CA4	2.27	114.79	108.69
20	C	268	PGV	O01-C02-C01	2.28	116.41	108.36
25	C	270	CDL	C82-C81-C80	2.29	126.34	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	271	CHD	C9-C10-C5	2.31	112.09	108.67
25	C	270	CDL	O1-C1-CB2	2.31	118.14	109.35
19	A	521	TGL	CB4-CB3-CB2	2.31	121.75	113.29
28	G	272	DMU	O61-C57-C4	2.31	118.98	111.33
22	B	1085	CHD	C14-C8-C7	2.31	114.95	111.74
19	N	1521	TGL	OG2-CB1-CB2	2.32	116.57	111.53
19	N	1522	TGL	OG2-CG2-CG3	2.33	116.56	108.36
25	T	1269	CDL	C82-C81-C80	2.35	126.65	114.53
28	Z	1526	DMU	C10-O1-C9	2.35	118.31	113.75
24	T	263	PEK	O03-C01-C02	2.38	115.09	108.69
28	P	1272	DMU	C10-C5-C7	2.38	114.67	109.97
22	C	271	CHD	C14-C8-C9	2.38	112.90	109.62
14	N	515	HEA	C26-C15-C16	2.39	119.06	115.41
14	A	515	HEA	C20-C19-C18	2.40	125.60	121.05
25	P	1270	CDL	CA6-OA8-CA7	2.40	123.58	116.85
28	Z	1526	DMU	C57-C4-C3	2.41	120.25	113.25
22	J	60	CHD	C13-C14-C8	2.41	117.86	114.75
19	L	522	TGL	CG3-OG3-CC1	2.41	123.60	116.85
28	P	1272	DMU	C57-C4-C3	2.42	120.29	113.25
19	N	1521	TGL	OG2-CG2-CG1	2.43	116.91	108.36
28	M	526	DMU	C1-C2-C3	2.43	114.93	109.60
28	P	1272	DMU	O16-C18-C19	2.44	119.57	109.88
22	C	271	CHD	C9-C8-C7	2.45	114.81	111.92
19	N	1521	TGL	OG2-CG2-CG3	2.45	116.98	108.36
19	Q	1523	TGL	OG1-CA1-CA2	2.46	119.38	111.90
24	T	1264	PEK	C3-C2-C1	2.47	123.31	113.59
14	A	516	HEA	CMB-C2B-C3B	2.48	130.20	125.14
28	M	526	DMU	O5-C6-O16	2.48	116.02	110.05
25	G	269	CDL	C19-C18-C17	2.48	127.33	114.53
20	C	267	PGV	O14-P-O13	2.48	125.98	112.53
25	T	1269	CDL	C39-C38-C37	2.48	127.36	114.53
25	C	270	CDL	OA8-CA7-C31	2.49	119.49	111.90
20	A	522	PGV	O03-C01-C02	2.49	115.40	108.69
19	N	1522	TGL	C15-CC9-CC8	2.50	127.43	114.53
28	M	526	DMU	C6-O5-C4	2.50	118.60	113.75
19	D	523	TGL	C10-CB9-CB8	2.50	127.45	114.53
22	B	1085	CHD	C2-C1-C10	2.51	117.31	112.84
22	P	1525	CHD	C5-C6-C7	2.52	117.25	114.44
19	Q	1523	TGL	OG2-CB1-CB2	2.53	117.02	111.53
22	O	229	CHD	C9-C11-C12	2.53	117.56	114.36
19	A	521	TGL	C15-CC9-CC8	2.54	127.64	114.53
28	Z	1526	DMU	O7-C3-C2	2.54	113.73	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	516	HEA	C16-C17-C18	2.55	118.37	111.69
28	G	272	DMU	O4-C7-C5	2.56	116.10	110.34
22	P	1525	CHD	C14-C8-C7	2.56	115.30	111.74
28	M	526	DMU	O55-C2-C3	2.56	115.94	109.87
28	Z	1526	DMU	O5-C6-O16	2.57	116.23	110.05
22	J	60	CHD	C17-C13-C14	2.57	102.65	100.05
24	G	1263	PEK	C02-O01-C1	2.57	124.05	117.89
25	T	1269	CDL	OA8-CA7-C31	2.57	119.74	111.90
28	G	272	DMU	C11-C9-C8	2.58	119.37	113.02
20	N	1524	PGV	O03-C19-C20	2.58	119.77	111.90
28	M	526	DMU	O4-C7-C5	2.59	116.16	110.34
28	Z	1526	DMU	C6-C1-C2	2.60	115.10	109.97
25	T	1269	CDL	C83-C82-C81	2.62	128.03	114.53
25	T	1269	CDL	OB8-CB7-C71	2.62	119.87	111.90
20	A	524	PGV	O01-C1-C2	2.62	117.22	111.53
19	D	523	TGL	OG2-CB1-OB1	2.63	130.74	123.67
25	C	270	CDL	CA6-OA8-CA7	2.64	124.22	116.85
14	A	515	HEA	CMC-C2C-C3C	2.64	130.25	125.09
22	O	229	CHD	C14-C8-C7	2.68	115.46	111.74
25	P	1270	CDL	OA8-CA7-C31	2.69	120.10	111.90
28	M	526	DMU	C6-C1-C2	2.69	115.28	109.97
22	O	229	CHD	C6-C7-C8	2.70	114.34	111.47
14	N	515	HEA	CMD-C2D-C3D	2.74	130.96	125.24
28	P	1272	DMU	C11-C9-C8	2.75	119.79	113.02
22	J	60	CHD	C14-C8-C9	2.77	113.43	109.62
25	G	269	CDL	C82-C81-C80	2.77	128.86	114.53
25	G	269	CDL	OB8-CB7-C71	2.78	120.37	111.90
22	C	271	CHD	C17-C13-C14	2.78	102.87	100.05
20	P	1267	PGV	O03-C19-C20	2.79	120.40	111.90
19	Q	1523	TGL	CG2-OG2-CB1	2.80	124.60	117.89
22	P	1525	CHD	C16-C17-C13	2.80	106.38	103.60
24	C	264	PEK	O04-C21-C22	2.80	134.93	123.72
19	N	1521	TGL	CG1-OG1-CA1	2.80	124.69	116.85
20	A	524	PGV	O03-C19-C20	2.81	120.45	111.90
26	E	229	PSC	C02-O01-C1	2.81	124.64	117.89
20	A	522	PGV	C02-O01-C1	2.82	124.67	117.89
22	B	1085	CHD	C21-C20-C17	2.82	117.66	112.96
20	N	1524	PGV	C02-O01-C1	2.83	124.68	117.89
25	T	1269	CDL	OB8-CB6-CB4	2.84	116.33	108.69
28	Z	1526	DMU	C10-C5-C7	2.84	115.58	109.97
28	G	272	DMU	O5-C6-O16	2.87	116.97	110.05
25	G	269	CDL	C80-C79-C78	2.88	129.40	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	P	1270	CDL	OB6-CB4-CB6	2.90	118.59	108.36
19	N	1521	TGL	OG3-CC1-CC2	2.93	120.82	111.90
14	N	515	HEA	C16-C17-C18	2.94	119.38	111.69
22	P	1271	CHD	C17-C13-C12	2.94	120.29	117.68
28	G	272	DMU	C10-O1-C9	2.96	119.49	113.75
14	N	515	HEA	CBA-CAA-C2A	2.96	117.83	112.53
24	G	1263	PEK	C01-O03-C21	2.96	125.13	116.85
19	N	1522	TGL	OG1-CG1-CG2	2.97	116.69	108.69
22	P	1525	CHD	C9-C8-C7	3.00	115.47	111.92
19	L	522	TGL	CC3-CC2-CC1	3.01	125.44	113.59
20	A	524	PGV	C01-O03-C19	3.01	125.28	116.85
28	Z	1526	DMU	O3-C5-C7	3.02	117.13	110.34
19	D	523	TGL	CG3-OG3-CC1	3.02	125.30	116.85
14	N	516	HEA	C3B-C4B-NB	3.03	116.67	110.94
19	Q	1523	TGL	OG2-CG2-CG3	3.04	119.06	108.36
19	N	1522	TGL	OG3-CC1-CC2	3.05	121.19	111.90
19	N	1522	TGL	OG1-CA1-CA2	3.06	121.22	111.90
24	T	263	PEK	C01-O03-C21	3.07	125.42	116.85
22	P	1525	CHD	C11-C9-C10	3.07	116.98	113.79
14	A	516	HEA	C4B-C3B-C11	3.07	130.34	127.01
20	A	524	PGV	O01-C02-C03	3.08	119.23	108.36
19	Q	1523	TGL	CG3-OG3-CC1	3.09	125.48	116.85
28	G	272	DMU	C10-C5-C7	3.10	116.08	109.97
26	R	1229	PSC	O03-C19-C20	3.11	121.38	111.90
24	S	1265	PEK	O03-C01-C02	3.13	117.11	108.69
25	G	269	CDL	CB6-OB8-CB7	3.16	125.70	116.85
19	Q	1523	TGL	CG1-OG1-CA1	3.17	125.70	116.85
25	T	1269	CDL	CB6-OB8-CB7	3.18	125.73	116.85
28	M	526	DMU	C57-C4-C3	3.21	122.57	113.25
24	G	1263	PEK	O03-C21-C22	3.23	121.73	111.90
19	N	1522	TGL	OG3-CG3-CG2	3.24	117.41	108.69
28	P	1272	DMU	C10-O1-C9	3.25	120.05	113.75
14	N	516	HEA	C12-C11-C3B	3.26	119.33	112.59
24	T	263	PEK	O03-C21-C22	3.30	121.95	111.90
22	P	1525	CHD	C1-C2-C3	3.30	115.79	110.43
22	J	60	CHD	C9-C8-C7	3.31	115.83	111.92
22	C	525	CHD	C15-C16-C17	3.34	111.86	105.12
24	C	264	PEK	C11-C10-C9	3.34	123.13	112.00
14	A	515	HEA	C3C-C4C-NC	3.35	113.54	109.21
20	N	1266	PGV	O03-C01-C02	3.36	117.73	108.69
22	B	1085	CHD	C11-C9-C10	3.36	117.28	113.79
22	C	271	CHD	C21-C20-C17	3.39	118.60	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	229	CHD	C15-C14-C13	3.42	107.00	103.60
20	C	268	PGV	C01-O03-C19	3.43	126.45	116.85
22	P	1525	CHD	C14-C8-C9	3.44	114.35	109.62
19	D	523	TGL	CG2-OG2-CB1	3.44	126.15	117.89
28	P	1272	DMU	O7-C3-C4	3.44	118.38	109.32
14	A	516	HEA	CAA-C2A-C1A	3.46	130.76	127.01
14	N	516	HEA	C3C-C4C-NC	3.49	113.72	109.21
28	G	272	DMU	C1-C2-C3	3.49	117.26	109.60
28	Z	1526	DMU	C1-C2-C3	3.49	117.27	109.60
28	M	526	DMU	C10-C5-C7	3.49	116.85	109.97
28	P	1272	DMU	C18-O16-C6	3.50	120.06	113.94
28	P	1272	DMU	O5-C6-O16	3.51	118.51	110.05
22	B	1085	CHD	C9-C11-C12	3.52	118.81	114.36
19	N	1521	TGL	OG1-CA1-CA2	3.53	122.67	111.90
19	Q	1523	TGL	OG3-CC1-CC2	3.53	122.67	111.90
19	D	523	TGL	OG1-CA1-CA2	3.55	122.70	111.90
22	J	60	CHD	C11-C9-C10	3.55	117.48	113.79
19	L	522	TGL	OG2-CB1-CB2	3.55	119.25	111.53
28	P	1272	DMU	C6-O5-C4	3.57	120.67	113.75
28	G	272	DMU	O7-C10-C5	3.57	116.80	108.10
22	P	1525	CHD	C13-C17-C20	3.58	123.86	119.50
19	A	521	TGL	OG2-CG2-CG3	3.59	121.02	108.36
28	G	272	DMU	O7-C3-C2	3.60	116.46	107.17
22	C	525	CHD	C5-C6-C7	3.61	118.47	114.44
22	P	1525	CHD	C9-C11-C12	3.63	118.94	114.36
28	Z	1526	DMU	C6-O5-C4	3.72	120.97	113.75
22	C	525	CHD	C14-C8-C9	3.72	114.74	109.62
28	M	526	DMU	C7-C8-C9	3.72	116.69	110.20
20	N	1266	PGV	O03-C19-C20	3.73	123.27	111.90
28	G	272	DMU	C6-O5-C4	3.74	121.00	113.75
19	A	521	TGL	OG1-CG1-CG2	3.74	118.77	108.69
26	R	1229	PSC	O01-C1-C2	3.75	119.68	111.53
22	W	1059	CHD	C11-C9-C8	3.77	116.09	110.73
14	A	516	HEA	C21-C20-C19	3.77	125.01	112.71
19	A	521	TGL	OG2-CG2-CG1	3.82	121.83	108.36
14	A	516	HEA	CAD-CBD-CGD	3.83	119.77	112.75
25	G	269	CDL	CA6-OA8-CA7	3.86	127.63	116.85
28	Z	1526	DMU	C7-C8-C9	3.89	116.98	110.20
20	A	522	PGV	O03-C19-C20	3.91	123.82	111.90
22	P	1525	CHD	C11-C12-C13	3.91	115.18	111.20
19	L	522	TGL	OG1-CA1-CA2	3.95	123.92	111.90
28	P	1272	DMU	C1-C2-C3	3.95	118.27	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	M	526	DMU	O7-C3-C2	3.95	117.36	107.17
24	S	1265	PEK	O01-C1-C2	3.95	120.12	111.53
19	N	1522	TGL	CG3-OG3-CC1	3.96	127.93	116.85
22	C	525	CHD	C11-C9-C8	3.98	116.38	110.73
28	M	526	DMU	O3-C5-C7	3.99	119.33	110.34
28	M	526	DMU	O16-C6-C1	4.00	113.09	108.04
22	B	1085	CHD	C15-C14-C8	4.01	124.14	118.32
24	T	263	PEK	O01-C1-C2	4.03	120.29	111.53
28	P	1272	DMU	C2-C3-C4	4.03	119.96	110.84
28	M	526	DMU	C8-C7-C5	4.03	118.32	110.79
28	G	272	DMU	O7-C3-C4	4.04	119.95	109.32
22	P	1271	CHD	C17-C13-C14	4.05	104.14	100.05
24	G	265	PEK	O01-C1-C2	4.07	120.38	111.53
25	G	269	CDL	OA8-CA7-C31	4.08	124.34	111.90
22	J	60	CHD	C22-C20-C17	4.08	118.82	110.24
22	B	1085	CHD	O3-C3-C4	4.09	118.00	109.86
25	T	1269	CDL	OA6-CA5-C11	4.12	120.48	111.53
14	A	516	HEA	CBD-CAD-C3D	4.14	119.95	112.53
22	W	1059	CHD	C17-C13-C12	4.16	121.37	117.68
25	C	270	CDL	OB8-CB7-C71	4.16	124.58	111.90
19	A	521	TGL	OG1-CA1-CA2	4.17	124.60	111.90
14	N	516	HEA	C21-C20-C19	4.17	126.29	112.71
22	P	1271	CHD	C13-C17-C20	4.19	124.61	119.50
22	B	1085	CHD	C9-C8-C7	4.23	116.92	111.92
22	C	525	CHD	C13-C14-C8	4.25	120.23	114.75
28	G	272	DMU	C7-C8-C9	4.31	117.72	110.20
28	M	526	DMU	O5-C4-C57	4.33	117.31	106.36
22	C	525	CHD	C2-C1-C10	4.34	120.59	112.84
22	P	1525	CHD	C2-C1-C10	4.35	120.61	112.84
28	M	526	DMU	O1-C9-C11	4.36	117.37	106.36
22	P	1525	CHD	O3-C3-C4	4.38	118.57	109.86
28	G	272	DMU	C6-C1-C2	4.39	118.62	109.97
22	B	1085	CHD	C16-C17-C20	4.42	119.94	112.05
19	D	523	TGL	CG1-OG1-CA1	4.45	129.29	116.85
22	P	1271	CHD	C9-C11-C12	4.49	120.04	114.36
25	P	1270	CDL	OA6-CA5-C11	4.51	121.33	111.53
19	N	1522	TGL	OG2-CB1-CB2	4.51	121.34	111.53
22	W	1059	CHD	C9-C8-C7	4.51	117.25	111.92
28	P	1272	DMU	O7-C10-C5	4.52	119.09	108.10
22	B	1085	CHD	C11-C9-C8	4.52	117.16	110.73
20	N	1524	PGV	C01-O03-C19	4.53	129.51	116.85
25	P	1270	CDL	OB8-CB7-C71	4.55	125.76	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	P	1272	DMU	C7-C8-C9	4.55	118.13	110.20
28	G	272	DMU	O1-C9-C11	4.55	117.86	106.36
24	G	1263	PEK	O01-C1-C2	4.57	121.46	111.53
20	N	1524	PGV	O01-C1-C2	4.58	121.48	111.53
25	G	269	CDL	OA6-CA5-C11	4.60	121.52	111.53
22	C	525	CHD	C9-C11-C12	4.60	120.17	114.36
19	L	522	TGL	OG1-CG1-CG2	4.63	121.15	108.69
28	P	1272	DMU	O5-C4-C57	4.64	118.08	106.36
28	P	1272	DMU	C6-C1-C2	4.64	119.12	109.97
19	L	522	TGL	OG3-CC1-CC2	4.66	126.08	111.90
28	Z	1526	DMU	C2-C3-C4	4.66	121.39	110.84
22	J	60	CHD	C9-C10-C5	4.67	115.58	108.67
22	O	229	CHD	C16-C17-C20	4.67	120.39	112.05
22	J	60	CHD	C14-C8-C7	4.68	118.23	111.74
14	A	516	HEA	C27-C19-C20	4.69	122.57	115.41
22	W	1059	CHD	C11-C9-C10	4.72	118.70	113.79
28	G	272	DMU	C2-C3-C4	4.75	121.58	110.84
22	C	271	CHD	C14-C8-C7	4.78	118.37	111.74
19	L	522	TGL	CG2-OG2-CB1	4.81	129.44	117.89
19	N	1522	TGL	CG2-OG2-CB1	4.82	129.45	117.89
28	P	1272	DMU	O5-C6-C1	4.84	120.21	110.28
22	C	271	CHD	C9-C11-C12	4.86	120.50	114.36
28	P	1272	DMU	O1-C9-C11	4.87	118.67	106.36
28	Z	1526	DMU	O1-C9-C11	4.88	118.70	106.36
28	M	526	DMU	O5-C4-C3	4.89	120.08	109.75
28	G	272	DMU	C8-C7-C5	4.90	119.93	110.79
25	C	270	CDL	OA6-CA5-C11	4.96	122.30	111.53
22	O	229	CHD	C14-C8-C9	4.96	116.45	109.62
24	S	1265	PEK	O03-C21-C22	4.97	127.05	111.90
24	G	265	PEK	O03-C21-C22	4.99	127.11	111.90
22	B	1085	CHD	C4-C3-C2	5.00	116.89	110.52
28	G	272	DMU	O5-C6-C1	5.01	120.56	110.28
22	C	271	CHD	C2-C1-C10	5.03	121.82	112.84
28	Z	1526	DMU	O5-C4-C57	5.03	119.08	106.36
19	N	1521	TGL	CG3-OG3-CC1	5.06	131.01	116.85
19	A	521	TGL	CG3-OG3-CC1	5.06	131.01	116.85
22	W	1059	CHD	C9-C10-C5	5.07	116.17	108.67
20	A	524	PGV	C02-O01-C1	5.09	130.11	117.89
20	C	268	PGV	O03-C19-C20	5.10	127.44	111.90
28	Z	1526	DMU	C8-C7-C5	5.10	120.32	110.79
22	P	1271	CHD	C4-C5-C10	5.12	118.30	112.66
14	A	515	HEA	C26-C15-C16	5.14	123.26	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Z	1526	DMU	O5-C4-C3	5.15	120.62	109.75
14	N	515	HEA	C27-C19-C20	5.16	123.28	115.41
22	J	60	CHD	C2-C1-C10	5.17	122.06	112.84
22	J	60	CHD	C11-C9-C8	5.19	118.11	110.73
22	P	1271	CHD	C2-C1-C10	5.21	122.14	112.84
28	P	1272	DMU	C8-C7-C5	5.24	120.57	110.79
22	J	60	CHD	C15-C14-C8	5.27	125.96	118.32
22	J	60	CHD	C9-C11-C12	5.27	121.02	114.36
22	O	229	CHD	C2-C1-C10	5.31	122.32	112.84
28	G	272	DMU	O5-C4-C3	5.32	120.98	109.75
22	W	1059	CHD	C22-C20-C17	5.33	121.43	110.24
22	J	60	CHD	C16-C17-C20	5.34	121.58	112.05
22	C	525	CHD	C5-C4-C3	5.36	120.89	112.91
22	P	1525	CHD	C17-C13-C14	5.40	105.51	100.05
22	C	525	CHD	O3-C3-C4	5.45	120.70	109.86
25	T	1269	CDL	OB6-CB5-C51	5.46	123.40	111.53
20	P	1268	PGV	O03-C19-C20	5.47	128.55	111.90
14	A	516	HEA	C3B-C4B-NB	5.49	121.31	110.94
22	P	1271	CHD	C1-C2-C3	5.49	119.34	110.43
22	C	525	CHD	C11-C9-C10	5.50	119.50	113.79
28	G	272	DMU	C18-O16-C6	5.50	123.56	113.94
14	A	516	HEA	O11-C11-C12	5.51	123.19	109.73
22	O	229	CHD	C9-C8-C7	5.51	118.43	111.92
20	C	268	PGV	O01-C1-C2	5.53	123.54	111.53
22	W	1059	CHD	C2-C1-C10	5.54	122.73	112.84
22	B	1085	CHD	C6-C7-C8	5.58	117.39	111.47
14	N	516	HEA	C20-C21-C22	5.59	126.32	111.69
28	P	1272	DMU	O5-C4-C3	5.62	121.62	109.75
14	A	516	HEA	C17-C18-C19	5.64	140.04	127.76
22	P	1271	CHD	C16-C17-C20	5.70	122.22	112.05
22	C	271	CHD	C4-C3-C2	5.71	117.80	110.52
22	C	271	CHD	C1-C2-C3	5.74	119.75	110.43
22	P	1271	CHD	C15-C14-C13	5.75	109.32	103.60
28	G	272	DMU	O5-C4-C57	5.77	120.94	106.36
22	B	1085	CHD	C1-C2-C3	5.78	119.80	110.43
22	C	525	CHD	C11-C12-C13	5.80	117.09	111.20
22	W	1059	CHD	C11-C12-C13	5.80	117.10	111.20
22	P	1271	CHD	C11-C12-C13	5.82	117.11	111.20
28	M	526	DMU	C2-C3-C4	5.83	124.01	110.84
22	B	1085	CHD	C11-C12-C13	5.83	117.12	111.20
22	O	229	CHD	C5-C6-C7	5.83	120.94	114.44
22	B	1085	CHD	C17-C13-C14	5.84	105.95	100.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	1059	CHD	C4-C5-C10	5.86	119.11	112.66
22	B	1085	CHD	C14-C8-C9	5.87	117.70	109.62
22	J	60	CHD	C1-C10-C5	5.88	117.48	107.81
22	P	1271	CHD	C14-C8-C7	5.89	119.91	111.74
22	W	1059	CHD	C1-C10-C5	5.90	117.50	107.81
19	N	1521	TGL	CG2-OG2-CB1	5.91	132.06	117.89
22	P	1271	CHD	C14-C13-C12	5.91	112.68	107.39
22	W	1059	CHD	C1-C2-C3	5.91	120.03	110.43
22	C	271	CHD	C11-C9-C8	5.94	119.18	110.73
22	J	60	CHD	C5-C4-C3	5.95	121.76	112.91
22	J	60	CHD	C4-C3-C2	6.00	118.18	110.52
22	J	60	CHD	C11-C12-C13	6.01	117.30	111.20
22	O	229	CHD	C11-C12-C13	6.03	117.32	111.20
22	W	1059	CHD	C4-C3-C2	6.04	118.22	110.52
20	P	1268	PGV	O01-C1-C2	6.04	124.66	111.53
22	J	60	CHD	C15-C14-C13	6.07	109.63	103.60
22	J	60	CHD	C13-C17-C20	6.09	126.92	119.50
22	C	525	CHD	C14-C13-C12	6.12	112.87	107.39
22	C	271	CHD	C17-C13-C12	6.16	123.14	117.68
22	W	1059	CHD	C9-C11-C12	6.19	122.18	114.36
22	J	60	CHD	C1-C2-C3	6.20	120.50	110.43
19	A	521	TGL	OG2-CB1-CB2	6.24	125.10	111.53
22	C	271	CHD	C4-C5-C10	6.24	119.53	112.66
25	G	269	CDL	OB6-CB5-C51	6.25	125.12	111.53
26	E	229	PSC	O01-C1-C2	6.28	125.17	111.53
22	C	271	CHD	C1-C10-C5	6.29	118.15	107.81
22	P	1271	CHD	C4-C3-C2	6.30	118.55	110.52
22	C	525	CHD	C15-C14-C13	6.30	109.87	103.60
28	P	1272	DMU	O1-C9-C8	6.31	121.53	109.68
22	O	229	CHD	C15-C14-C8	6.33	127.51	118.32
24	C	264	PEK	C2-C3-C4	6.35	125.96	113.30
22	W	1059	CHD	C5-C4-C3	6.38	122.41	112.91
22	W	1059	CHD	C6-C5-C10	6.45	119.76	112.66
22	C	271	CHD	C5-C4-C3	6.45	122.51	112.91
22	J	60	CHD	C16-C17-C13	6.45	110.02	103.60
22	P	1525	CHD	C11-C9-C8	6.47	119.93	110.73
22	P	1271	CHD	C1-C10-C5	6.49	118.47	107.81
22	C	525	CHD	C17-C13-C14	6.49	106.61	100.05
22	J	60	CHD	C6-C5-C10	6.51	119.83	112.66
22	P	1271	CHD	C5-C4-C3	6.57	122.69	112.91
22	P	1271	CHD	C16-C17-C13	6.58	110.14	103.60
22	W	1059	CHD	C6-C7-C8	6.58	118.45	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	1059	CHD	C15-C14-C8	6.61	127.92	118.32
28	G	272	DMU	O1-C10-C5	6.62	123.86	110.28
22	C	271	CHD	C6-C7-C8	6.65	118.53	111.47
22	J	60	CHD	C4-C5-C10	6.67	120.01	112.66
22	P	1525	CHD	C4-C3-C2	6.67	119.03	110.52
28	Z	1526	DMU	O5-C6-C1	6.71	124.04	110.28
22	J	60	CHD	C5-C6-C7	6.75	121.97	114.44
22	C	271	CHD	C15-C14-C13	6.80	110.36	103.60
22	P	1271	CHD	C6-C7-C8	6.83	118.71	111.47
22	P	1525	CHD	C5-C4-C3	6.83	123.07	112.91
22	C	525	CHD	C9-C8-C7	6.87	120.04	111.92
22	O	229	CHD	C11-C9-C8	6.91	120.55	110.73
22	O	229	CHD	C17-C13-C14	6.92	107.05	100.05
22	W	1059	CHD	C15-C14-C13	6.93	110.49	103.60
28	Z	1526	DMU	O1-C9-C8	6.96	122.74	109.68
28	G	272	DMU	O1-C9-C8	6.97	122.76	109.68
22	C	271	CHD	C11-C12-C13	7.02	118.33	111.20
22	C	525	CHD	C13-C17-C20	7.05	128.09	119.50
22	C	271	CHD	C16-C17-C13	7.06	110.62	103.60
28	P	1272	DMU	O1-C10-C5	7.13	124.91	110.28
28	Z	1526	DMU	O16-C6-C1	7.16	117.08	108.04
19	A	521	TGL	OG3-CC1-CC2	7.17	133.75	111.90
22	P	1271	CHD	C11-C9-C8	7.18	120.94	110.73
22	O	229	CHD	C4-C3-C2	7.19	119.68	110.52
22	W	1059	CHD	C14-C13-C12	7.22	113.86	107.39
28	M	526	DMU	O1-C10-C5	7.24	125.14	110.28
22	P	1525	CHD	C6-C7-C8	7.26	119.17	111.47
22	B	1085	CHD	C5-C4-C3	7.28	123.74	112.91
28	Z	1526	DMU	O1-C10-C5	7.29	125.23	110.28
22	J	60	CHD	C6-C7-C8	7.31	119.22	111.47
22	P	1271	CHD	C5-C6-C7	7.31	122.59	114.44
22	C	271	CHD	C16-C17-C20	7.39	125.23	112.05
22	C	271	CHD	C14-C13-C12	7.62	114.22	107.39
28	M	526	DMU	C18-O16-C6	7.64	127.29	113.94
22	P	1271	CHD	C15-C14-C8	7.65	129.43	118.32
22	B	1085	CHD	C15-C14-C13	7.69	111.24	103.60
22	C	271	CHD	C5-C6-C7	7.73	123.06	114.44
22	P	1271	CHD	C6-C5-C10	7.89	121.34	112.66
22	P	1525	CHD	C15-C14-C13	7.89	111.44	103.60
14	N	516	HEA	C26-C15-C16	7.91	127.49	115.41
28	G	272	DMU	O16-C6-C1	7.97	118.10	108.04
28	M	526	DMU	O1-C9-C8	7.99	124.69	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	516	HEA	C26-C15-C16	8.01	127.64	115.41
28	M	526	DMU	O5-C6-C1	8.02	126.73	110.28
22	W	1059	CHD	C5-C6-C7	8.03	123.39	114.44
22	C	271	CHD	C6-C5-C10	8.05	121.53	112.66
22	C	271	CHD	C15-C14-C8	8.23	130.27	118.32
22	P	1525	CHD	C17-C13-C12	8.26	125.00	117.68
14	N	516	HEA	CMC-C2C-C3C	8.33	141.38	125.09
22	O	229	CHD	C17-C13-C12	8.33	125.06	117.68
22	J	60	CHD	C17-C13-C12	8.41	125.14	117.68
22	W	1059	CHD	C14-C8-C7	8.42	123.42	111.74
28	P	1272	DMU	O16-C6-C1	8.58	118.87	108.04
22	C	525	CHD	C10-C9-C8	8.61	121.33	111.88
22	P	1525	CHD	C10-C9-C8	8.68	121.40	111.88
19	A	521	TGL	CG2-OG2-CB1	8.85	139.12	117.89
22	J	60	CHD	C14-C13-C12	8.86	115.33	107.39
22	C	525	CHD	C4-C3-C2	8.87	121.83	110.52
24	T	1264	PEK	C2-C3-C4	9.15	131.53	113.30
22	W	1059	CHD	C16-C17-C13	9.28	112.83	103.60
22	P	1525	CHD	C6-C5-C10	9.35	122.96	112.66
22	P	1525	CHD	C1-C10-C5	9.45	123.35	107.81
22	O	229	CHD	C5-C4-C3	9.46	126.98	112.91
22	B	1085	CHD	C10-C9-C8	9.73	122.56	111.88
22	O	229	CHD	C10-C9-C8	9.81	122.64	111.88
22	W	1059	CHD	C13-C17-C20	9.90	131.56	119.50
22	B	1085	CHD	C14-C13-C12	10.19	116.52	107.39
22	O	229	CHD	C6-C5-C10	10.20	123.89	112.66
22	C	525	CHD	C17-C13-C12	10.31	126.82	117.68
22	J	60	CHD	C10-C9-C8	10.55	123.46	111.88
22	O	229	CHD	C1-C10-C5	10.62	125.26	107.81
22	W	1059	CHD	C10-C9-C8	10.84	123.78	111.88
22	C	525	CHD	C1-C10-C5	11.10	126.05	107.81
22	B	1085	CHD	C1-C10-C5	11.20	126.22	107.81
22	B	1085	CHD	C17-C13-C12	11.32	127.71	117.68
22	B	1085	CHD	C6-C5-C10	11.87	125.73	112.66
22	C	525	CHD	C6-C5-C10	12.23	126.13	112.66
22	O	229	CHD	C14-C13-C12	12.28	118.38	107.39
22	P	1525	CHD	C14-C13-C12	12.55	118.63	107.39
22	C	271	CHD	C10-C9-C8	13.34	126.52	111.88
22	P	1271	CHD	C10-C9-C8	13.89	127.12	111.88

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C5
28	P	1272	DMU	C6
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C2
28	P	1272	DMU	C10
22	W	1059	CHD	C17
22	W	1059	CHD	C9
28	M	526	DMU	C2
28	M	526	DMU	C4
28	M	526	DMU	C9
28	M	526	DMU	C5
22	J	60	CHD	C17
22	J	60	CHD	C9
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
28	G	272	DMU	C5
28	G	272	DMU	C6
28	G	272	DMU	C9
28	G	272	DMU	C4
28	G	272	DMU	C2
28	G	272	DMU	C3
22	P	1271	CHD	C9
28	Z	1526	DMU	C2
28	Z	1526	DMU	C4
28	Z	1526	DMU	C9
28	Z	1526	DMU	C6
28	Z	1526	DMU	C5
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
22	C	271	CHD	C9

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C02-O01-C1-C2
20	N	1524	PGV	C02-O01-C1-O02
20	N	1524	PGV	P-O11-C03-C02
20	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

42 monomers are involved in 341 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	5	0
14	A	516	HEA	8	0
19	A	521	TGL	7	0
20	A	522	PGV	2	0
20	A	524	PGV	8	0
22	B	1085	CHD	3	0
24	C	264	PEK	3	0
20	C	267	PGV	3	0
20	C	268	PGV	3	0
25	C	270	CDL	21	0
22	C	271	CHD	3	0
22	C	525	CHD	1	0
19	D	523	TGL	13	0
26	E	229	PSC	16	0
24	G	1263	PEK	11	0
24	G	265	PEK	13	0
25	G	269	CDL	28	0
28	G	272	DMU	3	0
22	J	60	CHD	2	0
19	L	522	TGL	15	0
28	M	526	DMU	1	0
19	N	1521	TGL	7	0
19	N	1522	TGL	15	0
20	N	1524	PGV	7	0
14	N	515	HEA	3	0
14	N	516	HEA	10	0
15	N	520	CYN	2	0
22	O	229	CHD	1	0
20	P	1267	PGV	3	0
20	P	1268	PGV	2	0
25	P	1270	CDL	19	0
22	P	1271	CHD	4	0
28	P	1272	DMU	5	0
22	P	1525	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	1523	TGL	10	0
26	R	1229	PSC	14	0
24	S	1265	PEK	16	0
24	T	1264	PEK	9	0
25	T	1269	CDL	34	0
24	T	263	PEK	19	0
22	W	1059	CHD	6	0
28	Z	1526	DMU	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	0.58	56 (10%) 7 8	23, 29, 40, 63	0
1	N	513/514 (99%)	0.35	33 (6%) 23 26	30, 36, 47, 68	0
2	B	226/227 (99%)	-0.29	4 (1%) 71 76	24, 35, 59, 78	0
2	O	226/227 (99%)	-0.01	6 (2%) 58 64	33, 45, 70, 88	0
3	C	259/261 (99%)	-0.39	1 (0%) 93 94	26, 32, 43, 62	0
3	P	259/261 (99%)	-0.40	3 (1%) 81 84	29, 36, 47, 67	0
4	D	144/147 (97%)	-0.40	1 (0%) 89 91	30, 37, 56, 70	0
4	Q	144/147 (97%)	1.33	31 (21%) 1 1	39, 52, 76, 118	0
5	E	105/109 (96%)	0.03	2 (1%) 70 75	31, 38, 63, 99	0
5	R	105/109 (96%)	0.29	5 (4%) 34 40	36, 43, 68, 103	0
6	F	98/98 (100%)	0.40	9 (9%) 11 12	29, 39, 80, 127	0
6	S	98/98 (100%)	0.57	11 (11%) 7 7	34, 43, 86, 123	0
7	G	83/85 (97%)	0.78	15 (18%) 2 2	29, 39, 110, 113	0
7	T	83/85 (97%)	0.76	18 (21%) 1 1	29, 42, 102, 110	0
8	H	79/85 (92%)	0.38	12 (15%) 3 3	30, 41, 90, 112	0
8	U	79/85 (92%)	0.95	17 (21%) 1 1	37, 48, 94, 113	0
9	I	72/73 (98%)	0.27	7 (9%) 10 11	34, 46, 80, 83	0
9	V	72/73 (98%)	0.85	13 (18%) 2 2	39, 55, 82, 85	0
10	J	58/59 (98%)	0.27	8 (13%) 4 4	31, 41, 65, 96	0
10	W	58/59 (98%)	0.61	11 (18%) 2 1	34, 45, 69, 107	0
11	K	49/56 (87%)	-0.33	0 100 100	33, 41, 52, 62	0
11	X	49/56 (87%)	1.23	13 (26%) 1 0	44, 51, 64, 76	0
12	L	46/47 (97%)	-0.40	2 (4%) 39 44	29, 34, 50, 79	0
12	Y	46/47 (97%)	0.10	3 (6%) 22 25	34, 45, 61, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.18	3 (6%) 19 22	30, 34, 71, 101	0
13	Z	43/46 (93%)	0.52	8 (18%) 2 1	41, 46, 90, 112	0
All	All	3550/3614 (98%)	0.25	292 (8%) 14 16	23, 38, 69, 127	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	32.3
4	Q	5	VAL	14.3
6	S	97	ALA	14.2
4	Q	4	SER	13.0
6	F	96	LEU	11.3
7	G	2	SER	11.0
6	F	97	ALA	10.9
6	F	98	HIS	10.7
4	Q	8	SER	10.5
7	G	3	ALA	10.4
4	Q	7	LYS	10.0
8	U	7	LYS	9.8
6	F	2	SER	9.1
7	T	1	ALA	8.5
6	S	96	LEU	8.4
13	Z	43	SER	8.2
8	H	46	LYS	8.1
8	U	8	ILE	8.1
10	J	58	LYS	7.9
6	F	1	ALA	7.7
8	H	44	THR	7.5
10	W	58	LYS	7.5
6	S	94	HIS	7.3
6	S	2	SER	7.1
8	H	47	GLY	6.8
5	R	109	VAL	6.5
7	G	5	LYS	6.4
7	G	42	ARG	6.4
11	X	7	PRO	6.3
5	R	5	HIS	6.1
6	F	95	GLN	6.0
8	H	7	LYS	6.0
11	X	6	ALA	5.9
8	H	45	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
10	J	1	PHE	5.9
7	T	5	LYS	5.8
6	S	98	HIS	5.8
6	S	1	ALA	5.7
11	X	13	TYR	5.6
13	M	43	SER	5.6
5	E	5	HIS	5.6
8	U	44	THR	5.4
7	T	42	ARG	5.2
9	V	30	GLY	5.2
7	T	36	TRP	5.0
9	I	25	PHE	4.9
7	T	2	SER	4.8
1	A	66	ILE	4.7
8	U	45	ALA	4.6
13	Z	32	TRP	4.6
5	E	109	VAL	4.6
4	Q	147	LYS	4.6
7	T	4	ALA	4.6
9	V	29	LEU	4.6
7	G	40	GLY	4.5
7	G	1	ALA	4.5
7	G	8	HIS	4.4
7	T	40	GLY	4.4
7	T	39	SER	4.4
9	I	37	PHE	4.4
10	W	52	TRP	4.3
9	V	37	PHE	4.3
10	W	57	HIS	4.3
1	A	73	ILE	4.2
2	O	113	TYR	4.1
12	Y	47	LYS	4.1
1	N	3	ILE	4.1
8	H	43	MET	4.1
5	R	96	LEU	4.0
9	I	30	GLY	4.0
9	V	2	THR	4.0
9	I	29	LEU	4.0
8	U	9	LYS	4.0
4	Q	58	GLU	4.0
4	Q	53	ILE	4.0
8	U	10	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
9	V	33	THR	3.8
6	S	95	GLN	3.8
1	A	195	LEU	3.7
13	Z	40	TYR	3.7
13	Z	35	TYR	3.7
7	G	84	LYS	3.7
12	L	2	HIS	3.7
1	N	66	ILE	3.7
1	A	202	LEU	3.7
8	U	47	GLY	3.6
6	S	93	PRO	3.6
1	A	243	VAL	3.6
1	A	199	LEU	3.6
4	Q	46	ALA	3.6
4	Q	62	LEU	3.5
7	T	8	HIS	3.5
10	W	26	ALA	3.5
10	J	52	TRP	3.5
8	H	48	GLY	3.5
8	U	48	GLY	3.5
7	G	37	LEU	3.5
1	N	62	ALA	3.4
4	Q	48	TRP	3.4
8	U	55	TRP	3.4
4	Q	138	TRP	3.4
4	Q	33	LEU	3.4
8	U	42	ALA	3.3
4	Q	30	VAL	3.3
1	A	75	ILE	3.3
1	A	64	VAL	3.3
7	T	84	LYS	3.2
7	G	4	ALA	3.2
13	Z	39	ASN	3.2
1	A	237	PHE	3.2
11	X	23	THR	3.2
3	P	3	HIS	3.2
1	N	75	ILE	3.2
7	G	7	ASP	3.2
8	U	49	ASP	3.2
4	Q	51	LEU	3.2
1	N	377	PHE	3.2
1	A	67	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
6	F	3	GLY	3.1
1	A	70	VAL	3.1
2	O	217	LYS	3.1
6	F	94	HIS	3.1
11	X	16	ALA	3.1
1	N	70	VAL	3.1
13	Z	13	LYS	3.1
4	Q	102	TYR	3.0
8	H	8	ILE	3.0
1	A	194	LEU	3.0
11	X	52	GLU	3.0
4	Q	39	ALA	3.0
7	T	6	GLY	3.0
7	T	10	GLY	3.0
1	N	373	VAL	3.0
8	U	11	TYR	3.0
1	N	2	PHE	3.0
10	W	1	PHE	3.0
9	V	26	MET	3.0
1	A	62	ALA	3.0
7	T	3	ALA	3.0
7	T	43	GLU	2.9
9	V	25	PHE	2.9
4	Q	40	LEU	2.9
1	N	246	LEU	2.9
9	I	33	THR	2.9
13	Z	42	LYS	2.9
1	A	197	LEU	2.9
8	U	43	MET	2.9
1	N	201	VAL	2.9
12	Y	19	TRP	2.9
13	M	40	TYR	2.9
4	Q	97	ILE	2.8
10	W	30	ILE	2.8
2	B	59	GLN	2.8
1	A	235	PHE	2.8
1	A	246	LEU	2.8
1	A	71	MET	2.8
7	T	41	HIS	2.8
10	J	57	HIS	2.8
1	A	236	TRP	2.8
1	A	385	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	161	ALA	2.7
1	A	193	VAL	2.7
4	Q	49	SER	2.7
1	N	67	PHE	2.7
1	N	193	VAL	2.7
7	G	9	GLY	2.7
3	P	38	ASN	2.7
7	G	43	GLU	2.7
1	A	65	MET	2.7
1	N	202	LEU	2.6
1	A	153	ALA	2.6
10	W	55	PHE	2.6
10	J	2	GLU	2.6
1	N	243	VAL	2.6
2	O	47	THR	2.6
4	Q	43	LYS	2.6
1	N	71	MET	2.6
4	Q	124	LEU	2.6
1	N	388	ALA	2.6
8	H	42	ALA	2.6
1	A	241	PRO	2.5
7	T	37	LEU	2.5
4	D	147	LYS	2.5
1	A	238	PHE	2.5
5	R	52	LEU	2.5
1	A	126	TRP	2.5
10	W	56	PRO	2.5
1	A	192	ALA	2.5
9	V	31	PHE	2.5
1	A	201	VAL	2.5
8	H	50	VAL	2.5
1	N	384	GLY	2.5
1	A	196	LEU	2.5
9	V	53	ASN	2.5
7	T	33	LEU	2.5
10	J	56	PRO	2.5
10	J	30	ILE	2.5
1	N	383	MET	2.4
10	W	48	TYR	2.4
3	C	92	LEU	2.4
3	P	91	VAL	2.4
1	A	74	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	241	PRO	2.4
8	U	46	LYS	2.4
12	Y	20	ARG	2.4
1	N	197	LEU	2.4
6	S	44	GLU	2.4
11	X	19	ALA	2.4
11	X	35	GLN	2.4
9	I	34	PHE	2.4
11	X	9	PHE	2.4
1	A	386	VAL	2.4
1	A	203	ALA	2.4
1	N	245	ILE	2.4
10	W	2	GLU	2.4
1	A	440	TYR	2.4
4	Q	140	TYR	2.4
1	A	191	THR	2.4
1	A	188	VAL	2.4
1	A	389	ILE	2.4
10	J	48	TYR	2.4
6	S	3	GLY	2.3
2	B	199	ILE	2.3
11	X	15	ASN	2.3
1	A	68	PHE	2.3
1	N	285	PHE	2.3
4	Q	134	PHE	2.3
9	V	34	PHE	2.3
1	A	381	LEU	2.3
1	A	78	PHE	2.3
1	N	385	ALA	2.3
4	Q	52	SER	2.3
7	T	9	GLY	2.3
8	U	52	VAL	2.3
8	U	85	ILE	2.3
1	A	198	SER	2.3
9	V	65	LYS	2.3
1	N	158	ILE	2.3
1	N	199	LEU	2.3
7	G	41	HIS	2.3
7	G	6	GLY	2.2
1	N	196	LEU	2.2
1	A	63	PHE	2.2
1	A	383	MET	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	128	VAL	2.2
1	N	73	ILE	2.2
1	A	377	PHE	2.2
5	R	11	PHE	2.2
4	Q	44	GLU	2.2
8	H	9	LYS	2.2
11	X	36	ILE	2.2
1	A	388	ALA	2.2
4	Q	10	ASP	2.2
1	N	126	TRP	2.2
1	N	381	LEU	2.2
2	B	60	GLU	2.2
6	S	43	LYS	2.2
1	A	105	LEU	2.2
10	W	4	ARG	2.2
8	H	49	ASP	2.2
1	A	373	VAL	2.2
9	V	39	VAL	2.2
1	A	200	PRO	2.2
2	O	226	MET	2.1
13	M	39	ASN	2.1
1	A	157	SER	2.1
1	N	392	GLY	2.1
13	Z	17	ILE	2.1
11	X	47	ARG	2.1
1	A	72	PRO	2.1
1	A	154	GLY	2.1
1	A	384	GLY	2.1
1	N	72	PRO	2.1
4	Q	35	ALA	2.1
1	A	239	GLY	2.1
1	A	245	ILE	2.1
1	A	337	ALA	2.1
2	O	59	GLN	2.1
2	O	40	TYR	2.1
11	X	12	LYS	2.0
12	L	47	LYS	2.0
1	N	382	SER	2.0
8	U	51	SER	2.0
1	A	102	PHE	2.0
6	F	43	LYS	2.0
2	B	200	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	Q	78	TRP	2.0
9	I	26	MET	2.0
9	V	45	LYS	2.0
1	N	237	PHE	2.0
1	A	76	GLY	2.0
4	Q	125	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.45	0.32	-	74,82,105,105	0
1	FME	A	1	10/11	0.92	0.14	-	46,51,63,76	0
2	FME	O	1	10/11	0.95	0.14	-	41,42,49,55	0
7	TPO	T	11	11/12	0.53	0.26	-	75,82,101,102	0
9	SAC	V	1	9/10	0.15	0.56	-	88,90,92,93	0
9	SAC	I	1	9/10	0.80	0.28	-	77,82,84,85	0
1	FME	N	1	10/11	0.87	0.23	-	50,54,74,77	0
2	FME	B	1	10/11	0.96	0.13	-	31,33,40,56	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMU	G	272	33/33	0.54	0.31	9.31	85,116,119,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	PGV	A	524	51/51	0.75	0.28	8.83	45,75,117,118	0
25	CDL	P	1270	100/100	0.68	0.37	6.51	46,100,119,122	0
20	PGV	N	1524	51/51	0.68	0.33	5.06	54,81,117,119	0
22	CHD	W	1059	29/29	0.67	0.47	4.99	107,115,119,120	0
22	CHD	J	60	29/29	0.72	0.28	4.67	105,109,113,114	0
25	CDL	C	270	100/100	0.75	0.31	4.63	49,96,120,122	0
19	TGL	N	1522	63/63	0.55	0.33	4.08	54,76,92,95	0
28	DMU	P	1272	33/33	0.56	0.35	3.96	104,118,124,125	0
19	TGL	D	523	63/63	0.77	0.22	3.79	48,70,93,94	0
19	TGL	L	522	63/63	0.69	0.27	3.32	43,68,84,87	0
25	CDL	T	1269	100/100	0.65	0.32	2.86	66,96,122,126	0
25	CDL	G	269	100/100	0.64	0.34	2.76	72,99,122,124	0
19	TGL	N	1521	63/63	0.76	0.23	2.67	71,92,105,109	0
19	TGL	A	521	63/63	0.81	0.21	2.53	49,82,106,110	0
26	PSC	R	1229	52/52	0.67	0.32	2.52	53,109,133,136	0
26	PSC	E	229	52/52	0.72	0.33	2.40	53,106,131,133	0
20	PGV	P	1268	51/51	0.66	0.31	2.23	64,100,119,121	0
22	CHD	P	1271	29/29	0.91	0.22	1.75	68,86,90,91	0
22	CHD	C	271	29/29	0.85	0.31	1.73	72,84,87,90	0
24	PEK	T	263	53/53	0.54	0.38	1.69	54,103,127,128	0
19	TGL	Q	1523	63/63	0.72	0.22	1.61	67,83,98,100	0
28	DMU	Z	1526	33/33	0.78	0.26	1.55	44,59,75,75	0
20	PGV	P	1267	51/51	0.97	0.13	1.51	29,40,77,85	0
28	DMU	M	526	33/33	0.89	0.16	1.34	36,51,69,71	0
24	PEK	S	1265	53/53	0.58	0.30	1.08	50,87,111,114	0
20	PGV	C	268	51/51	0.69	0.29	1.04	60,91,117,117	0
24	PEK	T	1264	53/53	0.94	0.15	1.04	30,54,83,85	0
20	PGV	C	267	51/51	0.96	0.13	0.93	23,36,72,75	0
24	PEK	G	1263	53/53	0.66	0.37	0.87	59,107,131,132	0
14	HEA	N	515	60/60	0.97	0.20	0.72	30,36,50,52	0
24	PEK	C	264	53/53	0.95	0.13	0.71	27,50,76,79	0
24	PEK	G	265	53/53	0.55	0.27	0.70	51,91,109,114	0
20	PGV	A	522	51/51	0.97	0.17	0.57	25,36,68,72	0
14	HEA	N	516	60/60	0.96	0.19	0.50	32,40,54,57	0
17	MG	A	518	1/1	0.98	0.17	0.44	25,25,25,25	0
20	PGV	N	1266	51/51	0.97	0.15	0.42	28,43,70,75	0
14	HEA	A	515	60/60	0.98	0.20	0.25	18,27,40,45	0
14	HEA	A	516	60/60	0.97	0.17	0.01	23,35,51,52	0
22	CHD	B	1085	29/29	0.95	0.09	-0.40	29,34,40,50	0
27	ZN	F	99	1/1	0.99	0.07	-0.40	35,35,35,35	0
22	CHD	C	525	29/29	0.96	0.11	-0.41	25,35,39,46	0
22	CHD	O	229	29/29	0.95	0.08	-0.42	27,34,42,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	MG	N	518	1/1	0.92	0.12	-0.44	33,33,33,33	0
27	ZN	S	99	1/1	0.99	0.07	-0.45	38,38,38,38	0
22	CHD	P	1525	29/29	0.94	0.11	-0.57	28,38,43,51	0
21	CUA	B	228	2/2	0.99	0.13	-0.74	28,28,28,28	0
18	NA	A	519	1/1	0.97	0.09	-1.08	30,30,30,30	0
21	CUA	O	228	2/2	0.98	0.09	-1.31	36,36,36,37	0
15	CYN	A	520	2/2	0.98	0.13	-1.45	31,31,31,31	0
18	NA	N	519	1/1	0.92	0.06	-1.73	40,40,40,40	0
15	CYN	N	520	2/2	0.88	0.15	-1.84	42,42,42,43	0
16	CU	N	517	1/1	0.99	0.16	-	37,37,37,37	0
23	UNX	C	262	1/1	0.64	0.58	-	49,49,49,49	0
16	CU	A	517	1/1	1.00	0.17	-	31,31,31,31	0
23	UNX	P	262	1/1	0.80	0.60	-	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.