Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:24 PM GMT

PDB ID	:	3X2Q
Title	:	X-ray structure of cyanide-bound bovine heart cytochrome c oxidase in the fully oxidized state at 2.0 angstrom resolution
Authors	:	Yano, N.; Muramoto, K.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2014-12-26
Resolution	:	2.00 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:

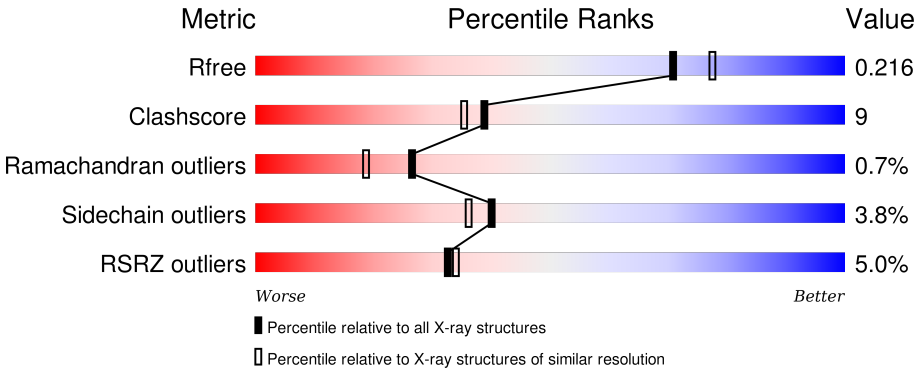
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	81% 18%
1	N	514	84% 14%
2	B	227	78% 19%
2	O	227	80% 18%
3	C	261	83% 16%

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Mol	Chain	Length	Quality of chain
3	P	261	2% 84% 14%
4	D	147	% 79% 16%
4	Q	147	14% 82% 12%
5	E	109	2% 82% 13%
5	R	109	4% 86% 7%
6	F	98	8% 79% 18%
6	S	98	10% 76% 17% 7%
7	G	85	19% 72% 16% 11%
7	T	85	20% 68% 20% 11%
8	H	85	9% 76% 12% 7%
8	U	85	11% 74% 14% 7%
9	I	73	5% 86% 10%
9	V	73	11% 85% 12%
10	J	59	14% 90% 7%
10	W	59	14% 93%
11	K	56	79% 9% 13%
11	X	56	30% 77% 9% 13%
12	L	47	79% 17%
12	Y	47	2% 77% 19%
13	M	46	11% 74% 17% 7%
13	Z	46	17% 78% 15% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	A	602	X	-	-	-
15	HEA	A	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	N	602	X	-	-	-
15	HEA	N	603	X	-	-	-
17	MG	A	605	-	-	-	X
17	MG	N	605	-	-	-	X
18	NA	A	606	-	-	-	X
18	NA	N	606	-	-	-	X
19	TGL	A	607	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	L	101	-	-	-	X
19	TGL	N	609	-	-	-	X
19	TGL	N	610	-	-	-	X
19	TGL	Q	201	-	-	-	X
20	PGV	A	609	-	-	-	X
20	PGV	C	307	-	-	-	X
20	PGV	N	607	-	-	-	X
20	PGV	P	302	-	-	-	X
22	CHD	C	304	-	-	-	X
24	CDL	C	303	-	-	-	X
24	CDL	G	103	-	-	X	X
24	CDL	P	306	-	-	-	X
24	CDL	T	102	-	-	X	X
25	PEK	G	104	-	-	-	X
25	PEK	T	101	-	-	X	X
26	PSC	E	201	-	-	-	X
26	PSC	O	303	-	-	-	X
28	DMU	G	101	-	-	-	X
28	DMU	P	301	-	-	-	X
28	DMU	Z	101	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32060 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	3	0
			4051	2708	626	681	36			
1	N	514	Total	C	N	O	S	0	3	0
			4051	2708	626	681	36			

- 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	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

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

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, mitochondrial.

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, mitochondrial.

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, mitochondrial.

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 subunit 7A1, mitochondrial.

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, mitochondrial.

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			

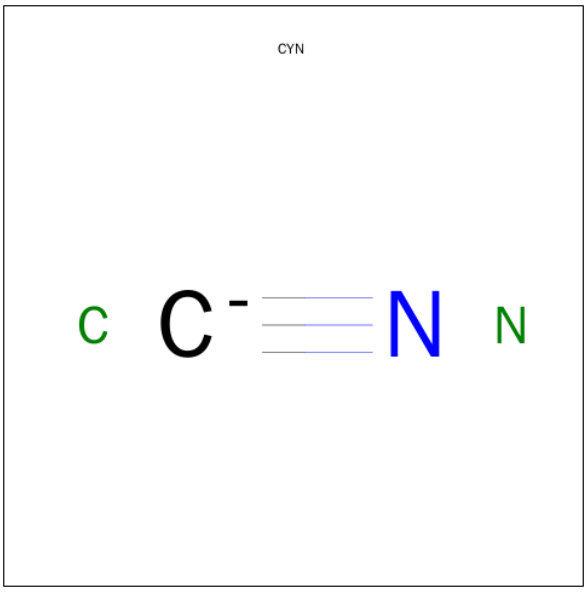
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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, mitochondrial.

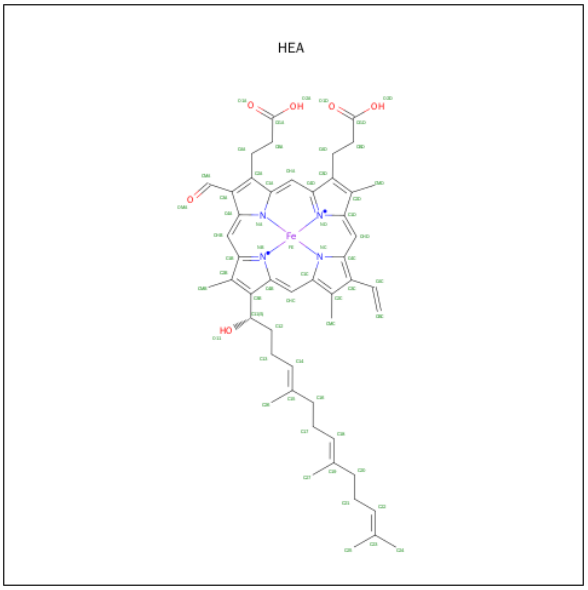
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 15 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

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

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

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

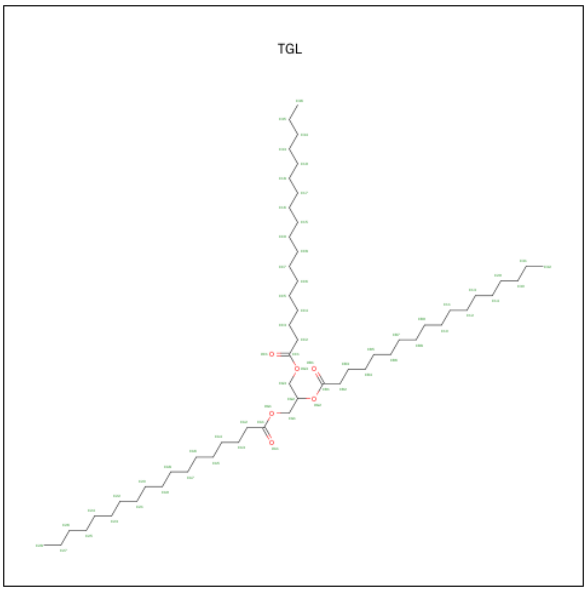
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

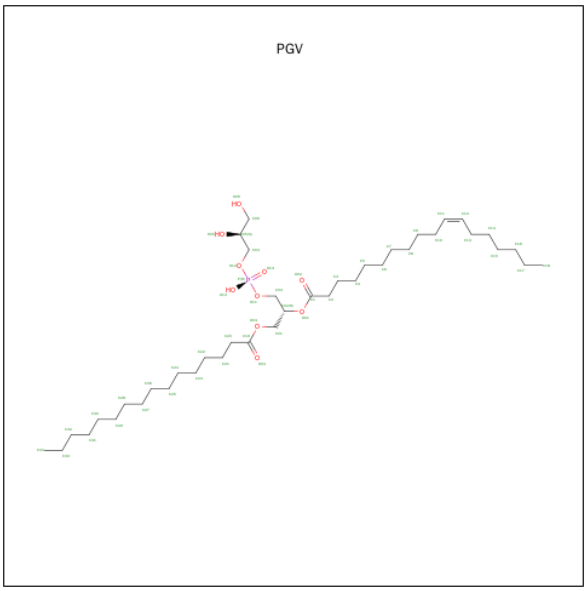
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

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



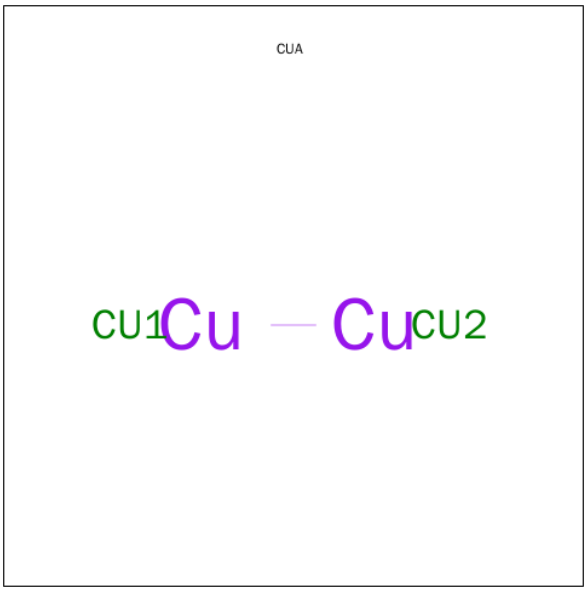
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0

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



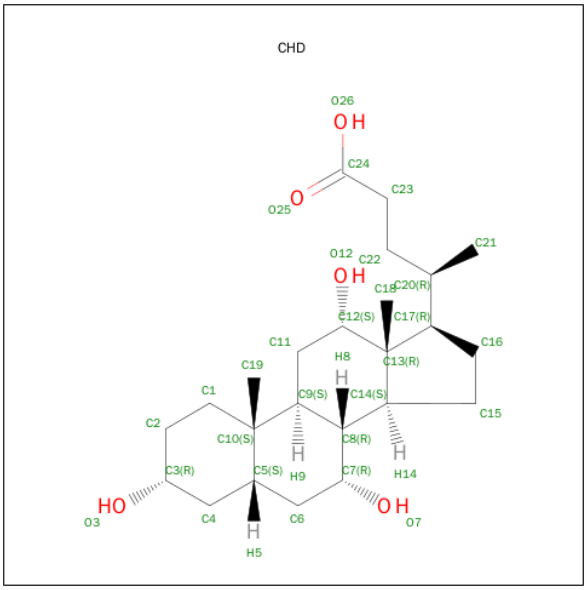
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			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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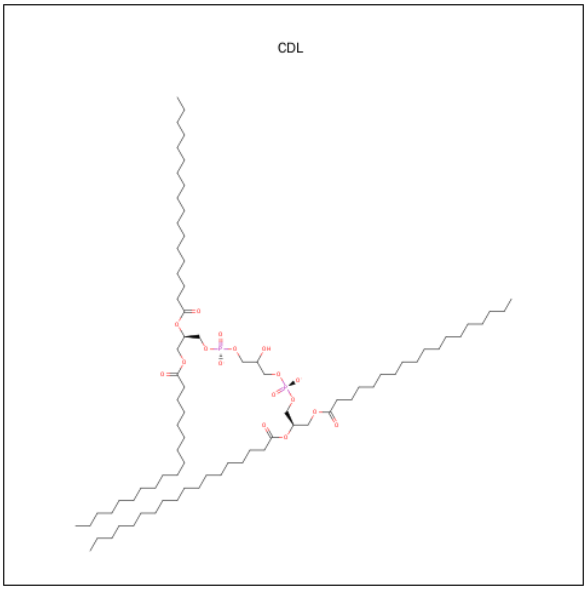
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0

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



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

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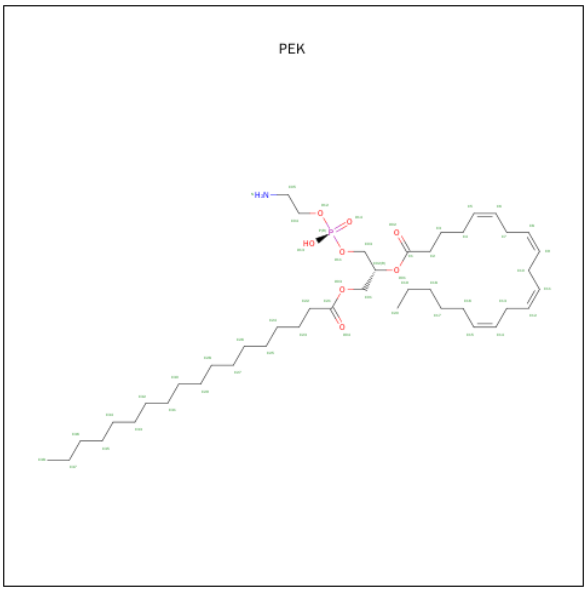
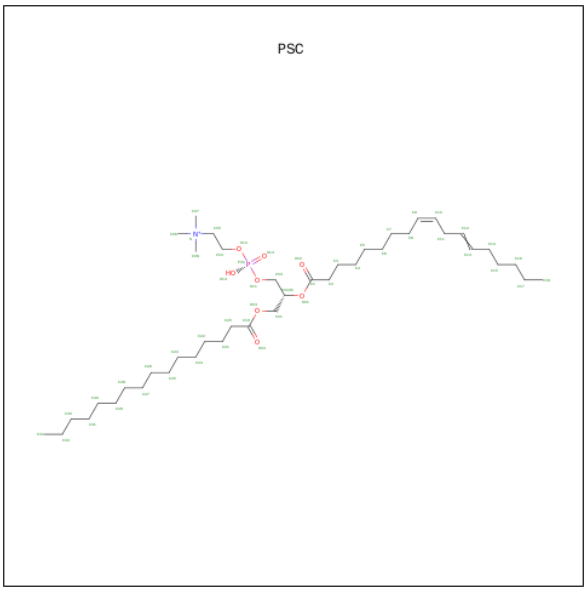
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	T	1	Total	C	O	P	0	0
			100	81	17	2		

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



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

- Molecule 26 is (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: $C_{42}H_{81}NO_8P$).

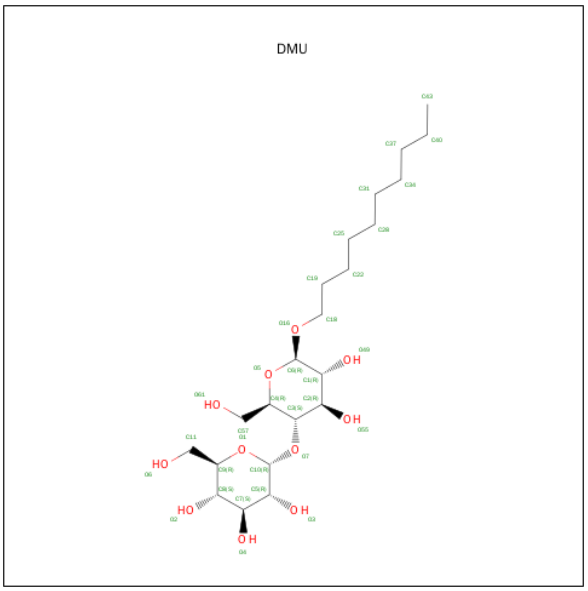


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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	188	Total O 188 188	0	0
29	B	121	Total O 121 121	0	0
29	C	77	Total O 77 77	0	0
29	D	78	Total O 78 78	0	0
29	E	58	Total O 58 58	0	0
29	F	58	Total O 58 58	0	0
29	G	27	Total O 27 27	0	0
29	H	34	Total O 34 34	0	0

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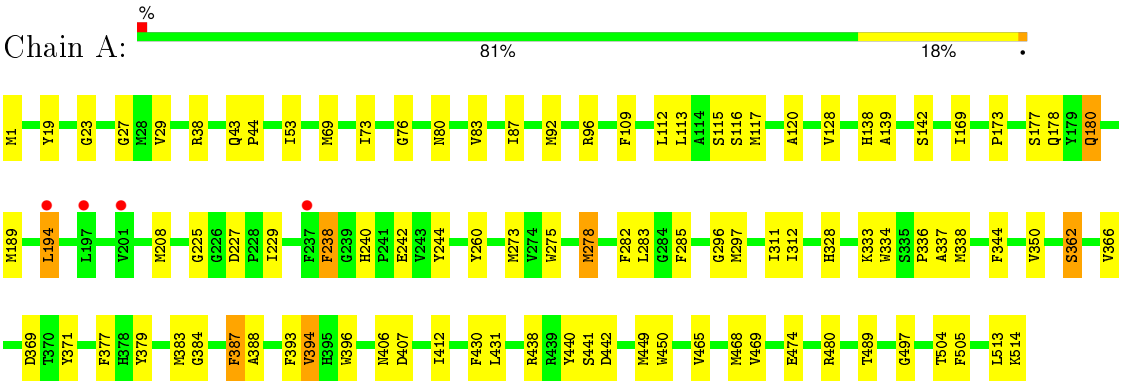
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	29	Total O 29 29	0	0
29	J	15	Total O 15 15	0	0
29	K	20	Total O 20 20	0	0
29	L	16	Total O 16 16	0	0
29	M	14	Total O 14 14	0	0
29	N	156	Total O 156 156	0	0
29	O	91	Total O 91 91	0	0
29	P	76	Total O 76 76	0	0
29	Q	46	Total O 46 46	0	0
29	R	42	Total O 42 42	0	0
29	S	38	Total O 38 38	0	0
29	T	23	Total O 23 23	0	0
29	U	28	Total O 28 28	0	0
29	V	14	Total O 14 14	0	0
29	W	4	Total O 4 4	0	0
29	X	15	Total O 15 15	0	0
29	Y	11	Total O 11 11	0	0
29	Z	7	Total O 7 7	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.

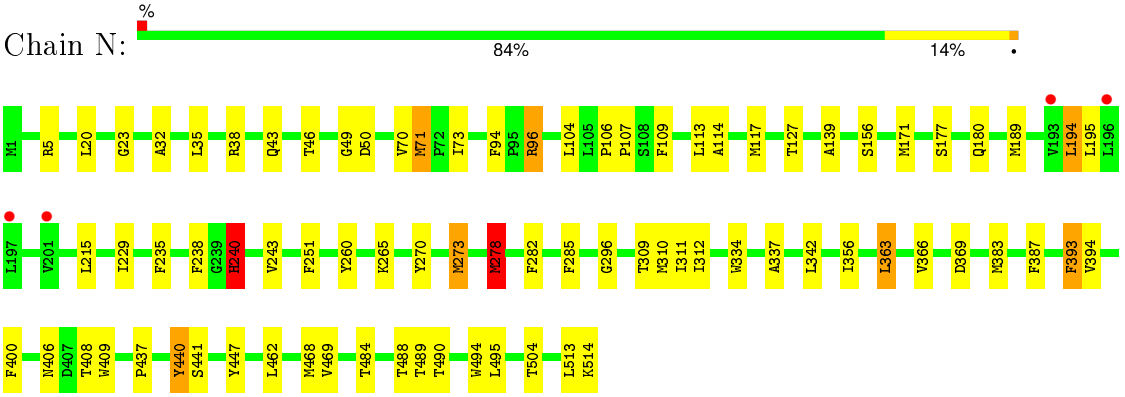
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



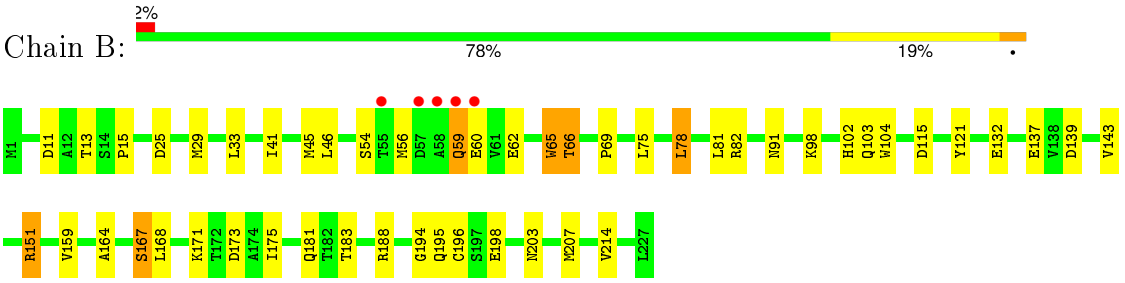
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



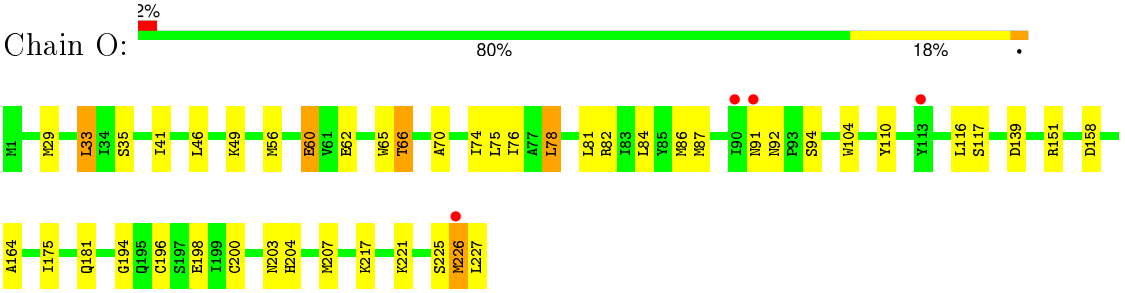
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



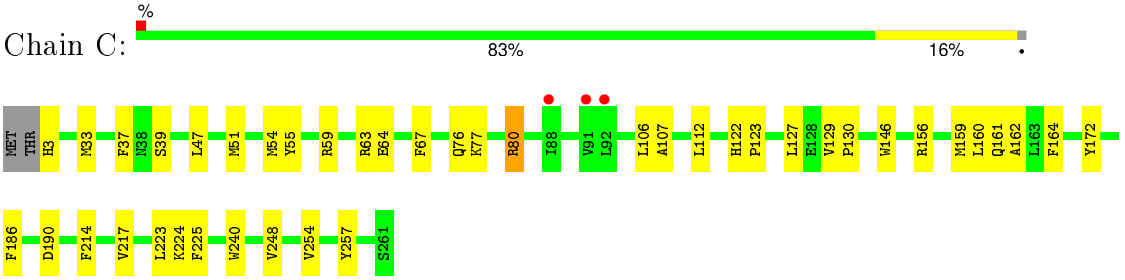
- Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



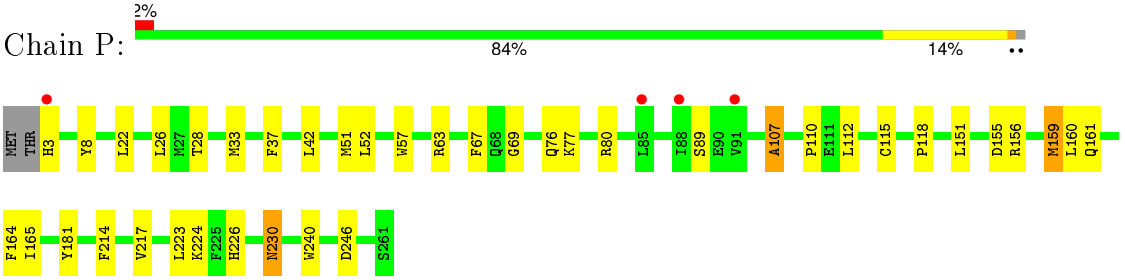
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



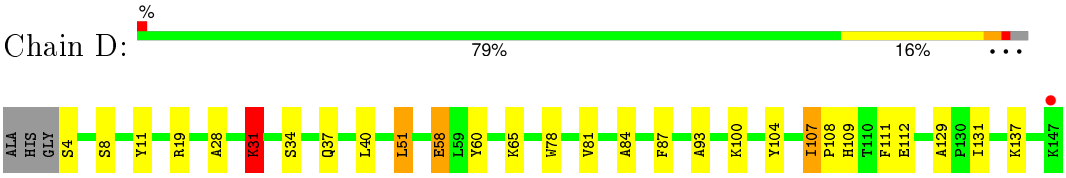
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



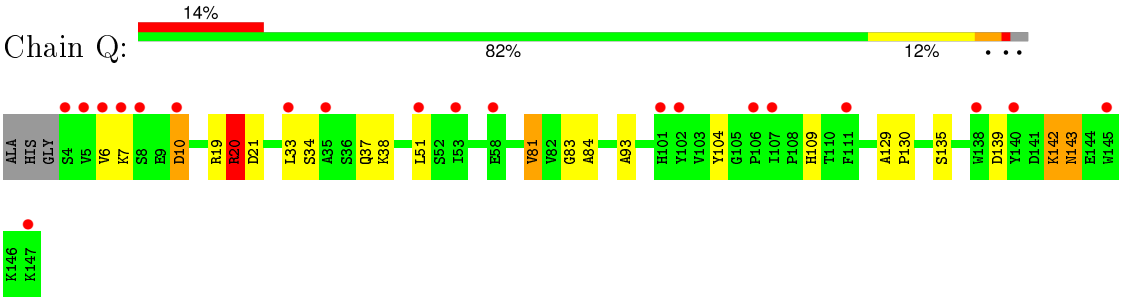
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



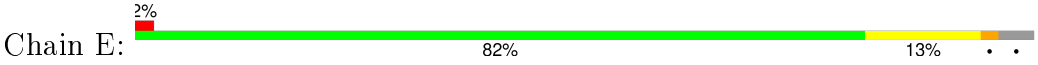
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

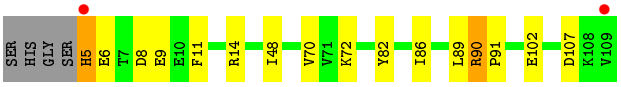
Chain Q:



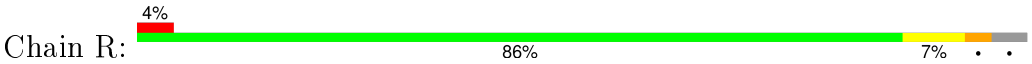
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:

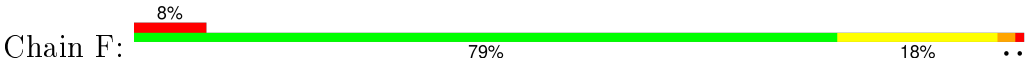


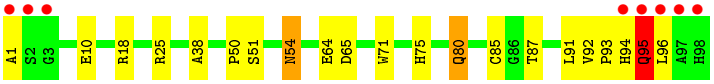


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

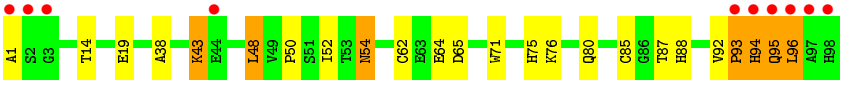


• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

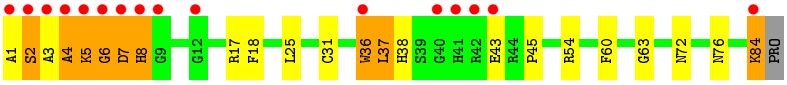




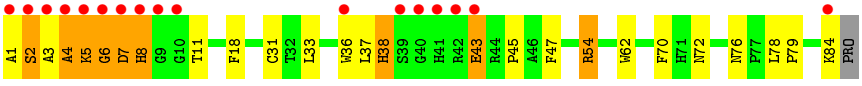
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



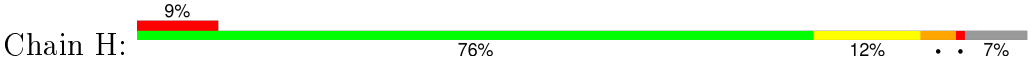
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

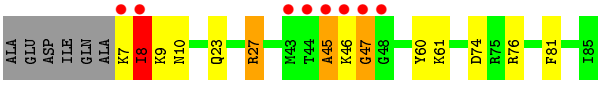


• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

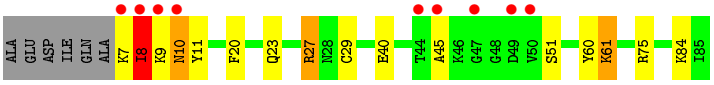


• Molecule 8: Cytochrome c oxidase subunit 6B1

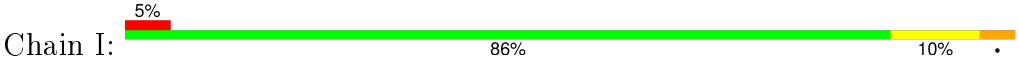


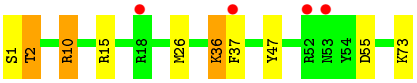


• Molecule 8: Cytochrome c oxidase subunit 6B1

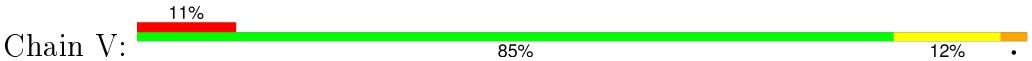


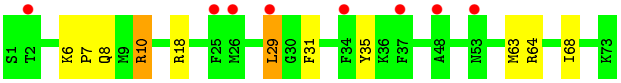
• Molecule 9: Cytochrome c oxidase subunit 6C



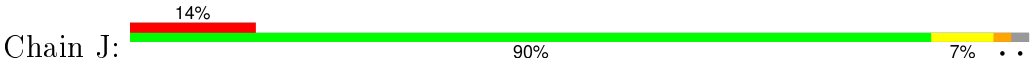


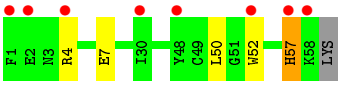
• Molecule 9: Cytochrome c oxidase subunit 6C



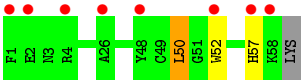


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

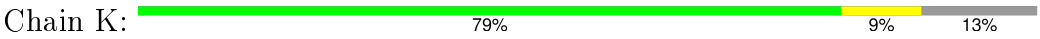


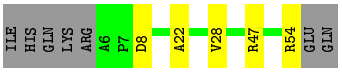


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

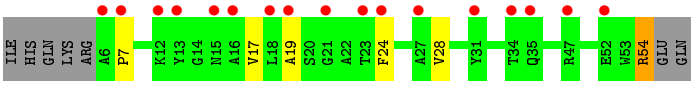


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

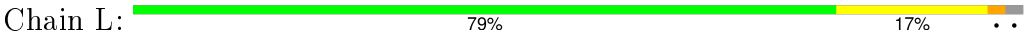


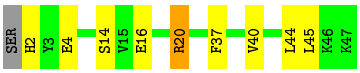


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

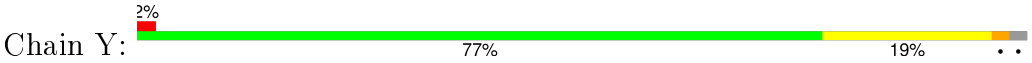


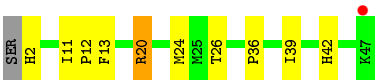
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



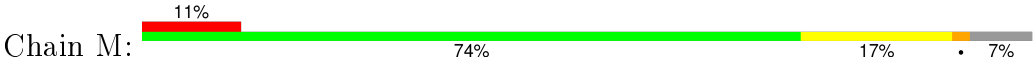


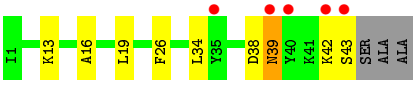
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



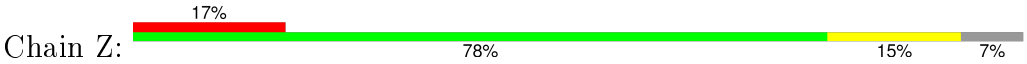


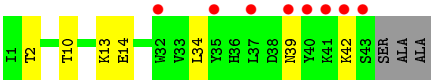
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial





• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.68Å 206.68Å 178.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 81.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.00) 99.9 (81.64-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.214 0.188 , 0.216	Depositor DCC
R_{free} test set	22863 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.5	EDS
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 451733 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32060	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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	1.51	29/4180 (0.7%)	1.15	18/5710 (0.3%)
1	N	1.34	15/4180 (0.4%)	0.99	10/5710 (0.2%)
2	B	1.45	11/1860 (0.6%)	1.16	13/2534 (0.5%)
2	O	1.14	3/1860 (0.2%)	1.01	3/2534 (0.1%)
3	C	1.35	5/2221 (0.2%)	0.96	1/3035 (0.0%)
3	P	1.31	6/2221 (0.3%)	0.93	2/3035 (0.1%)
4	D	1.48	10/1229 (0.8%)	1.14	6/1658 (0.4%)
4	Q	1.03	1/1229 (0.1%)	0.92	3/1658 (0.2%)
5	E	1.27	3/871 (0.3%)	1.11	3/1182 (0.3%)
5	R	1.15	3/871 (0.3%)	0.97	2/1182 (0.2%)
6	F	1.31	0/765	1.08	2/1038 (0.2%)
6	S	1.20	0/765	1.02	0/1038
7	G	1.33	3/690 (0.4%)	1.01	4/937 (0.4%)
7	T	1.31	4/690 (0.6%)	1.07	2/937 (0.2%)
8	H	1.26	1/682 (0.1%)	1.01	3/921 (0.3%)
8	U	1.04	0/682	0.91	1/921 (0.1%)
9	I	1.36	0/605	1.11	2/802 (0.2%)
9	V	1.09	0/605	1.06	3/802 (0.4%)
10	J	1.21	0/471	0.94	0/636
10	W	1.07	0/471	0.92	0/636
11	K	1.38	1/398 (0.3%)	1.11	2/546 (0.4%)
11	X	1.07	1/398 (0.3%)	0.85	0/546
12	L	1.38	3/393 (0.8%)	1.02	1/526 (0.2%)
12	Y	1.16	0/393	0.82	0/526
13	M	1.38	2/345 (0.6%)	1.04	0/470
13	Z	1.05	0/345	0.87	0/470
All	All	1.32	101/29420 (0.3%)	1.03	81/39990 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	6

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CG-CD	9.50	1.66	1.51
2	B	167	SER	CB-OG	-8.83	1.30	1.42
1	A	371	TYR	CD1-CE1	8.27	1.51	1.39
7	T	36	TRP	CB-CG	8.23	1.65	1.50
5	R	80	GLU	CB-CG	8.14	1.67	1.52
7	G	36	TRP	CB-CG	7.93	1.64	1.50
2	O	198	GLU	C-O	7.50	1.37	1.23
1	A	139	ALA	CA-CB	7.40	1.68	1.52
1	N	70	VAL	CB-CG2	7.32	1.68	1.52
1	N	260	TYR	CE1-CZ	7.21	1.48	1.38
1	A	242	GLU	CG-CD	7.10	1.62	1.51
3	P	181	TYR	CD1-CE1	7.02	1.49	1.39
1	N	139	ALA	CA-CB	6.95	1.67	1.52
1	A	393	PHE	CE1-CZ	6.94	1.50	1.37
1	A	275	TRP	CG-CD1	6.93	1.46	1.36
11	X	19	ALA	CA-CB	6.93	1.67	1.52
13	M	26	PHE	CE2-CZ	6.88	1.50	1.37
4	D	112	GLU	CG-CD	6.78	1.62	1.51
4	D	31	LYS	CD-CE	6.75	1.68	1.51
13	M	16	ALA	CA-CB	6.66	1.66	1.52
1	A	377	PHE	CE2-CZ	6.60	1.49	1.37
3	P	115	CYS	CB-SG	6.43	1.93	1.82
2	B	143	VAL	CB-CG2	6.43	1.66	1.52
1	A	244	TYR	CE1-CZ	6.41	1.46	1.38
2	B	214	VAL	CB-CG1	6.31	1.66	1.52
4	D	100	LYS	CD-CE	6.29	1.67	1.51
1	N	273	MET	CB-CG	6.28	1.71	1.51
3	P	57	TRP	CB-CG	6.27	1.61	1.50
5	E	70	VAL	CB-CG2	6.24	1.66	1.52
1	N	189	MET	CB-CG	6.23	1.71	1.51

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	102	GLU	CB-CG	6.14	1.63	1.52
12	L	4	GLU	CG-CD	6.13	1.61	1.51
11	K	22	ALA	CA-CB	6.12	1.65	1.52
4	D	11	TYR	CB-CG	6.06	1.60	1.51
2	B	121	TYR	CE2-CZ	6.03	1.46	1.38
5	E	9	GLU	CG-CD	6.01	1.60	1.51
2	B	159	VAL	CB-CG2	5.97	1.65	1.52
1	A	19	TYR	CD2-CE2	5.97	1.48	1.39
3	C	64	GLU	CG-CD	5.92	1.60	1.51
2	B	59	GLN	CG-CD	5.90	1.64	1.51
1	A	465	VAL	CB-CG1	5.87	1.65	1.52
8	H	81	PHE	CE2-CZ	5.87	1.48	1.37
1	N	494	TRP	CZ3-CH2	5.87	1.49	1.40
4	D	19	ARG	CZ-NH2	5.85	1.40	1.33
3	C	172	TYR	CD2-CE2	5.83	1.48	1.39
1	A	505	PHE	CE2-CZ	5.78	1.48	1.37
4	D	104	TYR	CD1-CE1	5.76	1.48	1.39
1	A	388	ALA	CA-CB	5.75	1.64	1.52
1	A	441	SER	C-O	5.74	1.34	1.23
2	B	198	GLU	CD-OE1	-5.71	1.19	1.25
2	B	198	GLU	CB-CG	5.71	1.62	1.52
7	T	47	PHE	CE1-CZ	5.68	1.48	1.37
1	A	396	TRP	CE3-CZ3	5.67	1.48	1.38
1	A	83	VAL	CB-CG2	5.66	1.64	1.52
3	C	257	TYR	CE2-CZ	5.64	1.45	1.38
1	N	251	PHE	CE2-CZ	5.62	1.48	1.37
1	N	366	VAL	CB-CG1	-5.56	1.41	1.52
3	P	107	ALA	CA-CB	5.53	1.64	1.52
4	D	28	ALA	CA-CB	5.53	1.64	1.52
1	A	238	PHE	CE2-CZ	5.52	1.47	1.37
1	A	394	VAL	CB-CG2	-5.51	1.41	1.52
1	N	94	PHE	CD1-CE1	5.50	1.50	1.39
3	C	240	TRP	CG-CD1	5.46	1.44	1.36
1	A	260	TYR	CD2-CE2	5.46	1.47	1.39
2	B	98	LYS	CD-CE	5.40	1.64	1.51
5	R	80	GLU	CD-OE1	5.40	1.31	1.25
1	A	387	PHE	CD2-CE2	5.37	1.50	1.39
7	T	5	LYS	CB-CG	5.33	1.67	1.52
2	O	110	TYR	CD1-CE1	5.32	1.47	1.39
1	A	120	ALA	CA-CB	5.31	1.63	1.52
1	A	128	VAL	CB-CG1	5.31	1.64	1.52
3	C	225	PHE	CD2-CE2	5.29	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	60	GLU	CG-CD	5.28	1.59	1.51
1	A	469	VAL	CB-CG1	5.25	1.63	1.52
1	N	447	TYR	CD2-CE2	5.25	1.47	1.39
3	P	89	SER	CB-OG	5.24	1.49	1.42
4	Q	81	VAL	CB-CG1	5.20	1.63	1.52
12	L	37	PHE	CE2-CZ	5.20	1.47	1.37
4	D	100	LYS	CE-NZ	5.18	1.62	1.49
1	A	260	TYR	CE2-CZ	5.18	1.45	1.38
1	A	362	SER	CB-OG	-5.17	1.35	1.42
1	A	29	VAL	CB-CG1	5.14	1.63	1.52
1	N	270	TYR	CD1-CE1	5.12	1.47	1.39
2	B	159	VAL	CB-CG1	5.12	1.63	1.52
7	G	60	PHE	CE1-CZ	5.11	1.47	1.37
7	T	70	PHE	CG-CD2	5.10	1.46	1.38
3	P	240	TRP	CE3-CZ3	5.10	1.47	1.38
4	D	87	PHE	CD2-CE2	5.09	1.49	1.39
7	G	5	LYS	CB-CG	5.08	1.66	1.52
1	A	497	GLY	C-O	5.07	1.31	1.23
1	A	92	MET	CB-CG	5.07	1.67	1.51
4	D	60	TYR	CG-CD1	5.06	1.45	1.39
2	B	198	GLU	C-O	5.05	1.32	1.23
1	N	469	VAL	CB-CG2	5.05	1.63	1.52
1	N	440	TYR	CD2-CE2	5.03	1.46	1.39
1	N	393	PHE	CE1-CZ	5.03	1.47	1.37
12	L	16	GLU	CG-CD	5.03	1.59	1.51
1	A	371	TYR	CD2-CE2	5.02	1.46	1.39
1	A	379	TYR	CG-CD1	5.02	1.45	1.39
1	A	474	GLU	CB-CG	5.01	1.61	1.52
1	N	441	SER	C-O	5.01	1.32	1.23

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	MET	CG-SD-CE	-19.27	69.37	100.20
4	D	19	ARG	NE-CZ-NH1	-13.36	113.62	120.30
1	A	96	ARG	NE-CZ-NH2	-11.58	114.51	120.30
4	Q	20	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	278	MET	CG-SD-CE	-9.12	85.61	100.20
5	E	90	ARG	NE-CZ-NH1	9.08	124.84	120.30
9	V	10	ARG	NE-CZ-NH2	-8.69	115.96	120.30
11	K	47	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	N	5	ARG	NE-CZ-NH2	-8.25	116.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	90	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	N	278	MET	CG-SD-CE	-8.11	87.22	100.20
7	T	33	LEU	CA-CB-CG	8.04	133.78	115.30
1	A	208	MET	CG-SD-CE	7.98	112.96	100.20
6	F	18	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	194	LEU	CB-CG-CD2	7.19	123.22	111.00
1	N	194	LEU	CB-CG-CD2	7.16	123.17	111.00
4	D	19	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	N	71	MET	CG-SD-CE	-7.02	88.97	100.20
1	A	227	ASP	CB-CG-OD2	6.88	124.49	118.30
5	E	107	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	366	VAL	CG1-CB-CG2	-6.85	99.94	110.90
3	C	80	ARG	CG-CD-NE	-6.82	97.48	111.80
1	A	480	ARG	NE-CZ-NH2	-6.70	116.95	120.30
5	R	90	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	227	ASP	CB-CG-OD1	-6.42	112.52	118.30
2	B	188	ARG	NE-CZ-NH2	-6.34	117.13	120.30
9	V	10	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	168	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	407	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	189	MET	CA-CB-CG	-6.24	102.70	113.30
2	B	25	ASP	CB-CG-OD1	6.01	123.71	118.30
2	B	198	GLU	OE1-CD-OE2	-6.01	116.08	123.30
1	A	438	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	B	139	ASP	CB-CG-OD2	5.95	123.66	118.30
2	B	151	ARG	NE-CZ-NH1	5.92	123.26	120.30
3	P	155	ASP	CB-CG-OD1	5.92	123.62	118.30
2	B	65	TRP	CB-CA-C	5.85	122.11	110.40
1	N	189	MET	CA-CB-CG	-5.83	103.39	113.30
8	H	76	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	480	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	244	TYR	CA-CB-CG	-5.74	102.50	113.40
8	H	27	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	96	ARG	NE-CZ-NH1	5.69	123.14	120.30
9	I	55	ASP	CB-CG-OD1	5.68	123.41	118.30
4	D	65	LYS	CD-CE-NZ	-5.67	98.66	111.70
1	N	96	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	P	80	ARG	CG-CD-NE	-5.66	99.91	111.80
4	D	137	LYS	CD-CE-NZ	-5.62	98.77	111.70
2	B	173	ASP	CB-CG-OD1	5.57	123.31	118.30
2	B	167	SER	CB-CA-C	-5.51	99.63	110.10
1	A	438	ARG	NE-CZ-NH1	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	74	ASP	CB-CG-OD1	5.44	123.20	118.30
4	Q	20	ARG	CG-CD-NE	-5.40	100.46	111.80
7	G	7	ASP	N-CA-C	5.39	125.55	111.00
6	F	18	ARG	NE-CZ-NH1	5.33	122.96	120.30
7	G	8	HIS	N-CA-C	5.31	125.34	111.00
11	K	47	ARG	CD-NE-CZ	5.29	131.01	123.60
2	O	139	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	442	ASP	CB-CG-OD2	5.27	123.04	118.30
4	D	51	LEU	CA-CB-CG	5.26	127.40	115.30
2	B	151	ARG	NE-CZ-NH2	-5.22	117.69	120.30
9	V	64	ARG	NE-CZ-NH1	-5.18	117.71	120.30
8	U	75	ARG	NE-CZ-NH2	-5.13	117.73	120.30
7	G	17	ARG	NE-CZ-NH1	-5.13	117.74	120.30
2	B	102	HIS	CB-CA-C	-5.12	100.15	110.40
7	G	6	GLY	N-CA-C	5.12	125.90	113.10
2	B	11	ASP	CB-CG-OD2	5.11	122.89	118.30
4	D	107	ILE	CB-CG1-CD1	-5.10	99.61	113.90
9	I	10	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	O	226	MET	CG-SD-CE	5.09	108.35	100.20
1	N	50	ASP	CB-CG-OD2	5.08	122.88	118.30
4	Q	20	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	N	5	ARG	CG-CD-NE	-5.07	101.16	111.80
5	R	90	ARG	CG-CD-NE	-5.06	101.17	111.80
1	N	363	LEU	CB-CG-CD2	5.04	119.58	111.00
7	T	54	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	B	82	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	N	240	HIS	N-CA-CB	5.03	119.66	110.60
2	O	158	ASP	CB-CG-OD1	5.02	122.82	118.30
12	L	20	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	449	MET	CA-CB-CG	-5.00	104.80	113.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
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	4051	0	4029	55	0
1	N	4051	0	4029	56	0
2	B	1824	0	1833	26	0
2	O	1824	0	1833	31	0
3	C	2134	0	2051	31	0
3	P	2134	0	2051	36	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	11	0
5	R	852	0	845	8	0
6	F	748	0	728	16	0
6	S	748	0	728	29	0
7	G	675	0	643	27	0
7	T	675	0	643	45	0
8	H	662	0	623	7	0
8	U	662	0	623	12	0
9	I	601	0	613	12	0
9	V	601	0	613	10	0
10	J	460	0	459	4	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	15	0
13	M	335	0	352	2	0
13	Z	335	0	352	2	0
14	A	2	0	0	0	0
14	N	2	0	0	0	0
15	A	120	0	108	9	0
15	N	120	0	108	8	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	1	0
18	N	1	0	0	0	0
19	A	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	12	0
19	L	63	0	110	14	0
19	N	126	0	220	22	0
19	Q	63	0	110	2	0
20	A	102	0	152	8	0
20	C	102	0	152	5	0
20	N	102	0	152	10	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	39	2	0
22	C	58	0	78	6	0
22	O	29	0	39	1	0
22	P	58	0	78	8	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	100	0	156	17	0
24	G	100	0	156	26	0
24	P	100	0	156	20	0
24	T	100	0	156	27	0
25	C	53	0	77	6	0
25	G	106	0	154	13	0
25	P	106	0	154	13	0
25	T	53	0	77	22	0
26	E	52	0	80	16	0
26	O	52	0	80	17	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	41	4	0
28	M	33	0	42	0	0
28	P	33	0	42	3	0
28	Z	33	0	42	0	0
29	A	188	0	0	10	0
29	B	121	0	0	3	0
29	C	77	0	0	1	0
29	D	78	0	0	4	0
29	E	58	0	0	2	0
29	F	58	0	0	4	0
29	G	27	0	0	3	0
29	H	34	0	0	0	0
29	I	29	0	0	4	0
29	J	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	20	0	0	1	0
29	L	16	0	0	2	0
29	M	14	0	0	0	0
29	N	156	0	0	3	0
29	O	91	0	0	3	0
29	P	76	0	0	9	0
29	Q	46	0	0	4	0
29	R	42	0	0	1	0
29	S	38	0	0	3	0
29	T	23	0	0	2	0
29	U	28	0	0	3	0
29	V	14	0	0	0	0
29	W	4	0	0	0	0
29	X	15	0	0	1	0
29	Y	11	0	0	0	0
29	Z	7	0	0	0	0
All	All	32060	0	31341	561	0

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

All (561) 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)
25:P:309:PEK:H383	24:T:102:CDL:C27	1.43	1.46
1:A:297:MET:SD	1:A:297:MET:CE	2.04	1.45
25:C:306:PEK:H383	24:G:103:CDL:C27	1.49	1.38
1:A:312[A]:ILE:HD12	29:A:740:HOH:O	1.21	1.31
6:S:43:LYS:CD	6:S:43:LYS:H	1.43	1.26
6:F:95:GLN:HA	29:F:256:HOH:O	1.34	1.25
19:N:610:TGL:HC32	12:Y:20:ARG:NH2	1.53	1.22
24:G:103:CDL:H241	24:G:103:CDL:H541	1.25	1.17
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.08	1.16
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.60	1.15
1:A:27:GLY:HA3	15:A:602:HEA:C27	1.78	1.13
25:C:306:PEK:H383	24:G:103:CDL:H273	1.18	1.12
26:E:201:PSC:H072	9:I:10:ARG:HH21	1.10	1.12
19:L:101:TGL:HC62	19:L:101:TGL:HC22	1.32	1.08
25:P:309:PEK:C38	24:T:102:CDL:C27	2.31	1.08
8:U:9:LYS:HG3	8:U:10:ASN:H	1.14	1.08
7:G:45:PRO:HD2	29:G:221:HOH:O	1.53	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:309:PEK:H383	24:T:102:CDL:H272	1.33	1.07
3:P:67:PHE:HE1	24:P:306:CDL:H1	1.15	1.06
25:P:309:PEK:H383	24:T:102:CDL:H273	1.10	1.06
6:S:43:LYS:H	6:S:43:LYS:HD3	1.21	1.05
7:T:5:LYS:HB2	25:T:101:PEK:H362	1.05	1.04
24:G:103:CDL:C54	24:G:103:CDL:H241	1.86	1.04
2:B:41:ILE:HD13	26:E:201:PSC:H342	1.36	1.04
19:L:101:TGL:HC41	19:L:101:TGL:OC1	1.53	1.02
6:S:43:LYS:H	6:S:43:LYS:HD2	1.23	1.01
1:A:27:GLY:HA3	15:A:602:HEA:H273	1.38	1.01
7:G:5:LYS:HG3	25:G:104:PEK:H383	1.38	1.01
6:S:85:CYS:SG	6:S:87:THR:HG23	2.01	1.00
20:P:305:PGV:H182	24:P:306:CDL:H671	1.43	0.98
25:C:306:PEK:C38	24:G:103:CDL:H273	1.94	0.97
6:S:43:LYS:CD	6:S:43:LYS:N	2.26	0.96
25:C:306:PEK:H383	24:G:103:CDL:H271	1.47	0.95
6:S:43:LYS:HE2	29:S:220:HOH:O	1.65	0.95
25:C:306:PEK:C38	24:G:103:CDL:C27	2.44	0.94
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.30	0.94
24:G:103:CDL:C24	24:G:103:CDL:H541	1.97	0.94
24:P:306:CDL:H522	24:P:306:CDL:OB9	1.68	0.94
1:N:400:PHE:HB3	19:N:610:TGL:H283	1.48	0.93
7:T:5:LYS:CD	25:T:101:PEK:H371	1.98	0.93
28:G:101:DMU:H30	28:G:101:DMU:H36	1.47	0.93
18:A:606:NA:NA	29:A:709:HOH:O	1.41	0.93
26:E:201:PSC:C07	9:I:10:ARG:HH21	1.83	0.92
25:P:304:PEK:H32	25:P:304:PEK:H71	1.51	0.92
3:C:67:PHE:HE1	24:C:303:CDL:H1	1.32	0.92
3:P:3:HIS:HB3	29:P:456:HOH:O	1.71	0.91
7:T:31:CYS:SG	24:T:102:CDL:H532	2.12	0.90
7:T:5:LYS:HB2	25:T:101:PEK:C36	1.99	0.90
7:T:5:LYS:HD2	25:T:101:PEK:H371	1.52	0.89
3:C:63:ARG:HE	24:C:303:CDL:HA22	1.37	0.89
6:S:75:HIS:H	6:S:80:GLN:HE22	1.15	0.89
15:N:602:HEA:C16	15:N:602:HEA:H273	2.00	0.89
19:N:610:TGL:HC32	12:Y:20:ARG:HH22	1.39	0.88
1:A:27:GLY:CA	15:A:602:HEA:H273	2.03	0.88
6:F:85:CYS:SG	6:F:87:THR:HG23	2.14	0.88
20:N:607:PGV:O14	20:N:607:PGV:H02	1.71	0.88
19:L:101:TGL:CC2	19:L:101:TGL:HC62	2.03	0.86
6:S:19:GLU:HG2	29:S:232:HOH:O	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:CE1	24:P:306:CDL:H1	2.08	0.86
1:N:117[A]:MET:HE2	12:Y:42:HIS:CD2	2.09	0.86
7:T:5:LYS:HD2	25:T:101:PEK:C38	2.06	0.86
19:N:610:TGL:HC32	12:Y:20:ARG:HH21	1.33	0.86
25:P:309:PEK:C38	24:T:102:CDL:H273	2.02	0.85
29:P:463:HOH:O	6:S:96:LEU:HD13	1.77	0.85
25:P:309:PEK:C38	24:T:102:CDL:H272	2.00	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.84
26:E:201:PSC:H072	9:I:10:ARG:NH2	1.92	0.83
6:F:75:HIS:H	6:F:80:GLN:HE22	1.26	0.83
3:P:160:LEU:HD13	22:P:307:CHD:H181	1.59	0.83
20:P:305:PGV:H182	24:P:306:CDL:C67	2.08	0.83
7:T:2:SER:OG	25:T:101:PEK:H301	1.78	0.82
19:L:101:TGL:OG3	19:L:101:TGL:OA1	1.97	0.82
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.80	0.82
29:P:475:HOH:O	6:S:1:ALA:HB2	1.80	0.82
1:A:406:ASN:HD21	20:A:609:PGV:H22	1.44	0.82
1:A:27:GLY:HA3	15:A:602:HEA:H271	1.59	0.82
7:T:5:LYS:HD2	25:T:101:PEK:C37	2.09	0.81
8:U:9:LYS:HG3	8:U:10:ASN:N	1.93	0.81
1:A:297:MET:HB2	29:A:884:HOH:O	1.80	0.81
24:T:102:CDL:H111	24:T:102:CDL:HA21	1.63	0.80
24:P:306:CDL:H652	29:P:468:HOH:O	1.81	0.79
7:G:72:ASN:H	7:G:76:ASN:HD22	1.27	0.79
25:P:304:PEK:HN2	7:T:76:ASN:HD21	1.31	0.78
6:F:54:ASN:HD22	6:F:54:ASN:H	1.31	0.78
28:G:101:DMU:H30	28:G:101:DMU:C10	2.13	0.78
6:F:1:ALA:HB2	29:F:251:HOH:O	1.82	0.78
3:C:161:GLN:HE22	25:C:306:PEK:H22	1.48	0.78
8:U:7:LYS:O	8:U:8:ILE:HB	1.83	0.78
20:P:305:PGV:H172	29:P:468:HOH:O	1.84	0.77
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.20	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.34	0.76
7:T:45:PRO:HD2	29:T:223:HOH:O	1.85	0.75
19:D:201:TGL:CG3	29:D:323:HOH:O	2.33	0.75
6:S:43:LYS:N	6:S:43:LYS:HD2	1.91	0.75
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.69	0.75
7:T:37:LEU:CD2	24:T:102:CDL:H361	2.16	0.75
5:E:8:ASP:HA	26:E:201:PSC:H071	1.69	0.75
3:C:160:LEU:HD13	22:C:304:CHD:H181	1.69	0.75
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:610:TGL:H231	19:N:610:TGL:HA92	1.68	0.74
6:F:64:GLU:O	6:F:65:ASP:HB2	1.86	0.74
2:O:56:MET:HA	26:O:303:PSC:H202	1.69	0.74
8:H:9:LYS:O	8:H:10:ASN:HB2	1.87	0.74
15:N:602:HEA:H161	15:N:602:HEA:H273	1.69	0.74
1:N:513:LEU:O	1:N:514:LYS:HB2	1.88	0.74
12:L:2:HIS:CD2	29:L:209:HOH:O	2.40	0.74
19:N:610:TGL:H161	12:Y:24:MET:SD	2.28	0.74
20:A:609:PGV:H221	20:A:609:PGV:C01	2.17	0.74
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.53	0.73
8:H:45:ALA:O	8:H:47:GLY:N	2.18	0.73
7:T:5:LYS:CB	25:T:101:PEK:H362	2.01	0.73
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.88	0.73
1:N:117[A]:MET:HE3	12:Y:39:ILE:HG23	1.71	0.72
4:D:81:VAL:HG11	19:D:201:TGL:HB52	1.70	0.72
9:I:26:MET:HE3	29:I:128:HOH:O	1.89	0.72
7:T:31:CYS:SG	24:T:102:CDL:H551	2.29	0.72
9:I:1:SAC:OAC	9:I:2:THR:HG22	1.89	0.72
2:O:217:LYS:HG3	29:O:485:HOH:O	1.88	0.72
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.72	0.71
8:U:9:LYS:CG	8:U:10:ASN:H	1.98	0.71
8:U:20:PHE:CE2	8:U:27:ARG:HG2	2.26	0.71
3:P:165:ILE:HG12	25:P:309:PEK:H102	1.72	0.71
24:T:102:CDL:C11	24:T:102:CDL:HA21	2.20	0.71
4:Q:109:HIS:HD2	29:Q:338:HOH:O	1.72	0.71
15:N:602:HEA:HBC1	15:N:602:HEA:HMC1	1.73	0.70
6:S:43:LYS:N	6:S:43:LYS:HD3	1.99	0.70
1:A:312[A]:ILE:CD1	29:A:740:HOH:O	2.01	0.70
7:G:5:LYS:HB2	25:G:104:PEK:H362	1.74	0.70
7:G:38:HIS:CE1	24:G:103:CDL:H111	2.27	0.70
1:N:273:MET:HE2	29:N:735:HOH:O	1.92	0.70
24:C:303:CDL:H242	24:C:303:CDL:H661	1.73	0.70
26:O:303:PSC:H212	26:O:303:PSC:O01	1.92	0.70
8:H:7:LYS:O	8:H:8:ILE:HB	1.91	0.70
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.38	0.69
19:N:609:TGL:H302	19:N:609:TGL:H122	1.74	0.69
24:C:303:CDL:H521	24:C:303:CDL:OB9	1.92	0.69
2:O:41:ILE:HD13	26:O:303:PSC:H342	1.75	0.69
3:C:63:ARG:HE	24:C:303:CDL:CA2	2.05	0.69
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.75	0.68
1:A:468:MET:HG3	29:A:735:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:609:PGV:H221	20:A:609:PGV:H012	1.73	0.68
26:O:303:PSC:C07	9:V:10:ARG:HH21	2.07	0.67
1:A:27:GLY:CA	15:A:602:HEA:C27	2.66	0.67
3:P:107:ALA:HB2	20:P:302:PGV:H031	1.77	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.67
24:T:102:CDL:H231	24:T:102:CDL:H541	1.76	0.67
3:P:63:ARG:HE	24:P:306:CDL:CA2	2.07	0.67
20:A:609:PGV:C06	29:A:822:HOH:O	2.43	0.67
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.77	0.66
3:P:246:ASP:HB2	29:P:428:HOH:O	1.94	0.66
2:B:183:THR:HG22	29:B:424:HOH:O	1.96	0.66
7:T:37:LEU:HD21	24:T:102:CDL:H361	1.78	0.66
1:N:406:ASN:HD21	20:N:607:PGV:H21	1.58	0.66
7:G:45:PRO:CD	29:G:221:HOH:O	2.26	0.66
24:C:303:CDL:PA1	24:C:303:CDL:HB22	2.35	0.66
3:P:63:ARG:HE	24:P:306:CDL:HA22	1.58	0.66
7:G:3:ALA:HB1	25:G:104:PEK:H382	1.78	0.66
26:E:201:PSC:C07	9:I:10:ARG:NH2	2.55	0.66
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.76	0.66
7:T:5:LYS:HD3	25:T:101:PEK:H371	1.78	0.66
24:G:103:CDL:C23	24:G:103:CDL:H541	2.25	0.65
24:G:103:CDL:H571	24:G:103:CDL:H792	1.77	0.65
26:O:303:PSC:C02	26:O:303:PSC:H212	2.26	0.65
1:N:117[A]:MET:CE	12:Y:42:HIS:CD2	2.79	0.65
24:G:103:CDL:H241	24:G:103:CDL:H542	1.77	0.65
3:P:160:LEU:HD13	22:P:307:CHD:C18	2.27	0.65
1:N:117[B]:MET:HE3	10:W:50:LEU:HD21	1.77	0.64
1:N:177:SER:H	1:N:180:GLN:NE2	1.94	0.64
19:L:101:TGL:CC4	19:L:101:TGL:OC1	2.36	0.64
26:O:303:PSC:H072	9:V:10:ARG:HH21	1.63	0.64
24:G:103:CDL:H201	1:N:311:ILE:CD1	2.27	0.64
24:P:306:CDL:H262	24:P:306:CDL:H672	1.79	0.64
19:N:609:TGL:H111	2:O:35:SER:HB3	1.80	0.64
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.63	0.64
29:O:452:HOH:O	8:U:61:LYS:HD3	1.98	0.64
7:G:5:LYS:CG	25:G:104:PEK:H383	2.19	0.64
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.64
2:B:78:LEU:HD12	24:T:102:CDL:H352	1.80	0.63
1:A:406:ASN:HD21	20:A:609:PGV:C2	2.11	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.95	0.63
3:P:3:HIS:HD2	29:P:465:HOH:O	1.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:201:TGL:C24	19:D:201:TGL:HA91	2.29	0.63
5:E:11:PHE:CB	26:E:201:PSC:H073	2.28	0.62
6:S:94:HIS:CD2	6:S:95:GLN:H	2.16	0.62
19:D:201:TGL:HG32	29:D:323:HOH:O	1.98	0.62
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.80	0.62
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.81	0.62
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.80	0.62
19:D:201:TGL:H242	19:D:201:TGL:HA91	1.81	0.62
8:U:9:LYS:O	8:U:10:ASN:HB2	2.01	0.61
26:O:303:PSC:H21	26:O:303:PSC:C22	2.30	0.61
7:T:8:HIS:CD2	25:T:101:PEK:H252	2.36	0.61
5:E:11:PHE:HB3	26:E:201:PSC:H073	1.83	0.61
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.01	0.61
7:G:72:ASN:H	7:G:76:ASN:ND2	1.96	0.61
1:A:273:MET:HE2	29:A:738:HOH:O	2.00	0.61
7:T:3:ALA:HB3	25:T:101:PEK:H361	1.83	0.60
19:A:607:TGL:H252	19:A:607:TGL:HA91	1.82	0.60
29:N:790:HOH:O	4:Q:20:ARG:HG2	2.01	0.60
19:L:101:TGL:CA9	19:L:101:TGL:H231	2.31	0.60
1:A:311:ILE:CD1	24:T:102:CDL:H201	2.32	0.60
19:N:610:TGL:CC3	12:Y:20:ARG:HH22	2.14	0.59
6:S:64:GLU:O	6:S:65:ASP:HB2	2.02	0.59
26:O:303:PSC:H071	5:R:8:ASP:HA	1.84	0.59
7:T:3:ALA:O	7:T:4:ALA:CB	2.50	0.59
1:N:309:THR:O	1:N:312[B]:ILE:HG22	2.02	0.59
2:B:41:ILE:HD13	26:E:201:PSC:C34	2.23	0.59
3:P:224:LYS:CD	24:P:306:CDL:HB31	2.32	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.67	0.59
5:R:79:LYS:HE2	29:R:219:HOH:O	2.03	0.59
5:E:91:PRO:HD2	29:E:335:HOH:O	2.03	0.59
19:A:607:TGL:C28	19:A:607:TGL:H101	2.33	0.58
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.84	0.58
20:C:302:PGV:H182	24:C:303:CDL:H671	1.85	0.58
20:A:609:PGV:H311	13:M:19:LEU:HD23	1.85	0.58
4:D:40:LEU:HD22	4:D:58:GLU:HG2	1.85	0.58
11:K:8:ASP:HB2	29:K:108:HOH:O	2.03	0.58
11:X:54:ARG:HD3	29:X:114:HOH:O	2.03	0.58
24:G:103:CDL:H231	24:G:103:CDL:H541	1.85	0.58
20:C:302:PGV:H172	24:C:303:CDL:H651	1.85	0.58
6:F:1:ALA:HB3	6:S:65:ASP:OD1	2.03	0.58
1:A:1:FME:HA	1:A:1:FME:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.69	0.58
2:B:62:GLU:O	2:B:66:THR:HB	2.04	0.58
24:P:306:CDL:PA1	24:P:306:CDL:HB22	2.44	0.57
1:A:513:LEU:O	1:A:514:LYS:HB2	2.05	0.57
9:I:15:ARG:HD3	29:I:122:HOH:O	2.04	0.57
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.03	0.57
1:A:430:PHE:HE1	19:A:607:TGL:HB21	1.69	0.57
2:O:225:SER:C	2:O:227:LEU:H	2.06	0.57
20:N:608:PGV:H182	3:P:28:THR:HG22	1.86	0.57
19:D:201:TGL:HG32	19:D:201:TGL:OB1	2.04	0.57
5:E:90:ARG:HD2	29:E:347:HOH:O	2.04	0.57
9:I:26:MET:HG3	29:I:128:HOH:O	2.03	0.57
26:O:303:PSC:H061	5:R:8:ASP:OD1	2.05	0.57
1:N:468:MET:HG3	29:N:732:HOH:O	2.04	0.57
24:G:103:CDL:H112	24:G:103:CDL:HA21	1.87	0.56
3:C:67:PHE:CE1	24:C:303:CDL:H1	2.25	0.56
26:O:303:PSC:H343	26:O:303:PSC:H142	1.88	0.56
24:T:102:CDL:OA7	24:T:102:CDL:H342	2.06	0.56
7:G:38:HIS:HE1	24:G:103:CDL:H111	1.69	0.56
3:P:164:PHE:CD1	22:P:307:CHD:H192	2.40	0.56
10:J:7:GLU:HG3	29:J:110:HOH:O	2.04	0.56
7:T:2:SER:OG	25:T:101:PEK:C30	2.53	0.56
1:A:334:TRP:HB2	19:D:201:TGL:HG11	1.88	0.56
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.05	0.56
7:T:37:LEU:HD23	24:T:102:CDL:H361	1.88	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
3:C:59:ARG:HG3	24:C:303:CDL:H511	1.88	0.56
7:T:5:LYS:HD2	25:T:101:PEK:H383	1.88	0.55
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.55
5:E:8:ASP:HA	26:E:201:PSC:C07	2.36	0.55
6:F:54:ASN:HB3	29:F:226:HOH:O	2.06	0.55
3:P:33[A]:MET:HE1	3:P:42:LEU:N	2.12	0.55
20:N:607:PGV:H011	20:N:607:PGV:C21	2.37	0.55
2:O:29:MET:HG3	9:V:35:TYR:CD2	2.42	0.55
20:A:609:PGV:H221	20:A:609:PGV:H011	1.89	0.55
20:A:609:PGV:H321	20:A:609:PGV:H152	1.87	0.54
26:O:303:PSC:H21	26:O:303:PSC:H221	1.89	0.54
1:N:310:MET:CE	1:N:356:ILE:HG23	2.37	0.54
3:C:106:LEU:HD13	20:C:307:PGV:H22	1.88	0.54
12:L:2:HIS:CG	29:L:209:HOH:O	2.57	0.54
3:P:161:GLN:HE22	25:P:309:PEK:H22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:63:GLY:H	28:G:101:DMU:H34	1.73	0.54
24:P:306:CDL:H642	24:P:306:CDL:H242	1.89	0.54
7:T:38:HIS:HE2	24:T:102:CDL:H111	1.73	0.54
5:E:72:LYS:HB2	5:E:82:TYR:CD2	2.43	0.54
1:N:117[A]:MET:HE2	12:Y:42:HIS:HD2	1.67	0.54
4:Q:7:LYS:HB2	4:Q:10:ASP:OD1	2.06	0.54
24:G:103:CDL:H511	24:G:103:CDL:H181	1.89	0.53
3:C:164:PHE:CD1	22:C:304:CHD:H192	2.43	0.53
7:G:31:CYS:SG	24:G:103:CDL:H532	2.48	0.53
8:U:9:LYS:HG3	29:U:123:HOH:O	2.07	0.53
25:G:104:PEK:H051	3:P:77:LYS:HZ1	1.73	0.53
26:E:201:PSC:H083	26:E:201:PSC:O13	2.09	0.53
19:N:609:TGL:C30	19:N:609:TGL:C12	2.86	0.53
2:B:13:THR:OG1	2:B:167:SER:HB3	2.08	0.53
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.53
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.43	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.08	0.53
1:N:383:MET:O	1:N:387:PHE:HB2	2.07	0.53
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.08	0.53
6:S:54:ASN:C	6:S:54:ASN:HD22	2.11	0.53
15:A:602:HEA:HHC	15:A:602:HEA:H122	1.91	0.53
15:N:602:HEA:H122	15:N:602:HEA:HHC	1.91	0.52
7:T:2:SER:O	25:T:101:PEK:H322	2.10	0.52
20:N:607:PGV:H011	20:N:607:PGV:H211	1.91	0.52
3:P:156:ARG:HE	22:P:307:CHD:C24	2.22	0.52
2:O:56:MET:CA	26:O:303:PSC:H202	2.39	0.52
3:C:107:ALA:HB2	20:C:307:PGV:H031	1.90	0.52
6:F:64:GLU:O	6:F:65:ASP:CB	2.53	0.52
28:P:301:DMU:H30	7:T:62:TRP:HB3	1.91	0.52
19:N:610:TGL:CC3	12:Y:20:ARG:NH2	2.47	0.52
4:D:31:LYS:NZ	29:D:359:HOH:O	2.26	0.52
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.75	0.52
3:C:254:VAL:CG2	24:G:103:CDL:H672	2.40	0.52
3:C:156:ARG:HE	22:C:304:CHD:C24	2.22	0.52
4:D:109:HIS:HD2	29:D:314:HOH:O	1.93	0.52
25:P:304:PEK:H161	25:P:304:PEK:H102	1.92	0.51
3:P:224:LYS:HD3	24:P:306:CDL:HB31	1.92	0.51
4:D:131:ILE:HD13	9:I:47:TYR:CE2	2.45	0.51
24:C:303:CDL:OA5	24:C:303:CDL:HB22	2.10	0.51
2:O:164:ALA:O	2:O:194:GLY:HA3	2.10	0.51
2:B:56:MET:HG2	26:E:201:PSC:H211	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:603:HEA:HMC1	15:A:603:HEA:HBC1	1.93	0.51
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.92	0.51
1:A:112:LEU:HG	29:A:742:HOH:O	2.11	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
1:A:311:ILE:HD12	24:T:102:CDL:H201	1.91	0.51
19:N:610:TGL:HG11	12:Y:12:PRO:HG2	1.93	0.51
26:O:303:PSC:H212	26:O:303:PSC:C01	2.41	0.51
26:O:303:PSC:H21	26:O:303:PSC:H222	1.91	0.51
8:H:9:LYS:O	8:H:10:ASN:CB	2.57	0.50
12:L:14:SER:H	19:L:101:TGL:HC31	1.75	0.50
2:B:41:ILE:CD1	26:E:201:PSC:H342	2.26	0.50
19:D:201:TGL:CG3	19:D:201:TGL:OB1	2.59	0.50
8:U:51:SER:HB2	29:U:122:HOH:O	2.10	0.50
19:N:610:TGL:HC31	12:Y:13:PHE:HA	1.93	0.50
15:N:603:HEA:HMC1	15:N:603:HEA:HBC1	1.92	0.50
7:G:3:ALA:O	7:G:4:ALA:CB	2.59	0.50
26:E:201:PSC:O01	26:E:201:PSC:H212	2.12	0.50
25:G:102:PEK:H71	25:G:102:PEK:H32	1.94	0.50
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.93	0.50
7:G:3:ALA:CB	25:G:104:PEK:H382	2.40	0.50
22:C:305:CHD:H152	20:C:307:PGV:H11	1.93	0.50
1:N:20:LEU:HB3	19:N:610:TGL:H221	1.92	0.50
12:L:20:ARG:HH22	19:L:101:TGL:CC3	2.01	0.50
2:B:56:MET:HA	26:E:201:PSC:H202	1.94	0.50
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.94	0.50
2:O:41:ILE:CD1	26:O:303:PSC:H342	2.41	0.49
3:C:33[A]:MET:HG2	3:C:39:SER:HB3	1.94	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.57	0.49
3:C:224:LYS:CD	24:C:303:CDL:HB31	2.42	0.49
6:S:48:LEU:HG	6:S:92:VAL:HG11	1.94	0.49
7:G:5:LYS:CB	25:G:104:PEK:H362	2.43	0.49
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.49
1:A:169:ILE:HD12	7:T:7:ASP:O	2.12	0.49
3:C:254:VAL:HG23	24:G:103:CDL:H672	1.94	0.49
1:A:328:HIS:HB2	2:B:45:MET:SD	2.53	0.49
3:C:217:VAL:HG22	24:C:303:CDL:H732	1.95	0.49
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.43	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.49
8:H:7:LYS:O	8:H:8:ILE:CB	2.61	0.49
1:A:177:SER:H	1:A:180:GLN:HE21	1.61	0.49
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:LYS:HB3	29:I:121:HOH:O	2.13	0.48
3:C:55:TYR:CE1	24:C:303:CDL:H532	2.48	0.48
6:F:50:PRO:HG2	29:F:244:HOH:O	2.13	0.48
5:E:5:HIS:HB3	5:E:6:GLU:HG2	1.95	0.48
6:S:19:GLU:CG	29:S:232:HOH:O	2.49	0.48
9:I:1:SAC:OAC	9:I:2:THR:CG2	2.59	0.48
19:N:610:TGL:HA22	12:Y:13:PHE:HB3	1.96	0.48
28:G:101:DMU:C57	28:G:101:DMU:H36	2.30	0.48
19:N:609:TGL:H302	19:N:609:TGL:C12	2.40	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.96	0.48
7:G:2:SER:O	25:G:104:PEK:H321	2.13	0.48
3:P:224:LYS:HD2	24:P:306:CDL:HB31	1.95	0.48
2:B:66:THR:HG21	22:B:302:CHD:H3	1.94	0.48
20:N:607:PGV:H221	20:N:607:PGV:H22	1.95	0.48
7:T:1:ALA:N	29:T:222:HOH:O	2.47	0.48
29:A:855:HOH:O	3:C:77:LYS:HE3	2.12	0.48
3:P:52:LEU:HD21	24:P:306:CDL:H411	1.96	0.47
6:S:94:HIS:CD2	6:S:95:GLN:N	2.82	0.47
12:L:20:ARG:HH21	19:L:101:TGL:HC32	1.69	0.47
6:S:94:HIS:HD2	6:S:95:GLN:H	1.60	0.47
24:T:102:CDL:H592	24:T:102:CDL:H561	1.63	0.47
19:A:607:TGL:H101	19:A:607:TGL:H281	1.96	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.14	0.47
6:S:52:ILE:O	6:S:94:HIS:CE1	2.67	0.47
1:N:106:PRO:N	1:N:107:PRO:HD2	2.30	0.47
4:Q:109:HIS:CD2	29:Q:338:HOH:O	2.56	0.47
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.96	0.47
26:O:303:PSC:H343	26:O:303:PSC:C14	2.44	0.47
19:N:609:TGL:H101	19:N:609:TGL:C28	2.44	0.47
7:T:8:HIS:CE1	25:T:101:PEK:H332	2.49	0.47
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.96	0.46
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.97	0.46
13:M:39:ASN:O	13:M:43:SER:HB2	2.15	0.46
29:O:456:HOH:O	4:Q:129:ALA:HB2	2.15	0.46
10:J:52:TRP:O	10:J:57:HIS:HE1	1.98	0.46
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.98	0.46
24:T:102:CDL:H631	24:T:102:CDL:H662	1.69	0.46
26:E:201:PSC:H62	26:E:201:PSC:H241	1.98	0.46
3:P:164:PHE:CE1	22:P:307:CHD:H192	2.50	0.46
6:S:43:LYS:HD2	6:S:88:HIS:CE1	2.51	0.46
3:P:63:ARG:HE	24:P:306:CDL:HA21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:VAL:HG22	25:T:101:PEK:H15	1.98	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.14	0.46
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.51	0.45
6:S:75:HIS:H	6:S:80:GLN:NE2	1.99	0.45
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.99	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.45
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.45
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.34	0.45
3:P:22:LEU:O	3:P:26:LEU:HG	2.16	0.45
24:G:103:CDL:H332	2:O:78:LEU:HD12	1.99	0.45
1:A:283:LEU:HB2	1:A:312[B]:ILE:HD12	1.99	0.45
19:L:101:TGL:CC6	19:L:101:TGL:HC22	2.23	0.45
1:A:178:GLN:CB	7:T:7:ASP:OD2	2.65	0.45
1:A:113:LEU:HB3	1:A:117[B]:MET:CE	2.46	0.45
6:F:92:VAL:O	6:F:92:VAL:HG23	2.16	0.45
4:Q:93:ALA:HB3	11:X:28:VAL:HG22	1.98	0.45
15:N:602:HEA:H172	15:N:602:HEA:H272	1.31	0.45
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.45
24:G:103:CDL:H561	24:G:103:CDL:H592	1.69	0.44
24:G:103:CDL:H452	2:O:70:ALA:HB1	1.99	0.44
5:R:106:LEU:HA	5:R:106:LEU:HD23	1.79	0.44
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.99	0.44
3:P:51[B]:MET:HB3	24:P:306:CDL:H381	2.00	0.44
1:N:488:THR:HB	1:N:495:LEU:HD13	1.98	0.44
1:N:240:HIS:O	1:N:243:VAL:HG22	2.18	0.44
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.99	0.44
25:P:304:PEK:H32	25:P:304:PEK:C7	2.31	0.44
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.44
24:T:102:CDL:H362	24:T:102:CDL:H122	2.00	0.44
2:B:41:ILE:O	2:B:45:MET:HG2	2.17	0.44
22:P:307:CHD:H12A	22:P:307:CHD:H112	1.84	0.44
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.53	0.44
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.44
7:T:3:ALA:HB1	25:T:101:PEK:H382	2.00	0.44
20:N:607:PGV:H011	20:N:607:PGV:H221	1.99	0.44
1:N:409:TRP:CE2	20:N:607:PGV:H61	2.53	0.44
26:O:303:PSC:H031	26:O:303:PSC:O02	2.17	0.44
1:N:437:PRO:HG2	1:N:440:TYR:CE1	2.53	0.44
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.83	0.44
7:T:31:CYS:HG	24:T:102:CDL:H532	1.82	0.43
9:V:29:LEU:HA	9:V:29:LEU:HD12	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
24:T:102:CDL:C23	24:T:102:CDL:H541	2.43	0.43
24:P:306:CDL:OB6	24:P:306:CDL:HB21	2.18	0.43
7:G:5:LYS:HB3	1:N:278:MET:SD	2.58	0.43
19:D:201:TGL:H132	19:D:201:TGL:H302	1.72	0.43
4:Q:143:ASN:ND2	29:Q:309:HOH:O	2.50	0.43
1:A:116:SER:HB3	29:A:746:HOH:O	2.17	0.43
3:C:54:MET:HE3	24:C:303:CDL:H612	2.00	0.43
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.91	0.43
19:N:609:TGL:H111	2:O:35:SER:CB	2.48	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.00	0.43
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	0.43
24:T:102:CDL:CA2	24:T:102:CDL:H111	2.43	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.43
24:G:103:CDL:H351	2:O:81:LEU:HD12	2.01	0.43
22:C:304:CHD:H12A	22:C:304:CHD:H112	1.77	0.43
15:A:603:HEA:H243	2:B:69:PRO:HB3	2.00	0.43
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.99	0.43
7:T:3:ALA:HB1	25:T:101:PEK:C38	2.49	0.43
1:N:393:PHE:CD1	15:N:602:HEA:H241	2.53	0.43
22:B:302:CHD:H212	22:B:302:CHD:H12	2.00	0.43
19:N:609:TGL:C30	19:N:609:TGL:H122	2.43	0.43
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.54	0.43
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.43
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.18	0.43
2:B:81:LEU:HD13	24:T:102:CDL:H121	2.00	0.43
24:G:103:CDL:H662	24:G:103:CDL:H631	1.78	0.43
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.18	0.43
11:X:24:PHE:O	11:X:28:VAL:HG12	2.19	0.43
5:E:48:ILE:HG21	5:E:89:LEU:HD11	2.00	0.43
3:P:217:VAL:HG22	24:P:306:CDL:H732	2.01	0.43
4:D:107:ILE:HB	4:D:108:PRO:CD	2.48	0.43
5:R:108:LYS:HB2	5:R:108:LYS:NZ	2.34	0.43
3:C:122:HIS:HA	3:C:123:PRO:HD3	1.88	0.43
19:L:101:TGL:H231	19:L:101:TGL:HA91	1.99	0.42
3:C:223:LEU:HD21	22:C:304:CHD:H183	2.02	0.42
1:A:430:PHE:CE1	19:A:607:TGL:HB21	2.52	0.42
4:Q:139:ASP:OD2	4:Q:142:LYS:HG3	2.19	0.42
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.00	0.42
1:N:113:LEU:HD13	19:N:610:TGL:H292	2.01	0.42
3:P:69:GLY:HA3	6:S:14:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:G:103:CDL:H152	24:G:103:CDL:H182	1.69	0.42
25:T:101:PEK:H282	25:T:101:PEK:H312	1.73	0.42
7:T:3:ALA:CB	25:T:101:PEK:H382	2.50	0.42
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.42
3:P:230:ASN:HB2	29:P:459:HOH:O	2.19	0.42
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.36	0.42
3:C:76:GLN:NE2	3:C:80:ARG:HH21	2.17	0.42
7:T:38:HIS:ND1	7:T:38:HIS:N	2.68	0.42
3:P:226:HIS:CE1	24:P:306:CDL:HB32	2.55	0.42
7:T:2:SER:HG	25:T:101:PEK:H301	1.81	0.42
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.66	0.42
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.01	0.42
2:B:69:PRO:HG2	29:B:474:HOH:O	2.19	0.42
9:V:6:LYS:HA	9:V:7:PRO:HD3	1.87	0.42
2:O:116:LEU:HD12	2:O:117:SER:N	2.34	0.42
2:B:78:LEU:CD1	24:T:102:CDL:H352	2.47	0.42
1:A:297:MET:CE	1:A:297:MET:CB	2.97	0.42
19:L:101:TGL:CA9	19:L:101:TGL:C23	2.97	0.42
15:A:602:HEA:HBC1	15:A:602:HEA:HMC1	2.01	0.42
7:G:3:ALA:HB3	25:G:104:PEK:H361	2.01	0.42
1:N:408:THR:HB	20:N:607:PGV:H51	2.01	0.42
1:N:114:ALA:HA	1:N:117[B]:MET:HE3	2.01	0.42
6:F:54:ASN:H	6:F:54:ASN:ND2	2.07	0.42
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.42
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.85	0.42
1:N:310:MET:HE1	2:O:76:ILE:HG21	2.02	0.42
28:P:301:DMU:H30	7:T:62:TRP:CB	2.48	0.42
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.83	0.42
3:P:76:GLN:NE2	29:P:414:HOH:O	2.47	0.42
1:N:309:THR:HG22	15:N:603:HEA:HMB2	2.02	0.42
2:B:29:MET:SD	9:I:36:LYS:HE3	2.60	0.42
4:D:93:ALA:HB3	11:K:28:VAL:HG22	2.00	0.42
1:N:215:LEU:HD11	25:P:304:PEK:H271	2.02	0.41
6:S:95:GLN:HG3	6:S:96:LEU:H	1.85	0.41
9:V:18:ARG:CG	9:V:18:ARG:HH11	2.32	0.41
28:P:301:DMU:C57	7:T:62:TRP:HB3	2.50	0.41
25:G:104:PEK:H341	29:G:227:HOH:O	2.18	0.41
3:C:224:LYS:HD2	24:C:303:CDL:HB31	2.01	0.41
8:H:8:ILE:HG23	8:H:8:ILE:O	2.20	0.41
19:N:609:TGL:C28	19:N:609:TGL:C10	2.98	0.41
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:302:CHD:H212	22:O:302:CHD:H12	2.02	0.41
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.41
7:G:1:ALA:N	20:P:302:PGV:H321	2.35	0.41
1:A:412:ILE:HG12	4:D:84:ALA:HB3	2.01	0.41
2:O:82:ARG:HH11	2:O:86:MET:HE3	1.85	0.41
1:N:43:GLN:OE1	4:Q:104:TYR:HB3	2.20	0.41
10:J:4:ARG:HD3	10:J:7:GLU:OE2	2.20	0.41
5:R:5:HIS:CD2	5:R:6:GLU:HG2	2.55	0.41
2:O:74:ILE:HG22	2:O:78:LEU:HD22	2.02	0.41
19:N:610:TGL:H272	12:Y:11:ILE:CG2	2.50	0.41
1:A:334:TRP:CB	19:D:201:TGL:HG11	2.50	0.41
3:C:186:PHE:HA	3:C:190:ASP:OD2	2.19	0.41
7:G:84:LYS:HD2	7:G:84:LYS:H	1.86	0.41
3:C:3:HIS:N	29:C:475:HOH:O	2.52	0.41
2:O:62:GLU:O	2:O:66:THR:HB	2.21	0.41
19:Q:201:TGL:OB1	29:Q:308:HOH:O	2.22	0.41
1:N:342:LEU:HD13	2:O:46:LEU:HD11	2.03	0.41
2:O:29:MET:HG3	9:V:35:TYR:CG	2.56	0.41
7:G:5:LYS:HG3	25:G:104:PEK:C38	2.28	0.41
24:C:303:CDL:H222	24:C:303:CDL:H641	2.02	0.41
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.51	0.41
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.02	0.41
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.03	0.41
2:O:200:CYS:SG	2:O:204:HIS:HA	2.61	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
8:U:9:LYS:CG	29:U:123:HOH:O	2.66	0.41
1:A:169:ILE:CD1	7:T:7:ASP:O	2.69	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
7:T:11:TPO:HA	7:T:11:TPO:O2P	2.21	0.41
7:T:6:GLY:O	25:T:101:PEK:H311	2.21	0.41
3:P:223:LEU:HD21	22:P:307:CHD:H183	2.03	0.41
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	2.03	0.41
1:A:115:SER:HB2	1:A:142:SER:O	2.20	0.41
29:B:490:HOH:O	4:D:129:ALA:HB2	2.21	0.41
1:A:489:THR:HA	6:F:71:TRP:O	2.21	0.41
12:L:44:LEU:HA	12:L:44:LEU:HD23	1.87	0.41
1:N:104:LEU:HB2	1:N:156:SER:HB2	2.03	0.41
2:B:103:GLN:HA	2:B:104:TRP:HA	1.88	0.41
22:P:308:CHD:H212	22:P:308:CHD:H12	2.03	0.41
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.37	0.40
4:Q:81:VAL:HG11	19:Q:201:TGL:HB51	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.49	0.40
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.51	0.40
20:N:607:PGV:H92	4:Q:84:ALA:HB2	2.02	0.40
1:A:350:VAL:HG13	19:A:607:TGL:HB81	2.04	0.40
5:R:79:LYS:HD2	5:R:79:LYS:N	2.35	0.40
5:E:86:ILE:O	5:E:90:ARG:HG2	2.22	0.40
1:N:46:THR:HG23	1:N:49:GLY:O	2.21	0.40
4:Q:33:LEU:HB2	4:Q:38:LYS:HE2	2.02	0.40
1:A:344:PHE:C	1:A:344:PHE:CD1	2.95	0.40
2:O:84:LEU:HA	2:O:87:MET:HE2	2.03	0.40
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	515/514 (100%)	502 (98%)	12 (2%)	1 (0%)	52 48
1	N	515/514 (100%)	501 (97%)	14 (3%)	0	100 100
2	B	225/227 (99%)	216 (96%)	9 (4%)	0	100 100
2	O	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	39 33
3	C	260/261 (100%)	256 (98%)	4 (2%)	0	100 100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100 100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100 100
4	Q	142/147 (97%)	132 (93%)	10 (7%)	0	100 100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
5	R	103/109 (94%)	103 (100%)	0	0	100 100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	9 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	5 1
7	G	81/85 (95%)	70 (86%)	6 (7%)	5 (6%)	2 0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	2 0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	2 0
8	U	77/85 (91%)	71 (92%)	2 (3%)	4 (5%)	2 0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100 100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100 100
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	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	3516/3614 (97%)	3386 (96%)	105 (3%)	25 (1%)	26 19

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
8	H	8	ILE
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	8	ILE
6	F	95	GLN
7	G	37	LEU
7	T	43	GLU
8	U	45	ALA
8	H	47	GLY

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Mol	Chain	Res	Type
6	S	95	GLN
8	U	11	TYR
7	G	8	HIS
7	T	6	GLY
7	G	6	GLY
8	U	10	ASN
1	A	384	GLY
2	O	92	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/426 (101%)	418 (97%)	11 (3%)	54	54
1	N	429/426 (101%)	421 (98%)	8 (2%)	65	67
2	B	210/210 (100%)	198 (94%)	12 (6%)	25	19
2	O	210/210 (100%)	200 (95%)	10 (5%)	31	26
3	C	227/226 (100%)	224 (99%)	3 (1%)	76	79
3	P	227/226 (100%)	223 (98%)	4 (2%)	66	69
4	D	128/129 (99%)	123 (96%)	5 (4%)	39	35
4	Q	128/129 (99%)	122 (95%)	6 (5%)	32	27
5	E	92/95 (97%)	91 (99%)	1 (1%)	80	83
5	R	92/95 (97%)	88 (96%)	4 (4%)	35	30
6	F	81/81 (100%)	77 (95%)	4 (5%)	31	25
6	S	81/81 (100%)	77 (95%)	4 (5%)	31	25
7	G	67/68 (98%)	61 (91%)	6 (9%)	12	7
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	7
8	H	71/75 (95%)	67 (94%)	4 (6%)	26	20
8	U	71/75 (95%)	64 (90%)	7 (10%)	10	5
9	I	57/57 (100%)	54 (95%)	3 (5%)	28	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	V	57/57 (100%)	55 (96%)	2 (4%)	43 40
10	J	49/50 (98%)	48 (98%)	1 (2%)	63 65
10	W	49/50 (98%)	48 (98%)	1 (2%)	63 65
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 54
11	X	39/46 (85%)	37 (95%)	2 (5%)	29 23
12	L	39/40 (98%)	39 (100%)	0	100 100
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16 10
13	M	37/38 (97%)	32 (86%)	5 (14%)	5 2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 4
All	All	3052/3082 (99%)	2935 (96%)	117 (4%)	40 36

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	333	LYS
1	A	336	PRO
1	A	338	MET
1	A	362	SER
1	A	369	ASP
1	A	504	THR
2	B	15	PRO
2	B	33	LEU
2	B	54	SER
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET

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Mol	Chain	Res	Type
3	C	214	PHE
4	D	4	SER
4	D	8	SER
4	D	31	LYS
4	D	51	LEU
4	D	58	GLU
5	E	5	HIS
6	F	54	ASN
6	F	80	GLN
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	27	ARG
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	36	LYS
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	96	ARG
1	N	109	PHE
1	N	238	PHE
1	N	278	MET
1	N	363	LEU
1	N	369	ASP
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP

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Mol	Chain	Res	Type
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	221	LYS
2	O	226	MET
3	P	110	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	6	VAL
4	Q	10	ASP
4	Q	20	ARG
4	Q	51	LEU
4	Q	142	LYS
4	Q	143	ASN
5	R	79	LYS
5	R	80	GLU
5	R	90	ARG
5	R	109	VAL
6	S	43	LYS
6	S	48	LEU
6	S	50	PRO
6	S	54	ASN
7	T	2	SER
7	T	18	PHE
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS
8	U	8	ILE
8	U	27	ARG
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU
11	X	7	PRO

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Mol	Chain	Res	Type
11	X	54	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	39	ASN
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	503	HIS
2	B	22	HIS
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	149	HIS
3	C	161	GLN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	76	ASN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN

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Mol	Chain	Res	Type
3	P	68	GLN
4	Q	37	GLN
4	Q	143	ASN
5	R	5	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
11	X	35	GLN
12	Y	42	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	1.18	1 (12%)	5,9,11	2.39	3 (60%)
2	FME	B	1	2	8,9,10	2.14	2 (25%)	5,9,11	5.84	3 (60%)
7	TPO	G	11	7	7,10,11	1.78	2 (28%)	10,14,16	1.58	2 (20%)
9	SAC	I	1	9	7,8,9	3.25	2 (28%)	7,9,11	3.70	4 (57%)
1	FME	N	1	1	8,9,10	1.55	1 (12%)	5,9,11	3.56	3 (60%)
2	FME	O	1	2	8,9,10	0.97	0	5,9,11	2.60	2 (40%)
7	TPO	T	11	7	7,10,11	2.00	3 (42%)	10,14,16	1.86	2 (20%)
9	SAC	V	1	9	7,8,9	2.33	2 (28%)	7,9,11	2.18	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-2.43	1.14	1.22
1	A	1	FME	O1-CN	-2.24	1.15	1.22
7	T	11	TPO	CB-CA	2.04	1.57	1.54
7	G	11	TPO	P-O2P	2.08	1.61	1.54
7	T	11	TPO	P-O3P	2.16	1.62	1.54
7	G	11	TPO	P-O1P	3.05	1.60	1.50
9	I	1	SAC	CA-N	3.25	1.50	1.46
7	T	11	TPO	P-O1P	3.29	1.61	1.50
1	N	1	FME	CA-N	3.63	1.51	1.46
9	V	1	SAC	CA-N	4.09	1.52	1.46
9	V	1	SAC	OAC-C1A	4.31	1.33	1.23
2	B	1	FME	CA-N	4.80	1.53	1.46
9	I	1	SAC	OAC-C1A	7.81	1.41	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	SAC	C2A-C1A-N	-6.84	102.98	116.10
2	B	1	FME	CG-CB-CA	-4.96	98.15	113.07
9	I	1	SAC	OG-CB-CA	-4.78	100.16	111.18
2	O	1	FME	O1-CN-N	-4.11	118.51	124.80
2	O	1	FME	CG-CB-CA	-2.85	104.50	113.07
2	B	1	FME	O-C-CA	-2.75	118.17	125.69
9	V	1	SAC	CB-CA-N	-2.74	104.69	110.70
9	V	1	SAC	O-C-CA	-2.23	119.61	125.69
7	T	11	TPO	O-C-CA	-2.17	119.75	125.69
1	A	1	FME	CG-CB-CA	-2.14	106.64	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	O-C-CA	-2.09	119.99	125.69
9	I	1	SAC	OAC-C1A-C2A	2.16	126.05	122.07
9	V	1	SAC	CA-N-C1A	2.56	130.13	121.32
1	N	1	FME	CE-SD-CG	2.64	109.52	100.36
1	A	1	FME	O1-CN-N	2.69	128.91	124.80
7	G	11	TPO	O2P-P-OG1	2.87	115.21	106.62
9	V	1	SAC	C2A-C1A-N	2.95	121.74	116.10
7	G	11	TPO	CG2-CB-CA	3.28	119.70	113.15
1	A	1	FME	CE-SD-CG	3.77	113.47	100.36
7	T	11	TPO	CG2-CB-CA	4.35	121.83	113.15
9	I	1	SAC	OAC-C1A-N	4.47	130.95	121.84
1	N	1	FME	O1-CN-N	7.15	135.74	124.80
2	B	1	FME	O1-CN-N	11.64	142.60	124.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CYN	A	601	16	0,1,1	0.00	-	0,0,0	0.00	-
15	HEA	A	602	1	40,67,67	1.67	9 (22%)	36,103,103	2.95	10 (27%)
15	HEA	A	603	1	40,67,67	1.32	5 (12%)	36,103,103	2.78	11 (30%)
19	TGL	A	607	-	62,62,62	1.34	7 (11%)	65,65,65	2.29	16 (24%)
20	PGV	A	608	-	50,50,50	0.95	2 (4%)	51,56,56	1.45	5 (9%)
20	PGV	A	609	-	50,50,50	1.21	2 (4%)	51,56,56	1.50	9 (17%)
21	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	B	302	-	29,32,32	1.07	3 (10%)	48,51,51	1.68	9 (18%)
20	PGV	C	302	-	50,50,50	0.91	3 (6%)	51,56,56	1.09	5 (9%)
24	CDL	C	303	-	99,99,99	1.37	12 (12%)	101,111,111	1.43	13 (12%)
22	CHD	C	304	-	29,32,32	0.66	0	48,51,51	2.77	22 (45%)
22	CHD	C	305	-	29,32,32	1.16	3 (10%)	48,51,51	1.79	11 (22%)
25	PEK	C	306	-	51,52,52	1.13	2 (3%)	52,57,57	1.29	5 (9%)
20	PGV	C	307	-	50,50,50	1.39	4 (8%)	51,56,56	1.47	6 (11%)
19	TGL	D	201	-	62,62,62	1.42	7 (11%)	65,65,65	1.49	11 (16%)
26	PSC	E	201	-	51,51,51	1.27	3 (5%)	55,59,59	1.28	4 (7%)
28	DMU	G	101	-	34,34,34	0.83	2 (5%)	45,45,45	2.45	12 (26%)
25	PEK	G	102	-	51,52,52	0.97	3 (5%)	52,57,57	1.67	9 (17%)
24	CDL	G	103	-	99,99,99	1.39	12 (12%)	101,111,111	1.44	16 (15%)
25	PEK	G	104	-	51,52,52	1.11	2 (3%)	52,57,57	1.21	6 (11%)
19	TGL	L	101	-	62,62,62	1.49	7 (11%)	65,65,65	1.67	15 (23%)
28	DMU	M	101	-	34,34,34	0.59	0	45,45,45	1.92	12 (26%)
14	CYN	N	601	16	0,1,1	0.00	-	0,0,0	0.00	-
15	HEA	N	602	1	40,67,67	1.17	6 (15%)	36,103,103	2.98	10 (27%)
15	HEA	N	603	1	40,67,67	1.15	3 (7%)	36,103,103	2.31	13 (36%)
20	PGV	N	607	-	50,50,50	1.00	2 (4%)	51,56,56	1.57	6 (11%)
20	PGV	N	608	-	50,50,50	1.01	2 (4%)	51,56,56	1.27	5 (9%)
19	TGL	N	609	-	62,62,62	1.27	6 (9%)	65,65,65	1.47	9 (13%)
19	TGL	N	610	-	62,62,62	1.50	6 (9%)	65,65,65	1.68	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	302	-	29,32,32	1.08	3 (10%)	48,51,51	1.69	8 (16%)
26	PSC	O	303	-	51,51,51	1.17	3 (5%)	55,59,59	1.36	6 (10%)
28	DMU	P	301	-	34,34,34	0.90	1 (2%)	45,45,45	2.60	12 (26%)
20	PGV	P	302	-	50,50,50	1.12	2 (4%)	51,56,56	1.27	3 (5%)
25	PEK	P	304	-	51,52,52	0.84	2 (3%)	52,57,57	1.79	9 (17%)
20	PGV	P	305	-	50,50,50	0.87	2 (4%)	51,56,56	1.15	4 (7%)
24	CDL	P	306	-	99,99,99	1.37	12 (12%)	101,111,111	1.40	11 (10%)
22	CHD	P	307	-	29,32,32	0.71	0	48,51,51	3.12	23 (47%)
22	CHD	P	308	-	29,32,32	1.13	3 (10%)	48,51,51	2.03	17 (35%)
25	PEK	P	309	-	51,52,52	1.19	2 (3%)	52,57,57	1.22	4 (7%)
19	TGL	Q	201	-	62,62,62	1.30	6 (9%)	65,65,65	1.48	8 (12%)
25	PEK	T	101	-	51,52,52	1.21	2 (3%)	52,57,57	1.31	6 (11%)
24	CDL	T	102	-	99,99,99	1.33	12 (12%)	101,111,111	1.38	12 (11%)
28	DMU	Z	101	-	34,34,34	0.63	0	45,45,45	1.92	10 (22%)

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	CYN	A	601	16	-	0/0/0/0	0/0/0/0
15	HEA	A	602	1	2/2/7/16	0/24/76/76	0/0/8/8
15	HEA	A	603	1	2/2/7/16	0/24/76/76	0/0/8/8
19	TGL	A	607	-	-	0/65/65/65	0/0/0/0
20	PGV	A	608	-	-	0/55/55/55	0/0/0/0
20	PGV	A	609	-	-	2/55/55/55	0/0/0/0
21	CUA	B	301	2	-	0/0/0/0	0/0/0/0
22	CHD	B	302	-	-	0/7/74/74	0/4/4/4
20	PGV	C	302	-	-	0/55/55/55	0/0/0/0
24	CDL	C	303	-	-	0/110/110/110	0/0/0/0
22	CHD	C	304	-	-	0/7/74/74	0/4/4/4
22	CHD	C	305	-	-	0/7/74/74	0/4/4/4
25	PEK	C	306	-	-	0/56/56/56	0/0/0/0
20	PGV	C	307	-	-	0/55/55/55	0/0/0/0
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0
26	PSC	E	201	-	-	0/55/55/55	0/0/0/0
28	DMU	G	101	-	-	0/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	G	102	-	-	0/56/56/56	0/0/0/0
24	CDL	G	103	-	-	0/110/110/110	0/0/0/0
25	PEK	G	104	-	-	0/56/56/56	0/0/0/0
19	TGL	L	101	-	-	0/65/65/65	0/0/0/0
28	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	CYN	N	601	16	-	0/0/0/0	0/0/0/0
15	HEA	N	602	1	3/3/7/16	0/24/76/76	0/0/8/8
15	HEA	N	603	1	2/2/7/16	0/24/76/76	0/0/8/8
20	PGV	N	607	-	-	1/55/55/55	0/0/0/0
20	PGV	N	608	-	-	0/55/55/55	0/0/0/0
19	TGL	N	609	-	-	0/65/65/65	0/0/0/0
19	TGL	N	610	-	-	0/65/65/65	0/0/0/0
21	CUA	O	301	2	-	0/0/0/0	0/0/0/0
22	CHD	O	302	-	-	0/7/74/74	0/4/4/4
26	PSC	O	303	-	-	0/55/55/55	0/0/0/0
28	DMU	P	301	-	-	0/19/59/59	0/2/2/2
20	PGV	P	302	-	-	0/55/55/55	0/0/0/0
25	PEK	P	304	-	-	0/56/56/56	0/0/0/0
20	PGV	P	305	-	-	0/55/55/55	0/0/0/0
24	CDL	P	306	-	-	0/110/110/110	0/0/0/0
22	CHD	P	307	-	-	0/7/74/74	0/4/4/4
22	CHD	P	308	-	-	0/7/74/74	0/4/4/4
25	PEK	P	309	-	-	0/56/56/56	0/0/0/0
19	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
25	PEK	T	101	-	-	0/56/56/56	0/0/0/0
24	CDL	T	102	-	-	0/110/110/110	0/0/0/0
28	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	C20-CA9	-3.76	1.30	1.51
15	A	602	HEA	C3A-C2A	-3.50	1.35	1.40
25	P	304	PEK	O03-C01	-3.43	1.37	1.45
19	N	610	TGL	C20-CA9	-3.41	1.32	1.51
24	C	303	CDL	C59-C58	-3.40	1.32	1.51
15	A	602	HEA	C1A-NA	-3.38	1.32	1.36
24	G	103	CDL	C59-C58	-3.36	1.32	1.51
19	N	609	TGL	C10-CB9	-3.32	1.32	1.51
24	P	306	CDL	C59-C58	-3.27	1.32	1.51
24	C	303	CDL	C79-C78	-3.26	1.32	1.51
19	N	610	TGL	C10-CB9	-3.24	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	102	CDL	C59-C58	-3.21	1.33	1.51
24	T	102	CDL	C42-C41	-3.20	1.33	1.51
24	T	102	CDL	C62-C61	-3.15	1.33	1.51
15	A	603	HEA	C3C-C2C	-3.15	1.36	1.40
24	C	303	CDL	C62-C61	-3.14	1.33	1.51
24	P	306	CDL	C79-C78	-3.14	1.33	1.51
24	P	306	CDL	C82-C81	-3.13	1.33	1.51
19	A	607	TGL	C10-CB9	-3.11	1.33	1.51
24	G	103	CDL	C62-C61	-3.10	1.33	1.51
24	P	306	CDL	C62-C61	-3.07	1.34	1.51
15	N	602	HEA	C3C-C2C	-3.01	1.36	1.40
19	N	609	TGL	C20-CA9	-3.00	1.34	1.51
24	P	306	CDL	C19-C18	-2.98	1.34	1.51
19	A	607	TGL	C20-CA9	-2.97	1.34	1.51
24	C	303	CDL	C82-C81	-2.96	1.34	1.51
24	P	306	CDL	C22-C21	-2.95	1.34	1.51
19	Q	201	TGL	C20-CA9	-2.95	1.34	1.51
24	T	102	CDL	C19-C18	-2.94	1.34	1.51
24	C	303	CDL	C22-C21	-2.93	1.34	1.51
24	P	306	CDL	C39-C38	-2.92	1.34	1.51
24	C	303	CDL	C19-C18	-2.91	1.34	1.51
24	G	103	CDL	C42-C41	-2.90	1.35	1.51
24	G	103	CDL	C19-C18	-2.89	1.35	1.51
19	D	201	TGL	C15-CC9	-2.88	1.35	1.51
24	T	102	CDL	C39-C38	-2.88	1.35	1.51
19	L	101	TGL	C10-CB9	-2.87	1.35	1.51
24	T	102	CDL	C79-C78	-2.83	1.35	1.51
24	T	102	CDL	C82-C81	-2.82	1.35	1.51
24	G	103	CDL	C22-C21	-2.80	1.35	1.51
24	C	303	CDL	C39-C38	-2.80	1.35	1.51
19	Q	201	TGL	C10-CB9	-2.79	1.35	1.51
24	C	303	CDL	C42-C41	-2.75	1.35	1.51
19	Q	201	TGL	C15-CC9	-2.73	1.35	1.51
24	G	103	CDL	C39-C38	-2.72	1.36	1.51
24	T	102	CDL	C22-C21	-2.72	1.36	1.51
19	D	201	TGL	C20-CA9	-2.71	1.36	1.51
19	N	609	TGL	C15-CC9	-2.69	1.36	1.51
24	G	103	CDL	C82-C81	-2.65	1.36	1.51
19	L	101	TGL	C15-CC9	-2.60	1.36	1.51
24	G	103	CDL	C79-C78	-2.59	1.36	1.51
19	D	201	TGL	C10-CB9	-2.58	1.36	1.51
24	P	306	CDL	C42-C41	-2.56	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	610	TGL	C15-CC9	-2.56	1.36	1.51
15	N	602	HEA	C4A-NA	-2.54	1.33	1.36
25	G	102	PEK	O03-C01	-2.48	1.39	1.45
19	A	607	TGL	C15-CC9	-2.46	1.37	1.51
19	A	607	TGL	OC1-CC1	-2.35	1.15	1.22
15	N	603	HEA	C3C-C2C	-2.32	1.37	1.40
15	N	603	HEA	C4B-NB	-2.24	1.33	1.36
20	C	302	PGV	P-O14	-2.16	1.45	1.55
15	N	602	HEA	C1C-CHC	2.02	1.45	1.40
15	A	602	HEA	CMD-C2D	2.06	1.56	1.51
15	A	603	HEA	C18-C19	2.07	1.38	1.32
22	C	305	CHD	C4-C5	2.09	1.57	1.53
22	B	302	CHD	C19-C10	2.12	1.58	1.54
15	A	602	HEA	CAA-C2A	2.15	1.55	1.52
15	N	602	HEA	C4D-CHA	2.16	1.45	1.40
15	N	602	HEA	C4C-CHD	2.18	1.46	1.40
20	P	305	PGV	O01-C1	2.20	1.40	1.34
28	G	101	DMU	O1-C10	2.22	1.47	1.41
20	C	307	PGV	P-O11	2.23	1.68	1.59
15	A	603	HEA	OMA-CMA	2.23	1.29	1.21
22	C	305	CHD	C8-C14	2.25	1.58	1.53
22	O	302	CHD	C11-C12	2.25	1.57	1.53
25	P	304	PEK	O01-C1	2.32	1.41	1.34
20	C	307	PGV	C03-C02	2.35	1.57	1.50
22	P	308	CHD	C6-C5	2.39	1.57	1.53
22	B	302	CHD	C4-C3	2.42	1.56	1.51
22	P	308	CHD	C6-C7	2.48	1.56	1.52
22	O	302	CHD	C6-C7	2.51	1.56	1.52
20	N	608	PGV	O01-C1	2.53	1.41	1.34
15	A	603	HEA	O11-C11	2.56	1.48	1.42
19	L	101	TGL	CG3-CG2	2.56	1.58	1.50
22	O	302	CHD	C11-C9	2.58	1.58	1.53
19	D	201	TGL	OB1-CB1	2.64	1.30	1.22
15	A	603	HEA	C12-C13	2.70	1.62	1.53
15	N	603	HEA	C12-C13	2.70	1.62	1.53
15	A	602	HEA	C12-C13	2.71	1.62	1.53
15	N	602	HEA	C12-C13	2.72	1.62	1.53
22	P	308	CHD	C8-C7	2.73	1.58	1.53
22	B	302	CHD	C6-C7	2.75	1.57	1.52
25	G	102	PEK	O03-C21	2.80	1.41	1.33
22	C	305	CHD	C8-C9	2.86	1.59	1.53
15	A	602	HEA	C1C-CHC	2.89	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	302	PGV	O01-C1	2.96	1.43	1.34
28	G	101	DMU	O16-C6	2.98	1.45	1.40
15	A	602	HEA	CMC-C2C	3.01	1.57	1.51
20	A	608	PGV	O01-C1	3.05	1.43	1.34
24	T	102	CDL	OA8-CA7	3.26	1.43	1.33
19	N	609	TGL	OG3-CC1	3.45	1.43	1.33
20	C	302	PGV	O03-C19	3.47	1.43	1.33
25	G	102	PEK	O01-C1	3.47	1.44	1.34
19	A	607	TGL	OG3-CC1	3.50	1.43	1.33
20	P	305	PGV	O03-C19	3.68	1.44	1.33
15	A	602	HEA	O11-C11	3.72	1.51	1.42
26	O	303	PSC	C13-C12	3.81	1.54	1.31
24	C	303	CDL	OB6-CB5	3.85	1.45	1.34
20	N	607	PGV	O01-C1	3.85	1.45	1.34
26	E	201	PSC	C13-C12	3.85	1.54	1.31
28	P	301	DMU	O16-C6	3.86	1.47	1.40
20	N	607	PGV	O03-C19	3.95	1.45	1.33
15	A	602	HEA	C27-C19	4.04	1.61	1.50
26	O	303	PSC	O03-C19	4.16	1.45	1.33
19	D	201	TGL	OG2-CB1	4.16	1.46	1.34
24	G	103	CDL	OA8-CA7	4.21	1.45	1.33
19	Q	201	TGL	OG3-CC1	4.29	1.46	1.33
20	A	608	PGV	O03-C19	4.31	1.46	1.33
24	P	306	CDL	OB8-CB7	4.32	1.46	1.33
25	G	104	PEK	O01-C1	4.33	1.47	1.34
24	C	303	CDL	OB8-CB7	4.34	1.46	1.33
20	N	608	PGV	O03-C19	4.34	1.46	1.33
26	O	303	PSC	O01-C1	4.35	1.47	1.34
24	P	306	CDL	OA6-CA5	4.36	1.47	1.34
24	P	306	CDL	OB6-CB5	4.37	1.47	1.34
19	Q	201	TGL	OG1-CA1	4.45	1.46	1.33
20	P	302	PGV	O03-C19	4.52	1.46	1.33
24	T	102	CDL	OB6-CB5	4.53	1.47	1.34
24	C	303	CDL	OA6-CA5	4.54	1.47	1.34
19	N	609	TGL	OG1-CA1	4.57	1.46	1.33
19	A	607	TGL	OG2-CB1	4.57	1.47	1.34
20	A	609	PGV	O01-C1	4.72	1.48	1.34
25	C	306	PEK	O03-C21	4.73	1.47	1.33
19	Q	201	TGL	OG2-CB1	4.73	1.48	1.34
26	E	201	PSC	O01-C1	4.75	1.48	1.34
24	T	102	CDL	OB8-CB7	4.77	1.47	1.33
24	G	103	CDL	OA6-CA5	4.77	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	101	PEK	O01-C1	4.83	1.48	1.34
24	T	102	CDL	OA6-CA5	4.84	1.48	1.34
25	P	309	PEK	O03-C21	4.86	1.47	1.33
25	G	104	PEK	O03-C21	4.88	1.47	1.33
19	N	609	TGL	OG2-CB1	4.88	1.48	1.34
20	P	302	PGV	O01-C1	4.92	1.48	1.34
20	A	609	PGV	O03-C19	4.93	1.48	1.33
26	E	201	PSC	O03-C19	4.94	1.48	1.33
24	G	103	CDL	OB6-CB5	4.97	1.48	1.34
19	D	201	TGL	OG3-CC1	4.97	1.48	1.33
25	P	309	PEK	O01-C1	4.99	1.49	1.34
25	C	306	PEK	O01-C1	4.99	1.49	1.34
19	N	610	TGL	OG1-CA1	5.01	1.48	1.33
19	L	101	TGL	OG1-CA1	5.02	1.48	1.33
24	G	103	CDL	OB8-CB7	5.03	1.48	1.33
25	T	101	PEK	O03-C21	5.09	1.48	1.33
24	C	303	CDL	OA8-CA7	5.11	1.48	1.33
19	D	201	TGL	OG1-CA1	5.11	1.48	1.33
19	L	101	TGL	OG3-CC1	5.16	1.48	1.33
19	A	607	TGL	OG1-CA1	5.23	1.48	1.33
19	N	610	TGL	OG3-CC1	5.32	1.49	1.33
24	P	306	CDL	OA8-CA7	5.33	1.49	1.33
19	L	101	TGL	OG2-CB1	5.73	1.51	1.34
20	C	307	PGV	O03-C19	5.74	1.50	1.33
20	C	307	PGV	O01-C1	5.81	1.51	1.34
19	N	610	TGL	OG2-CB1	5.82	1.51	1.34

All (398) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	602	HEA	C20-C19-C18	-11.33	99.87	120.98
15	N	602	HEA	C17-C18-C19	-11.15	103.15	127.75
15	A	603	HEA	C13-C12-C11	-10.99	101.82	114.74
22	C	304	CHD	C6-C5-C4	-7.60	102.91	111.07
15	N	602	HEA	C27-C19-C18	-6.76	110.48	123.58
15	N	603	HEA	C13-C12-C11	-6.37	107.24	114.74
22	P	308	CHD	C23-C22-C20	-6.12	107.22	114.79
22	P	307	CHD	C18-C13-C12	-6.09	103.00	109.09
28	G	101	DMU	C8-C7-C5	-5.89	99.94	110.79
15	A	603	HEA	C20-C19-C18	-5.69	110.38	120.98
28	M	101	DMU	O2-C8-C9	-5.44	94.89	109.23
22	B	302	CHD	C18-C13-C12	-5.42	103.67	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	101	DMU	C7-C8-C9	-5.37	100.65	110.23
22	P	307	CHD	C6-C5-C4	-5.28	105.40	111.07
28	Z	101	DMU	C8-C7-C5	-4.98	101.61	110.79
20	N	607	PGV	C3-C2-C1	-4.82	94.76	113.57
25	P	304	PEK	O03-C01-C02	-4.81	95.71	108.70
15	N	603	HEA	CAD-CBD-CGD	-4.69	103.66	112.78
20	A	608	PGV	O03-C19-O04	-4.68	111.24	123.51
22	P	307	CHD	C14-C8-C9	-4.59	103.16	109.63
28	Z	101	DMU	C7-C8-C9	-4.56	102.09	110.23
25	G	102	PEK	C24-C23-C22	-4.41	96.97	113.30
22	C	304	CHD	C19-C10-C1	-4.41	100.76	108.23
22	C	305	CHD	C5-C4-C3	-4.35	106.43	112.88
19	A	607	TGL	OG3-CC1-OC1	-4.35	112.10	123.51
19	A	607	TGL	OB1-CB1-CB2	-4.30	107.29	123.76
22	C	305	CHD	C1-C2-C3	-4.27	104.74	110.41
15	A	603	HEA	CAD-CBD-CGD	-4.25	104.51	112.78
15	A	602	HEA	C20-C21-C22	-4.22	100.54	111.61
25	P	304	PEK	O01-C1-O02	-4.19	112.26	123.67
22	O	302	CHD	O12-C12-C13	-4.17	104.16	111.12
20	N	608	PGV	O03-C19-O04	-3.93	113.20	123.51
25	G	102	PEK	O03-C01-C02	-3.91	98.15	108.70
22	O	302	CHD	C6-C5-C4	-3.91	106.88	111.07
22	P	307	CHD	C19-C10-C9	-3.91	106.03	111.20
22	P	307	CHD	C23-C22-C20	-3.81	110.08	114.79
28	P	301	DMU	O5-C6-C1	-3.80	102.39	110.28
22	C	304	CHD	C18-C13-C12	-3.78	105.31	109.09
28	Z	101	DMU	O49-C1-C2	-3.74	101.92	110.36
22	C	304	CHD	C14-C8-C9	-3.71	104.40	109.63
28	M	101	DMU	C18-O16-C6	-3.67	107.58	114.00
22	B	302	CHD	C13-C14-C8	-3.55	110.06	114.73
28	P	301	DMU	C8-C7-C5	-3.50	104.33	110.79
22	C	304	CHD	C23-C22-C20	-3.47	110.50	114.79
22	P	308	CHD	C21-C20-C22	-3.44	104.73	110.33
19	L	101	TGL	CB4-CB3-CB2	-3.38	100.81	113.30
19	N	609	TGL	OG3-CC1-OC1	-3.36	114.70	123.51
28	P	301	DMU	C7-C8-C9	-3.33	104.28	110.23
15	N	602	HEA	C13-C14-C15	-3.29	120.50	127.75
24	C	303	CDL	OB8-CB7-OB9	-3.25	115.00	123.51
22	C	305	CHD	C23-C22-C20	-3.25	110.78	114.79
25	P	309	PEK	O03-C21-O04	-3.21	115.09	123.51
20	N	607	PGV	O03-C19-O04	-3.16	115.23	123.51
24	P	306	CDL	OB8-CB7-OB9	-3.15	115.26	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	603	HEA	CAA-CBA-CGA	-3.14	106.68	112.78
15	A	603	HEA	C12-C11-C3B	-3.10	106.18	112.59
15	N	603	HEA	C3C-CAC-CBC	-3.07	120.23	126.40
20	P	305	PGV	O12-P-O13	-3.06	96.70	109.21
15	N	602	HEA	C13-C12-C11	-3.04	111.17	114.74
24	G	103	CDL	OA6-CA5-OA7	-3.03	115.41	123.67
19	A	607	TGL	CB3-CB2-CB1	-3.03	101.73	113.57
22	P	307	CHD	C19-C10-C1	-3.01	103.14	108.23
19	Q	201	TGL	OG1-CA1-OA1	-2.98	115.69	123.51
25	P	304	PEK	C24-C23-C22	-2.96	102.33	113.30
25	C	306	PEK	C2-C3-C4	-2.94	108.25	113.65
19	L	101	TGL	OG3-CC1-OC1	-2.94	115.80	123.51
20	P	302	PGV	O03-C19-O04	-2.92	115.86	123.51
25	G	102	PEK	O01-C1-O02	-2.91	115.76	123.67
24	P	306	CDL	CB6-CB4-CB3	-2.90	105.32	112.08
15	N	602	HEA	C3C-CAC-CBC	-2.90	120.57	126.40
20	A	609	PGV	C8-C9-C10	-2.89	102.05	113.79
22	C	305	CHD	C9-C11-C12	-2.88	110.76	114.38
24	T	102	CDL	OA8-CA7-OA9	-2.88	115.97	123.51
24	T	102	CDL	CA6-CA4-CA3	-2.87	105.40	112.08
25	P	304	PEK	C30-C29-C28	-2.83	99.84	114.54
19	Q	201	TGL	OG3-CC1-OC1	-2.81	116.14	123.51
19	D	201	TGL	OG1-CA1-OA1	-2.81	116.15	123.51
24	T	102	CDL	OA6-CA5-OA7	-2.80	116.06	123.67
15	N	603	HEA	OMA-CMA-C3A	-2.79	118.64	125.03
24	C	303	CDL	C54-C53-C52	-2.78	100.12	114.54
22	P	308	CHD	C22-C20-C17	-2.77	104.40	110.24
20	A	609	PGV	O03-C19-O04	-2.77	116.24	123.51
22	C	304	CHD	C19-C10-C9	-2.77	107.53	111.20
19	N	610	TGL	C25-C24-C23	-2.75	100.25	114.54
24	P	306	CDL	OA6-CA5-OA7	-2.75	116.20	123.67
22	P	308	CHD	C6-C5-C4	-2.74	108.13	111.07
20	N	608	PGV	O01-C1-O02	-2.70	116.33	123.67
25	G	102	PEK	C26-C25-C24	-2.70	100.52	114.54
19	N	610	TGL	C26-C25-C24	-2.68	100.64	114.54
15	N	603	HEA	C20-C19-C18	-2.67	116.01	120.98
28	Z	101	DMU	C22-C25-C28	-2.67	100.69	114.54
22	P	308	CHD	C5-C4-C3	-2.66	108.95	112.88
26	O	303	PSC	O01-C1-O02	-2.66	116.45	123.67
25	T	101	PEK	O01-C1-O02	-2.65	116.47	123.67
15	A	603	HEA	CAA-C2A-C3A	-2.63	121.14	128.66
22	B	302	CHD	C6-C5-C4	-2.62	108.26	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	609	TGL	OB1-CB1-CB2	-2.61	113.77	123.76
20	P	305	PGV	C03-C02-C01	-2.61	106.01	112.08
20	C	302	PGV	C22-C21-C20	-2.60	103.68	113.30
22	C	305	CHD	C5-C6-C7	-2.59	111.49	114.44
22	P	307	CHD	C5-C4-C3	-2.59	109.05	112.88
19	N	610	TGL	OG3-CC1-OC1	-2.55	116.82	123.51
25	P	304	PEK	C03-C02-C01	-2.55	106.14	112.08
20	N	607	PGV	C5-C4-C3	-2.52	101.44	114.54
20	P	305	PGV	C8-C9-C10	-2.52	103.54	113.79
15	A	602	HEA	C13-C12-C11	-2.52	111.78	114.74
25	P	304	PEK	C28-C27-C26	-2.51	101.48	114.54
24	P	306	CDL	C53-C52-C51	-2.51	104.00	113.30
22	P	308	CHD	C4-C5-C10	-2.51	109.97	112.66
28	M	101	DMU	O7-C3-C4	-2.50	102.66	109.33
15	A	602	HEA	CAA-CBA-CGA	-2.50	107.92	112.78
28	M	101	DMU	C7-C8-C9	-2.50	105.78	110.23
19	L	101	TGL	OB1-CB1-CB2	-2.49	114.22	123.76
20	C	302	PGV	O03-C19-O04	-2.47	117.05	123.51
24	C	303	CDL	CB4-OB6-CB5	-2.44	111.86	117.91
19	D	201	TGL	OG3-CC1-OC1	-2.41	117.18	123.51
20	C	302	PGV	C8-C9-C10	-2.40	104.02	113.79
24	C	303	CDL	OA6-CA5-OA7	-2.38	117.19	123.67
19	L	101	TGL	C26-C25-C24	-2.35	102.31	114.54
19	A	607	TGL	CB7-CB6-CB5	-2.33	102.43	114.54
24	C	303	CDL	C52-C51-CB5	-2.31	104.56	113.57
22	P	308	CHD	C16-C15-C14	-2.29	100.52	105.11
25	G	102	PEK	C25-C24-C23	-2.27	102.75	114.54
19	N	609	TGL	CB3-CB2-CB1	-2.27	104.73	113.57
19	N	610	TGL	OB1-CB1-CB2	-2.25	115.15	123.76
22	P	308	CHD	C11-C9-C10	-2.22	111.46	113.77
19	L	101	TGL	OG1-CA1-OA1	-2.22	117.69	123.51
22	P	308	CHD	C17-C13-C14	-2.21	97.84	100.08
19	A	607	TGL	OA1-CA1-CA2	-2.21	115.31	123.76
15	N	603	HEA	C12-C13-C14	-2.20	106.16	112.42
28	Z	101	DMU	O2-C8-C9	-2.19	103.45	109.23
24	G	103	CDL	OB8-CB7-OB9	-2.18	117.79	123.51
19	L	101	TGL	OC1-CC1-CC2	-2.16	115.48	123.76
22	C	304	CHD	C9-C11-C12	-2.16	111.67	114.38
20	C	307	PGV	O04-C19-C20	-2.16	115.50	123.76
25	T	101	PEK	O03-C21-O04	-2.15	117.88	123.51
25	G	104	PEK	O01-C1-O02	-2.14	117.84	123.67
28	M	101	DMU	C22-C25-C28	-2.14	103.42	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	607	TGL	OG1-CA1-OA1	-2.12	117.94	123.51
25	G	104	PEK	O03-C21-O04	-2.12	117.95	123.51
15	N	603	HEA	CAA-CBA-CGA	-2.09	108.72	112.78
15	A	603	HEA	C13-C14-C15	-2.09	123.14	127.75
19	L	101	TGL	CA3-CA2-CA1	-2.09	105.43	113.57
26	O	303	PSC	C29-C28-C27	-2.08	103.73	114.54
19	Q	201	TGL	OG2-CB1-OB1	-2.08	118.02	123.67
20	C	302	PGV	O06-C06-C05	-2.07	99.46	109.97
19	N	610	TGL	OG1-CA1-OA1	-2.07	118.08	123.51
22	P	307	CHD	O7-C7-C6	-2.05	105.02	110.02
26	O	303	PSC	C11-C12-C13	-2.04	112.10	124.38
20	N	608	PGV	O01-C02-C01	-2.03	101.25	108.36
20	A	608	PGV	O01-C1-O02	-2.02	118.16	123.67
22	C	305	CHD	C22-C23-C24	-2.02	104.81	113.05
28	M	101	DMU	O1-C10-C5	-2.02	106.08	110.28
20	A	609	PGV	C6-C5-C4	-2.02	104.05	114.54
24	C	303	CDL	C61-C60-C59	-2.02	104.05	114.54
24	G	103	CDL	OA8-CA7-OA9	-2.02	118.22	123.51
26	O	303	PSC	O03-C19-O04	-2.02	118.22	123.51
15	N	603	HEA	C26-C15-C14	-2.01	119.68	123.58
25	G	102	PEK	C28-C27-C26	-2.01	104.11	114.54
25	C	306	PEK	O03-C21-O04	-2.01	118.25	123.51
19	A	607	TGL	C16-C15-CC9	2.01	124.97	114.54
22	P	308	CHD	C9-C8-C7	2.01	114.31	111.89
20	C	302	PGV	O01-C1-C2	2.02	115.79	111.53
24	T	102	CDL	C80-C79-C78	2.03	125.09	114.54
19	N	609	TGL	C15-CC9-CC8	2.03	125.09	114.54
24	G	103	CDL	C80-C79-C78	2.06	125.25	114.54
24	P	306	CDL	OB6-CB4-CB6	2.06	115.61	108.36
15	N	603	HEA	CMC-C2C-C3C	2.07	129.13	125.09
19	D	201	TGL	C21-C20-CA9	2.08	125.36	114.54
15	A	603	HEA	OMA-CMA-C3A	2.08	129.81	125.03
19	N	610	TGL	OG2-CG2-CG3	2.11	115.76	108.36
28	G	101	DMU	C10-O1-C9	2.13	117.92	113.74
24	G	103	CDL	C40-C39-C38	2.14	125.64	114.54
22	B	302	CHD	C14-C8-C9	2.14	112.64	109.63
25	G	102	PEK	C01-O03-C21	2.14	123.38	117.00
19	L	101	TGL	CG3-OG3-CC1	2.14	123.38	117.00
26	E	201	PSC	C08-N-C06	2.15	114.52	108.96
22	P	308	CHD	C16-C17-C13	2.15	105.66	103.59
22	B	302	CHD	C11-C12-C13	2.15	113.39	111.22
22	C	305	CHD	C14-C8-C9	2.16	112.68	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	103	CDL	C82-C81-C80	2.17	125.81	114.54
24	T	102	CDL	C82-C81-C80	2.17	125.81	114.54
24	C	303	CDL	OA8-CA6-CA4	2.19	114.61	108.70
24	G	103	CDL	C79-C78-C77	2.19	125.91	114.54
19	N	610	TGL	C15-CC9-CC8	2.19	125.94	114.54
19	L	101	TGL	C15-CC9-CC8	2.21	126.02	114.54
22	C	305	CHD	C15-C14-C8	2.23	121.64	118.34
22	P	308	CHD	C16-C17-C20	2.23	115.69	112.12
22	B	302	CHD	C10-C9-C8	2.23	114.27	111.86
20	P	305	PGV	C01-O03-C19	2.24	123.68	117.00
25	P	309	PEK	O03-C01-C02	2.24	114.76	108.70
22	O	302	CHD	C15-C14-C13	2.26	105.77	103.59
22	C	304	CHD	C16-C17-C13	2.26	105.77	103.59
28	P	301	DMU	O1-C10-C5	2.27	115.00	110.28
24	G	103	CDL	CA6-OA8-CA7	2.28	123.78	117.00
22	C	304	CHD	C21-C20-C17	2.31	116.55	112.99
22	C	304	CHD	C4-C3-C2	2.31	113.48	110.53
24	T	102	CDL	OB8-CB7-C71	2.32	118.98	111.85
28	M	101	DMU	O16-C6-C1	2.32	110.86	108.00
22	P	307	CHD	C21-C20-C17	2.32	116.57	112.99
28	G	101	DMU	O3-C5-C10	2.32	115.16	110.01
25	P	304	PEK	O01-C1-C2	2.35	116.47	111.53
25	T	101	PEK	O03-C01-C02	2.35	115.04	108.70
24	C	303	CDL	C39-C38-C37	2.36	126.79	114.54
24	P	306	CDL	C42-C41-C40	2.38	126.88	114.54
15	A	603	HEA	C3C-C4C-NC	2.38	112.29	109.21
20	N	608	PGV	O01-C1-C2	2.38	116.55	111.53
15	A	602	HEA	C3C-C4C-NC	2.39	112.30	109.21
20	C	307	PGV	O01-C02-C03	2.40	116.78	108.36
28	G	101	DMU	O1-C10-C5	2.40	115.27	110.28
22	O	302	CHD	C15-C16-C17	2.41	109.95	105.11
19	N	610	TGL	OG3-CG3-CG2	2.42	115.24	108.70
24	G	103	CDL	C83-C82-C81	2.43	127.19	114.54
20	A	609	PGV	O03-C01-C02	2.44	115.30	108.70
25	G	104	PEK	O03-C01-C02	2.45	115.33	108.70
24	C	303	CDL	CA6-OA8-CA7	2.47	124.36	117.00
19	N	610	TGL	CC3-CC2-CC1	2.47	123.20	113.57
19	D	201	TGL	C11-C10-CB9	2.47	127.38	114.54
22	P	308	CHD	C6-C5-C10	2.48	115.31	112.66
28	P	301	DMU	O7-C10-C5	2.50	114.34	108.12
22	O	302	CHD	C14-C8-C7	2.51	115.37	111.77
19	A	607	TGL	CG1-OG1-CA1	2.53	124.54	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	609	PGV	O01-C02-C03	2.54	117.28	108.36
19	A	607	TGL	C15-CC9-CC8	2.55	127.81	114.54
20	C	307	PGV	C01-O03-C19	2.56	124.62	117.00
22	C	304	CHD	C16-C17-C20	2.56	116.22	112.12
22	B	302	CHD	C1-C10-C5	2.58	110.60	107.76
24	T	102	CDL	C83-C82-C81	2.58	127.93	114.54
19	L	101	TGL	OG3-CG3-CG2	2.60	115.72	108.70
28	Z	101	DMU	O5-C4-C57	2.61	113.15	106.38
24	P	306	CDL	CA6-OA8-CA7	2.63	124.84	117.00
24	T	102	CDL	OA8-CA7-C31	2.67	120.07	111.85
28	P	301	DMU	O1-C9-C11	2.67	113.31	106.38
24	P	306	CDL	OA8-CA7-C31	2.68	120.10	111.85
15	N	603	HEA	C21-C20-C19	2.69	121.52	112.61
24	G	103	CDL	C43-C42-C41	2.70	128.58	114.54
24	G	103	CDL	OB8-CB7-C71	2.71	120.20	111.85
22	P	307	CHD	C16-C17-C13	2.71	106.20	103.59
19	N	609	TGL	OG3-CC1-CC2	2.72	120.22	111.85
24	G	103	CDL	OB8-CB6-CB4	2.75	116.12	108.70
28	Z	101	DMU	O3-C5-C7	2.76	116.58	110.36
20	A	608	PGV	O03-C01-C02	2.76	116.16	108.70
25	G	104	PEK	C01-O03-C21	2.76	125.23	117.00
28	M	101	DMU	O5-C4-C57	2.77	113.56	106.38
24	T	102	CDL	CB6-OB8-CB7	2.79	125.31	117.00
24	T	102	CDL	OB8-CB6-CB4	2.83	116.33	108.70
22	P	307	CHD	C15-C14-C13	2.83	106.32	103.59
24	C	303	CDL	OA8-CA7-C31	2.84	120.59	111.85
28	M	101	DMU	O7-C10-C5	2.84	115.18	108.12
19	D	201	TGL	C10-CB9-CB8	2.85	129.37	114.54
22	P	307	CHD	C9-C10-C5	2.87	112.77	108.68
19	L	101	TGL	OG1-CG1-CG2	2.88	116.47	108.70
25	C	306	PEK	C01-O03-C21	2.88	125.59	117.00
19	D	201	TGL	CG2-OG2-CB1	2.89	125.05	117.91
15	A	602	HEA	C3C-CAC-CBC	2.90	132.22	126.40
22	C	304	CHD	C5-C6-C7	2.90	117.75	114.44
19	Q	201	TGL	OG2-CG2-CG3	2.91	118.58	108.36
24	C	303	CDL	OB6-CB5-C51	2.91	117.67	111.53
24	G	103	CDL	OA8-CA7-C31	2.92	120.83	111.85
28	P	301	DMU	C1-C2-C3	2.93	116.10	109.63
19	N	610	TGL	OG1-CG1-CG2	2.93	116.62	108.70
19	D	201	TGL	OG3-CC1-CC2	2.94	120.89	111.85
25	T	101	PEK	O03-C21-C22	2.94	120.90	111.85
20	A	609	PGV	C01-O03-C19	2.95	125.77	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	307	CHD	C11-C12-C13	2.95	114.19	111.22
24	P	306	CDL	OB6-CB5-C51	2.95	117.75	111.53
19	N	609	TGL	OG1-CA1-CA2	2.95	120.94	111.85
15	N	602	HEA	CBA-CAA-C2A	2.99	117.71	112.47
22	B	302	CHD	C17-C13-C12	3.00	120.31	117.68
28	P	301	DMU	C11-C9-C8	3.00	120.51	112.99
22	P	308	CHD	C15-C14-C13	3.02	106.50	103.59
15	A	603	HEA	C3C-CAC-CBC	3.03	132.49	126.40
26	E	201	PSC	O03-C19-C20	3.06	121.27	111.85
28	G	101	DMU	C10-C5-C7	3.08	116.09	109.98
28	Z	101	DMU	O1-C9-C8	3.14	115.66	109.67
22	P	308	CHD	C11-C9-C8	3.15	115.30	110.77
25	G	102	PEK	C11-C10-C9	3.18	122.75	112.17
19	L	101	TGL	OG1-CA1-CA2	3.19	121.67	111.85
26	E	201	PSC	C02-O01-C1	3.20	125.81	117.91
22	O	302	CHD	C11-C9-C8	3.22	115.41	110.77
28	P	301	DMU	O3-C5-C10	3.24	117.19	110.01
19	Q	201	TGL	OG1-CA1-CA2	3.24	121.82	111.85
15	N	602	HEA	C20-C19-C18	3.26	127.04	120.98
19	N	610	TGL	OG3-CC1-CC2	3.26	121.88	111.85
22	O	302	CHD	O7-C7-C6	3.29	118.06	110.02
15	N	603	HEA	C17-C18-C19	3.30	135.03	127.75
25	C	306	PEK	O03-C21-C22	3.34	122.14	111.85
25	G	104	PEK	O03-C21-C22	3.37	122.22	111.85
22	C	304	CHD	C5-C4-C3	3.37	117.88	112.88
28	M	101	DMU	O1-C9-C11	3.38	115.13	106.38
22	C	305	CHD	C15-C14-C13	3.42	106.88	103.59
28	G	101	DMU	C6-O5-C4	3.42	120.44	113.74
25	T	101	PEK	C01-O03-C21	3.43	127.23	117.00
19	D	201	TGL	CG3-OG3-CC1	3.44	127.25	117.00
20	N	607	PGV	O01-C02-C03	3.45	120.49	108.36
15	A	602	HEA	C27-C19-C20	3.46	120.64	115.37
19	Q	201	TGL	OG3-CC1-CC2	3.46	122.51	111.85
22	C	304	CHD	C15-C14-C13	3.47	106.93	103.59
19	N	609	TGL	CG3-OG3-CC1	3.47	127.33	117.00
22	P	308	CHD	C11-C12-C13	3.49	114.74	111.22
28	G	101	DMU	C18-O16-C6	3.50	120.12	114.00
20	C	307	PGV	O03-C01-C02	3.51	118.17	108.70
28	P	301	DMU	C10-O1-C9	3.54	120.68	113.74
22	O	302	CHD	C9-C8-C7	3.55	116.18	111.89
20	N	607	PGV	O03-C19-C20	3.56	122.79	111.85
19	Q	201	TGL	CG3-OG3-CC1	3.57	127.63	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	305	CHD	C9-C8-C7	3.58	116.22	111.89
28	Z	101	DMU	O1-C9-C11	3.59	115.67	106.38
19	D	201	TGL	CG1-OG1-CA1	3.59	127.70	117.00
20	A	608	PGV	O01-C1-C2	3.60	119.10	111.53
19	N	610	TGL	OG1-CA1-CA2	3.64	123.04	111.85
22	C	304	CHD	C6-C5-C10	3.65	116.57	112.66
19	A	607	TGL	OG2-CG2-CG1	3.66	121.23	108.36
22	C	304	CHD	C14-C13-C12	3.67	110.69	107.37
28	M	101	DMU	O3-C5-C7	3.68	118.65	110.36
28	G	101	DMU	O7-C10-C5	3.73	117.40	108.12
19	N	609	TGL	CG2-OG2-CB1	3.75	127.17	117.91
19	D	201	TGL	OG1-CA1-CA2	3.76	123.41	111.85
24	G	103	CDL	CB6-OB8-CB7	3.77	128.23	117.00
19	N	610	TGL	CG3-OG3-CC1	3.78	128.27	117.00
22	C	304	CHD	C6-C7-C8	3.79	115.48	111.46
22	P	307	CHD	C10-C9-C8	3.81	115.97	111.86
22	P	307	CHD	C5-C6-C7	3.85	118.83	114.44
22	C	305	CHD	C11-C12-C13	3.88	115.13	111.22
22	P	307	CHD	C2-C1-C10	3.90	119.80	112.81
20	A	609	PGV	O03-C19-C20	3.93	123.93	111.85
22	P	307	CHD	C15-C14-C8	3.95	124.20	118.34
20	A	609	PGV	O01-C1-C2	3.96	119.88	111.53
15	A	602	HEA	C17-C18-C19	3.98	136.52	127.75
22	P	307	CHD	C9-C8-C7	3.99	116.71	111.89
25	P	304	PEK	C01-O03-C21	4.03	129.00	117.00
19	A	607	TGL	OG3-CC1-CC2	4.06	124.34	111.85
28	M	101	DMU	O1-C9-C8	4.07	117.42	109.67
19	L	101	TGL	CG2-OG2-CB1	4.11	128.08	117.91
19	D	201	TGL	OG2-CB1-CB2	4.11	120.20	111.53
25	P	309	PEK	O03-C21-C22	4.12	124.52	111.85
19	L	101	TGL	OG2-CB1-CB2	4.15	120.28	111.53
20	A	609	PGV	C02-O01-C1	4.18	128.24	117.91
24	P	306	CDL	OB8-CB7-C71	4.20	124.76	111.85
20	N	608	PGV	O03-C19-C20	4.20	124.79	111.85
28	Z	101	DMU	O16-C6-C1	4.23	113.21	108.00
26	O	303	PSC	O03-C19-C20	4.24	124.89	111.85
19	N	610	TGL	CG2-OG2-CB1	4.30	128.53	117.91
22	C	304	CHD	C15-C14-C8	4.30	124.71	118.34
22	C	304	CHD	C4-C5-C10	4.35	117.32	112.66
19	N	610	TGL	OG2-CB1-CB2	4.36	120.72	111.53
24	C	303	CDL	OB8-CB7-C71	4.39	125.37	111.85
15	N	603	HEA	C26-C15-C16	4.40	122.08	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	304	CHD	C14-C8-C7	4.42	118.09	111.77
15	N	603	HEA	C27-C19-C20	4.46	122.16	115.37
19	A	607	TGL	OG3-CG3-CG2	4.50	120.84	108.70
20	P	302	PGV	O03-C19-C20	4.52	125.77	111.85
28	G	101	DMU	O3-C5-C7	4.56	120.63	110.36
22	B	302	CHD	C6-C7-C8	4.56	116.29	111.46
15	A	602	HEA	C25-C23-C24	4.56	125.69	114.61
15	N	602	HEA	C3C-C4C-NC	4.58	115.13	109.21
25	P	309	PEK	O01-C1-C2	4.58	121.17	111.53
25	C	306	PEK	O01-C1-C2	4.59	121.21	111.53
26	E	201	PSC	O01-C1-C2	4.61	121.23	111.53
20	C	307	PGV	O03-C19-C20	4.61	126.05	111.85
22	P	307	CHD	C14-C8-C7	4.63	118.38	111.77
15	N	602	HEA	C27-C19-C20	4.66	122.47	115.37
15	A	603	HEA	C27-C19-C20	4.70	122.53	115.37
28	G	101	DMU	O16-C6-C1	4.82	113.93	108.00
20	A	608	PGV	O03-C19-C20	4.82	126.69	111.85
19	A	607	TGL	OG1-CA1-CA2	4.84	126.74	111.85
22	C	304	CHD	C10-C9-C8	4.84	117.09	111.86
19	A	607	TGL	CG3-OG3-CC1	4.91	131.63	117.00
26	O	303	PSC	O01-C1-C2	4.98	122.01	111.53
25	G	104	PEK	O01-C1-C2	4.98	122.03	111.53
20	C	307	PGV	O01-C1-C2	5.05	122.18	111.53
22	P	308	CHD	C1-C10-C5	5.08	113.36	107.76
22	P	307	CHD	C1-C10-C5	5.12	113.41	107.76
20	P	302	PGV	O01-C1-C2	5.19	122.46	111.53
24	G	103	CDL	OB6-CB5-C51	5.20	122.49	111.53
19	N	609	TGL	OG2-CB1-CB2	5.20	122.49	111.53
24	T	102	CDL	OA6-CA5-C11	5.23	122.54	111.53
20	N	607	PGV	O01-C1-C2	5.33	122.76	111.53
24	T	102	CDL	OB6-CB5-C51	5.36	122.83	111.53
25	T	101	PEK	O01-C1-C2	5.40	122.90	111.53
24	G	103	CDL	OA6-CA5-C11	5.45	123.02	111.53
19	L	101	TGL	OG3-CC1-CC2	5.48	128.71	111.85
24	P	306	CDL	OA6-CA5-C11	5.68	123.50	111.53
15	N	602	HEA	C16-C17-C18	5.71	126.61	111.61
24	C	303	CDL	OA6-CA5-C11	5.93	124.03	111.53
22	C	304	CHD	C1-C10-C5	6.05	114.43	107.76
25	P	304	PEK	C2-C3-C4	6.05	124.75	113.65
22	P	307	CHD	C6-C5-C10	6.29	119.40	112.66
19	Q	201	TGL	OG2-CB1-CB2	6.33	124.86	111.53
25	G	102	PEK	C2-C3-C4	6.41	125.41	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	307	CHD	C14-C13-C12	6.80	113.52	107.37
28	P	301	DMU	C18-O16-C6	7.01	126.25	114.00
19	A	607	TGL	OG2-CB1-CB2	7.59	127.52	111.53
28	G	101	DMU	O1-C9-C11	7.80	126.60	106.38
22	P	307	CHD	C6-C7-C8	8.09	120.03	111.46
15	A	602	HEA	C27-C19-C18	8.20	139.47	123.58
19	A	607	TGL	CG2-OG2-CB1	8.81	139.70	117.91
28	P	301	DMU	O16-C6-C1	11.85	122.58	108.00

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	N	602	HEA	ND
15	N	602	HEA	NA
15	N	602	HEA	NB
15	A	603	HEA	ND
15	A	603	HEA	NB
15	A	602	HEA	ND
15	A	602	HEA	NB
15	N	603	HEA	ND
15	N	603	HEA	NB

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	609	PGV	C02-O01-C1-O02
20	N	607	PGV	C02-O01-C1-C2
20	A	609	PGV	C02-O01-C1-C2

There are no ring outliers.

37 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	602	HEA	7	0
15	A	603	HEA	2	0
19	A	607	TGL	6	0
20	A	609	PGV	8	0
22	B	302	CHD	2	0
20	C	302	PGV	2	0
24	C	303	CDL	17	0
22	C	304	CHD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	305	CHD	1	0
25	C	306	PEK	6	0
20	C	307	PGV	3	0
19	D	201	TGL	12	0
26	E	201	PSC	16	0
28	G	101	DMU	4	0
25	G	102	PEK	2	0
24	G	103	CDL	26	0
25	G	104	PEK	11	0
19	L	101	TGL	14	0
15	N	602	HEA	6	0
15	N	603	HEA	2	0
20	N	607	PGV	9	0
20	N	608	PGV	1	0
19	N	609	TGL	8	0
19	N	610	TGL	14	0
22	O	302	CHD	1	0
26	O	303	PSC	17	0
28	P	301	DMU	3	0
20	P	302	PGV	2	0
25	P	304	PEK	5	0
20	P	305	PGV	3	0
24	P	306	CDL	20	0
22	P	307	CHD	7	0
22	P	308	CHD	1	0
25	P	309	PEK	8	0
19	Q	201	TGL	2	0
25	T	101	PEK	22	0
24	T	102	CDL	27	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	-0.05	4 (0%) 87 88	21, 27, 35, 67	0
1	N	513/514 (99%)	-0.06	4 (0%) 87 88	26, 35, 47, 76	0
2	B	226/227 (99%)	-0.39	5 (2%) 65 66	24, 33, 55, 80	0
2	O	226/227 (99%)	-0.17	4 (1%) 71 72	34, 45, 69, 95	0
3	C	259/261 (99%)	-0.27	3 (1%) 81 81	25, 33, 44, 64	0
3	P	259/261 (99%)	-0.21	4 (1%) 76 77	29, 37, 49, 69	0
4	D	144/147 (97%)	-0.44	1 (0%) 89 89	28, 36, 52, 69	0
4	Q	144/147 (97%)	1.08	20 (13%) 4 4	41, 58, 83, 130	0
5	E	105/109 (96%)	-0.20	2 (1%) 70 70	29, 36, 59, 99	0
5	R	105/109 (96%)	0.23	4 (3%) 44 45	36, 47, 66, 104	0
6	F	98/98 (100%)	0.70	8 (8%) 14 15	29, 39, 97, 134	0
6	S	98/98 (100%)	0.71	10 (10%) 9 9	31, 45, 103, 128	0
7	G	83/85 (97%)	1.02	16 (19%) 2 2	31, 39, 110, 123	0
7	T	83/85 (97%)	0.98	17 (20%) 1 1	32, 47, 104, 119	0
8	H	79/85 (92%)	0.14	8 (10%) 9 10	30, 40, 88, 113	0
8	U	79/85 (92%)	0.45	9 (11%) 7 7	39, 50, 97, 125	0
9	I	72/73 (98%)	0.16	4 (5%) 28 29	34, 44, 65, 71	0
9	V	72/73 (98%)	0.71	8 (11%) 7 8	35, 60, 75, 102	0
10	J	58/59 (98%)	0.62	8 (13%) 4 4	33, 43, 72, 103	0
10	W	58/59 (98%)	0.71	8 (13%) 4 4	41, 52, 85, 125	0
11	K	49/56 (87%)	-0.29	0 100 100	34, 40, 52, 57	0
11	X	49/56 (87%)	1.52	17 (34%) 0 1	47, 59, 76, 84	0
12	L	46/47 (97%)	-0.32	0 100 100	28, 33, 55, 83	0
12	Y	46/47 (97%)	-0.05	1 (2%) 65 66	38, 50, 74, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.18	5 (11%) 6 7	29, 34, 90, 114	0
13	Z	43/46 (93%)	0.53	8 (18%) 2 2	46, 54, 122, 136	0
All	All	3550/3614 (98%)	0.10	178 (5%) 32 34	21, 38, 72, 136	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	25.4
4	Q	6	VAL	23.8
6	S	97	ALA	17.4
6	F	97	ALA	14.5
6	S	96	LEU	13.6
6	F	1	ALA	12.9
6	S	1	ALA	12.9
6	F	98	HIS	12.7
6	F	96	LEU	12.1
7	G	2	SER	11.1
6	S	2	SER	10.8
10	J	1	PHE	10.7
6	F	95	GLN	10.5
6	F	2	SER	10.4
7	G	3	ALA	9.6
7	G	1	ALA	9.4
4	Q	7	LYS	8.7
10	W	58	LYS	8.6
10	W	1	PHE	8.3
6	S	94	HIS	8.1
7	T	1	ALA	8.1
6	S	98	HIS	7.7
7	T	3	ALA	7.7
10	J	58	LYS	7.6
4	Q	4	SER	7.4
5	R	5	HIS	7.1
4	Q	8	SER	7.0
8	U	7	LYS	7.0
8	H	7	LYS	7.0
7	G	5	LYS	6.6
8	U	8	ILE	6.1
8	H	8	ILE	6.0
7	G	42	ARG	6.0
7	T	2	SER	6.0

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Mol	Chain	Res	Type	RSRZ
13	M	43	SER	5.9
6	F	94	HIS	5.8
9	V	2	THR	5.6
8	U	10	ASN	5.5
6	S	95	GLN	5.5
7	T	42	ARG	5.5
13	Z	43	SER	5.4
4	Q	147	LYS	5.4
7	T	36	TRP	5.3
7	T	41	HIS	5.3
13	Z	42	LYS	5.2
7	G	4	ALA	5.1
5	R	109	VAL	5.1
7	G	40	GLY	5.1
6	F	3	GLY	5.1
9	I	37	PHE	5.0
7	T	4	ALA	5.0
7	T	5	LYS	4.9
7	T	40	GLY	4.8
13	Z	35	TYR	4.7
8	H	45	ALA	4.7
11	X	13	TYR	4.7
7	G	41	HIS	4.5
7	T	8	HIS	4.5
7	G	9	GLY	4.4
6	S	93	PRO	4.3
13	M	40	TYR	4.3
7	T	84	LYS	4.3
13	Z	39	ASN	4.3
11	X	23	THR	4.2
13	Z	40	TYR	4.2
7	G	8	HIS	4.2
7	T	39	SER	4.1
8	H	44	THR	4.1
7	G	6	GLY	4.0
2	O	113	TYR	4.0
13	Z	37	LEU	3.9
9	V	37	PHE	3.9
7	G	36	TRP	3.9
8	H	46	LYS	3.8
11	X	27	ALA	3.8
12	Y	47	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
8	U	9	LYS	3.7
6	S	3	GLY	3.7
10	J	2	GLU	3.7
2	B	59	GLN	3.7
2	O	91	ASN	3.7
5	E	109	VAL	3.7
13	M	42	LYS	3.6
4	Q	102	TYR	3.6
7	G	43	GLU	3.5
4	Q	53	ILE	3.5
11	X	6	ALA	3.5
4	Q	51	LEU	3.4
11	X	7	PRO	3.4
8	H	47	GLY	3.3
5	E	5	HIS	3.2
2	B	60	GLU	3.2
8	H	43	MET	3.2
7	G	7	ASP	3.2
10	W	52	TRP	3.2
3	P	91	VAL	3.2
8	U	45	ALA	3.1
10	J	57	HIS	3.1
10	W	26	ALA	3.1
11	X	19	ALA	3.0
4	Q	107	ILE	3.0
10	W	57	HIS	3.0
13	M	39	ASN	3.0
10	J	48	TYR	3.0
7	G	84	LYS	3.0
10	W	48	TYR	2.9
4	Q	101	HIS	2.9
10	W	4	ARG	2.9
11	X	16	ALA	2.9
7	T	10	GLY	2.9
2	O	226	MET	2.9
7	T	43	GLU	2.9
8	U	44	THR	2.9
11	X	34	THR	2.8
7	T	6	GLY	2.8
10	J	52	TRP	2.8
1	N	201	VAL	2.8
2	O	90	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
9	V	25	PHE	2.8
11	X	24	PHE	2.8
4	Q	58	GLU	2.8
4	Q	33	LEU	2.8
3	P	3	HIS	2.7
13	Z	32	TRP	2.7
3	C	92	LEU	2.7
5	R	52	LEU	2.7
4	Q	138	TRP	2.6
10	W	2	GLU	2.6
13	Z	41	LYS	2.6
8	U	50	VAL	2.6
4	D	147	LYS	2.6
5	R	96	LEU	2.5
10	J	4	ARG	2.5
11	X	35	GLN	2.5
1	A	197	LEU	2.5
11	X	52	GLU	2.5
11	X	18	LEU	2.4
10	J	30	ILE	2.4
1	N	197	LEU	2.4
11	X	47	ARG	2.4
9	V	53	ASN	2.4
9	V	34	PHE	2.4
7	T	9	GLY	2.4
4	Q	140	TYR	2.4
2	B	57	ASP	2.3
3	P	88	ILE	2.3
9	I	52	ARG	2.3
1	N	193	VAL	2.3
11	X	15	ASN	2.3
4	Q	10	ASP	2.3
4	Q	106	PRO	2.3
8	U	49	ASP	2.3
4	Q	111	PHE	2.3
4	Q	35	ALA	2.3
3	P	85	LEU	2.2
2	B	58	ALA	2.2
13	M	35	TYR	2.2
9	V	26	MET	2.2
11	X	21	GLY	2.2
11	X	12	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	55	THR	2.2
3	C	91	VAL	2.2
9	V	48	ALA	2.1
9	V	29	LEU	2.1
9	I	18	ARG	2.1
1	A	201	VAL	2.1
4	Q	145	TRP	2.1
6	S	44	GLU	2.1
8	U	47	GLY	2.1
3	C	88	ILE	2.1
7	T	7	ASP	2.1
1	N	196	LEU	2.0
1	A	237	PHE	2.0
7	G	12	GLY	2.0
9	I	53	ASN	2.0
11	X	31	TYR	2.0
1	A	194	LEU	2.0
8	H	48	GLY	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
2	FME	B	1	10/11	0.97	0.12	-	32,34,43,59	0
2	FME	O	1	10/11	0.98	0.14	-	45,47,58,65	0
1	FME	A	1	10/11	0.93	0.14	-	44,53,74,81	0
7	TPO	G	11	11/12	0.53	0.38	-	83,91,111,114	0
7	TPO	T	11	11/12	0.56	0.35	-	87,95,113,113	0
9	SAC	I	1	9/10	0.80	0.18	-	68,71,73,74	0
9	SAC	V	1	9/10	0.25	0.59	-	113,117,118,119	0
1	FME	N	1	10/11	0.95	0.18	-	52,58,75,76	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	101	33/33	0.53	0.29	19.75	103,146,153,154	0
28	DMU	P	301	33/33	0.31	0.45	15.97	132,165,171,171	0
18	NA	A	606	1/1	0.87	0.29	11.89	45,45,45,45	0
20	PGV	A	609	51/51	0.73	0.28	10.14	34,78,100,106	0
19	TGL	N	610	63/63	0.66	0.32	7.48	57,80,98,100	0
24	CDL	P	306	100/100	0.67	0.37	6.82	57,103,125,132	0
19	TGL	L	101	63/63	0.77	0.27	6.69	38,61,82,85	0
24	CDL	T	102	100/100	0.61	0.35	6.57	68,101,133,137	0
18	NA	N	606	1/1	0.85	0.32	5.97	53,53,53,53	0
24	CDL	C	303	100/100	0.74	0.39	5.57	44,96,128,130	0
19	TGL	N	609	63/63	0.83	0.22	5.37	57,84,100,103	0
19	TGL	D	201	63/63	0.75	0.22	5.15	46,69,82,83	0
19	TGL	A	607	63/63	0.84	0.21	4.53	49,77,97,100	0
20	PGV	N	607	51/51	0.72	0.32	4.36	54,92,119,123	0
17	MG	N	605	1/1	0.84	0.15	3.82	39,39,39,39	0
19	TGL	Q	201	63/63	0.71	0.25	3.81	64,87,97,100	0
24	CDL	G	103	100/100	0.57	0.37	3.32	73,101,133,138	0
26	PSC	E	201	52/52	0.72	0.34	2.86	53,106,127,129	0
17	MG	A	605	1/1	0.97	0.13	2.31	27,27,27,27	0
26	PSC	O	303	52/52	0.58	0.34	2.30	57,105,133,136	0
25	PEK	T	101	53/53	0.52	0.48	2.19	62,105,129,130	0
20	PGV	C	307	51/51	0.65	0.41	2.12	62,90,111,112	0
28	DMU	Z	101	33/33	0.81	0.30	2.08	57,70,87,91	0
20	PGV	P	302	51/51	0.64	0.42	1.94	74,105,119,121	0
22	CHD	C	304	29/29	0.70	0.48	1.79	92,125,126,127	0
22	CHD	P	307	29/29	0.71	0.37	1.55	91,121,122,124	0
25	PEK	G	104	53/53	0.58	0.51	1.54	60,112,135,137	0
25	PEK	P	304	53/53	0.93	0.17	1.42	38,60,93,95	0
21	CUA	B	301	2/2	0.99	0.13	1.31	26,26,26,27	0
25	PEK	P	309	53/53	0.55	0.36	1.28	47,97,125,127	0
28	DMU	M	101	33/33	0.91	0.16	1.24	43,49,68,70	0
25	PEK	G	102	53/53	0.95	0.14	1.12	29,50,79,81	0
20	PGV	P	305	51/51	0.95	0.14	1.12	31,47,86,89	0
22	CHD	C	305	29/29	0.90	0.15	0.84	37,44,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	PEK	C	306	53/53	0.48	0.30	0.84	53,92,130,133	0
27	ZN	F	101	1/1	1.00	0.09	0.81	35,35,35,35	0
14	CYN	N	601	2/2	0.99	0.15	0.72	30,30,30,31	0
20	PGV	A	608	51/51	0.96	0.13	0.58	24,41,65,70	0
20	PGV	C	302	51/51	0.96	0.12	0.57	26,37,79,82	0
20	PGV	N	608	51/51	0.96	0.14	0.46	30,49,74,76	0
14	CYN	A	601	2/2	0.99	0.15	0.27	20,20,20,24	0
21	CUA	O	301	2/2	0.99	0.10	0.25	38,38,38,38	0
15	HEA	N	603	60/60	0.99	0.13	0.20	25,30,39,42	0
22	CHD	P	308	29/29	0.92	0.13	0.04	41,47,50,50	0
15	HEA	A	602	60/60	0.98	0.13	-0.15	17,23,51,55	0
15	HEA	A	603	60/60	0.99	0.12	-0.33	18,23,33,35	0
22	CHD	O	302	29/29	0.97	0.10	-0.34	33,37,43,45	0
22	CHD	B	302	29/29	0.97	0.09	-0.43	33,37,42,53	0
15	HEA	N	602	60/60	0.97	0.10	-0.60	15,31,57,63	0
27	ZN	S	101	1/1	1.00	0.08	-0.66	40,40,40,40	0
23	UNX	C	301	1/1	0.73	0.24	-	38,38,38,38	0
23	UNX	P	303	1/1	0.92	0.30	-	35,35,35,35	0
16	CU	A	604	1/1	1.00	0.13	-	25,25,25,25	0
16	CU	N	604	1/1	1.00	0.13	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.