



Full wwPDB X-ray Structure Validation Report

Jul 16, 2014 – 05:16 PM EDT

PDB ID : 4OGQ
Title : Internal Lipid Architecture of the Hetero-Oligomeric Cytochrome b6f Complex
Authors : Hasan, S.S.; Cramer, W.A.
Deposited on : 2014-01-16
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

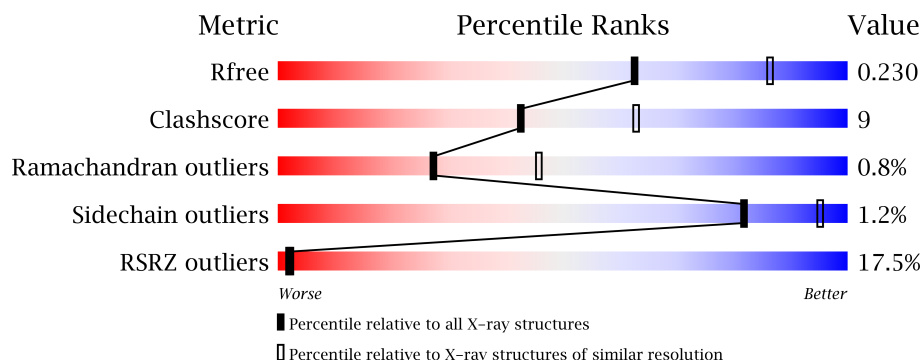
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	215	
2	B	160	
3	C	333	
4	D	179	
5	E	31	
6	F	34	
7	G	37	
8	H	29	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	UMQ	A	304	-	X
10	UMQ	B	203[B]	-	X
10	UMQ	D	201	-	X
10	UMQ	G	101	-	X
11	7PH	A	305	-	X
11	7PH	B	206	-	X
11	7PH	C	303	-	X
11	7PH	F	104	-	X
12	8K6	A	306	-	X
12	8K6	A	307	-	X
12	8K6	A	308	-	X
12	8K6	B	202[A]	-	X
15	OPC	B	205	-	X
17	MYS	D	202	-	X
20	2WD	D	206	-	X
22	2WA	F	101	-	X
23	OCT	F	102	-	X
24	1O2	F	103	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 8396 atoms, of which 0 are hydrogen and 0 are deuterium.

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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1708	1139	271	288	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1232	825	194	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2137	1361	355	415	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1250	791	213	240	6			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			228	157	35	35	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			231	156	36	38	1			

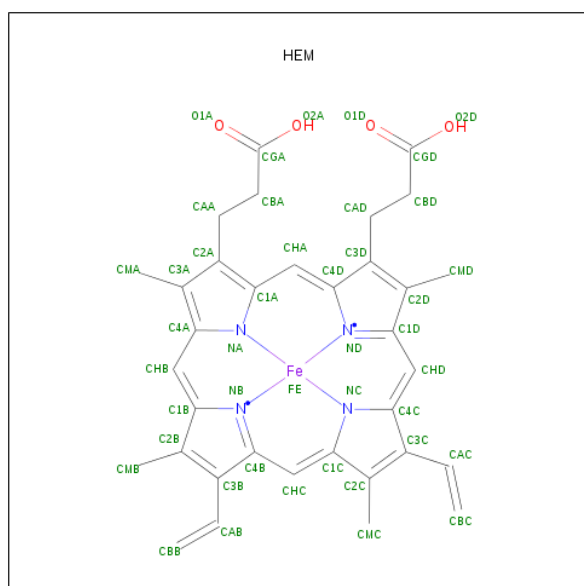
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	0	0	0
			282	188	44	49	1			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

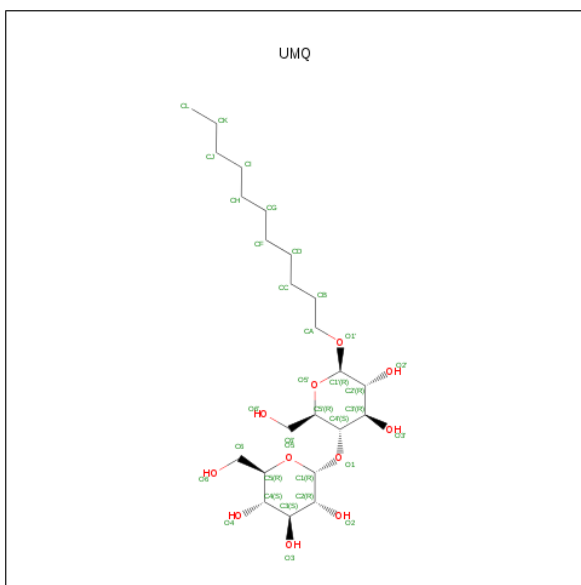
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			228	155	36	35	2			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



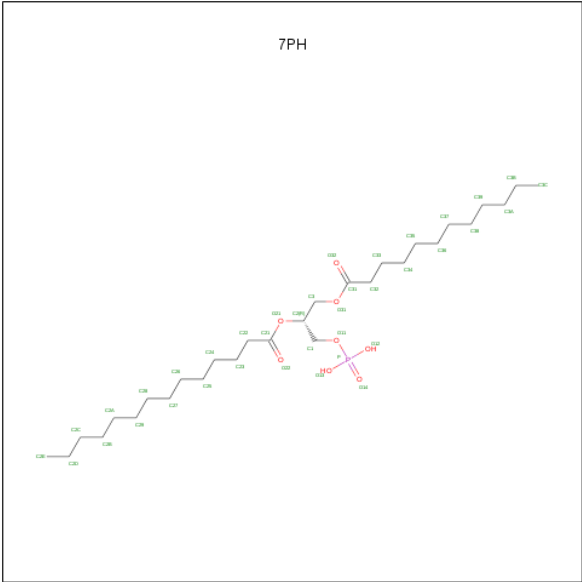
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



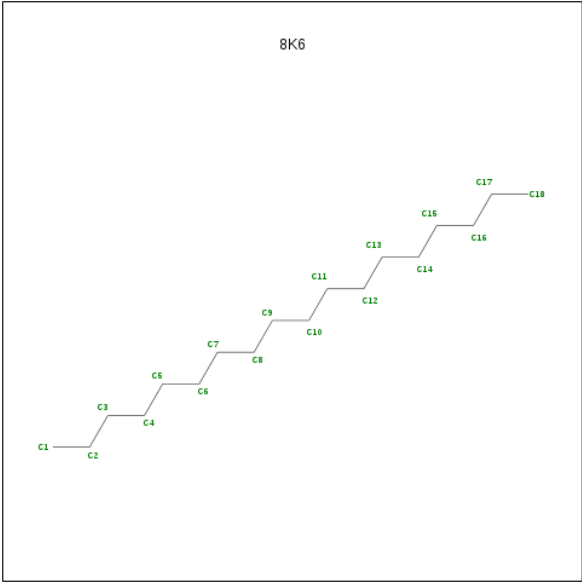
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			34	23	11		
10	B	1	Total	C	O	0	0
			34	23	11		
10	B	1	Total	C	O	0	1
			34	23	11		
10	D	1	Total	C	O	0	0
			34	23	11		
10	G	1	Total	C	O	0	0
			34	23	11		

- Molecule 11 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: C₂₉H₅₇O₈P).



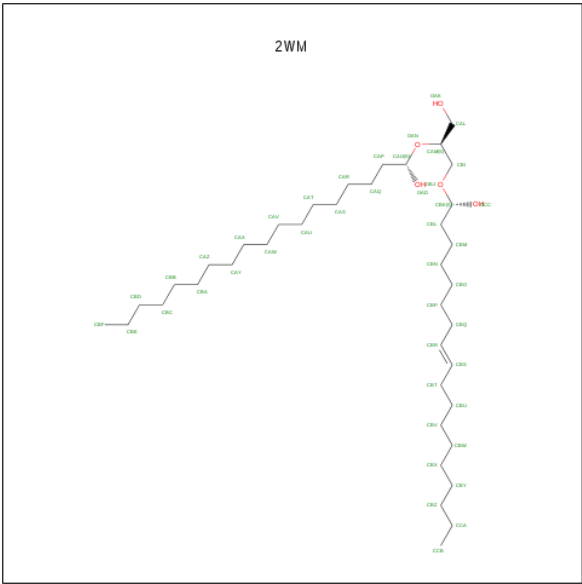
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			32	27	5		
11	B	1	Total	C	O	0	0
			32	27	5		
11	C	1	Total	C	O	0	0
			32	27	5		
11	D	1	Total	C	O	0	0
			32	27	5		
11	F	1	Total	C	O	0	0
			32	27	5		

- Molecule 12 is OCTADECANE (three-letter code: 8K6) (formula: C₁₈H₃₈).



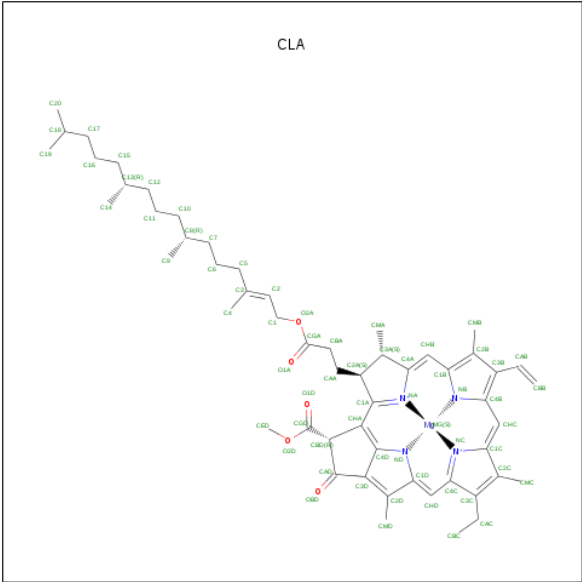
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C 18 18	0	0
12	A	1	Total C 18 18	0	0
12	A	1	Total C 14 14	0	0
12	B	1	Total C 18 18	0	1

- Molecule 13 is (1S,8E)-1-{[(2S)-3-HYDROXY-2-{[(1S)-1-HYDROXYOCTADECYL]OXY}PROPYL]OXY}OCTADEC-8-EN-1-OL (three-letter code: 2WM) (formula: C₃₉H₇₈O₅).



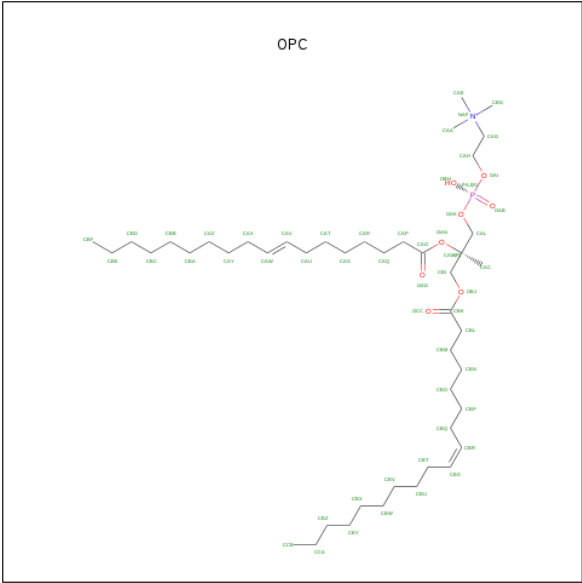
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 44 39 5	0	0

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 15 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM4-OXIDE (three-letter code: OPC) (formula: C₄₅H₈₇NO₈P).

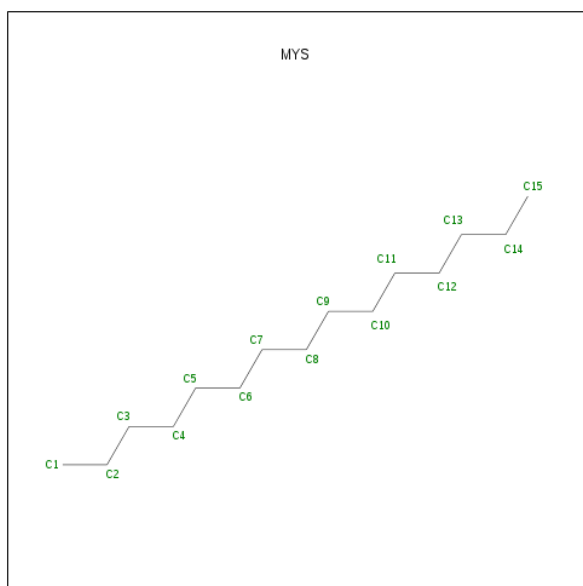


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 16 is CADMIUM ION (three-letter code: CD) (formula: Cd).

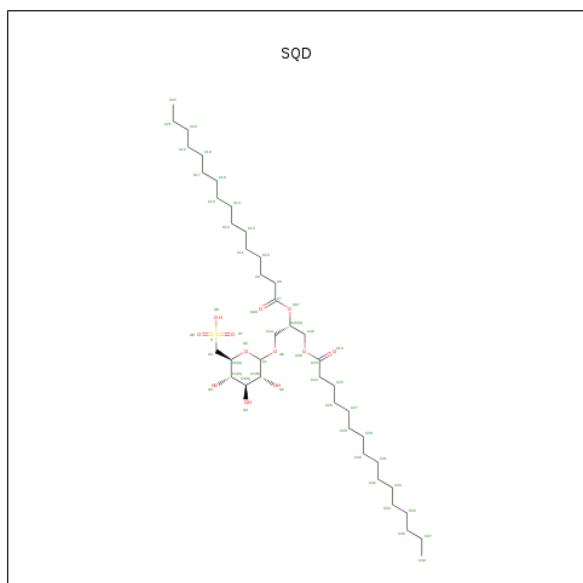
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	Cd	0	0
			1	1		

- Molecule 17 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



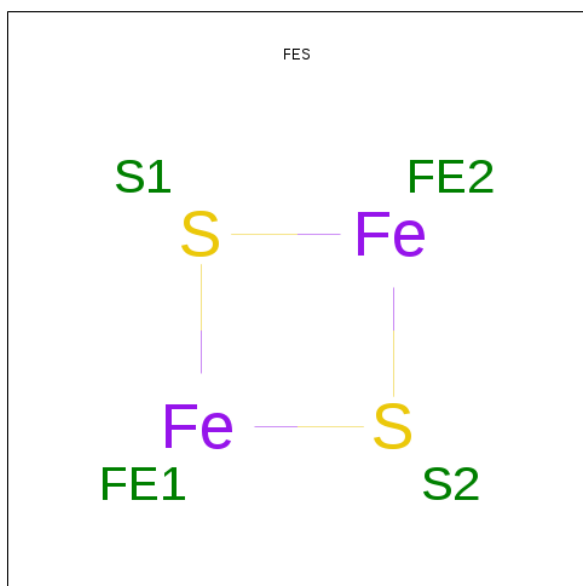
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	D	1	Total	C	0	0
			15	15		

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



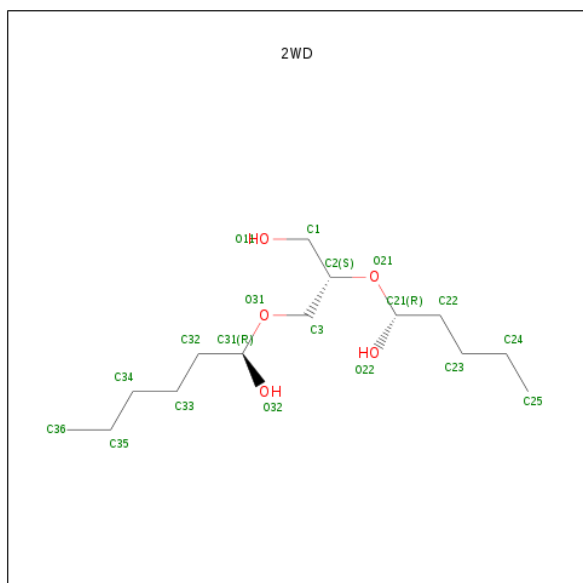
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



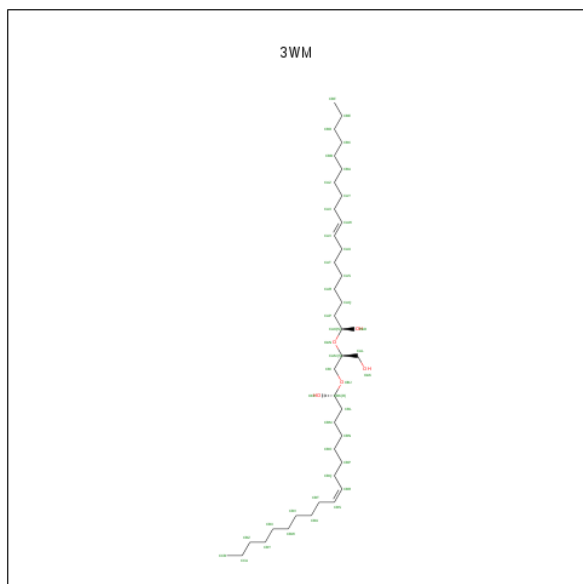
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is (1R)-1-{[(2S)-3-HYDROXY-2-{[(1R)-1-HYDROXYPENTYL]OXY}PROPYL]OXY}HEXAN-1-OL (three-letter code: 2WD) (formula: C₁₄H₃₀O₅).



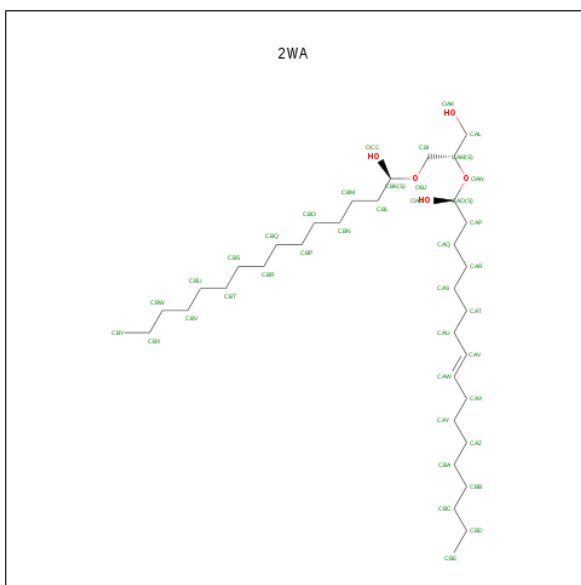
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total	C	O	0	0
			19	14	5		

- Molecule 21 is (1S,8E,1'R,8'Z)-1,1'-{[(2S)-3-HYDROXYPROPANE-1,2-DIYL]BIS(OXY)} BIS(OCTADEC-8-EN-1-OL (three-letter code: 3WM) (formula: C₃₉H₇₆O₅).



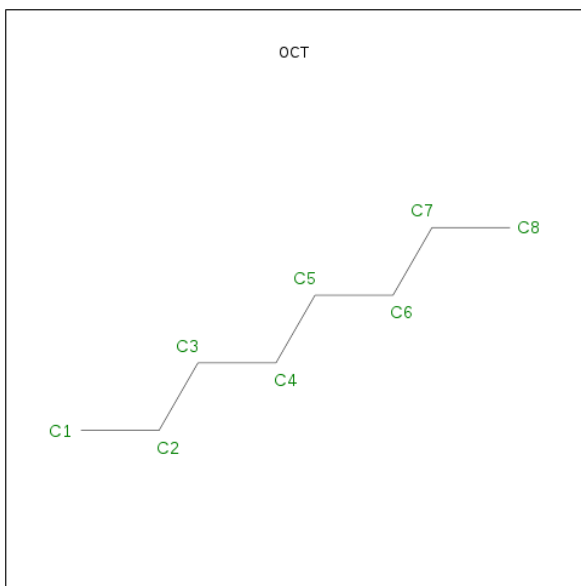
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	C	O	0	0
			44	39	5		

- Molecule 22 is (1S,8E)-1-{[(2S)-1-HYDROXY-3-{[(1S)-1-HYDROXPENTADECYL]OXY}PROPAN-2-YL]OXY}HEPTADEC-8-EN-1-OL (three-letter code: 2WA) (formula: C₃₅H₇₀O₅).



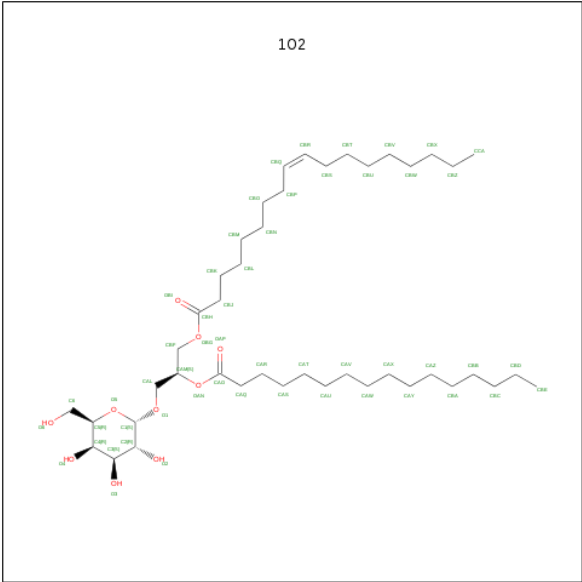
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	F	1	Total	C	O	0	0
			40	35	5		

- Molecule 23 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



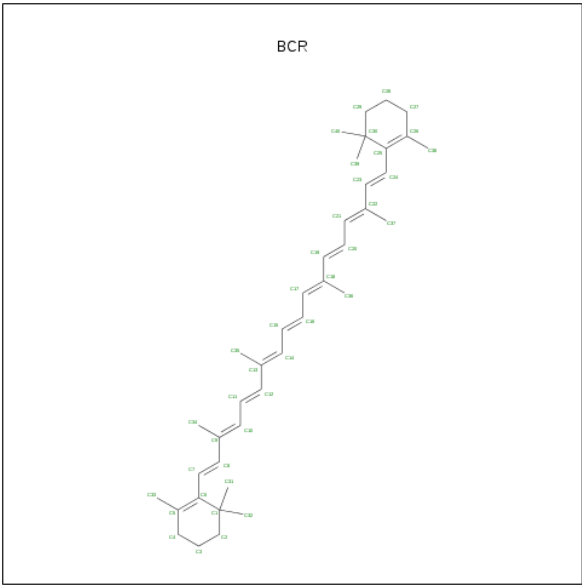
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	F	1	Total C 8 8	0	0

- Molecule 24 is (2S)-3-(ALPHA-D-GALACTOPYRANOSYLOXY)-2-(HEXADECANOYLOXY)PROPYL(9Z)-OCTADEC-9-ENOATE (three-letter code: 1O2) (formula: C₄₃H₈₀O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	F	1	Total	C	O	0	0
			49	39	10		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	1	Total	C	0	0
			40	40		

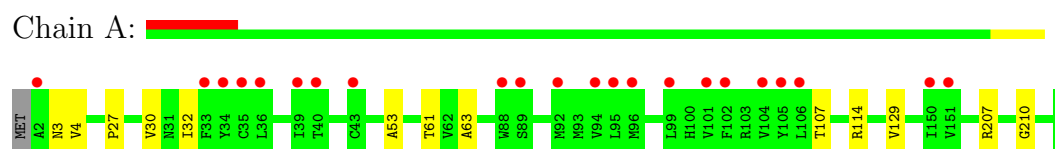
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	21	Total 21	O 21	0	0
26	B	25	Total 25	O 25	0	0
26	C	38	Total 38	O 38	0	0
26	D	1	Total 1	O 1	0	0
26	F	1	Total 1	O 1	0	0
26	G	7	Total 7	O 7	0	0

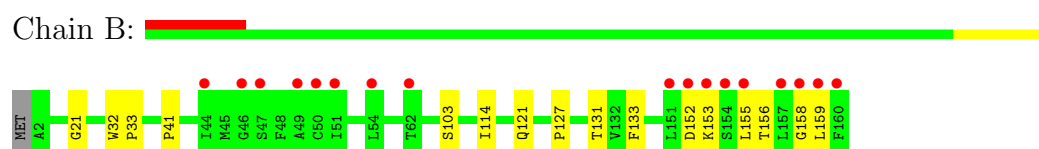
3 Residue-property plots

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.

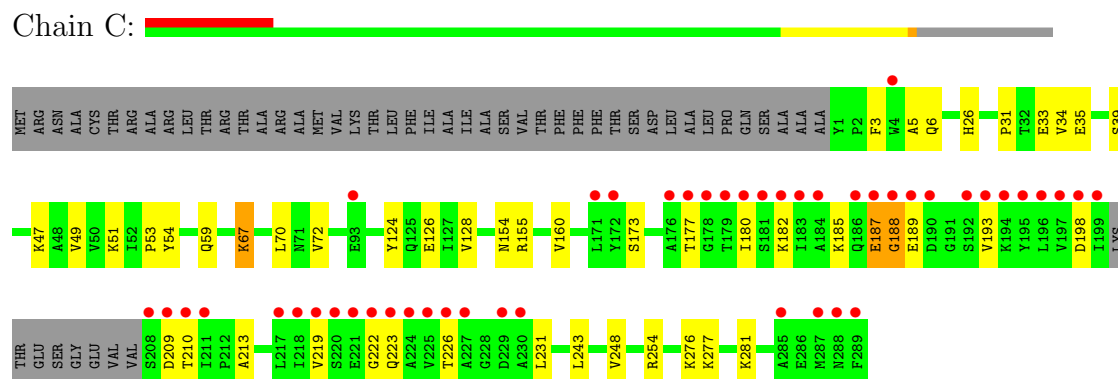
• Molecule 1: Cytochrome b6



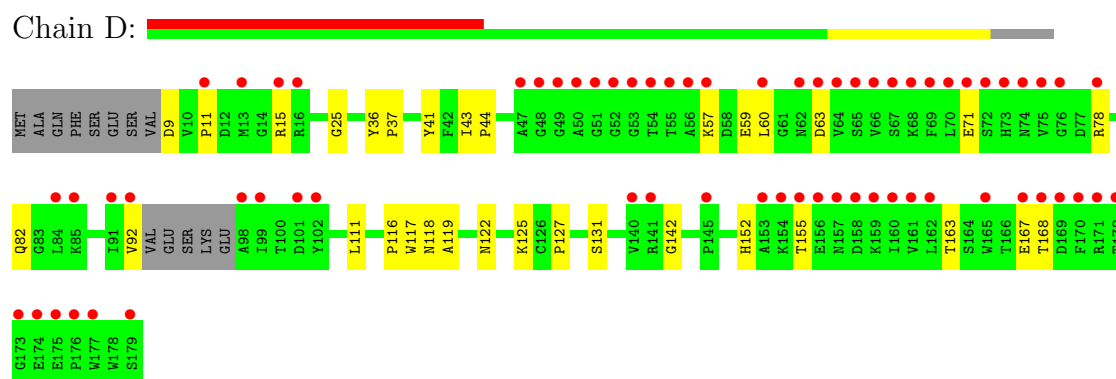
• Molecule 2: Cytochrome b6-f complex subunit 4



• Molecule 3: Apocytochrome f



• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1



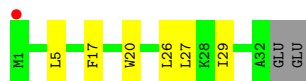
- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E: 



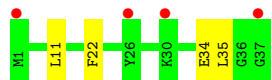
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F: 



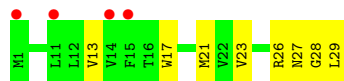
- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G: 



- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.23Å 159.23Å 365.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.50 39.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.57-2.50) 89.3 (39.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.201 , 0.232 0.198 , 0.230	Depositor DCC
R_{free} test set	4287 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 93415 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2WA, 2WD, 1O2, 3WM, MYS, CLA, 2WM, BCR, 7PH, FES, OPC, UMQ, CD, 8K6, OCT, HEM, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1761	0.41	0/2401
2	B	0.23	0/1271	0.38	0/1742
3	C	0.22	0/2182	0.38	0/2972
4	D	0.22	0/1281	0.40	0/1745
5	E	0.25	0/231	0.65	0/309
6	F	0.22	0/234	0.33	0/315
7	G	0.23	0/287	0.34	0/387
8	H	0.26	0/234	0.39	0/319
All	All	0.23	0/7481	0.40	0/10190

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
5	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1721	11	0
2	B	1232	0	1278	14	0
3	C	2137	0	2122	28	0
4	D	1250	0	1208	19	0
5	E	228	0	257	8	0
6	F	231	0	252	6	0
7	G	282	0	303	3	0
8	H	228	0	243	7	0
9	A	129	0	90	9	0
9	C	43	0	30	3	0
10	A	34	0	44	9	0
10	B	68	0	87	17	0
10	D	34	0	44	4	0
10	G	34	0	44	4	0
11	A	32	0	45	1	0
11	B	32	0	45	5	0
11	C	32	0	45	4	0
11	D	32	0	45	1	0
11	F	32	0	45	5	0
12	A	50	0	103	8	0
12	B	18	0	38	2	0
13	A	44	0	0	0	0
14	B	65	0	72	3	0
15	B	54	0	83	5	0
16	C	1	0	0	0	0
17	D	15	0	32	1	0
18	D	54	0	77	2	0
19	D	4	0	0	0	0
20	D	19	0	0	0	0
21	E	44	0	0	0	0
22	F	40	0	0	0	0
23	F	8	0	18	0	0
24	F	49	0	69	9	0
25	G	40	0	56	2	0
26	A	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	25	0	0	1	0
26	C	38	0	0	1	0
26	D	1	0	0	0	0
26	F	1	0	0	0	0
26	G	7	0	0	0	0
All	All	8396	0	8496	150	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:G:101:UMQ:C5'	10:G:101:UMQ:O5'	1.63	1.46
10:A:304:UMQ:C5'	10:A:304:UMQ:O5'	1.63	1.45
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C5'	1.63	1.44
10:B:201:UMQ:C1'	10:B:201:UMQ:O5'	1.69	1.41
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C1'	1.69	1.38
10:D:201:UMQ:C1'	10:D:201:UMQ:O5'	1.69	1.38
10:A:304:UMQ:C1'	10:A:304:UMQ:O5'	1.69	1.38
10:G:101:UMQ:O5'	10:G:101:UMQ:C1'	1.69	1.37
10:D:201:UMQ:C1'	10:D:201:UMQ:C5'	2.46	0.93
10:G:101:UMQ:C5'	10:G:101:UMQ:C1'	2.47	0.93
10:B:203[B]:UMQ:C1'	10:B:203[B]:UMQ:C5'	2.47	0.92
10:A:304:UMQ:C1'	10:A:304:UMQ:C5'	2.48	0.92
10:B:201:UMQ:C5'	10:B:201:UMQ:C1'	2.48	0.92
10:A:304:UMQ:H6'2	10:A:304:UMQ:H11	1.59	0.83
3:C:34:VAL:HG23	3:C:243:LEU:HD23	1.70	0.73
9:A:303:HEM:HHD	9:A:303:HEM:HBC2	1.71	0.72
11:C:303:7PH:H25	11:C:303:7PH:H35A	1.70	0.72
2:B:41:PRO:HG3	12:B:202[A]:8K6:H92C	1.73	0.71
10:B:201:UMQ:H6'1	10:B:201:UMQ:H51	1.73	0.71
1:A:61:THR:HG22	1:A:63:ALA:H	1.56	0.70
8:H:26:ARG:HE	8:H:29:LEU:HD11	1.57	0.70
3:C:31:PRO:O	3:C:155:ARG:NH2	2.26	0.69
1:A:4:VAL:HG13	11:A:305:7PH:H34	1.74	0.69
4:D:131:SER:HA	4:D:142:GLY:HA3	1.76	0.67
1:A:114:ARG:NH1	1:A:210:GLY:O	2.29	0.66
10:D:201:UMQ:H51	10:D:201:UMQ:H4'1	1.79	0.65
3:C:26:HIS:CG	3:C:154:ASN:HD21	2.14	0.64
3:C:33:GLU:HB2	3:C:51:LYS:HB2	1.81	0.62
10:D:201:UMQ:C5	10:D:201:UMQ:H4'1	2.30	0.62
9:C:301:HEM:HBB2	9:C:301:HEM:HMB1	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:F:103:1O2:HAZA	24:F:103:1O2:HBSA	1.82	0.60
24:F:103:1O2:HBQ	24:F:103:1O2:HAY	1.83	0.60
4:D:15:ARG:HH12	5:E:29:LYS:HE3	1.67	0.59
9:A:302:HEM:HBC2	9:A:302:HEM:HMC2	1.84	0.59
3:C:281:LYS:NZ	4:D:9:ASP:O	2.29	0.59
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C6'	2.47	0.58
24:F:103:1O2:CBQ	24:F:103:1O2:HAY	2.33	0.58
3:C:3:PHE:HA	3:C:6:GLN:HG2	1.84	0.58
2:B:32:TRP:CE2	10:B:201:UMQ:HC2	2.39	0.58
6:F:29:ILE:HG22	24:F:103:1O2:HAS	1.85	0.57
10:B:203[B]:UMQ:H6'1	10:B:203[B]:UMQ:H11	1.85	0.57
11:B:206:7PH:H29A	11:B:206:7PH:H24	1.86	0.57
2:B:114:ILE:HD13	15:B:205:OPC:HAT2	1.88	0.56
10:A:304:UMQ:C6'	10:A:304:UMQ:O5'	2.47	0.55
3:C:59:GLN:HB3	3:C:67:LYS:HG3	1.89	0.55
2:B:127:PRO:HD2	15:B:205:OPC:HAG1	1.88	0.55
10:G:101:UMQ:C6'	10:G:101:UMQ:O5'	2.48	0.54
3:C:180:ILE:HB	3:C:223:GLN:H	1.73	0.54
3:C:70:LEU:HD13	3:C:155:ARG:HB3	1.90	0.54
5:E:10:PHE:H	5:E:11:LEU:HB2	1.73	0.54
1:A:32:ILE:N	8:H:29:LEU:HD13	2.23	0.54
6:F:26:LEU:HD13	6:F:29:ILE:HD11	1.90	0.53
5:E:10:PHE:CD2	8:H:13:VAL:HG11	2.44	0.53
4:D:11:PRO:HA	4:D:15:ARG:HD2	1.91	0.53
12:A:308:8K6:H112	12:A:308:8K6:H72C	1.90	0.52
4:D:59:GLU:HG2	4:D:60:LEU:HD12	1.90	0.52
7:G:34:GLU:HG2	7:G:35:LEU:HG	1.91	0.52
10:A:304:UMQ:HL3	10:B:201:UMQ:HK2	1.91	0.51
2:B:133:PHE:HA	14:B:204:CLA:HBB1	1.93	0.51
12:A:308:8K6:H72C	12:A:308:8K6:C13	2.40	0.51
2:B:33:PRO:HG3	18:D:204:SQD:H4	1.91	0.51
11:C:303:7PH:C35	11:C:303:7PH:H25	2.39	0.50
3:C:180:ILE:HG13	3:C:219:VAL:HG11	1.92	0.50
8:H:23:VAL:HG13	8:H:28:GLY:HA2	1.93	0.50
4:D:78:ARG:HD3	4:D:92:VAL:HG22	1.93	0.50
9:A:301:HEM:HBB2	9:A:301:HEM:HMB1	1.92	0.49
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.47	0.49
9:A:303:HEM:C1A	10:B:203[B]:UMQ:H62	2.47	0.49
10:A:304:UMQ:CJ	10:A:304:UMQ:HF2	2.42	0.49
11:B:206:7PH:H29A	11:B:206:7PH:C24	2.44	0.48
5:E:9:GLY:HA2	5:E:12:ALA:HB3	1.95	0.48
1:A:27:PRO:HG2	1:A:30:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:17:PHE:CE1	11:F:104:7PH:H29	2.49	0.47
3:C:5:ALA:HB2	9:C:301:HEM:HHC	1.97	0.47
12:A:306:8K6:H101	12:A:306:8K6:H61C	1.97	0.47
12:A:308:8K6:H72C	12:A:308:8K6:H131	1.97	0.47
24:F:103:1O2:HAWA	24:F:103:1O2:HBQ	1.97	0.47
1:A:129:VAL:HG21	14:B:204:CLA:H43	1.96	0.46
4:D:57:LYS:NZ	4:D:63:ASP:OD1	2.49	0.46
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.96	0.46
6:F:5:LEU:HD21	7:G:11:LEU:HD12	1.98	0.46
24:F:103:1O2:HBMA	24:F:103:1O2:HBJA	1.74	0.46
4:D:57:LYS:O	4:D:82:GLN:N	2.45	0.46
2:B:153:LYS:HG3	2:B:158:GLY:H	1.81	0.45
2:B:41:PRO:HG3	10:B:203[B]:UMQ:HF1	1.97	0.45
15:B:205:OPC:HAA3	15:B:205:OPC:HAH2	1.61	0.45
4:D:118:ASN:HD22	4:D:125:LYS:HE2	1.80	0.45
24:F:103:1O2:HBSA	24:F:103:1O2:CAZ	2.45	0.45
4:D:25:GLY:HA2	18:D:204:SQD:H311	1.99	0.45
5:E:10:PHE:HD2	8:H:13:VAL:HG21	1.81	0.45
11:C:303:7PH:H33A	11:C:303:7PH:H36	1.74	0.45
3:C:209:ASP:OD1	3:C:210:THR:N	2.50	0.45
5:E:11:LEU:HA	5:E:11:LEU:HD22	1.78	0.45
1:A:53:ALA:HB1	4:D:41:TYR:CE1	2.52	0.45
2:B:131:THR:HG23	11:B:206:7PH:H25	1.98	0.45
6:F:27:LEU:HD21	8:H:27:ASN:HA	1.98	0.45
1:A:129:VAL:HG21	14:B:204:CLA:H11	1.99	0.45
3:C:160:VAL:O	9:C:301:HEM:HAC	2.17	0.45
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.99	0.45
11:B:206:7PH:H38	11:B:206:7PH:H35A	1.68	0.44
4:D:117:TRP:HE1	4:D:119:ALA:HB2	1.83	0.44
6:F:20:TRP:CD2	11:F:104:7PH:H34A	2.52	0.44
9:A:303:HEM:HBA2	10:B:203[B]:UMQ:H41	2.00	0.44
3:C:182:LYS:HB2	3:C:198:ASP:H	1.82	0.44
11:F:104:7PH:H39A	11:F:104:7PH:H36	1.72	0.44
2:B:156:THR:HG22	2:B:159:LEU:H	1.81	0.44
9:A:302:HEM:HBB2	9:A:302:HEM:HMB1	2.00	0.43
10:A:304:UMQ:HB1	10:A:304:UMQ:H2'1	2.01	0.43
2:B:103:SER:OG	15:B:205:OPC:HBD2	2.18	0.43
3:C:54:TYR:HB3	3:C:155:ARG:HD3	1.99	0.43
3:C:193:VAL:HB	3:C:213:ALA:HB2	2.00	0.43
12:A:308:8K6:H171	12:A:308:8K6:H142	1.68	0.43
3:C:59:GLN:CB	3:C:67:LYS:HG3	2.49	0.43
11:F:104:7PH:H27A	25:G:102:BCR:C22	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:B:202[A]:8K6:H142	12:B:202[A]:8K6:H112	1.64	0.43
9:A:303:HEM:HMB1	9:A:303:HEM:HBB2	2.00	0.42
25:G:102:BCR:H361	25:G:102:BCR:H20C	1.80	0.42
15:B:205:OPC:HBP1	15:B:205:OPC:HBS	1.79	0.42
5:E:16:GLY:CA	24:F:103:1O2:HBUA	2.49	0.42
4:D:116:PRO:HD2	4:D:127:PRO:HD3	2.01	0.42
12:A:308:8K6:H132	12:A:308:8K6:H62C	2.01	0.42
3:C:177:THR:HG23	3:C:226:THR:HA	2.01	0.42
4:D:167:GLU:HG2	4:D:168:THR:H	1.85	0.42
9:A:301:HEM:HMC1	9:A:301:HEM:HBC2	2.01	0.42
3:C:51:LYS:HG2	3:C:126:GLU:HG2	2.01	0.42
3:C:53:PRO:HD2	3:C:155:ARG:HH21	1.85	0.42
3:C:277:LYS:NZ	26:C:402:HOH:O	2.53	0.42
9:A:303:HEM:C2A	10:B:203[B]:UMQ:H62	2.54	0.41
4:D:152:HIS:HB2	4:D:163:THR:OG1	2.21	0.41
11:B:206:7PH:H35	7:G:22:PHE:CD2	2.54	0.41
12:A:307:8K6:H152	12:A:307:8K6:H121	1.84	0.41
2:B:32:TRP:NE1	10:B:201:UMQ:HA2	2.35	0.41
1:A:207:ARG:NH1	10:B:203[B]:UMQ:O2	2.54	0.41
12:A:306:8K6:H132	12:A:307:8K6:H81C	2.03	0.41
4:D:122:ASN:ND2	4:D:122:ASN:O	2.54	0.41
3:C:187:GLU:HB2	3:C:188:GLY:H	1.72	0.41
26:B:310:HOH:O	3:C:276:LYS:NZ	2.53	0.41
3:C:35:GLU:HB2	3:C:49:VAL:HB	2.03	0.41
3:C:39:SER:HB3	3:C:248:VAL:HB	2.02	0.41
1:A:114:ARG:NH2	2:B:21:GLY:O	2.54	0.41
3:C:254:ARG:HA	11:D:203:7PH:H25	2.03	0.41
11:C:303:7PH:O32	11:C:303:7PH:H34	2.15	0.41
3:C:72:VAL:HG21	3:C:124:TYR:O	2.21	0.41
10:A:304:UMQ:CL	10:B:201:UMQ:HI2	2.51	0.41
8:H:17:TRP:O	8:H:21:MET:HG2	2.21	0.41
1:A:107:THR:O	2:B:121:GLN:HB3	2.21	0.40
5:E:16:GLY:HA3	24:F:103:1O2:HBUA	2.03	0.40
17:D:202:MYS:H82	17:D:202:MYS:H112	1.64	0.40
4:D:43:ILE:HA	4:D:44:PRO:HD3	1.91	0.40
11:F:104:7PH:H29A	11:F:104:7PH:H2C	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	38	60
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	C	277/333 (83%)	249 (90%)	23 (8%)	5 (2%)	13	20
4	D	162/179 (90%)	147 (91%)	15 (9%)	0	100	100
5	E	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	6	7
6	F	30/34 (88%)	30 (100%)	0	0	100	100
7	G	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	929/1018 (91%)	865 (93%)	57 (6%)	7 (1%)	27	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	173	SER
1	A	3	ASN
3	C	185	LYS
5	E	11	LEU
3	C	189	GLU
3	C	222	GLY
3	C	188	GLY

5.3.2 Protein sidechains ⓘ

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	183/184 (100%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	133/134 (99%)	131 (98%)	2 (2%)	76	93
3	C	231/272 (85%)	228 (99%)	3 (1%)	80	94
4	D	133/145 (92%)	130 (98%)	3 (2%)	63	87
5	E	21/21 (100%)	20 (95%)	1 (5%)	35	60
6	F	22/24 (92%)	22 (100%)	0	100	100
7	G	29/29 (100%)	29 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
All	All	776/833 (93%)	767 (99%)	9 (1%)	82	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	152	ASP
2	B	155	LEU
3	C	67	LYS
3	C	187	GLU
3	C	231	LEU
4	D	71	GLU
4	D	111	LEU
4	D	155	THR
5	E	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	154	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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$
9	HEM	A	301	1	42,50,50	3.52	13 (30%)	27,82,82	1.29	3 (11%)
9	HEM	A	302	1	42,50,50	3.53	13 (30%)	27,82,82	1.30	3 (11%)
9	HEM	A	303	1,26	42,50,50	3.77	14 (33%)	27,82,82	1.27	3 (11%)
10	UMQ	A	304	-	35,35,35	3.63	17 (48%)	46,46,46	2.12	8 (17%)
11	7PH	A	305	-	31,31,37	1.46	3 (9%)	33,33,42	1.31	3 (9%)
12	8K6	A	306	-	17,17,17	0.11	0	16,16,16	0.83	0
12	8K6	A	307	-	17,17,17	0.10	0	16,16,16	0.87	0
12	8K6	A	308	-	13,13,17	2.28	1 (7%)	12,12,16	0.83	0
13	2WM	A	309	-	43,43,43	0.64	2 (4%)	45,45,45	0.52	0
10	UMQ	B	201	-	35,35,35	3.62	17 (48%)	46,46,46	2.15	6 (13%)
12	8K6	B	202[A]	-	17,17,17	0.10	0	16,16,16	0.84	0
10	UMQ	B	203[B]	-	35,35,35	3.63	17 (48%)	46,46,46	2.15	8 (17%)
14	CLA	B	204	26	73,73,73	1.63	10 (13%)	96,113,113	1.19	11 (11%)
15	OPC	B	205	-	51,53,54	1.01	2 (3%)	55,61,64	0.98	2 (3%)
11	7PH	B	206	-	31,31,37	1.47	3 (9%)	33,33,42	1.28	3 (9%)
9	HEM	C	301	3	42,50,50	3.48	12 (28%)	27,82,82	1.26	3 (11%)
11	7PH	C	303	-	31,31,37	1.47	3 (9%)	33,33,42	1.33	3 (9%)
10	UMQ	D	201	-	35,35,35	3.64	17 (48%)	46,46,46	2.19	9 (19%)
17	MYS	D	202	-	14,14,14	0.11	0	13,13,13	0.82	0
11	7PH	D	203	-	31,31,37	1.50	3 (9%)	33,33,42	1.25	3 (9%)
18	SQD	D	204	-	54,54,54	0.93	4 (7%)	65,65,65	1.69	10 (15%)
19	FES	D	205	4	0,4,4	0.00	-	0,4,4	0.00	-
20	2WD	D	206	-	18,18,18	1.16	1 (5%)	20,20,20	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	3WM	E	101	-	43,43,43	0.79	1 (2%)	45,45,45	0.63	1 (2%)
22	2WA	F	101	-	39,39,39	0.88	1 (2%)	41,41,41	0.57	0
23	OCT	F	102	-	7,7,7	0.15	0	6,6,6	0.69	0
24	1O2	F	103	-	49,49,53	1.52	6 (12%)	57,57,61	1.15	8 (14%)
11	7PH	F	104	-	31,31,37	1.49	3 (9%)	33,33,42	1.31	3 (9%)
10	UMQ	G	101	-	35,35,35	3.63	17 (48%)	46,46,46	2.16	8 (17%)
25	BCR	G	102	-	41,41,41	1.02	2 (4%)	56,56,56	1.13	4 (7%)

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
9	HEM	A	301	1	-	0/14/114/114	0/0/8/8
9	HEM	A	302	1	-	0/14/114/114	0/0/8/8
9	HEM	A	303	1,26	-	0/14/114/114	0/0/8/8
10	UMQ	A	304	-	-	0/20/60/60	0/2/2/2
11	7PH	A	305	-	-	0/33/33/39	0/0/0/0
12	8K6	A	306	-	-	0/15/15/15	0/0/0/0
12	8K6	A	307	-	-	0/15/15/15	0/0/0/0
12	8K6	A	308	-	-	0/11/11/15	0/0/0/0
13	2WM	A	309	-	-	0/45/45/45	0/0/0/0
10	UMQ	B	201	-	-	0/20/60/60	0/2/2/2
12	8K6	B	202[A]	-	-	0/15/15/15	0/0/0/0
10	UMQ	B	203[B]	-	-	1/20/60/60	0/2/2/2
14	CLA	B	204	26	-	0/37/135/135	0/0/9/9
15	OPC	B	205	-	-	0/55/57/60	0/0/0/0
11	7PH	B	206	-	-	0/33/33/39	0/0/0/0
9	HEM	C	301	3	-	0/14/114/114	0/0/8/8
11	7PH	C	303	-	-	0/33/33/39	0/0/0/0
10	UMQ	D	201	-	-	0/20/60/60	0/2/2/2
17	MYS	D	202	-	-	0/12/12/12	0/0/0/0
11	7PH	D	203	-	-	0/33/33/39	0/0/0/0
18	SQD	D	204	-	-	0/49/69/69	0/1/1/1
19	FES	D	205	4	-	0/0/4/4	0/1/1/1
20	2WD	D	206	-	-	0/20/20/20	0/0/0/0
21	3WM	E	101	-	-	0/45/45/45	0/0/0/0
22	2WA	F	101	-	-	0/41/41/41	0/0/0/0
23	OCT	F	102	-	-	0/5/5/5	0/0/0/0
24	1O2	F	103	-	1/1/8/10	0/44/64/68	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	7PH	F	104	-	-	0/33/33/39	0/0/0/0
10	UMQ	G	101	-	-	0/20/60/60	0/2/2/2
25	BCR	G	102	-	-	0/29/63/63	0/2/2/2

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	HEM	C3C-C2C	-14.94	1.33	1.45
9	A	301	HEM	C3C-C2C	-13.21	1.35	1.45
9	C	301	HEM	C3C-C2C	-13.18	1.35	1.45
9	A	302	HEM	C3C-C2C	-12.99	1.35	1.45
9	A	303	HEM	C3B-C2B	-10.90	1.35	1.45
9	A	302	HEM	C3B-C2B	-10.82	1.35	1.45
10	B	203[B]	UMQ	O5'-C1'	10.77	1.69	1.41
9	A	301	HEM	C3B-C2B	-10.77	1.35	1.45
10	G	101	UMQ	O5'-C1'	10.77	1.69	1.41
10	A	304	UMQ	O5'-C1'	10.77	1.69	1.41
10	D	201	UMQ	O5'-C1'	10.77	1.69	1.41
10	B	201	UMQ	O5'-C1'	10.73	1.69	1.41
9	C	301	HEM	C3B-C2B	-10.69	1.35	1.45
10	B	201	UMQ	O3'-C3'	8.29	1.63	1.43
10	G	101	UMQ	O3'-C3'	8.26	1.63	1.43
10	B	203[B]	UMQ	O3'-C3'	8.23	1.62	1.43
12	A	308	8K6	C5-C6	-8.22	1.51	1.55
10	A	304	UMQ	O3'-C3'	8.20	1.62	1.43
10	D	201	UMQ	O3'-C3'	8.18	1.62	1.43
10	A	304	UMQ	O5'-C5'	7.66	1.63	1.44
10	G	101	UMQ	O5'-C5'	7.63	1.63	1.44
10	B	203[B]	UMQ	O5'-C5'	7.62	1.63	1.44
10	D	201	UMQ	O5'-C5'	7.57	1.63	1.44
10	B	201	UMQ	O5'-C5'	7.51	1.63	1.44
14	B	204	CLA	C3B-C4B	7.37	1.50	1.41
10	D	201	UMQ	O5-C5	6.04	1.59	1.44
9	A	303	HEM	CMB-C2B	6.00	1.55	1.45
9	A	301	HEM	CMC-C2C	5.97	1.55	1.45
9	A	302	HEM	CMB-C2B	5.90	1.55	1.45
9	C	301	HEM	CMB-C2B	5.89	1.55	1.45
10	A	304	UMQ	O5-C5	5.86	1.59	1.44
10	B	203[B]	UMQ	O5-C5	5.86	1.59	1.44
9	A	303	HEM	CMD-C2D	5.83	1.55	1.45
9	A	301	HEM	CMB-C2B	5.81	1.55	1.45
10	B	201	UMQ	O5-C5	5.79	1.58	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	101	UMQ	O5-C5	5.79	1.58	1.44
9	A	302	HEM	CMC-C2C	5.78	1.54	1.45
9	A	302	HEM	CMD-C2D	5.74	1.54	1.45
9	A	303	HEM	CMC-C2C	5.73	1.54	1.45
9	C	301	HEM	CMC-C2C	5.72	1.54	1.45
9	C	301	HEM	CMD-C2D	5.72	1.54	1.45
9	A	301	HEM	CMD-C2D	5.68	1.54	1.45
10	B	203[B]	UMQ	C6-C5	-5.54	1.32	1.52
10	B	201	UMQ	C6-C5	-5.51	1.32	1.52
10	D	201	UMQ	C6-C5	-5.50	1.32	1.52
10	A	304	UMQ	C6-C5	-5.49	1.32	1.52
10	G	101	UMQ	C6-C5	-5.47	1.32	1.52
11	D	203	7PH	C3B-C3A	4.82	1.57	1.55
14	B	204	CLA	C4B-NB	4.75	1.42	1.34
9	A	301	HEM	C3B-CAB	4.72	1.55	1.40
9	A	301	HEM	C3C-CAC	4.72	1.55	1.40
11	F	104	7PH	C3B-C3A	4.70	1.57	1.55
9	A	303	HEM	C3B-CAB	4.69	1.55	1.40
9	A	302	HEM	C3B-CAB	4.66	1.55	1.40
9	C	301	HEM	C3C-CAC	4.66	1.55	1.40
9	A	302	HEM	C3C-CAC	4.65	1.55	1.40
24	F	103	1O2	CBQ-CBR	4.64	1.57	1.31
9	C	301	HEM	C3B-CAB	4.64	1.55	1.40
9	A	303	HEM	FE-ND	4.59	2.14	1.95
9	A	303	HEM	C3C-CAC	4.58	1.55	1.40
11	B	206	7PH	C3B-C3A	4.55	1.57	1.55
11	A	305	7PH	C3B-C3A	4.54	1.57	1.55
11	C	303	7PH	C3B-C3A	4.47	1.56	1.55
9	A	302	HEM	FE-ND	4.45	2.13	1.95
10	A	304	UMQ	C3'-C4'	-4.44	1.39	1.52
10	B	201	UMQ	C3'-C4'	-4.41	1.39	1.52
10	G	101	UMQ	C3'-C4'	-4.39	1.40	1.52
10	D	201	UMQ	C3'-C4'	-4.38	1.40	1.52
10	B	201	UMQ	O1'-C1'	-4.38	1.32	1.40
10	A	304	UMQ	O2-C2	4.37	1.53	1.43
10	B	203[B]	UMQ	C3'-C4'	-4.37	1.40	1.52
10	A	304	UMQ	O1'-C1'	-4.36	1.32	1.40
10	D	201	UMQ	O1'-C1'	-4.35	1.32	1.40
10	B	203[B]	UMQ	O2-C2	4.34	1.53	1.43
10	D	201	UMQ	O2-C2	4.34	1.53	1.43
10	G	101	UMQ	O1'-C1'	-4.33	1.32	1.40
10	B	201	UMQ	O2-C2	4.32	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	101	UMQ	O2-C2	4.31	1.53	1.43
10	B	203[B]	UMQ	O1'-C1'	-4.30	1.32	1.40
10	D	201	UMQ	C3-C2	-4.22	1.41	1.52
10	G	101	UMQ	C3-C2	-4.21	1.41	1.52
24	F	103	1O2	OBG-CBH	4.20	1.46	1.33
10	B	203[B]	UMQ	C3-C2	-4.18	1.41	1.52
10	A	304	UMQ	C3-C2	-4.14	1.41	1.52
10	B	201	UMQ	C3-C2	-4.12	1.41	1.52
11	C	303	7PH	O31-C31	4.10	1.45	1.33
11	D	203	7PH	O31-C31	4.09	1.45	1.33
11	F	104	7PH	O31-C31	4.08	1.45	1.33
11	B	206	7PH	O31-C31	4.06	1.45	1.33
11	A	305	7PH	O31-C31	4.02	1.45	1.33
9	C	301	HEM	C3D-C2D	4.01	1.54	1.43
9	A	303	HEM	C3D-C2D	3.97	1.53	1.43
24	F	103	1O2	OAN-CAO	3.90	1.46	1.34
11	D	203	7PH	O21-C21	3.90	1.46	1.34
11	C	303	7PH	O21-C21	3.89	1.46	1.34
11	F	104	7PH	O21-C21	3.88	1.46	1.34
9	A	301	HEM	C3D-C2D	3.88	1.53	1.43
9	A	302	HEM	C3D-C2D	3.87	1.53	1.43
11	B	206	7PH	O21-C21	3.87	1.46	1.34
11	A	305	7PH	O21-C21	3.87	1.46	1.34
14	B	204	CLA	CHB-C4A	3.86	1.38	1.33
14	B	204	CLA	C1A-NA	3.83	1.40	1.32
15	B	205	OPC	OBJ-CBK	3.64	1.44	1.33
10	G	101	UMQ	C4-C5	3.60	1.60	1.53
10	D	201	UMQ	C4-C5	3.59	1.60	1.53
14	B	204	CLA	C1B-C2B	3.55	1.49	1.43
10	B	201	UMQ	C4-C5	3.55	1.60	1.53
10	A	304	UMQ	C3'-C2'	-3.54	1.43	1.52
10	B	203[B]	UMQ	C4-C5	3.53	1.60	1.53
10	A	304	UMQ	C4-C5	3.53	1.60	1.53
9	C	301	HEM	FE-ND	3.51	2.09	1.95
10	B	201	UMQ	C3'-C2'	-3.49	1.43	1.52
10	G	101	UMQ	C3'-C2'	-3.48	1.43	1.52
10	B	203[B]	UMQ	C3'-C2'	-3.47	1.43	1.52
20	D	206	2WD	O21-C2	-3.46	1.39	1.44
10	D	201	UMQ	C3'-C2'	-3.44	1.43	1.52
24	F	103	1O2	CBV-CBU	-3.41	1.53	1.55
24	F	103	1O2	O5-C1	3.36	1.50	1.41
9	A	303	HEM	FE-NB	3.31	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	203[B]	UMQ	O3-C3	3.28	1.50	1.43
10	G	101	UMQ	O3-C3	3.26	1.50	1.43
10	B	201	UMQ	O3-C3	3.25	1.50	1.43
10	D	201	UMQ	O3-C3	3.23	1.50	1.43
10	A	304	UMQ	O3-C3	3.22	1.50	1.43
25	G	102	BCR	C1-C6	-3.21	1.49	1.53
18	D	204	SQD	O48-C23	3.10	1.42	1.33
10	A	304	UMQ	O1-C4'	3.09	1.51	1.43
10	B	203[B]	UMQ	O1-C4'	3.07	1.51	1.43
9	A	303	HEM	FE-NC	3.05	2.07	1.95
10	G	101	UMQ	O1-C4'	3.00	1.51	1.43
10	D	201	UMQ	O1-C4'	2.99	1.51	1.43
9	A	301	HEM	FE-NB	2.95	2.06	1.95
10	B	201	UMQ	O1-C4'	2.90	1.51	1.43
9	A	301	HEM	FE-ND	2.90	2.07	1.95
10	B	203[B]	UMQ	C6'-C5'	-2.90	1.41	1.52
10	G	101	UMQ	C6'-C5'	-2.83	1.41	1.52
10	D	201	UMQ	C6'-C5'	-2.82	1.41	1.52
10	B	201	UMQ	C6'-C5'	-2.81	1.41	1.52
24	F	103	1O2	CAQ-CAO	2.80	1.59	1.50
10	A	304	UMQ	C6'-C5'	-2.79	1.42	1.52
9	A	302	HEM	FE-NC	2.75	2.06	1.95
18	D	204	SQD	O47-C7	2.67	1.42	1.34
13	A	309	2WM	CAW-CAV	-2.67	1.35	1.51
25	G	102	BCR	C30-C25	-2.65	1.50	1.53
9	A	301	HEM	FE-NC	2.58	2.06	1.95
9	A	303	HEM	C1D-ND	2.53	1.40	1.33
15	B	205	OPC	OAN-CAO	2.53	1.42	1.36
10	B	203[B]	UMQ	C1-C2	-2.52	1.45	1.52
9	A	303	HEM	C4D-ND	2.51	1.40	1.33
10	G	101	UMQ	C1-C2	-2.50	1.45	1.52
10	D	201	UMQ	C1-C2	-2.50	1.45	1.52
10	B	201	UMQ	C1-C2	-2.48	1.45	1.52
14	B	204	CLA	CMB-C2B	-2.47	1.46	1.51
10	G	101	UMQ	O2'-C2'	2.46	1.48	1.43
10	B	201	UMQ	O2'-C2'	2.46	1.48	1.43
10	D	201	UMQ	O2'-C2'	2.45	1.48	1.43
9	A	301	HEM	C1D-ND	2.41	1.39	1.33
9	A	302	HEM	C1D-ND	2.41	1.39	1.33
10	A	304	UMQ	O2'-C2'	2.40	1.48	1.43
10	A	304	UMQ	C1-C2	-2.40	1.45	1.52
9	A	302	HEM	FE-NB	2.39	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	203[B]	UMQ	O2'-C2'	2.38	1.48	1.43
14	B	204	CLA	CHC-C1C	2.37	1.43	1.35
14	B	204	CLA	C1D-C2D	2.37	1.48	1.42
13	A	309	2WM	OAN-CAM	-2.35	1.41	1.44
14	B	204	CLA	C4D-C3D	2.35	1.48	1.42
9	A	301	HEM	C4D-ND	2.33	1.39	1.33
9	C	301	HEM	FE-NB	2.33	2.03	1.95
21	E	101	3WM	OAN-CAM	-2.32	1.41	1.44
9	A	302	HEM	C4D-ND	2.30	1.39	1.33
9	C	301	HEM	C4D-ND	2.30	1.39	1.33
14	B	204	CLA	CMD-C2D	-2.25	1.46	1.51
9	C	301	HEM	C1D-ND	2.25	1.39	1.33
10	D	201	UMQ	O5-C1	2.24	1.47	1.41
10	A	304	UMQ	O5-C1	2.19	1.47	1.41
10	B	203[B]	UMQ	O5-C1	2.14	1.47	1.41
18	D	204	SQD	O2-C2	-2.11	1.37	1.43
10	G	101	UMQ	O5-C1	2.09	1.47	1.41
9	A	303	HEM	C4C-NC	2.08	1.39	1.33
10	B	201	UMQ	O5-C1	2.05	1.47	1.41
22	F	101	2WA	CBS-CBR	-2.04	1.39	1.51
18	D	204	SQD	O3-C3	-2.01	1.38	1.43

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	201	UMQ	C1'-O5'-C5'	-9.46	95.44	113.73
10	G	101	UMQ	C1'-O5'-C5'	-9.12	96.10	113.73
10	B	203[B]	UMQ	C1'-O5'-C5'	-8.96	96.41	113.73
10	A	304	UMQ	C1'-O5'-C5'	-8.91	96.50	113.73
10	B	201	UMQ	C1'-O5'-C5'	-8.87	96.57	113.73
10	B	203[B]	UMQ	C2'-C3'-C4'	7.38	125.58	109.59
10	D	201	UMQ	C2'-C3'-C4'	7.33	125.47	109.59
10	B	201	UMQ	C2'-C3'-C4'	7.20	125.20	109.59
10	A	304	UMQ	C2'-C3'-C4'	7.18	125.15	109.59
10	G	101	UMQ	C2'-C3'-C4'	7.16	125.12	109.59
18	D	204	SQD	O9-S-C6	5.19	111.42	106.83
18	D	204	SQD	O7-S-C6	5.02	111.26	106.83
10	B	201	UMQ	O5-C5-C4	-4.10	102.11	109.73
24	F	103	1O2	OAN-CAO-CAQ	4.05	120.17	111.54
10	G	101	UMQ	O5-C5-C4	-3.97	102.35	109.73
10	A	304	UMQ	O5-C5-C4	-3.94	102.40	109.73
11	C	303	7PH	O21-C21-C22	3.91	119.86	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	204	SQD	C5-C6-S	-3.89	108.96	114.40
18	D	204	SQD	O6-C1-C2	3.86	113.10	108.15
18	D	204	SQD	O8-S-C6	3.83	110.45	105.89
11	F	104	7PH	O21-C21-C22	3.79	119.62	111.54
11	A	305	7PH	O21-C21-C22	3.78	119.60	111.54
18	D	204	SQD	O47-C7-C8	3.71	119.44	111.54
10	B	201	UMQ	C1-O1-C4'	-3.68	108.65	118.00
10	G	101	UMQ	C1-O1-C4'	-3.63	108.79	118.00
18	D	204	SQD	O9-S-O7	-3.58	101.02	113.45
14	B	204	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
11	B	206	7PH	O21-C21-C22	3.55	119.10	111.54
9	A	302	HEM	CBD-CAD-C3D	-3.53	106.85	114.51
10	B	203[B]	UMQ	C1-O1-C4'	-3.35	109.50	118.00
10	B	203[B]	UMQ	O5-C5-C4	-3.32	103.56	109.73
11	D	203	7PH	O21-C21-C22	3.15	118.26	111.54
9	A	301	HEM	CBD-CAD-C3D	-3.13	107.72	114.51
10	A	304	UMQ	C1-O1-C4'	-3.07	110.21	118.00
15	B	205	OPC	OAN-CAO-CAP	3.00	119.74	110.50
10	D	201	UMQ	O5-C5-C4	-2.98	104.19	109.73
11	D	203	7PH	O11-C1-C2	-2.89	109.25	113.35
11	F	104	7PH	O11-C1-C2	-2.85	109.30	113.35
11	C	303	7PH	O11-C1-C2	-2.84	109.32	113.35
14	B	204	CLA	O2D-CGD-O1D	-2.81	118.15	123.79
11	A	305	7PH	O11-C1-C2	-2.79	109.39	113.35
10	D	201	UMQ	O5-C1-C2	2.77	115.97	110.30
11	B	206	7PH	O11-C1-C2	-2.74	109.46	113.35
24	F	103	1O2	OBG-CBH-CBJ	2.71	120.20	111.90
10	A	304	UMQ	C1-C2-C3	2.69	115.20	109.99
14	B	204	CLA	C3D-C4D-CHA	2.69	112.47	108.16
14	B	204	CLA	C2D-C3D-CAD	2.69	145.89	134.94
25	G	102	BCR	C27-C26-C25	2.67	126.38	122.86
11	C	303	7PH	O31-C31-C32	2.66	120.05	111.90
15	B	205	OPC	OBJ-CBK-CBL	2.65	120.03	111.90
18	D	204	SQD	O48-C23-C24	2.64	119.99	111.90
11	B	206	7PH	O31-C31-C32	2.64	119.97	111.90
11	F	104	7PH	O31-C31-C32	2.63	119.95	111.90
10	G	101	UMQ	C1-C2-C3	2.63	115.07	109.99
10	D	201	UMQ	C1-C2-C3	2.61	115.04	109.99
9	A	303	HEM	CAD-CBD-CGD	-2.59	108.65	113.53
11	A	305	7PH	O31-C31-C32	2.58	119.78	111.90
14	B	204	CLA	CMB-C2B-C3B	2.57	130.01	125.16
18	D	204	SQD	C44-O6-C1	2.56	118.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	102	BCR	C33-C5-C6	-2.54	121.62	124.50
14	B	204	CLA	CBD-CHA-C1A	2.51	132.05	128.77
14	B	204	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
14	B	204	CLA	CHD-C4C-NC	2.46	126.00	124.28
9	A	302	HEM	C3A-C4A-NA	-2.45	107.86	109.50
10	B	203[B]	UMQ	C1-C2-C3	2.44	114.72	109.99
9	A	301	HEM	C3A-C4A-NA	-2.44	107.87	109.50
9	C	301	HEM	C3A-C4A-NA	-2.42	107.88	109.50
21	E	101	3WM	CBT-CBS-CBR	-2.38	111.16	125.44
9	C	301	HEM	CBA-CAA-C2A	-2.37	108.68	112.63
11	D	203	7PH	O31-C31-C32	2.32	118.99	111.90
24	F	103	1O2	C1-C2-C3	2.31	114.46	109.99
10	B	203[B]	UMQ	O5-C5-C6	2.30	112.06	106.34
14	B	204	CLA	CHB-C4A-NA	2.29	127.58	124.38
25	G	102	BCR	C7-C8-C9	-2.28	122.81	126.22
10	D	201	UMQ	C1-O5-C5	2.28	118.14	113.73
10	G	101	UMQ	C3-C4-C5	2.25	114.21	110.17
10	B	201	UMQ	C1-C2-C3	2.24	114.32	109.99
10	D	201	UMQ	C1-O1-C4'	-2.23	112.34	118.00
9	A	303	HEM	C3A-C4A-NA	-2.21	108.02	109.50
10	B	203[B]	UMQ	O5'-C5'-C4'	2.20	114.31	109.71
18	D	204	SQD	O5-C5-C4	2.19	113.81	109.73
10	D	201	UMQ	O3'-C3'-C2'	-2.19	105.47	110.36
25	G	102	BCR	C24-C23-C22	-2.18	122.95	126.22
9	A	303	HEM	CBD-CAD-C3D	-2.18	109.79	114.51
24	F	103	1O2	O5-C1-C2	2.17	114.75	110.30
9	C	301	HEM	CBD-CAD-C3D	-2.17	109.81	114.51
24	F	103	1O2	CBP-CBQ-CBR	-2.13	112.64	125.44
10	A	304	UMQ	O5-C1-C2	2.13	114.66	110.30
14	B	204	CLA	CMD-C2D-C3D	2.12	129.16	125.16
10	B	201	UMQ	O3'-C3'-C2'	-2.12	105.63	110.36
9	A	301	HEM	C4A-C3A-C2A	2.10	108.45	107.00
10	D	201	UMQ	C3-C4-C5	2.07	113.89	110.17
24	F	103	1O2	CBS-CBR-CBQ	-2.06	113.06	125.44
14	B	204	CLA	C4A-NA-C1A	2.06	109.28	106.38
9	A	302	HEM	CMC-C2C-C3C	2.06	129.12	124.26
24	F	103	1O2	C3-C4-C5	2.05	113.85	110.17
10	A	304	UMQ	O5-C5-C6	2.04	111.43	106.34
10	G	101	UMQ	O5-C1-C2	2.03	114.47	110.30
10	A	304	UMQ	O3'-C3'-C2'	-2.03	105.82	110.36
10	B	203[B]	UMQ	O3'-C3'-C2'	-2.03	105.83	110.36
24	F	103	1O2	C4-C3-C2	2.02	114.52	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	101	UMQ	O3'-C3'-C2'	-2.01	105.86	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	F	103	1O2	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	203[B]	UMQ	CA-O1'-C1'-O5'

There are no ring outliers.

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, 95th 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	214/215 (99%)	0.40	22 (10%) 7 6	43, 59, 97, 186	0
2	B	159/160 (99%)	0.50	17 (10%) 6 6	52, 77, 124, 195	0
3	C	281/333 (84%)	0.83	47 (16%) 2 2	57, 85, 191, 249	0
4	D	166/179 (92%)	2.01	66 (39%) 1 0	50, 145, 205, 239	0
5	E	31/31 (100%)	0.46	4 (12%) 4 4	81, 98, 123, 153	0
6	F	32/34 (94%)	0.25	1 (3%) 47 48	69, 87, 131, 169	0
7	G	37/37 (100%)	0.95	4 (10%) 6 6	57, 74, 144, 155	0
8	H	29/29 (100%)	1.09	4 (13%) 4 3	59, 71, 100, 144	0
All	All	949/1018 (93%)	0.87	165 (17%) 2 2	43, 81, 185, 249	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	199	ILE	11.9
2	B	160	PHE	10.9
3	C	188	GLY	9.2
3	C	192	SER	9.2
3	C	183	ILE	8.9
3	C	196	LEU	8.9
4	D	69	PHE	8.8
4	D	50	ALA	8.7
3	C	189	GLU	8.4
4	D	49	GLY	8.3
3	C	190	ASP	7.8
3	C	176	ALA	7.8
4	D	70	LEU	7.7
4	D	75	VAL	7.6
4	D	56	ALA	7.3
3	C	186	GLN	7.2

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Mol	Chain	Res	Type	RSRZ
4	D	92	VAL	7.0
4	D	48	GLY	6.8
4	D	160	ILE	6.7
2	B	159	LEU	6.5
3	C	225	VAL	6.5
4	D	67	SER	6.4
4	D	55	THR	6.4
4	D	66	VAL	6.2
4	D	64	VAL	6.2
4	D	98	ALA	6.1
4	D	51	GLY	5.9
3	C	218	ILE	5.8
3	C	193	VAL	5.8
3	C	184	ALA	5.8
4	D	159	LYS	5.7
4	D	85	LYS	5.6
4	D	62	ASN	5.6
3	C	197	VAL	5.5
4	D	102	TYR	5.5
4	D	99	ILE	5.4
3	C	220	SER	5.4
4	D	179	SER	5.3
4	D	172	THR	5.3
3	C	224	ALA	5.2
3	C	198	ASP	5.2
4	D	175	GLU	5.2
4	D	161	VAL	5.2
4	D	174	GLU	5.2
4	D	156	GLU	5.1
7	G	37	GLY	5.0
3	C	177	THR	5.0
4	D	173	GLY	5.0
4	D	63	ASP	4.9
4	D	60	LEU	4.9
3	C	182	LYS	4.9
4	D	71	GLU	4.8
3	C	208	SER	4.8
5	E	31	LEU	4.7
3	C	221	GLU	4.7
4	D	57	LYS	4.7
4	D	158	ASP	4.6
4	D	157	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	180	ILE	4.6
2	B	157	LEU	4.5
4	D	52	GLY	4.5
3	C	209	ASP	4.4
4	D	53	GLY	4.4
2	B	153	LYS	4.3
2	B	50	CYS	4.2
4	D	168	THR	4.2
3	C	219	VAL	4.2
4	D	72	SER	4.1
4	D	154	LYS	4.0
4	D	76	GLY	4.0
4	D	54	THR	3.9
2	B	47	SER	3.9
6	F	1	MET	3.9
3	C	226	THR	3.8
4	D	140	VAL	3.8
4	D	91	ILE	3.7
3	C	285	ALA	3.7
3	C	288	ASN	3.7
3	C	195	TYR	3.7
4	D	73	HIS	3.6
4	D	162	LEU	3.6
3	C	179	THR	3.6
3	C	194	LYS	3.6
1	A	2	ALA	3.6
4	D	155	THR	3.5
4	D	171	ARG	3.4
1	A	35	CYS	3.4
3	C	181	SER	3.4
4	D	47	ALA	3.3
3	C	210	THR	3.3
1	A	43	CYS	3.3
2	B	46	GLY	3.3
1	A	92	MET	3.2
4	D	141	ARG	3.2
1	A	99	LEU	3.2
3	C	172	TYR	3.2
4	D	65	SER	3.1
4	D	170	PHE	3.1
3	C	187	GLU	3.1
3	C	211	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	217	LEU	3.1
2	B	152	ASP	3.1
4	D	165	TRP	3.0
4	D	13	MET	3.0
1	A	96	MET	3.0
1	A	95	LEU	2.9
5	E	27	SER	2.9
1	A	34	TYR	2.9
4	D	74	ASN	2.9
5	E	29	LYS	2.9
1	A	36	LEU	2.8
1	A	104	VAL	2.8
4	D	169	ASP	2.8
4	D	176	PRO	2.8
1	A	101	VAL	2.7
3	C	229	ASP	2.7
3	C	223	GLN	2.7
2	B	151	LEU	2.7
8	H	1	MET	2.7
4	D	167	GLU	2.6
3	C	289	PHE	2.6
4	D	84	LEU	2.6
3	C	93	GLU	2.6
1	A	150	ILE	2.6
1	A	151	VAL	2.6
4	D	68	LYS	2.6
1	A	39	ILE	2.5
2	B	51	ILE	2.5
7	G	26	TYR	2.5
4	D	16	ARG	2.5
3	C	178	GLY	2.5
5	E	10	PHE	2.5
2	B	54	LEU	2.5
3	C	171	LEU	2.4
3	C	222	GLY	2.4
2	B	62	THR	2.4
2	B	154	SER	2.4
4	D	101	ASP	2.3
7	G	30	LYS	2.3
8	H	15	PHE	2.3
2	B	49	ALA	2.2
3	C	227	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	287	MET	2.2
1	A	40	THR	2.2
1	A	89	SER	2.2
4	D	177	TRP	2.2
4	D	15	ARG	2.2
2	B	158	GLY	2.2
1	A	33	PHE	2.1
1	A	94	VAL	2.1
2	B	44	ILE	2.1
1	A	88	TRP	2.1
2	B	155	LEU	2.1
4	D	145	PRO	2.1
1	A	106	LEU	2.1
7	G	1	MET	2.1
4	D	11	PRO	2.1
1	A	105	TYR	2.1
3	C	4	TRP	2.1
8	H	14	VAL	2.1
1	A	102	PHE	2.1
8	H	11	LEU	2.1
4	D	78	ARG	2.0
3	C	230	ALA	2.0
4	D	153	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	2WD	D	206	19/19	0.70	20.20	75,123,142,145	0
11	7PH	B	206	32/38	0.73	17.72	77,132,182,184	0
23	OCT	F	102	8/8	0.58	15.13	101,106,110,116	0
12	8K6	A	306	18/18	0.36	11.60	93,113,147,148	0
24	1O2	F	103	49/53	0.70	10.29	80,127,216,220	0
17	MYS	D	202	15/15	0.45	10.27	93,107,121,126	0
12	8K6	A	307	18/18	0.37	8.00	76,108,124,127	0
10	UMQ	D	201	34/34	0.69	7.78	102,210,248,264	0
11	7PH	C	303	32/38	0.53	7.18	73,117,149,150	0
10	UMQ	A	304	34/34	0.47	6.15	127,146,201,254	0
10	UMQ	G	101	34/34	0.65	5.24	81,173,199,284	0
10	UMQ	B	203[B]	34/34	0.39	4.08	80,103,132,144	34
12	8K6	B	202[A]	18/18	0.41	3.78	47,102,122,122	18
22	2WA	F	101	40/40	0.43	3.71	70,111,169,182	0
11	7PH	F	104	32/38	0.33	3.56	81,101,172,175	0
12	8K6	A	308	14/18	0.25	3.04	62,82,95,99	0
15	OPC	B	205	54/55	0.24	2.57	55,92,121,137	0
11	7PH	A	305	32/38	0.39	2.22	93,126,189,190	0
21	3WM	E	101	44/44	0.34	1.44	60,97,122,125	0
11	7PH	D	203	32/38	0.23	1.40	54,81,153,157	0
18	SQD	D	204	54/54	0.27	1.39	73,116,159,177	0
13	2WM	A	309	44/44	0.25	1.36	70,96,152,158	0
25	BCR	G	102	40/40	0.34	1.10	49,74,116,122	0
10	UMQ	B	201	34/34	0.28	0.90	64,114,151,224	0
14	CLA	B	204	65/65	0.20	0.62	59,79,107,117	0
9	HEM	A	302	43/43	0.26	0.50	34,57,71,76	0
9	HEM	A	301	43/43	0.18	0.05	31,50,65,78	0
9	HEM	A	303	43/43	0.21	-0.00	47,66,85,95	0
9	HEM	C	301	43/43	0.15	-0.01	46,69,96,113	0
16	CD	C	302	1/1	0.10	-0.91	136,136,136,136	1
19	FES	D	205	4/4	0.08	-1.84	96,97,100,102	0

6.5 Other polymers ⓘ

There are no such residues in this entry.