



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:44 am GMT

PDB ID : 4H13
Title : Crystal Structure of the Cytochrome b6f Complex from *Mastigocladus laminosus* with TDS
Authors : Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on : 2012-09-10
Resolution : 3.07 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

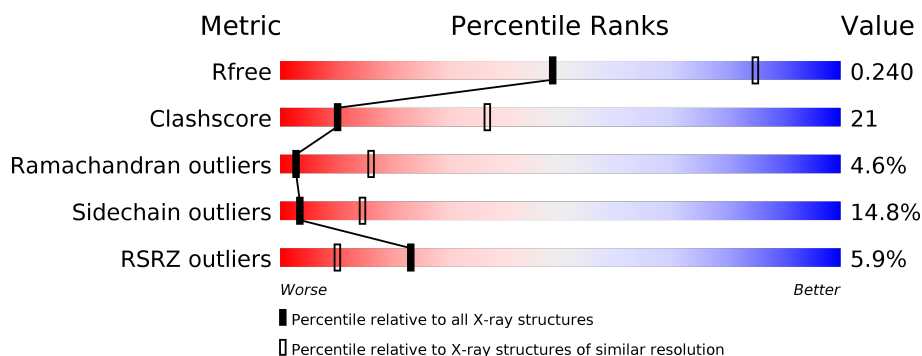
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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}	100719	1116 (3.10-3.06)
Clashscore	112137	1220 (3.10-3.06)
Ramachandran outliers	110173	1176 (3.10-3.06)
Sidechain outliers	110143	1176 (3.10-3.06)
RSRZ outliers	101464	1123 (3.10-3.06)

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 $\leq 5\%$. 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	215	<div> <div>0%</div> <div>68% 26% 6%</div> </div>
2	B	160	<div> <div>3%</div> <div>60% 37% .</div> </div>
3	C	289	<div> <div>9%</div> <div>50% 40% 10%</div> </div>
4	D	179	<div> <div>13%</div> <div>48% 37% 7% . 6%</div> </div>
5	E	32	<div> <div>56% 34% 9%</div> </div>
6	F	35	<div> <div>3%</div> <div>54% 17% 17% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	37	
8	H	29	

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
11	OPC	A	305	-	-	-	X
11	OPC	B	204	-	-	-	X
12	MYS	A	306	-	-	-	X
13	8K6	A	307	-	-	-	X
14	UMQ	A	308	X	-	-	X
14	UMQ	B	202	X	-	-	X
16	CLA	B	203	X	-	-	X
17	7PH	C	301	-	-	-	X
18	SQD	D	201	X	-	-	X
20	BCR	G	101	-	-	-	X
21	OCT	F	101	-	-	-	X

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 16526 atoms, of which 8399 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 b6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	0	0
			3449	1140	1738	272	288	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	160	Total	C	H	N	O	S	0	0	0
			2558	841	1309	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	288	Total	C	H	N	O	S	0	0	0
			4451	1415	2235	369	424	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	SEE REMARK 999	UNP P83793

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	168	Total	C	H	N	O	S	0	0	0
			2563	823	1275	221	237	7			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	32	Total	C	H	N	O	S	0	0	0
			532	179	284	34	34	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	31	Total	C	H	N	O	S	0	0	0
			483	160	249	34	39	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	H	N	O	S	0	0	0
			572	188	289	44	50	1			

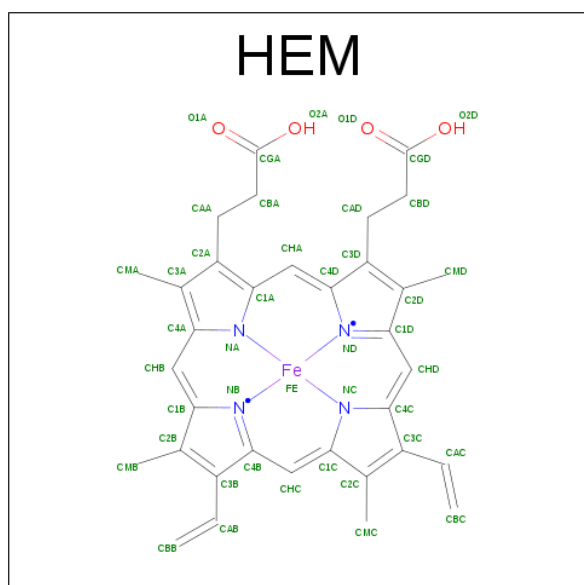
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	29	Total	C	H	N	O	S	0	0	0
			469	156	239	36	36	2			

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

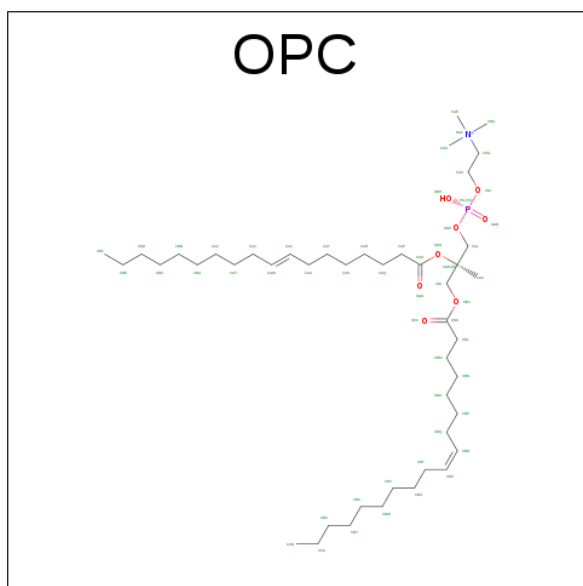
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cd	0	0
			1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



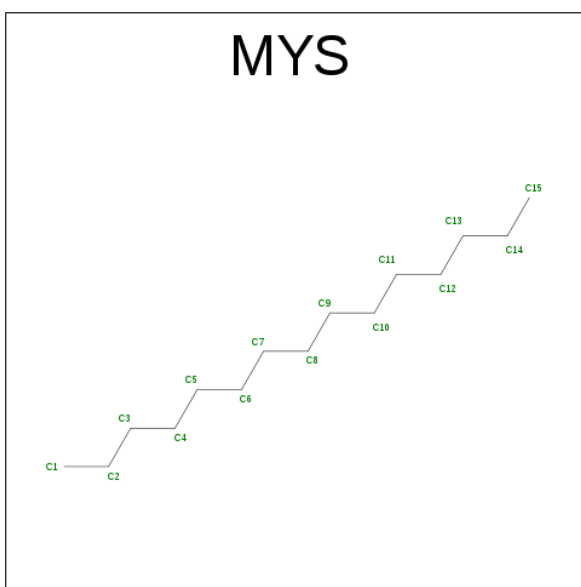
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 11 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-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: C₄₅H₈₇NO₈P).



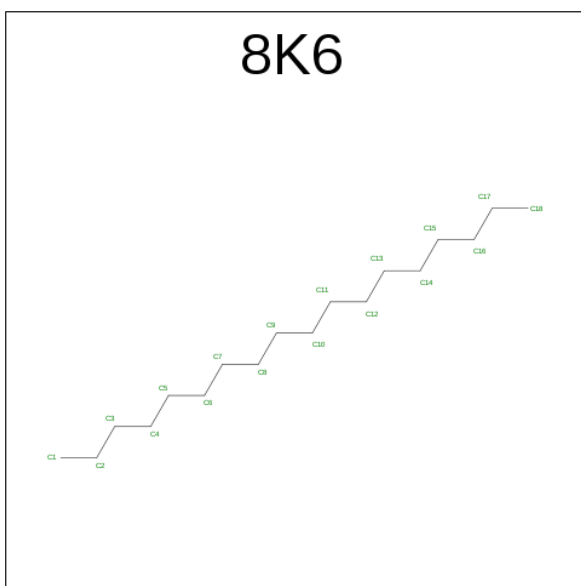
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
11	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 12 is PENTADECANE (three-letter code: MYS) (formula: C₁₅H₃₂).



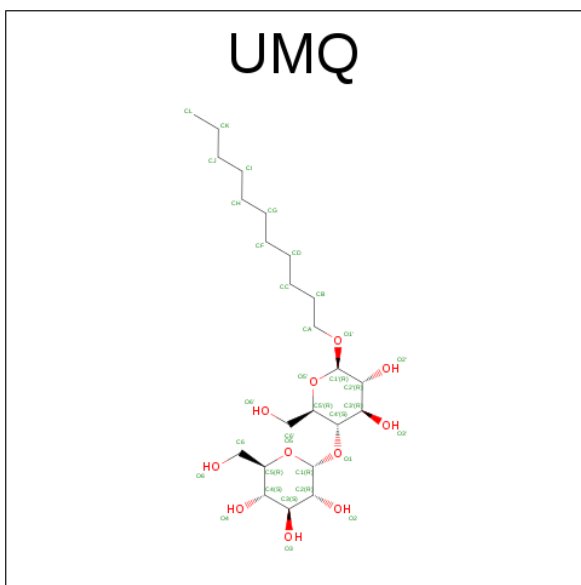
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	H	0	0
			47	15	32		

- Molecule 13 is OCTADECANE (three-letter code: 8K6) (formula: $C_{18}H_{38}$).



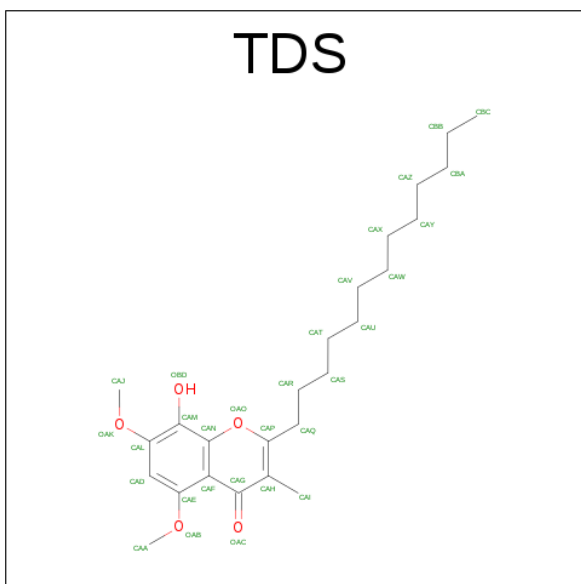
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	H	0	0
			56	18	38		

- Molecule 14 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total 77	C 23	H 43	O 11	0	0
14	B	1	Total 77	C 23	H 43	O 11	0	0

- Molecule 15 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (three-letter code: TDS) (formula: $C_{25}H_{38}O_5$).



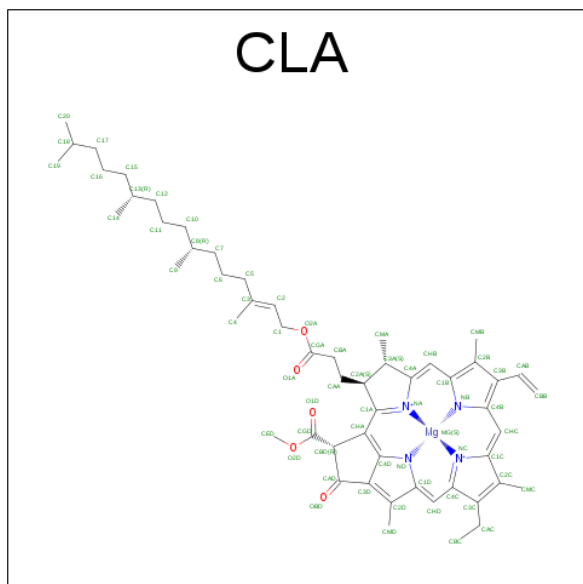
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			68	25	38	5		

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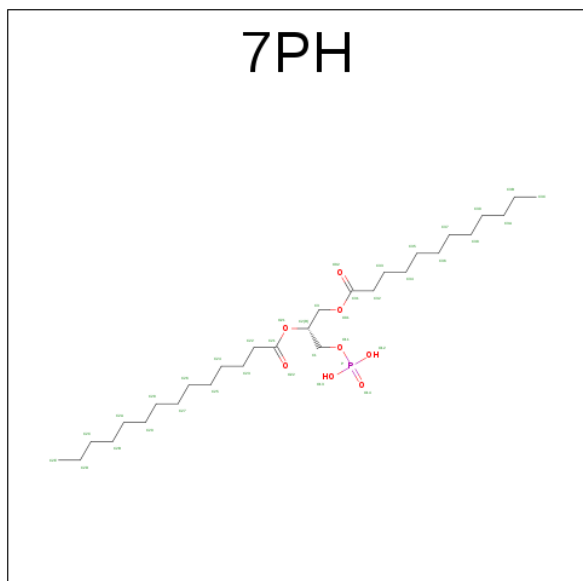
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	H	O	0	0
			68	25	38	5		

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



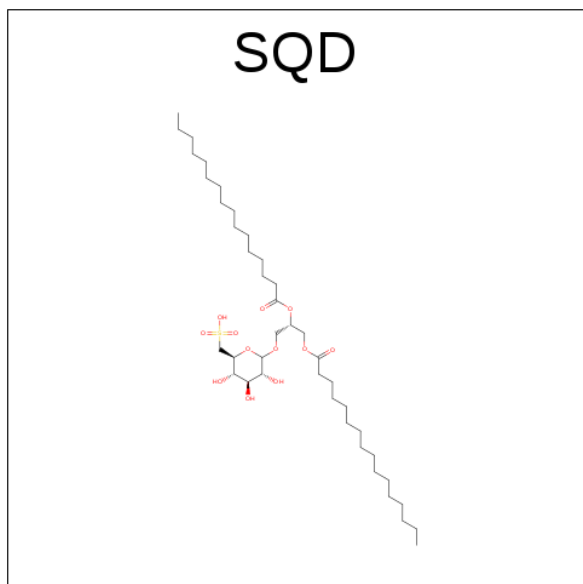
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 17 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



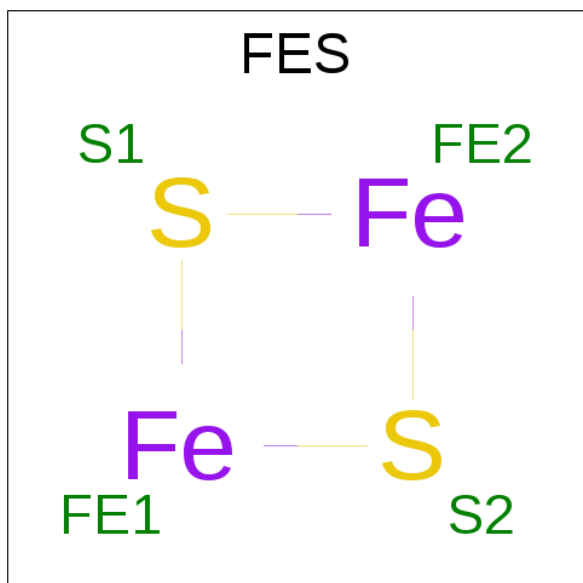
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	H	O	0	0
			81	27	49	5		

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



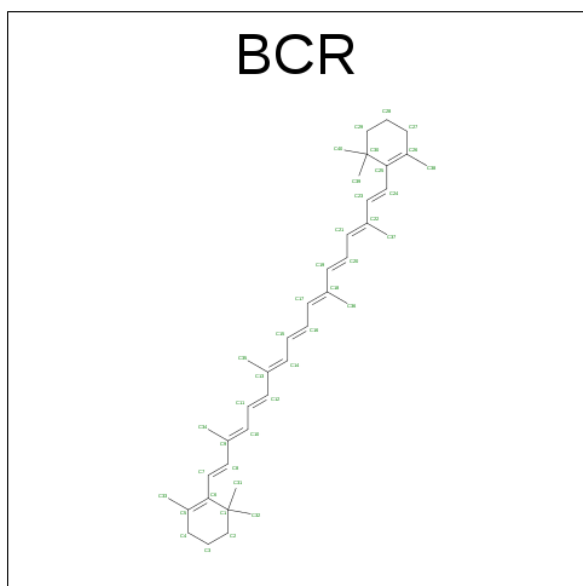
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	H	O	S	1	0
			131	41	78	11	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



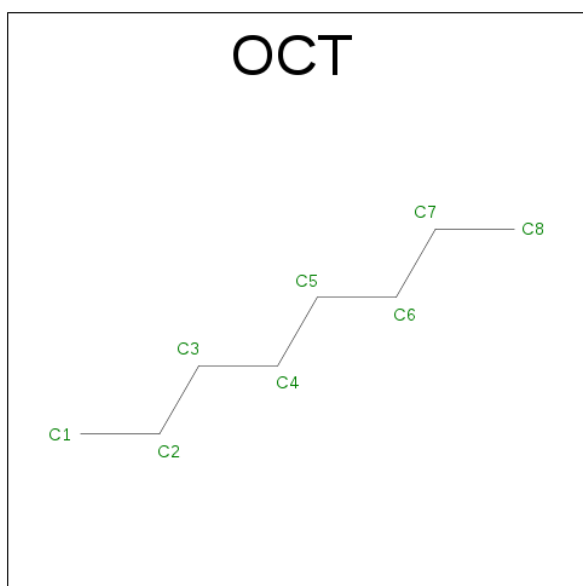
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	G	1	Total	C	H	0	0
			96	40	56		

- Molecule 21 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	F	1	Total	C	H	0	0
			26	8	18		

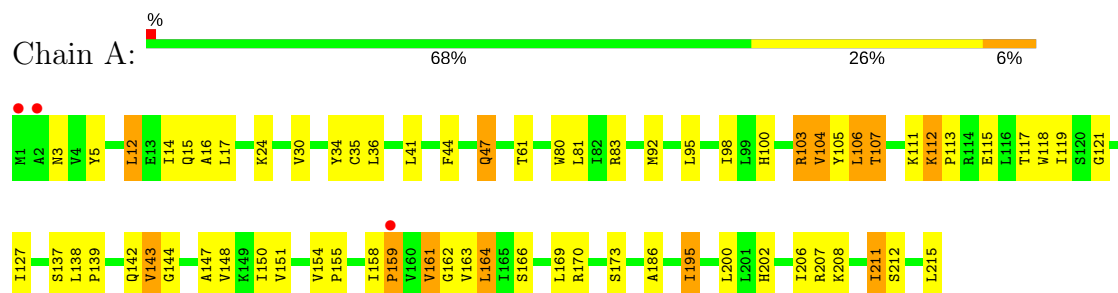
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	12	Total	O	0	0
			12	12		
22	B	6	Total	O	0	0
			6	6		
22	C	4	Total	O	0	0
			4	4		
22	F	1	Total	O	0	0
			1	1		
22	G	1	Total	O	0	0
			1	1		

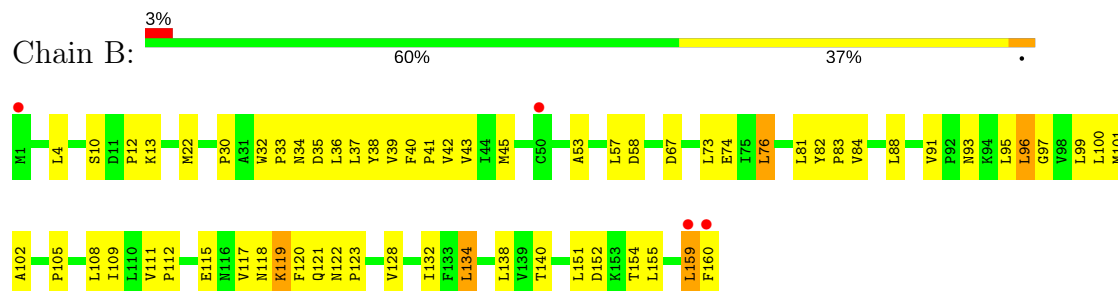
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

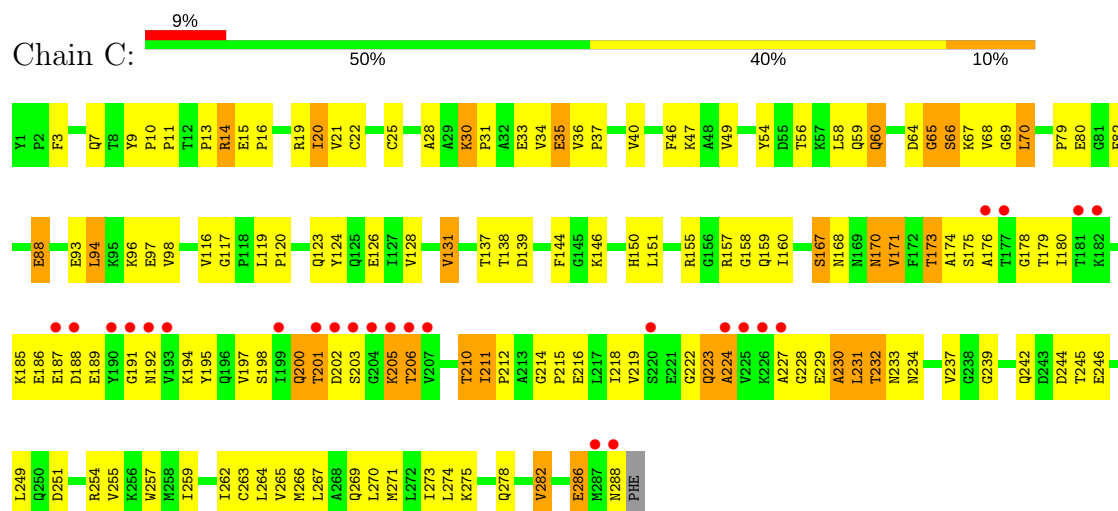
• Molecule 1: Cytochrome b6



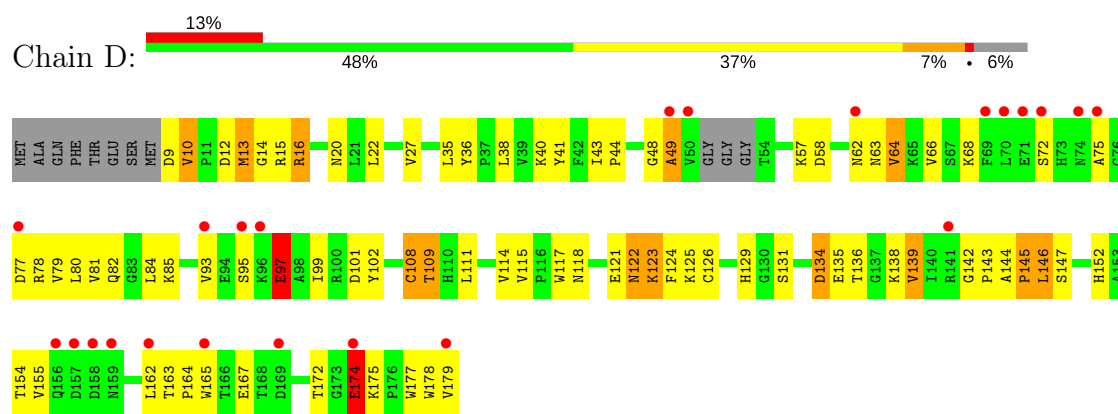
• Molecule 2: Cytochrome b6-f complex subunit 4



• Molecule 3: Apocytochrome f



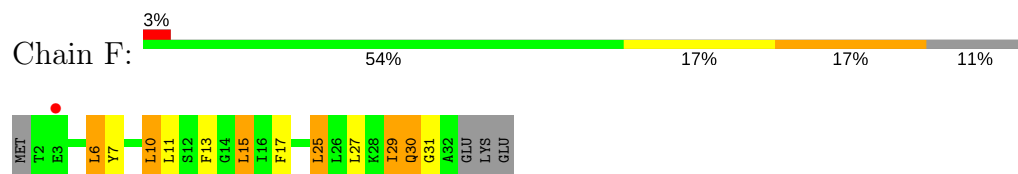
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



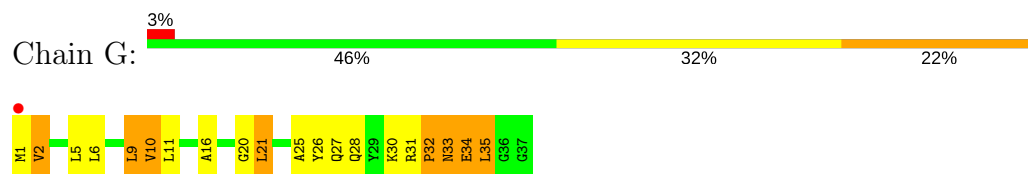
- Molecule 5: Cytochrome b6-f complex subunit 6



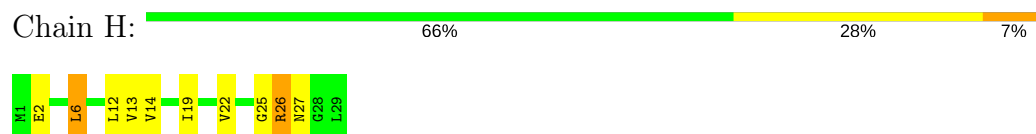
- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5



- Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.20Å 157.20Å 363.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.57 – 3.07 34.57 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.57-3.07) 99.1 (34.57-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.214 , 0.238 0.209 , 0.240	Depositor DCC
R_{free} test set	2542 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	91.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16526	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, MYS, CLA, CD, 7PH, FES, OPC, TDS, HEM, 8K6, OCT, BCR, 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	0.29	0/1763	0.50	0/2405
2	B	0.29	0/1288	0.53	0/1765
3	C	0.27	0/2264	0.56	0/3082
4	D	0.25	0/1320	0.51	0/1798
5	E	0.34	0/253	0.63	0/340
6	F	0.30	0/238	0.51	0/321
7	G	0.31	0/289	0.62	0/391
8	H	0.31	0/236	0.54	0/323
All	All	0.28	0/7651	0.53	0/10425

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
4	D	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
4	D	97	GLU	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	1711	1738	1737	67	0
2	B	1249	1309	1308	62	0
3	C	2216	2235	2233	109	0
4	D	1288	1275	1273	52	0
5	E	248	284	284	16	0
6	F	234	249	248	12	0
7	G	283	289	289	20	0
8	H	230	239	239	10	0
9	A	1	0	0	0	0
10	A	129	90	90	23	0
10	C	43	30	30	10	0
11	A	54	83	83	5	0
11	B	54	83	83	1	0
12	A	15	32	32	5	0
13	A	18	38	38	0	0
14	A	34	43	41	0	0
14	B	34	43	41	1	0
15	A	30	38	38	4	0
15	B	30	38	37	4	0
16	B	65	62	71	5	0
17	C	32	49	45	1	0
18	D	53	78	75	3	0
19	D	4	0	0	1	0
20	G	40	56	56	7	0
21	F	8	18	18	0	0
22	A	12	0	0	5	0
22	B	6	0	0	1	0
22	C	4	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
All	All	8127	8399	8389	345	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 21.

All (345) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:CYS:SG	10:A:304:HEM:CAB	2.57	0.92
3:C:25:CYS:SG	10:C:302:HEM:CAC	2.58	0.92
20:G:101:BCR:H321	20:G:101:BCR:HC8	1.53	0.89
10:A:303:HEM:O1A	22:A:403:HOH:O	1.98	0.81
1:A:117:THR:OG1	22:A:404:HOH:O	2.01	0.79
10:A:304:HEM:HBD1	10:A:304:HEM:HHA	1.65	0.79
1:A:35:CYS:SG	10:A:304:HEM:CBB	2.71	0.78
3:C:25:CYS:SG	10:C:302:HEM:CBC	2.72	0.78
3:C:157:ARG:HB2	10:C:302:HEM:HAD2	1.68	0.74
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.23	0.73
16:B:203:CLA:HMB1	16:B:203:CLA:HBB1	1.71	0.71
7:G:20:GLY:N	20:G:101:BCR:H363	2.06	0.69
3:C:171:VAL:HG12	3:C:234:ASN:HA	1.74	0.69
3:C:19:ARG:O	3:C:20:ILE:HB	1.93	0.68
1:A:30:VAL:HG22	1:A:34:TYR:CD1	2.29	0.68
3:C:34:VAL:HG21	3:C:151:LEU:HB2	1.74	0.68
1:A:112:LYS:CB	1:A:113:PRO:CD	2.72	0.67
11:B:204:OPC:HAE2	11:B:204:OPC:OAI	1.94	0.67
1:A:35:CYS:HG	10:A:304:HEM:CAB	2.08	0.67
3:C:200:GLN:HA	3:C:205:LYS:HB3	1.76	0.67
1:A:83:ARG:NH1	10:A:302:HEM:O2A	2.28	0.66
2:B:119:LYS:O	2:B:119:LYS:HG2	1.96	0.66
3:C:70:LEU:N	3:C:70:LEU:HD23	2.11	0.66
3:C:211:ILE:O	3:C:211:ILE:HG13	1.96	0.66
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.78	0.65
15:A:309:TDS:HAQ2	2:B:81:LEU:HD13	1.80	0.64
2:B:82:TYR:OH	22:B:305:HOH:O	2.14	0.64
2:B:151:LEU:O	2:B:154:THR:HG22	1.98	0.64
11:A:305:OPC:HBV1	7:G:9:LEU:HD21	1.80	0.64
2:B:33:PRO:HB3	2:B:38:TYR:CE1	2.33	0.63
7:G:1:MET:O	7:G:2:VAL:HG13	1.99	0.63
4:D:78:ARG:HD2	4:D:117:TRP:CD1	2.33	0.63
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.81	0.63
4:D:129:HIS:HB2	19:D:202:FES:S1	2.38	0.63
3:C:65:GLY:O	3:C:66:SER:O	2.16	0.62
3:C:200:GLN:HG2	3:C:201:THR:N	2.14	0.62
10:A:302:HEM:HBB2	10:A:302:HEM:HMB2	1.81	0.62
4:D:134:ASP:OD1	4:D:135:GLU:N	2.32	0.62
2:B:159:LEU:HD23	2:B:159:LEU:N	2.14	0.62
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.80	0.62
2:B:35:ASP:HA	2:B:39:VAL:HG13	1.83	0.61
10:A:303:HEM:HBC2	10:A:303:HEM:HMC2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:O	2:B:154:THR:CG2	2.50	0.60
10:A:304:HEM:HBC2	10:A:304:HEM:HHD	1.83	0.60
3:C:180:ILE:HG22	3:C:222:GLY:O	2.01	0.60
5:E:10:VAL:O	5:E:14:LEU:HB2	2.01	0.60
1:A:112:LYS:CB	1:A:113:PRO:HD3	2.32	0.60
3:C:257:TRP:HB2	17:C:301:7PH:H26A	1.82	0.60
4:D:108:CYS:CB	4:D:115:VAL:CG2	2.80	0.60
1:A:112:LYS:HB3	1:A:113:PRO:HD3	1.83	0.59
1:A:112:LYS:HB2	1:A:113:PRO:CD	2.32	0.59
2:B:30:PRO:HG2	2:B:34:ASN:OD1	2.01	0.59
7:G:31:ARG:N	7:G:32:PRO:CD	2.65	0.59
1:A:211:ILE:HD12	1:A:212:SER:H	1.66	0.59
3:C:230:ALA:O	3:C:232:THR:N	2.35	0.59
3:C:60:GLN:HE22	3:C:157:ARG:HG2	1.68	0.59
3:C:170:ASN:OD1	3:C:170:ASN:N	2.35	0.59
10:A:302:HEM:HBC2	10:A:302:HEM:HMC1	1.85	0.59
4:D:146:LEU:HD12	4:D:177:TRP:CD2	2.38	0.59
2:B:40:PHE:HB2	2:B:41:PRO:HD3	1.84	0.58
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.39	0.58
7:G:1:MET:O	7:G:2:VAL:HG22	2.04	0.57
1:A:100:HIS:ND1	22:A:410:HOH:O	2.26	0.57
3:C:262:ILE:HG22	3:C:263:CYS:N	2.19	0.57
3:C:40:VAL:HG11	3:C:46:PHE:CD2	2.39	0.57
4:D:12:ASP:O	4:D:14:GLY:N	2.36	0.57
20:G:101:BCR:H323	8:H:19:ILE:HG13	1.86	0.57
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.85	0.57
2:B:22:MET:HG3	2:B:22:MET:O	2.05	0.57
10:C:302:HEM:HBC2	10:C:302:HEM:HMC2	1.87	0.57
3:C:167:SER:OG	3:C:168:ASN:N	2.36	0.57
3:C:200:GLN:CG	3:C:201:THR:N	2.68	0.57
5:E:29:ILE:O	5:E:29:ILE:HG22	2.03	0.57
2:B:159:LEU:O	2:B:160:PHE:HB3	2.05	0.56
2:B:33:PRO:CB	2:B:38:TYR:CE1	2.88	0.56
5:E:12:ILE:O	5:E:15:PHE:N	2.38	0.56
2:B:40:PHE:CB	2:B:41:PRO:HD3	2.36	0.56
12:A:306:MYS:H101	12:A:306:MYS:H61	1.88	0.56
6:F:7:TYR:O	6:F:11:LEU:HD12	2.04	0.56
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.87	0.56
3:C:59:GLN:HB2	3:C:67:LYS:CE	2.35	0.56
15:A:309:TDS:HAJ2	2:B:76:LEU:O	2.05	0.56
2:B:96:LEU:HD13	2:B:100:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:139:VAL:HG22	4:D:147:SER:CA	2.36	0.56
3:C:46:PHE:CZ	3:C:131:VAL:CG2	2.89	0.55
4:D:108:CYS:HB2	4:D:115:VAL:CG2	2.37	0.55
1:A:112:LYS:O	1:A:115:GLU:OE1	2.25	0.55
1:A:92:MET:HE2	11:A:305:OPC:HBY1	1.87	0.55
3:C:34:VAL:HG21	3:C:151:LEU:CB	2.36	0.55
2:B:119:LYS:O	2:B:119:LYS:CG	2.55	0.55
2:B:40:PHE:HZ	15:B:201:TDS:OBD	1.90	0.54
3:C:22:CYS:HB2	10:C:302:HEM:CAB	2.37	0.54
3:C:237:VAL:HG22	3:C:237:VAL:O	2.06	0.54
2:B:91:VAL:O	2:B:91:VAL:HG12	2.07	0.54
2:B:36:LEU:O	2:B:40:PHE:HB2	2.08	0.54
3:C:15:GLU:HB3	3:C:16:PRO:CD	2.38	0.54
4:D:152:HIS:O	4:D:162:LEU:HA	2.08	0.54
4:D:13:MET:HA	4:D:16:ARG:HD3	1.90	0.53
7:G:16:ALA:O	20:G:101:BCR:H16C	2.09	0.53
3:C:46:PHE:CZ	3:C:131:VAL:HG22	2.44	0.53
1:A:100:HIS:HA	22:A:410:HOH:O	2.09	0.53
3:C:160:ILE:O	10:C:302:HEM:HMD2	2.09	0.53
3:C:19:ARG:O	3:C:20:ILE:CB	2.56	0.53
2:B:32:TRP:NE1	18:D:201:SQD:O3	2.42	0.53
4:D:152:HIS:CE1	4:D:165:TRP:CE3	2.97	0.53
6:F:11:LEU:O	6:F:15:LEU:HD12	2.08	0.53
2:B:84:VAL:CG1	2:B:101:MET:SD	2.97	0.52
10:A:303:HEM:HBA1	10:A:303:HEM:HHA	1.92	0.52
4:D:63:ASN:O	4:D:64:VAL:C	2.47	0.52
3:C:150:HIS:ND1	3:C:244:ASP:OD1	2.42	0.52
2:B:154:THR:HG23	2:B:155:LEU:N	2.24	0.52
4:D:57:LYS:HB2	4:D:82:GLN:HB2	1.91	0.52
3:C:28:ALA:HB3	3:C:239:GLY:HA2	1.92	0.52
2:B:154:THR:HG23	2:B:155:LEU:HG	1.91	0.52
3:C:282:VAL:HG12	4:D:10:VAL:HG13	1.91	0.52
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.45	0.52
4:D:48:GLY:O	4:D:49:ALA:C	2.48	0.52
5:E:18:ILE:O	5:E:22:ILE:HG22	2.10	0.52
1:A:211:ILE:HG23	1:A:212:SER:O	2.10	0.51
5:E:8:TYR:OH	6:F:15:LEU:HD23	2.09	0.51
1:A:41:LEU:HD23	10:A:304:HEM:CBC	2.40	0.51
1:A:30:VAL:HG22	1:A:34:TYR:CE1	2.46	0.51
10:A:304:HEM:HMB1	10:A:304:HEM:HBB2	1.92	0.51
2:B:151:LEU:C	2:B:151:LEU:HD13	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ILE:O	5:E:13:ALA:C	2.49	0.51
6:F:6:LEU:O	6:F:10:LEU:HB2	2.11	0.51
2:B:93:ASN:OD1	2:B:96:LEU:HB2	2.11	0.51
10:C:302:HEM:HMB2	10:C:302:HEM:HBB2	1.91	0.51
1:A:138:LEU:N	1:A:139:PRO:CD	2.73	0.50
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.46	0.50
4:D:99:ILE:HD11	4:D:155:VAL:HG23	1.94	0.50
1:A:186:ALA:HB2	12:A:306:MYS:H81	1.93	0.50
3:C:211:ILE:CG1	3:C:211:ILE:O	2.59	0.50
6:F:30:GLN:HG3	6:F:31:GLY:N	2.26	0.50
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.94	0.50
1:A:215:LEU:HD22	2:B:121:GLN:CB	2.42	0.50
1:A:111:LYS:HE2	2:B:115:GLU:O	2.12	0.50
7:G:34:GLU:O	7:G:35:LEU:HB2	2.11	0.50
1:A:24:LYS:HE2	22:A:407:HOH:O	2.11	0.49
3:C:35:GLU:HG3	3:C:49:VAL:HB	1.93	0.49
3:C:68:VAL:HG22	3:C:69:GLY:N	2.27	0.49
1:A:47:GLN:HG3	10:A:302:HEM:C3B	2.47	0.49
3:C:70:LEU:N	3:C:70:LEU:CD2	2.76	0.49
1:A:103:ARG:O	1:A:104:VAL:C	2.50	0.49
4:D:109:THR:HG22	4:D:144:ALA:HB1	1.93	0.49
7:G:10:VAL:HG12	7:G:11:LEU:N	2.26	0.49
2:B:96:LEU:HD13	2:B:100:LEU:CD1	2.42	0.49
3:C:117:GLY:HA2	3:C:119:LEU:HD12	1.94	0.49
4:D:12:ASP:O	4:D:13:MET:C	2.51	0.49
6:F:13:PHE:CE2	6:F:17:PHE:HE1	2.30	0.49
1:A:144:GLY:O	1:A:148:VAL:HG23	2.13	0.49
3:C:214:GLY:N	3:C:215:PRO:CD	2.75	0.49
3:C:9:TYR:CD1	3:C:21:VAL:HB	2.48	0.49
1:A:211:ILE:HD12	1:A:212:SER:N	2.27	0.49
14:B:202:UMQ:H6'1	18:D:201:SQD:H3	1.94	0.49
3:C:158:GLY:C	3:C:159:GLN:NE2	2.67	0.48
10:A:303:HEM:HMB1	10:A:303:HEM:HBB2	1.94	0.48
4:D:36:TYR:OH	4:D:40:LYS:HE3	2.12	0.48
5:E:12:ILE:O	5:E:14:LEU:N	2.46	0.48
5:E:24:PHE:CZ	6:F:29:ILE:HD12	2.49	0.48
3:C:60:GLN:OE1	3:C:70:LEU:HB3	2.13	0.48
4:D:143:PRO:O	4:D:145:PRO:HD3	2.14	0.48
2:B:102:ALA:O	2:B:105:PRO:HG2	2.13	0.48
3:C:19:ARG:O	3:C:242:GLN:OE1	2.32	0.48
3:C:206:THR:O	3:C:206:THR:CG2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:GLU:HG2	3:C:34:VAL:N	2.28	0.48
3:C:197:VAL:HG12	3:C:198:SER:N	2.29	0.48
3:C:270:LEU:C	3:C:270:LEU:HD13	2.33	0.48
4:D:142:GLY:HA2	4:D:144:ALA:H	1.79	0.48
7:G:34:GLU:O	7:G:35:LEU:CB	2.61	0.48
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.94	0.48
4:D:134:ASP:C	4:D:134:ASP:OD1	2.52	0.48
3:C:222:GLY:O	3:C:223:GLN:O	2.31	0.48
3:C:88:GLU:O	3:C:88:GLU:HG2	2.14	0.47
7:G:1:MET:C	7:G:2:VAL:HG22	2.35	0.47
1:A:107:THR:O	1:A:107:THR:HG23	2.13	0.47
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.95	0.47
3:C:200:GLN:HG2	3:C:201:THR:H	1.77	0.47
3:C:286:GLU:OE1	3:C:286:GLU:N	2.48	0.47
2:B:160:PHE:CD1	2:B:160:PHE:C	2.88	0.47
1:A:105:TYR:CE1	16:B:203:CLA:HBB1	2.49	0.47
3:C:266:MET:SD	8:H:13:VAL:HG12	2.54	0.47
1:A:142:GLN:HE22	2:B:67:ASP:HB3	1.80	0.47
2:B:159:LEU:O	2:B:160:PHE:CB	2.63	0.47
3:C:138:THR:OG1	3:C:139:ASP:N	2.48	0.47
6:F:25:LEU:O	6:F:29:ILE:HG23	2.15	0.47
3:C:79:PRO:HG2	3:C:82:PHE:CE1	2.50	0.47
4:D:163:THR:HG22	4:D:164:PRO:HD2	1.97	0.46
2:B:40:PHE:O	2:B:43:VAL:N	2.49	0.46
3:C:13:PRO:O	3:C:20:ILE:HA	2.15	0.46
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.44	0.46
7:G:31:ARG:N	7:G:32:PRO:HD3	2.31	0.46
3:C:259:ILE:CD1	8:H:6:LEU:HD13	2.46	0.46
4:D:139:VAL:HG22	4:D:147:SER:HA	1.96	0.46
4:D:142:GLY:HA2	4:D:144:ALA:N	2.31	0.46
4:D:78:ARG:HD2	4:D:117:TRP:CG	2.50	0.46
4:D:85:LYS:O	4:D:85:LYS:HG2	2.15	0.46
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.51	0.46
3:C:15:GLU:CB	3:C:16:PRO:CD	2.94	0.46
4:D:117:TRP:CH2	4:D:123:LYS:N	2.84	0.46
2:B:84:VAL:HG11	2:B:101:MET:SD	2.54	0.46
1:A:147:ALA:O	1:A:151:VAL:HG13	2.16	0.45
12:A:306:MYS:H101	12:A:306:MYS:C6	2.47	0.45
1:A:202:HIS:O	1:A:206:ILE:HG13	2.16	0.45
1:A:35:CYS:SG	10:A:304:HEM:C3B	3.04	0.45
2:B:128:VAL:O	2:B:132:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:101:BCR:C8	20:G:101:BCR:H321	2.36	0.45
20:G:101:BCR:H323	8:H:19:ILE:CG1	2.46	0.45
12:A:306:MYS:C10	12:A:306:MYS:H61	2.46	0.45
1:A:44:PHE:O	1:A:47:GLN:HB2	2.16	0.45
2:B:154:THR:HG23	2:B:155:LEU:H	1.81	0.45
1:A:111:LYS:NZ	2:B:120:PHE:O	2.41	0.45
7:G:2:VAL:HG23	7:G:2:VAL:O	2.16	0.45
1:A:127:ILE:CG2	1:A:195:ILE:HG13	2.47	0.45
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.52	0.45
3:C:173:THR:O	3:C:231:LEU:CD2	2.65	0.45
3:C:259:ILE:HD13	8:H:6:LEU:HD13	1.99	0.45
11:A:305:OPC:HBQ1	8:H:12:LEU:HD21	1.98	0.45
1:A:161:VAL:O	1:A:163:VAL:N	2.49	0.45
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.32	0.45
4:D:146:LEU:HD23	4:D:146:LEU:N	2.32	0.45
3:C:14:ARG:CZ	3:C:150:HIS:CD2	3.00	0.45
3:C:278:GLN:HG3	5:E:31:LEU:O	2.18	0.45
3:C:25:CYS:SG	10:C:302:HEM:C3C	3.10	0.45
3:C:60:GLN:NE2	3:C:157:ARG:HG2	2.32	0.44
3:C:93:GLU:O	3:C:97:GLU:HG3	2.17	0.44
3:C:201:THR:O	3:C:203:SER:N	2.50	0.44
3:C:49:VAL:HG13	3:C:126:GLU:HG3	1.99	0.44
3:C:274:LEU:HD11	5:E:22:ILE:HG23	1.98	0.44
1:A:24:LYS:HB3	15:B:201:TDS:HAA1	1.98	0.44
4:D:139:VAL:HG22	4:D:147:SER:N	2.32	0.44
3:C:275:LYS:HE2	4:D:20:ASN:OD1	2.18	0.44
1:A:107:THR:O	1:A:107:THR:CG2	2.65	0.44
1:A:215:LEU:HD22	2:B:121:GLN:HB2	1.98	0.44
3:C:194:LYS:O	3:C:195:TYR:C	2.56	0.44
6:F:27:LEU:HA	6:F:30:GLN:HG2	1.98	0.44
4:D:108:CYS:CB	4:D:115:VAL:HG22	2.47	0.44
12:A:306:MYS:H101	12:A:306:MYS:H41	1.99	0.44
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.18	0.44
2:B:40:PHE:CB	2:B:41:PRO:CD	2.96	0.44
3:C:9:TYR:CE1	3:C:21:VAL:HB	2.53	0.44
3:C:160:ILE:O	10:C:302:HEM:HHD	2.18	0.44
3:C:245:THR:OG1	3:C:246:GLU:N	2.50	0.44
4:D:139:VAL:HG22	4:D:146:LEU:C	2.37	0.44
2:B:109:ILE:O	2:B:112:PRO:HD2	2.17	0.43
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.80	0.43
1:A:105:TYR:CZ	16:B:203:CLA:CBB	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:GLU:OE1	3:C:19:ARG:HB3	2.18	0.43
3:C:34:VAL:CG2	3:C:151:LEU:HB2	2.43	0.43
4:D:93:VAL:HG12	4:D:97:GLU:HB3	2.00	0.43
2:B:111:VAL:N	2:B:112:PRO:CD	2.81	0.43
3:C:119:LEU:HB3	3:C:120:PRO:HD2	1.99	0.43
3:C:94:LEU:O	3:C:98:VAL:HG23	2.17	0.43
1:A:34:TYR:CZ	1:A:103:ARG:NH1	2.85	0.43
4:D:134:ASP:OD2	4:D:138:LYS:HB3	2.18	0.43
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.83	0.43
3:C:119:LEU:HD22	3:C:124:TYR:CE1	2.54	0.43
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.54	0.43
3:C:273:ILE:HG23	8:H:25:GLY:HA2	2.00	0.43
3:C:30:LYS:HB3	3:C:31:PRO:HD2	2.01	0.43
3:C:64:ASP:OD2	3:C:65:GLY:N	2.52	0.43
1:A:137:SER:HB2	1:A:148:VAL:CG2	2.48	0.43
2:B:37:LEU:HD12	15:B:201:TDS:HBB1	2.00	0.43
4:D:178:TRP:CD1	4:D:179:VAL:HB	2.54	0.43
4:D:75:ALA:HB1	4:D:95:SER:HA	2.01	0.43
4:D:80:LEU:C	4:D:81:VAL:CG2	2.86	0.43
15:A:309:TDS:HAW1	16:B:203:CLA:H93	2.00	0.43
2:B:30:PRO:O	2:B:34:ASN:HB2	2.18	0.43
4:D:108:CYS:HB3	4:D:115:VAL:HG22	2.00	0.43
4:D:174:GLU:HB2	4:D:175:LYS:H	1.68	0.43
20:G:101:BCR:C32	8:H:19:ILE:HG12	2.48	0.43
2:B:97:GLY:HA2	2:B:100:LEU:HD12	2.02	0.42
8:H:22:VAL:O	8:H:26:ARG:HG2	2.19	0.42
3:C:34:VAL:CG2	3:C:151:LEU:CB	2.96	0.42
3:C:34:VAL:CG2	3:C:151:LEU:HD22	2.47	0.42
3:C:160:ILE:O	10:C:302:HEM:HAC	2.19	0.42
5:E:23:ILE:O	5:E:27:LYS:N	2.52	0.42
1:A:83:ARG:NH1	10:A:302:HEM:CGA	2.82	0.42
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.49	0.42
4:D:115:VAL:CG1	4:D:124:PHE:HB3	2.49	0.42
3:C:229:GLU:HG3	3:C:230:ALA:CB	2.49	0.42
3:C:36:VAL:HG23	3:C:37:PRO:O	2.19	0.42
1:A:143:VAL:HG12	1:A:144:GLY:N	2.34	0.42
1:A:211:ILE:HG12	10:A:304:HEM:HMA3	2.02	0.42
1:A:47:GLN:OE1	1:A:47:GLN:HA	2.20	0.42
3:C:229:GLU:O	3:C:231:LEU:N	2.43	0.42
1:A:106:LEU:HD12	7:G:21:LEU:HD23	2.02	0.42
1:A:118:TRP:CD1	2:B:112:PRO:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:O	2:B:42:VAL:HB	2.20	0.42
4:D:108:CYS:HB2	4:D:115:VAL:HG21	2.01	0.42
1:A:12:LEU:HB2	1:A:14:ILE:CD1	2.49	0.42
2:B:117:VAL:HG23	2:B:118:ASN:N	2.34	0.42
3:C:231:LEU:HD12	3:C:231:LEU:C	2.40	0.42
3:C:255:VAL:O	3:C:259:ILE:HG13	2.19	0.42
3:C:265:VAL:O	3:C:269:GLN:HG3	2.20	0.42
10:A:303:HEM:CMB	10:A:303:HEM:HBB2	2.50	0.42
3:C:15:GLU:HB3	3:C:16:PRO:HD2	2.02	0.42
18:D:201:SQD:H162	18:D:201:SQD:H131	1.78	0.42
2:B:10:SER:O	2:B:12:PRO:HD3	2.19	0.42
3:C:194:LYS:HD3	3:C:210:THR:CG2	2.50	0.42
4:D:102:TYR:OH	4:D:136:THR:HG22	2.20	0.42
4:D:121:GLU:O	4:D:122:ASN:C	2.59	0.42
2:B:117:VAL:HG23	2:B:118:ASN:H	1.85	0.41
2:B:95:LEU:HD23	2:B:99:LEU:CD1	2.50	0.41
4:D:38:LEU:O	4:D:41:TYR:HB3	2.20	0.41
5:E:22:ILE:O	5:E:22:ILE:HG13	2.19	0.41
1:A:161:VAL:O	1:A:164:LEU:N	2.52	0.41
3:C:10:PRO:HD2	3:C:11:PRO:HD3	2.02	0.41
4:D:43:ILE:HA	4:D:44:PRO:HD3	1.93	0.41
3:C:266:MET:CE	5:E:15:PHE:CD1	3.03	0.41
1:A:112:LYS:HB3	1:A:113:PRO:CD	2.45	0.41
2:B:82:TYR:N	2:B:83:PRO:CD	2.84	0.41
6:F:13:PHE:CE2	6:F:17:PHE:CE1	3.07	0.41
1:A:215:LEU:HD22	2:B:121:GLN:HB3	2.03	0.41
10:A:304:HEM:HAB	2:B:43:VAL:HG21	2.02	0.41
2:B:37:LEU:HD23	2:B:38:TYR:CZ	2.56	0.41
7:G:21:LEU:HA	7:G:21:LEU:HD12	1.89	0.41
7:G:33:ASN:O	7:G:34:GLU:O	2.39	0.41
4:D:115:VAL:HG12	4:D:124:PHE:HB3	2.02	0.41
7:G:35:LEU:HD23	7:G:35:LEU:N	2.35	0.41
1:A:98:ILE:HD11	16:B:203:CLA:HED3	2.02	0.41
11:A:305:OPC:CBV	7:G:9:LEU:HD21	2.50	0.41
1:A:105:TYR:C	1:A:107:THR:H	2.23	0.41
1:A:121:GLY:HA3	10:A:303:HEM:C3C	2.56	0.41
1:A:207:ARG:NH1	15:B:201:TDS:HA11	2.35	0.41
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.91	0.41
3:C:176:ALA:HB1	3:C:205:LYS:NZ	2.35	0.41
3:C:288:ASN:C	3:C:288:ASN:OD1	2.58	0.41
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:THR:O	3:C:231:LEU:HD23	2.21	0.41
3:C:178:GLY:O	3:C:224:ALA:HA	2.21	0.41
3:C:229:GLU:HG3	3:C:230:ALA:HB2	2.03	0.41
3:C:206:THR:O	3:C:206:THR:HG22	2.20	0.41
1:A:15:GLN:O	1:A:16:ALA:C	2.58	0.40
2:B:58:ASP:OD2	3:C:146:LYS:CE	2.68	0.40
4:D:118:ASN:ND2	4:D:121:GLU:OE2	2.54	0.40
4:D:58:ASP:N	4:D:62:ASN:O	2.53	0.40
5:E:24:PHE:CZ	6:F:29:ILE:CD1	3.04	0.40
4:D:15:ARG:HB3	5:E:31:LEU:HD23	2.03	0.40
6:F:27:LEU:HD11	8:H:27:ASN:HA	2.03	0.40
1:A:139:PRO:HG3	10:A:302:HEM:O2A	2.22	0.40
2:B:53:ALA:O	2:B:57:LEU:HG	2.21	0.40
1:A:150:ILE:HD13	15:A:309:TDS:HAA3	2.03	0.40
1:A:92:MET:HB3	11:A:305:OPC:HCB2	2.03	0.40
7:G:26:TYR:O	7:G:28:GLN:N	2.54	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	213/215 (99%)	190 (89%)	17 (8%)	6 (3%)	6	28
2	B	158/160 (99%)	137 (87%)	21 (13%)	0	100	100
3	C	286/289 (99%)	229 (80%)	36 (13%)	21 (7%)	1	7
4	D	164/179 (92%)	135 (82%)	21 (13%)	8 (5%)	2	15
5	E	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	4	24
6	F	29/35 (83%)	26 (90%)	3 (10%)	0	100	100
7	G	35/37 (95%)	22 (63%)	6 (17%)	7 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	942/976 (96%)	791 (84%)	108 (12%)	43 (5%)	3	16

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
1	A	162	GLY
3	C	66	SER
3	C	192	ASN
3	C	201	THR
3	C	202	ASP
3	C	205	LYS
4	D	13	MET
4	D	49	ALA
4	D	64	VAL
7	G	2	VAL
7	G	32	PRO
7	G	34	GLU
3	C	20	ILE
3	C	186	GLU
3	C	223	GLN
3	C	224	ALA
3	C	227	ALA
3	C	228	GLY
3	C	230	ALA
3	C	231	LEU
4	D	122	ASN
4	D	123	LYS
7	G	10	VAL
7	G	27	GLN
1	A	3	ASN
3	C	173	THR
3	C	187	GLU
3	C	191	GLY
3	C	200	GLN
3	C	206	THR
4	D	97	GLU
4	D	145	PRO
3	C	174	ALA
3	C	212	PRO
7	G	33	ASN

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Mol	Chain	Res	Type
7	G	35	LEU
1	A	104	VAL
1	A	159	PRO
1	A	106	LEU
4	D	174	GLU
5	E	13	ALA
3	C	65	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	184/184 (100%)	164 (89%)	20 (11%)	7	29
2	B	137/137 (100%)	123 (90%)	14 (10%)	8	31
3	C	242/243 (100%)	202 (84%)	40 (16%)	2	11
4	D	139/146 (95%)	112 (81%)	27 (19%)	1	7
5	E	25/25 (100%)	22 (88%)	3 (12%)	6	23
6	F	23/27 (85%)	17 (74%)	6 (26%)	0	1
7	G	28/28 (100%)	23 (82%)	5 (18%)	2	9
8	H	24/24 (100%)	20 (83%)	4 (17%)	2	11
All	All	802/814 (98%)	683 (85%)	119 (15%)	3	15

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	12	LEU
1	A	17	LEU
1	A	36	LEU
1	A	47	GLN
1	A	61	THR
1	A	81	LEU
1	A	95	LEU

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Mol	Chain	Res	Type
1	A	103	ARG
1	A	107	THR
1	A	119	ILE
1	A	143	VAL
1	A	161	VAL
1	A	164	LEU
1	A	169	LEU
1	A	173	SER
1	A	195	ILE
1	A	200	LEU
1	A	208	LYS
1	A	211	ILE
2	B	4	LEU
2	B	13	LYS
2	B	73	LEU
2	B	74	GLU
2	B	76	LEU
2	B	88	LEU
2	B	96	LEU
2	B	108	LEU
2	B	119	LYS
2	B	134	LEU
2	B	138	LEU
2	B	140	THR
2	B	152	ASP
2	B	159	LEU
3	C	3	PHE
3	C	7	GLN
3	C	14	ARG
3	C	30	LYS
3	C	35	GLU
3	C	54	TYR
3	C	56	THR
3	C	58	LEU
3	C	60	GLN
3	C	70	LEU
3	C	80	GLU
3	C	88	GLU
3	C	94	LEU
3	C	96	LYS
3	C	116	VAL
3	C	123	GLN

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Mol	Chain	Res	Type
3	C	131	VAL
3	C	137	THR
3	C	155	ARG
3	C	167	SER
3	C	170	ASN
3	C	171	VAL
3	C	175	SER
3	C	179	THR
3	C	185	LYS
3	C	188	ASP
3	C	189	GLU
3	C	210	THR
3	C	211	ILE
3	C	216	GLU
3	C	218	ILE
3	C	219	VAL
3	C	232	THR
3	C	233	ASN
3	C	249	LEU
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	282	VAL
3	C	286	GLU
4	D	9	ASP
4	D	10	VAL
4	D	16	ARG
4	D	22	LEU
4	D	35	LEU
4	D	66	VAL
4	D	68	LYS
4	D	72	SER
4	D	77	ASP
4	D	79	VAL
4	D	84	LEU
4	D	97	GLU
4	D	101	ASP
4	D	108	CYS
4	D	109	THR
4	D	111	LEU
4	D	114	VAL
4	D	125	LYS

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Mol	Chain	Res	Type
4	D	126	CYS
4	D	131	SER
4	D	134	ASP
4	D	139	VAL
4	D	146	LEU
4	D	154	THR
4	D	167	GLU
4	D	172	THR
4	D	174	GLU
5	E	11	PHE
5	E	12	ILE
5	E	14	LEU
6	F	6	LEU
6	F	10	LEU
6	F	15	LEU
6	F	25	LEU
6	F	29	ILE
6	F	30	GLN
7	G	5	LEU
7	G	6	LEU
7	G	9	LEU
7	G	21	LEU
7	G	30	LYS
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL
8	H	26	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	60	GLN
3	C	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z > 2$
10	HEM	A	302	1	28,50,50	2.13	6 (21%)	17,82,82	1.75	3 (17%)
10	HEM	A	303	1	28,50,50	2.16	6 (21%)	17,82,82	1.52	4 (23%)
10	HEM	A	304	15,22	28,50,50	2.28	6 (21%)	17,82,82	1.44	4 (23%)
11	OPC	A	305	-	53,53,54	0.98	4 (7%)	58,61,64	1.10	3 (5%)
12	MYS	A	306	-	14,14,14	0.30	0	13,13,13	0.77	0
13	8K6	A	307	-	17,17,17	0.20	0	16,16,16	0.54	0
14	UMQ	A	308	-	35,35,35	1.25	5 (14%)	46,46,46	2.58	18 (39%)
15	TDS	A	309	-	30,31,31	0.87	1 (3%)	33,40,40	2.48	9 (27%)
15	TDS	B	201	10	30,31,31	0.87	1 (3%)	33,40,40	2.34	10 (30%)
14	UMQ	B	202	-	35,35,35	1.21	4 (11%)	46,46,46	2.80	15 (32%)
16	CLA	B	203	22	56,73,73	1.12	4 (7%)	65,113,113	1.31	11 (16%)
11	OPC	B	204	-	53,53,54	1.05	3 (5%)	58,61,64	1.03	4 (6%)
17	7PH	C	301	-	31,31,37	0.93	2 (6%)	33,33,42	1.22	3 (9%)
10	HEM	C	302	3	28,50,50	2.13	6 (21%)	17,82,82	1.59	5 (29%)
18	SQD	D	201	-	52,53,54	3.34	18 (34%)	61,63,65	2.48	15 (24%)
19	FES	D	202	4	0,4,4	0.00	-	0,4,4	0.00	-
21	OCT	F	101	-	7,7,7	0.23	0	6,6,6	0.63	0
20	BCR	G	101	-	41,41,41	2.25	22 (53%)	56,56,56	2.20	20 (35%)

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
10	HEM	A	302	1	-	0/6/54/54	0/0/8/8
10	HEM	A	303	1	-	0/6/54/54	0/0/8/8
10	HEM	A	304	15,22	-	0/6/54/54	0/0/8/8
11	OPC	A	305	-	-	0/57/57/60	0/0/0/0
12	MYS	A	306	-	-	0/12/12/12	0/0/0/0
13	8K6	A	307	-	-	0/15/15/15	0/0/0/0
14	UMQ	A	308	-	3/3/10/10	0/20/60/60	0/2/2/2
15	TDS	A	309	-	-	0/16/17/17	0/2/2/2
15	TDS	B	201	10	-	0/16/17/17	0/2/2/2
14	UMQ	B	202	-	2/2/10/10	0/20/60/60	0/2/2/2
16	CLA	B	203	22	3/3/22/25	0/37/135/135	0/0/9/9
11	OPC	B	204	-	-	0/57/57/60	0/0/0/0
17	7PH	C	301	-	-	0/33/33/39	0/0/0/0
10	HEM	C	302	3	-	0/6/54/54	0/0/8/8
18	SQD	D	201	-	2/2/9/9	0/49/65/69	0/1/1/1
19	FES	D	202	4	-	0/0/4/4	0/1/1/1
21	OCT	F	101	-	-	0/5/5/5	0/0/0/0
20	BCR	G	101	-	-	0/29/63/63	0/2/2/2

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	201	SQD	C2-C3	-11.64	1.34	1.52
18	D	201	SQD	C4-C5	-6.70	1.38	1.53
10	A	304	HEM	C3C-C2C	-5.19	1.33	1.40
18	D	201	SQD	C46-C45	-5.10	1.36	1.50
10	A	303	HEM	C3C-C2C	-4.54	1.34	1.40
10	A	304	HEM	C3B-C2B	-4.51	1.34	1.40
10	A	302	HEM	C3C-C2C	-4.40	1.34	1.40
10	A	303	HEM	C3B-C2B	-4.38	1.34	1.40
10	C	302	HEM	C3C-C2C	-4.37	1.34	1.40
10	C	302	HEM	C3B-C2B	-4.07	1.35	1.40
10	A	302	HEM	C3B-C2B	-4.06	1.35	1.40
18	D	201	SQD	C2-C1	-3.60	1.43	1.51
17	C	301	7PH	O21-C2	-3.14	1.38	1.46
18	D	201	SQD	O48-C46	-2.94	1.38	1.45
14	B	202	UMQ	O5'-C5'	-2.86	1.37	1.44
17	C	301	7PH	O31-C3	-2.83	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	201	TDS	CAH-CAP	-2.70	1.36	1.39
20	G	101	BCR	C32-C1	-2.67	1.48	1.53
14	B	202	UMQ	O3'-C3'	-2.52	1.37	1.43
15	A	309	TDS	CAH-CAP	-2.51	1.36	1.39
14	A	308	UMQ	O2'-C2'	-2.48	1.37	1.43
14	A	308	UMQ	O3'-C3'	-2.47	1.37	1.43
16	B	203	CLA	CMB-C2B	-2.44	1.46	1.51
11	A	305	OPC	OBJ-CBI	-2.41	1.39	1.45
14	A	308	UMQ	O5'-C5'	-2.40	1.38	1.44
14	B	202	UMQ	O2'-C2'	-2.38	1.37	1.43
14	A	308	UMQ	C4-C5	-2.35	1.48	1.53
20	G	101	BCR	C40-C30	-2.30	1.48	1.53
16	B	203	CLA	CMD-C2D	-2.28	1.46	1.51
14	A	308	UMQ	C3-C4	-2.21	1.46	1.52
18	D	201	SQD	O4-C4	-2.06	1.38	1.43
20	G	101	BCR	C31-C1	-2.05	1.49	1.53
20	G	101	BCR	C29-C28	-2.03	1.47	1.52
14	B	202	UMQ	C4'-C5'	-2.02	1.47	1.52
20	G	101	BCR	C39-C30	-2.01	1.49	1.53
18	D	201	SQD	C18-C17	2.00	1.63	1.51
18	D	201	SQD	O6-C1	2.04	1.47	1.40
10	A	303	HEM	C4D-ND	2.12	1.39	1.36
20	G	101	BCR	C11-C12	2.15	1.40	1.34
20	G	101	BCR	C5-C6	2.15	1.38	1.34
20	G	101	BCR	C24-C23	2.22	1.39	1.33
11	A	305	OPC	CAV-CAW	2.22	1.44	1.31
10	A	302	HEM	C4D-ND	2.25	1.39	1.36
11	A	305	OPC	OBJ-CBK	2.25	1.39	1.33
11	B	204	OPC	CAV-CAW	2.27	1.44	1.31
20	G	101	BCR	C20-C19	2.31	1.40	1.34
18	D	201	SQD	C10-C9	2.38	1.65	1.51
16	B	203	CLA	CHC-C1C	2.56	1.42	1.35
18	D	201	SQD	C9-C8	2.63	1.62	1.52
20	G	101	BCR	C8-C9	2.64	1.51	1.45
10	C	302	HEM	C4D-ND	2.70	1.40	1.36
20	G	101	BCR	C10-C9	2.72	1.39	1.35
18	D	201	SQD	O5-C5	2.94	1.51	1.44
10	A	304	HEM	C4D-ND	2.98	1.40	1.36
20	G	101	BCR	C26-C25	3.06	1.39	1.34
11	B	204	OPC	OBJ-CBK	3.08	1.42	1.33
20	G	101	BCR	C16-C17	3.14	1.53	1.43
20	G	101	BCR	C12-C13	3.15	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	101	BCR	C23-C22	3.17	1.52	1.45
20	G	101	BCR	C11-C10	3.19	1.53	1.43
20	G	101	BCR	C19-C18	3.19	1.52	1.45
20	G	101	BCR	C15-C14	3.22	1.53	1.43
20	G	101	BCR	C14-C13	3.25	1.40	1.35
11	B	204	OPC	OAN-CAO	3.26	1.43	1.34
18	D	201	SQD	C6-S	3.35	1.90	1.77
20	G	101	BCR	C20-C21	3.36	1.53	1.43
20	G	101	BCR	C21-C22	3.41	1.40	1.35
11	A	305	OPC	OAN-CAO	3.42	1.44	1.34
10	A	302	HEM	C3B-CAB	3.49	1.54	1.47
20	G	101	BCR	C17-C18	3.50	1.40	1.35
10	A	302	HEM	C3C-CAC	3.62	1.54	1.47
10	A	304	HEM	C3B-CAB	3.63	1.55	1.47
10	A	303	HEM	C3B-CAB	3.64	1.55	1.47
10	A	304	HEM	C3C-CAC	3.66	1.55	1.47
10	C	302	HEM	C3B-CAB	3.70	1.55	1.47
10	A	303	HEM	C3C-CAC	3.79	1.55	1.47
10	C	302	HEM	C3C-CAC	3.91	1.55	1.47
16	B	203	CLA	CHB-C4A	4.31	1.39	1.33
18	D	201	SQD	O47-C45	4.36	1.57	1.46
10	C	302	HEM	C3D-C2D	5.27	1.53	1.37
10	A	303	HEM	C3D-C2D	5.37	1.53	1.37
10	A	302	HEM	C3D-C2D	5.39	1.53	1.37
10	A	304	HEM	C3D-C2D	5.45	1.53	1.37
18	D	201	SQD	C3-C4	5.70	1.60	1.52
18	D	201	SQD	O47-C7	5.73	1.50	1.34
18	D	201	SQD	O5-C1	5.92	1.57	1.42
18	D	201	SQD	C8-C7	7.89	1.73	1.50
18	D	201	SQD	O6-C44	9.82	1.61	1.43

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	101	BCR	C16-C17-C18	-5.03	120.13	127.31
20	G	101	BCR	C23-C24-C25	-4.68	114.14	127.25
15	A	309	TDS	OAK-CAL-CAD	-4.43	116.71	124.17
20	G	101	BCR	C15-C14-C13	-4.41	121.02	127.31
20	G	101	BCR	C8-C7-C6	-3.72	116.84	127.25
10	A	302	HEM	CBA-CAA-C2A	-3.72	105.38	112.48
20	G	101	BCR	C20-C21-C22	-3.72	122.01	127.31
14	A	308	UMQ	O5'-C1'-C2'	-3.60	103.35	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	201	SQD	O9-S-O7	-3.52	101.64	113.86
20	G	101	BCR	C33-C5-C6	-3.50	120.59	124.51
16	B	203	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
15	B	201	TDS	OAK-CAL-CAD	-3.19	118.79	124.17
18	D	201	SQD	C5-C6-S	-3.15	109.95	114.34
20	G	101	BCR	C11-C10-C9	-3.02	123.00	127.31
14	A	308	UMQ	C1-O5-C5	-2.97	108.13	113.72
20	G	101	BCR	C34-C9-C10	-2.96	118.78	122.92
14	B	202	UMQ	C3'-C4'-C5'	-2.90	104.71	110.88
14	A	308	UMQ	C1'-O5'-C5'	-2.90	108.25	113.72
20	G	101	BCR	C38-C26-C25	-2.90	121.27	124.51
16	B	203	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
20	G	101	BCR	C4-C5-C6	-2.77	118.68	122.74
20	G	101	BCR	C7-C8-C9	-2.76	122.06	126.21
15	B	201	TDS	OAO-CAN-CAF	-2.65	118.72	121.11
16	B	203	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
10	A	302	HEM	C1D-C2D-C3D	-2.61	105.18	107.00
10	A	303	HEM	C1D-C2D-C3D	-2.61	105.18	107.00
14	B	202	UMQ	C1-O5-C5	-2.61	108.80	113.72
15	B	201	TDS	CAQ-CAP-CAH	-2.56	117.29	120.35
15	A	309	TDS	OAO-CAN-CAF	-2.51	118.86	121.11
14	B	202	UMQ	C1'-O5'-C5'	-2.50	109.00	113.72
11	B	204	OPC	OAN-CAO-OAD	-2.50	117.45	123.68
14	B	202	UMQ	C6-C5-C4	-2.49	107.17	113.00
10	C	302	HEM	CAD-CBD-CGD	-2.49	108.41	112.66
10	A	304	HEM	CBA-CAA-C2A	-2.41	107.88	112.48
16	B	203	CLA	CAA-C2A-C1A	-2.40	104.10	111.97
20	G	101	BCR	C1-C6-C5	-2.37	119.26	122.59
15	A	309	TDS	OAB-CAE-CAD	-2.34	119.61	123.49
20	G	101	BCR	C27-C26-C25	-2.33	119.33	122.74
15	B	201	TDS	CAG-CAF-CAE	-2.32	121.31	124.94
10	A	304	HEM	CAD-C3D-C2D	-2.29	122.47	129.00
10	A	303	HEM	CBD-CAD-C3D	-2.26	108.16	112.47
10	A	304	HEM	CMA-C3A-C4A	-2.25	125.01	128.46
15	B	201	TDS	OAB-CAE-CAD	-2.24	119.78	123.49
20	G	101	BCR	C20-C19-C18	-2.22	120.17	126.42
11	A	305	OPC	CBI-CAM-CAL	-2.22	106.85	111.86
20	G	101	BCR	C35-C13-C14	-2.21	119.82	122.92
10	C	302	HEM	CAA-CBA-CGA	-2.18	108.93	112.66
16	B	203	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
20	G	101	BCR	C10-C11-C12	-2.16	116.62	123.23
10	A	303	HEM	CAD-CBD-CGD	-2.15	108.98	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	302	HEM	C1D-C2D-C3D	-2.14	105.50	107.00
14	A	308	UMQ	C1-C2-C3	-2.13	106.03	109.98
17	C	301	7PH	O21-C21-O22	-2.08	118.50	123.68
10	A	304	HEM	CMB-C2B-C3B	2.03	128.66	124.89
10	C	302	HEM	CMC-C2C-C3C	2.09	128.77	124.89
14	A	308	UMQ	C6-C5-C4	2.16	118.05	113.00
16	B	203	CLA	O2D-CGD-CBD	2.17	115.17	111.30
14	A	308	UMQ	O1'-C1'-C2'	2.20	111.82	108.23
14	A	308	UMQ	C3'-C4'-C5'	2.27	115.70	110.88
11	B	204	OPC	CBI-CAM-CAL	2.30	117.03	111.86
17	C	301	7PH	O31-C31-C32	2.31	118.61	111.90
16	B	203	CLA	C9-C8-C10	2.32	119.83	111.36
16	B	203	CLA	CHB-C4A-NA	2.42	127.85	124.51
10	A	303	HEM	CMC-C2C-C3C	2.42	129.39	124.89
10	C	302	HEM	CMB-C2B-C3B	2.49	129.52	124.89
11	A	305	OPC	OBJ-CBK-CBL	2.53	119.25	111.90
15	B	201	TDS	CAE-CAF-CAN	2.57	120.50	115.03
10	A	302	HEM	CMB-C2B-C3B	2.57	129.67	124.89
16	B	203	CLA	CMD-C2D-C3D	2.61	129.74	124.89
14	A	308	UMQ	C3-C4-C5	2.62	114.83	110.22
15	A	309	TDS	CAE-CAF-CAN	2.64	120.65	115.03
16	B	203	CLA	C4A-NA-C1A	2.68	109.77	106.45
16	B	203	CLA	CMB-C2B-C3B	2.72	129.93	124.89
18	D	201	SQD	O48-C23-C24	2.78	119.99	111.90
20	G	101	BCR	C29-C30-C25	2.87	114.97	110.48
15	B	201	TDS	OAB-CAE-CAF	2.89	120.28	115.91
14	A	308	UMQ	O5'-C5'-C4'	2.91	115.70	109.75
14	A	308	UMQ	O5-C1-C2	2.96	116.01	110.30
11	B	204	OPC	OBJ-CBK-CBL	3.04	120.75	111.90
18	D	201	SQD	O8-S-C6	3.05	109.73	106.01
20	G	101	BCR	C38-C26-C27	3.14	119.41	113.45
14	A	308	UMQ	C1'-C2'-C3'	3.37	116.24	109.98
15	A	309	TDS	OAB-CAE-CAF	3.56	121.28	115.91
11	B	204	OPC	OAN-CAO-CAP	3.60	119.04	111.55
14	B	202	UMQ	O1-C4'-C3'	3.61	115.89	107.19
17	C	301	7PH	O21-C21-C22	3.65	119.12	111.55
15	A	309	TDS	CAJ-OAK-CAL	3.65	122.79	117.54
14	B	202	UMQ	O2'-C2'-C3'	3.74	118.50	110.36
14	A	308	UMQ	CA-O1'-C1'	3.79	120.37	113.87
18	D	201	SQD	O7-S-C6	3.83	110.10	106.83
20	G	101	BCR	C33-C5-C4	3.84	120.73	113.45
14	B	202	UMQ	CA-O1'-C1'	3.86	120.49	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	202	UMQ	O1-C1-O5	3.92	120.21	110.70
14	B	202	UMQ	O2'-C2'-C1'	4.02	118.44	110.03
18	D	201	SQD	O5-C1-C2	4.05	117.08	110.83
18	D	201	SQD	C44-O6-C1	4.15	122.23	113.84
18	D	201	SQD	O47-C7-C8	4.21	120.30	111.55
18	D	201	SQD	O4-C4-C5	4.40	120.38	109.28
14	A	308	UMQ	O5-C5-C6	4.60	117.43	106.41
18	D	201	SQD	O5-C5-C4	4.62	118.17	109.66
14	A	308	UMQ	O1-C1-O5	4.66	122.02	110.70
18	D	201	SQD	C2-C3-C4	4.70	116.73	110.59
20	G	101	BCR	C2-C1-C6	4.77	117.93	110.48
11	A	305	OPC	OAN-CAO-CAP	4.78	121.47	111.55
14	B	202	UMQ	C3-C4-C5	4.82	118.70	110.22
18	D	201	SQD	C1-C2-C3	4.90	119.58	111.24
14	A	308	UMQ	O2'-C2'-C3'	4.98	121.20	110.36
15	A	309	TDS	OAO-CAN-CAM	5.01	121.97	116.03
14	B	202	UMQ	O5-C5-C4	5.04	118.95	109.66
15	A	309	TDS	OAO-CAP-CAQ	5.34	118.52	111.94
18	D	201	SQD	O4-C4-C3	5.62	120.25	110.02
15	B	201	TDS	OAO-CAN-CAM	5.65	122.73	116.03
14	A	308	UMQ	O1-C1-C2	5.66	120.87	108.11
14	A	308	UMQ	O2'-C2'-C1'	5.68	121.90	110.03
14	B	202	UMQ	O2-C2-C3	5.74	122.84	110.36
15	B	201	TDS	OAK-CAL-CAM	6.06	120.49	114.49
14	B	202	UMQ	C1'-C2'-C3'	6.43	121.93	109.98
14	B	202	UMQ	O2-C2-C1	6.46	123.55	110.03
18	D	201	SQD	O9-S-C6	6.52	112.40	106.83
15	B	201	TDS	OAO-CAP-CAQ	6.85	120.38	111.94
14	A	308	UMQ	O5-C5-C4	7.61	123.68	109.66
14	B	202	UMQ	O1-C1-C2	8.08	126.31	108.11
15	A	309	TDS	OAK-CAL-CAM	8.22	122.62	114.49
18	D	201	SQD	C3-C4-C5	8.76	118.67	109.91

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	B	202	UMQ	C2'
14	B	202	UMQ	C2
16	B	203	CLA	NC
16	B	203	CLA	ND
16	B	203	CLA	NA
14	A	308	UMQ	C2'

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Mol	Chain	Res	Type	Atom
14	A	308	UMQ	C5
14	A	308	UMQ	C1
18	D	201	SQD	C4
18	D	201	SQD	C5

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	302	HEM	7	0
10	A	303	HEM	6	0
10	A	304	HEM	10	0
11	A	305	OPC	5	0
12	A	306	MYS	5	0
15	A	309	TDS	4	0
15	B	201	TDS	4	0
14	B	202	UMQ	1	0
16	B	203	CLA	5	0
11	B	204	OPC	1	0
17	C	301	7PH	1	0
10	C	302	HEM	10	0
18	D	201	SQD	3	0
19	D	202	FES	1	0
20	G	101	BCR	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	215/215 (100%)	-0.07	3 (1%) 75 56	49, 69, 105, 222	0
2	B	160/160 (100%)	-0.02	4 (2%) 58 34	61, 90, 131, 186	0
3	C	288/289 (99%)	0.18	25 (8%) 11 4	64, 100, 224, 256	1 (0%)
4	D	168/179 (93%)	0.64	23 (13%) 3 1	63, 138, 207, 236	0
5	E	32/32 (100%)	-0.02	0 100 100	86, 105, 135, 150	0
6	F	31/35 (88%)	-0.16	1 (3%) 48 25	78, 93, 150, 158	0
7	G	37/37 (100%)	0.01	1 (2%) 55 30	71, 87, 178, 205	0
8	H	29/29 (100%)	0.21	0 100 100	76, 85, 103, 141	0
All	All	960/976 (98%)	0.15	57 (5%) 23 10	49, 93, 201, 256	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	95	SER	8.6
4	D	96	LYS	7.1
4	D	50	VAL	6.1
1	A	1	MET	5.6
4	D	157	ASP	5.4
3	C	206	THR	4.8
3	C	288	ASN	4.7
3	C	207	VAL	4.7
2	B	160	PHE	4.6
3	C	203	SER	4.5
4	D	156	GLN	4.2
3	C	202	ASP	4.2
3	C	191	GLY	4.1
3	C	204	GLY	4.0
4	D	179	VAL	3.9
4	D	74	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	158	ASP	3.7
4	D	159	ASN	3.7
1	A	2	ALA	3.7
3	C	287	MET	3.6
3	C	181	THR	3.3
2	B	159	LEU	3.2
3	C	201	THR	3.2
3	C	225	VAL	3.2
4	D	70	LEU	3.2
4	D	77	ASP	3.2
4	D	49	ALA	3.1
3	C	192	ASN	3.0
3	C	226	LYS	3.0
3	C	220	SER	2.9
3	C	177	THR	2.9
3	C	176	ALA	2.9
4	D	93	VAL	2.8
4	D	69	PHE	2.8
2	B	1	MET	2.7
4	D	75	ALA	2.6
7	G	1	MET	2.6
4	D	174	GLU	2.6
4	D	62	ASN	2.5
6	F	3	GLU	2.5
4	D	162	LEU	2.4
3	C	205	LYS	2.4
4	D	141	ARG	2.4
3	C	224	ALA	2.4
4	D	71	GLU	2.3
3	C	190	TYR	2.3
3	C	182	LYS	2.3
4	D	72	SER	2.3
3	C	193	VAL	2.2
3	C	199	ILE	2.2
4	D	169	ASP	2.2
3	C	227	ALA	2.2
3	C	187	GLU	2.2
4	D	165	TRP	2.2
3	C	188	ASP	2.2
1	A	159	PRO	2.0
2	B	50	CYS	2.0

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

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

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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
18	SQD	D	201	53/54	0.61	0.61	9.23	0,163,195,201	1
21	OCT	F	101	8/8	0.71	0.53	8.96	98,124,131,132	0
13	8K6	A	307	18/18	0.67	0.37	6.13	83,115,138,142	0
12	MYS	A	306	15/15	0.83	0.34	4.78	72,101,126,129	0
17	7PH	C	301	32/38	0.70	0.46	4.72	73,108,165,198	0
14	UMQ	B	202	34/34	0.65	0.49	4.63	104,171,232,247	0
20	BCR	G	101	40/40	0.63	0.52	3.95	61,105,223,230	0
11	OPC	A	305	54/55	0.70	0.50	2.83	77,127,224,237	0
11	OPC	B	204	54/55	0.87	0.36	2.53	91,133,171,184	0
16	CLA	B	203	65/65	0.87	0.34	2.24	73,104,147,157	0
14	UMQ	A	308	34/34	0.76	0.41	1.84	108,160,202,212	0
15	TDS	A	309	30/30	0.87	0.28	0.99	90,119,165,167	0
10	HEM	A	302	43/43	0.98	0.26	0.62	44,66,93,112	0
10	HEM	C	302	43/43	0.96	0.24	0.49	71,95,139,149	0
10	HEM	A	303	43/43	0.98	0.26	0.44	49,68,84,87	0
15	TDS	B	201	30/30	0.93	0.25	0.40	73,115,141,159	0
10	HEM	A	304	43/43	0.97	0.25	0.00	61,90,109,123	0
19	FES	D	202	4/4	0.99	0.12	-1.88	80,95,101,103	0
9	CD	A	301	1/1	1.00	0.10	-	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.