



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 03:59 PM GMT

PDB ID : 2E74
Title : Crystal Structure of the Cytochrome b6f Complex from M.laminosus
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on : 2007-01-05
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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>

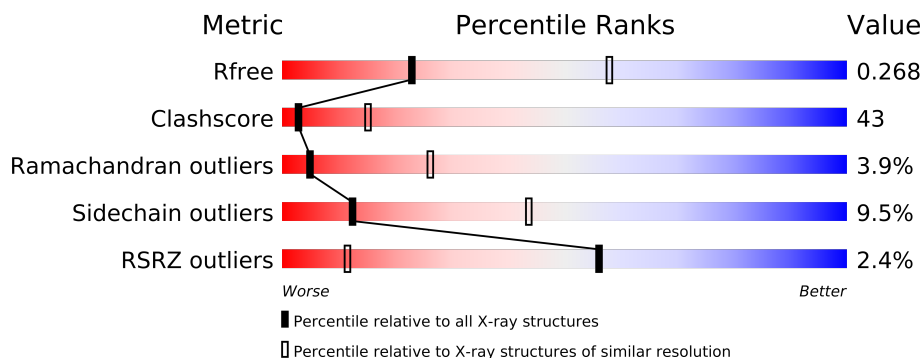
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	289	
4	D	179	
5	E	32	
6	F	35	
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
11	UMQ	A	1101	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
11	UMQ	A	1102	-	X
15	SQD	D	201	-	X
16	BCR	G	101	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 8025 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	215	Total	C	N	O	S	0	0	0
			1711	1140	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	N	O	S	0	0	0
			1249	841	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2216	1415	369	424	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1260	805	218	230	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	N	O	S	0	0	0
			248	179	34	34	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
			242	165	35	40	2			

- 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
			283	188	44	50	1			

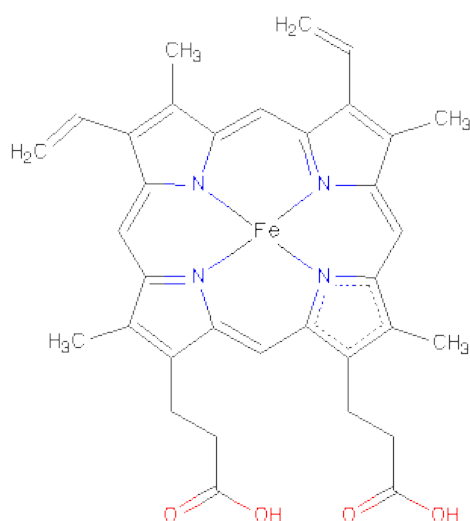
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			230	156	36	36	2			

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

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

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



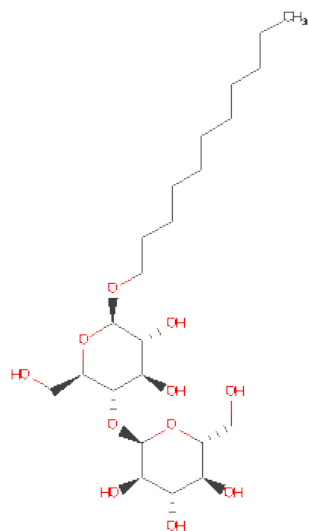
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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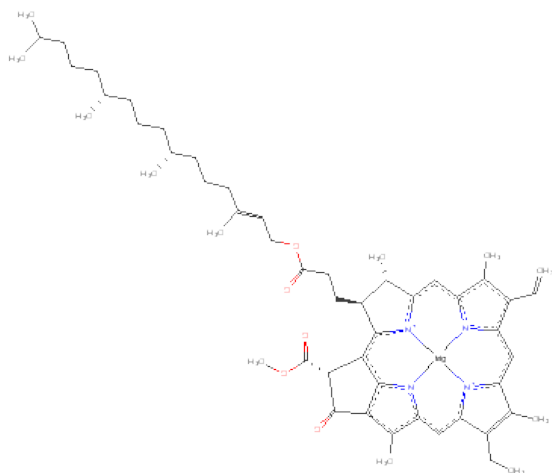
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



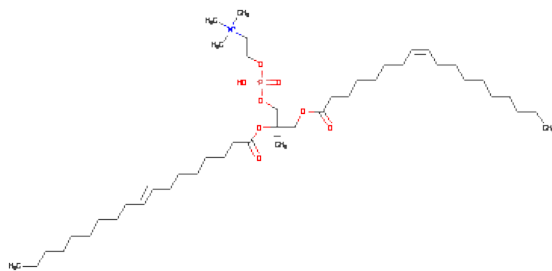
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O		
			34	23	11	0	0
11	A	1	Total	C	O		
			34	23	11	0	0
11	A	1	Total	C	O		
			34	23	11	0	0
11	A	1	Total	C	O		
			34	23	11	0	0

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



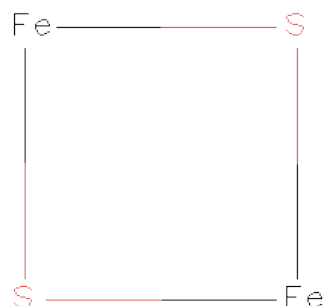
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 13 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).



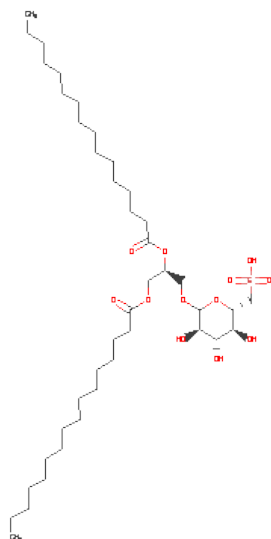
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
13	H	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



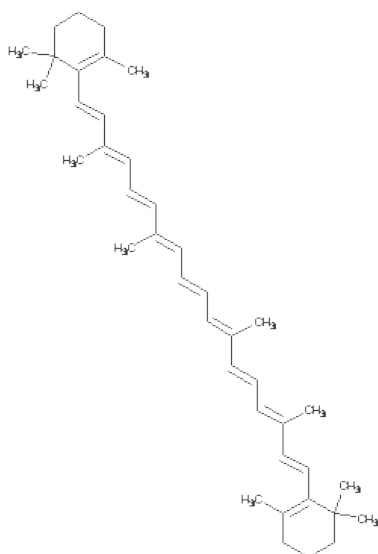
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

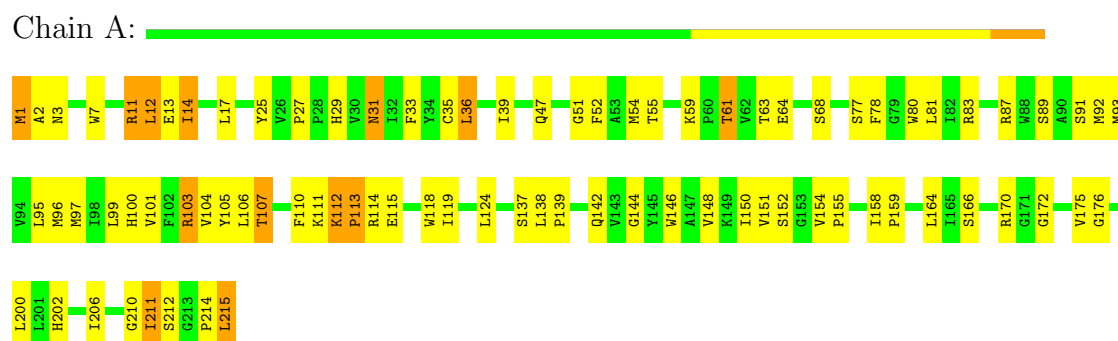
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	2	Total O 2 2	0	0
17	B	2	Total O 2 2	0	0
17	C	1	Total O 1 1	0	0

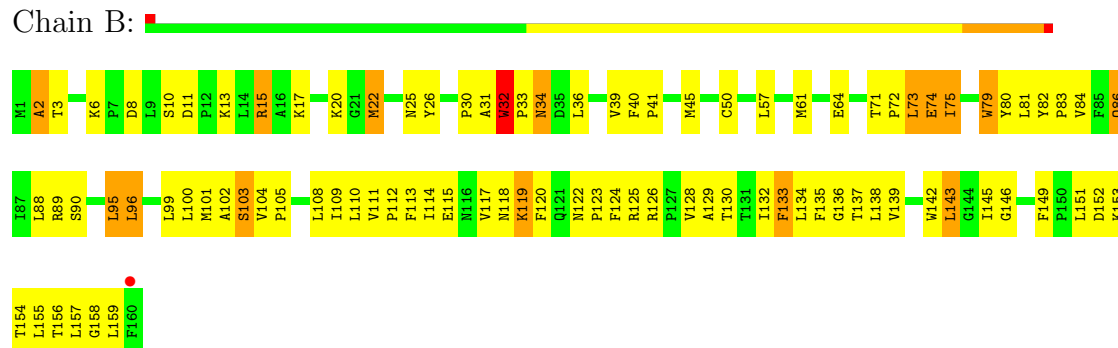
3 Residue-property plots

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.

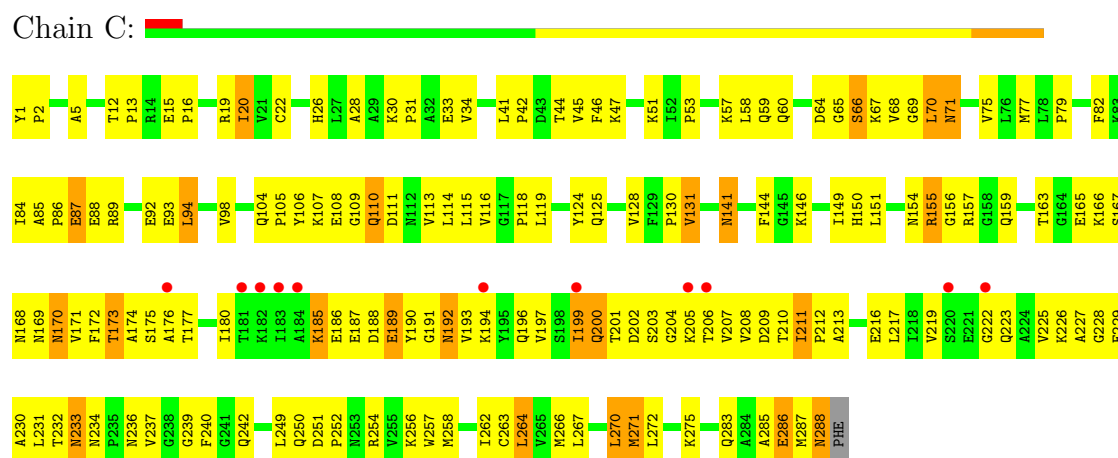
• Molecule 1: Cytochrome b6



• Molecule 2: Cytochrome b6-f complex subunit 4

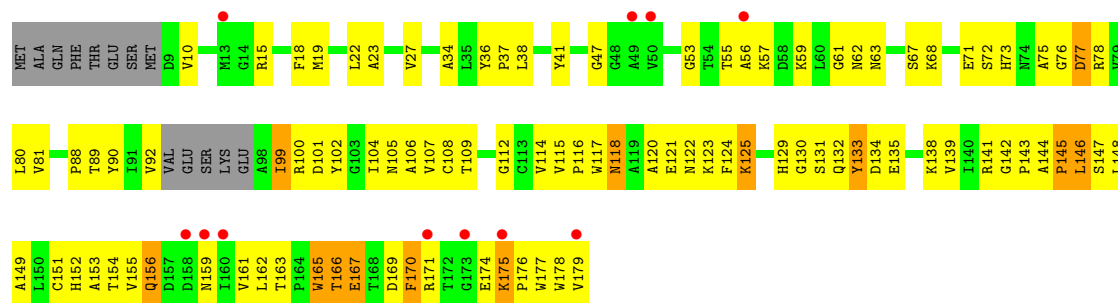


• Molecule 3: Apocytochrome f



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

Chain D:



- 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	158.34Å 158.34Å 361.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.30 – 3.00 39.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.30-3.00) 99.7 (39.27-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.268 0.221 , 0.268	Depositor DCC
R_{free} test set	2740 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 54187 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8025	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: UMQ, CLA, CD, FES, OPC, HEM, 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	0.78	1/1763 (0.1%)	0.81	1/2405 (0.0%)
2	B	0.75	0/1288	0.87	3/1765 (0.2%)
3	C	0.57	1/2264 (0.0%)	0.66	0/3082
4	D	0.45	0/1292	0.57	0/1760
5	E	0.55	0/253	0.76	0/340
6	F	0.66	0/246	0.74	0/331
7	G	0.67	0/289	0.73	0/391
8	H	0.79	0/236	0.78	0/323
All	All	0.65	2/7631 (0.0%)	0.74	4/10397 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	87	GLU	CG-CD	5.81	1.60	1.51
1	A	113	PRO	CB-CG	5.09	1.75	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	ARG	NE-CZ-NH2	-5.49	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	126	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	113	PRO	CA-N-CD	5.15	118.92	111.70
2	B	126	ARG	NE-CZ-NH1	5.13	122.86	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TRP	Peptide
8	H	27	ASN	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	1711	0	1736	138	1
2	B	1249	0	1308	135	0
3	C	2216	0	2232	199	2
4	D	1260	0	1243	121	0
5	E	248	0	284	27	0
6	F	242	0	260	27	0
7	G	283	0	289	42	1
8	H	230	0	239	21	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	129	0	90	24	0
10	C	43	0	30	8	0
11	A	136	0	164	13	0
12	B	65	0	72	4	0
13	B	54	0	83	2	0
13	H	54	0	83	24	0
14	D	4	0	0	2	0
15	D	54	0	57	12	0
16	G	40	0	52	11	0
17	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	2	0	0	0	0
17	C	1	0	0	0	0
All	All	8025	0	8222	692	2

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 43.

The worst 5 of 692 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:D:201:SQD:C4	15:D:201:SQD:C3	1.85	1.54
1:A:113:PRO:CG	1:A:113:PRO:CB	1.75	1.41
15:D:201:SQD:C2	15:D:201:SQD:C4	2.11	1.27
2:B:151:LEU:O	2:B:154:THR:HG22	1.25	1.25
2:B:151:LEU:O	2:B:154:THR:CG2	1.86	1.23

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:108:GLU:OE1	7:G:33:ASN:CB[8_565]	1.89	0.31
1:A:112:LYS:CE	3:C:87:GLU:OE1[8_665]	2.14	0.06

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	213/215 (99%)	185 (87%)	26 (12%)	2 (1%)	25	73
2	B	158/160 (99%)	126 (80%)	25 (16%)	7 (4%)	4	22
3	C	286/289 (99%)	244 (85%)	31 (11%)	11 (4%)	5	27
4	D	162/179 (90%)	124 (76%)	28 (17%)	10 (6%)	2	13
5	E	30/32 (94%)	23 (77%)	6 (20%)	1 (3%)	6	32
6	F	30/35 (86%)	25 (83%)	5 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	1
8	H	27/29 (93%)	24 (89%)	2 (7%)	1 (4%)	5	28
All	All	941/976 (96%)	767 (82%)	137 (15%)	37 (4%)	5	26

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
2	B	32	TRP
2	B	74	GLU
2	B	125	ARG
3	C	66	SER

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%)	167 (91%)	17 (9%)	13	46
2	B	137/137 (100%)	123 (90%)	14 (10%)	11	38
3	C	242/243 (100%)	222 (92%)	20 (8%)	16	52
4	D	134/146 (92%)	126 (94%)	8 (6%)	27	69
5	E	25/25 (100%)	23 (92%)	2 (8%)	17	53
6	F	24/27 (89%)	17 (71%)	7 (29%)	0	2
7	G	28/28 (100%)	25 (89%)	3 (11%)	10	35
8	H	24/24 (100%)	19 (79%)	5 (21%)	2	8
All	All	798/814 (98%)	722 (90%)	76 (10%)	12	44

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	94	LEU
3	C	249	LEU
7	G	21	LEU
3	C	131	VAL

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Mol	Chain	Res	Type
3	C	166	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	123	GLN
3	C	192	ASN
4	D	159	ASN
3	C	141	ASN
3	C	196	GLN

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
11	UMQ	A	1101	-	35,35,35	1.43	4 (11%)	46,46,46	2.33	9 (19%)
11	UMQ	A	1102	-	35,35,35	1.57	4 (11%)	46,46,46	2.40	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	UMQ	A	1103	-	35,35,35	1.46	4 (11%)	46,46,46	2.28	9 (19%)
11	UMQ	A	1104	-	35,35,35	1.38	3 (8%)	46,46,46	2.23	7 (15%)
10	HEM	A	301	1	49,50,50	2.11	10 (20%)	46,82,82	2.34	17 (36%)
10	HEM	A	302	1	49,50,50	2.56	13 (26%)	46,82,82	1.62	7 (15%)
10	HEM	A	303	1	49,50,50	2.36	14 (28%)	46,82,82	2.13	9 (19%)
12	CLA	B	201	-	73,73,73	1.99	17 (23%)	95,113,113	2.88	32 (33%)
13	OPC	B	202	-	51,53,54	1.92	14 (27%)	55,61,64	2.45	16 (29%)
10	HEM	C	301	3	49,50,50	2.24	13 (26%)	46,82,82	2.23	10 (21%)
14	FES	D	200	4	0,4,4	0.00	-	0,4,4	0.00	-
15	SQD	D	201	-	54,54,54	4.25	24 (44%)	65,65,65	4.47	26 (40%)
16	BCR	G	101	-	41,41,41	2.81	13 (31%)	56,56,56	6.85	16 (28%)
13	OPC	H	1002	-	51,53,54	2.00	14 (27%)	55,61,64	2.41	20 (36%)

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
11	UMQ	A	1101	-	2/2/10/10	0/20/60/60	0/2/2/2
11	UMQ	A	1102	-	2/2/10/10	0/20/60/60	0/2/2/2
11	UMQ	A	1103	-	2/2/10/10	0/20/60/60	0/2/2/2
11	UMQ	A	1104	-	2/2/10/10	0/20/60/60	0/2/2/2
10	HEM	A	301	1	-	0/14/114/114	0/0/8/8
10	HEM	A	302	1	-	0/14/114/114	0/0/8/8
10	HEM	A	303	1	-	0/14/114/114	0/0/8/8
12	CLA	B	201	-	1/1/20/25	0/37/135/135	0/0/9/9
13	OPC	B	202	-	-	0/55/57/60	0/0/0/0
10	HEM	C	301	3	-	0/14/114/114	0/0/8/8
14	FES	D	200	4	-	0/0/4/4	0/0/1/1
15	SQD	D	201	-	1/1/9/9	0/49/69/69	0/1/1/1
16	BCR	G	101	-	-	0/29/63/63	0/2/2/2
13	OPC	H	1002	-	-	1/55/57/60	0/0/0/0

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	201	SQD	C6-S	-17.39	1.58	1.77
15	D	201	SQD	C6-C5	-16.15	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	201	SQD	C4-C3	12.37	1.85	1.52
10	A	302	HEM	C2B-C1B	8.77	1.46	1.44
16	G	101	BCR	C8-C9	-8.64	1.26	1.45

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	101	BCR	C24-C23-C22	33.41	176.20	126.22
16	G	101	BCR	C7-C8-C9	29.30	170.05	126.22
15	D	201	SQD	C4-C3-C2	-18.44	76.74	110.82
16	G	101	BCR	C23-C24-C25	16.11	174.90	127.32
16	G	101	BCR	C8-C7-C6	15.62	173.47	127.32

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1103	UMQ	C2'
11	A	1103	UMQ	C1'
11	A	1102	UMQ	C2'
11	A	1102	UMQ	C1'
15	D	201	SQD	C5

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	H	1002	OPC	CAO-OAN-CAM-CBI

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	215/215 (100%)	-0.32	0 100 100	21, 41, 72, 160	0
2	B	160/160 (100%)	-0.27	1 (0%) 86 32	32, 57, 103, 135	0
3	C	288/289 (99%)	0.05	11 (3%) 38 7	20, 54, 114, 130	1 (0%)
4	D	166/179 (92%)	0.33	11 (6%) 18 4	38, 91, 125, 171	0
5	E	32/32 (100%)	-0.13	0 100 100	60, 75, 106, 122	0
6	F	32/35 (91%)	-0.22	0 100 100	47, 69, 124, 139	0
7	G	37/37 (100%)	-0.19	0 100 100	42, 57, 123, 131	0
8	H	29/29 (100%)	-0.15	0 100 100	40, 52, 76, 118	0
All	All	959/976 (98%)	-0.07	23 (2%) 56 11	20, 57, 115, 171	1 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	50	VAL	3.8
4	D	49	ALA	3.6
3	C	205	LYS	3.6
3	C	206	THR	3.4
3	C	184	ALA	3.2

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(Å ²)	Q<0.9
11	UMQ	A	1102	34/34	0.42	4.53	62,119,148,149	0
11	UMQ	A	1101	34/34	0.38	4.47	35,109,146,149	0
16	BCR	G	101	40/40	0.43	4.03	33,70,131,136	0
15	SQD	D	201	54/54	0.64	2.95	67,164,194,196	0
13	OPC	H	1002	54/55	0.29	1.58	41,93,187,196	0
13	OPC	B	202	54/55	0.25	1.33	48,82,157,162	0
9	CD	B	161	1/1	0.25	1.19	166,166,166,166	0
11	UMQ	A	1103	34/34	0.30	0.98	76,112,134,135	0
12	CLA	B	201	65/65	0.22	0.79	41,60,91,99	0
10	HEM	A	302	43/43	0.24	0.57	9,34,57,74	0
10	HEM	A	301	43/43	0.20	0.47	9,32,51,75	0
11	UMQ	A	1104	34/34	0.30	0.17	86,134,171,175	0
10	HEM	A	303	43/43	0.21	0.09	26,59,68,76	0
10	HEM	C	301	43/43	0.18	-0.19	29,54,89,97	0
9	CD	A	1001	1/1	0.16	-0.41	65,65,65,65	0
14	FES	D	200	4/4	0.08	-1.74	96,101,102,113	0

6.5 Other polymers ⓘ

There are no such residues in this entry.