



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 12:04 AM GMT

PDB ID : 1VF5
Title : Crystal Structure of Cytochrome b6f Complex from M.laminosus
Authors : Kurisu, G.; Zhang, H.; Smith, J.L.; Cramer, W.A.
Deposited on : 2004-04-08
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>

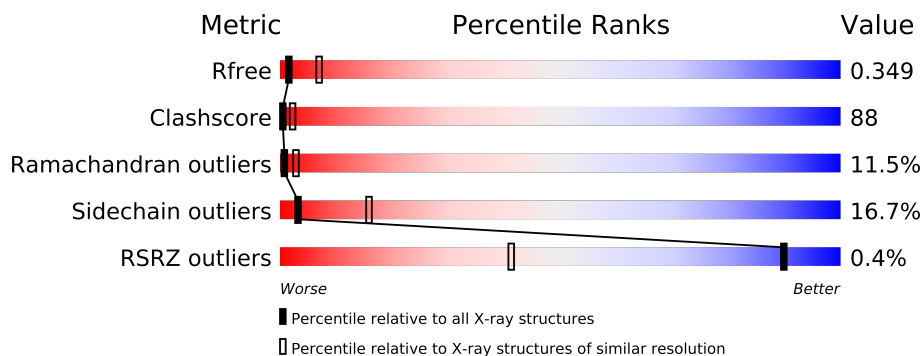
The following versions of software and data (see [references](#)) were used in the production of this report:

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.



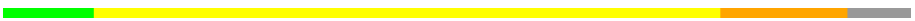
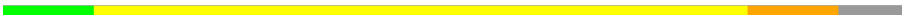
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	
1	N	215	
2	B	160	
2	O	160	
3	C	289	
3	P	289	
4	D	179	
4	Q	179	
5	E	32	
5	R	32	
6	F	35	
6	S	35	
7	G	37	
7	T	37	

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Mol	Chain	Length	Quality of chain
8	H	29	
8	U	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	TDS	N	1304	-	X
11	PL9	A	305	-	X
13	CLA	B	201	-	X
15	BCR	E	101	-	X
15	BCR	R	1101	-	X
9	HEM	A	301	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 15091 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	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			
1	N	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			

- Molecule 2 is a protein called SUBUNIT IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1075	727	165	178	5			
2	O	138	Total	C	N	O	S	0	0	0
			1075	727	165	178	5			

- Molecule 3 is a protein called CYTOCHROME F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			
3	P	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			

- Molecule 4 is a protein called RIESKE IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			
4	Q	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			

- Molecule 5 is a protein called PROTEIN PET L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			
5	R	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called PROTEIN PET M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			251	170	36	43	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

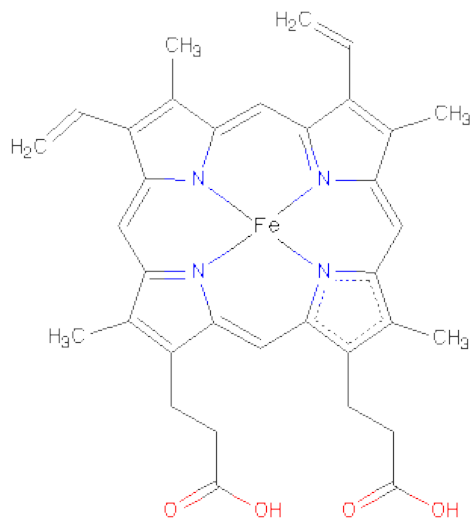
- Molecule 7 is a protein called PROTEIN PET G.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	23	Total	C	N	O	0	0	0
			184	126	29	29			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

- Molecule 8 is a protein called PROTEIN PET N.

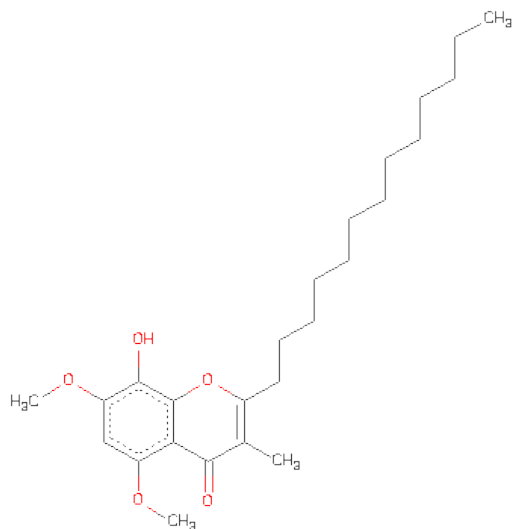
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

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



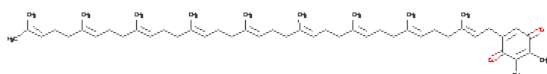
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	N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

- Molecule 10 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (three-letter code: TDS) (formula: C₂₅H₃₈O₅).



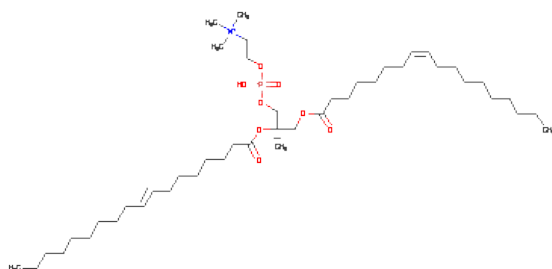
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			30	25	5		
10	N	1	Total	C	O	0	0
			30	25	5		

- Molecule 11 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



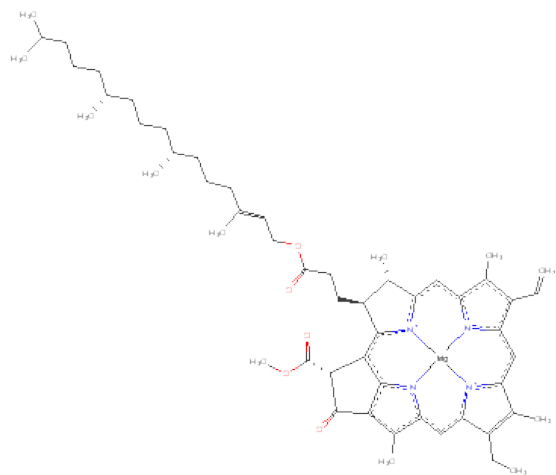
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			55	53	2		
11	Q	1	Total	C	O	0	0
			55	53	2		

- Molecule 12 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).



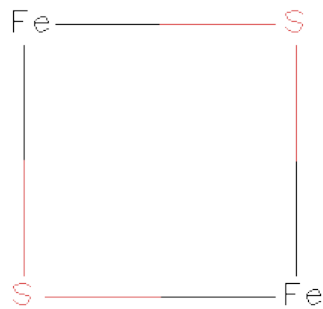
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	N	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	Q	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



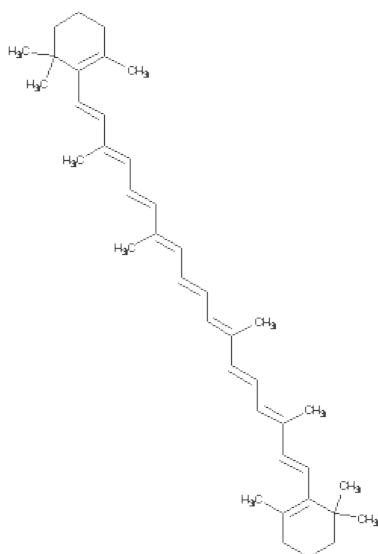
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total C 40 40	0	0
15	R	1	Total C 40 40	0	0

- Molecule 16 is water.

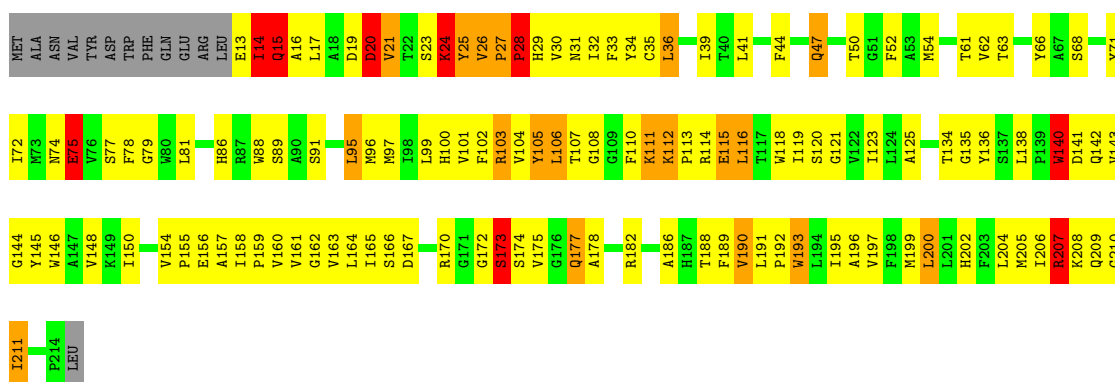
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 1 1	0	0
16	N	1	Total O 1 1	0	0

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.

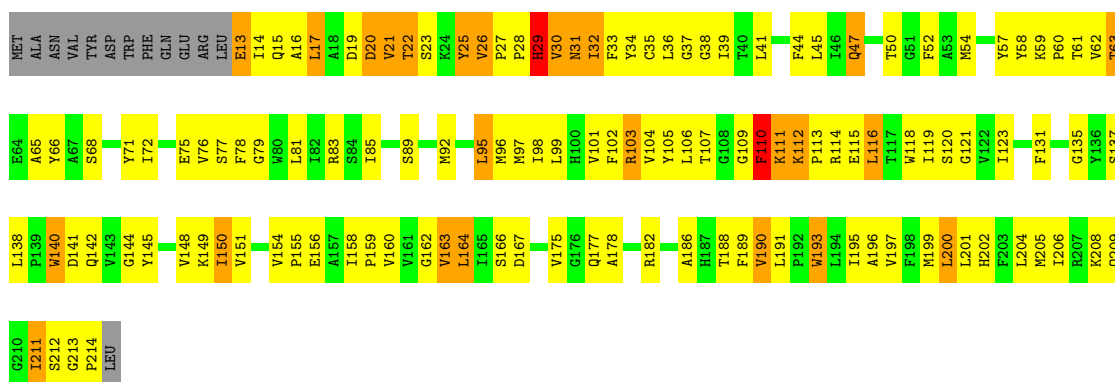
• Molecule 1: CYTOCHROME B6

Chain A:



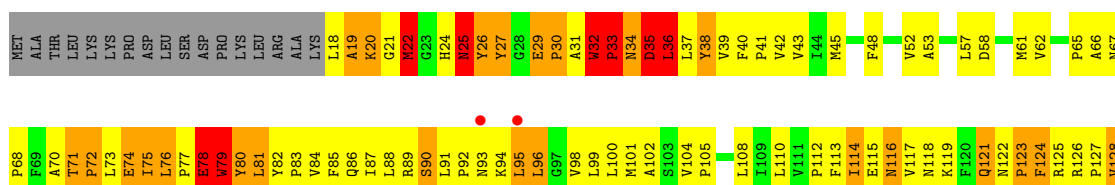
• Molecule 1: CYTOCHROME B6

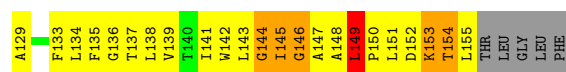
Chain N:



• Molecule 2: SUBUNIT IV

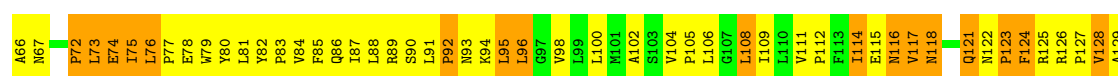
Chain B:





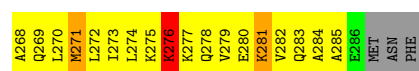
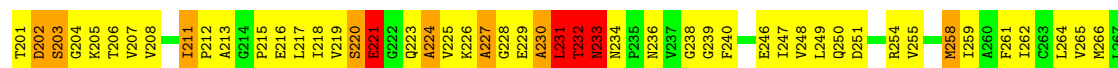
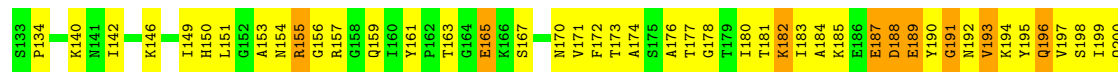
• Molecule 2: SUBUNIT IV

Chain O:



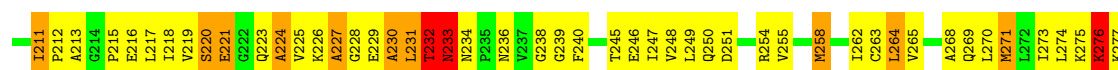
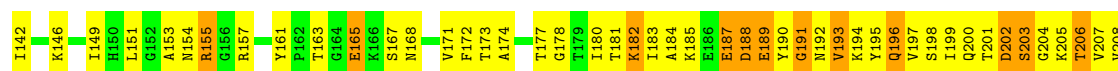
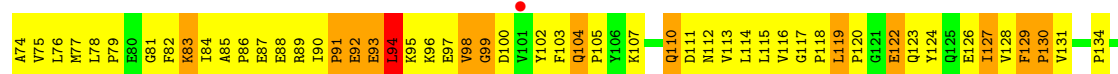
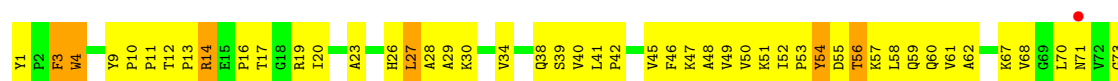
• Molecule 3: CYTOCHROME F

Chain C:



• Molecule 3: CYTOCHROME F

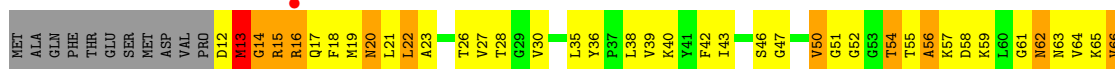
Chain P:





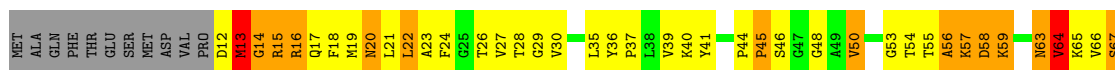
• Molecule 4: RIESKE IRON-SULFUR PROTEIN

Chain D:



• Molecule 4: RIESKE IRON-SULFUR PROTEIN

Chain Q:



• Molecule 5: PROTEIN PET L

Chain E:



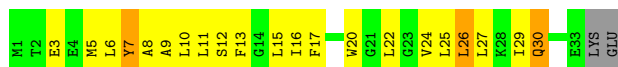
• Molecule 5: PROTEIN PET L

Chain R:



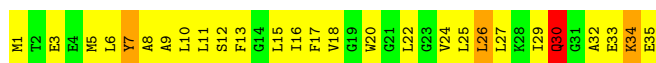
• Molecule 6: PROTEIN PET M

Chain F:



• Molecule 6: PROTEIN PET M

Chain S:



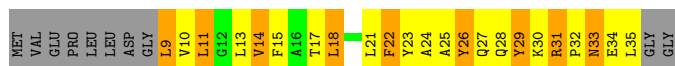
- Molecule 7: PROTEIN PET G

Chain G:



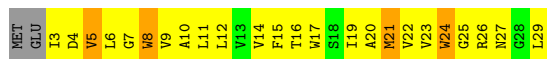
- Molecule 7: PROTEIN PET G

Chain T:



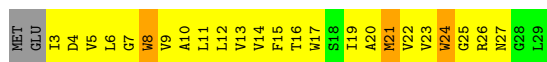
- Molecule 8: PROTEIN PET N

Chain H:



- Molecule 8: PROTEIN PET N

Chain U:



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	157.54Å 157.54Å 360.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 3.00 48.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.16-3.00) 99.8 (48.16-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.346 0.259 , 0.349	Depositor DCC
R_{free} test set	2788 reflections (2.85%)	DCC
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 110.1	EDS
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 100543 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15091	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: CLA, PL9, FES, OPC, TDS, HEM, BCR

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	0.55	0/1641	0.77	2/2239 (0.1%)
1	N	0.56	0/1641	0.81	2/2239 (0.1%)
2	B	0.54	0/1110	0.88	3/1526 (0.2%)
2	O	0.58	0/1110	0.99	8/1526 (0.5%)
3	C	0.44	0/2248	0.73	1/3061 (0.0%)
3	P	0.45	0/2248	0.72	0/3061
4	D	0.47	0/1312	0.86	2/1786 (0.1%)
4	Q	0.47	0/1312	0.76	0/1786
5	E	0.67	0/253	0.80	0/340
5	R	0.64	0/253	0.77	0/340
6	F	0.58	0/255	0.66	0/343
6	S	0.52	0/274	0.61	0/366
7	G	0.64	0/188	0.91	0/253
7	T	0.63	0/221	0.95	0/299
8	H	0.61	0/220	0.83	1/301 (0.3%)
8	U	0.59	0/220	0.81	0/301
All	All	0.52	0/14506	0.80	19/19767 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	63	GLY	N-CA-C	7.67	132.29	113.10
2	B	36	LEU	N-CA-C	-7.09	91.85	111.00
2	O	64	GLU	N-CA-C	6.99	129.88	111.00
2	O	36	LEU	N-CA-C	-6.86	92.47	111.00
1	N	20	ASP	N-CA-C	6.33	128.08	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	105	TYR	Sidechain

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	1593	0	1623	242	0
1	N	1593	0	1623	230	0
2	B	1075	0	1117	258	0
2	O	1075	0	1117	284	0
3	C	2200	0	2216	355	0
3	P	2200	0	2216	338	0
4	D	1280	0	1263	317	0
4	Q	1280	0	1263	380	0
5	E	248	0	284	72	0
5	R	248	0	284	113	0
6	F	251	0	266	39	0
6	S	270	0	285	42	0
7	G	184	0	190	104	0
7	T	216	0	220	70	0
8	H	214	0	221	42	0
8	U	214	0	221	43	0
9	A	129	0	90	18	0
9	C	43	0	30	0	0
9	N	129	0	90	17	0
9	P	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	30	0	37	13	0
10	N	30	0	37	12	0
11	A	55	0	80	18	0
11	Q	55	0	80	23	0
12	B	54	0	83	14	0
12	D	54	0	83	24	0
12	N	54	0	83	10	0
12	Q	54	0	83	30	0
13	B	65	0	70	8	0
13	O	65	0	70	20	0
14	D	4	0	0	1	0
14	Q	4	0	0	1	0
15	E	40	0	56	7	0
15	R	40	0	56	7	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
All	All	15091	0	15467	2688	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 88.

The worst 5 of 2688 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:38:TYR:HB3	3:P:276:LYS:HG2	1.22	1.20
1:A:14:ILE:HA	1:A:17:LEU:HB2	1.26	1.18
1:N:214:PRO:HB3	5:R:29:ILE:HG22	1.19	1.17
4:D:166:THR:HA	4:D:179:VAL:HG13	1.22	1.17
2:B:71:THR:HB	2:B:72:PRO:HD3	1.28	1.15

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	200/215 (93%)	152 (76%)	29 (14%)	19 (10%)	1	4
1	N	200/215 (93%)	155 (78%)	32 (16%)	13 (6%)	2	11
2	B	136/160 (85%)	80 (59%)	31 (23%)	25 (18%)	0	1
2	O	136/160 (85%)	67 (49%)	38 (28%)	31 (23%)	0	0
3	C	284/289 (98%)	206 (72%)	47 (16%)	31 (11%)	1	3
3	P	284/289 (98%)	213 (75%)	44 (16%)	27 (10%)	1	4
4	D	166/179 (93%)	123 (74%)	25 (15%)	18 (11%)	1	3
4	Q	166/179 (93%)	85 (51%)	49 (30%)	32 (19%)	0	0
5	E	30/32 (94%)	22 (73%)	6 (20%)	2 (7%)	2	10
5	R	30/32 (94%)	23 (77%)	5 (17%)	2 (7%)	2	10
6	F	31/35 (89%)	25 (81%)	5 (16%)	1 (3%)	6	33
6	S	33/35 (94%)	25 (76%)	5 (15%)	3 (9%)	1	5
7	G	21/37 (57%)	15 (71%)	5 (24%)	1 (5%)	4	20
7	T	25/37 (68%)	18 (72%)	6 (24%)	1 (4%)	5	25
8	H	25/29 (86%)	18 (72%)	7 (28%)	0	100	100
8	U	25/29 (86%)	19 (76%)	6 (24%)	0	100	100
All	All	1792/1952 (92%)	1246 (70%)	340 (19%)	206 (12%)	1	3

5 of 206 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	TYR
1	A	28	PRO
1	A	111	LYS
1	A	160	VAL
1	A	173	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	172/184 (94%)	147 (86%)	25 (14%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	172/184 (94%)	153 (89%)	19 (11%)	9	34
2	B	117/136 (86%)	93 (80%)	24 (20%)	2	9
2	O	117/136 (86%)	98 (84%)	19 (16%)	3	17
3	C	240/243 (99%)	207 (86%)	33 (14%)	5	24
3	P	240/243 (99%)	206 (86%)	34 (14%)	5	22
4	D	136/146 (93%)	113 (83%)	23 (17%)	3	15
4	Q	136/146 (93%)	113 (83%)	23 (17%)	3	15
5	E	25/25 (100%)	15 (60%)	10 (40%)	0	0
5	R	25/25 (100%)	14 (56%)	11 (44%)	0	0
6	F	25/27 (93%)	22 (88%)	3 (12%)	7	30
6	S	27/27 (100%)	23 (85%)	4 (15%)	4	21
7	G	17/28 (61%)	9 (53%)	8 (47%)	0	0
7	T	21/28 (75%)	12 (57%)	9 (43%)	0	0
8	H	22/24 (92%)	18 (82%)	4 (18%)	2	13
8	U	22/24 (92%)	18 (82%)	4 (18%)	2	13
All	All	1514/1626 (93%)	1261 (83%)	253 (17%)	3	16

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	30	LYS
1	N	116	LEU
5	R	27	LYS
6	F	30	GLN
8	H	21	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	152	HIS
1	N	209	GLN
4	Q	122	ASN
8	H	27	ASN
2	O	86	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 ⓘ

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	HEM	A	301	1	49,50,50	3.94	15 (30%)	46,82,82	1.60	10 (21%)
9	HEM	A	302	1	49,50,50	3.38	16 (32%)	46,82,82	2.86	11 (23%)
9	HEM	A	303	1,16	49,50,50	4.10	16 (32%)	46,82,82	2.21	14 (30%)
10	TDS	A	304	-	31,31,31	2.60	6 (19%)	38,40,40	4.54	12 (31%)
11	PL9	A	305	-	55,55,55	3.53	21 (38%)	69,69,69	2.45	21 (30%)
13	CLA	B	201	-	73,73,73	1.74	14 (19%)	95,113,113	2.18	23 (24%)
12	OPC	B	307	-	51,53,54	1.37	6 (11%)	55,61,64	1.06	6 (10%)
9	HEM	C	301	3	49,50,50	2.93	17 (34%)	46,82,82	1.49	9 (19%)
14	FES	D	200	4	0,4,4	0.00	-	0,4,4	0.00	-
12	OPC	D	306	-	51,53,54	1.38	6 (11%)	55,61,64	1.14	4 (7%)
15	BCR	E	101	-	41,41,41	2.09	8 (19%)	56,56,56	2.44	23 (41%)
10	TDS	N	1304	-	31,31,31	2.58	6 (19%)	38,40,40	4.27	13 (34%)
12	OPC	N	1306	-	51,53,54	1.37	6 (11%)	55,61,64	1.27	8 (14%)
9	HEM	N	301	1	49,50,50	3.32	17 (34%)	46,82,82	1.67	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEM	N	302	1	49,50,50	2.95	17 (34%)	46,82,82	2.88	13 (28%)
9	HEM	N	303	1,16	49,50,50	4.25	19 (38%)	46,82,82	1.82	8 (17%)
13	CLA	O	1201	-	73,73,73	1.76	13 (17%)	95,113,113	2.23	22 (23%)
9	HEM	P	301	3	49,50,50	3.36	19 (38%)	46,82,82	1.49	7 (15%)
14	FES	Q	1200	4	0,4,4	0.00	-	0,4,4	0.00	-
11	PL9	Q	1305	-	55,55,55	3.52	21 (38%)	69,69,69	2.56	22 (31%)
12	OPC	Q	1307	-	51,53,54	1.37	6 (11%)	55,61,64	1.11	5 (9%)
15	BCR	R	1101	-	41,41,41	2.03	8 (19%)	56,56,56	2.45	22 (39%)

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	1,16	-	0/14/114/114	0/0/8/8
10	TDS	A	304	-	-	0/16/17/17	0/0/2/2
11	PL9	A	305	-	-	1/53/73/73	0/1/1/1
13	CLA	B	201	-	2/2/20/25	0/37/135/135	0/0/9/9
12	OPC	B	307	-	-	2/55/57/60	0/0/0/0
9	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
12	OPC	D	306	-	-	3/55/57/60	0/0/0/0
15	BCR	E	101	-	-	0/29/63/63	0/2/2/2
10	TDS	N	1304	-	-	0/16/17/17	0/0/2/2
12	OPC	N	1306	-	-	3/55/57/60	0/0/0/0
9	HEM	N	301	1	-	0/14/114/114	0/0/8/8
9	HEM	N	302	1	-	0/14/114/114	0/0/8/8
9	HEM	N	303	1,16	-	0/14/114/114	0/0/8/8
13	CLA	O	1201	-	3/3/20/25	0/37/135/135	0/0/9/9
9	HEM	P	301	3	-	0/14/114/114	0/0/8/8
14	FES	Q	1200	4	-	0/0/4/4	0/0/1/1
11	PL9	Q	1305	-	-	1/53/73/73	0/1/1/1
12	OPC	Q	1307	-	-	2/55/57/60	0/0/0/0
15	BCR	R	1101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	C2D-C1D	22.13	1.50	1.44
9	A	302	HEM	C2D-C1D	18.41	1.49	1.44
9	N	303	HEM	C2D-C1D	17.62	1.49	1.44
9	N	301	HEM	C2D-C1D	17.05	1.48	1.44
9	A	303	HEM	C2D-C1D	15.67	1.48	1.44

The worst 5 of 262 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	304	TDS	CAP-OAO-CAN	-21.65	115.01	122.07
10	N	1304	TDS	CAP-OAO-CAN	-18.60	116.01	122.07
9	N	302	HEM	CBA-CAA-C2A	-15.21	85.90	112.69
9	A	302	HEM	CBA-CAA-C2A	-14.90	86.43	112.69
10	N	1304	TDS	OAO-CAP-CAQ	11.80	117.17	110.58

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	201	CLA	C8
13	B	201	CLA	C3A
13	O	1201	CLA	C8
13	O	1201	CLA	C2A
13	O	1201	CLA	C3A

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	Q	1307	OPC	CAM-OAN-CAO-CAP
12	Q	1307	OPC	CAM-OAN-CAO-OAD
12	B	307	OPC	CAM-OAN-CAO-OAD
12	B	307	OPC	CAM-OAN-CAO-CAP
12	D	306	OPC	CAM-OAN-CAO-CAP

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	202/215 (93%)	-0.13	0	100	100	22, 55, 101, 174	0
1	N	202/215 (93%)	-0.14	0	100	100	19, 53, 86, 121	0
2	B	138/160 (86%)	-0.16	2 (1%)	72	18	24, 65, 122, 194	0
2	O	138/160 (86%)	-0.11	0	100	100	28, 62, 139, 184	0
3	C	286/289 (98%)	-0.08	2 (0%)	84	28	5, 82, 153, 200	1 (0%)
3	P	286/289 (98%)	-0.02	2 (0%)	84	28	14, 85, 154, 200	1 (0%)
4	D	168/179 (93%)	-0.04	2 (1%)	75	20	36, 117, 179, 200	0
4	Q	168/179 (93%)	-0.09	0	100	100	33, 109, 165, 192	0
5	E	32/32 (100%)	0.10	0	100	100	30, 76, 149, 177	0
5	R	32/32 (100%)	0.13	0	100	100	37, 81, 149, 171	0
6	F	33/35 (94%)	-0.08	0	100	100	39, 63, 140, 177	0
6	S	35/35 (100%)	-0.13	0	100	100	41, 78, 152, 167	0
7	G	23/37 (62%)	0.01	0	100	100	33, 71, 128, 171	0
7	T	27/37 (72%)	-0.07	0	100	100	37, 65, 100, 152	0
8	H	27/29 (93%)	-0.11	0	100	100	33, 71, 130, 165	0
8	U	27/29 (93%)	-0.08	0	100	100	46, 81, 152, 157	0
All	All	1824/1952 (93%)	-0.08	8 (0%)	90	41	5, 74, 155, 200	2 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	117	GLY	3.2
2	B	93	ASN	2.5
4	D	16	ARG	2.4
3	P	101	VAL	2.3
3	P	71	ASN	2.2

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
10	TDS	N	1304	30/30	0.45	3.75	80,80,80,80	0
11	PL9	A	305	55/55	0.41	3.47	98,98,98,98	0
15	BCR	R	1101	40/40	0.56	3.46	91,91,91,91	0
15	BCR	E	101	40/40	0.47	3.16	77,77,77,77	0
9	HEM	A	301	43/43	0.28	2.33	45,45,45,45	0
13	CLA	B	201	65/65	0.28	2.19	45,56,56,56	0
9	HEM	N	302	43/43	0.28	1.91	48,56,56,56	0
12	OPC	N	1306	54/55	0.32	1.87	87,87,87,87	0
9	HEM	N	301	43/43	0.28	1.83	41,50,50,50	0
9	HEM	A	302	43/43	0.29	1.67	62,62,62,62	0
11	PL9	Q	1305	55/55	0.29	1.31	85,85,85,85	0
10	TDS	A	304	30/30	0.34	1.26	52,52,52,52	0
13	CLA	O	1201	65/65	0.27	1.05	22,72,72,72	0
12	OPC	D	306	54/55	0.29	1.04	86,86,86,86	0
9	HEM	A	303	43/43	0.25	0.40	55,81,81,81	0
9	HEM	C	301	43/43	0.26	0.11	62,83,83,83	0
12	OPC	B	307	54/55	0.24	0.10	84,84,84,84	0
9	HEM	N	303	43/43	0.22	-0.19	61,61,61,64	0
9	HEM	P	301	43/43	0.24	-0.26	47,56,56,56	0
12	OPC	Q	1307	54/55	0.20	-0.69	72,72,72,72	0
14	FES	Q	1200	4/4	0.15	-0.92	94,94,98,98	0
14	FES	D	200	4/4	0.10	-1.56	144,144,170,170	0

6.5 Other polymers ⓘ

There are no such residues in this entry.