



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 11:22 PM EDT

PDB ID : 1P84
Title : HDBT inhibited Yeast Cytochrome bc1 Complex
Authors : Palsdottir, H.; Lojero, C.G.; Trumpower, B.L.; Hunte, C.
Deposited on : unknown
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure 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/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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

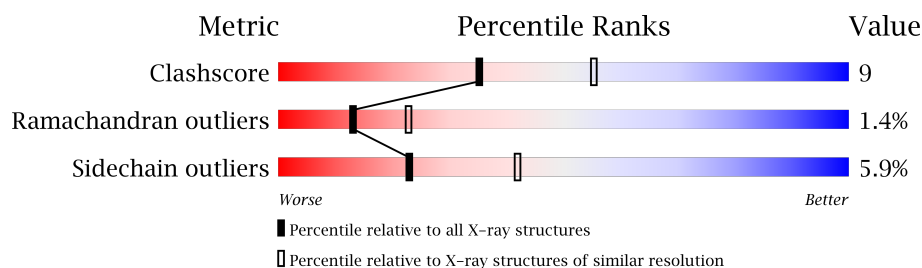
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	352	
3	C	385	
4	D	246	
5	E	185	
6	F	74	
7	G	125	

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Mol	Chain	Length	Quality of chain
8	H	93	<div><div></div><div>85%</div><div>13%</div><div></div></div>
9	I	55	<div><div></div><div>85%</div><div>11%</div><div></div></div>
10	J	127	<div><div></div><div>69%</div><div>26%</div><div>5%</div></div>
11	K	107	<div><div></div><div>60%</div><div>35%</div><div>6%</div></div>

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 18069 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquinol-cytochrome C reductase complex core protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	CONFLICT	UNP P07256

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	THR	ILE	CONFLICT	UNP P00163

- Molecule 4 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	246	Total	C	N	O	S	0	0	0
			1941	1237	334	361	9			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 17 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase complex 7.3 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			449	298	75	76			

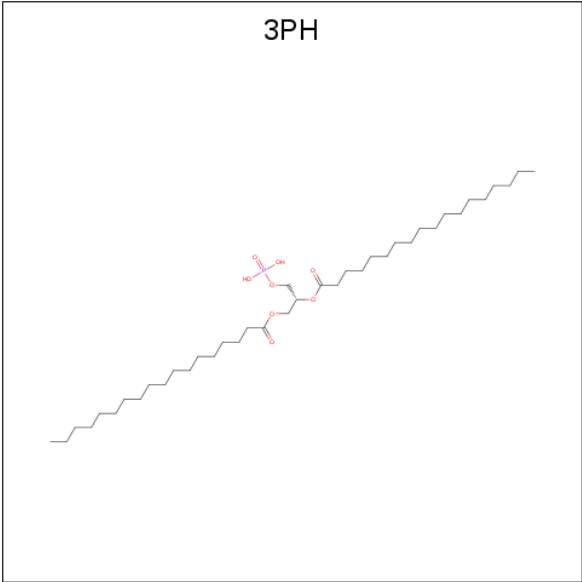
- Molecule 10 is a protein called Heavy Chain (Vh) Of Fv-Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Light Chain (Vl) Of Fv-Fragment.

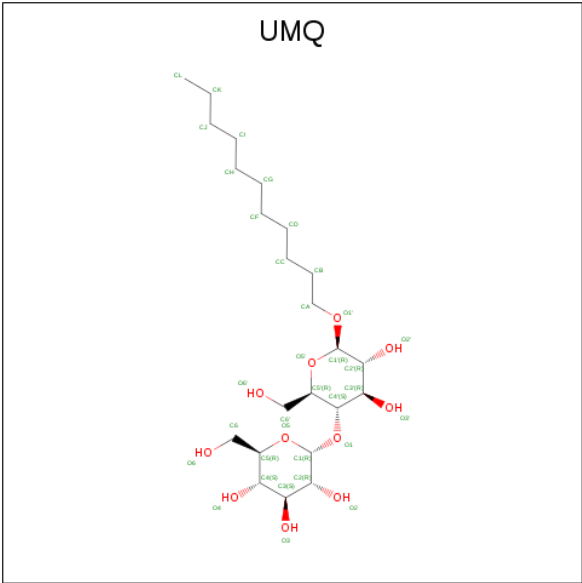
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			40	31	8	1		
12	D	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 13 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



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

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

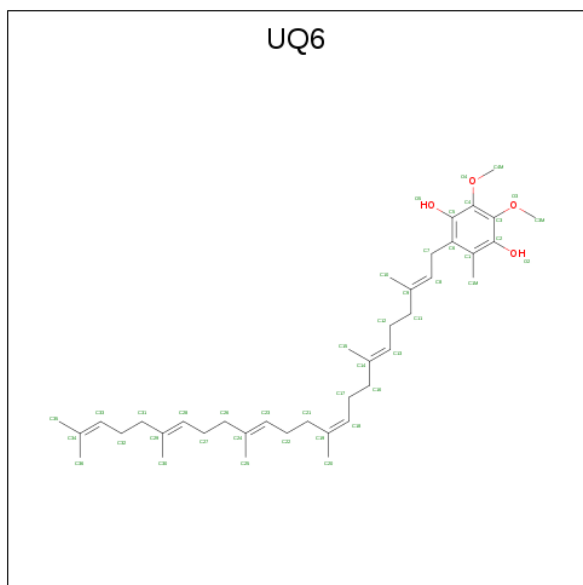
HEM

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

-
- Chemical structure of DBT (Dibenzothiophene) with atom labels. The structure shows a benzothienyl core with a butyl chain. Atoms are labeled: O6 (hydroxyl oxygen), O7 (carbonyl oxygen), O4 (carbonyl oxygen), S1 (sulfur), N3 (nitrogen), C2, C4A, C7A, C6, C5, C8, C9, C10, C11, C12, C13, C14. The butyl chain is attached at C8.

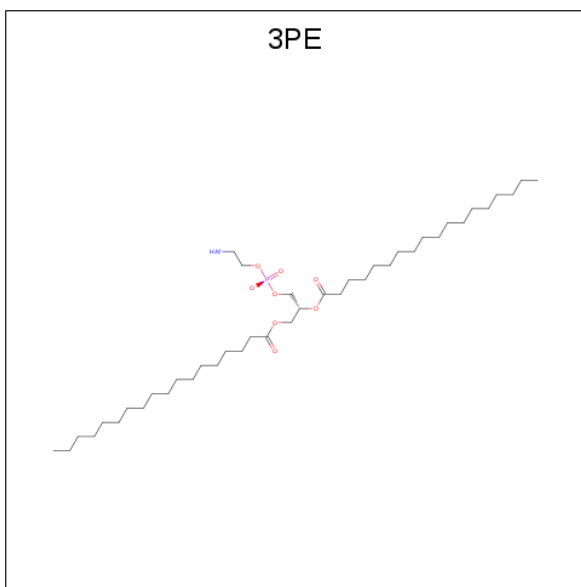
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			19	14	1	3	1		

- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: C₃₉H₆₀O₄).



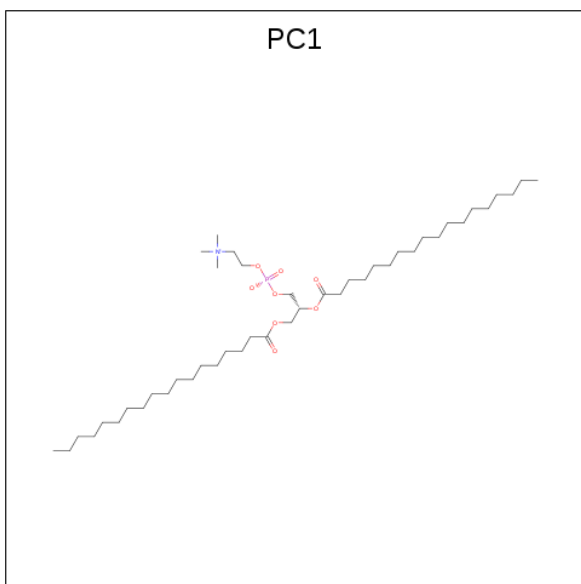
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



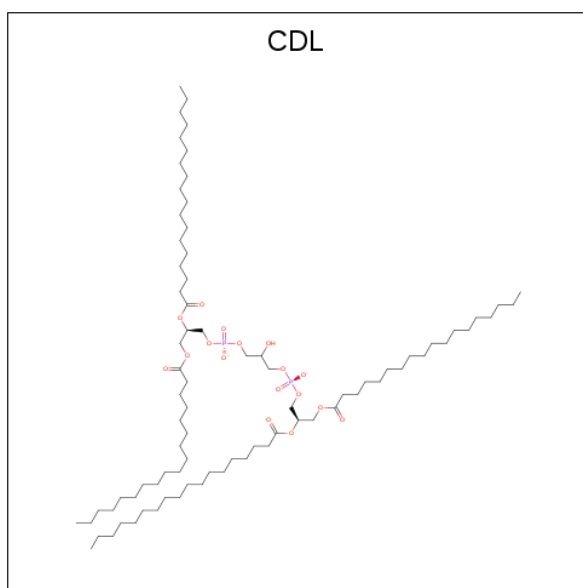
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



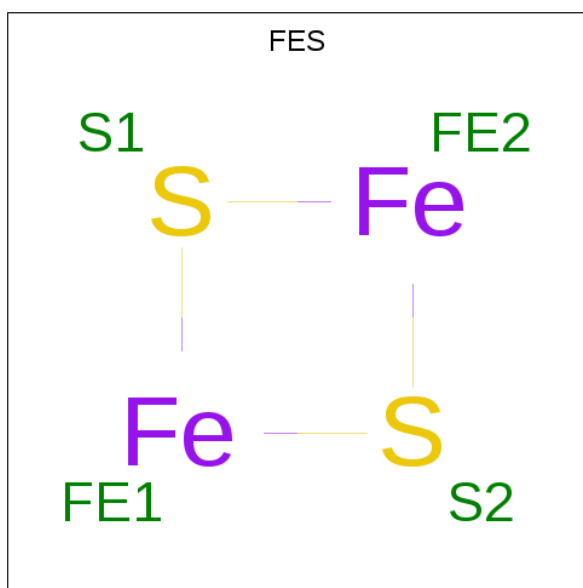
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			76	57	17	2		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

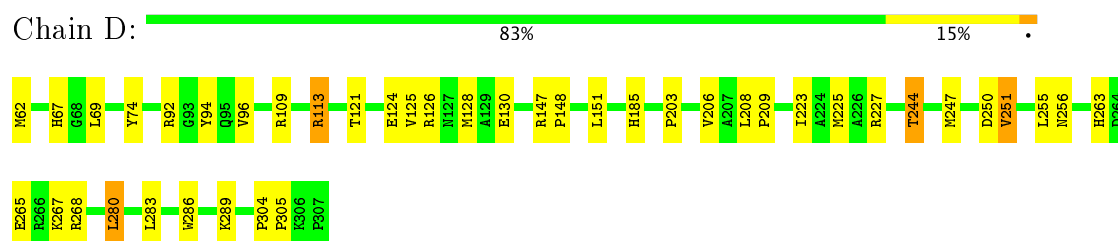


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	E	1	Total	Fe	S	0	0
			4	2	2		

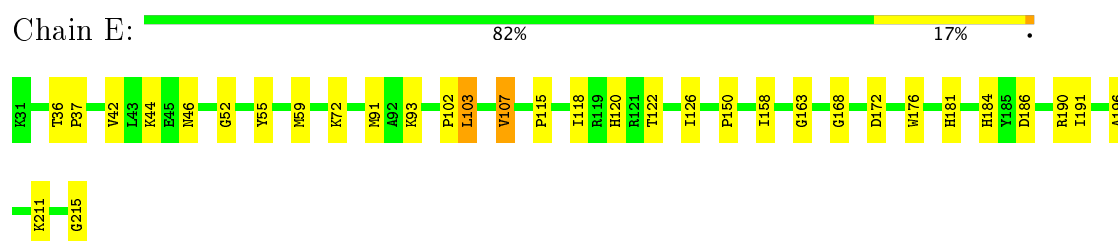
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	55	Total 55	O 55	0	0
21	B	11	Total 11	O 11	0	0
21	C	110	Total 110	O 110	0	0
21	D	62	Total 62	O 62	0	0
21	E	25	Total 25	O 25	0	0
21	F	4	Total 4	O 4	0	0
21	G	32	Total 32	O 32	0	0
21	H	20	Total 20	O 20	0	0
21	I	2	Total 2	O 2	0	0
21	J	3	Total 3	O 3	0	0
21	K	2	Total 2	O 2	0	0

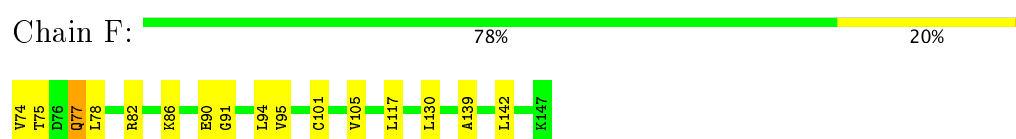
- Molecule 4: Cytochrome c1, heme protein



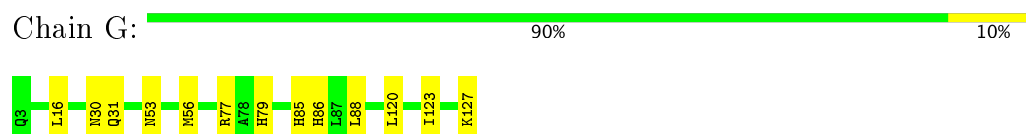
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit



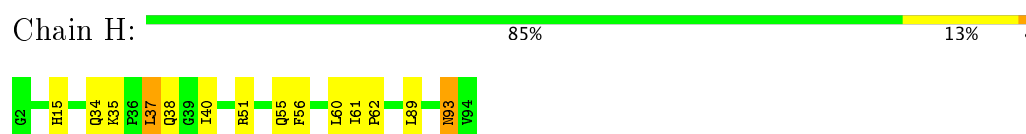
- Molecule 6: Ubiquinol-cytochrome C reductase complex 17 kDa protein



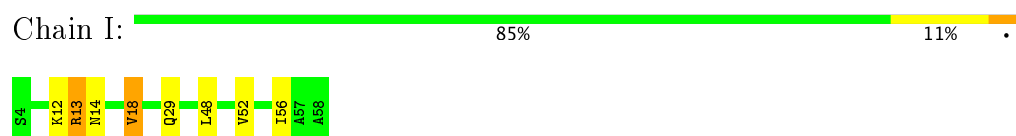
- Molecule 7: Ubiquinol-cytochrome C reductase complex 14 kDa protein



- Molecule 8: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

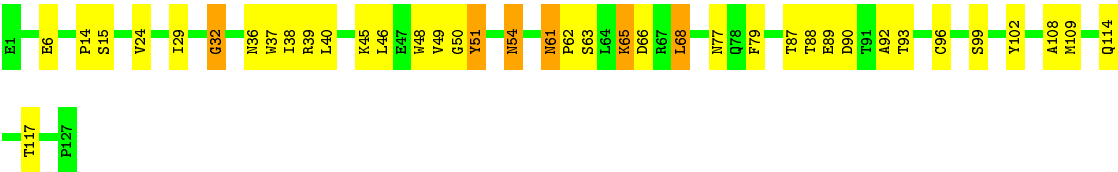


- Molecule 9: Ubiquinol-cytochrome C reductase complex 7.3 kDa protein

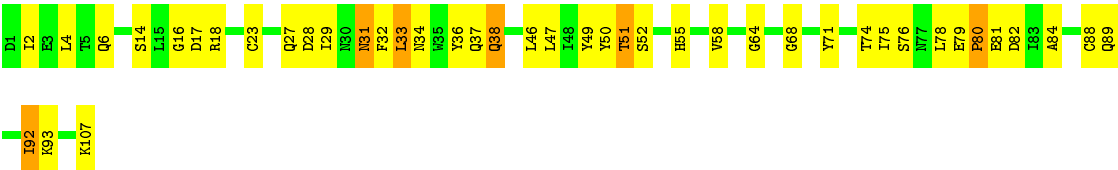
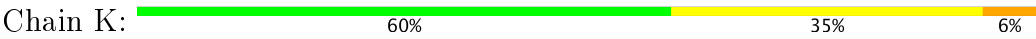


- Molecule 10: Heavy Chain (Vh) Of Fv-Fragment





• Molecule 11: Light Chain (VI) Of Fv-Fragment



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.00Å 165.09Å 147.53Å 90.00° 117.33° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.5 (25.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18069	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

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, CDL, PC1, 3PE, 3PH, FES, HEM, DBT, UQ6

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	0.36	0/3405	0.59	0/4614
2	B	0.33	0/2781	0.59	0/3764
3	C	0.45	0/3191	0.64	1/4353 (0.0%)
4	D	0.37	0/2002	0.60	0/2726
5	E	0.35	0/1444	0.61	1/1957 (0.1%)
6	F	0.34	0/638	0.54	0/858
7	G	0.37	0/1032	0.64	0/1397
8	H	0.40	0/804	0.52	0/1088
9	I	0.41	0/462	0.50	0/622
10	J	0.35	0/1043	0.64	1/1422 (0.1%)
11	K	0.33	0/863	0.57	0/1172
All	All	0.37	0/17665	0.60	3/23973 (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
4	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	32	GLY	N-CA-C	6.55	129.48	113.10
3	C	346	VAL	N-CA-C	5.96	127.08	111.00
5	E	163	GLY	N-CA-C	5.45	126.73	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

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	3344	0	3321	70	0
2	B	2735	0	2774	83	0
3	C	3089	0	3125	33	0
4	D	1941	0	1862	25	0
5	E	1411	0	1386	24	0
6	F	624	0	581	11	0
7	G	1012	0	1026	9	0
8	H	773	0	736	12	0
9	I	449	0	445	6	0
10	J	1015	0	959	30	0
11	K	842	0	820	25	0
12	A	40	0	53	4	0
12	D	38	0	49	3	0
13	A	34	0	44	2	0
14	C	86	0	60	1	0
14	D	43	0	30	0	0
15	C	19	0	17	1	0
16	C	43	0	58	8	0
17	C	87	0	128	3	0
18	D	38	0	50	3	0
19	D	76	0	99	5	0
20	E	4	0	0	1	0
21	A	55	0	0	1	0
21	B	11	0	0	0	0
21	C	110	0	0	5	0
21	D	62	0	0	0	0
21	E	25	0	0	0	0
21	F	4	0	0	1	0
21	G	32	0	0	1	0
21	H	20	0	0	1	0
21	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	3	0	0	0	0
21	K	2	0	0	0	0
All	All	18069	0	17623	328	0

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

The worst 5 of 328 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)
16:C:706:UQ6:H1M1	16:C:706:UQ6:H103	1.31	1.10
6:F:77:GLN:H	6:F:77:GLN:HE21	1.01	0.98
17:C:710:3PE:H111	8:H:51:ARG:HD2	1.53	0.90
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.58	0.86
6:F:77:GLN:H	6:F:77:GLN:NE2	1.75	0.85

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	429/431 (100%)	391 (91%)	33 (8%)	5 (1%)	15	27
2	B	350/352 (99%)	304 (87%)	39 (11%)	7 (2%)	9	14
3	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	44	66
4	D	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
5	E	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	11	19
6	F	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	G	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	78 (86%)	9 (10%)	4 (4%)	3	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	53/55 (96%)	49 (92%)	2 (4%)	2 (4%)	4	4
10	J	125/127 (98%)	114 (91%)	8 (6%)	3 (2%)	7	11
11	K	105/107 (98%)	88 (84%)	11 (10%)	6 (6%)	2	2
All	All	2158/2180 (99%)	1983 (92%)	144 (7%)	31 (1%)	13	23

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	335	PRO
3	C	223	SER
8	H	93	ASN
11	K	80	PRO

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	370/370 (100%)	343 (93%)	27 (7%)	16	31
2	B	301/301 (100%)	277 (92%)	24 (8%)	14	27
3	C	338/338 (100%)	316 (94%)	22 (6%)	20	37
4	D	204/204 (100%)	196 (96%)	8 (4%)	37	63
5	E	151/151 (100%)	148 (98%)	3 (2%)	60	84
6	F	67/67 (100%)	63 (94%)	4 (6%)	22	41
7	G	109/109 (100%)	105 (96%)	4 (4%)	39	66
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	45/45 (100%)	42 (93%)	3 (7%)	19	35
10	J	112/112 (100%)	104 (93%)	8 (7%)	17	32
11	K	93/93 (100%)	85 (91%)	8 (9%)	12	23
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	23	42

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	LEU
3	C	218	ARG
10	J	89	GLU
3	C	5	LYS
3	C	89	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	252	GLN
3	C	208	ASN
10	J	78	GLN
2	B	258	ASN
3	C	43	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 ⓘ

13 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
12	3PH	A	713	-	39,39,47	1.15	3 (7%)	43,44,52	1.61	5 (11%)
13	UMQ	A	721	-	35,35,35	1.04	2 (5%)	46,46,46	1.74	8 (17%)
14	HEM	C	701	3	28,50,50	1.76	5 (17%)	17,82,82	1.17	2 (11%)
14	HEM	C	702	3	28,50,50	1.52	5 (17%)	17,82,82	1.45	5 (29%)
15	DBT	C	705	-	17,20,20	1.23	2 (11%)	13,27,27	0.85	0
16	UQ6	C	706	-	43,43,43	3.14	18 (41%)	52,55,55	2.14	14 (26%)
17	3PE	C	710	-	46,46,50	1.14	7 (15%)	48,51,55	1.30	4 (8%)
17	3PE	C	711	-	39,39,50	0.82	1 (2%)	41,44,55	1.05	2 (4%)
14	HEM	D	703	4	28,50,50	1.68	5 (17%)	17,82,82	1.08	1 (5%)
12	3PH	D	714	-	37,37,47	1.03	1 (2%)	41,42,52	1.61	9 (21%)
18	PC1	D	715	-	37,37,53	2.00	8 (21%)	42,45,61	1.59	8 (19%)
19	CDL	D	731	-	75,75,99	1.62	14 (18%)	77,87,111	1.42	7 (9%)
20	FES	E	704	5	0,4,4	0.00	-	0,4,4	0.00	-

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
12	3PH	A	713	-	-	0/41/41/49	0/0/0/0
13	UMQ	A	721	-	-	0/20/60/60	0/2/2/2
14	HEM	C	701	3	-	0/6/54/54	0/0/8/8
14	HEM	C	702	3	-	0/6/54/54	0/0/8/8
15	DBT	C	705	-	-	0/7/27/27	0/2/2/2
16	UQ6	C	706	-	-	0/39/39/39	0/1/1/1
17	3PE	C	710	-	-	0/50/50/54	0/0/0/0
17	3PE	C	711	-	-	0/43/43/54	0/0/0/0
14	HEM	D	703	4	-	0/6/54/54	0/0/8/8
12	3PH	D	714	-	-	0/39/39/49	0/0/0/0
18	PC1	D	715	-	-	1/41/41/57	0/0/0/0
19	CDL	D	731	-	-	2/86/86/110	0/0/0/0
20	FES	E	704	5	-	0/0/4/4	0/1/1/1

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	731	CDL	OA8-CA6	-5.23	1.33	1.45
16	C	706	UQ6	O2-C2	-5.00	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	701	HEM	C3C-CAC	-4.67	1.38	1.47
16	C	706	UQ6	O5-C5	-4.12	1.27	1.37
14	D	703	HEM	C3B-C2B	-4.02	1.35	1.40

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	721	UMQ	CA-O1'-C1'	-7.77	100.54	113.87
19	D	731	CDL	CB4-OB6-CB5	-6.53	102.45	117.88
18	D	715	PC1	C3-C2-C1	-4.74	101.17	111.86
19	D	731	CDL	CA6-CA4-CA3	-4.13	102.55	111.86
17	C	710	3PE	C2-O21-C21	-4.09	108.21	117.88

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	731	CDL	CA4-OA6-CA5-OA7
19	D	731	CDL	CA4-OA6-CA5-C11
18	D	715	PC1	P-O13-C11-C12

There are no ring outliers.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	713	3PH	4	0
13	A	721	UMQ	2	0
14	C	702	HEM	1	0
15	C	705	DBT	1	0
16	C	706	UQ6	8	0
17	C	710	3PE	3	0
12	D	714	3PH	3	0
18	D	715	PC1	3	0
19	D	731	CDL	5	0
20	E	704	FES	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.