



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SQV
Title : Crystal Structure Analysis of Bovine Bcl with UHDBT
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on : 2004-03-19
Resolution : 2.85 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

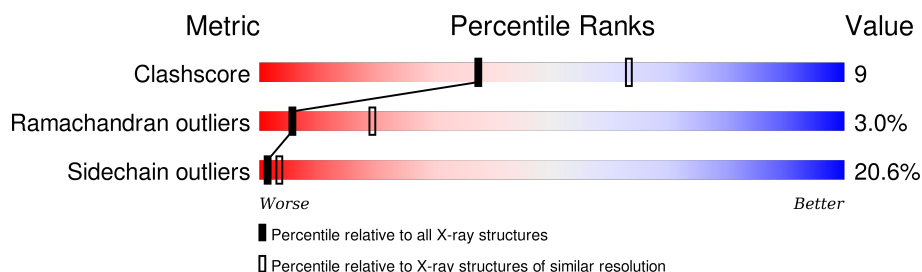
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	

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Mol	Chain	Length	Quality of chain
8	H	78	<div><div></div><div>58%</div><div>21%</div><div>8%</div><div>14%</div></div>
9	I	78	<div><div></div><div>18%</div><div>36%</div><div>12%</div><div>8%</div><div>27%</div></div>
10	J	62	<div><div></div><div>52%</div><div>44%</div><div></div><div></div></div>
11	K	56	<div><div></div><div>59%</div><div>25%</div><div>5%</div><div></div><div>9%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16953 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase complex 8 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

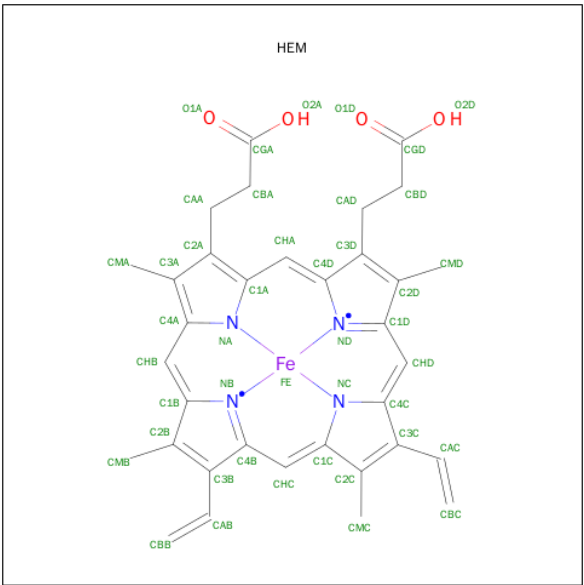
- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	S	0	0	0
			502	329	87	86				

- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

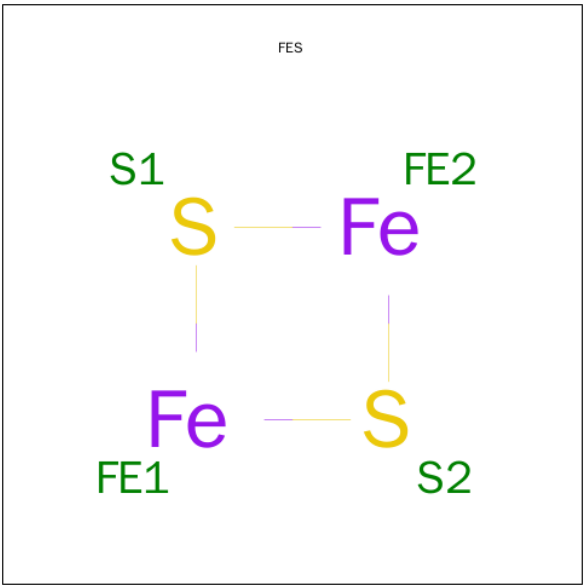
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			418	278	75	64	1			

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



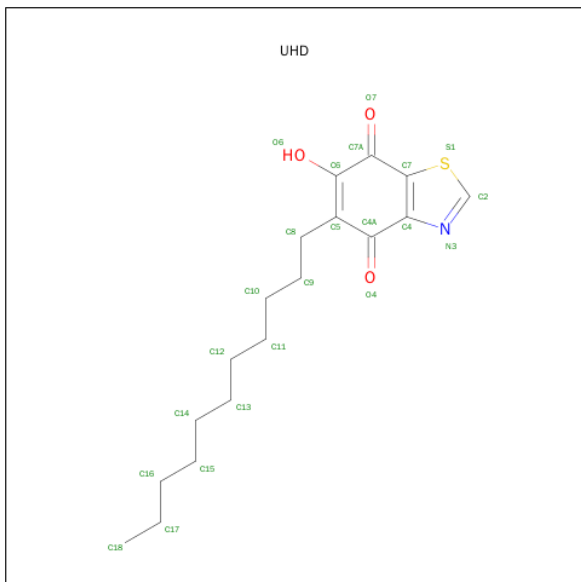
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



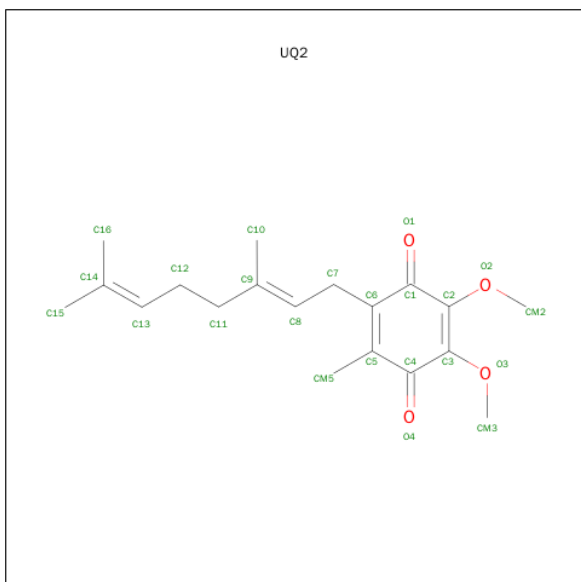
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is 6-HYDROXY-5-UNDECYL-1,3-BENZOTHIAZOLE-4,7-DIONE (three-letter code: UHD) (formula: $C_{18}H_{25}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	S	0	0
			23	18	1	3	1		

- Molecule 15 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			23	19	4		

- Molecule 16 is water.

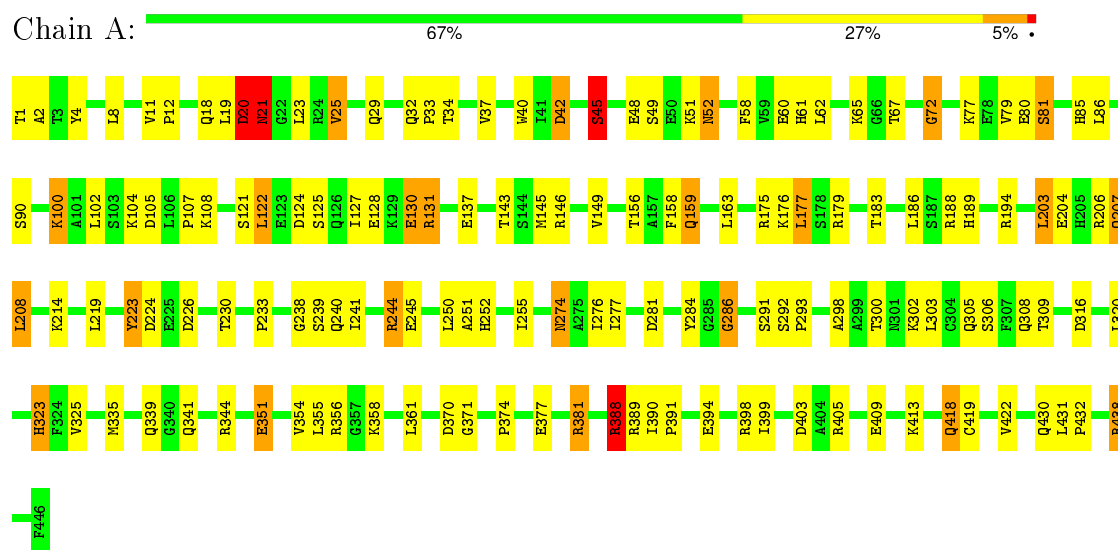
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	70	Total 70	O 70	0	0
16	B	103	Total 103	O 103	0	0
16	C	26	Total 26	O 26	0	0
16	D	21	Total 21	O 21	0	0
16	E	8	Total 8	O 8	0	0
16	F	31	Total 31	O 31	0	0
16	G	16	Total 16	O 16	0	0
16	I	10	Total 10	O 10	0	0
16	K	6	Total 6	O 6	0	0

3 Residue-property plots

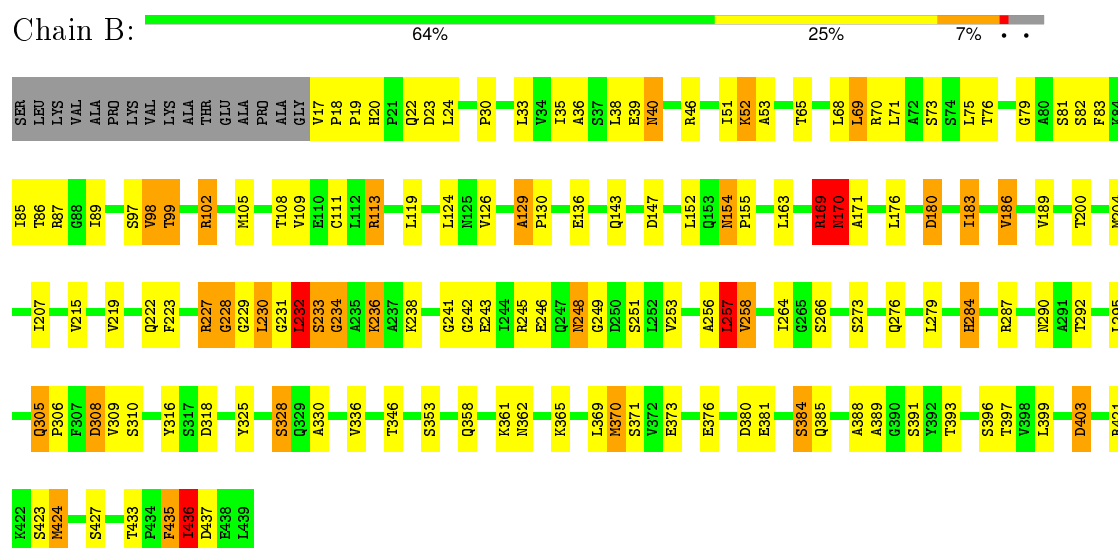
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

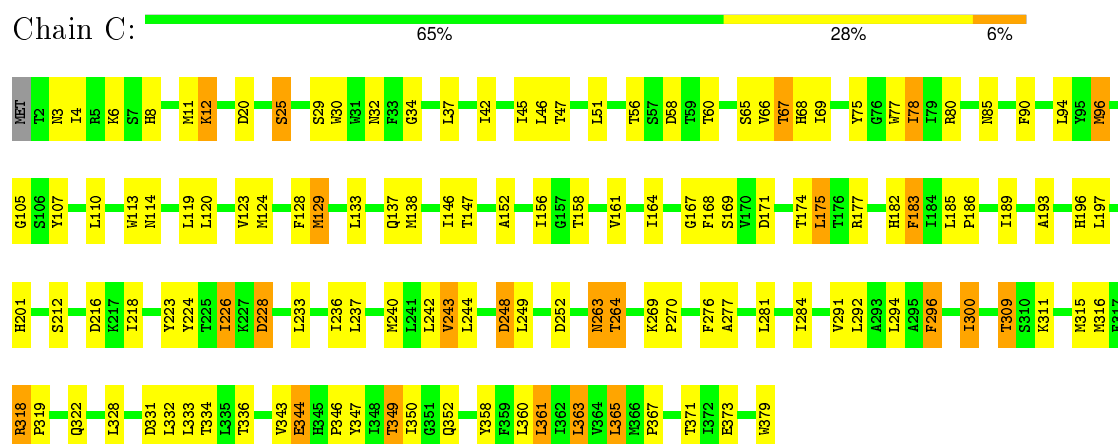
- Molecule 1: Ubiquinol-cytochrome c reductase complex core protein I, mitochondrial



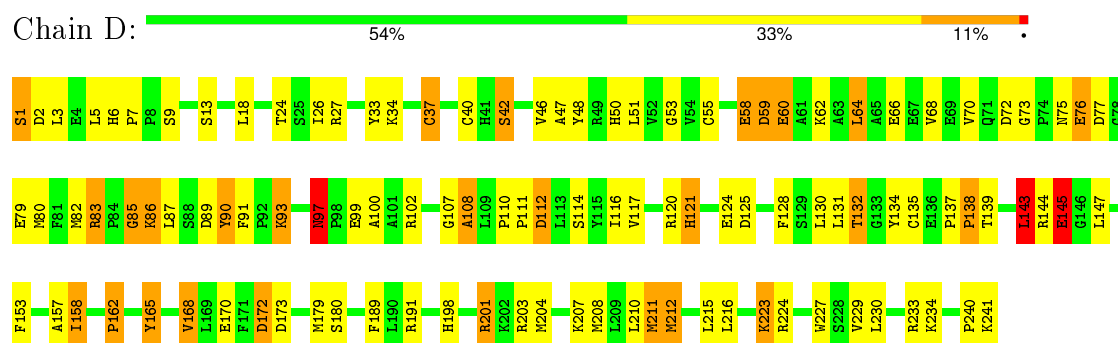
- Molecule 2: Ubiquinol-cytochrome c reductase complex core protein 2, mitochondrial



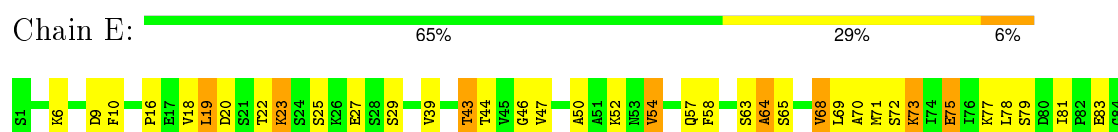
- Molecule 3: Cytochrome b



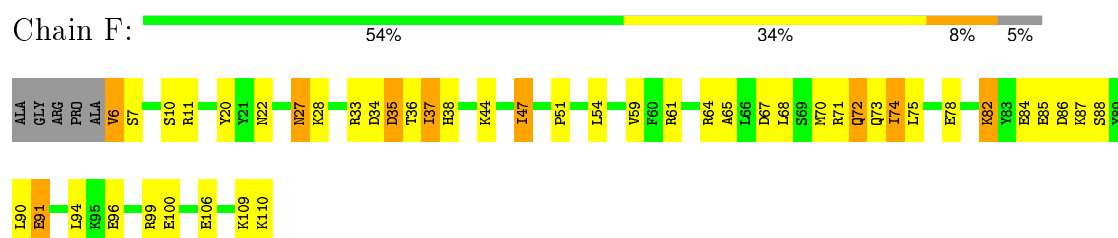
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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

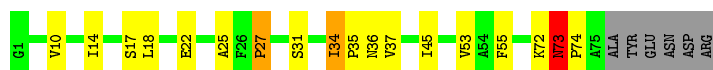


- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:  70% 19% 7%



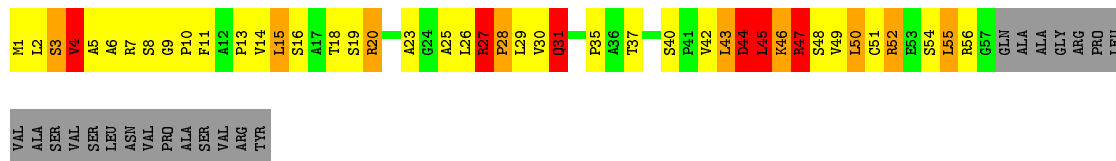
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:  58% 21% 8% 14%



- Molecule 9: Ubiquinol-cytochrome C reductase complex 8 kDa protein

Chain I:  18% 36% 12% 8% 27%



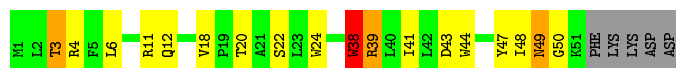
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:  52% 44% 2%



- Molecule 11: Ubiquinol-cytochrome C reductase complex 6.4 kDa protein

Chain K:  59% 25% 5% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.67Å 153.67Å 589.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.5 (40.00-2.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16953	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, UHD, UQ2, FES

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	0.47	0/3531	0.89	5/4792 (0.1%)
2	B	0.52	0/3232	0.92	8/4386 (0.2%)
3	C	0.51	0/3100	0.88	3/4242 (0.1%)
4	D	0.46	0/1977	0.89	4/2684 (0.1%)
5	E	0.46	0/1553	0.86	4/2100 (0.2%)
6	F	0.52	0/930	0.94	3/1246 (0.2%)
7	G	0.57	0/649	0.87	0/878
8	H	0.50	1/553 (0.2%)	0.96	2/741 (0.3%)
9	I	0.62	0/411	1.22	2/558 (0.4%)
10	J	0.52	0/515	0.83	0/696
11	K	0.49	0/433	0.91	1/594 (0.2%)
All	All	0.50	1/16884 (0.0%)	0.90	32/22917 (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	A	0	8
2	B	0	12
3	C	0	3
4	D	0	21
5	E	0	5
6	F	0	1
8	H	0	5
9	I	0	16
10	J	0	1
11	K	0	3
All	All	0	75

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	57	GLU	CD-OE2	5.20	1.31	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	203	LEU	CA-CB-CG	6.19	129.53	115.30
9	I	45	LEU	CA-CB-CG	6.17	129.48	115.30
2	B	180	ASP	CB-CG-OD2	6.16	123.84	118.30
2	B	147	ASP	CB-CG-OD2	6.00	123.70	118.30

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ASP	Peptide
1	A	137	GLU	Mainchain
1	A	20	ASP	Peptide
1	A	45	SER	Peptide
1	A	52	ASN	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	3458	0	3356	71	0
2	B	3172	0	3152	86	0
3	C	3003	0	3065	65	0
4	D	1918	0	1870	36	0
5	E	1519	0	1503	19	0
6	F	911	0	904	18	0
7	G	628	0	636	7	0
8	H	548	0	530	4	0
9	I	406	0	437	36	0
10	J	502	0	505	8	0
11	K	418	0	425	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	86	0	60	10	0
12	D	43	0	30	5	0
13	E	4	0	0	0	0
14	C	23	0	24	3	0
15	C	23	0	26	4	0
16	A	70	0	0	3	0
16	B	103	0	0	5	0
16	C	26	0	0	1	0
16	D	21	0	0	0	0
16	E	8	0	0	0	0
16	F	31	0	0	2	0
16	G	16	0	0	0	0
16	I	10	0	0	2	0
16	K	6	0	0	0	0
All	All	16953	0	16523	308	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 308 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:B:623:HOH:O	9:I:11:PHE:HB2	1.70	0.92
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.52	0.90
16:B:627:HOH:O	9:I:4:VAL:HG21	1.75	0.85
2:B:385:GLN:HA	9:I:2:LEU:HD12	1.60	0.81
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.64	0.80

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	444/446 (100%)	397 (89%)	37 (8%)	10 (2%)	8	26
2	B	421/439 (96%)	383 (91%)	26 (6%)	12 (3%)	6	20
3	C	376/379 (99%)	332 (88%)	39 (10%)	5 (1%)	15	42
4	D	239/241 (99%)	199 (83%)	30 (13%)	10 (4%)	3	11
5	E	194/196 (99%)	168 (87%)	21 (11%)	5 (3%)	7	23
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	10	32
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	6	22
8	H	65/78 (83%)	57 (88%)	7 (11%)	1 (2%)	13	38
9	I	55/78 (70%)	28 (51%)	17 (31%)	10 (18%)	0	0
10	J	59/62 (95%)	48 (81%)	8 (14%)	3 (5%)	2	7
11	K	49/56 (88%)	42 (86%)	4 (8%)	3 (6%)	2	5
All	All	2078/2166 (96%)	1818 (88%)	197 (10%)	63 (3%)	5	19

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
2	B	52	LYS
2	B	232	LEU
2	B	437	ASP
3	C	347	TYR

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%)	307 (83%)	63 (17%)	2	6
2	B	332/343 (97%)	280 (84%)	52 (16%)	3	8
3	C	326/327 (100%)	267 (82%)	59 (18%)	2	5
4	D	206/206 (100%)	145 (70%)	61 (30%)	0	1
5	E	168/168 (100%)	130 (77%)	38 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	96/98 (98%)	73 (76%)	23 (24%)	1	2
7	G	66/71 (93%)	56 (85%)	10 (15%)	3	9
8	H	64/74 (86%)	50 (78%)	14 (22%)	1	3
9	I	44/60 (73%)	29 (66%)	15 (34%)	0	0
10	J	51/52 (98%)	34 (67%)	17 (33%)	0	0
11	K	41/46 (89%)	29 (71%)	12 (29%)	0	1
All	All	1764/1815 (97%)	1400 (79%)	364 (21%)	1	3

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	343	VAL
4	D	97	ASN
10	J	5	LEU
3	C	361	LEU
4	D	37	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	305	GLN
3	C	32	ASN
7	G	23	GLN
2	B	385	GLN
3	C	85	ASN

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

6 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	HEM	C	381	3	30,50,50	2.97	10 (33%)	24,82,82	3.99	10 (41%)
12	HEM	C	382	3	30,50,50	2.84	9 (30%)	24,82,82	3.34	12 (50%)
14	UHD	C	383	-	20,24,24	2.48	7 (35%)	16,31,31	1.46	1 (6%)
15	UQ2	C	384	-	23,23,23	2.04	5 (21%)	28,31,31	1.40	4 (14%)
12	HEM	D	242	4	30,50,50	2.92	10 (33%)	24,82,82	3.06	11 (45%)
13	FES	E	197	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	HEM	C	381	3	-	0/10/54/54	0/0/8/8
12	HEM	C	382	3	-	0/10/54/54	0/0/8/8
14	UHD	C	383	-	-	0/11/31/31	0/2/2/2
15	UQ2	C	384	-	-	0/15/39/39	0/1/1/1
12	HEM	D	242	4	-	0/10/54/54	0/0/8/8
13	FES	E	197	5	-	0/0/4/4	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C3D-C4D	-9.02	1.40	1.51
12	D	242	HEM	C3D-C4D	-8.68	1.40	1.51
12	C	382	HEM	C3D-C4D	-8.21	1.41	1.51
14	C	383	UHD	C4-C4A	-7.80	1.40	1.49
12	C	382	HEM	C3B-C4B	-6.73	1.45	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	C	381	HEM	C3B-CAB-CBB	-12.21	105.73	124.46
12	C	382	HEM	C3B-CAB-CBB	-9.21	110.32	124.46
12	C	381	HEM	C3C-CAC-CBC	-9.10	110.50	124.46
12	D	242	HEM	C3C-CAC-CBC	-8.20	111.88	124.46
12	C	382	HEM	C1D-CHD-C4C	-6.41	115.10	125.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	3	0
12	C	382	HEM	7	0
14	C	383	UHD	3	0
15	C	384	UQ2	4	0
12	D	242	HEM	5	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.