wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:36 PM GMT

PDB ID	:	1L0N
Title	:	native structure of bovine mitochondrial cytochrome bc1 complex
Authors	:	Gao, X.; Wen, X.; Yu, C.A.; Esser, L.; Tsao, S.; Quinn, B.; Zhang, L.; Yu, L.; Xia, D.
Deposited on	:	2002-02-11
Resolution	:	2.60 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 (i) symbol.

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

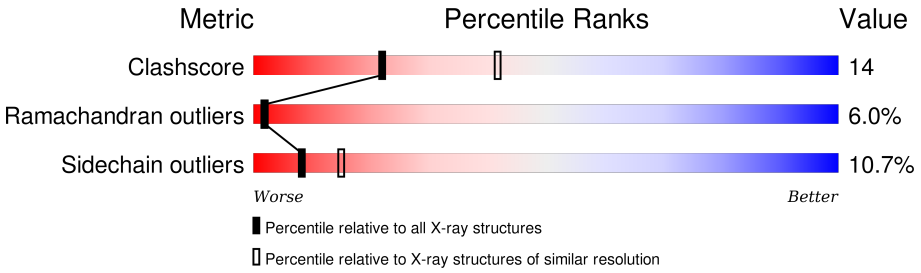
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 <=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	72% 23% •
2	B	439	69% 22% 5% • •
3	C	379	74% 20% 6% ••
4	D	241	52% 33% 13% •
5	E	196	49% 36% 12% •
6	F	110	59% 28% 8% 5%
7	G	81	63% 20% 7% • 7%

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Mol	Chain	Length	Quality of chain
8	H	78	50% 31% 8% • 10%
9	I	78	22% 21% 24% 6% 27%
10	J	62	55% 29% 8% • 6%
11	K	56	54% 21% 7% 5% 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16577 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
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2.

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

- Molecule 3 is a protein called Cytochrome B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	377	2996	2009	470	499	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

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

- 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	70	Total	C	N	O	S	0	0	0
			575	347	102	121	5			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE 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	58	Total	C	N	O	0	0	0
			473	311	83	79			

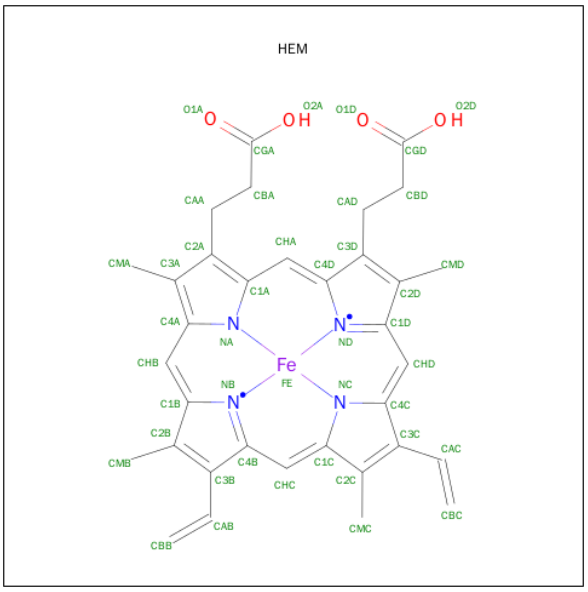
- Molecule 11 is a protein called cytochrome b-c1 complex 6.4K protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			387	251	71	64	1			

There is a discrepancy between the modelled and reference sequences:

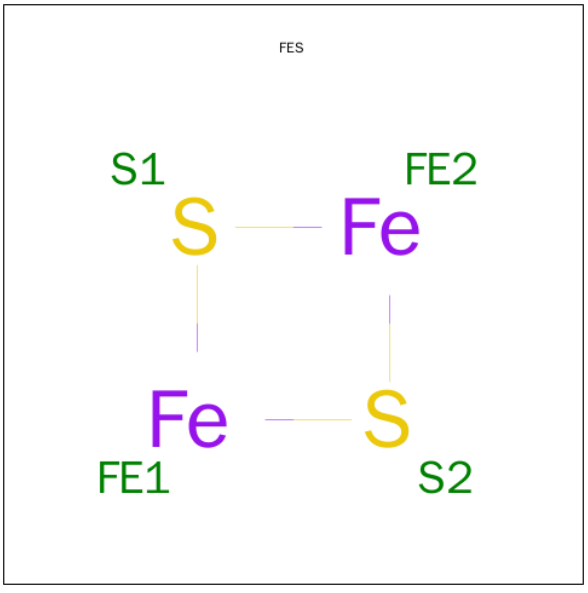
Chain	Residue	Modelled	Actual	Comment	Reference
K	47	THR	TYR	CONFLICT	UNP P07552

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

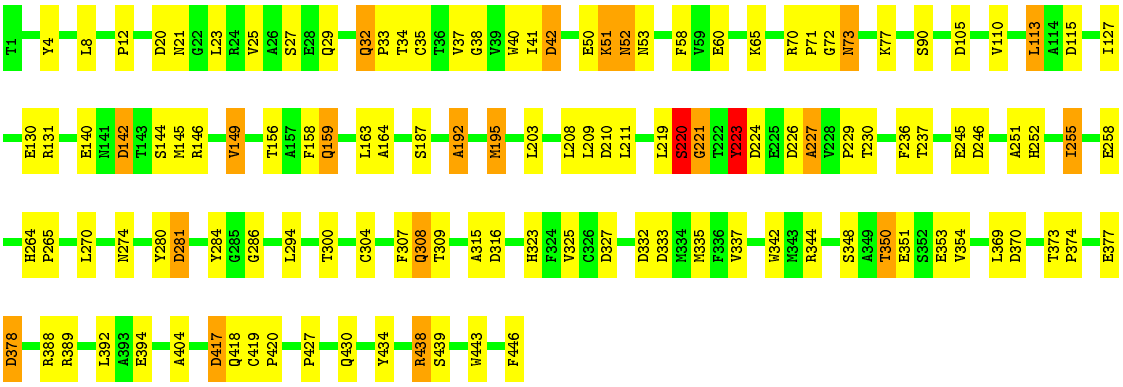
3 Residue-property plots (i)

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.

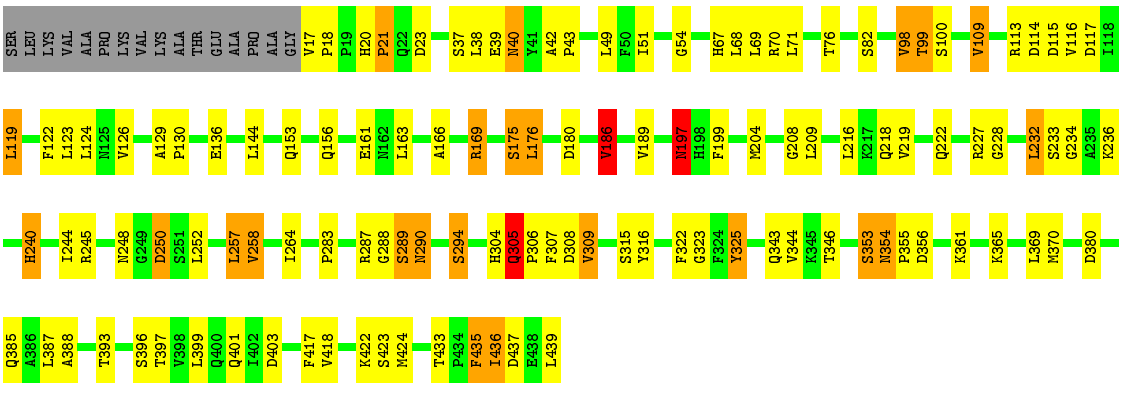
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

Chain A:



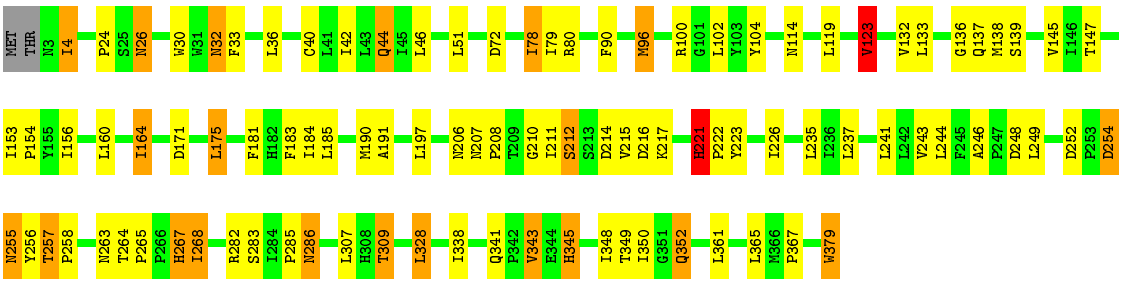
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



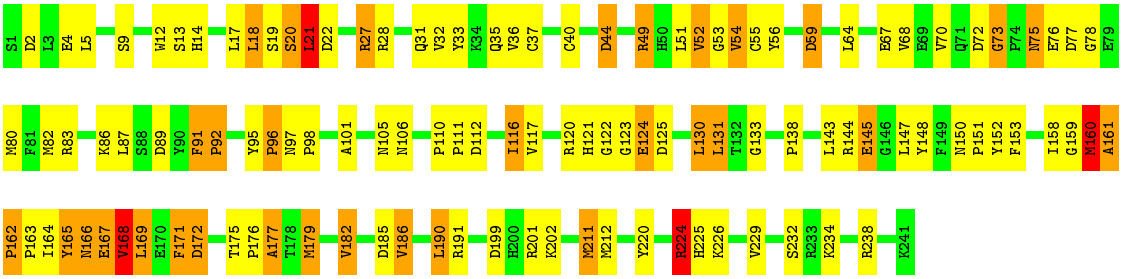
• Molecule 3: Cytochrome B

Chain C:



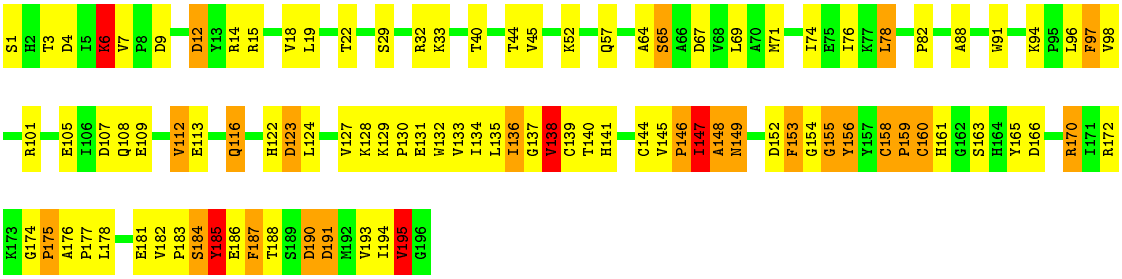
• Molecule 4: Cytochrome c1, heme protein

Chain D:



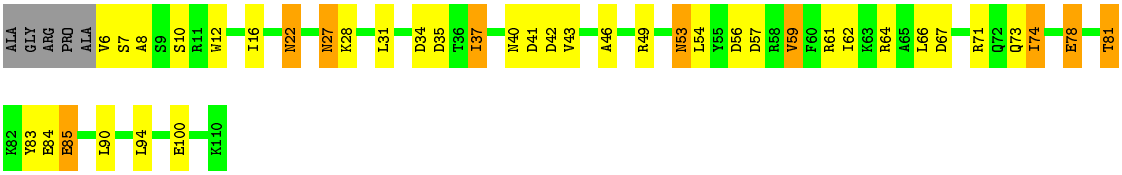
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E:



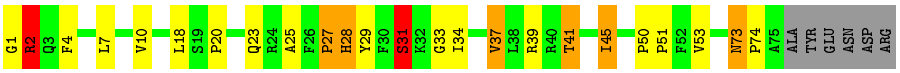
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



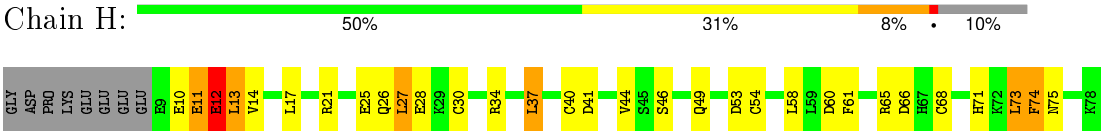
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



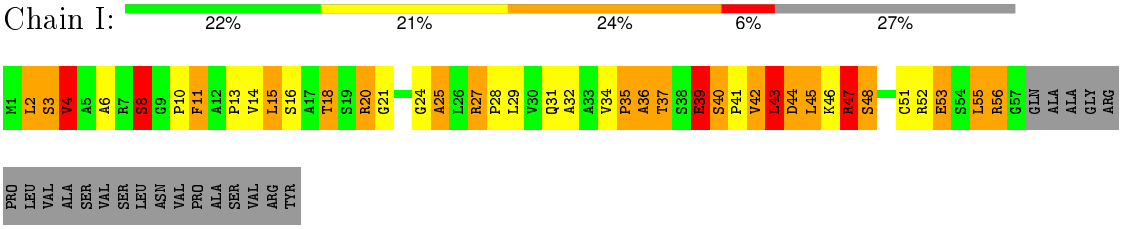
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



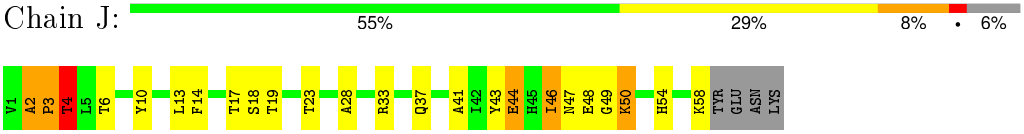
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN

Chain I:



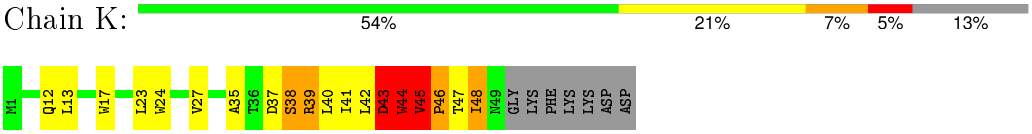
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



• Molecule 11: cytochrome b-c1 complex 6.4K protein

Chain K:



4 Data and refinement statistics (i)

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	153.83Å 153.83Å 596.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (28.99-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.261 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16577	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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, 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	0.98	4/3531 (0.1%)	0.89	17/4792 (0.4%)
2	B	1.22	9/3232 (0.3%)	0.98	18/4386 (0.4%)
3	C	0.89	3/3093 (0.1%)	0.85	7/4232 (0.2%)
4	D	0.80	3/1978 (0.2%)	1.17	19/2684 (0.7%)
5	E	0.82	3/1553 (0.2%)	0.98	11/2100 (0.5%)
6	F	1.01	1/930 (0.1%)	0.97	6/1246 (0.5%)
7	G	0.93	0/649	0.87	1/878 (0.1%)
8	H	0.70	0/580	0.97	5/777 (0.6%)
9	I	1.24	3/411 (0.7%)	1.50	8/558 (1.4%)
10	J	0.79	0/485	0.80	1/655 (0.2%)
11	K	0.77	0/397	0.97	3/544 (0.6%)
All	All	0.97	26/16839 (0.2%)	0.97	96/22852 (0.4%)

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
3	C	0	1
4	D	1	0
All	All	1	1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	26	ASN	CB-CG	-7.32	1.34	1.51
9	I	25	ALA	CA-CB	-7.28	1.37	1.52
4	D	92	PRO	CB-CG	-7.26	1.13	1.50
2	B	325	TYR	CE2-CZ	-6.84	1.29	1.38
3	C	379	TRP	CB-CG	-6.41	1.38	1.50

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	91	PHE	C-N-CD	-23.89	68.03	120.60
9	I	42	VAL	O-C-N	12.05	141.98	122.70
4	D	168	VAL	O-C-N	10.28	139.15	122.70
4	D	92	PRO	CA-N-CD	-10.23	97.18	111.50
9	I	42	VAL	CA-C-N	-10.16	94.85	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	171	PHE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Peptide

5.2 Too-close contacts (i)

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	85	0
3	C	2996	0	3058	57	0
4	D	1919	0	1867	82	0
5	E	1519	0	1505	72	0
6	F	911	0	904	24	0
7	G	628	0	636	18	0
8	H	575	0	550	15	0
9	I	406	0	437	62	0
10	J	473	0	484	22	0
11	K	387	0	400	19	0
12	C	86	0	60	2	0
12	D	43	0	30	5	0
13	E	4	0	0	1	0
All	All	16577	0	16439	460	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 14.

The worst 5 of 460 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)
2:B:305:GLN:NE2	2:B:305:GLN:HA	1.52	1.10
5:E:52:LYS:HE2	11:K:35:ALA:HA	1.22	1.10
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.28	1.08
4:D:167:GLU:HG2	4:D:169:LEU:HD23	1.08	1.05
4:D:167:GLU:HG2	4:D:169:LEU:CD2	1.86	1.05

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%)	407 (92%)	23 (5%)	14 (3%)	5 8
2	B	421/439 (96%)	391 (93%)	22 (5%)	8 (2%)	10 19
3	C	375/379 (99%)	335 (89%)	28 (8%)	12 (3%)	5 8
4	D	239/241 (99%)	177 (74%)	36 (15%)	26 (11%)	0 0
5	E	194/196 (99%)	127 (66%)	43 (22%)	24 (12%)	0 0
6	F	103/110 (94%)	96 (93%)	6 (6%)	1 (1%)	19 39
7	G	73/81 (90%)	62 (85%)	6 (8%)	5 (7%)	1 1
8	H	68/78 (87%)	50 (74%)	9 (13%)	9 (13%)	0 0
9	I	55/78 (70%)	26 (47%)	15 (27%)	14 (26%)	0 0
10	J	56/62 (90%)	43 (77%)	7 (12%)	6 (11%)	0 0
11	K	47/56 (84%)	32 (68%)	9 (19%)	6 (13%)	0 0
All	All	2075/2166 (96%)	1746 (84%)	204 (10%)	125 (6%)	2 2

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	220	SER
1	A	227	ALA
2	B	305	GLN
3	C	212	SER

5.3.2 Protein sidechains (i)

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%)	342 (92%)	28 (8%)	16 32
2	B	332/343 (97%)	299 (90%)	33 (10%)	10 18
3	C	325/327 (99%)	298 (92%)	27 (8%)	14 27
4	D	206/206 (100%)	175 (85%)	31 (15%)	3 6
5	E	168/168 (100%)	148 (88%)	20 (12%)	6 11
6	F	96/98 (98%)	87 (91%)	9 (9%)	11 20
7	G	66/71 (93%)	58 (88%)	8 (12%)	6 11
8	H	67/74 (90%)	58 (87%)	9 (13%)	5 8
9	I	44/60 (73%)	35 (80%)	9 (20%)	1 2
10	J	48/52 (92%)	41 (85%)	7 (15%)	4 6
11	K	40/46 (87%)	32 (80%)	8 (20%)	1 2
All	All	1762/1815 (97%)	1573 (89%)	189 (11%)	8 15

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	350	ILE
4	D	124	GLU
10	J	4	THR
4	D	4	GLU
4	D	36	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	284	HIS
2	B	385	GLN
9	I	31	GLN
2	B	342	ASN
2	B	401	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

4 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	2.06	8 (26%)	24,82,82	2.43	12 (50%)
12	HEM	C	382	3	30,50,50	2.06	7 (23%)	24,82,82	2.45	10 (41%)
12	HEM	D	242	4	30,50,50	2.05	6 (20%)	24,82,82	2.40	8 (33%)
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
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 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C3B-C4B	-7.39	1.45	1.51
12	D	242	HEM	C3B-C4B	-6.92	1.45	1.51
12	C	382	HEM	C3B-C4B	-6.55	1.46	1.51
12	C	382	HEM	C3D-C4D	-4.79	1.45	1.51
12	C	381	HEM	C3D-C4D	-4.03	1.46	1.51

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	382	HEM	C3C-CAC-CBC	-4.83	117.05	124.46
12	D	242	HEM	CAA-CBA-CGA	-3.75	105.86	112.75
12	C	382	HEM	C3B-CAB-CBB	-3.24	119.49	124.46
12	C	381	HEM	CAA-CBA-CGA	-3.18	106.92	112.75
12	D	242	HEM	C3B-CAB-CBB	-2.92	119.98	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	2	0
12	D	242	HEM	5	0
13	E	197	FES	1	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.