



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:15 am GMT

PDB ID : 2FYU
Title : Crystal structure of bovine heart mitochondrial bc1 with jg144 inhibitor
Authors : Xia, D.; Esser, L.
Deposited on : 2006-02-08
Resolution : 2.26 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)
Xtrriage (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) : recalc28949

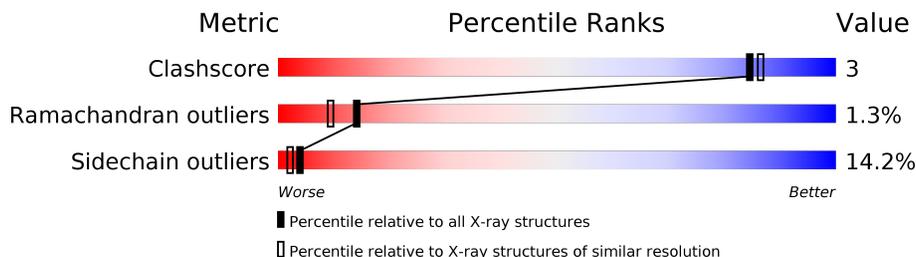
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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	80% 16% .
2	B	439	76% 18% . .
3	C	379	79% 18% .
4	D	241	73% 23% 5%
5	E	196	80% 17% . .
6	F	110	78% 15% . .
7	G	81	73% 17% . . 7%

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Mol	Chain	Length	Quality of chain
8	H	78	 <p>54% 26% 18%</p>
9	I	78	 <p>35% 23% 12% 27%</p>
10	J	62	 <p>71% 24%</p>
11	K	56	 <p>63% 30% 5%</p>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16900 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
			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, mitochondrial.

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	378	3003	2013	471	501	18	0	0	0

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

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

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

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 Hypothetical protein LOC616871.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	106	Total	C	N	O	S	0	0	0
			916	579	166	169	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	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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

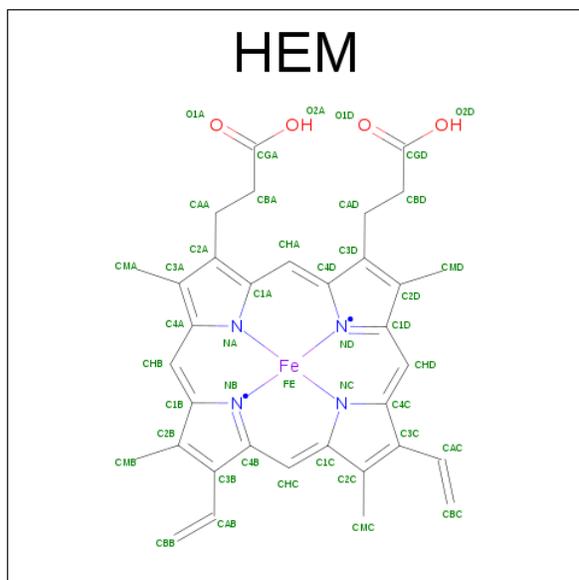
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

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

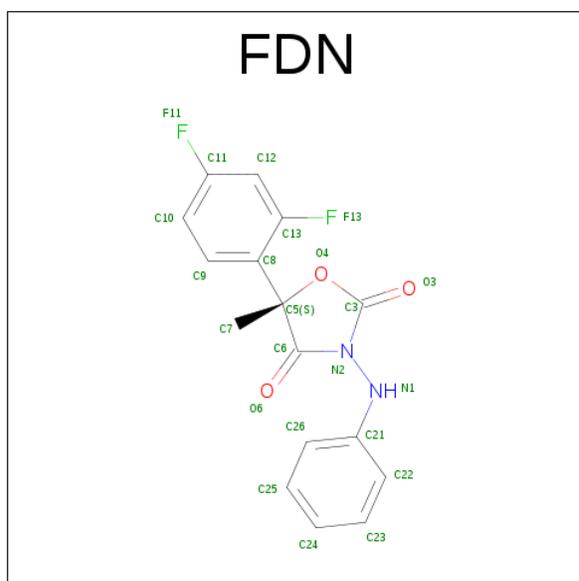
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			438	293	78	66	1			

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



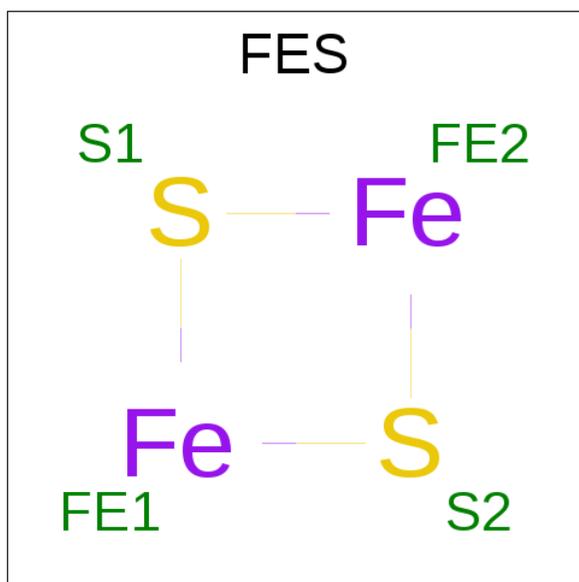
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is (5S)-3-ANILINO-5-(2,4-DIFLUOROPHENYL)-5-METHYL-1,3-OXAZOLIDINE-2,4-DIONE (three-letter code: FDN) (formula: $C_{16}H_{12}F_2N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
13	C	1	23	16	2	2	3	0	0

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



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	38	Total	O	0	0
			38	38		
15	B	53	Total	O	0	0
			53	53		
15	C	84	Total	O	0	0
			84	84		
15	D	34	Total	O	0	0
			34	34		
15	F	27	Total	O	0	0
			27	27		
15	G	13	Total	O	0	0
			13	13		
15	H	2	Total	O	0	0
			2	2		
15	I	6	Total	O	0	0
			6	6		

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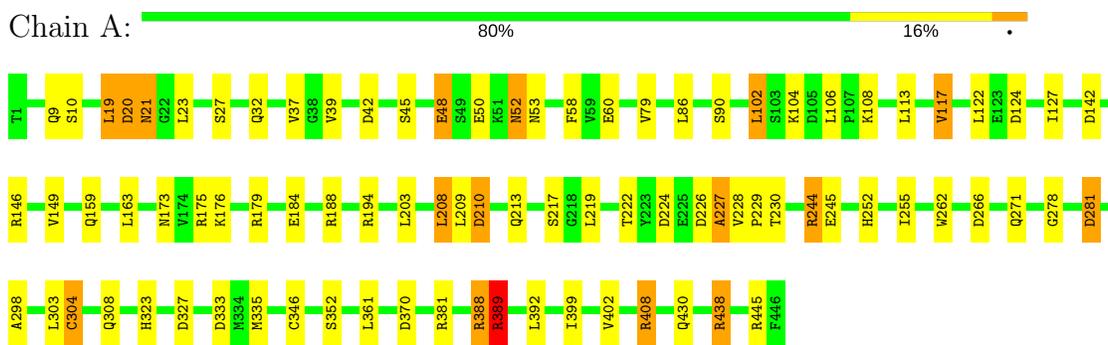
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	J	7	Total O 7 7	0	0
15	K	3	Total O 3 3	0	0

3 Residue-property plots [i](#)

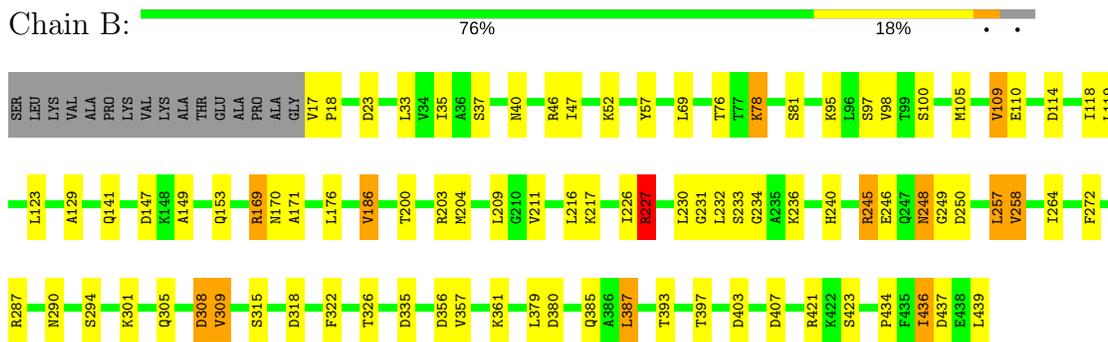
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

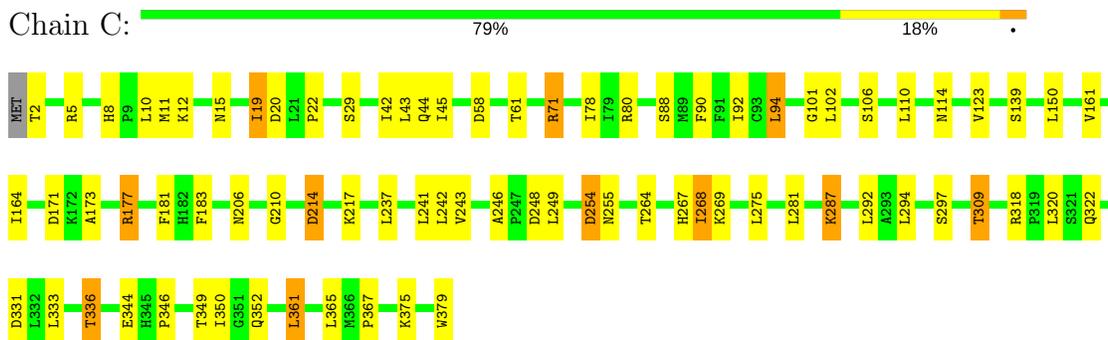
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial



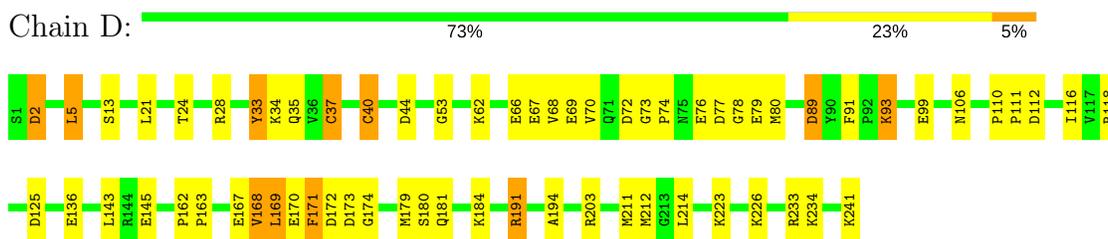
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



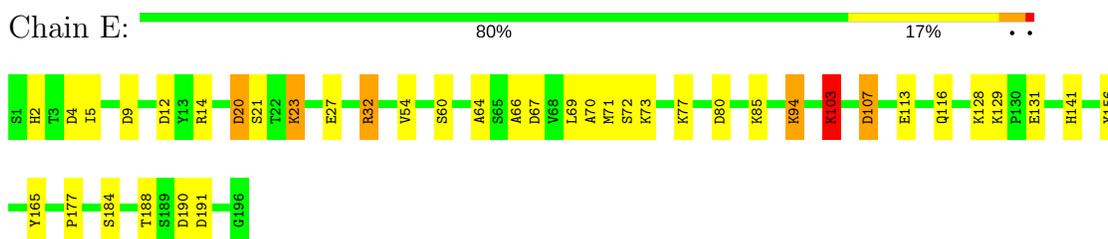
- Molecule 3: Cytochrome b



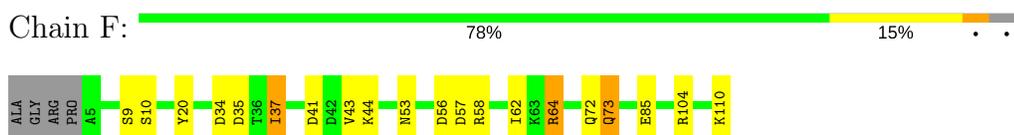
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



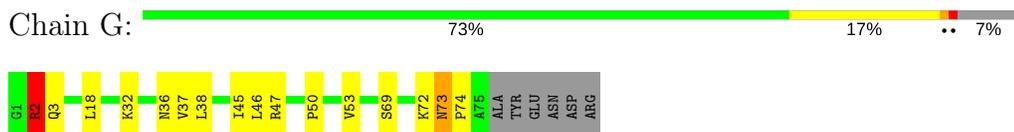
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



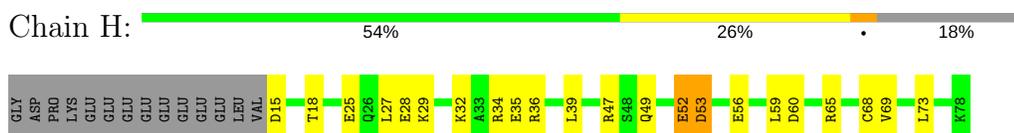
- Molecule 6: Hypothetical protein LOC616871



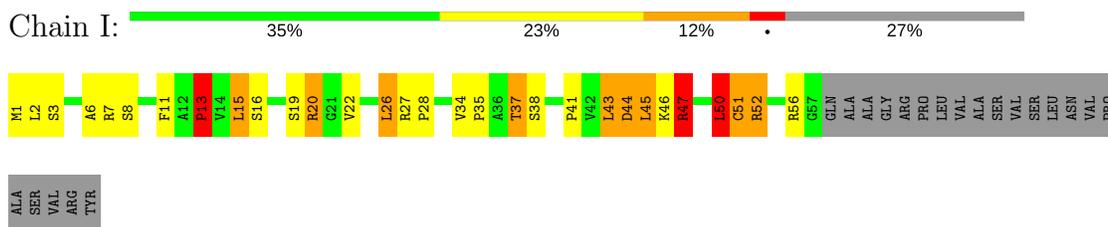
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



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



- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



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

Chain J:  71% 24% ••



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

Chain K:  63% 30% • 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.26Å 154.26Å 590.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.26	Depositor
% Data completeness (in resolution range)	96.9 (40.00-2.26)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.248 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16900	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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, FDN

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	0.97	0/3531	1.06	15/4792 (0.3%)
2	B	1.01	3/3232 (0.1%)	1.04	13/4386 (0.3%)
3	C	1.12	0/3100	1.00	10/4242 (0.2%)
4	D	1.08	0/1977	1.04	11/2684 (0.4%)
5	E	1.07	1/1553 (0.1%)	1.01	8/2100 (0.4%)
6	F	1.09	0/935	1.12	6/1253 (0.5%)
7	G	1.26	0/649	1.07	2/878 (0.2%)
8	H	0.88	0/529	1.07	2/708 (0.3%)
9	I	1.01	0/411	1.24	3/558 (0.5%)
10	J	1.18	0/508	1.02	2/686 (0.3%)
11	K	1.20	0/454	1.02	1/621 (0.2%)
All	All	1.06	4/16879 (0.0%)	1.05	73/22908 (0.3%)

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	12
2	B	0	14
3	C	0	7
4	D	0	9
5	E	0	6
6	F	0	2
8	H	0	1
9	I	0	13
10	J	0	3
11	K	0	4
All	All	0	71

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	103	LYS	CE-NZ	7.62	1.68	1.49
2	B	105	MET	SD-CE	-5.54	1.46	1.77
2	B	272	PHE	CE2-CZ	5.17	1.47	1.37
2	B	57	TYR	CG-CD2	5.05	1.45	1.39

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	ARG	NE-CZ-NH2	-8.73	115.93	120.30
6	F	57	ASP	CB-CG-OD2	8.38	125.84	118.30
1	A	244	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	389	ARG	NE-CZ-NH2	-8.13	116.23	120.30
6	F	34	ASP	CB-CG-OD2	7.91	125.42	118.30

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ASP	Peptide
1	A	227	ALA	Peptide
1	A	228	VAL	Peptide
1	A	229	PRO	Peptide
1	A	48	GLU	Mainchain

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	17	0
2	B	3172	0	3152	22	0
3	C	3003	0	3065	22	0
4	D	1918	0	1870	13	0
5	E	1519	0	1503	9	0
6	F	916	0	909	3	0
7	G	628	0	636	5	0
8	H	524	0	504	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	406	0	437	5	0
10	J	495	0	493	2	0
11	K	438	0	447	2	0
12	C	86	0	60	2	0
12	D	43	0	30	2	0
13	C	23	0	12	1	0
14	E	4	0	0	0	0
15	A	38	0	0	0	0
15	B	53	0	0	1	0
15	C	84	0	0	0	0
15	D	34	0	0	0	0
15	F	27	0	0	0	0
15	G	13	0	0	0	0
15	H	2	0	0	0	0
15	I	6	0	0	0	0
15	J	7	0	0	0	0
15	K	3	0	0	0	0
All	All	16900	0	16474	89	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 3.

The worst 5 of 89 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)
5:E:103:LYS:CE	5:E:103:LYS:NZ	1.68	1.53
2:B:385:GLN:HE22	2:B:393:THR:H	1.22	0.88
3:C:217:LYS:HE3	7:G:2:ARG:HH22	1.48	0.76
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.73	0.70
2:B:248:ASN:HB3	2:B:250:ASP:HB2	1.79	0.65

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%)	427 (96%)	12 (3%)	5 (1%)	17	12
2	B	421/439 (96%)	396 (94%)	22 (5%)	3 (1%)	25	25
3	C	376/379 (99%)	356 (95%)	18 (5%)	2 (0%)	32	33
4	D	239/241 (99%)	215 (90%)	21 (9%)	3 (1%)	14	9
5	E	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	12	7
6	F	104/110 (94%)	102 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	68 (93%)	3 (4%)	2 (3%)	6	3
8	H	62/78 (80%)	60 (97%)	2 (3%)	0	100	100
9	I	55/78 (70%)	36 (66%)	11 (20%)	8 (14%)	0	0
10	J	58/62 (94%)	51 (88%)	7 (12%)	0	100	100
11	K	51/56 (91%)	45 (88%)	4 (8%)	2 (4%)	3	1
All	All	2077/2166 (96%)	1939 (93%)	110 (5%)	28 (1%)	14	9

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	224	ASP
2	B	437	ASP
3	C	29	SER
5	E	67	ASP

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%)	325 (88%)	45 (12%)	6	4
2	B	332/343 (97%)	297 (90%)	35 (10%)	8	6
3	C	326/327 (100%)	284 (87%)	42 (13%)	5	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	170 (82%)	36 (18%)	2	1
5	E	168/168 (100%)	149 (89%)	19 (11%)	7	5
6	F	96/98 (98%)	86 (90%)	10 (10%)	8	6
7	G	66/71 (93%)	56 (85%)	10 (15%)	3	2
8	H	61/74 (82%)	43 (70%)	18 (30%)	0	0
9	I	44/60 (73%)	27 (61%)	17 (39%)	0	0
10	J	50/52 (96%)	41 (82%)	9 (18%)	2	1
11	K	43/46 (94%)	33 (77%)	10 (23%)	1	0
All	All	1762/1815 (97%)	1511 (86%)	251 (14%)	4	2

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	309	THR
4	D	116	ILE
9	I	56	ARG
3	C	336	THR
4	D	35	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	ASN
2	B	313	ASN
9	I	31	GLN
2	B	276	GLN
2	B	342	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	28,50,50	1.73	8 (28%)	17,82,82	1.04	1 (5%)
12	HEM	C	382	3	28,50,50	1.62	7 (25%)	17,82,82	1.39	2 (11%)
13	FDN	C	400	-	24,25,25	2.17	7 (29%)	24,37,37	1.74	6 (25%)
12	HEM	D	242	4	28,50,50	1.81	9 (32%)	17,82,82	1.32	2 (11%)
14	FES	E	200	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	-	0/6/54/54	0/0/8/8
12	HEM	C	382	3	-	0/6/54/54	0/0/8/8
13	FDN	C	400	-	-	0/10/29/29	0/3/3/3
12	HEM	D	242	4	-	0/6/54/54	0/0/8/8
14	FES	E	200	5	-	0/0/4/4	0/1/1/1

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C3C-C2C	-3.56	1.35	1.40
13	C	400	FDN	C21-N1	-2.97	1.36	1.41
13	C	400	FDN	N1-N2	-2.94	1.34	1.40
12	D	242	HEM	C3C-C2C	-2.69	1.36	1.40
12	D	242	HEM	C3B-C2B	-2.53	1.37	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	400	FDN	C12-C13-C8	-3.04	120.67	124.07
12	C	382	HEM	CBD-CAD-C3D	-2.41	107.87	112.47
13	C	400	FDN	O6-C6-C5	-2.39	123.99	126.08
12	C	381	HEM	CBD-CAD-C3D	-2.18	108.31	112.47
13	C	400	FDN	C10-C11-C12	-2.14	120.48	123.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	2	0
13	C	400	FDN	1	0
12	D	242	HEM	2	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 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.