wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:19 PM GMT

PDB ID	:	1EZV
Title	:	STRUCTURE OF THE YEAST CYTOCHROME BC1 COMPLEX CO-CRYSTALLIZED WITH AN ANTIBODY FV-FRAGMENT
Authors	:	Hunte, C.; Koepke, J.; Lange, C.; Rossmanith, T.; Michel, H.
Deposited on	:	2000-05-12
Resolution	:	2.30 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:

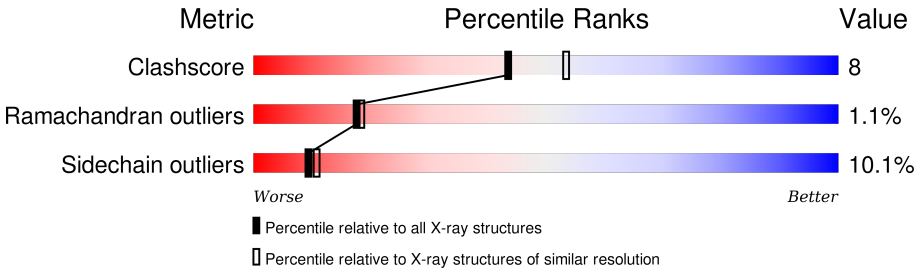
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	430	71% 25%
2	B	352	60% 34% 6%
3	C	385	84% 15%
4	D	245	85% 14%
5	E	185	82% 17%
6	H	74	78% 16% 5%
7	F	125	81% 15%

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Mol	Chain	Length	Quality of chain
8	G	93	
9	I	55	
10	X	127	
11	Y	107	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	SMA	C	505	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 17781 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	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP P07256
A	152	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			

- Molecule 4 is a protein called CYTOCHROME C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1934	1232	333	360	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 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	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 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	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	G	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 KD PROTEIN.

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

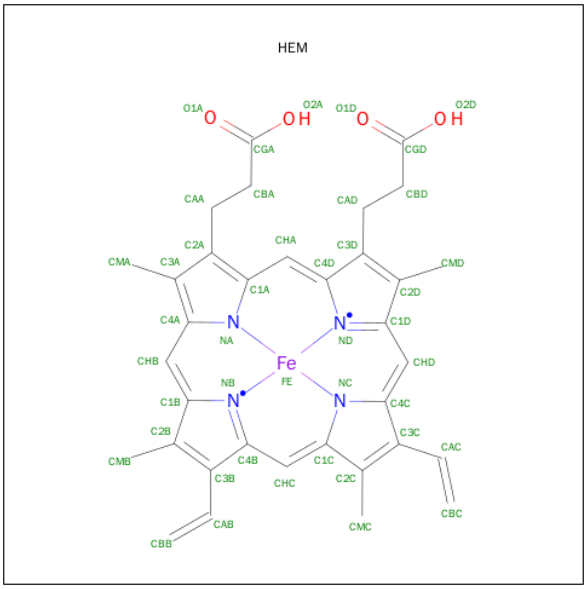
- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	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.

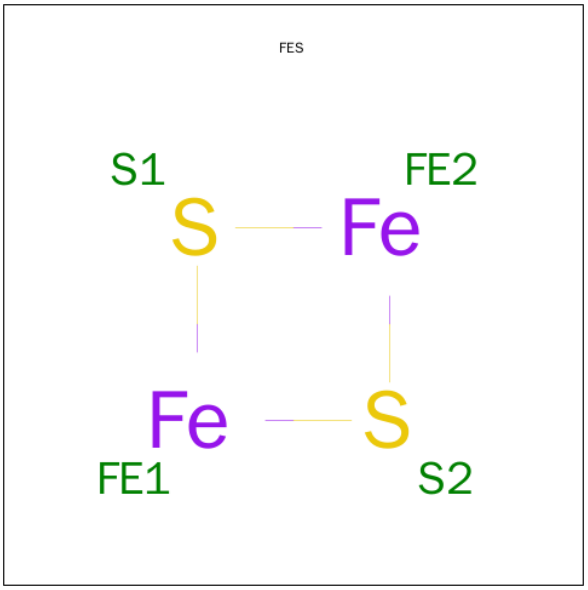
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

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



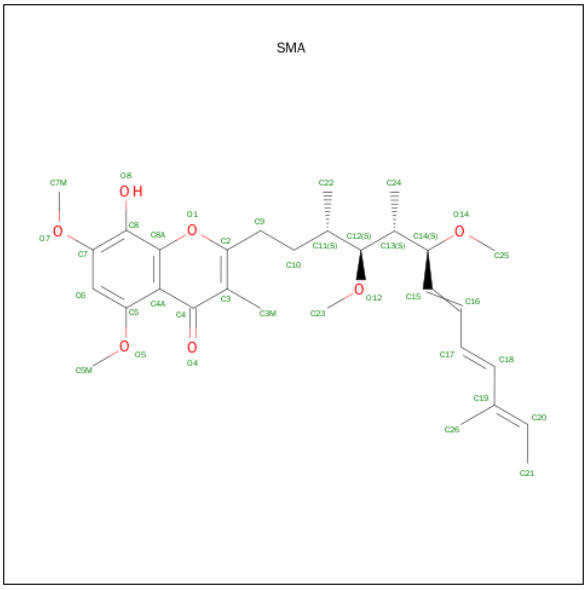
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



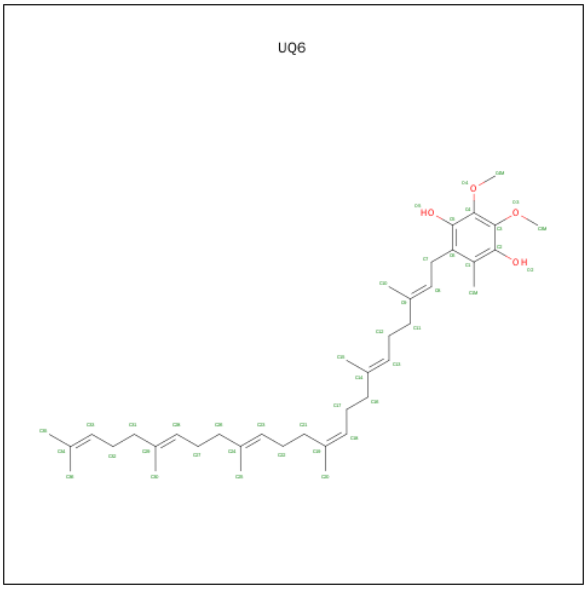
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	E	1	Total Fe S 4 2 2	0	0

- Molecule 14 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C O 37 30 7	0	0

- Molecule 15 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$).



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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	47	Total O 47 47	0	0
16	B	11	Total O 11 11	0	0
16	C	114	Total O 114 114	0	0
16	D	71	Total O 71 71	0	0
16	E	33	Total O 33 33	0	0
16	F	36	Total O 36 36	0	0
16	G	20	Total O 20 20	0	0
16	H	6	Total O 6 6	0	0
16	I	1	Total O 1 1	0	0
16	X	5	Total O 5 5	0	0
16	Y	2	Total O 2 2	0	0

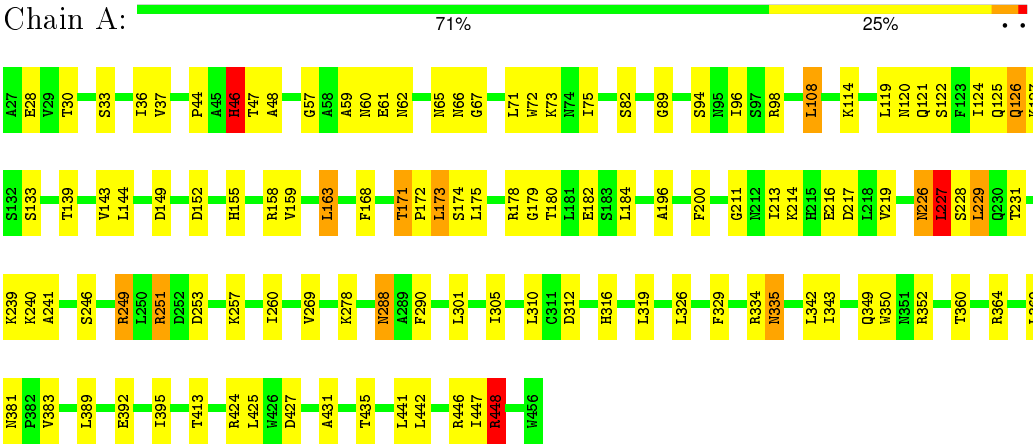
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

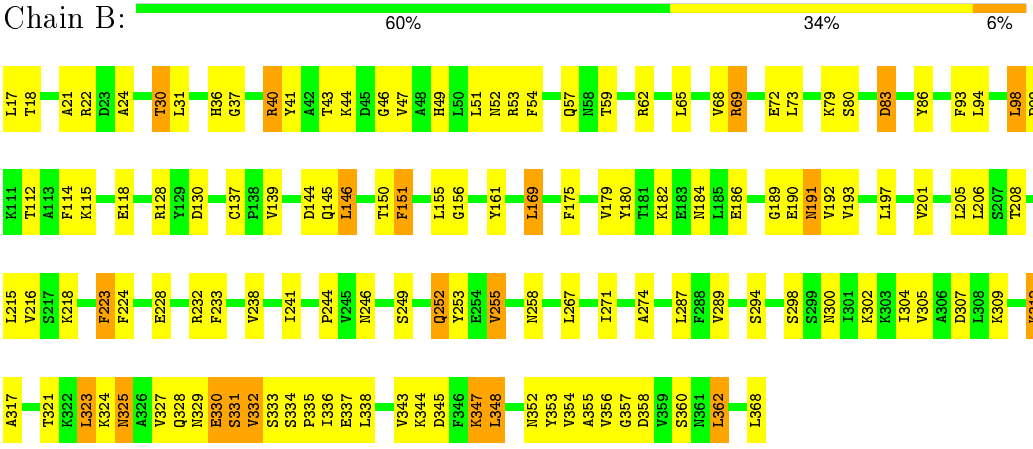
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

Chain A:



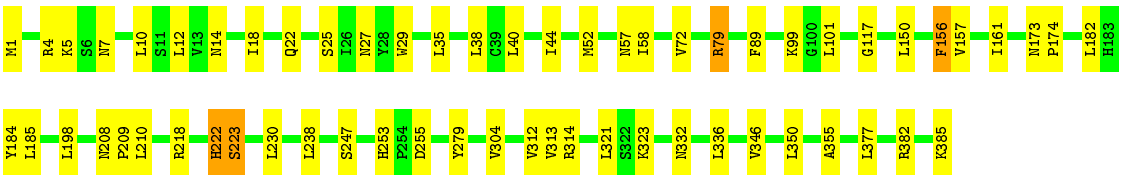
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



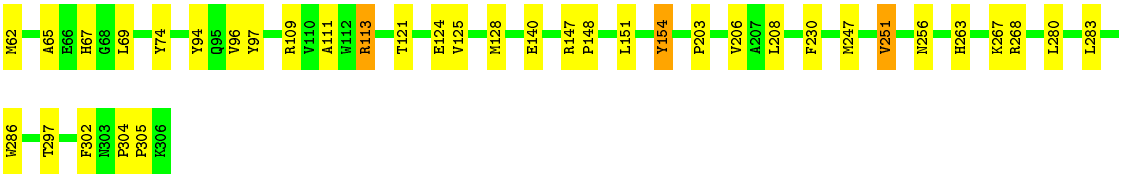
• Molecule 3: CYTOCHROME B

Chain C:



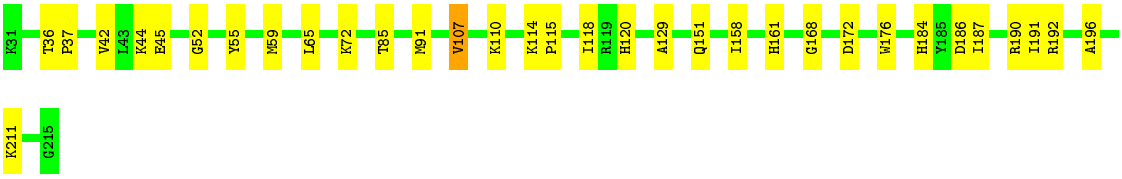
• Molecule 4: CYTOCHROME C1

Chain D:



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

Chain E:



• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain H:

• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain F:

• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

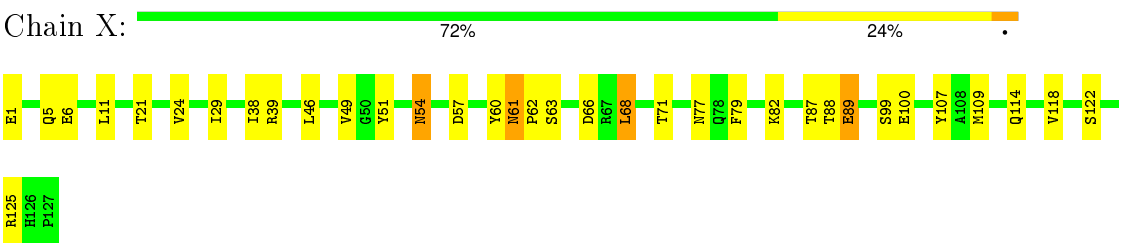
Chain G:

• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:

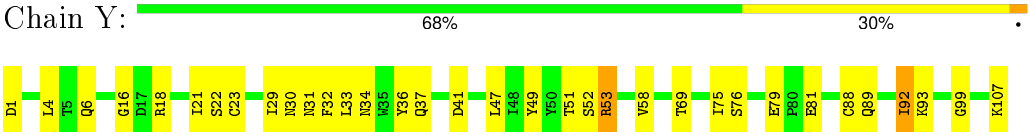
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain X:



• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain Y:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	214.47Å 163.92Å 147.27Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	84.7 (15.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17781	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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, SMA, 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	0.34	0/3399	0.49	0/4606
2	B	0.31	0/2781	0.47	0/3764
3	C	0.44	0/3191	0.53	0/4353
4	D	0.34	0/1994	0.48	0/2714
5	E	0.35	0/1444	0.52	0/1957
6	H	0.33	0/638	0.42	0/858
7	F	0.34	0/1032	0.52	1/1397 (0.1%)
8	G	0.38	0/804	0.43	0/1088
9	I	0.40	0/462	0.43	0/622
10	X	0.32	0/1043	0.47	0/1422
11	Y	0.31	0/863	0.43	0/1172
All	All	0.36	0/17651	0.49	1/23953 (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
1	A	0	4
2	B	0	2
3	C	0	5
4	D	0	4
5	E	0	1
6	H	0	1
7	F	0	1
8	G	0	1
10	X	0	1
11	Y	0	1
All	All	0	21

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	71	ARG	NE-CZ-NH1	-5.33	117.63	120.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	LEU	Peptide
1	A	249	ARG	Sidechain
1	A	446	ARG	Sidechain
1	A	448	ARG	Sidechain
2	B	69	ARG	Sidechain

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	3338	0	3316	66	0
2	B	2735	0	2774	79	0
3	C	3089	0	3125	27	0
4	D	1934	0	1855	18	0
5	E	1411	0	1386	22	0
6	H	624	0	581	9	0
7	F	1012	0	1026	14	0
8	G	773	0	736	6	0
9	I	449	0	445	7	0
10	X	1015	0	959	20	0
11	Y	842	0	820	16	0
12	C	86	0	60	3	0
12	D	43	0	30	0	0
13	E	4	0	0	0	0
14	C	37	0	40	5	0
15	C	43	0	58	12	0
16	A	47	0	0	1	0
16	B	11	0	0	0	0
16	C	114	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	D	71	0	0	0	0
16	E	33	0	0	0	0
16	F	36	0	0	2	0
16	G	20	0	0	1	0
16	H	6	0	0	0	0
16	I	1	0	0	0	0
16	X	5	0	0	1	0
16	Y	2	0	0	0	0
All	All	17781	0	17211	279	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 8.

The worst 5 of 279 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)
15:C:506:UQ6:H103	15:C:506:UQ6:H1M1	1.11	1.09
15:C:506:UQ6:H103	15:C:506:UQ6:C1M	1.93	0.98
15:C:506:UQ6:H1M1	15:C:506:UQ6:C10	1.97	0.92
6:H:77:GLN:H	6:H:77:GLN:HE21	1.11	0.91
2:B:347:LYS:HD3	2:B:347:LYS:H	1.43	0.82

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	428/430 (100%)	396 (92%)	27 (6%)	5 (1%)	16 16
2	B	350/352 (99%)	311 (89%)	31 (9%)	8 (2%)	8 6
3	C	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	46 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	243/245 (99%)	238 (98%)	5 (2%)	0	100 100
5	E	183/185 (99%)	174 (95%)	7 (4%)	2 (1%)	17 18
6	H	72/74 (97%)	68 (94%)	4 (6%)	0	100 100
7	F	123/125 (98%)	120 (98%)	3 (2%)	0	100 100
8	G	91/93 (98%)	76 (84%)	10 (11%)	5 (6%)	2 1
9	I	53/55 (96%)	50 (94%)	3 (6%)	0	100 100
10	X	125/127 (98%)	116 (93%)	9 (7%)	0	100 100
11	Y	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	6 3
All	All	2156/2178 (99%)	2009 (93%)	123 (6%)	24 (1%)	17 18

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	336	ILE
8	G	52	PHE
8	G	93	ASN
2	B	313	ASP
2	B	329	ASN

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	369/369 (100%)	323 (88%)	46 (12%)	6 6
2	B	301/301 (100%)	254 (84%)	47 (16%)	3 3
3	C	338/338 (100%)	312 (92%)	26 (8%)	16 20
4	D	203/203 (100%)	195 (96%)	8 (4%)	39 53
5	E	151/151 (100%)	145 (96%)	6 (4%)	38 52
6	H	67/67 (100%)	59 (88%)	8 (12%)	6 7
7	F	109/109 (100%)	100 (92%)	9 (8%)	14 17
8	G	77/77 (100%)	69 (90%)	8 (10%)	9 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	45/45 (100%)	41 (91%)	4 (9%)	12 14
10	X	112/112 (100%)	95 (85%)	17 (15%)	3 3
11	Y	93/93 (100%)	83 (89%)	10 (11%)	8 9
All	All	1865/1865 (100%)	1676 (90%)	189 (10%)	9 11

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

Mol	Chain	Res	Type
2	B	337	GLU
3	C	185	LEU
10	X	79	PHE
2	B	345	ASP
3	C	35	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	14	ASN
3	C	332	ASN
10	X	114	GLN
3	C	173	ASN
4	D	79	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)

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	401	3	30,50,50	3.02	11 (36%)	24,82,82	2.43	9 (37%)
12	HEM	C	402	3	30,50,50	2.80	12 (40%)	24,82,82	2.48	7 (29%)
14	SMA	C	505	-	35,38,38	1.90	8 (22%)	40,52,52	2.16	12 (30%)
15	UQ6	C	506	-	43,43,43	2.55	17 (39%)	52,55,55	2.28	17 (32%)
12	HEM	D	3	4	30,50,50	2.58	8 (26%)	24,82,82	3.23	8 (33%)
13	FES	E	4	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	401	3	-	0/10/54/54	0/0/8/8
12	HEM	C	402	3	-	0/10/54/54	0/0/8/8
14	SMA	C	505	-	2/2/5/10	0/33/34/34	0/2/2/2
15	UQ6	C	506	-	-	0/39/39/39	0/1/1/1
12	HEM	D	3	4	-	0/10/54/54	0/0/8/8
13	FES	E	4	5	-	0/0/4/4	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	402	HEM	C3B-C4B	-7.77	1.44	1.51
12	C	401	HEM	C3B-C4B	-7.77	1.44	1.51
12	D	3	HEM	C3B-C4B	-7.45	1.45	1.51
15	C	506	UQ6	O5-C5	-6.94	1.20	1.37
12	C	401	HEM	C3B-CAB	-6.64	1.38	1.51

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	3	HEM	C3B-CAB-CBB	-9.02	110.61	124.46
12	D	3	HEM	C3C-CAC-CBC	-8.18	111.91	124.46
14	C	505	SMA	C26-C19-C18	-5.95	108.19	118.10
12	C	401	HEM	C3C-CAC-CBC	-4.23	117.97	124.46
14	C	505	SMA	C3-C4-C4A	-4.21	115.51	121.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	505	SMA	C12
14	C	505	SMA	C14

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	401	HEM	2	0
12	C	402	HEM	1	0
14	C	505	SMA	5	0
15	C	506	UQ6	12	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.