wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1KYO
Title	:	YEAST CYTOCHROME BC1 COMPLEX WITH BOUND SUBSTRATE CYTOCHROME C
Authors	:	Lange, C.; Hunte, C.
Deposited on	:	2002-02-05
Resolution	:	2.97 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:

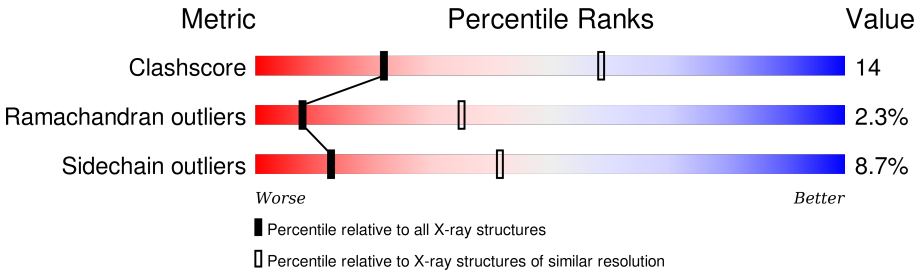
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.97 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	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)

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	70% 26% •
1	L	430	65% 30% 5%
2	B	352	58% 36% 6% •
2	M	352	58% 35% 7% •
3	C	385	70% 27% •
3	N	385	73% 23% •
4	D	248	80% 17% ••

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Mol	Chain	Length	Quality of chain
4	O	248	75% 23%
5	E	185	69% 28%
5	P	185	75% 24%
6	F	74	70% 28%
6	Q	74	73% 24%
7	G	126	77% 21%
7	R	126	74% 23%
8	H	93	63% 30% 5%
8	S	93	66% 27% 6%
9	I	57	65% 26% 7%
9	T	57	74% 16% 7%
10	J	127	51% 38% 10%
10	U	127	50% 43% 7%
11	K	107	56% 36% 7%
11	V	107	56% 39% 5%
12	W	108	61% 31% 7%

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
15	SMA	C	505	X	-	-	-
15	SMA	N	525	X	-	-	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 35643 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			
1	L	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			

There are 4 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
L	?	-	SER	DELETION	UNP P07256
L	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			
2	M	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			
3	N	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	270	VAL	ASP	SEE REMARK 999	UNP P00163
N	270	VAL	ASP	SEE REMARK 999	UNP P00163

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1929	1229	332	359	9			
4	O	245	Total	C	N	O	S	0	0	0
			1929	1229	332	359	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			
5	P	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	F	74	Total	C	N	O	S	0	0	0
			625	390	108	125	2			
6	Q	74	Total	C	N	O	S	0	0	0
			625	390	108	125	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	74	ASP	VAL	CONFLICT	UNP P00127
Q	74	ASP	VAL	CONFLICT	UNP P00127

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			
7	R	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	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	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	53	Total	C	N	O	0	0	0
			436	292	71	73			
9	T	53	Total	C	N	O	0	0	0
			436	292	71	73			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	55	LYS	ARG	CONFLICT	UNP P22289
T	55	LYS	ARG	CONFLICT	UNP P22289

- 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			
10	U	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			
11	V	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

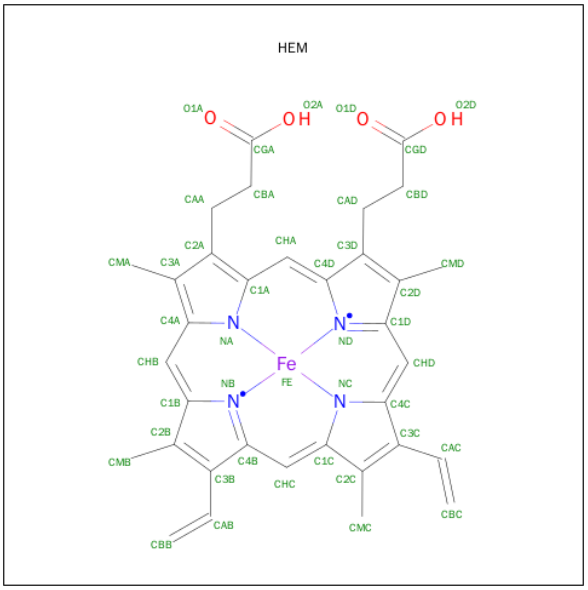
- Molecule 12 is a protein called CYTOCHROME C, ISO-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	0	0
			850	537	151	157	5			

There is a discrepancy between the modelled and reference sequences:

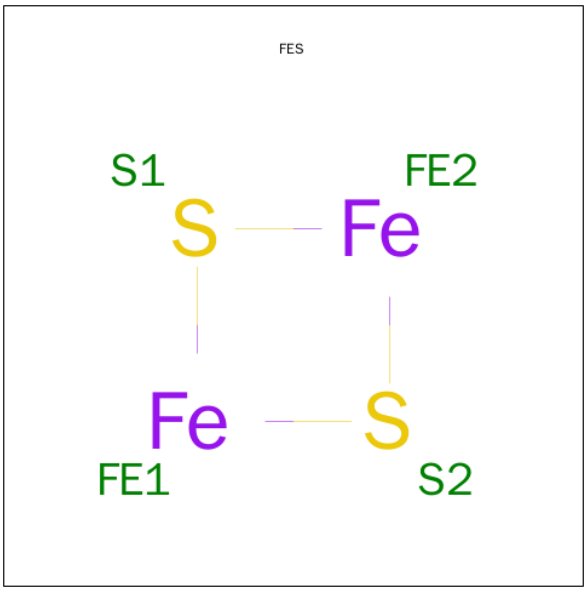
Chain	Residue	Modelled	Actual	Comment	Reference
W	77	M3L	LYS	MODIFIED RESIDUE	UNP P00044

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



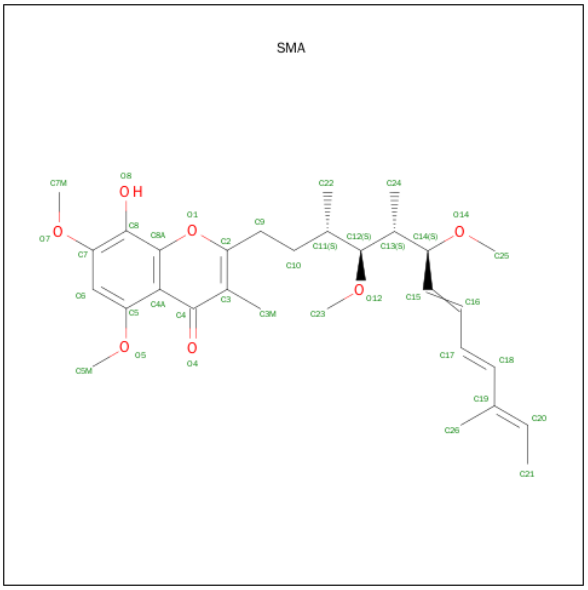
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4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

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 15 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



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

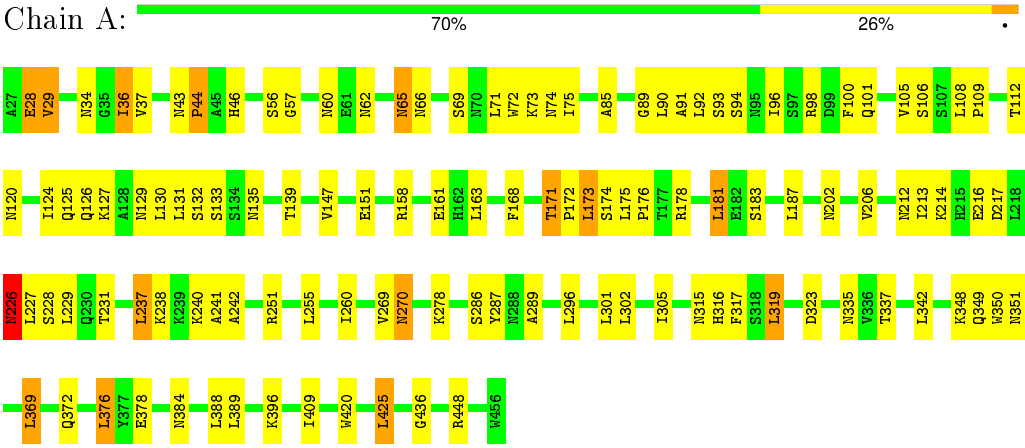
3 Residue-property plots (i)

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.

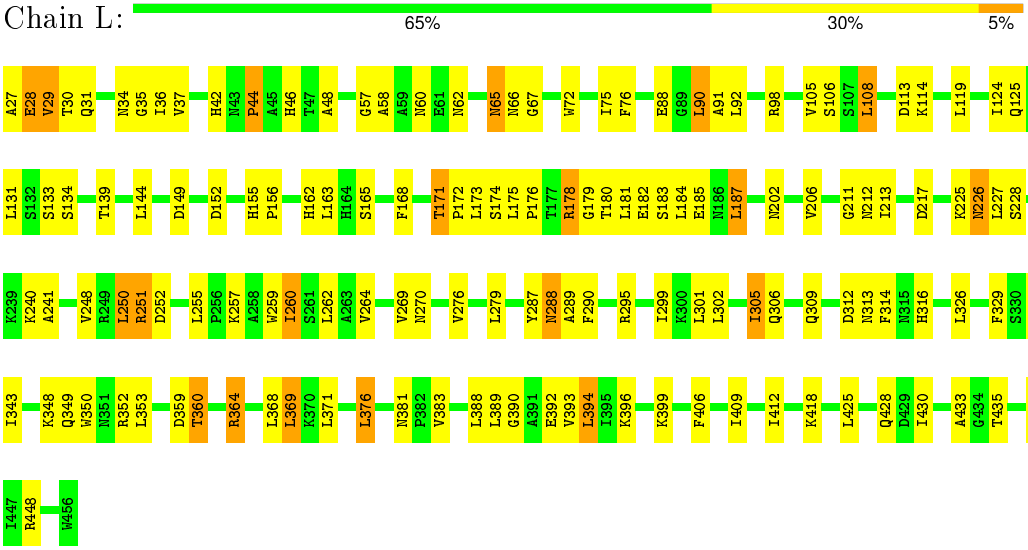
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

Chain A:



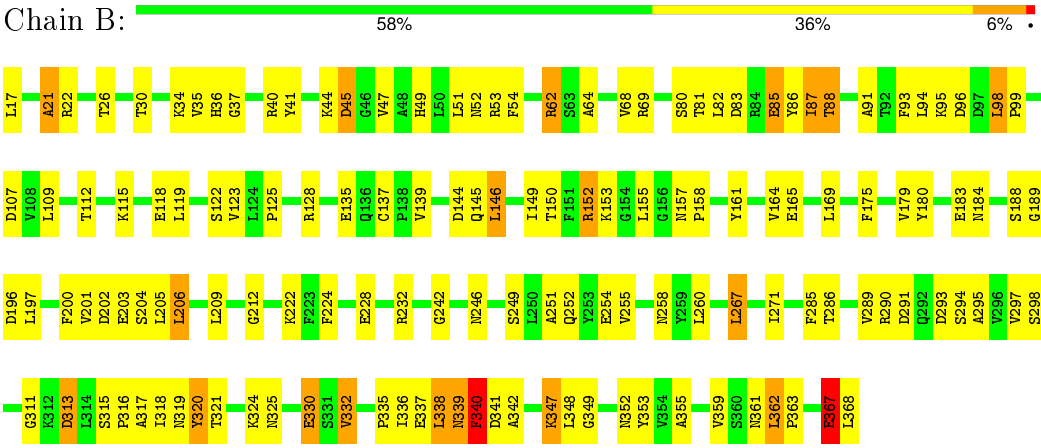
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

Chain L:



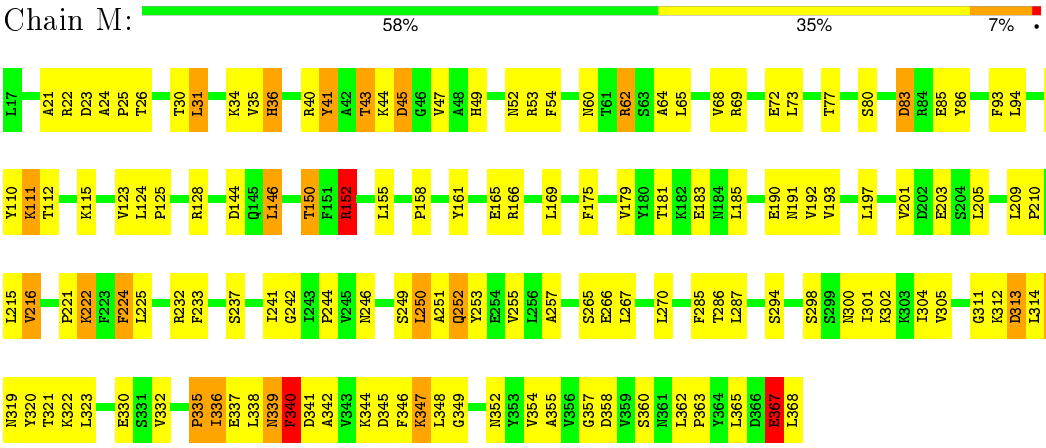
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



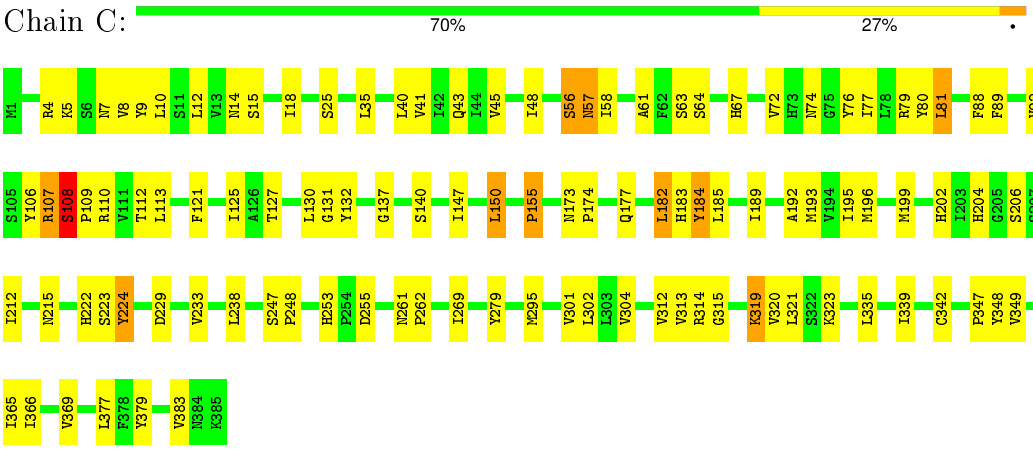
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain M:



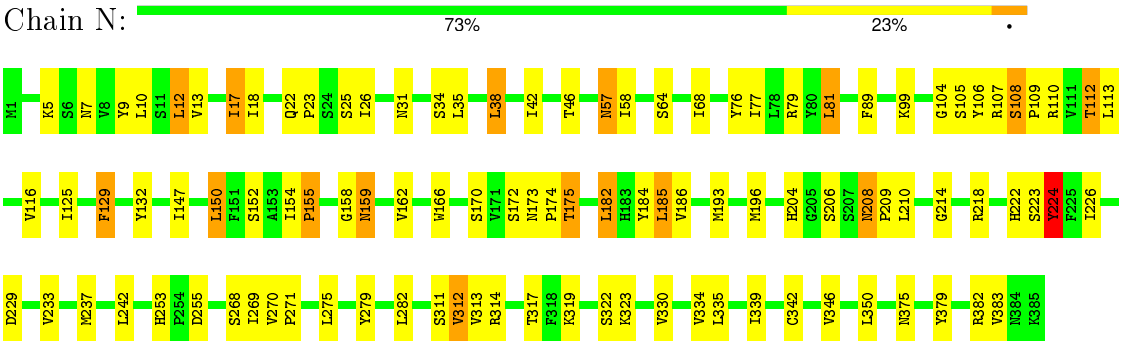
• Molecule 3: CYTOCHROME B

Chain C:



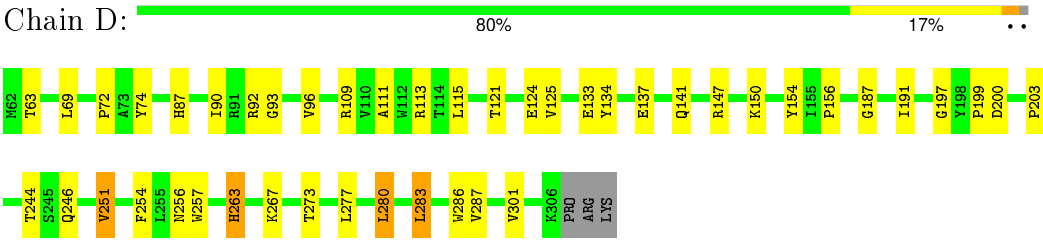
• Molecule 3: CYTOCHROME B

Chain N:



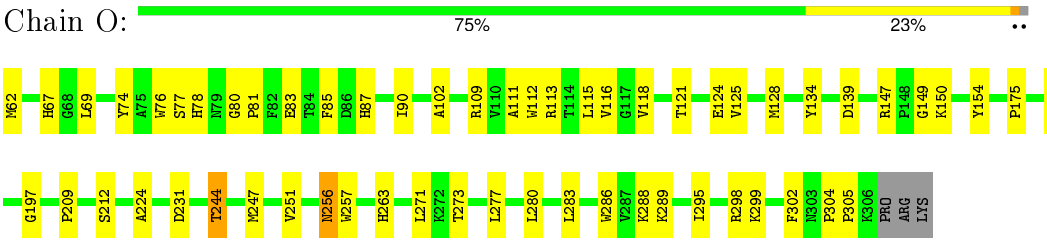
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain D:



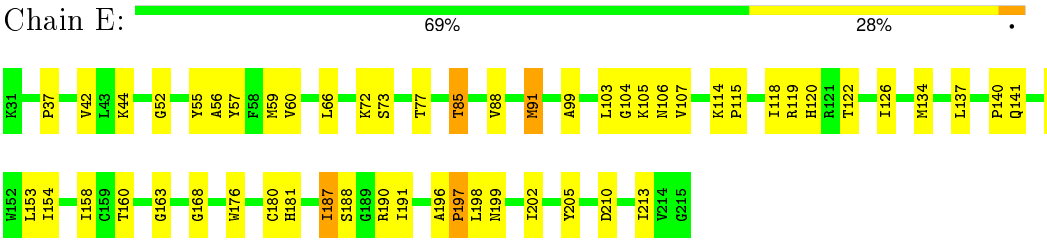
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain O:



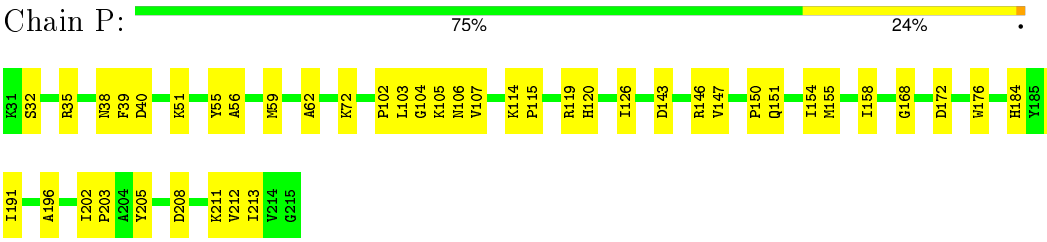
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E:



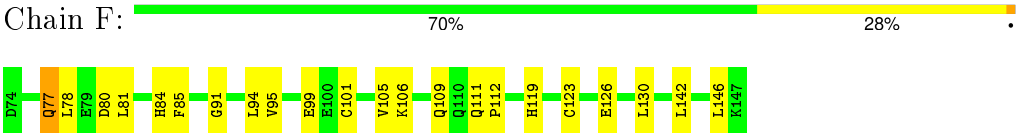
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain P:



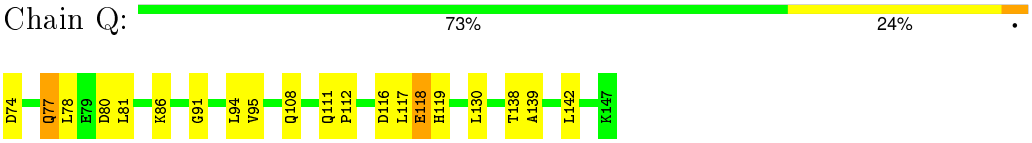
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain F:



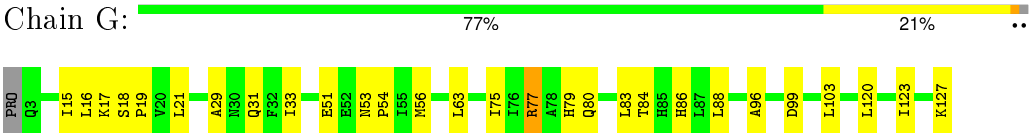
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain Q:



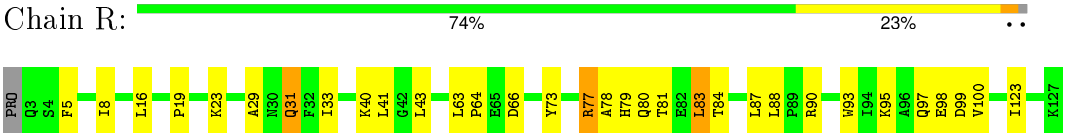
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain G:



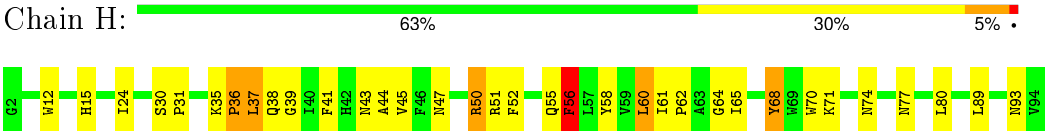
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain R:



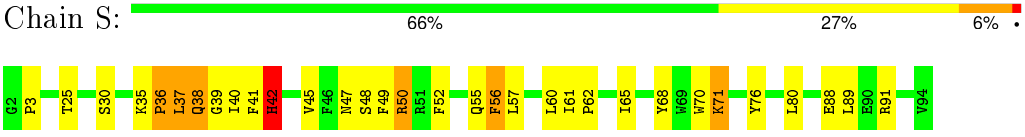
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain H:



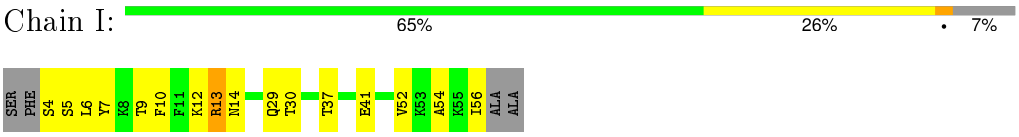
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain S:



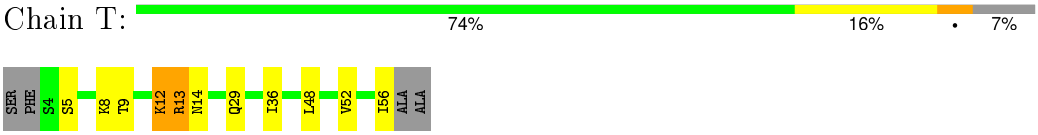
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:



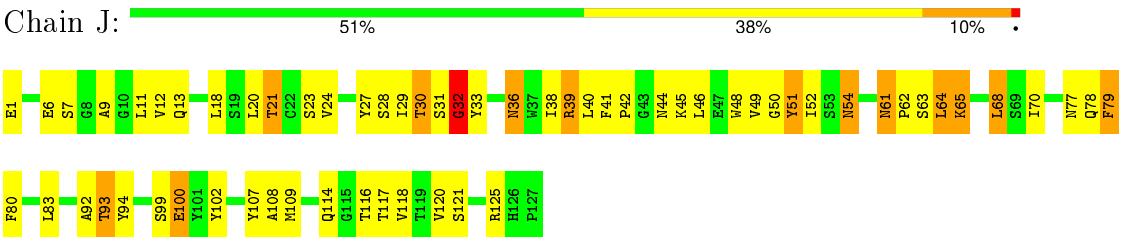
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain T:



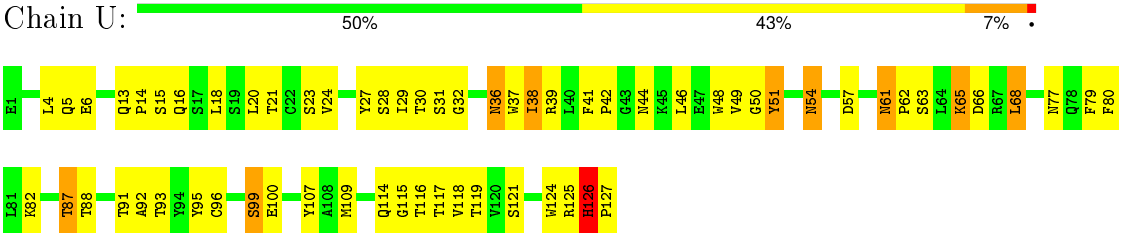
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J:



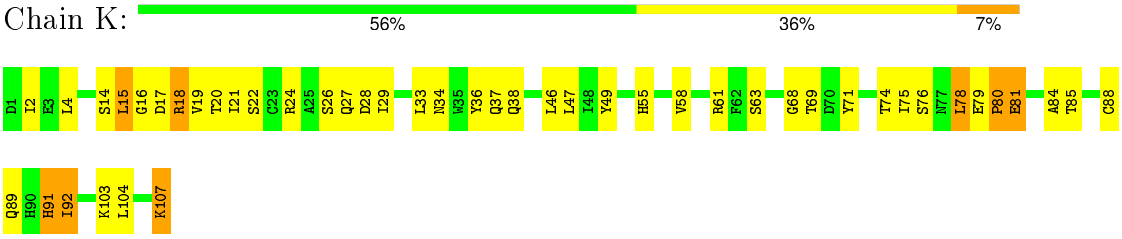
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain U:



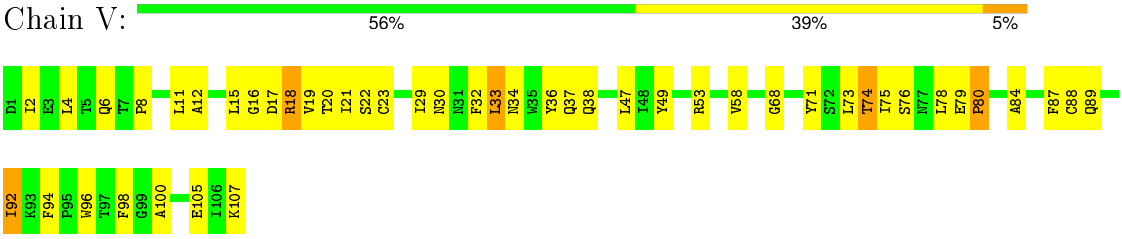
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K:



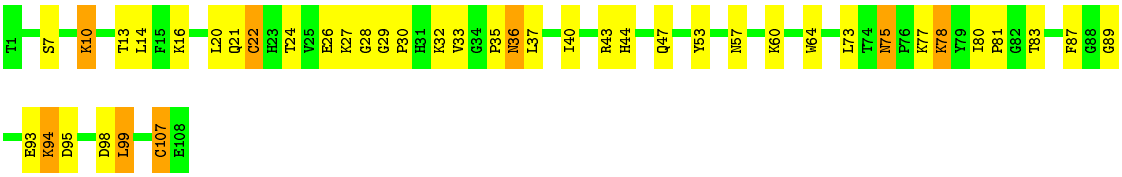
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain V:



• Molecule 12: CYTOCHROME C, ISO-1

Chain W:


T1
S7
K10
T13
L14
F15
K16
L20
Q21
C22
H23
T24
V25
E26
K27
G28
G29
P30
H31
K32
V33
G34
P35
N36
L37
I40
R43
H44
Q47
Y53
N57
K60
W64
L73
T74
N75
P76
K77
K78
Y79
I80
P81
G82
T83
F87
G88
G89
E93
K94
D95
D98
L99
C107
E108

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	147.22Å 165.53Å 195.89Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	29.64 – 2.97	Depositor
% Data completeness (in resolution range)	93.7 (29.64-2.97)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35643	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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, M3L, FES, SMA

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	0.40	0/3399	0.63	0/4606
1	L	0.40	0/3399	0.63	1/4606 (0.0%)
2	B	0.37	0/2781	0.68	2/3764 (0.1%)
2	M	0.38	0/2781	0.68	1/3764 (0.0%)
3	C	0.50	0/3191	0.68	0/4353
3	N	0.49	0/3191	0.70	0/4353
4	D	0.41	0/1989	0.64	0/2710
4	O	0.41	0/1989	0.63	0/2710
5	E	0.41	0/1444	0.67	1/1957 (0.1%)
5	P	0.39	0/1444	0.67	0/1957
6	F	0.39	0/639	0.59	0/859
6	Q	0.39	0/639	0.61	0/859
7	G	0.42	0/1032	0.69	0/1397
7	R	0.43	0/1032	0.68	0/1397
8	H	0.49	0/804	0.65	0/1088
8	S	0.52	0/804	0.61	0/1088
9	I	0.43	0/449	0.55	0/605
9	T	0.44	0/449	0.56	0/605
10	J	0.38	0/1043	0.68	1/1422 (0.1%)
10	U	0.38	0/1043	0.68	1/1422 (0.1%)
11	K	0.35	0/863	0.58	0/1172
11	V	0.36	0/863	0.62	0/1172
12	W	0.52	0/856	0.68	0/1145
All	All	0.42	0/36124	0.66	7/49011 (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
3	N	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	32	GLY	N-CA-C	8.27	133.77	113.10
10	J	32	GLY	N-CA-C	6.98	130.55	113.10
2	B	340	PHE	N-CA-C	-6.37	93.80	111.00
2	M	340	PHE	N-CA-C	-6.34	93.87	111.00
5	E	163	GLY	N-CA-C	5.42	126.66	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	224	TYR	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	87	0
1	L	3338	0	3316	101	0
2	B	2735	0	2774	98	0
2	M	2735	0	2774	107	0
3	C	3089	0	3125	87	0
3	N	3089	0	3125	84	0
4	D	1929	0	1844	25	0
4	O	1929	0	1844	43	0
5	E	1411	0	1386	49	0
5	P	1411	0	1386	38	0
6	F	625	0	576	11	0
6	Q	625	0	576	9	0
7	G	1012	0	1026	18	0
7	R	1012	0	1026	21	0
8	H	773	0	736	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	773	0	736	29	0
9	I	436	0	435	10	0
9	T	436	0	435	12	0
10	J	1015	0	959	48	0
10	U	1015	0	959	47	0
11	K	842	0	820	40	0
11	V	842	0	820	41	0
12	W	850	0	854	27	0
13	C	86	0	60	7	0
13	D	43	0	30	0	0
13	N	86	0	60	3	0
13	O	43	0	30	3	0
13	W	43	0	30	2	0
14	E	4	0	0	1	0
14	P	4	0	0	0	0
15	C	37	0	40	4	0
15	N	37	0	40	4	0
All	All	35643	0	35138	991	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 991 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:49:HIS:HD2	2:B:161:TYR:H	1.08	0.97
2:M:49:HIS:HD2	2:M:161:TYR:H	1.13	0.96
7:R:31:GLN:HE21	7:R:31:GLN:HA	1.31	0.96
1:L:62:ASN:H	1:L:65:ASN:HD21	1.13	0.95
1:A:62:ASN:HB2	1:A:65:ASN:HD21	1.31	0.95

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%)	374 (87%)	47 (11%)	7 (2%)	12	46
1	L	428/430 (100%)	384 (90%)	37 (9%)	7 (2%)	12	46
2	B	350/352 (99%)	286 (82%)	47 (13%)	17 (5%)	3	15
2	M	350/352 (99%)	283 (81%)	48 (14%)	19 (5%)	2	12
3	C	383/385 (100%)	357 (93%)	21 (6%)	5 (1%)	15	52
3	N	383/385 (100%)	354 (92%)	24 (6%)	5 (1%)	15	52
4	D	243/248 (98%)	222 (91%)	20 (8%)	1 (0%)	39	79
4	O	243/248 (98%)	225 (93%)	14 (6%)	4 (2%)	12	46
5	E	183/185 (99%)	161 (88%)	19 (10%)	3 (2%)	12	46
5	P	183/185 (99%)	163 (89%)	20 (11%)	0	100	100
6	F	72/74 (97%)	65 (90%)	7 (10%)	0	100	100
6	Q	72/74 (97%)	62 (86%)	10 (14%)	0	100	100
7	G	123/126 (98%)	113 (92%)	8 (6%)	2 (2%)	12	46
7	R	123/126 (98%)	120 (98%)	2 (2%)	1 (1%)	24	65
8	H	91/93 (98%)	79 (87%)	8 (9%)	4 (4%)	3	17
8	S	91/93 (98%)	73 (80%)	13 (14%)	5 (6%)	2	12
9	I	51/57 (90%)	45 (88%)	6 (12%)	0	100	100
9	T	51/57 (90%)	45 (88%)	5 (10%)	1 (2%)	9	39
10	J	125/127 (98%)	110 (88%)	11 (9%)	4 (3%)	5	25
10	U	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	7	34
11	K	105/107 (98%)	85 (81%)	14 (13%)	6 (6%)	2	11
11	V	105/107 (98%)	83 (79%)	17 (16%)	5 (5%)	3	15
12	W	105/108 (97%)	89 (85%)	14 (13%)	2 (2%)	10	41
All	All	4413/4476 (99%)	3885 (88%)	427 (10%)	101 (2%)	8	35

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
2	B	95	LYS
2	B	152	ARG
2	B	335	PRO

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Mol	Chain	Res	Type
2	B	336	ILE

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%)	333 (90%)	36 (10%)	10 35
1	L	369/369 (100%)	328 (89%)	41 (11%)	8 28
2	B	301/301 (100%)	272 (90%)	29 (10%)	10 36
2	M	301/301 (100%)	269 (89%)	32 (11%)	8 30
3	C	338/338 (100%)	311 (92%)	27 (8%)	15 45
3	N	338/338 (100%)	311 (92%)	27 (8%)	15 45
4	D	202/206 (98%)	190 (94%)	12 (6%)	24 61
4	O	202/206 (98%)	193 (96%)	9 (4%)	34 72
5	E	151/151 (100%)	141 (93%)	10 (7%)	21 56
5	P	151/151 (100%)	145 (96%)	6 (4%)	38 75
6	F	67/67 (100%)	60 (90%)	7 (10%)	9 31
6	Q	67/67 (100%)	58 (87%)	9 (13%)	5 19
7	G	109/110 (99%)	104 (95%)	5 (5%)	33 71
7	R	109/110 (99%)	101 (93%)	8 (7%)	17 51
8	H	77/77 (100%)	70 (91%)	7 (9%)	12 39
8	S	77/77 (100%)	69 (90%)	8 (10%)	9 31
9	I	45/47 (96%)	41 (91%)	4 (9%)	12 40
9	T	45/47 (96%)	44 (98%)	1 (2%)	60 87
10	J	112/112 (100%)	99 (88%)	13 (12%)	7 26
10	U	112/112 (100%)	96 (86%)	16 (14%)	4 17
11	K	93/93 (100%)	87 (94%)	6 (6%)	21 57
11	V	93/93 (100%)	87 (94%)	6 (6%)	21 57
12	W	88/88 (100%)	76 (86%)	12 (14%)	5 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3816/3830 (100%)	3485 (91%)	331 (9%)	13 41

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	100	GLU
1	L	331	THR
10	U	66	ASP
11	K	92	ILE
1	L	173	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	90	HIS
1	L	335	ASN
10	U	61	ASN
1	L	60	ASN
1	L	155	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	M3L	W	77	12	10,11,12	0.61	0	12,14,16	1.19	1 (8%)

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	M3L	W	77	12	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	W	77	M3L	CM3-NZ-CM2	-2.86	101.61	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	W	77	M3L	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
13	HEM	C	501	3	30,50,50	3.22	10 (33%)	24,82,82	2.39	10 (41%)
13	HEM	C	502	3	30,50,50	3.06	10 (33%)	24,82,82	2.44	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SMA	C	505	-	35,38,38	1.89	6 (17%)	40,52,52	2.14	12 (30%)
13	HEM	D	503	4	30,50,50	2.75	10 (33%)	24,82,82	3.69	11 (45%)
14	FES	E	504	5	0,4,4	0.00	-	0,4,4	0.00	-
13	HEM	N	521	3	30,50,50	3.09	10 (33%)	24,82,82	2.09	8 (33%)
13	HEM	N	522	3	30,50,50	2.66	10 (33%)	24,82,82	2.47	8 (33%)
15	SMA	N	525	-	35,38,38	1.91	7 (20%)	40,52,52	2.21	12 (30%)
13	HEM	O	523	4	30,50,50	2.77	8 (26%)	24,82,82	3.41	11 (45%)
14	FES	P	524	5	0,4,4	0.00	-	0,4,4	0.00	-
13	HEM	W	526	12	30,50,50	2.86	13 (43%)	24,82,82	3.66	8 (33%)

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
13	HEM	C	501	3	-	0/10/54/54	0/0/8/8
13	HEM	C	502	3	-	0/10/54/54	0/0/8/8
15	SMA	C	505	-	2/2/5/10	0/33/34/34	0/2/2/2
13	HEM	D	503	4	-	0/10/54/54	0/0/8/8
14	FES	E	504	5	-	0/0/4/4	0/1/1/1
13	HEM	N	521	3	-	0/10/54/54	0/0/8/8
13	HEM	N	522	3	-	0/10/54/54	0/0/8/8
15	SMA	N	525	-	2/2/5/10	0/33/34/34	0/2/2/2
13	HEM	O	523	4	-	0/10/54/54	0/0/8/8
14	FES	P	524	5	-	0/0/4/4	0/1/1/1
13	HEM	W	526	12	-	0/10/54/54	0/0/8/8

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	503	HEM	C3B-C4B	-8.53	1.44	1.51
13	C	502	HEM	C3B-C4B	-8.40	1.44	1.51
13	W	526	HEM	C3B-C4B	-8.34	1.44	1.51
13	C	501	HEM	C3B-C4B	-8.33	1.44	1.51
13	O	523	HEM	C3B-C4B	-8.17	1.44	1.51

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	503	HEM	C3C-CAC-CBC	-11.39	106.99	124.46
13	O	523	HEM	C3C-CAC-CBC	-11.35	107.05	124.46
13	W	526	HEM	C3C-CAC-CBC	-10.29	108.67	124.46
13	W	526	HEM	C3B-CAB-CBB	-9.40	110.04	124.46
13	D	503	HEM	C3B-CAB-CBB	-8.42	111.54	124.46

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	N	525	SMA	C12
15	N	525	SMA	C14
15	C	505	SMA	C12
15	C	505	SMA	C14

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	501	HEM	6	0
13	C	502	HEM	1	0
15	C	505	SMA	4	0
14	E	504	FES	1	0
13	N	521	HEM	1	0
13	N	522	HEM	2	0
15	N	525	SMA	4	0
13	O	523	HEM	3	0
13	W	526	HEM	2	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 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.