



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BGY
Title : CYTOCHROME BC1 COMPLEX FROM BOVINE
Authors : Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.
Deposited on : 1998-06-02
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

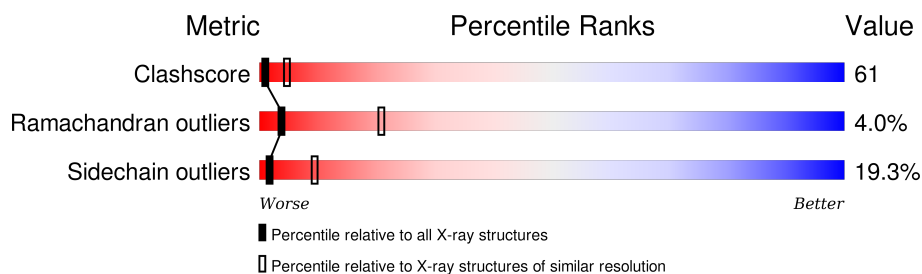
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	
1	M	446	
2	B	439	
2	N	439	
3	C	379	
3	O	379	
4	D	241	

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Mol	Chain	Length	Quality of chain
4	P	241	
5	E	196	
5	Q	196	
6	F	110	
6	R	110	
7	G	81	
7	S	81	
8	H	78	
8	T	78	
9	I	78	
9	U	78	
10	J	62	
10	V	62	
11	K	56	
11	W	56	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31486 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 CYTOCHROME BC1 COMPLEX.

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

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			
2	N	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			
3	O	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

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

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	75	Total	C	N	O	S	0	0	0
			566	352	94	118	2			
5	Q	196	Total	C	N	O	S	0	0	0
			1518	956	263	291	8			

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			
6	R	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			
7	S	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			
8	T	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			
9	U	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			

- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			512	335	89	88			

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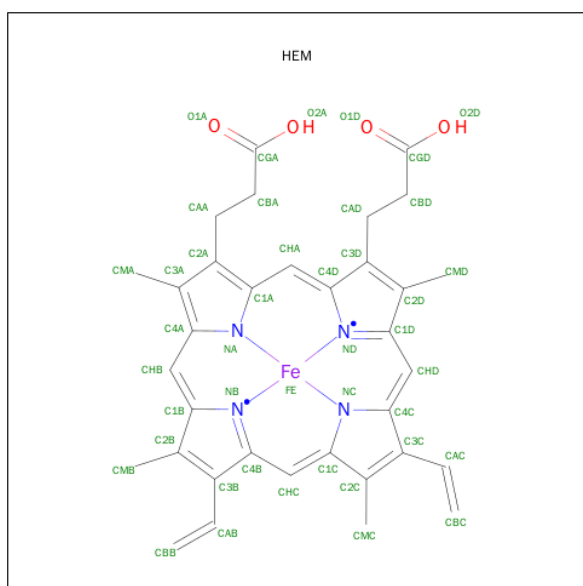
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	62	Total	C	N	O	0	0	0
			512	335	89	88			

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

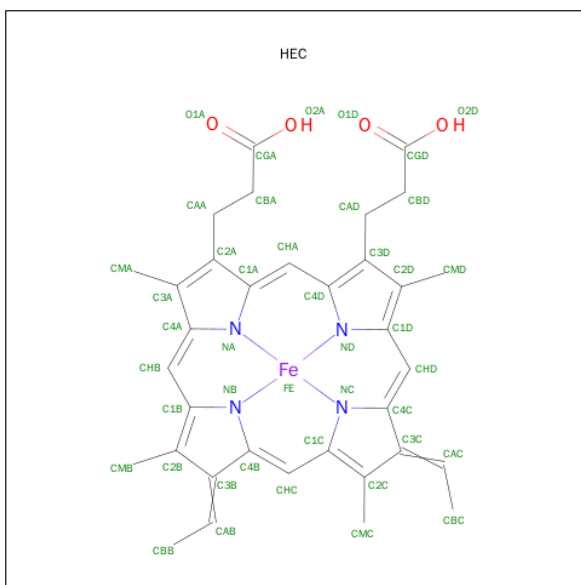
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	22	Total	C	N	O	0	0	0
			159	103	29	27			
11	W	22	Total	C	N	O	0	0	0
			159	103	29	27			

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



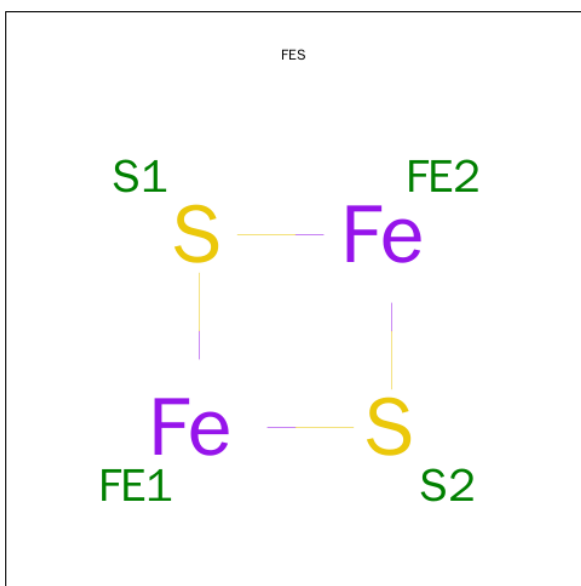
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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



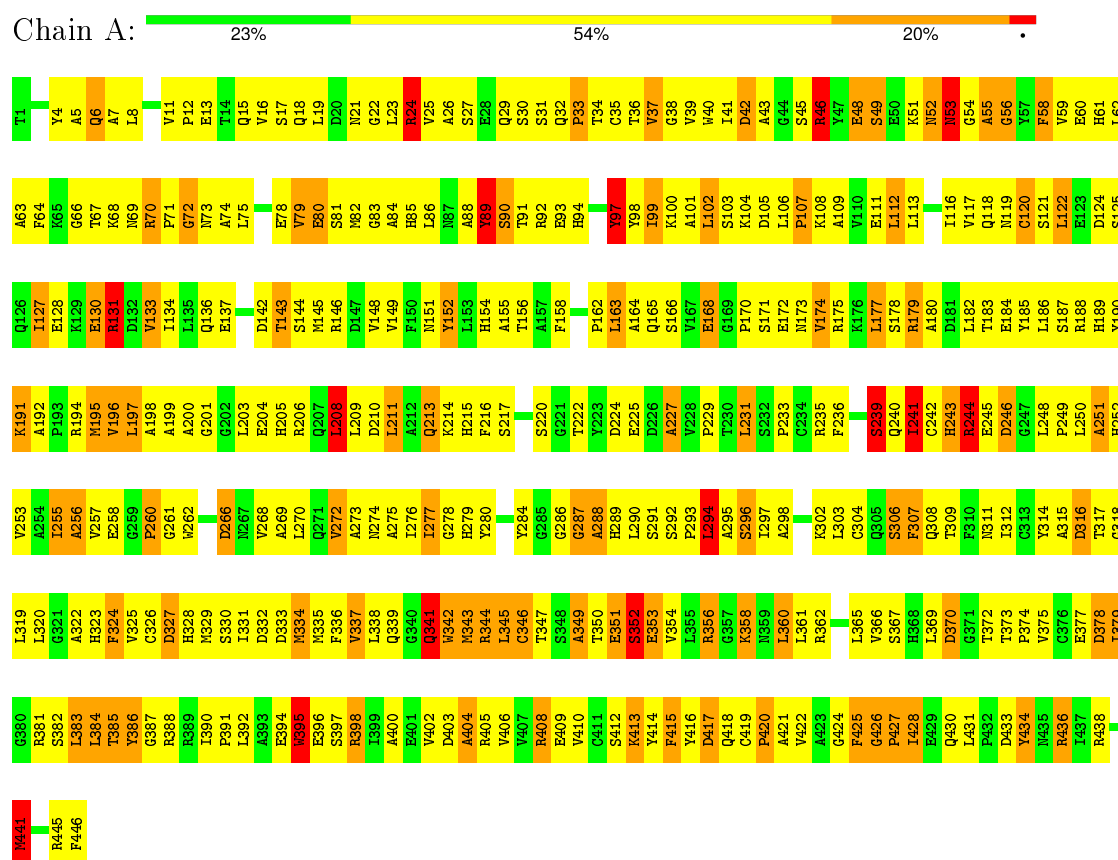
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	Q	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots

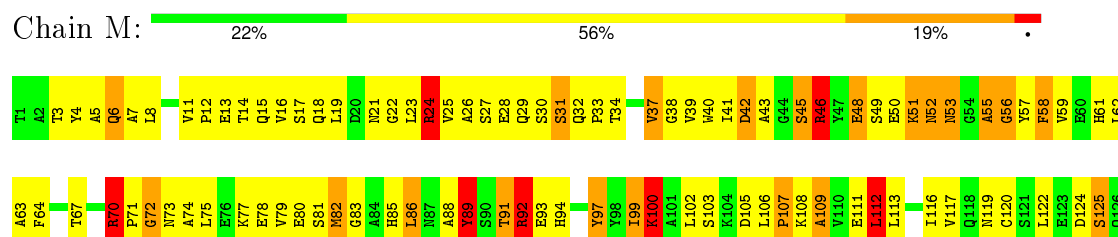
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

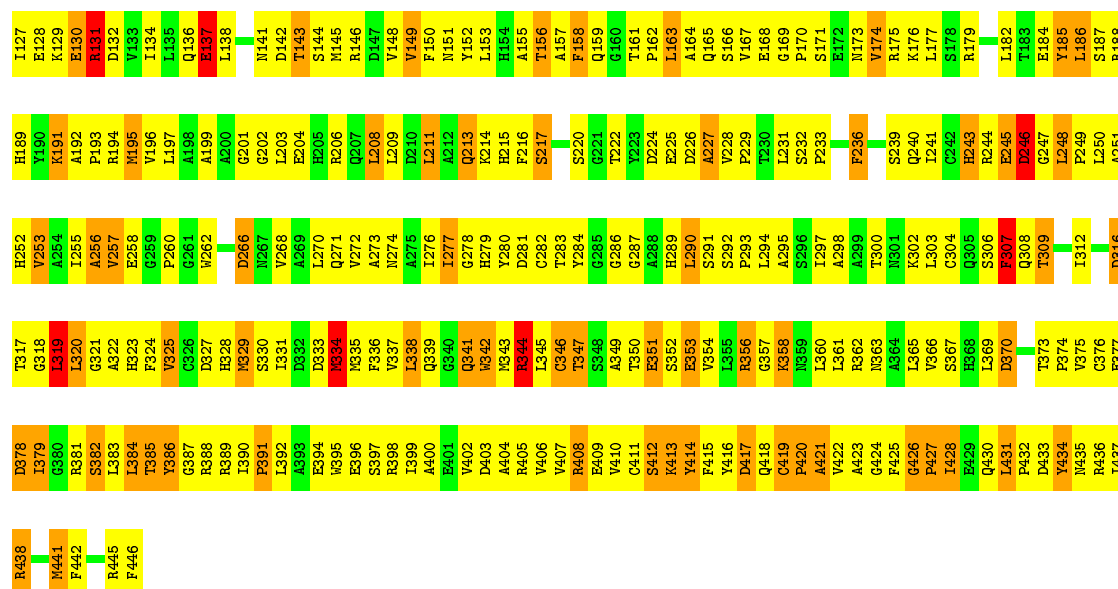
Note EDS was not executed.

• Molecule 1: CYTOCHROME BC1 COMPLEX



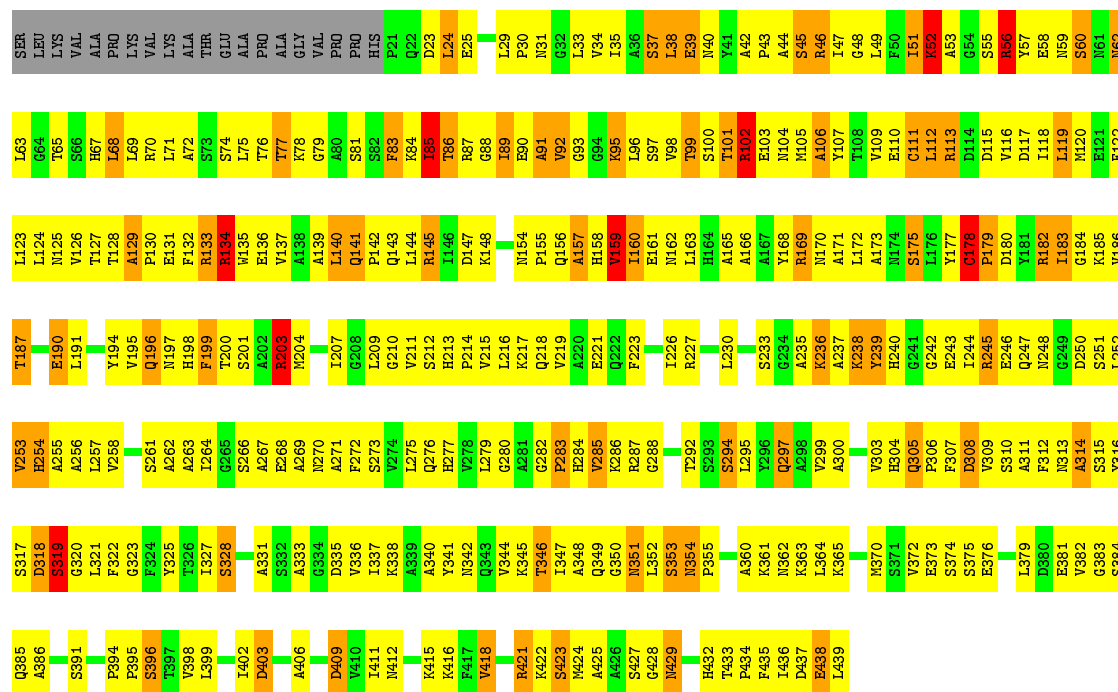
• Molecule 1: CYTOCHROME BC1 COMPLEX





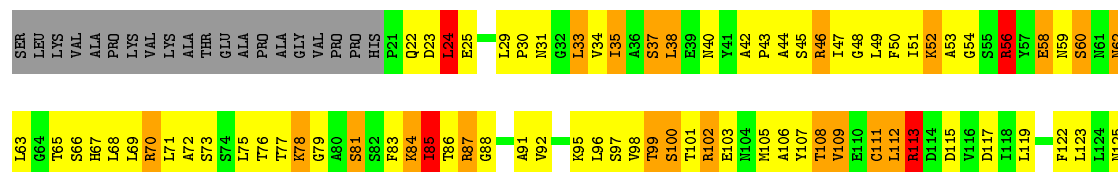
• Molecule 2: CYTOCHROME BC1 COMPLEX

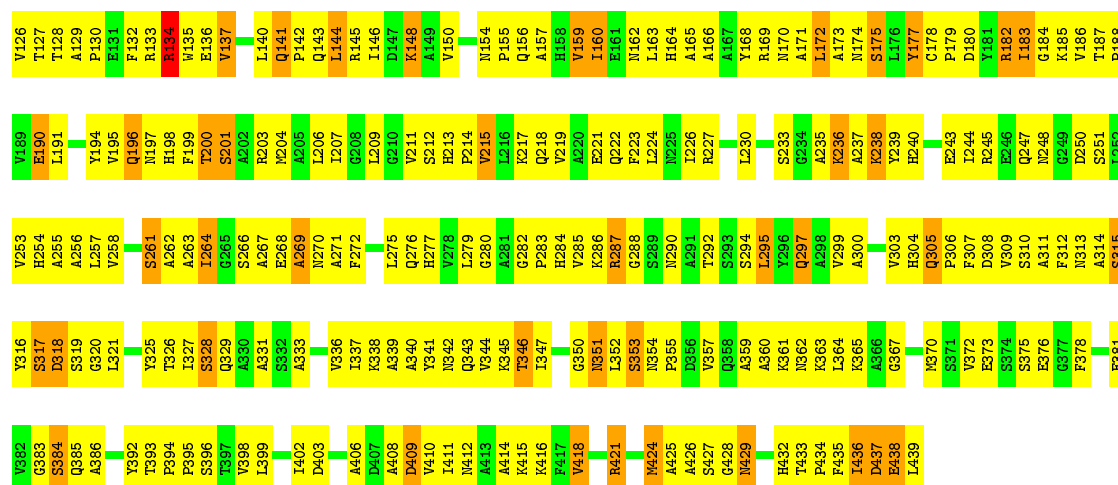
Chain B: 24% 54% 15% 5%



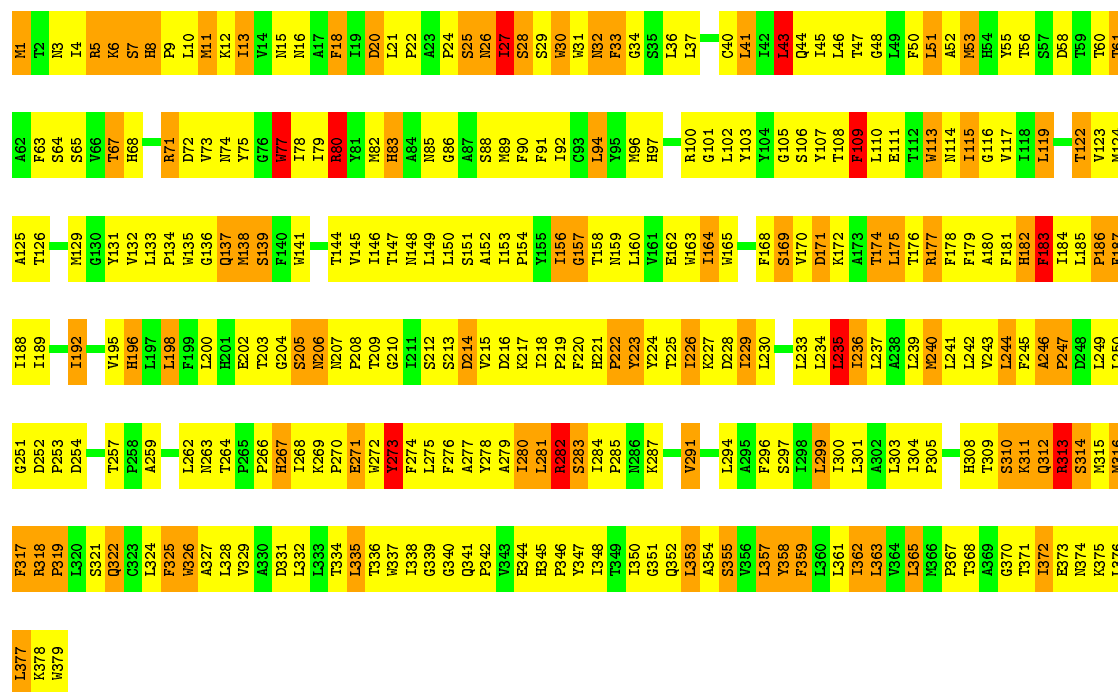
• Molecule 2: CYTOCHROME BC1 COMPLEX

Chain N: 26% 54% 14% 5%

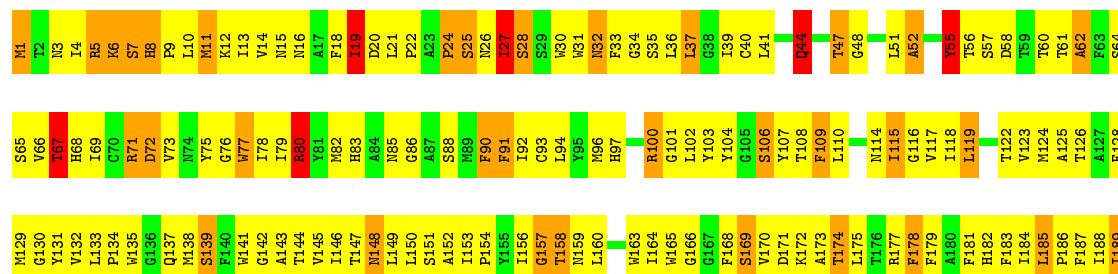


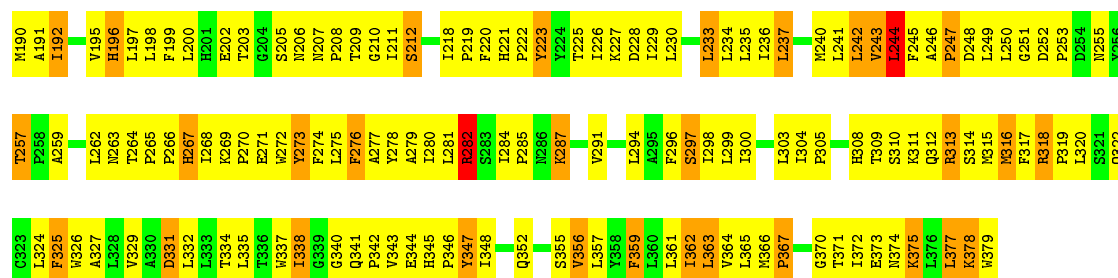


• Molecule 3: CYTOCHROME BC1 COMPLEX



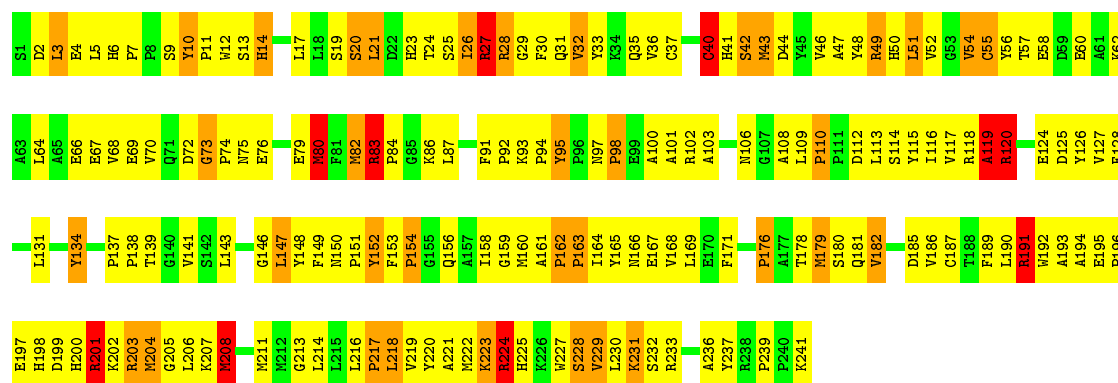
• Molecule 3: CYTOCHROME BC1 COMPLEX





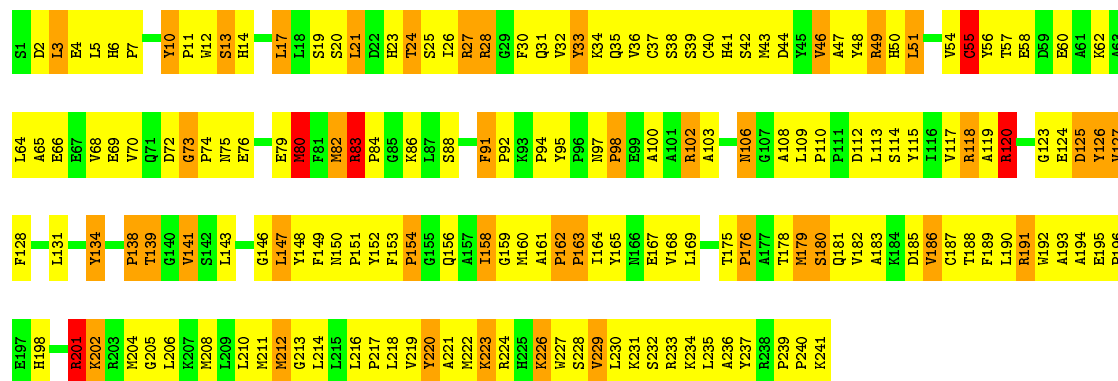
• Molecule 4: CYTOCHROME BC1 COMPLEX

Chain D: 26% 55% 15% .



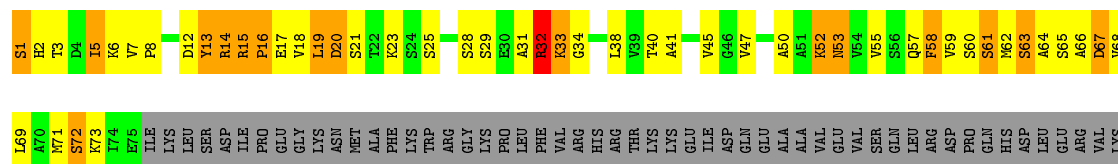
• Molecule 4: CYTOCHROME BC1 COMPLEX

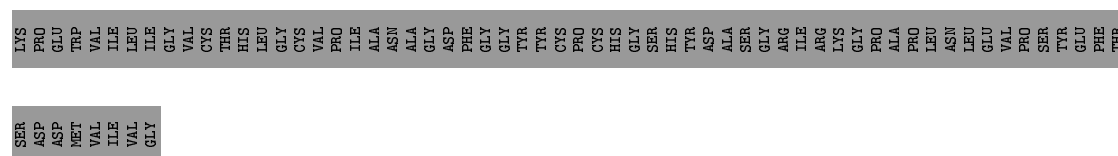
Chain P: 27% 54% 17% .



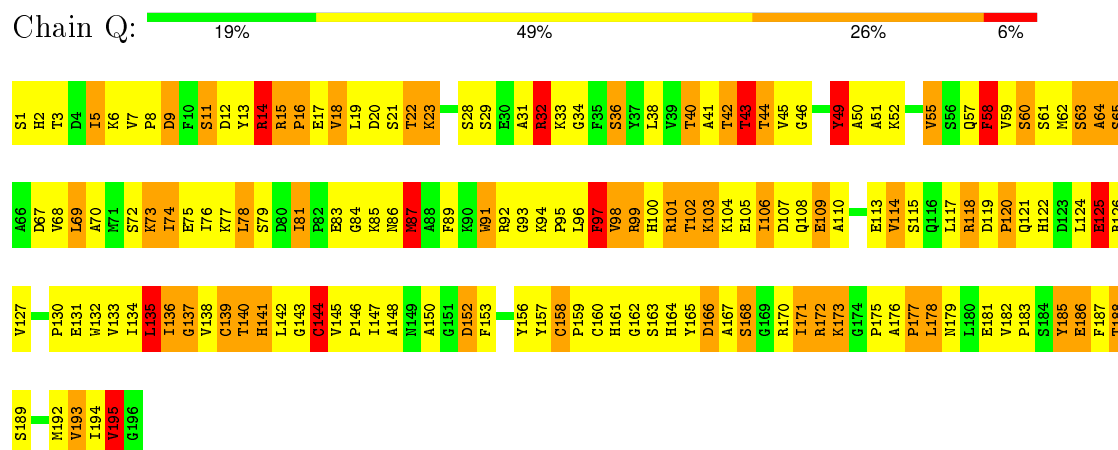
• Molecule 5: CYTOCHROME BC1 COMPLEX

Chain E: 13% 17% 8% 62% .

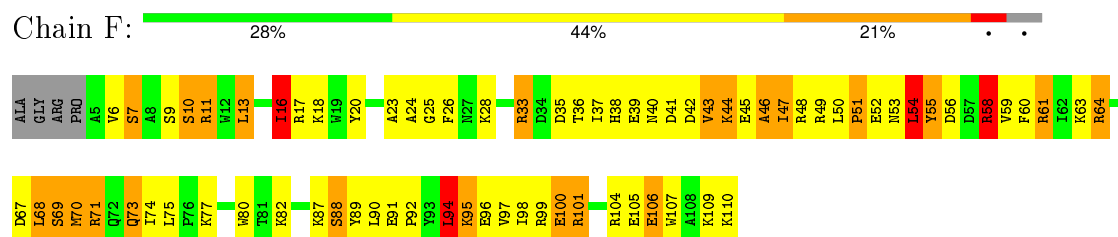




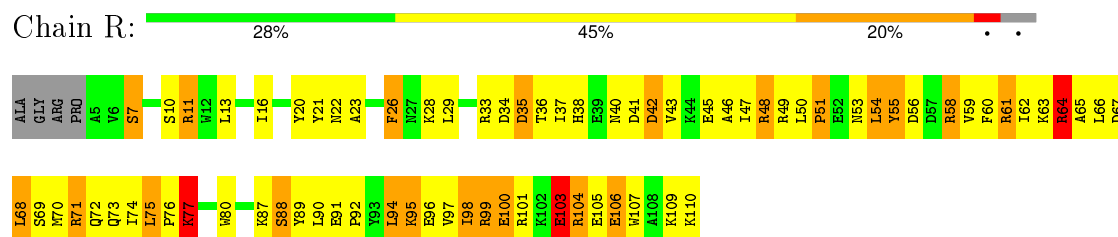
• Molecule 5: CYTOCHROME BC1 COMPLEX



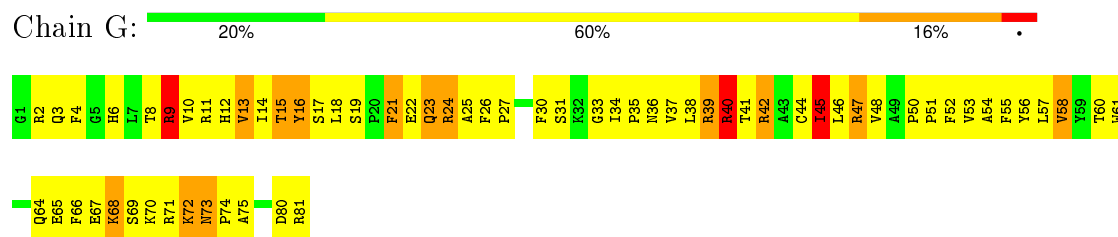
• Molecule 6: CYTOCHROME BC1 COMPLEX



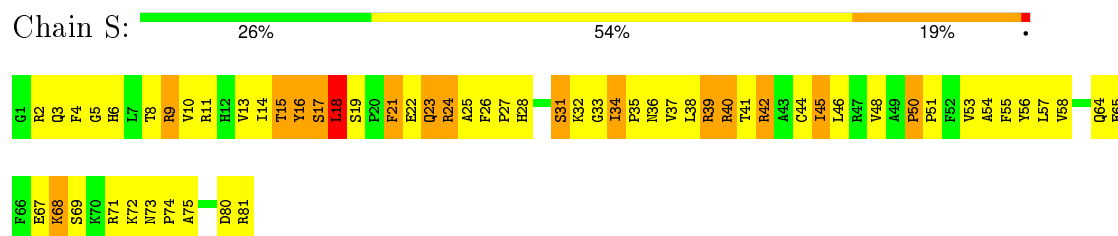
• Molecule 6: CYTOCHROME BC1 COMPLEX



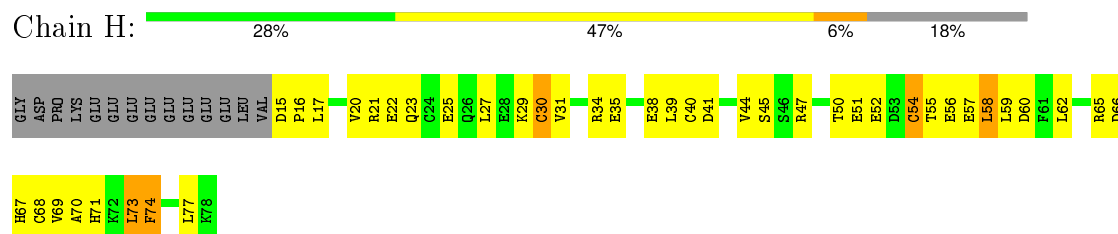
• Molecule 7: CYTOCHROME BC1 COMPLEX



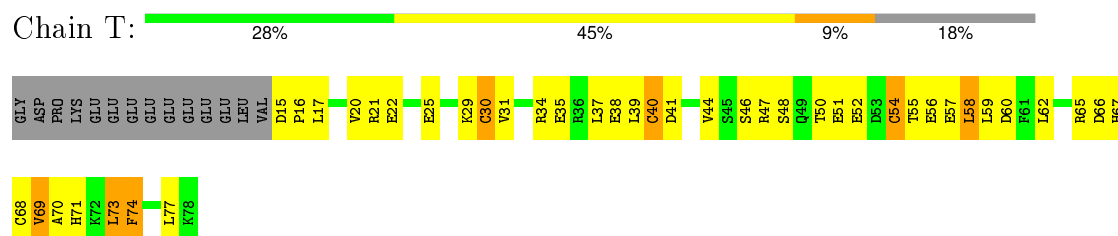
• Molecule 7: CYTOCHROME BC1 COMPLEX



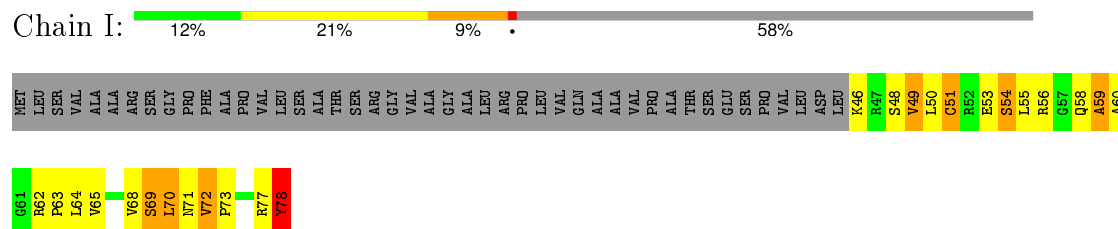
• Molecule 8: CYTOCHROME BC1 COMPLEX



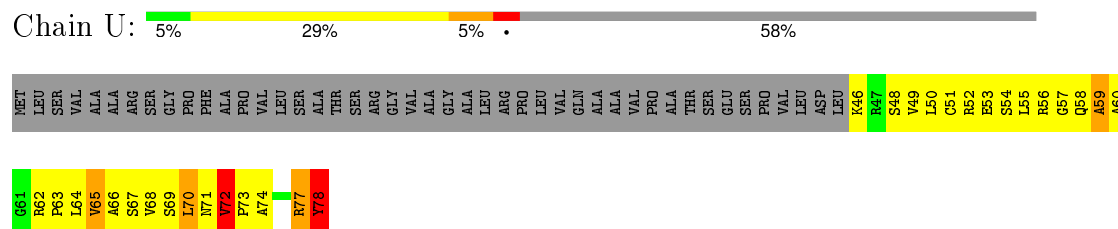
• Molecule 8: CYTOCHROME BC1 COMPLEX



• Molecule 9: CYTOCHROME BC1 COMPLEX

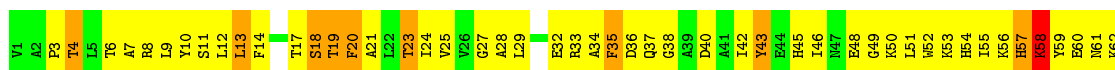


• Molecule 9: CYTOCHROME BC1 COMPLEX

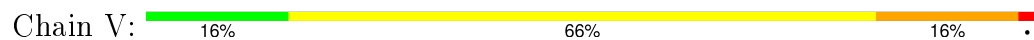


• Molecule 10: CYTOCHROME BC1 COMPLEX

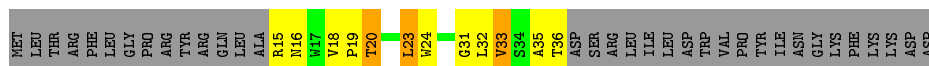




• Molecule 10: CYTOCHROME BC1 COMPLEX



• Molecule 11: CYTOCHROME BC1 COMPLEX



• Molecule 11: CYTOCHROME BC1 COMPLEX



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	130.11Å 130.11Å 720.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	74.0 (20.00-3.00)	Depositor
R_{merge}	0.92	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.320 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31486	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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, HEC

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	0.60	2/3531 (0.1%)	1.58	43/4792 (0.9%)
1	M	0.63	3/3531 (0.1%)	1.61	58/4792 (1.2%)
2	B	0.51	0/3198	1.46	31/4336 (0.7%)
2	N	0.51	0/3198	1.33	11/4336 (0.3%)
3	C	0.71	2/3108 (0.1%)	1.73	63/4252 (1.5%)
3	O	0.69	3/3108 (0.1%)	1.62	51/4252 (1.2%)
4	D	0.55	0/1978	1.50	23/2684 (0.9%)
4	P	0.55	0/1978	1.40	24/2684 (0.9%)
5	E	0.60	0/574	1.63	7/775 (0.9%)
5	Q	0.61	0/1551	1.68	28/2097 (1.3%)
6	F	0.57	0/935	1.56	18/1253 (1.4%)
6	R	0.57	0/935	1.66	24/1253 (1.9%)
7	G	0.61	1/704 (0.1%)	1.41	9/951 (0.9%)
7	S	0.59	0/704	1.31	5/951 (0.5%)
8	H	0.41	0/529	1.12	0/708
8	T	0.39	0/529	1.06	0/708
9	I	0.48	0/250	1.31	2/335 (0.6%)
9	U	0.48	0/250	1.32	1/335 (0.3%)
10	J	0.51	0/525	1.31	5/707 (0.7%)
10	V	0.51	0/525	1.42	6/707 (0.8%)
11	K	0.42	0/163	1.01	0/225
11	W	0.46	0/163	1.18	0/225
All	All	0.59	11/31967 (0.0%)	1.52	409/43358 (0.9%)

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	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	3
2	B	0	9
2	N	0	5
3	C	0	14
3	O	0	6
4	D	0	5
4	P	0	4
5	E	0	1
5	Q	0	9
6	F	0	2
7	G	0	2
7	S	0	3
8	T	0	1
9	I	0	1
9	U	0	1
10	J	0	1
11	W	0	1
All	All	0	81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	CYS	CB-SG	-7.17	1.70	1.82
1	M	253	VAL	C-O	6.79	1.36	1.23
1	A	104	LYS	CD-CE	6.57	1.67	1.51
1	M	169	GLY	N-CA	-6.53	1.36	1.46
3	O	106	SER	CB-OG	-6.43	1.33	1.42

The worst 5 of 409 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	46	ARG	NE-CZ-NH2	-19.34	110.63	120.30
4	D	120	ARG	NE-CZ-NH2	-16.26	112.17	120.30
2	B	70	ARG	NE-CZ-NH2	16.26	128.43	120.30
1	A	419	CYS	CA-CB-SG	16.23	143.21	114.00
2	B	245	ARG	NE-CZ-NH2	14.98	127.79	120.30

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLN	Mainchain
1	A	122	LEU	Mainchain
1	A	196	VAL	Mainchain
1	A	210	ASP	Mainchain
1	A	53	ASN	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	465	0
1	M	3458	0	3355	458	0
2	B	3141	0	3123	402	0
2	N	3141	0	3123	408	1
3	C	3011	0	3076	456	0
3	O	3011	0	3076	415	0
4	D	1919	0	1868	297	0
4	P	1919	0	1868	284	0
5	E	566	0	564	65	0
5	Q	1518	0	1499	264	1
6	F	916	0	909	91	0
6	R	916	0	909	91	1
7	G	682	0	679	104	0
7	S	682	0	679	100	0
8	H	524	0	504	71	1
8	T	524	0	504	75	0
9	I	248	0	265	52	0
9	U	248	0	265	66	0
10	J	512	0	518	66	0
10	V	512	0	518	74	0
11	K	159	0	159	26	0
11	W	159	0	159	26	0
12	C	86	0	60	20	0
12	O	86	0	60	25	0
13	D	43	0	30	7	0
13	P	43	0	30	3	0
14	Q	4	0	0	0	0
All	All	31486	0	31156	3839	2

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 61.

The worst 5 of 3839 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)
7:S:50:PRO:HB2	7:S:51:PRO:HD3	1.25	1.17
4:D:224:ARG:HB2	7:G:25:ALA:HB1	1.27	1.17
2:B:77:THR:HG22	2:B:130:PRO:HA	1.25	1.14
1:M:67:THR:HG23	1:M:70:ARG:H	1.13	1.14
1:M:426:GLY:CA	1:M:428:ILE:HG13	1.78	1.13

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:412:ASN:ND2	5:Q:122:HIS:NE2[6_554]	2.01	0.19
8:H:41:ASP:OD1	6:R:77:LYS:NZ[5_565]	2.19	0.01

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%)	355 (80%)	66 (15%)	23 (5%)	2	15
1	M	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	3	18
2	B	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	8	38
2	N	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	7	33
3	C	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	4	23
3	O	377/379 (100%)	317 (84%)	49 (13%)	11 (3%)	6	29
4	D	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	2	9
4	P	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	3	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	6	32
5	Q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	2	12
6	F	104/110 (94%)	89 (86%)	12 (12%)	3 (3%)	6	29
6	R	104/110 (94%)	86 (83%)	16 (15%)	2 (2%)	10	43
7	G	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	4	22
7	S	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	4	22
8	H	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	T	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	12	48
9	I	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	8
9	U	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	1	3
10	J	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	1	3
10	V	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	8
11	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	3	15
11	W	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	1	3
All	All	3933/4332 (91%)	3172 (81%)	603 (15%)	158 (4%)	4	21

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	A	426	GLY
1	A	427	PRO
2	B	141	GLN
2	B	183	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	289 (78%)	81 (22%)	1	6
1	M	370/370 (100%)	286 (77%)	84 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	328/343 (96%)	259 (79%)	69 (21%)	1	7
2	N	328/343 (96%)	262 (80%)	66 (20%)	1	8
3	C	327/327 (100%)	269 (82%)	58 (18%)	2	11
3	O	327/327 (100%)	276 (84%)	51 (16%)	3	16
4	D	206/206 (100%)	179 (87%)	27 (13%)	5	22
4	P	206/206 (100%)	179 (87%)	27 (13%)	5	22
5	E	65/168 (39%)	51 (78%)	14 (22%)	1	6
5	Q	167/168 (99%)	123 (74%)	44 (26%)	0	3
6	F	96/98 (98%)	74 (77%)	22 (23%)	1	5
6	R	96/98 (98%)	78 (81%)	18 (19%)	2	10
7	G	71/71 (100%)	58 (82%)	13 (18%)	2	11
7	S	71/71 (100%)	57 (80%)	14 (20%)	1	9
8	H	61/74 (82%)	51 (84%)	10 (16%)	3	14
8	T	61/74 (82%)	51 (84%)	10 (16%)	3	14
9	I	27/60 (45%)	19 (70%)	8 (30%)	0	2
9	U	27/60 (45%)	20 (74%)	7 (26%)	0	3
10	J	52/52 (100%)	46 (88%)	6 (12%)	7	28
10	V	52/52 (100%)	43 (83%)	9 (17%)	2	12
11	K	15/46 (33%)	12 (80%)	3 (20%)	1	8
11	W	15/46 (33%)	11 (73%)	4 (27%)	0	3
All	All	3338/3630 (92%)	2693 (81%)	645 (19%)	2	9

5 of 645 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	59	LEU
1	M	243	HIS
6	R	100	GLU
9	I	77	ARG
1	M	92	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	27	ASN
1	M	136	GLN
4	P	181	GLN
6	F	38	HIS
10	J	54	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](#)

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](#)

7 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	380	3	30,50,50	2.52	6 (20%)	24,82,82	3.51	11 (45%)
12	HEM	C	381	3	30,50,50	2.44	7 (23%)	24,82,82	3.33	12 (50%)
13	HEC	D	242	4	24,50,50	2.45	4 (16%)	19,82,82	2.95	8 (42%)
12	HEM	O	380	3	30,50,50	2.50	6 (20%)	24,82,82	3.23	16 (66%)
12	HEM	O	381	3	30,50,50	2.41	6 (20%)	24,82,82	2.89	11 (45%)
13	HEC	P	242	4	24,50,50	2.48	4 (16%)	19,82,82	2.88	11 (57%)
14	FES	Q	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	380	3	-	0/10/54/54	0/0/8/8
12	HEM	C	381	3	-	0/10/54/54	0/0/8/8
13	HEC	D	242	4	-	0/6/54/54	0/0/8/8
12	HEM	O	380	3	-	0/10/54/54	0/0/8/8
12	HEM	O	381	3	-	0/10/54/54	0/0/8/8
13	HEC	P	242	4	-	0/6/54/54	0/0/8/8
14	FES	Q	197	5	-	0/0/4/4	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	380	HEM	C3B-C4B	-8.52	1.44	1.51
12	O	381	HEM	C3B-C4B	-7.71	1.45	1.51
12	C	381	HEM	C3B-C4B	-7.63	1.45	1.51
12	O	380	HEM	C2D-C3D	-7.55	1.31	1.54
13	P	242	HEC	C3C-C2C	-7.16	1.33	1.40

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	380	HEM	C3B-CAB-CBB	-10.56	108.26	124.46
12	O	381	HEM	CAA-C2A-C1A	-6.87	119.55	127.01
12	C	381	HEM	CAA-C2A-C1A	-6.37	120.09	127.01
12	O	380	HEM	CMA-C3A-C4A	-6.31	117.92	128.36
13	D	242	HEC	CBC-CAC-C3C	-5.99	114.05	127.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	380	HEM	6	0
12	C	381	HEM	14	0
13	D	242	HEC	7	0
12	O	380	HEM	11	0
12	O	381	HEM	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	242	HEC	3	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.