wwPDB X-ray Structure Validation Summary Report (i)

Jul 18, 2016 – 01:22 PM EDT

PDB ID	:	5DJQ
Title	:	The structure of CBB3 cytochrome oxidase.
Authors	:	Buschmann, S.; Warkentin, E.; Xie, H.; Kohlstaedt, M.; Langer, J.D.; Ermler, U.; Michel, H.
Deposited on	:	2015-09-02
Resolution	:	3.20 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 (1)) were used in the production of this report:

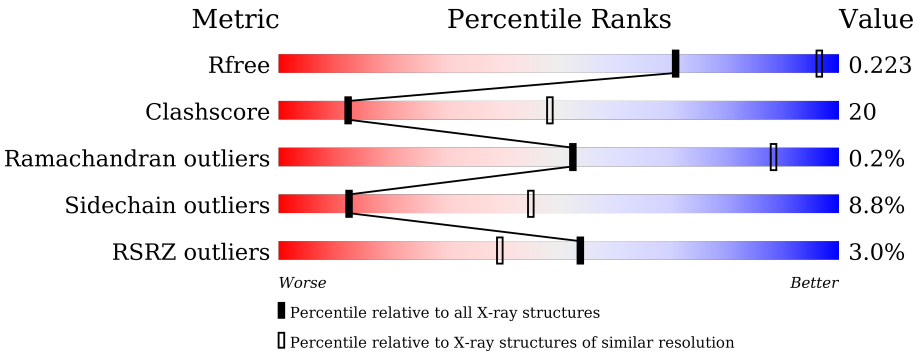
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 3.20 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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	474	64% 30%
1	D	474	4% 61% 34%
1	G	474	60% 34%
1	K	474	3% 63% 31%
2	B	203	67% 26%
2	E	203	3% 68% 26%

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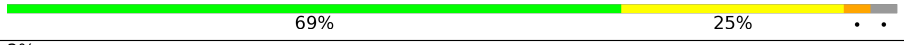
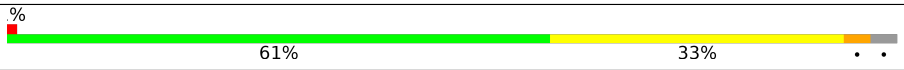
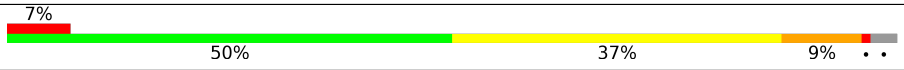
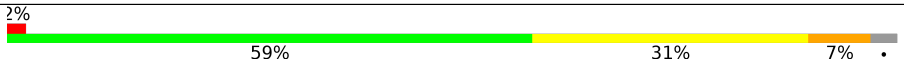
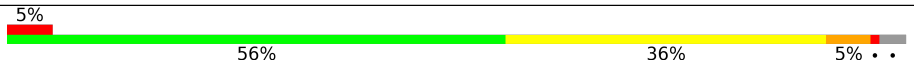
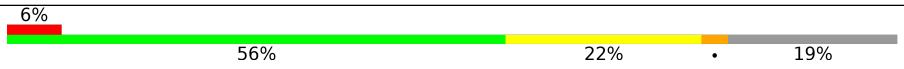
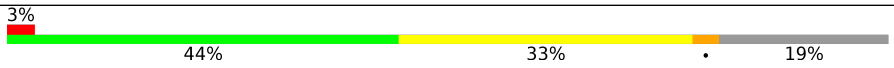
Mol	Chain	Length	Quality of chain
2	H	203	
2	L	203	
3	C	311	
3	F	311	
3	I	311	
3	M	311	
4	N	36	
4	O	36	
4	P	36	
4	Q	36	

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
11	FC6	F	403	-	-	-	X
9	PO4	K	506	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31974 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 Cbb3-type cytochrome c oxidase subunit CcoN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3683	2461	593	607	22			
1	D	463	Total	C	N	O	S	0	0	0
			3663	2450	590	601	22			
1	G	465	Total	C	N	O	S	0	0	0
			3676	2457	592	605	22			
1	K	465	Total	C	N	O	S	0	0	0
			3676	2457	592	605	22			

- Molecule 2 is a protein called Cbb3-type cytochrome c oxidase subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	E	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	H	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	L	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			

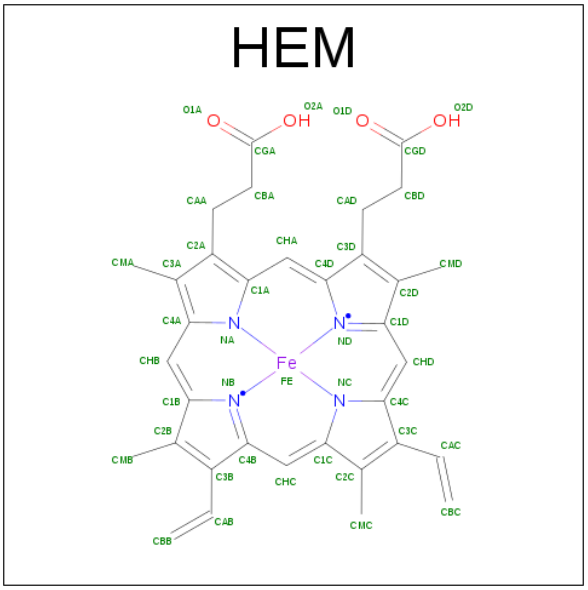
- Molecule 3 is a protein called Cbb3-type cytochrome c oxidase subunit CcoP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	F	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	I	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	M	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			
4	O	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			
4	P	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			
4	Q	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

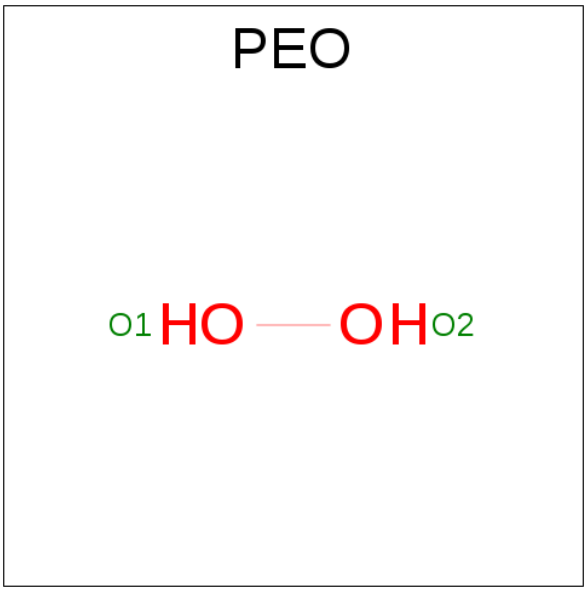
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Cu	0	0
			1	1		
6	A	1	Total	Cu	0	0
			1	1		
6	D	1	Total	Cu	0	0
			1	1		
6	K	1	Total	Cu	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

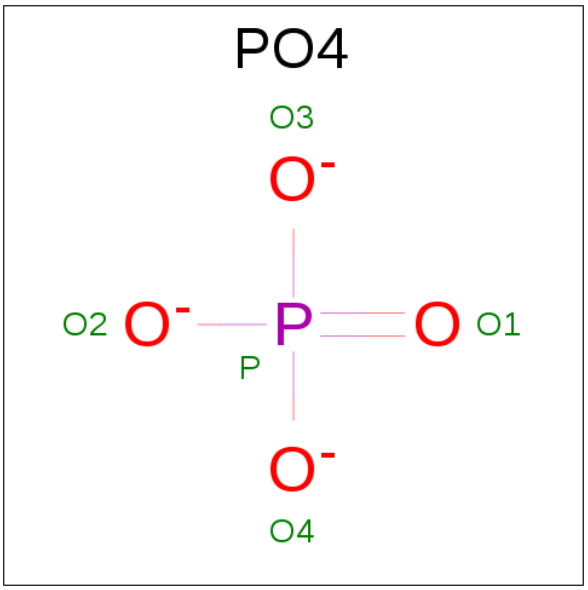
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	D	2	Total	Ca	0	0
			2	2		
7	K	2	Total	Ca	0	0
			2	2		

- Molecule 8 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



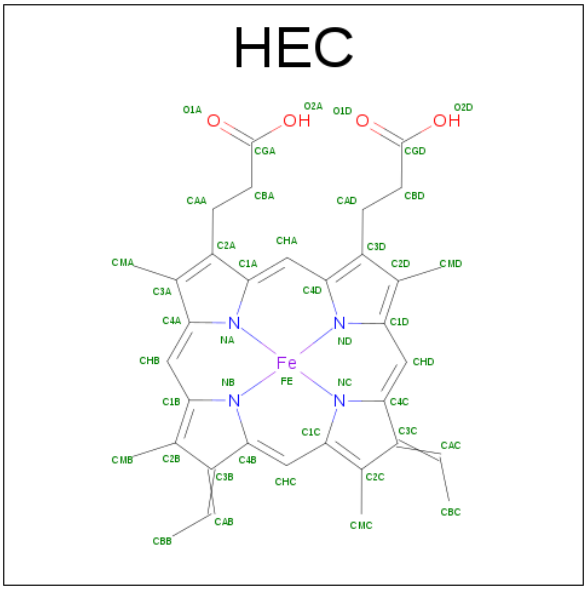
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	D	1	Total O 2 2	0	0
8	G	1	Total O 2 2	0	0
8	K	1	Total O 2 2	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O P 5 4 1	0	0
9	D	1	Total O P 5 4 1	0	0
9	G	1	Total O P 5 4 1	0	0
9	K	1	Total O P 5 4 1	0	0

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C Fe N O 43 34 1 4 4	0	0
10	C	1	Total C Fe N O 43 34 1 4 4	0	0
10	C	1	Total C Fe N O 43 34 1 4 4	0	0
10	E	1	Total C Fe N O 43 34 1 4 4	0	0
10	F	1	Total C Fe N O 43 34 1 4 4	0	0
10	F	1	Total C Fe N O 43 34 1 4 4	0	0
10	H	1	Total C Fe N O 43 34 1 4 4	0	0
10	I	1	Total C Fe N O 43 34 1 4 4	0	0

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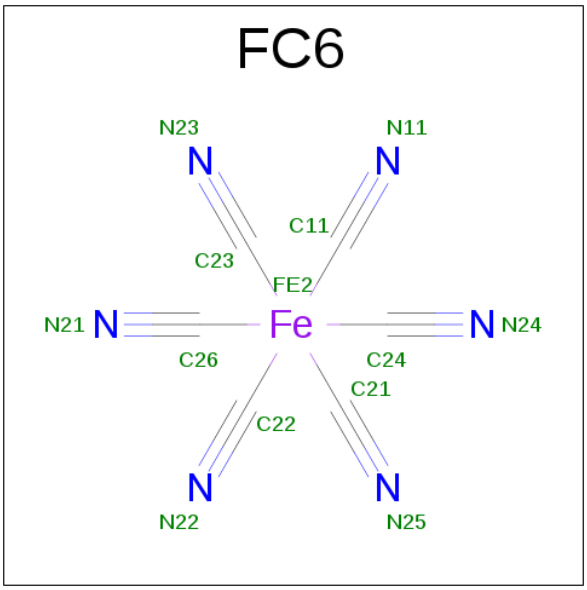
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is HEXACYANOFERRATE(3-) (three-letter code: FC6) (formula: C_6FeN_6).

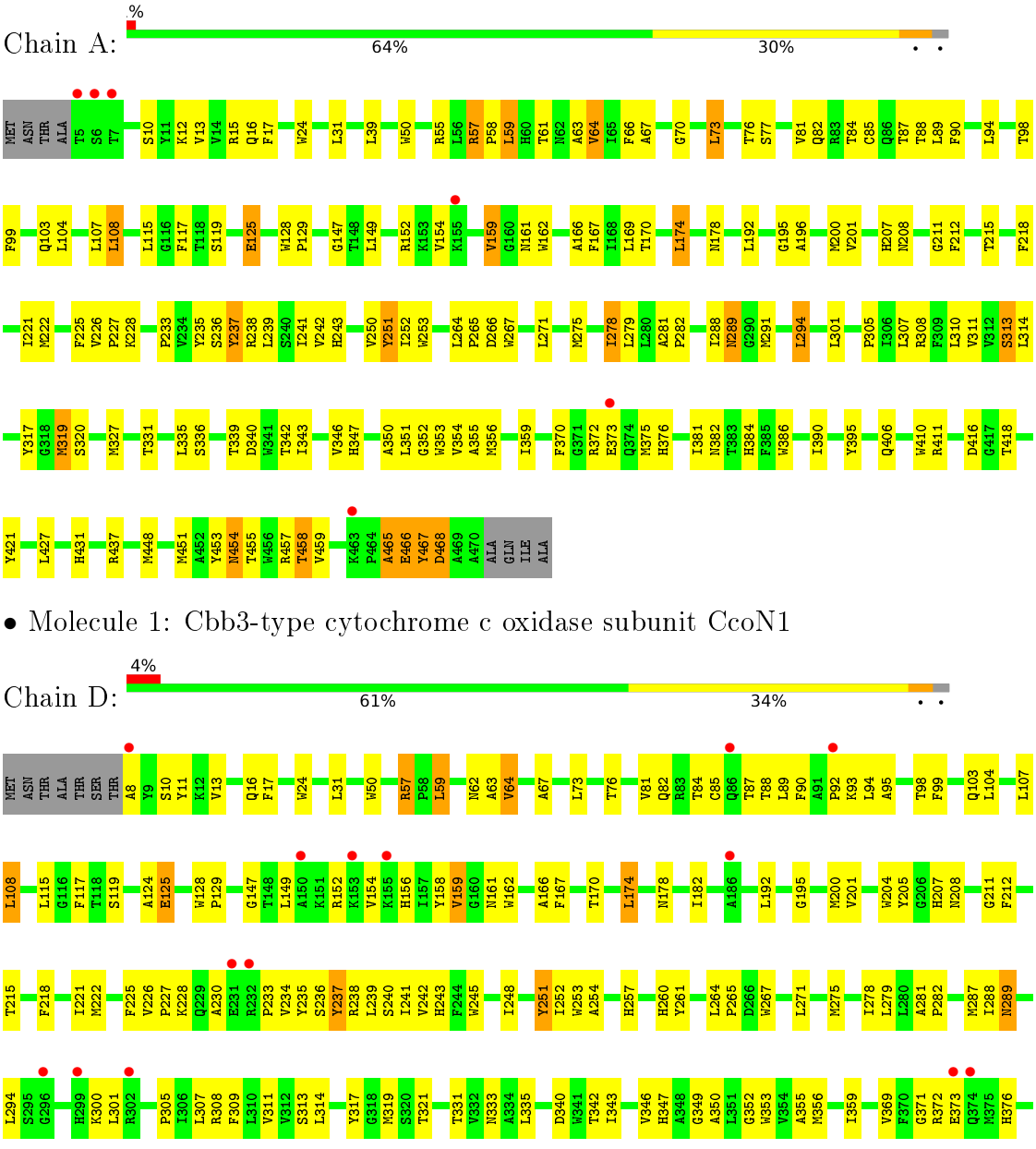


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	F	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	I	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	M	1	Total	C	Fe	N	0	0
			13	6	1	6		

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.

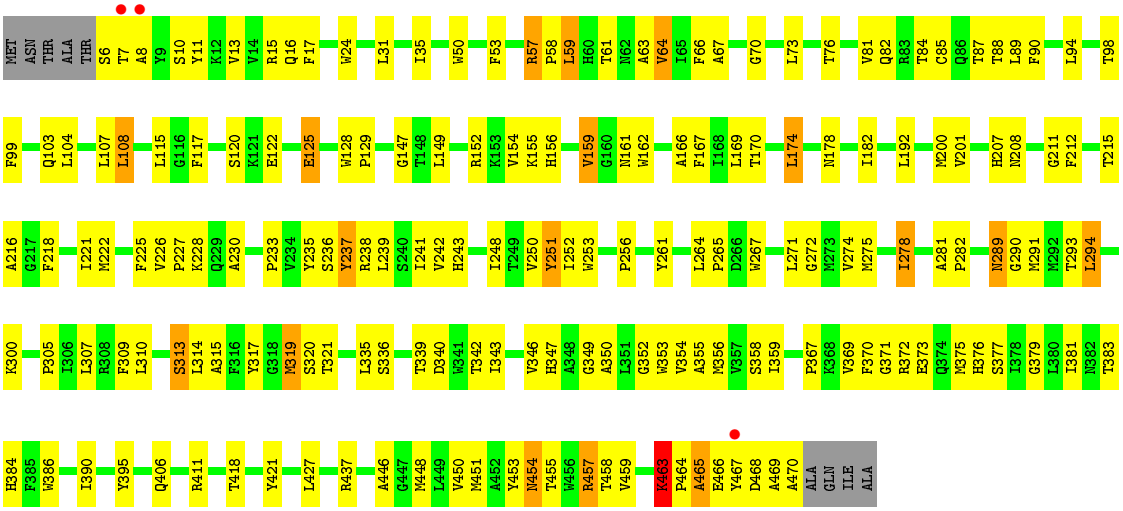
- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1



- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

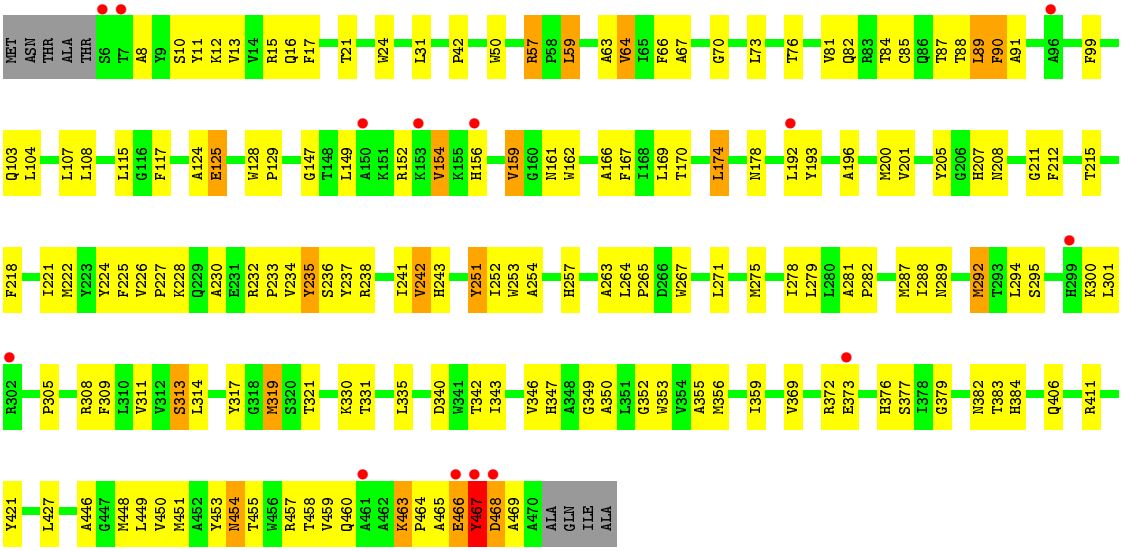
• Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

Chain G:



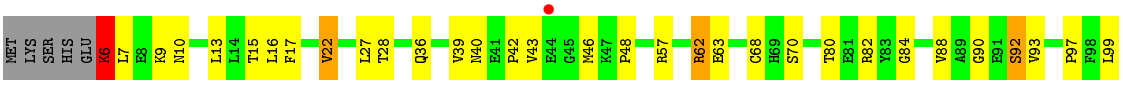
• Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

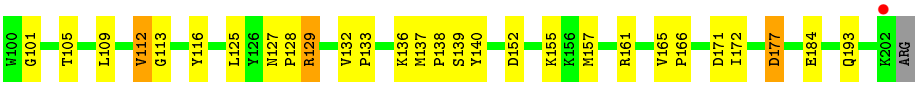
Chain K:



• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

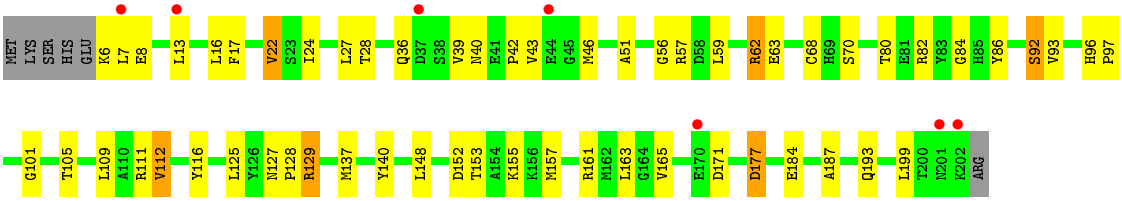
Chain B:





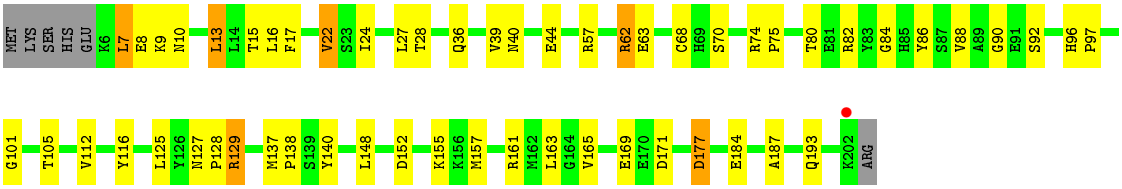
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

Chain E:



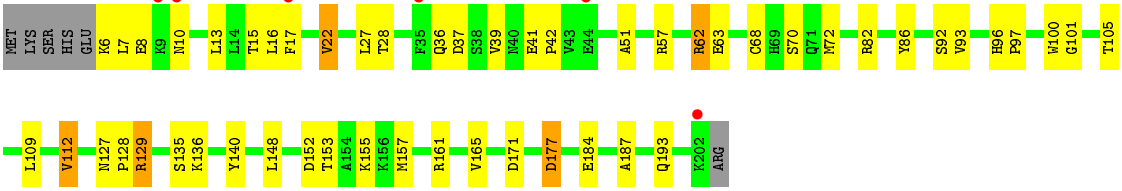
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

Chain H:



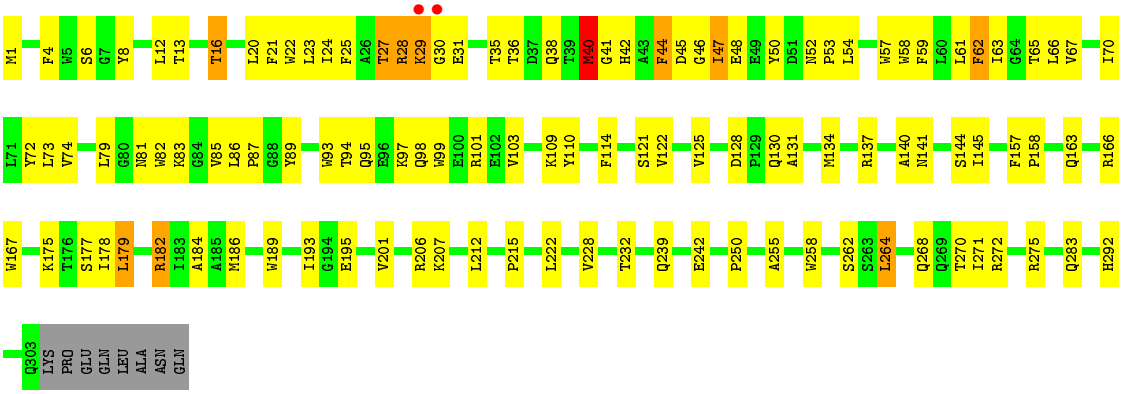
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

Chain L:



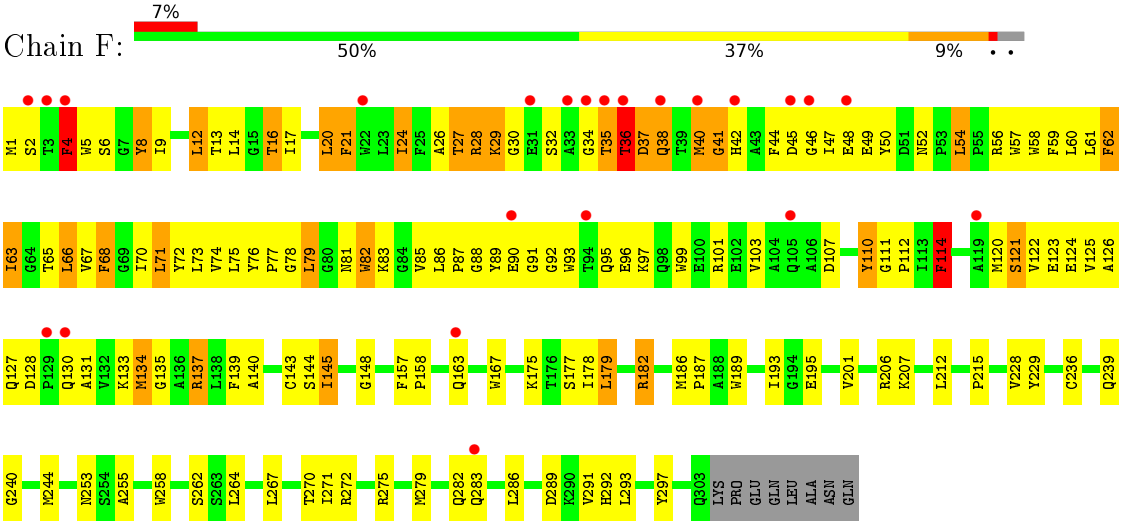
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain C:



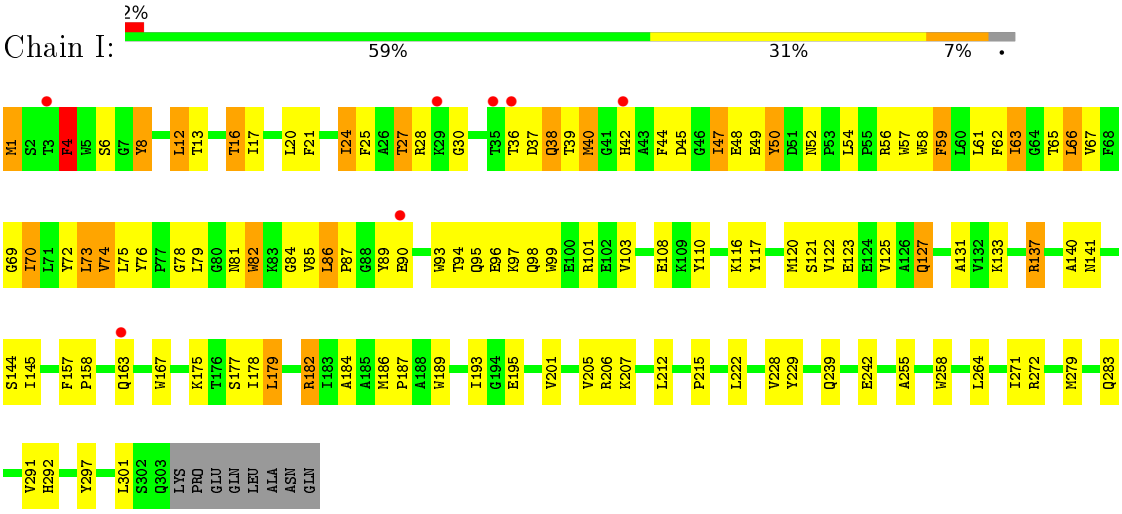
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain F:



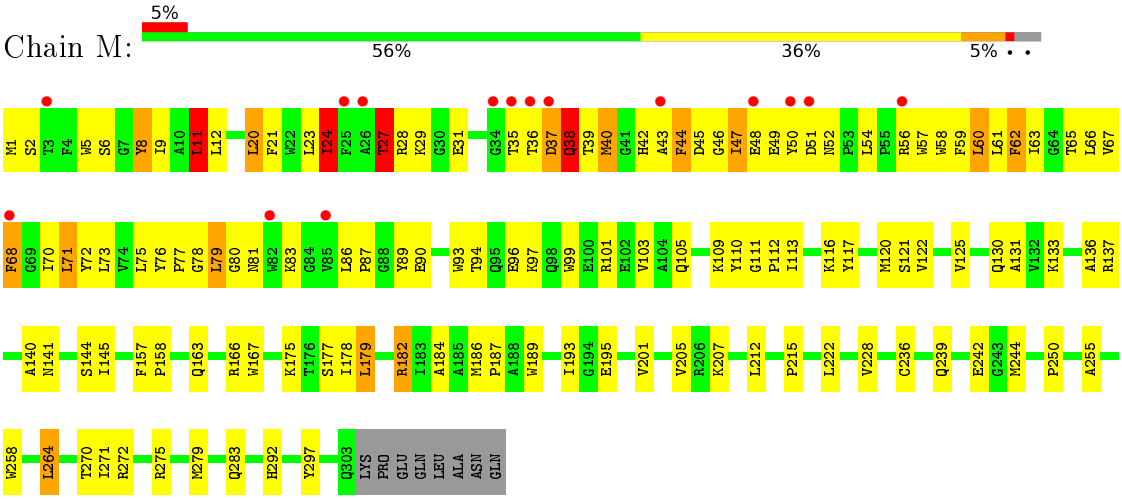
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain I:



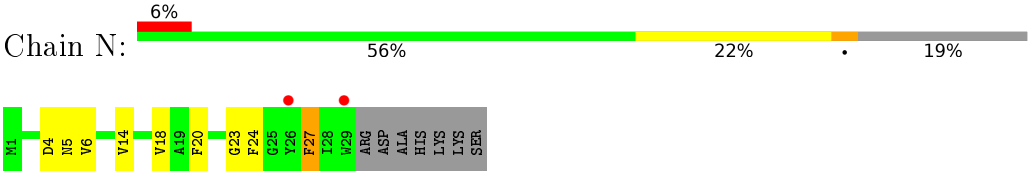
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain M:



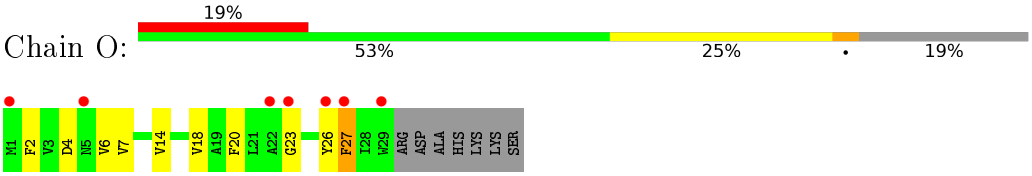
- Molecule 4: Putative uncharacterized protein

Chain N:



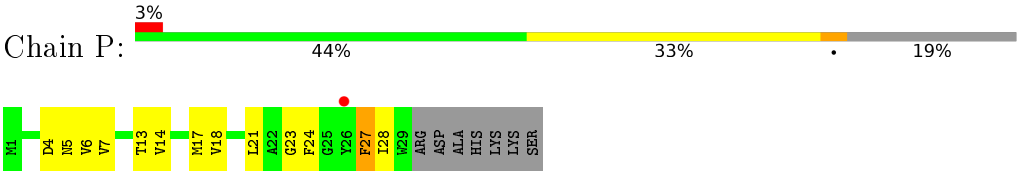
- Molecule 4: Putative uncharacterized protein

Chain O:



- Molecule 4: Putative uncharacterized protein

Chain P:



- Molecule 4: Putative uncharacterized protein

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	136.47Å 279.93Å 175.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.20 14.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (14.98-3.20) 98.8 (14.98-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.187 , 0.223 0.187 , 0.223	Depositor DCC
R_{free} test set	5482 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31974	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FC6, CA, PEO, HEC, HEM, PO4, CU

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	0.39	0/3811	0.64	5/5210 (0.1%)
1	D	0.36	0/3791	0.66	9/5182 (0.2%)
1	G	0.40	1/3804 (0.0%)	0.60	4/5200 (0.1%)
1	K	0.37	0/3804	0.60	4/5200 (0.1%)
2	B	0.38	0/1584	0.60	1/2146 (0.0%)
2	E	0.30	0/1584	0.53	0/2146
2	H	0.34	0/1584	0.57	0/2146
2	L	0.31	0/1584	0.52	0/2146
3	C	0.50	0/2374	0.89	9/3225 (0.3%)
3	F	0.56	2/2374 (0.1%)	1.02	10/3225 (0.3%)
3	I	0.54	1/2374 (0.0%)	0.91	12/3225 (0.4%)
3	M	0.54	0/2374	0.89	5/3225 (0.2%)
4	N	0.50	0/227	0.85	2/309 (0.6%)
4	O	0.47	0/227	0.82	2/309 (0.6%)
4	P	0.50	0/227	0.89	2/309 (0.6%)
4	Q	0.65	0/227	0.96	2/309 (0.6%)
All	All	0.43	4/31950 (0.0%)	0.73	67/43512 (0.2%)

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	2
1	G	0	1
3	C	0	1
3	F	0	2
3	I	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	110	TYR	CD2-CE2	-8.28	1.26	1.39
3	I	82	TRP	CB-CG	-7.12	1.37	1.50
3	F	110	TYR	CE2-CZ	-5.39	1.31	1.38
1	G	237	TYR	CD2-CE2	-5.10	1.31	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	44	PHE	CB-CG-CD1	-10.56	113.41	120.80
3	I	44	PHE	CB-CG-CD1	-10.03	113.78	120.80
3	F	66	LEU	CB-CG-CD1	-9.58	94.72	111.00
3	M	79	LEU	CB-CG-CD1	-9.16	95.42	111.00
1	D	462	ALA	N-CA-C	8.96	135.18	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ALA	Mainchain
1	A	467	TYR	Peptide
3	C	44	PHE	Sidechain
3	F	114	PHE	Sidechain
3	F	37	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3683	0	3663	134	0
1	D	3663	0	3644	161	0
1	G	3676	0	3656	150	0
1	K	3676	0	3656	158	0
2	B	1548	0	1526	46	0
2	E	1548	0	1526	48	0
2	H	1548	0	1526	42	0
2	L	1548	0	1526	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2312	0	2237	103	0
3	F	2312	0	2237	194	0
3	I	2312	0	2237	124	0
3	M	2312	0	2237	147	0
4	N	221	0	226	9	0
4	O	221	0	226	11	0
4	P	221	0	226	12	0
4	Q	221	0	226	12	0
5	A	86	0	60	12	0
5	D	86	0	60	13	0
5	G	86	0	60	13	0
5	K	86	0	60	13	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	K	1	0	0	0	0
7	A	2	0	0	0	0
7	D	2	0	0	0	0
7	G	2	0	0	0	0
7	K	2	0	0	0	0
8	A	2	0	0	0	0
8	D	2	0	0	0	0
8	G	2	0	0	0	0
8	K	2	0	0	0	0
9	A	5	0	0	1	0
9	D	5	0	0	1	0
9	G	5	0	0	1	0
9	K	5	0	0	4	0
10	B	43	0	30	5	0
10	C	86	0	60	11	0
10	E	43	0	30	6	0
10	F	86	0	60	10	0
10	H	43	0	30	6	0
10	I	86	0	60	11	0
10	L	43	0	30	4	0
10	M	86	0	60	11	0
11	C	13	0	0	2	0
11	F	13	0	0	2	0
11	I	13	0	0	1	0
11	M	13	0	0	2	0
All	All	31974	0	31175	1240	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 20.

The worst 5 of 1240 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)
1:D:207:HIS:NE2	1:D:251:TYR:CE1	1.70	1.59
1:A:207:HIS:NE2	1:A:251:TYR:CE1	1.70	1.56
1:G:207:HIS:NE2	1:G:251:TYR:CE1	1.70	1.56
1:K:207:HIS:NE2	1:K:251:TYR:CE1	1.70	1.53
1:K:207:HIS:NE2	1:K:251:TYR:HE1	1.02	1.33

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	464/474 (98%)	442 (95%)	20 (4%)	2 (0%)	39	80
1	D	461/474 (97%)	443 (96%)	17 (4%)	1 (0%)	52	88
1	G	463/474 (98%)	443 (96%)	19 (4%)	1 (0%)	52	88
1	K	463/474 (98%)	442 (96%)	19 (4%)	2 (0%)	39	80
2	B	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
2	E	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
2	H	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
2	L	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
3	C	301/311 (97%)	286 (95%)	15 (5%)	0	100	100
3	F	301/311 (97%)	286 (95%)	15 (5%)	0	100	100
3	I	301/311 (97%)	287 (95%)	14 (5%)	0	100	100
3	M	301/311 (97%)	284 (94%)	14 (5%)	3 (1%)	19	65
4	N	27/36 (75%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	O	27/36 (75%)	27 (100%)	0	0	100 100
4	P	27/36 (75%)	27 (100%)	0	0	100 100
4	Q	27/36 (75%)	27 (100%)	0	0	100 100
All	All	3943/4096 (96%)	3769 (96%)	165 (4%)	9 (0%)	52 88

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	GLU
1	A	468	ASP
1	G	465	ALA
1	K	466	GLU
1	K	468	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	374/379 (99%)	343 (92%)	31 (8%)	14 49
1	D	371/379 (98%)	339 (91%)	32 (9%)	13 46
1	G	373/379 (98%)	340 (91%)	33 (9%)	12 45
1	K	373/379 (98%)	339 (91%)	34 (9%)	12 42
2	B	166/172 (96%)	154 (93%)	12 (7%)	18 57
2	E	166/172 (96%)	155 (93%)	11 (7%)	21 61
2	H	166/172 (96%)	152 (92%)	14 (8%)	14 48
2	L	166/172 (96%)	155 (93%)	11 (7%)	21 61
3	C	227/234 (97%)	212 (93%)	15 (7%)	21 61
3	F	227/234 (97%)	197 (87%)	30 (13%)	5 23
3	I	227/234 (97%)	200 (88%)	27 (12%)	6 28
3	M	227/234 (97%)	203 (89%)	24 (11%)	8 34
4	N	22/28 (79%)	22 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	O	22/28 (79%)	22 (100%)	0	100 100
4	P	22/28 (79%)	21 (96%)	1 (4%)	34 74
4	Q	22/28 (79%)	19 (86%)	3 (14%)	5 22
All	All	3151/3252 (97%)	2873 (91%)	278 (9%)	12 45

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	163	GLN
1	G	289	ASN
3	M	35	THR
3	F	201	VAL
1	G	122	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	52	ASN
1	G	374	GLN
2	L	71	GLN
3	F	81	ASN
1	G	82	GLN

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)

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 for Mogul analysis.

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	$\#\|Z\| > 2$
5	HEM	A	501	1,8,7	24,50,50	2.39	6 (25%)	16,82,82	1.78	4 (25%)
5	HEM	A	502	1,7	24,50,50	2.50	6 (25%)	16,82,82	1.37	1 (6%)
8	PEO	A	505	5,6	1,1,1	0.44	0	0,0,0	0.00	-
9	PO4	A	506	-	4,4,4	0.74	0	6,6,6	0.22	0
10	HEC	B	301	2	24,50,50	2.50	12 (50%)	19,82,82	3.16	9 (47%)
10	HEC	C	401	3	24,50,50	2.67	11 (45%)	19,82,82	3.25	11 (57%)
10	HEC	C	402	3	24,50,50	2.66	11 (45%)	19,82,82	3.07	14 (73%)
11	FC6	C	403	-	12,12,12	2.56	6 (50%)	0,21,21	0.00	-
5	HEM	D	501	1,8,7	24,50,50	2.36	6 (25%)	16,82,82	1.42	2 (12%)
5	HEM	D	502	1,7	24,50,50	2.44	6 (25%)	16,82,82	1.53	2 (12%)
9	PO4	D	505	-	4,4,4	0.70	0	6,6,6	0.23	0
8	PEO	D	506	5,6	1,1,1	0.48	0	0,0,0	0.00	-
10	HEC	E	301	2	24,50,50	2.56	11 (45%)	19,82,82	2.90	9 (47%)
10	HEC	F	401	3	24,50,50	2.71	11 (45%)	19,82,82	3.00	8 (42%)
10	HEC	F	402	3	24,50,50	2.84	11 (45%)	19,82,82	2.75	10 (52%)
11	FC6	F	403	-	12,12,12	2.63	6 (50%)	0,21,21	0.00	-
5	HEM	G	501	1,8,7	24,50,50	2.32	6 (25%)	16,82,82	1.68	4 (25%)
5	HEM	G	502	1,7	24,50,50	2.46	6 (25%)	16,82,82	1.64	4 (25%)
8	PEO	G	505	5,6	1,1,1	0.55	0	0,0,0	0.00	-
9	PO4	G	506	-	4,4,4	0.75	0	6,6,6	0.23	0
10	HEC	H	301	2	24,50,50	2.58	12 (50%)	19,82,82	3.12	8 (42%)
11	FC6	I	401	-	12,12,12	2.65	6 (50%)	0,21,21	0.00	-
10	HEC	I	402	3	24,50,50	2.73	11 (45%)	19,82,82	3.13	12 (63%)
10	HEC	I	403	3	24,50,50	2.62	11 (45%)	19,82,82	3.01	12 (63%)
5	HEM	K	501	1,8,7	24,50,50	2.33	7 (29%)	16,82,82	1.40	1 (6%)
5	HEM	K	502	1,7	24,50,50	2.43	6 (25%)	16,82,82	1.56	3 (18%)
9	PO4	K	506	-	4,4,4	0.89	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	PEO	K	507	5,6	1,1,1	0.48	0	0,0,0	0.00	-
10	HEC	L	301	2	24,50,50	2.51	11 (45%)	19,82,82	3.07	10 (52%)
11	FC6	M	401	-	12,12,12	2.58	6 (50%)	0,21,21	0.00	-
10	HEC	M	402	3	24,50,50	2.60	11 (45%)	19,82,82	3.40	11 (57%)
10	HEC	M	403	3	24,50,50	2.66	10 (41%)	19,82,82	3.03	11 (57%)

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
5	HEM	A	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	A	502	1,7	-	0/6/54/54	0/0/8/8
8	PEO	A	505	5,6	-	0/0/0/0	0/0/0/0
9	PO4	A	506	-	-	0/0/0/0	0/0/0/0
10	HEC	B	301	2	-	0/6/54/54	0/0/8/8
10	HEC	C	401	3	-	0/6/54/54	0/0/8/8
10	HEC	C	402	3	-	0/6/54/54	0/0/8/8
11	FC6	C	403	-	-	0/0/30/30	0/0/0/0
5	HEM	D	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	D	502	1,7	-	0/6/54/54	0/0/8/8
9	PO4	D	505	-	-	0/0/0/0	0/0/0/0
8	PEO	D	506	5,6	-	0/0/0/0	0/0/0/0
10	HEC	E	301	2	-	0/6/54/54	0/0/8/8
10	HEC	F	401	3	-	0/6/54/54	0/0/8/8
10	HEC	F	402	3	-	0/6/54/54	0/0/8/8
11	FC6	F	403	-	-	0/0/30/30	0/0/0/0
5	HEM	G	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	G	502	1,7	-	0/6/54/54	0/0/8/8
8	PEO	G	505	5,6	-	0/0/0/0	0/0/0/0
9	PO4	G	506	-	-	0/0/0/0	0/0/0/0
10	HEC	H	301	2	-	0/6/54/54	0/0/8/8
11	FC6	I	401	-	-	0/0/30/30	0/0/0/0
10	HEC	I	402	3	-	0/6/54/54	0/0/8/8
10	HEC	I	403	3	-	0/6/54/54	0/0/8/8
5	HEM	K	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	K	502	1,7	-	0/6/54/54	0/0/8/8
9	PO4	K	506	-	-	0/0/0/0	0/0/0/0
8	PEO	K	507	5,6	-	0/0/0/0	0/0/0/0
10	HEC	L	301	2	-	0/6/54/54	0/0/8/8
11	FC6	M	401	-	-	0/0/30/30	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEC	M	402	3	-	0/6/54/54	0/0/8/8
10	HEC	M	403	3	-	0/6/54/54	0/0/8/8

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	HEM	C3C-C2C	-5.89	1.32	1.40
5	A	502	HEM	C3B-C2B	-5.78	1.33	1.40
5	G	502	HEM	C3C-C2C	-5.76	1.33	1.40
5	D	502	HEM	C3C-C2C	-5.52	1.33	1.40
5	K	502	HEM	C3C-C2C	-5.46	1.33	1.40

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	301	HEC	CBB-CAB-C3B	-7.64	110.64	127.34
10	E	301	HEC	CBB-CAB-C3B	-7.38	111.20	127.34
10	B	301	HEC	CBA-CAA-C2A	-7.34	99.59	112.47
10	L	301	HEC	CBB-CAB-C3B	-7.28	111.42	127.34
10	M	402	HEC	CAA-CBA-CGA	-7.21	98.75	112.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	HEM	3	0
5	A	502	HEM	9	0
9	A	506	PO4	1	0
10	B	301	HEC	5	0
10	C	401	HEC	8	0
10	C	402	HEC	3	0
11	C	403	FC6	2	0
5	D	501	HEM	5	0
5	D	502	HEM	8	0
9	D	505	PO4	1	0
10	E	301	HEC	6	0
10	F	401	HEC	7	0
10	F	402	HEC	3	0
11	F	403	FC6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	501	HEM	5	0
5	G	502	HEM	8	0
9	G	506	PO4	1	0
10	H	301	HEC	6	0
11	I	401	FC6	1	0
10	I	402	HEC	8	0
10	I	403	HEC	3	0
5	K	501	HEM	5	0
5	K	502	HEM	8	0
9	K	506	PO4	4	0
10	L	301	HEC	4	0
11	M	401	FC6	2	0
10	M	402	HEC	9	0
10	M	403	HEC	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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	466/474 (98%)	-0.75	6 (1%) 79 67	45, 76, 129, 206	0
1	D	463/474 (97%)	-0.25	20 (4%) 39 25	76, 153, 234, 310	0
1	G	465/474 (98%)	-0.68	3 (0%) 90 84	55, 90, 142, 254	0
1	K	465/474 (98%)	-0.33	14 (3%) 54 39	61, 145, 226, 280	0
2	B	197/203 (97%)	-0.77	2 (1%) 84 75	42, 70, 126, 169	0
2	E	197/203 (97%)	-0.19	7 (3%) 46 31	68, 138, 213, 279	0
2	H	197/203 (97%)	-0.71	1 (0%) 91 87	54, 83, 146, 202	0
2	L	197/203 (97%)	-0.47	6 (3%) 54 39	52, 110, 215, 322	0
3	C	303/311 (97%)	-0.63	2 (0%) 89 83	41, 83, 138, 192	0
3	F	303/311 (97%)	0.18	23 (7%) 17 9	72, 173, 260, 419	0
3	I	303/311 (97%)	-0.43	7 (2%) 64 49	52, 106, 166, 215	0
3	M	303/311 (97%)	-0.31	15 (4%) 32 19	43, 85, 243, 322	0
4	N	29/36 (80%)	-0.20	2 (6%) 20 11	65, 92, 167, 174	0
4	O	29/36 (80%)	0.86	7 (24%) 1 1	148, 172, 249, 263	0
4	P	29/36 (80%)	-0.12	1 (3%) 49 34	91, 109, 173, 191	0
4	Q	29/36 (80%)	0.47	3 (10%) 9 5	119, 142, 186, 199	0
All	All	3975/4096 (97%)	-0.42	119 (2%) 54 39	41, 107, 219, 419	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	466	GLU	9.3
2	E	201	ASN	9.1
2	E	44	GLU	7.7
3	F	3	THR	7.7
3	M	50	TYR	7.3

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	FC6	F	403	13/13	0.78	0.35	4.50	53,61,87,101	13
11	FC6	I	401	13/13	0.91	0.25	1.78	78,94,143,158	13
10	HEC	C	402	43/43	0.94	0.18	1.76	36,54,72,160	0
10	HEC	B	301	43/43	0.96	0.17	1.70	39,55,69,119	0
5	HEM	K	501	43/43	0.96	0.22	1.24	119,135,151,154	0
10	HEC	I	403	43/43	0.97	0.17	0.87	50,61,69,85	0
10	HEC	H	301	43/43	0.98	0.15	0.78	42,53,70,79	0
10	HEC	F	401	43/43	0.96	0.21	0.74	85,103,116,121	0
11	FC6	C	403	13/13	0.98	0.15	0.70	60,75,98,101	13
8	PEO	A	505	2/2	0.97	0.16	0.65	74,74,74,74	0
10	HEC	M	403	43/43	0.98	0.14	0.64	35,51,64,84	0
10	HEC	M	402	43/43	0.98	0.14	0.64	33,42,54,63	0
10	HEC	L	301	43/43	0.98	0.14	0.60	49,65,78,78	0
11	FC6	M	401	13/13	0.98	0.14	0.58	43,60,98,98	13
10	HEC	C	401	43/43	0.98	0.15	0.52	44,57,66,73	0
10	HEC	F	402	43/43	0.96	0.20	0.42	117,134,147,154	0
10	HEC	I	402	43/43	0.98	0.14	0.40	38,54,77,91	0
10	HEC	E	301	43/43	0.98	0.14	0.21	62,73,96,102	0
5	HEM	K	502	43/43	0.98	0.16	0.17	95,108,128,130	0
5	HEM	D	501	43/43	0.98	0.15	0.13	93,119,136,143	0
5	HEM	A	502	43/43	0.98	0.13	0.04	41,54,79,83	0
7	CA	D	504	1/1	0.89	0.21	0.01	151,151,151,151	0
5	HEM	D	502	43/43	0.98	0.15	-0.01	89,110,124,130	0
5	HEM	G	502	43/43	0.98	0.13	-0.23	54,66,77,86	0
9	PO4	D	505	5/5	0.72	0.24	-0.31	180,183,183,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	HEM	A	501	43/43	0.99	0.12	-0.36	45,63,72,76	0
5	HEM	G	501	43/43	0.99	0.11	-0.97	57,72,84,93	0
7	CA	D	507	1/1	0.98	0.10	-1.05	96,96,96,96	0
7	CA	K	505	1/1	0.95	0.12	-1.06	136,136,136,136	0
9	PO4	A	506	5/5	0.93	0.14	-1.09	60,68,75,88	0
9	PO4	K	506	5/5	0.78	0.16	-1.18	138,141,143,150	0
7	CA	G	507	1/1	0.98	0.09	-1.35	72,72,72,72	0
7	CA	A	504	1/1	0.82	0.09	-1.37	99,99,99,99	0
7	CA	G	504	1/1	0.95	0.08	-1.47	87,87,87,87	0
9	PO4	G	506	5/5	0.91	0.12	-1.65	130,132,139,152	0
8	PEO	K	507	2/2	0.98	0.12	-1.70	131,131,131,131	0
8	PEO	D	506	2/2	0.99	0.11	-1.90	145,145,145,147	0
8	PEO	G	505	2/2	0.99	0.10	-3.08	80,80,80,83	0
7	CA	K	504	1/1	0.96	0.05	-3.60	95,95,95,95	0
6	CU	G	503	1/1	0.98	0.03	-	74,74,74,74	0
7	CA	A	507	1/1	0.98	0.25	-	84,84,84,84	0
6	CU	D	503	1/1	0.94	0.06	-	118,118,118,118	0
6	CU	A	503	1/1	0.94	0.34	-	133,133,133,133	0
6	CU	K	503	1/1	0.91	0.10	-	133,133,133,133	0

6.5 Other polymers (i)

There are no such residues in this entry.