wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:42 AM GMT

PDB ID	:	3MK7
Title	:	The structure of CBB3 cytochrome oxidase
Authors	:	Buschmann, S.; Warkentin, E.; Michel, H.; Ermler, U.
Deposited on	:	2010-04-14
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:

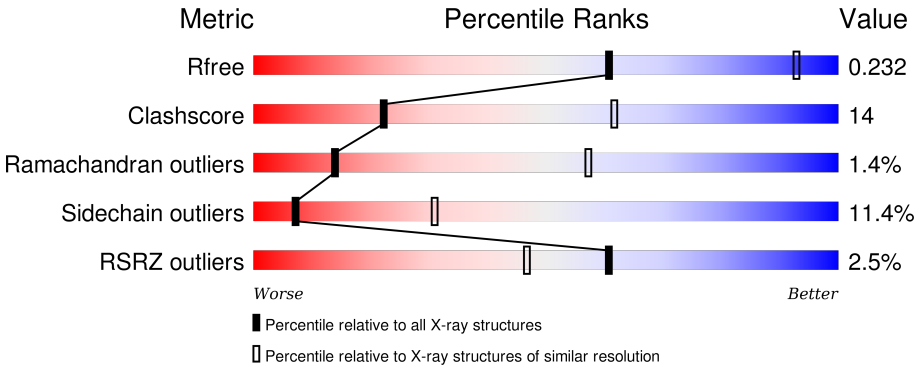
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 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% 64% 29%
1	G	474	62% 32% 5%
1	K	474	3% 66% 28%
2	B	203	68% 25%

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Mol	Chain	Length	Quality of chain
2	E	203	4% 70% 23%
2	H	203	2% 65% 29%
2	L	203	3% 72% 21%
3	C	311	% 68% 26%
3	F	311	5% 70% 22% 5%
3	I	311	2% 69% 24%
3	M	311	3% 68% 24%
4	U	30	73% 27%
4	X	30	93% 7%
4	Y	30	90% 10%
4	Z	30	80% 20%

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	C	323	-	-	X	-
11	FC6	F	323	-	-	X	X
11	FC6	I	323	-	-	X	X
9	PO4	G	506	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31690 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 c oxidase, cbb3-type, subunit N.

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 Cytochrome c oxidase, cbb3-type, subunit O.

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			

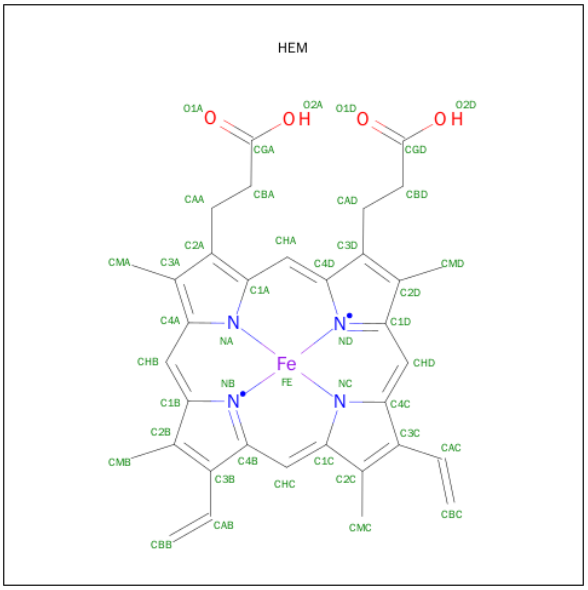
- Molecule 3 is a protein called Cytochrome c oxidase, cbb3-type, subunit P.

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 30-mer peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	U	30	Total C N O 150 90 30 30	0	0	0
4	X	30	Total C N O 150 90 30 30	0	0	0
4	Y	30	Total C N O 150 90 30 30	0	0	0
4	Z	30	Total C N O 150 90 30 30	0	0	0

- 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 43 34 1 4 4	0	0
5	A	1	Total C Fe N O 43 34 1 4 4	0	0
5	D	1	Total C Fe N O 43 34 1 4 4	0	0
5	D	1	Total C Fe N O 43 34 1 4 4	0	0
5	G	1	Total C Fe N O 43 34 1 4 4	0	0
5	G	1	Total C Fe N O 43 34 1 4 4	0	0

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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		

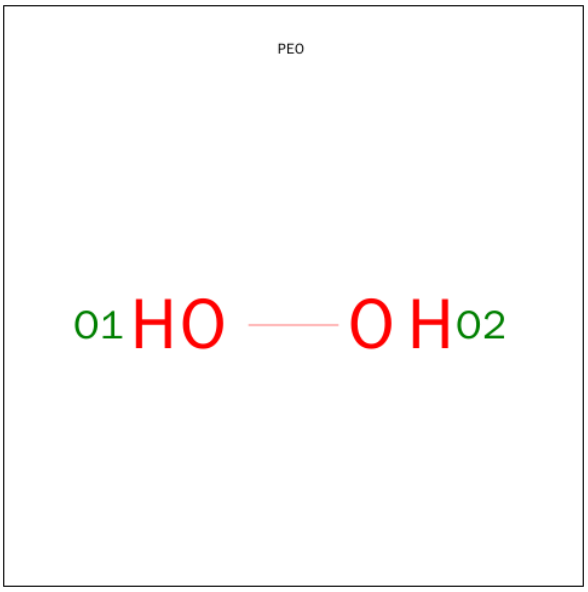
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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).

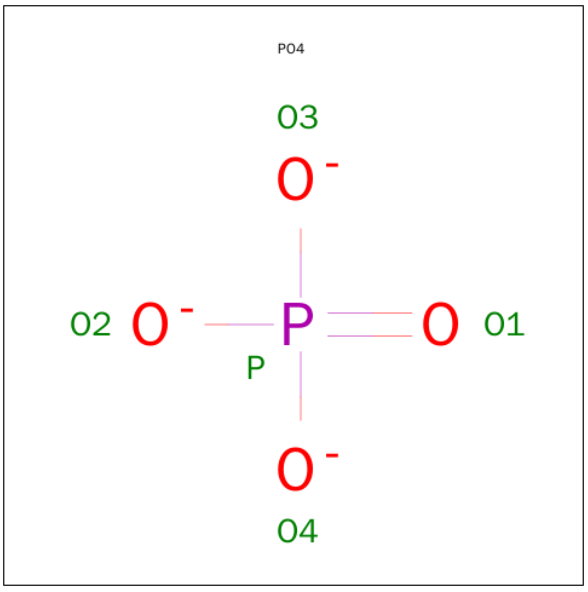
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total	Ca	0	0
			2	2		
7	D	1	Total	Ca	0	0
			1	1		
7	K	2	Total	Ca	0	0
			2	2		
7	E	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

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



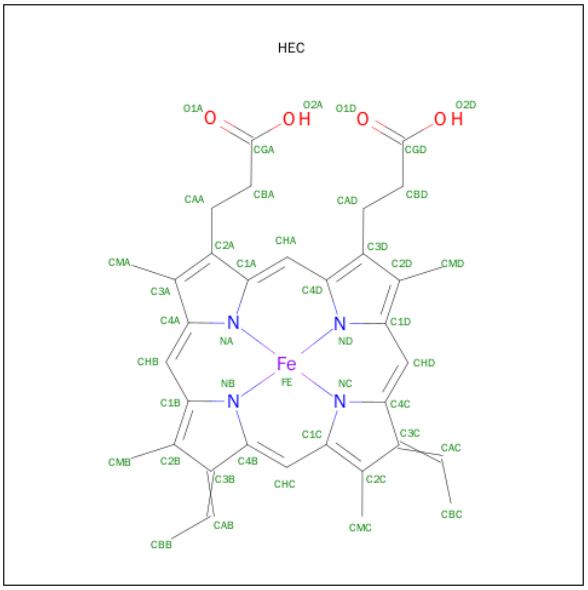
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	D	1	Total O 2 2	0	0
8	G	1	Total O 2 2	0	0
8	K	1	Total O 2 2	0	0

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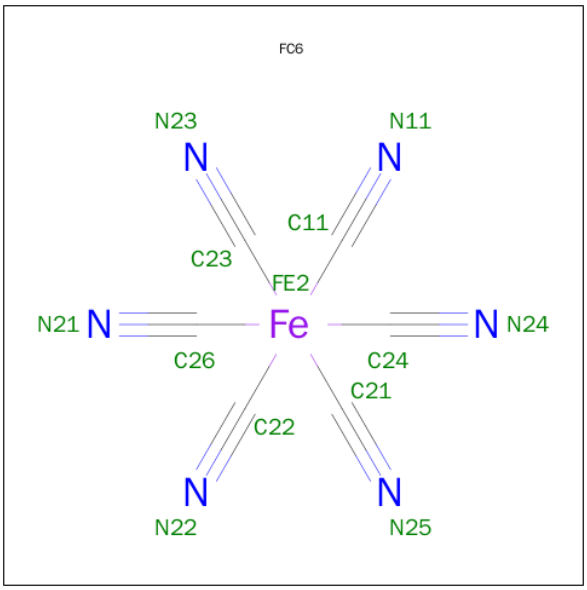
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



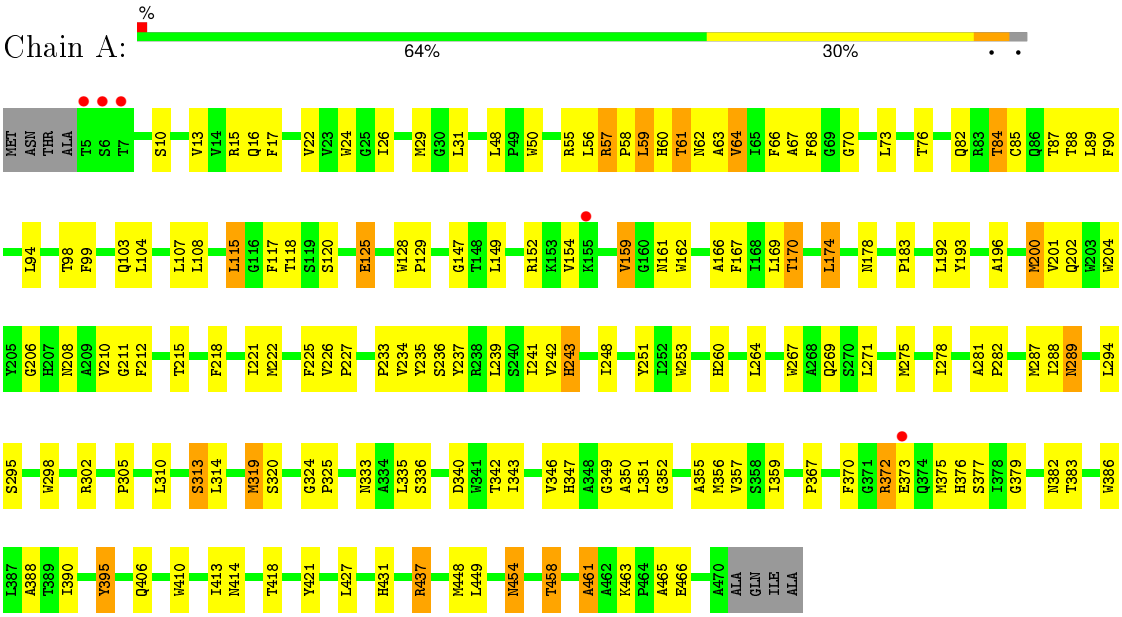
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	I	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	F	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	C	1	Total	C	Fe	N	0	0
			13	6	1	6		

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.

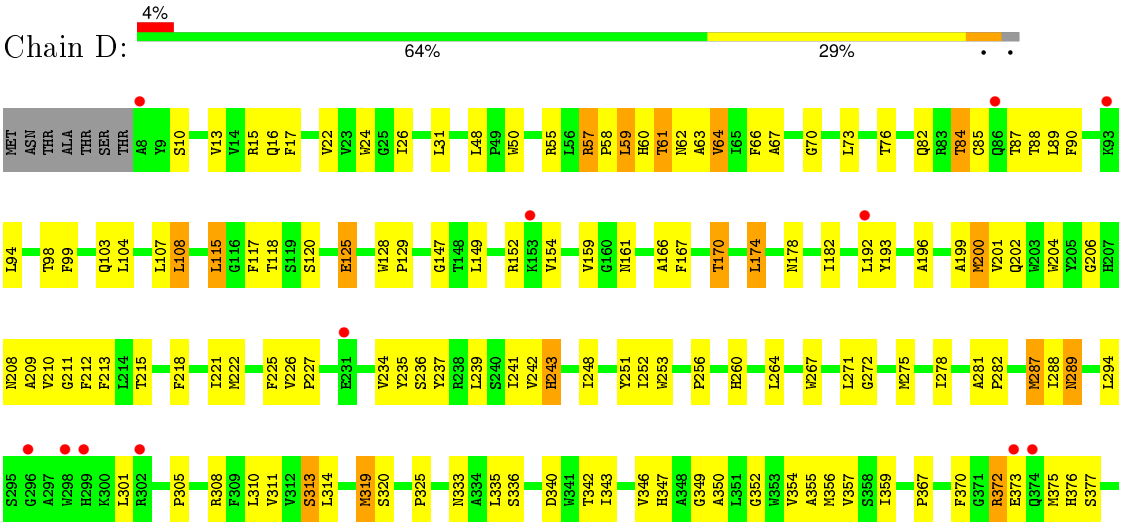
- Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N

Chain A:



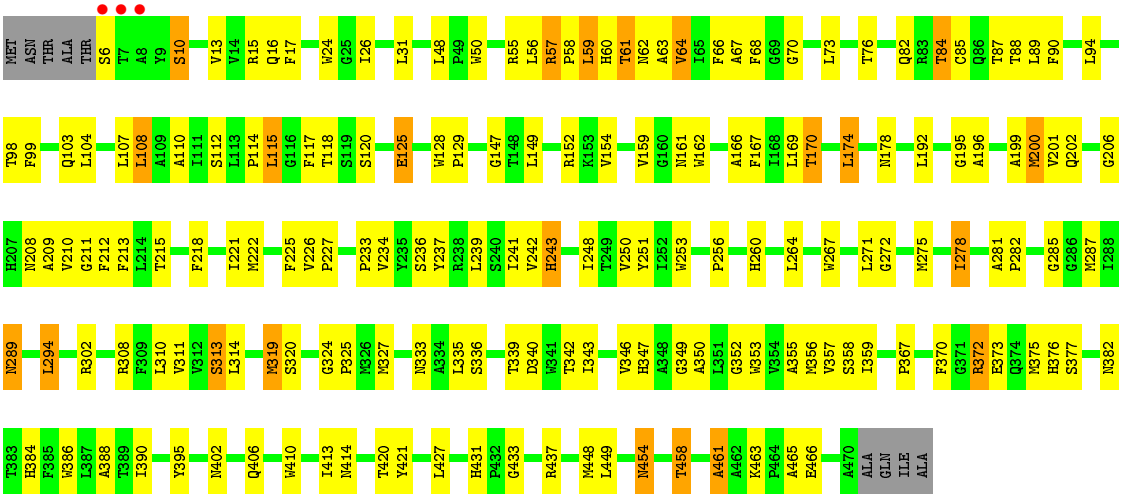
- Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N

Chain D:



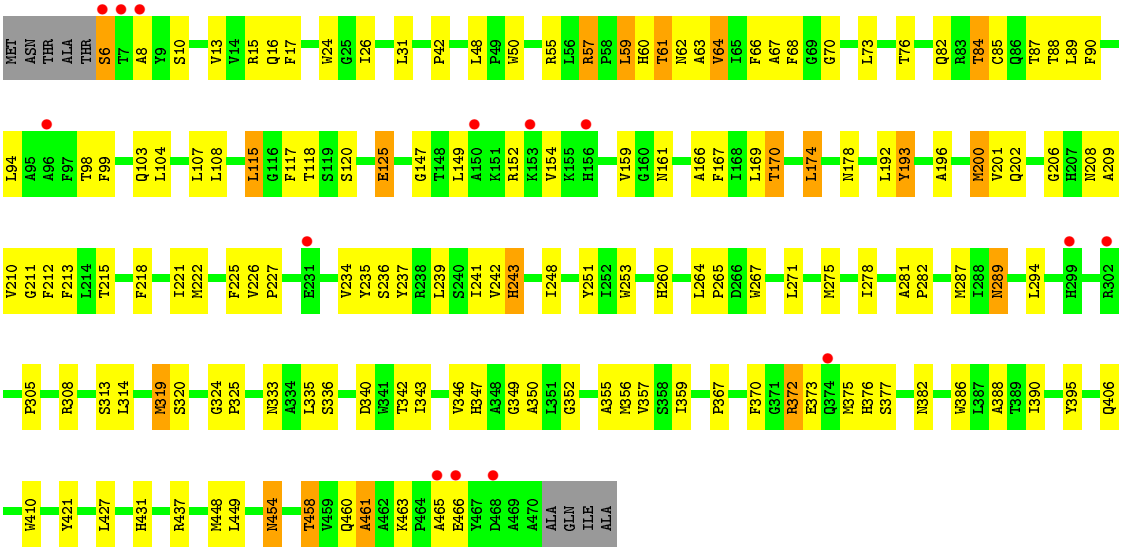
• Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N

Chain G:



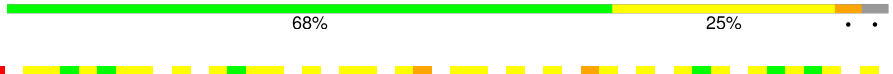
• Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N

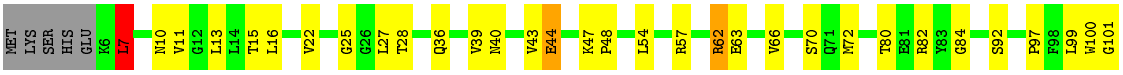
Chain K:



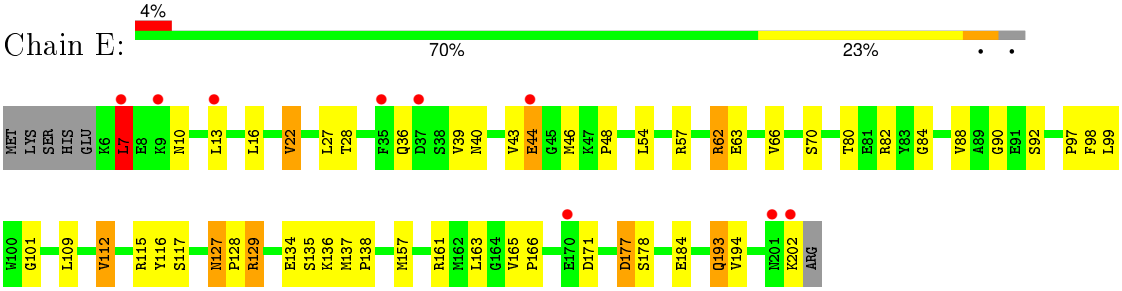
• Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O

Chain B:

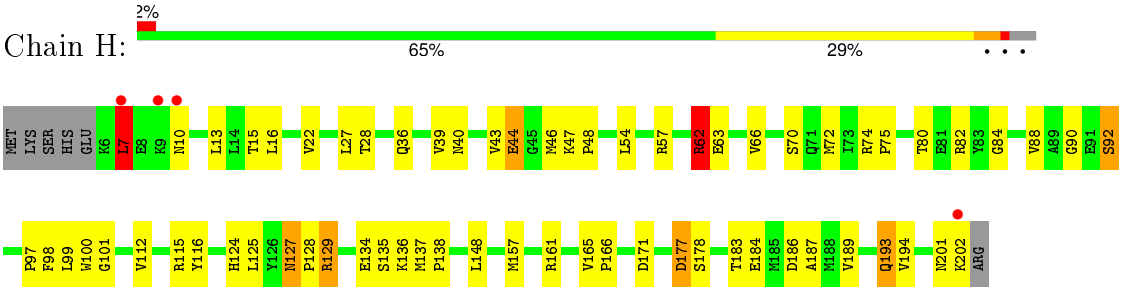




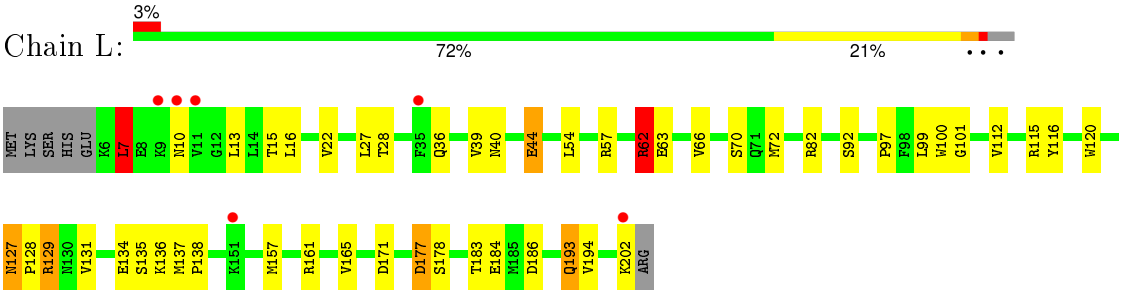
• Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O



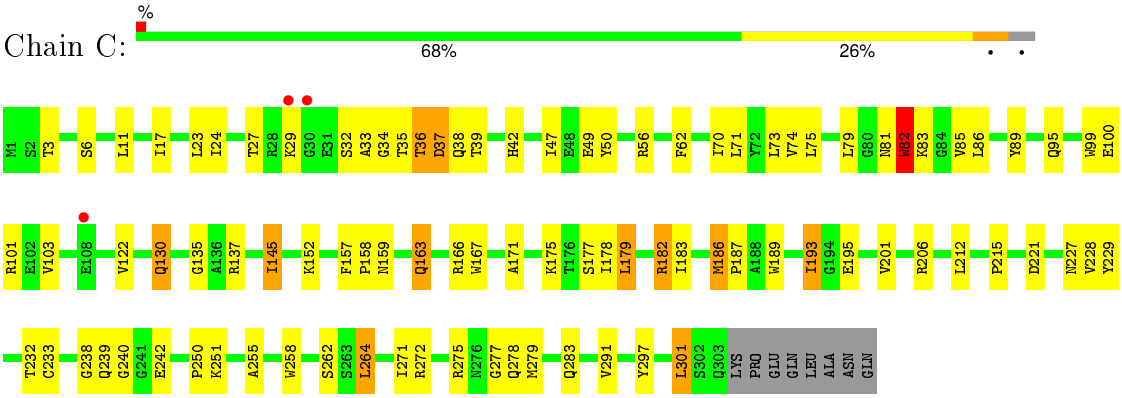
• Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O



• Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O

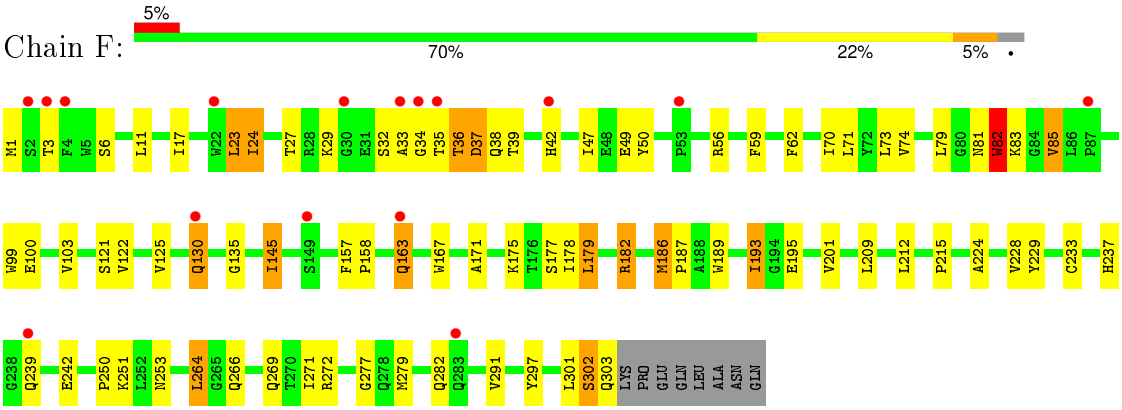


• Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P



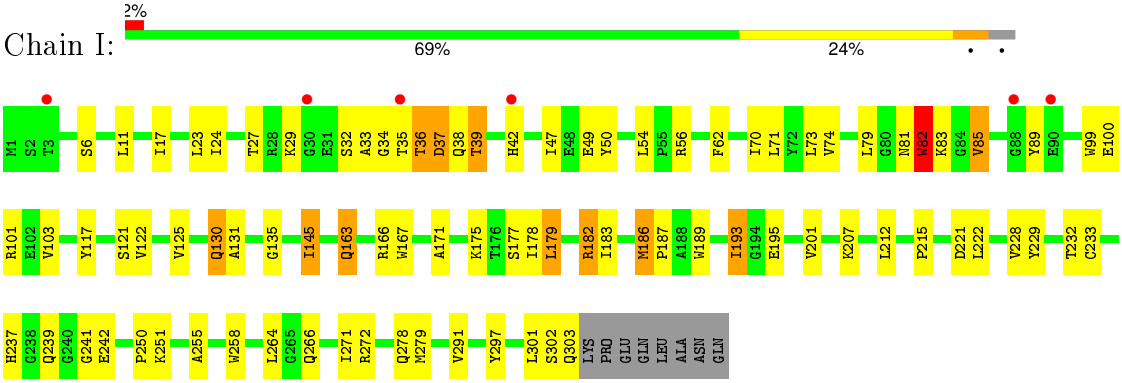
• Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P

Chain F:



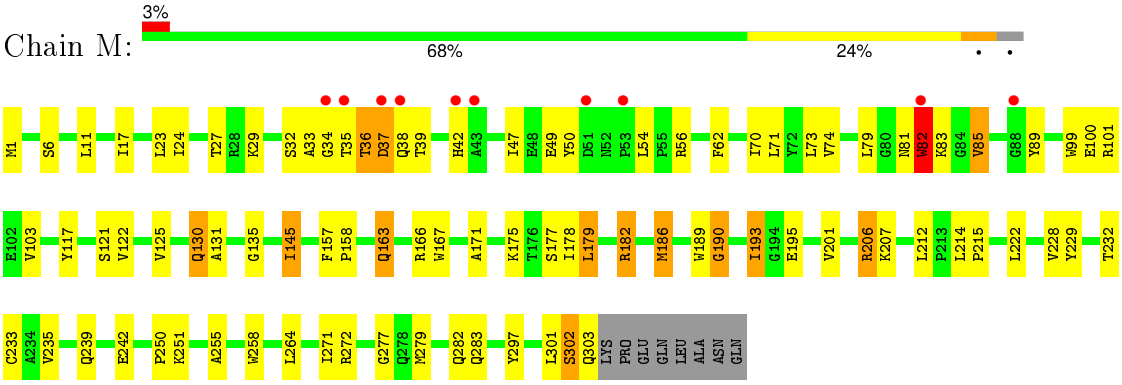
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P

Chain I:



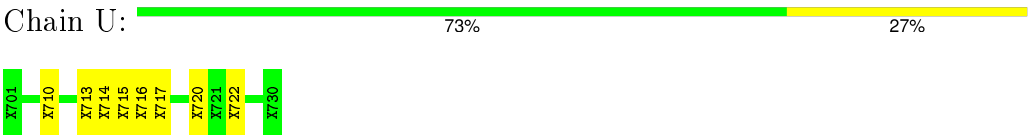
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P

Chain M:



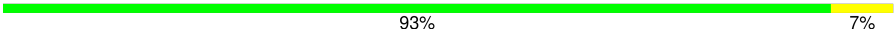
- Molecule 4: 30-mer peptide

Chain U:



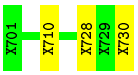
- Molecule 4: 30-mer peptide

Chain X:



• Molecule 4: 30-mer peptide

Chain Y:



• Molecule 4: 30-mer peptide

Chain Z:

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)	15.00 – 3.20 14.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-3.20) 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	REFMAC 5.6.0046	Depositor
R, R_{free}	0.189 , 0.223 0.198 , 0.232	Depositor DCC
R_{free} test set	5564 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	87.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 82.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	2 of 131746 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31690	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.58	0/3811	0.64	1/5210 (0.0%)
1	D	0.40	0/3791	0.54	0/5182
1	G	0.53	0/3804	0.60	0/5200
1	K	0.49	2/3804 (0.1%)	0.56	0/5200
2	B	0.68	0/1584	0.76	1/2146 (0.0%)
2	E	0.45	0/1584	0.64	1/2146 (0.0%)
2	H	0.62	0/1584	0.73	2/2146 (0.1%)
2	L	0.53	0/1584	0.69	2/2146 (0.1%)
3	C	0.61	0/2374	0.72	1/3225 (0.0%)
3	F	0.44	0/2374	0.59	0/3225
3	I	0.55	0/2374	0.66	0/3225
3	M	0.64	0/2374	0.71	1/3225 (0.0%)
All	All	0.54	2/31042 (0.0%)	0.64	9/42276 (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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	6	SER	CB-OG	-9.55	1.29	1.42
1	K	6	SER	CA-CB	7.86	1.64	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	ARG	NE-CZ-NH2	-7.53	116.54	120.30
3	C	275	ARG	NE-CZ-NH1	-6.66	116.97	120.30
2	H	62	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	L	62	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	E	7	LEU	CA-CB-CG	5.39	127.69	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	112	VAL	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	121	0
1	D	3663	0	3644	117	0
1	G	3676	0	3656	120	0
1	K	3676	0	3656	111	0
2	B	1548	0	1526	45	0
2	E	1548	0	1526	45	0
2	H	1548	0	1526	48	0
2	L	1548	0	1526	36	0
3	C	2312	0	2237	68	1
3	F	2312	0	2237	69	0
3	I	2312	0	2237	67	1
3	M	2312	0	2237	65	0
4	U	150	0	33	6	0
4	X	150	0	33	2	0
4	Y	150	0	33	4	0
4	Z	150	0	35	4	0
5	A	86	0	60	11	0
5	D	86	0	60	12	0
5	G	86	0	60	13	0
5	K	86	0	60	12	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	1	0	0	0	0
6	K	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	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	0	0
9	D	5	0	0	0	0
9	G	5	0	0	0	0
9	K	5	0	0	0	0
10	B	43	0	30	3	0
10	C	86	0	60	10	0
10	E	43	0	30	2	0
10	F	86	0	60	17	0
10	H	43	0	30	4	0
10	I	86	0	60	6	0
10	L	43	0	30	2	0
10	M	86	0	60	9	0
11	C	13	0	0	4	0
11	F	13	0	0	10	0
11	I	13	0	0	6	0
11	M	13	0	0	3	0
All	All	31690	0	30405	858	1

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 858 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:359:ILE:HD11	1:D:448:MET:HE1	1.18	1.17
1:K:359:ILE:HD11	1:K:448:MET:HE1	1.21	1.11
1:G:359:ILE:HD11	1:G:448:MET:HE1	1.19	1.11
1:A:359:ILE:HD11	1:A:448:MET:HE1	1.14	1.10
11:F:323:FC6:N24	3:I:215:PRO:HB3	1.66	1.10

All (1) 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)
3:C:34:GLY:CA	3:I:39:THR:OG1[1_556]	2.10	0.10

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%)	432 (93%)	27 (6%)	5 (1%)	17	62
1	D	461/474 (97%)	430 (93%)	26 (6%)	5 (1%)	17	62
1	G	463/474 (98%)	428 (92%)	30 (6%)	5 (1%)	17	62
1	K	463/474 (98%)	430 (93%)	28 (6%)	5 (1%)	17	62
2	B	195/203 (96%)	185 (95%)	8 (4%)	2 (1%)	19	65
2	E	195/203 (96%)	186 (95%)	7 (4%)	2 (1%)	19	65
2	H	195/203 (96%)	184 (94%)	9 (5%)	2 (1%)	19	65
2	L	195/203 (96%)	185 (95%)	8 (4%)	2 (1%)	19	65
3	C	301/311 (97%)	276 (92%)	17 (6%)	8 (3%)	6	39
3	F	301/311 (97%)	276 (92%)	19 (6%)	6 (2%)	9	48
3	I	301/311 (97%)	276 (92%)	19 (6%)	6 (2%)	9	48
3	M	301/311 (97%)	274 (91%)	20 (7%)	7 (2%)	8	44
All	All	3835/3952 (97%)	3562 (93%)	218 (6%)	55 (1%)	14	57

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ALA
1	A	465	ALA
2	B	44	GLU
3	C	29	LYS

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Mol	Chain	Res	Type
3	C	33	ALA

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%)	331 (88%)	43 (12%)	7	30
1	D	371/379 (98%)	328 (88%)	43 (12%)	7	30
1	G	373/379 (98%)	327 (88%)	46 (12%)	6	27
1	K	373/379 (98%)	330 (88%)	43 (12%)	7	30
2	B	166/172 (96%)	148 (89%)	18 (11%)	8	33
2	E	166/172 (96%)	148 (89%)	18 (11%)	8	33
2	H	166/172 (96%)	148 (89%)	18 (11%)	8	33
2	L	166/172 (96%)	148 (89%)	18 (11%)	8	33
3	C	227/234 (97%)	203 (89%)	24 (11%)	8	34
3	F	227/234 (97%)	200 (88%)	27 (12%)	6	28
3	I	227/234 (97%)	202 (89%)	25 (11%)	8	33
3	M	227/234 (97%)	200 (88%)	27 (12%)	6	28
All	All	3063/3140 (98%)	2713 (89%)	350 (11%)	7	31

5 of 350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	85	VAL
1	G	174	LEU
3	M	1	MET
3	F	163	GLN
1	G	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	105	GLN
1	G	178	ASN
2	L	29	GLN
3	F	130	GLN
1	G	16	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	30,50,50	2.08	4 (13%)	24,82,82	2.48	11 (45%)
5	HEM	A	502	1,7	30,50,50	2.19	6 (20%)	24,82,82	2.59	11 (45%)
9	PO4	A	506	-	4,4,4	0.39	0	6,6,6	0.32	0
8	PEO	A	508	5,6	1,1,1	0.38	0	0,0,0	0.00	-
10	HEC	B	211	2	24,50,50	2.70	3 (12%)	19,82,82	3.25	5 (26%)
10	HEC	C	321	3	24,50,50	2.56	4 (16%)	19,82,82	3.08	6 (31%)
10	HEC	C	322	3	24,50,50	2.46	3 (12%)	19,82,82	3.19	9 (47%)
11	FC6	C	323	-	12,12,12	1.17	1 (8%)	0,21,21	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	HEM	D	501	1,8,7	30,50,50	2.31	8 (26%)	24,82,82	2.31	9 (37%)
5	HEM	D	502	1,7	30,50,50	2.16	9 (30%)	24,82,82	2.54	10 (41%)
9	PO4	D	506	-	4,4,4	0.36	0	6,6,6	0.29	0
8	PEO	D	508	5,6	1,1,1	0.46	0	0,0,0	0.00	-
10	HEC	E	211	2	24,50,50	2.52	3 (12%)	19,82,82	2.84	4 (21%)
10	HEC	F	321	3	24,50,50	2.42	4 (16%)	19,82,82	3.01	7 (36%)
10	HEC	F	322	3	24,50,50	2.51	3 (12%)	19,82,82	2.80	7 (36%)
11	FC6	F	323	-	12,12,12	0.95	0	0,21,21	0.00	-
5	HEM	G	501	1,8,7	30,50,50	2.20	5 (16%)	24,82,82	2.47	11 (45%)
5	HEM	G	502	1,7	30,50,50	2.25	8 (26%)	24,82,82	2.66	11 (45%)
9	PO4	G	506	-	4,4,4	0.19	0	6,6,6	0.31	0
8	PEO	G	508	5,6	1,1,1	0.57	0	0,0,0	0.00	-
10	HEC	H	211	2	24,50,50	2.57	4 (16%)	19,82,82	3.12	7 (36%)
10	HEC	I	321	3	24,50,50	2.33	4 (16%)	19,82,82	3.20	6 (31%)
10	HEC	I	322	3	24,50,50	2.53	4 (16%)	19,82,82	2.77	8 (42%)
11	FC6	I	323	-	12,12,12	0.94	0	0,21,21	0.00	-
5	HEM	K	501	1,8,7	30,50,50	2.08	6 (20%)	24,82,82	2.36	10 (41%)
5	HEM	K	502	1,7	30,50,50	2.12	7 (23%)	24,82,82	2.48	11 (45%)
9	PO4	K	506	-	4,4,4	0.37	0	6,6,6	0.30	0
8	PEO	K	508	5,6	1,1,1	0.43	0	0,0,0	0.00	-
10	HEC	L	211	2	24,50,50	2.63	3 (12%)	19,82,82	2.95	6 (31%)
10	HEC	M	321	3	24,50,50	2.52	5 (20%)	19,82,82	3.50	7 (36%)
10	HEC	M	322	3	24,50,50	2.54	4 (16%)	19,82,82	2.94	7 (36%)
11	FC6	M	323	-	12,12,12	1.14	2 (16%)	0,21,21	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
5	HEM	A	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	A	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	A	506	-	-	0/0/0/0	0/0/0/0
8	PEO	A	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	B	211	2	-	0/6/54/54	0/0/8/8
10	HEC	C	321	3	-	0/6/54/54	0/0/8/8
10	HEC	C	322	3	-	0/6/54/54	0/0/8/8
11	FC6	C	323	-	-	0/0/30/30	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	D	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	D	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	D	506	-	-	0/0/0/0	0/0/0/0
8	PEO	D	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	E	211	2	-	0/6/54/54	0/0/8/8
10	HEC	F	321	3	-	0/6/54/54	0/0/8/8
10	HEC	F	322	3	-	0/6/54/54	0/0/8/8
11	FC6	F	323	-	-	0/0/30/30	0/0/0/0
5	HEM	G	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	G	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	G	506	-	-	0/0/0/0	0/0/0/0
8	PEO	G	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	H	211	2	-	0/6/54/54	0/0/8/8
10	HEC	I	321	3	-	0/6/54/54	0/0/8/8
10	HEC	I	322	3	-	0/6/54/54	0/0/8/8
11	FC6	I	323	-	-	0/0/30/30	0/0/0/0
5	HEM	K	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	K	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	K	506	-	-	0/0/0/0	0/0/0/0
8	PEO	K	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	L	211	2	-	0/6/54/54	0/0/8/8
10	HEC	M	321	3	-	0/6/54/54	0/0/8/8
10	HEC	M	322	3	-	0/6/54/54	0/0/8/8
11	FC6	M	323	-	-	0/0/30/30	0/0/0/0

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	211	HEC	C3C-C2C	-8.89	1.31	1.40
10	I	322	HEC	C3C-C2C	-7.92	1.32	1.40
5	G	502	HEM	C3B-C4B	-7.79	1.44	1.51
5	D	501	HEM	C3B-C4B	-7.79	1.44	1.51
10	M	321	HEC	C3C-C2C	-7.78	1.32	1.40

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	211	HEC	CBB-CAB-C3B	-10.07	104.97	127.35
10	M	321	HEC	CBB-CAB-C3B	-9.26	106.78	127.35
10	H	211	HEC	CBB-CAB-C3B	-8.86	107.66	127.35
10	E	211	HEC	CBB-CAB-C3B	-8.39	108.70	127.35
10	L	211	HEC	CBB-CAB-C3B	-8.23	109.06	127.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	HEM	5	0
5	A	502	HEM	6	0
10	B	211	HEC	3	0
10	C	321	HEC	7	0
10	C	322	HEC	3	0
11	C	323	FC6	4	0
5	D	501	HEM	4	0
5	D	502	HEM	8	0
10	E	211	HEC	2	0
10	F	321	HEC	11	0
10	F	322	HEC	6	0
11	F	323	FC6	10	0
5	G	501	HEM	6	0
5	G	502	HEM	7	0
10	H	211	HEC	4	0
10	I	321	HEC	4	0
10	I	322	HEC	2	0
11	I	323	FC6	6	0
5	K	501	HEM	5	0
5	K	502	HEM	7	0
10	L	211	HEC	2	0
10	M	321	HEC	5	0
10	M	322	HEC	4	0
11	M	323	FC6	3	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

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	5 (1%) 82 72	44, 75, 127, 177	0
1	D	463/474 (97%)	-0.28	20 (4%) 39 25	73, 156, 249, 313	0
1	G	465/474 (98%)	-0.68	3 (0%) 90 84	54, 88, 133, 176	0
1	K	465/474 (98%)	-0.37	14 (3%) 54 39	64, 145, 232, 269	0
2	B	197/203 (97%)	-0.79	1 (0%) 91 87	39, 64, 124, 172	0
2	E	197/203 (97%)	-0.18	9 (4%) 36 23	66, 140, 243, 290	0
2	H	197/203 (97%)	-0.68	4 (2%) 68 54	50, 78, 144, 200	0
2	L	197/203 (97%)	-0.52	6 (3%) 54 39	51, 105, 244, 304	0
3	C	303/311 (97%)	-0.64	3 (0%) 84 75	41, 77, 123, 179	0
3	F	303/311 (97%)	0.19	16 (5%) 30 17	71, 182, 279, 333	0
3	I	303/311 (97%)	-0.45	6 (1%) 68 54	48, 100, 158, 209	0
3	M	303/311 (97%)	-0.38	10 (3%) 50 35	43, 81, 279, 345	0
4	U	0/30	-	-	-	-
4	X	0/30	-	-	-	-
4	Y	0/30	-	-	-	-
4	Z	0/30	-	-	-	-
All	All	3859/4072 (94%)	-0.46	97 (2%) 61 47	39, 103, 235, 345	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	201	ASN	11.8
3	F	3	THR	9.0
2	E	202	LYS	8.2
1	K	299	HIS	7.3
3	F	34	GLY	5.8

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	I	323	13/13	0.89	0.36	4.78	52,57,68,80	13
11	FC6	F	323	13/13	0.86	0.31	3.51	37,40,42,46	13
9	PO4	G	506	5/5	0.94	0.27	2.52	27,29,32,35	0
11	FC6	C	323	13/13	0.96	0.25	1.60	33,39,46,55	13
5	HEM	K	501	43/43	0.95	0.22	1.22	117,127,147,153	0
10	HEC	F	322	43/43	0.94	0.25	1.08	34,43,47,50	0
9	PO4	A	506	5/5	0.95	0.19	0.99	21,22,23,24	0
8	PEO	K	508	2/2	0.99	0.17	0.65	130,130,130,135	0
10	HEC	F	321	43/43	0.94	0.23	0.65	20,24,28,35	0
11	FC6	M	323	13/13	0.97	0.17	0.42	28,30,38,39	13
10	HEC	E	211	43/43	0.97	0.15	0.32	16,18,27,32	0
5	HEM	K	502	43/43	0.97	0.16	0.23	85,102,115,125	0
5	HEM	D	502	43/43	0.98	0.15	0.18	83,96,110,112	0
5	HEM	A	502	43/43	0.98	0.14	0.10	43,52,61,72	0
10	HEC	L	211	43/43	0.97	0.12	-0.16	18,21,26,30	0
5	HEM	D	501	43/43	0.98	0.14	-0.26	96,121,137,149	0
5	HEM	G	502	43/43	0.98	0.12	-0.38	56,61,70,83	0
10	HEC	I	322	43/43	0.98	0.10	-0.47	24,28,31,36	0
10	HEC	B	211	43/43	0.98	0.10	-0.59	25,28,35,46	0
5	HEM	G	501	43/43	0.99	0.11	-0.65	56,71,81,89	0
10	HEC	I	321	43/43	0.98	0.10	-0.67	20,24,34,39	0
7	CA	G	505	1/1	0.93	0.12	-0.67	91,91,91,91	0
5	HEM	A	501	43/43	0.99	0.11	-0.68	47,57,64,71	0
10	HEC	H	211	43/43	0.98	0.10	-0.74	24,27,32,38	0
9	PO4	D	506	5/5	0.81	0.19	-0.83	177,178,188,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	HEC	C	321	43/43	0.99	0.08	-0.87	21,27,36,44	0
10	HEC	C	322	43/43	0.98	0.10	-0.91	22,28,34,36	0
10	HEC	M	322	43/43	0.98	0.09	-0.94	19,23,27,34	0
7	CA	A	505	1/1	0.71	0.11	-1.01	88,88,88,88	0
10	HEC	M	321	43/43	0.99	0.09	-1.10	18,25,35,43	0
8	PEO	D	508	2/2	0.99	0.12	-1.33	133,133,133,141	0
8	PEO	G	508	2/2	1.00	0.10	-1.52	71,71,71,74	0
7	CA	K	505	1/1	0.95	0.08	-1.58	133,133,133,133	0
7	CA	D	505	1/1	0.80	0.10	-1.62	138,138,138,138	0
7	CA	E	504	1/1	0.99	0.09	-1.63	105,105,105,105	0
9	PO4	K	506	5/5	0.95	0.08	-1.78	140,144,146,153	0
8	PEO	A	508	2/2	1.00	0.10	-1.84	57,57,57,63	0
7	CA	K	504	1/1	0.97	0.05	-2.82	99,99,99,99	0
7	CA	B	504	1/1	1.00	0.11	-	51,51,51,51	0
7	CA	G	504	1/1	0.98	0.08	-	74,74,74,74	0
6	CU	K	503	1/1	0.98	0.11	-	135,135,135,135	0
6	CU	G	503	1/1	0.99	0.05	-	77,77,77,77	0
6	CU	D	503	1/1	0.98	0.05	-	115,115,115,115	0
6	CU	A	503	1/1	1.00	0.09	-	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.