



wwPDB X-ray Structure Validation Summary Report i

Oct 21, 2014 – 08:06 PM EDT

PDB ID : 1PP9
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2003-06-16
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

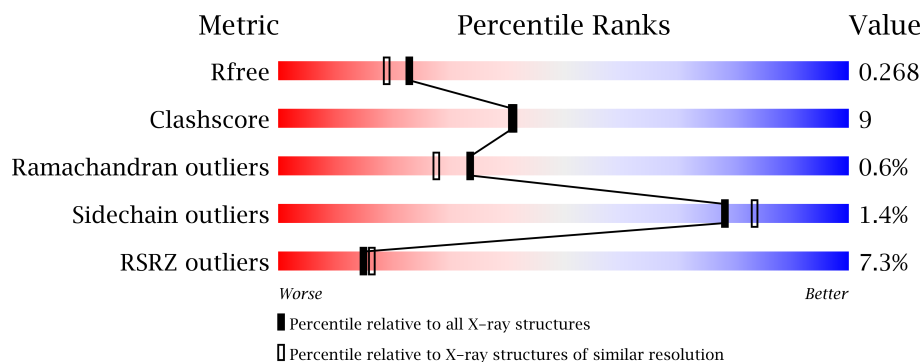
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24103
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
1	N	446	
2	B	439	
2	O	439	
3	C	379	
3	P	379	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	

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Mol	Chain	Length	Quality of chain
8	H	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	BHG	A	4002	-	X
11	BHG	C	2008	-	X
11	BHG	F	3011	-	X
11	BHG	F	4001	-	X
11	BHG	P	3008	-	X
11	BHG	S	2011	-	X
12	PO4	B	3010	-	X
13	AZI	A	4005	-	X
13	AZI	C	2014	-	X
13	AZI	D	4004	-	X
13	AZI	P	3014	X	X
18	UQ	P	3002	-	X
19	CDL	G	2003	-	X
19	CDL	G	2004	-	X
20	PEE	A	4003	-	X
20	PEE	C	2007	-	X
20	PEE	C	2012	-	X
20	PEE	D	2006	-	X
20	PEE	G	2005	-	X
20	PEE	Q	3006	-	X
20	PEE	T	3005	-	X
21	GOL	B	2013	-	X
21	GOL	C	2009	-	X
21	GOL	O	3013	-	X
21	GOL	P	3009	-	X

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33959 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	20			
1	N	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3177	1996	562	612	7			
2	O	424	Total	C	N	O	S	0	0	0
			3180	1998	562	613	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2892	1940	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2931	1968	455	490	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

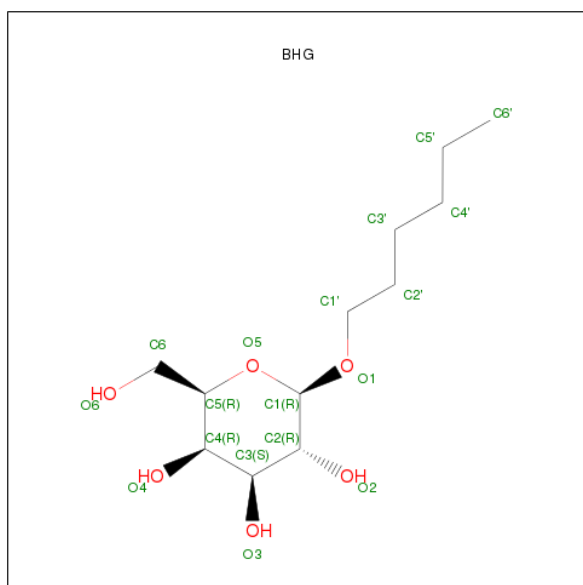
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			
9	V	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

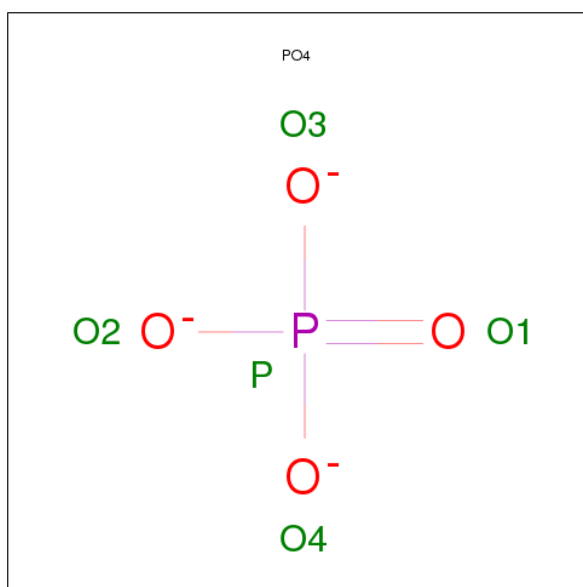
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			507	333	88	86			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: C₁₂H₂₄O₆).



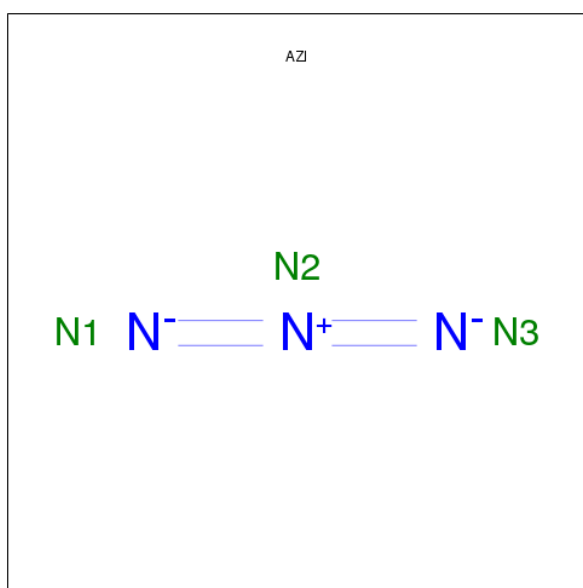
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	O	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula: N_3).



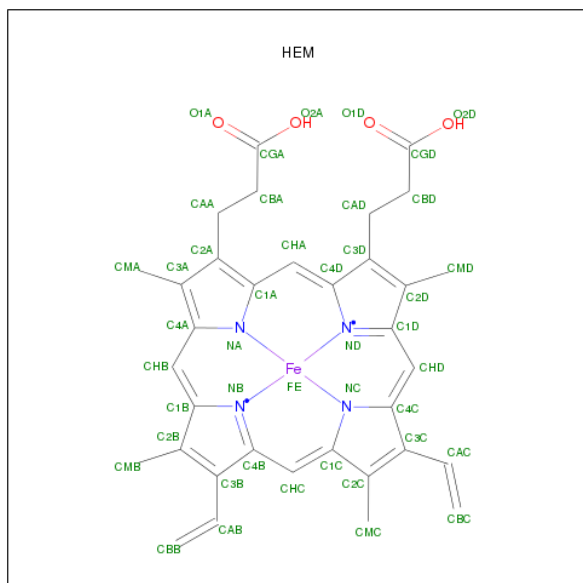
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	N	0	0
			3	3		
13	P	1	Total	N	0	0
			3	3		

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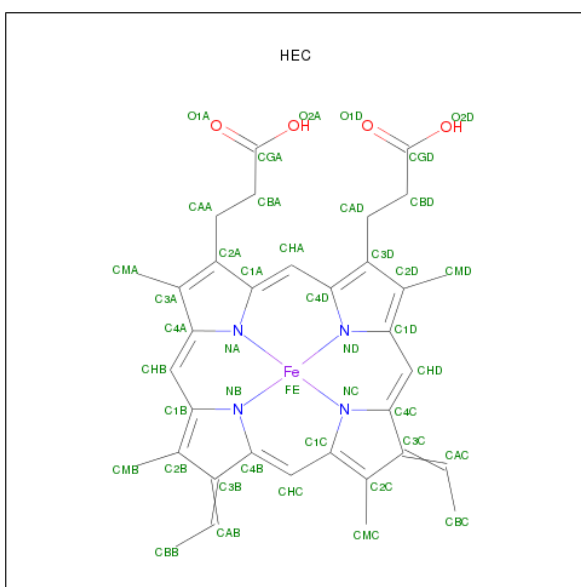
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total N 3 3	0	0
13	A	1	Total N 3 3	0	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



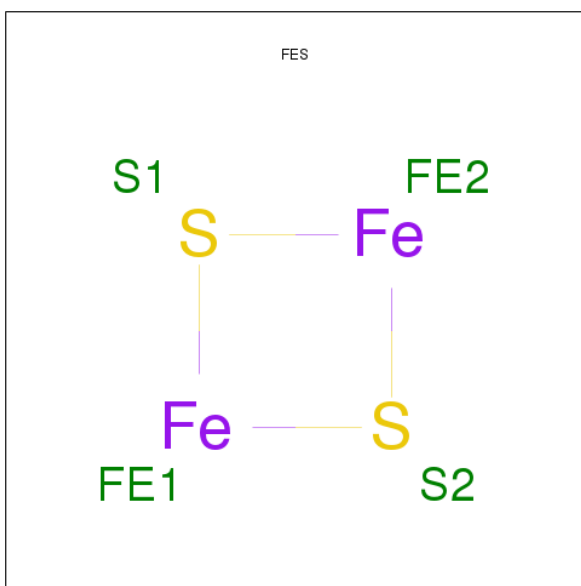
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

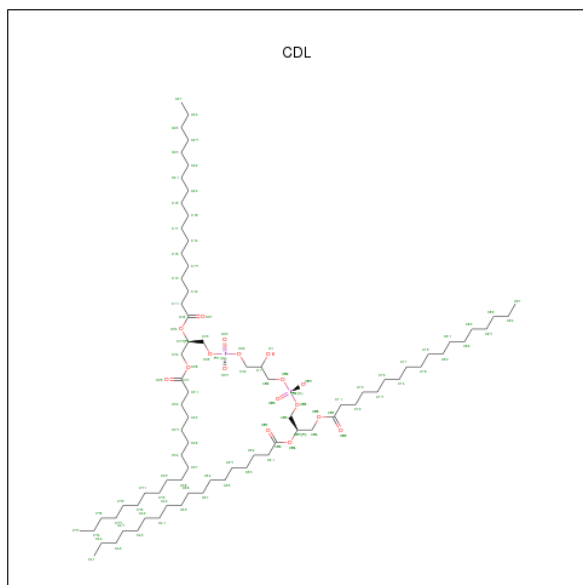
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- The chemical structure of SMA (Silymarin) is a complex molecule consisting of a flavanone core. The core is a chromone derivative with two methoxy groups (OCH₃) at positions 7 and 8. The side chain is a complex polyether structure with multiple stereocenters and a terminal diene system. The structure is labeled with atom numbers (C1 through C25) and oxygen atoms (O1 through O5). The side chain includes a methoxy group (OCH₃) at C14, a methoxy group (OCH₃) at C15, and a terminal diene system (C17-C18-C19-C20-C21). The structure is shown in a 2D representation with stereochemistry indicated by wedges and dashes.

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

- UQ
-
- The chemical structure of Ubiquinone (UQ) is shown, featuring a long hydrophobic chain with alternating double bonds and methoxy groups, and a head group consisting of a 1,4-naphthoquinone ring with two methoxy groups.

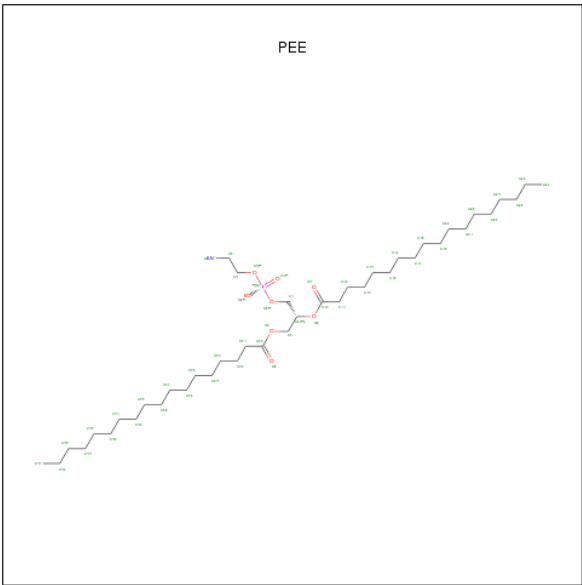
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			14	10	4		
18	P	1	Total	C	O	0	0
			14	10	4		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	G	1	Total	C	O	P	0	0
			50	31	17	2		
19	G	1	Total	C	O	P	0	0
			44	25	17	2		
19	Q	1	Total	C	O	P	0	0
			50	31	17	2		
19	T	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 20 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	G	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
20	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	C	1	Total	O	P			0	0
			5	4	1				
20	T	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
20	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	N	1	Total	O	P			0	0
			5	4	1				
20	A	1	Total	C	O			0	0
			6	3	3				

- Molecule 21 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	C	1	Total	C	O	0	0
			6	3	3		
21	B	1	Total	C	O	0	0
			6	3	3		
21	P	1	Total	C	O	0	0
			6	3	3		
21	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	187	Total	O	0	0
			187	187		
22	B	149	Total	O	0	0
			149	149		
22	C	125	Total	O	0	0
			125	125		
22	D	118	Total	O	0	0
			118	118		
22	E	54	Total	O	0	0
			54	54		
22	F	57	Total	O	0	0
			57	57		
22	G	24	Total	O	0	0
			24	24		
22	H	14	Total	O	0	0
			14	14		

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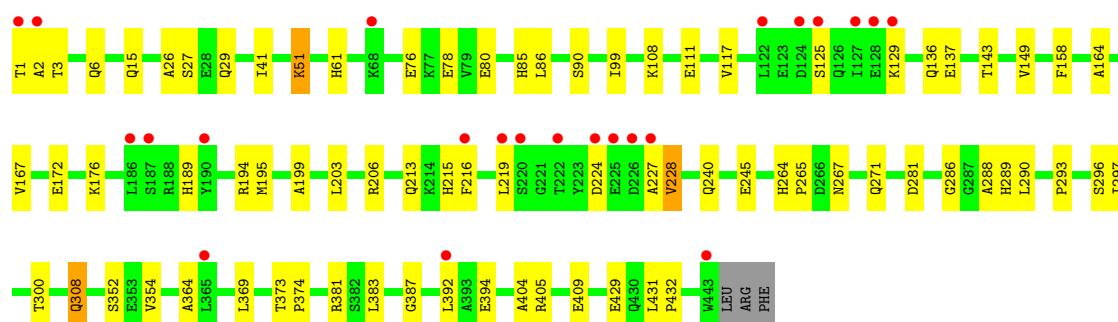
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	I	16	Total 16	O 16	0	0
22	J	5	Total 5	O 5	0	0
22	N	134	Total 134	O 134	0	0
22	O	130	Total 130	O 130	0	0
22	P	122	Total 122	O 122	0	0
22	Q	109	Total 109	O 109	0	0
22	R	64	Total 64	O 64	0	0
22	S	73	Total 73	O 73	0	0
22	T	21	Total 21	O 21	0	0
22	U	16	Total 16	O 16	0	0
22	V	10	Total 10	O 10	0	0
22	W	9	Total 9	O 9	0	0

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.

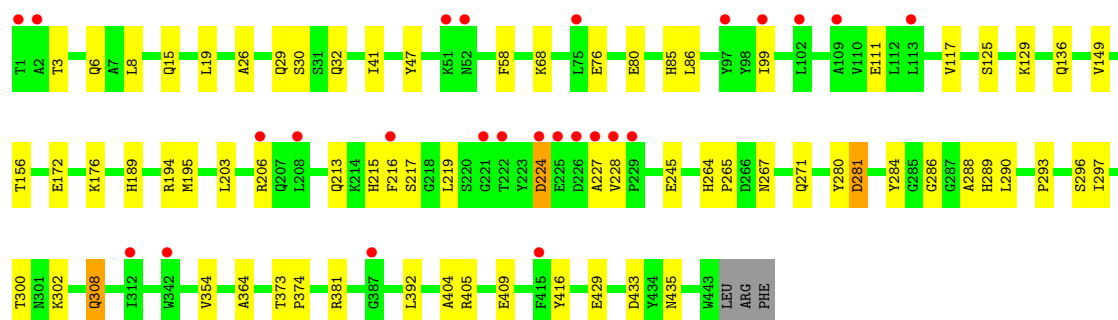
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A: 



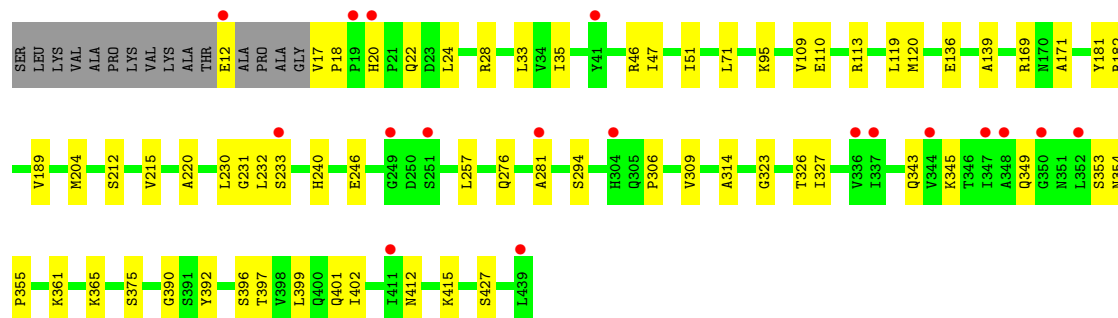
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain N: 



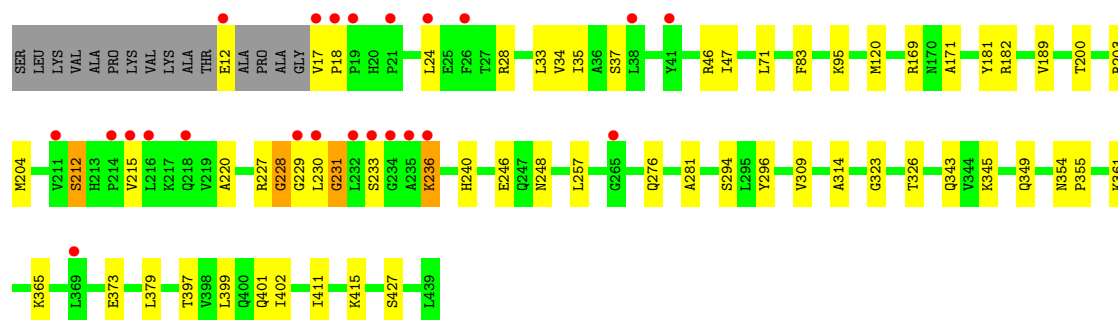
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain B: 



- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain O:



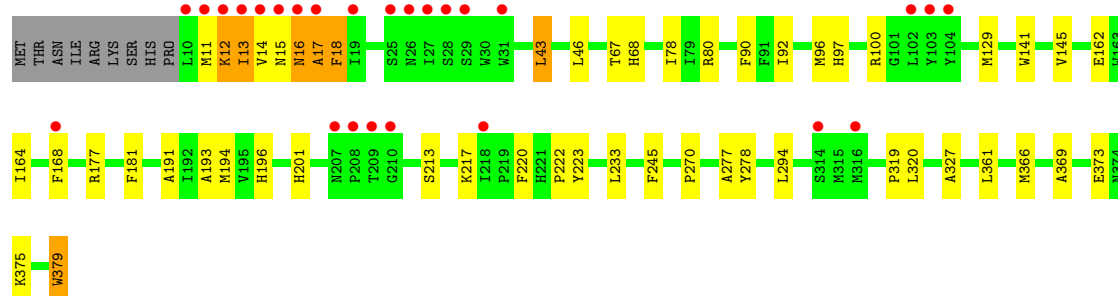
- Molecule 3: Cytochrome b

Chain C:



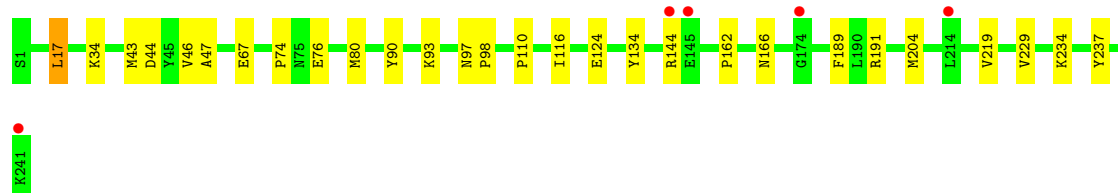
- Molecule 3: Cytochrome b

Chain P:



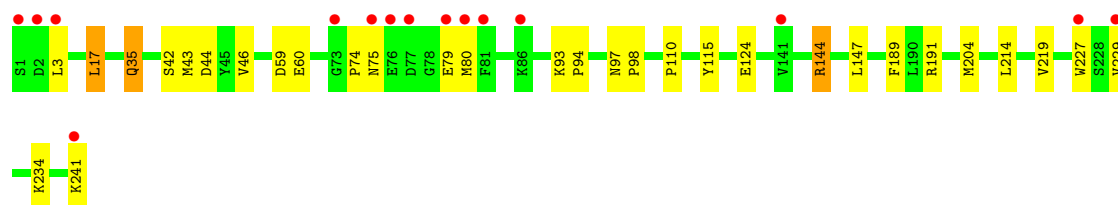
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



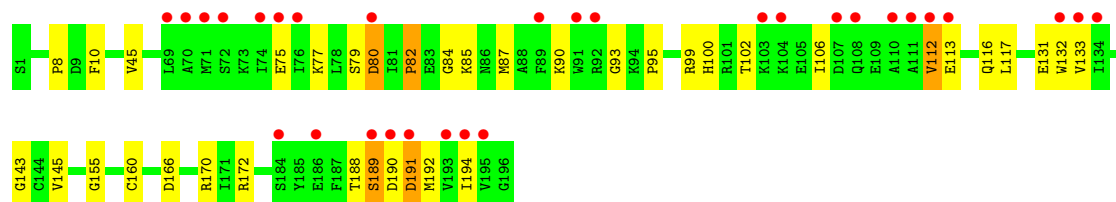
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



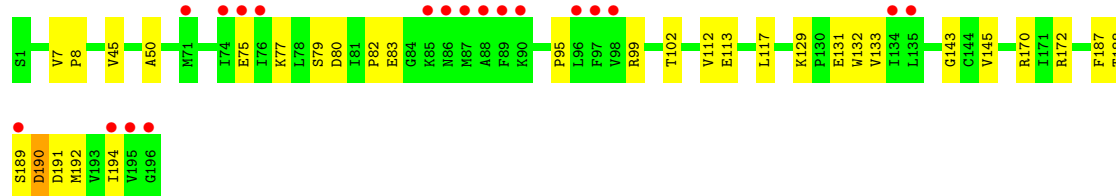
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain E:



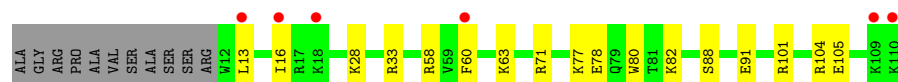
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain R:



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain S:



- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



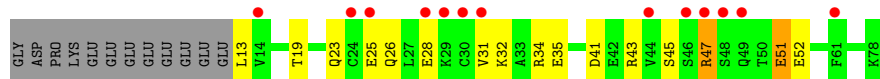
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain T:



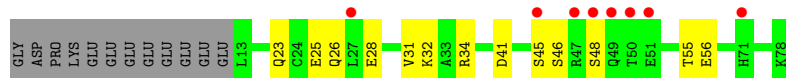
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



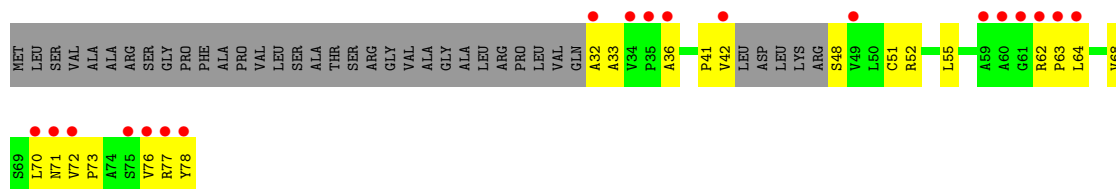
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain U:



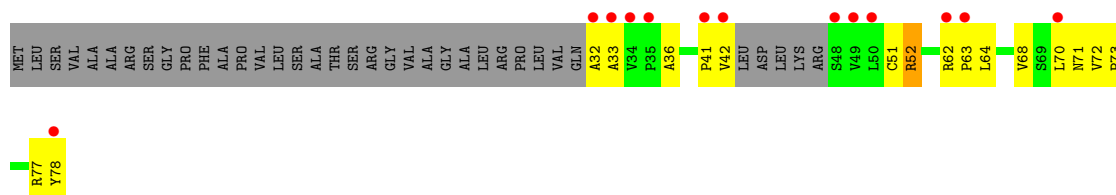
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain I:



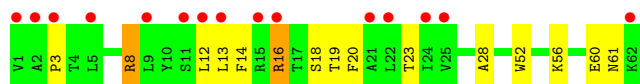
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain V:



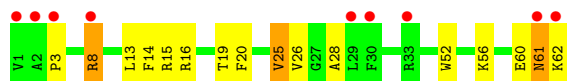
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain W:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.12Å 171.06Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.10 40.02 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.98-2.10) 96.1 (40.02-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.287 0.249 , 0.268	Depositor DCC
R_{free} test set	15323 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	2 of 308206 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33959	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, PO4, UQ, BHG, FES, HEC, HEM, PEE, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/3472	0.66	0/4714
1	N	0.33	0/3472	0.67	0/4714
2	B	0.32	0/3235	0.65	0/4387
2	O	0.31	0/3239	0.65	1/4393 (0.0%)
3	C	0.36	0/2986	0.65	1/4089 (0.0%)
3	P	0.35	0/3024	0.64	0/4137
4	D	0.34	0/1978	0.65	0/2684
4	Q	0.34	0/1978	0.65	0/2684
5	E	0.31	0/1553	0.67	1/2100 (0.0%)
5	R	0.35	0/1553	0.69	1/2100 (0.0%)
6	F	0.32	0/878	0.64	0/1175
6	S	0.32	0/878	0.65	0/1175
7	G	0.32	0/642	0.65	0/869
7	T	0.34	0/647	0.68	0/876
8	H	0.30	0/544	0.60	0/729
8	U	0.31	0/544	0.56	0/729
9	I	0.32	0/285	0.66	0/384
9	V	0.32	0/285	0.69	0/384
10	J	0.36	0/520	0.65	0/699
10	W	0.36	0/520	0.65	0/699
All	All	0.33	0/32233	0.65	4/43721 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	228	GLY	N-CA-C	-6.96	95.71	113.10
5	R	143	GLY	N-CA-C	5.70	127.36	113.10
5	E	143	GLY	N-CA-C	5.38	126.54	113.10
3	C	109	PHE	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3302	63	0
1	N	3403	0	3302	53	0
2	B	3177	0	3152	64	0
2	O	3180	0	3156	56	0
3	C	2892	0	2938	39	0
3	P	2931	0	2989	59	0
4	D	1919	0	1868	25	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	30	0
5	R	1519	0	1503	25	0
6	F	861	0	854	14	0
6	S	861	0	854	20	0
7	G	621	0	626	17	0
7	T	626	0	631	23	0
8	H	539	0	524	14	0
8	U	539	0	524	10	0
9	I	285	0	288	37	0
9	V	285	0	288	31	0
10	J	507	0	513	24	0
10	W	507	0	513	27	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0
11	S	18	0	24	8	0
12	B	5	0	0	0	0
12	O	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	D	3	0	0	0	0
13	P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	86	0	60	5	0
14	P	86	0	60	3	0
15	D	43	0	30	3	0
15	Q	43	0	30	2	0
16	E	4	0	0	0	0
16	R	4	0	0	0	0
17	C	37	0	42	1	0
17	P	37	0	42	2	0
18	C	14	0	9	3	0
18	P	14	0	9	5	0
19	G	94	0	76	5	0
19	Q	50	0	44	0	0
19	T	49	0	42	0	0
20	A	6	0	5	0	0
20	C	54	0	72	2	0
20	D	51	0	82	1	0
20	G	49	0	72	0	0
20	N	5	0	0	0	0
20	P	49	0	72	2	0
20	Q	51	0	82	9	0
20	T	49	0	72	1	0
21	B	6	0	8	0	0
21	C	6	0	8	0	0
21	O	6	0	8	0	0
21	P	6	0	8	0	0
22	A	187	0	0	8	0
22	B	149	0	0	2	0
22	C	125	0	0	4	0
22	D	118	0	0	2	0
22	E	54	0	0	2	0
22	F	57	0	0	3	0
22	G	24	0	0	1	0
22	H	14	0	0	0	0
22	I	16	0	0	1	0
22	J	5	0	0	0	0
22	N	134	0	0	1	0
22	O	130	0	0	1	0
22	P	122	0	0	6	0
22	Q	109	0	0	1	0
22	R	64	0	0	0	0
22	S	73	0	0	2	0
22	T	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	U	16	0	0	0	0
22	V	10	0	0	1	0
22	W	9	0	0	0	0
All	All	33959	0	32273	593	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 593 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.20	1.12
2:B:12:GLU:HG2	2:B:17:VAL:H	1.15	1.09
7:T:45:ILE:HG22	7:T:46:LEU:HD22	1.31	1.04
2:O:200:THR:HB	2:O:229:GLY:HA2	1.36	1.04
3:P:43:LEU:HD21	20:Q:3006:PEE:H192	1.40	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	38	33
1	N	441/446 (99%)	425 (96%)	15 (3%)	1 (0%)	56	57
2	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	56	57
2	O	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	38	33
3	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	27	20
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	16	9
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	11	4
5	R	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	38	33
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
6	S	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
7	G	73/81 (90%)	72 (99%)	1 (1%)	0	100	100
7	T	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	16	9
8	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
8	U	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	14	7
9	I	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	8	2
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	8	2
10	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	14	6
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	14	6
All	All	3980/4220 (94%)	3851 (97%)	104 (3%)	25 (1%)	33	28

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
3	C	16	ASN
3	C	17	ALA
9	I	41	PRO
10	J	61	ASN

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	364/370 (98%)	359 (99%)	5 (1%)	78	83
1	N	364/370 (98%)	359 (99%)	5 (1%)	78	83
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	332/343 (97%)	330 (99%)	2 (1%)	92	95
3	C	312/327 (95%)	307 (98%)	5 (2%)	75	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	316/327 (97%)	310 (98%)	6 (2%)	69	73
4	D	206/206 (100%)	203 (98%)	3 (2%)	76	81
4	Q	206/206 (100%)	203 (98%)	3 (2%)	76	81
5	E	168/168 (100%)	167 (99%)	1 (1%)	92	95
5	R	168/168 (100%)	166 (99%)	2 (1%)	82	87
6	F	90/98 (92%)	89 (99%)	1 (1%)	84	88
6	S	90/98 (92%)	89 (99%)	1 (1%)	84	88
7	G	66/71 (93%)	65 (98%)	1 (2%)	76	81
7	T	66/71 (93%)	64 (97%)	2 (3%)	53	55
8	H	63/74 (85%)	61 (97%)	2 (3%)	51	52
8	U	63/74 (85%)	62 (98%)	1 (2%)	75	79
9	I	28/60 (47%)	27 (96%)	1 (4%)	47	46
9	V	28/60 (47%)	26 (93%)	2 (7%)	21	16
10	J	51/52 (98%)	49 (96%)	2 (4%)	43	43
10	W	51/52 (98%)	49 (96%)	2 (4%)	43	43
All	All	3364/3538 (95%)	3317 (99%)	47 (1%)	78	83

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	58	PHE
2	O	212	SER
9	V	42	VAL
1	N	245	GLU
2	O	236	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	73	ASN
1	N	165	GLN
6	S	73	GLN
1	N	61	HIS
2	B	22	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

41 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$
11	BHG	A	4002	-	18,18,18	1.83	4 (22%)	23,23,23	0.77	1 (4%)
20	PEE	A	4003	-	5,5,50	1.53	1 (20%)	5,5,55	14.35	2 (40%)
13	AZI	A	4005	-	2,2,2	1.79	0	0,1,1	0.00	-
21	GOL	B	2013	-	5,5,5	1.20	0	5,5,5	0.71	0
12	PO4	B	3010	-	4,4,4	0.74	0	6,6,6	0.83	0
17	SMA	C	2001	-	38,38,38	1.83	7 (18%)	50,52,52	1.94	7 (14%)
18	UQ	C	2002	-	14,14,63	2.64	8 (57%)	18,20,79	0.71	0
20	PEE	C	2007	-	48,48,50	1.17	5 (10%)	53,53,55	0.87	5 (9%)
11	BHG	C	2008	-	18,18,18	1.75	5 (27%)	23,23,23	0.71	0
21	GOL	C	2009	-	5,5,5	1.24	0	5,5,5	0.69	0
20	PEE	C	2012	-	4,4,50	1.91	2 (50%)	6,6,55	0.79	0
13	AZI	C	2014	-	2,2,2	2.11	1 (50%)	0,1,1	0.00	-
14	HEM	C	501	3	42,50,50	2.99	18 (42%)	27,82,82	2.09	6 (22%)
14	HEM	C	502	3	42,50,50	2.74	19 (45%)	27,82,82	1.75	7 (25%)
20	PEE	D	2006	-	50,50,50	1.22	7 (14%)	55,55,55	0.94	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	AZI	D	4004	-	2,2,2	1.75	0	0,1,1	0.00	-
15	HEC	D	501	4	50,50,50	3.01	12 (24%)	56,82,82	2.19	12 (21%)
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	F	3011	-	18,18,18	1.83	4 (22%)	23,23,23	0.74	0
11	BHG	F	4001	-	18,18,18	1.73	5 (27%)	23,23,23	0.70	0
19	CDL	G	2003	-	47,49,99	1.15	2 (4%)	57,61,111	1.36	6 (10%)
19	CDL	G	2004	-	41,43,99	1.17	2 (4%)	50,55,111	1.53	7 (14%)
20	PEE	G	2005	-	48,48,50	1.27	7 (14%)	53,53,55	0.98	6 (11%)
20	PEE	N	3012	-	4,4,50	1.83	2 (50%)	6,6,55	0.75	0
12	PO4	O	2010	-	4,4,4	0.78	0	6,6,6	0.82	0
21	GOL	O	3013	-	5,5,5	1.20	0	5,5,5	0.77	0
17	SMA	P	3001	-	38,38,38	2.08	10 (26%)	50,52,52	1.99	7 (14%)
18	UQ	P	3002	-	14,14,63	2.52	8 (57%)	18,20,79	0.55	0
20	PEE	P	3007	-	48,48,50	1.22	5 (10%)	53,53,55	0.86	4 (7%)
11	BHG	P	3008	-	18,18,18	1.76	5 (27%)	23,23,23	0.70	0
21	GOL	P	3009	-	5,5,5	1.26	0	5,5,5	0.68	0
13	AZI	P	3014	-	2,2,2	2.48	2 (100%)	0,1,1	0.00	-
14	HEM	P	501	3	42,50,50	2.79	15 (35%)	27,82,82	1.84	6 (22%)
14	HEM	P	502	3	42,50,50	2.89	16 (38%)	27,82,82	2.12	8 (29%)
19	CDL	Q	3003	-	47,49,99	1.13	4 (8%)	57,61,111	1.42	6 (10%)
20	PEE	Q	3006	-	50,50,50	1.21	6 (12%)	55,55,55	0.91	4 (7%)
15	HEC	Q	501	4	50,50,50	3.08	8 (16%)	56,82,82	1.99	8 (14%)
16	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	S	2011	-	18,18,18	1.77	3 (16%)	23,23,23	0.78	0
19	CDL	T	3004	-	46,48,99	1.19	4 (8%)	56,60,111	1.39	5 (8%)
20	PEE	T	3005	-	48,48,50	1.29	8 (16%)	53,53,55	0.95	6 (11%)

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
11	BHG	A	4002	-	1/1/5/5	0/9/29/29	0/1/1/1
20	PEE	A	4003	-	-	0/4/4/54	0/0/0/0
13	AZI	A	4005	-	-	0/0/0/0	0/0/0/0
21	GOL	B	2013	-	-	0/4/4/4	0/0/0/0
12	PO4	B	3010	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
18	UQ	C	2002	-	-	0/4/28/87	0/1/1/1
20	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
11	BHG	C	2008	-	1/1/5/5	0/9/29/29	0/1/1/1
21	GOL	C	2009	-	-	0/4/4/4	0/0/0/0
20	PEE	C	2012	-	-	0/0/0/54	0/0/0/0
13	AZI	C	2014	-	-	0/0/0/0	0/0/0/0
14	HEM	C	501	3	-	0/14/114/114	0/0/8/8
14	HEM	C	502	3	-	0/14/114/114	0/0/8/8
20	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
13	AZI	D	4004	-	-	0/0/0/0	0/0/0/0
15	HEC	D	501	4	-	0/10/54/54	0/0/8/8
16	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	BHG	F	3011	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	F	4001	-	1/1/5/5	0/9/29/29	0/1/1/1
19	CDL	G	2003	-	1/1/9/9	0/58/58/110	0/0/0/0
19	CDL	G	2004	-	1/1/9/9	0/52/52/110	0/0/0/0
20	PEE	G	2005	-	-	0/52/52/54	0/0/0/0
20	PEE	N	3012	-	-	0/0/0/54	0/0/0/0
12	PO4	O	2010	-	-	0/0/0/0	0/0/0/0
21	GOL	O	3013	-	-	0/4/4/4	0/0/0/0
17	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
18	UQ	P	3002	-	-	0/4/28/87	0/1/1/1
20	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
11	BHG	P	3008	-	1/1/5/5	0/9/29/29	0/1/1/1
21	GOL	P	3009	-	-	0/4/4/4	0/0/0/0
13	AZI	P	3014	-	-	0/0/0/0	0/0/0/0
14	HEM	P	501	3	-	0/14/114/114	0/0/8/8
14	HEM	P	502	3	-	0/14/114/114	0/0/8/8
19	CDL	Q	3003	-	1/1/9/9	0/58/58/110	0/0/0/0
20	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
15	HEC	Q	501	4	-	0/10/54/54	0/0/8/8
16	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	BHG	S	2011	-	1/1/5/5	0/9/29/29	0/1/1/1
19	CDL	T	3004	-	1/1/9/9	0/57/57/110	0/0/0/0
20	PEE	T	3005	-	-	0/52/52/54	0/0/0/0

The worst 5 of 205 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	501	HEC	C3B-CAB	13.99	1.53	1.34
15	Q	501	HEC	C3C-CAC	12.42	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C3B-CAB	12.39	1.51	1.34
15	D	501	HEC	C3C-CAC	12.26	1.51	1.34
14	C	501	HEM	C3C-C2C	-9.63	1.37	1.45

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	4003	PEE	O2-C2-C1	-24.49	110.39	119.54
20	A	4003	PEE	O2-C2-C3	-20.68	111.82	119.54
15	D	501	HEC	CBB-CAB-C3B	-8.92	107.87	127.36
15	Q	501	HEC	CBB-CAB-C3B	-8.78	108.16	127.36
15	D	501	HEC	CBC-CAC-C3C	-8.03	109.80	127.36

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	F	3011	BHG	C4
19	Q	3003	CDL	CA4
11	S	2011	BHG	C4
11	P	3008	BHG	C4
11	C	2008	BHG	C4

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	442/446 (99%)	0.24	23 (5%) 26 29	27, 43, 65, 115	1 (0%)
1	N	442/446 (99%)	0.38	25 (5%) 23 25	28, 43, 63, 128	1 (0%)
2	B	424/439 (96%)	0.25	18 (4%) 35 39	29, 45, 67, 132	0
2	O	424/439 (96%)	0.25	23 (5%) 25 27	33, 47, 73, 162	0
3	C	365/379 (96%)	0.29	5 (1%) 72 76	25, 34, 47, 106	0
3	P	370/379 (97%)	0.41	26 (7%) 16 18	26, 34, 52, 165	0
4	D	241/241 (100%)	0.07	5 (2%) 60 65	28, 39, 59, 80	0
4	Q	241/241 (100%)	0.14	15 (6%) 20 22	28, 38, 59, 81	0
5	E	196/196 (100%)	0.72	30 (15%) 3 3	29, 54, 96, 117	0
5	R	196/196 (100%)	0.42	19 (9%) 8 9	29, 43, 61, 85	0
6	F	99/110 (90%)	0.35	6 (6%) 21 23	29, 44, 70, 80	0
6	S	99/110 (90%)	0.42	7 (7%) 16 17	28, 39, 79, 109	0
7	G	75/81 (92%)	0.39	4 (5%) 25 28	31, 50, 72, 80	0
7	T	76/81 (93%)	0.98	10 (13%) 4 5	30, 50, 97, 117	0
8	H	66/78 (84%)	1.04	13 (19%) 2 1	40, 55, 87, 101	0
8	U	66/78 (84%)	0.49	8 (12%) 5 6	40, 54, 79, 89	0
9	I	42/78 (53%)	2.18	19 (45%) 1 1	40, 75, 88, 93	0
9	V	42/78 (53%)	1.80	13 (30%) 1 1	45, 72, 92, 97	0
10	J	62/62 (100%)	1.14	15 (24%) 1 1	35, 60, 85, 116	0
10	W	62/62 (100%)	0.71	9 (14%) 3 3	34, 51, 80, 111	0
All	All	4030/4220 (95%)	0.39	293 (7%) 15 16	25, 42, 76, 165	2 (0%)

The worst 5 of 293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	76	ALA	28.3
10	J	1	VAL	17.7
1	N	1	THR	11.7
3	P	13	ILE	11.3
1	A	222	THR	10.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	BHG	A	4002	18/18	0.82	18.66	130,143,145,145	0
11	BHG	F	3011	18/18	0.45	17.32	114,118,122,122	0
11	BHG	S	2011	18/18	0.40	11.57	73,86,91,91	0
13	AZI	C	2014	3/3	0.38	9.99	53,53,57,59	0
20	PEE	T	3005	49/51	0.49	9.91	96,121,136,136	0
21	GOL	P	3009	6/6	0.32	9.43	59,65,67,68	0
11	BHG	P	3008	18/18	0.39	9.29	100,102,107,109	0
20	PEE	G	2005	49/51	0.52	9.14	105,123,129,129	0
21	GOL	C	2009	6/6	0.40	8.84	56,59,63,67	0
21	GOL	B	2013	6/6	0.94	7.18	145,148,148,149	0
11	BHG	C	2008	18/18	0.39	6.95	109,112,116,116	0
13	AZI	P	3014	3/3	0.38	6.43	54,54,55,61	0
11	BHG	F	4001	18/18	0.48	5.03	168,171,173,173	0
20	PEE	D	2006	51/51	0.24	4.84	52,66,94,95	0
21	GOL	O	3013	6/6	0.45	4.54	112,115,116,116	0
13	AZI	D	4004	3/3	0.29	3.83	69,69,72,73	0
20	PEE	C	2012	5/51	0.24	3.64	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	PEE	C	2007	49/51	0.30	3.63	39,53,68,69	0
12	PO4	B	3010	5/5	0.23	3.31	99,100,100,100	0
19	CDL	G	2003	50/100	0.27	3.27	62,96,113,113	0
19	CDL	G	2004	44/100	0.26	3.26	62,79,105,107	0
20	PEE	Q	3006	51/51	0.21	2.54	45,59,83,83	0
13	AZI	A	4005	3/3	0.38	2.51	72,72,73,74	0
18	UQ	P	3002	14/63	0.31	2.42	90,93,97,97	0
20	PEE	A	4003	6/51	0.19	2.18	110,111,112,113	0
19	CDL	T	3004	49/100	0.30	1.98	54,69,98,101	0
20	PEE	P	3007	49/51	0.26	1.60	35,54,62,63	0
18	UQ	C	2002	14/63	0.30	1.51	74,78,80,82	0
17	SMA	P	3001	37/37	0.17	0.94	24,32,37,37	0
19	CDL	Q	3003	50/100	0.22	0.72	55,78,90,92	0
20	PEE	N	3012	5/51	0.20	0.57	94,94,94,96	0
14	HEM	P	501	43/43	0.16	0.51	25,29,37,42	0
14	HEM	C	502	43/43	0.15	0.44	22,26,31,33	0
14	HEM	C	501	43/43	0.15	0.17	21,26,33,37	0
14	HEM	P	502	43/43	0.14	0.06	24,27,32,37	0
15	HEC	D	501	43/43	0.11	-0.08	29,33,36,38	0
16	FES	E	501	4/4	0.13	-0.10	34,35,37,37	0
17	SMA	C	2001	37/37	0.13	-0.25	25,30,32,38	0
16	FES	R	501	4/4	0.12	-0.38	31,31,33,33	0
15	HEC	Q	501	43/43	0.10	-0.44	32,35,36,37	0
12	PO4	O	2010	5/5	0.11	-0.48	106,106,107,108	0

6.5 Other polymers ⓘ

There are no such residues in this entry.