



wwPDB X-ray Structure Validation Summary Report i

Oct 21, 2014 – 06:14 PM EDT

PDB ID : 2A06
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2005-06-16
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>

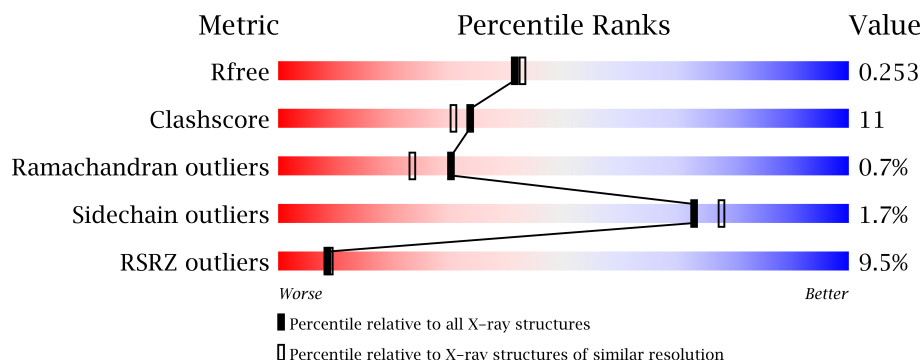
The following versions of software and data (see [references](#)) were used in the production of this report:

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	C	2011	-	X
11	BHG	F	3012	-	X
11	BHG	F	4003	-	X
11	BHG	P	3011	-	X
11	BHG	S	2012	-	X
12	AZI	A	4002	-	X
12	AZI	C	2005	-	X
12	AZI	G	4001	-	X
12	AZI	P	3005	-	X
13	PO4	A	2010	-	X
13	PO4	B	3009	-	X
13	PO4	D	4011	-	X
13	PO4	R	4013	-	X
13	PO4	R	4014	-	X
20	PEE	B	4017	-	X
20	PEE	C	2007	-	X
20	PEE	D	2006	-	X
20	PEE	Q	3006	-	X
21	UNL	A	4032	-	X
21	UNL	A	4035	-	X
21	UNL	A	4038	-	X
21	UNL	A	4048	-	X
21	UNL	A	4075	-	X
21	UNL	A	4076	-	X
21	UNL	A	4087	-	X
21	UNL	A	4091	-	X
21	UNL	B	4025	-	X
21	UNL	B	4026	-	X
21	UNL	B	4030	-	X
21	UNL	B	4034	-	X
21	UNL	B	4039	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
21	UNL	B	4051	-	X
21	UNL	B	4057	-	X
21	UNL	B	4079	-	X
21	UNL	B	4080	-	X
21	UNL	C	4018	-	X
21	UNL	C	4023	-	X
21	UNL	C	4045	-	X
21	UNL	C	4063	-	X
21	UNL	C	4068	-	X
21	UNL	C	4086	-	X
21	UNL	D	4027	-	X
21	UNL	D	4036	-	X
21	UNL	D	4054	-	X
21	UNL	D	4067	-	X
21	UNL	D	4083	-	X
21	UNL	E	4050	-	X
21	UNL	F	4028	-	X
21	UNL	G	4053	-	X
21	UNL	G	4064	-	X
21	UNL	I	4033	-	X
21	UNL	I	4072	-	X
21	UNL	N	4019	-	X
21	UNL	N	4022	-	X
21	UNL	N	4029	-	X
21	UNL	O	4031	-	X
21	UNL	O	4037	-	X
21	UNL	O	4041	-	X
21	UNL	O	4071	-	X
21	UNL	O	4084	-	X
21	UNL	P	4021	-	X
21	UNL	P	4040	-	X
21	UNL	P	4046	-	X
21	UNL	P	4058	-	X
21	UNL	P	4060	-	X
21	UNL	P	4074	-	X
21	UNL	P	4089	-	X
21	UNL	Q	4044	-	X
21	UNL	R	4069	-	X
21	UNL	T	4065	-	X
21	UNL	U	4049	-	X
21	UNL	U	4056	-	X
21	UNL	V	4078	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
21	UNL	V	4090	-	X
22	GOL	C	2008	-	X
22	GOL	E	4006	-	X
22	GOL	E	4007	-	X
22	GOL	O	4005	-	X
22	GOL	P	3008	-	X
22	GOL	P	4009	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33890 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
			3398	2118	602	658	20			
1	N	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	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, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2897	1945	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2936	1973	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
			1517	955	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			

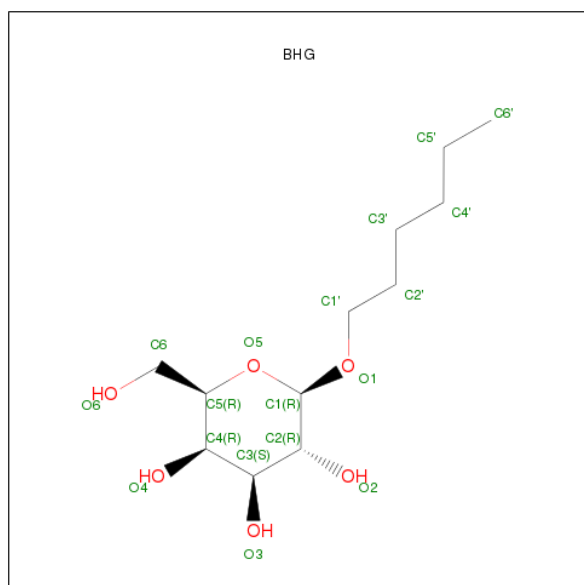
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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.

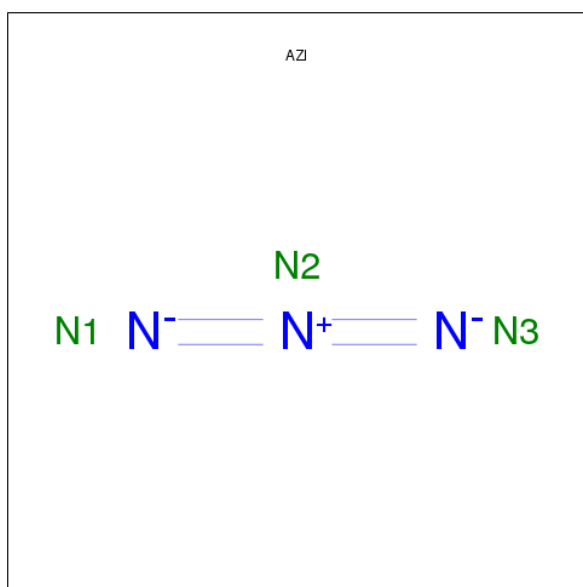
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

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



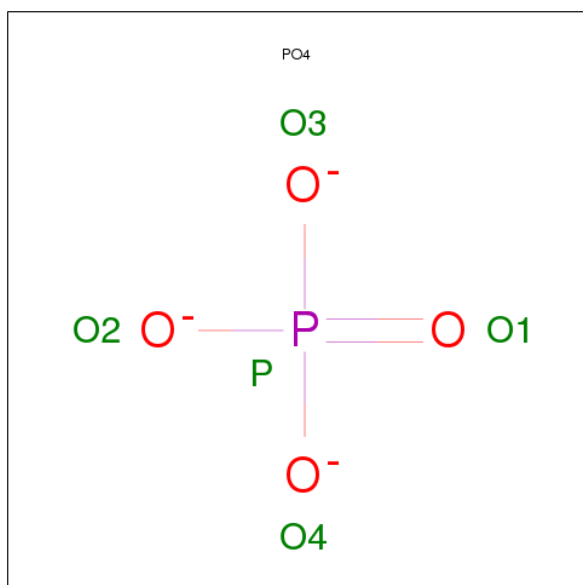
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is AZIDE ION (three-letter code: AZI) (formula: N₃).



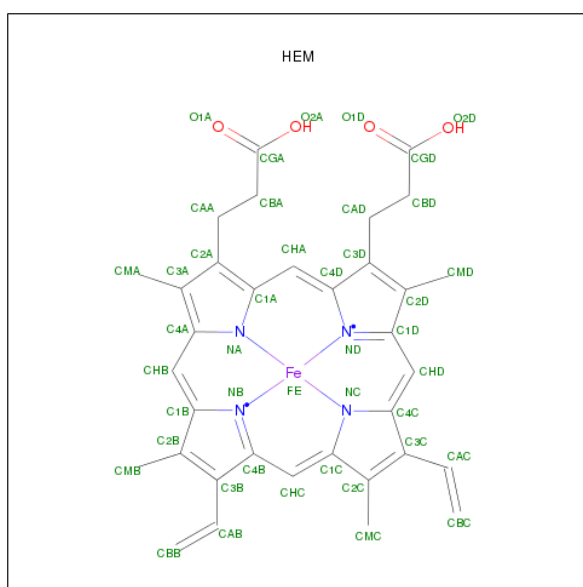
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0
12	G	1	Total N 3 3	0	0
12	A	1	Total N 3 3	0	0

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



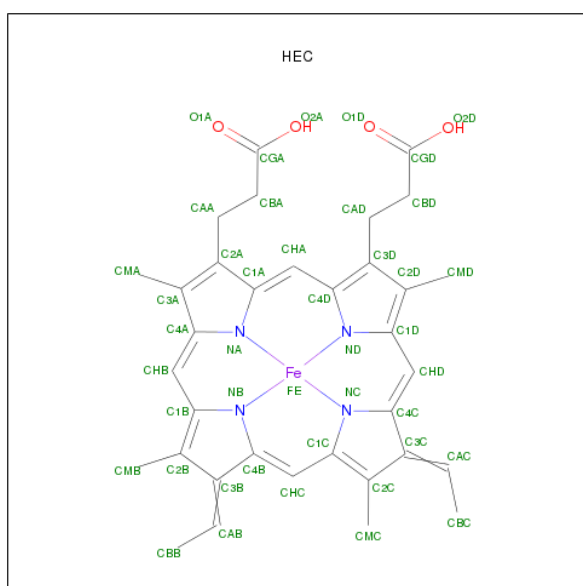
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	O	1	Total 5	O 4	P 1	0	0
13	A	1	Total 5	O 4	P 1	0	0
13	B	1	Total 5	O 4	P 1	0	0
13	P	1	Total 5	O 4	P 1	0	0
13	D	1	Total 5	O 4	P 1	0	0
13	D	1	Total 5	O 4	P 1	0	0
13	Q	1	Total 5	O 4	P 1	0	0
13	R	1	Total 5	O 4	P 1	0	0
13	R	1	Total 5	O 4	P 1	0	0
13	I	1	Total 5	O 4	P 1	0	0
13	T	1	Total 5	O 4	P 1	0	0

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



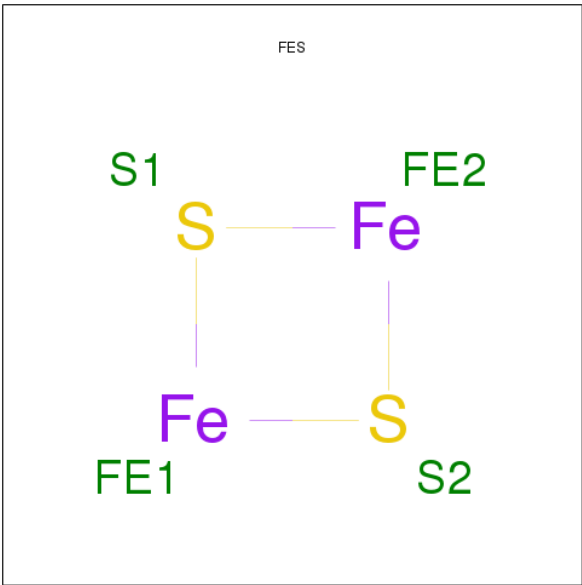
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



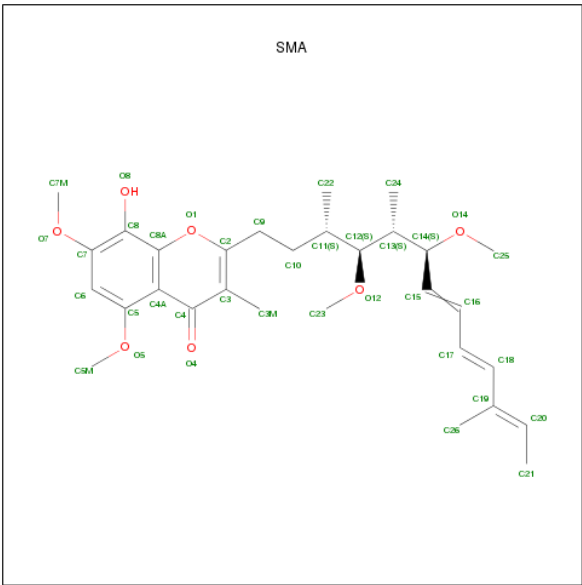
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
15	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



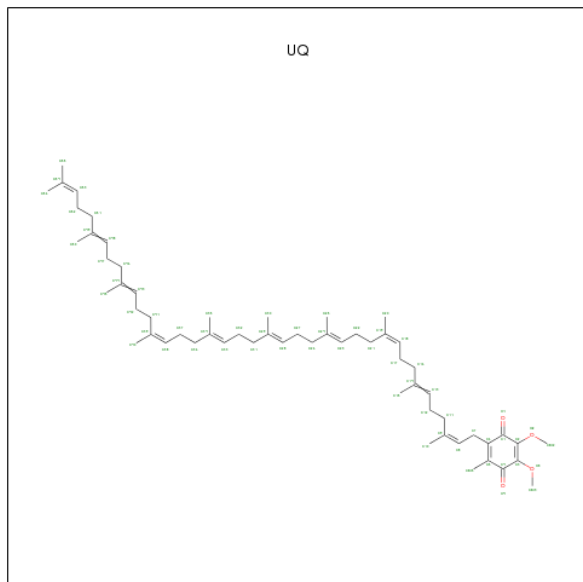
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		
16	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



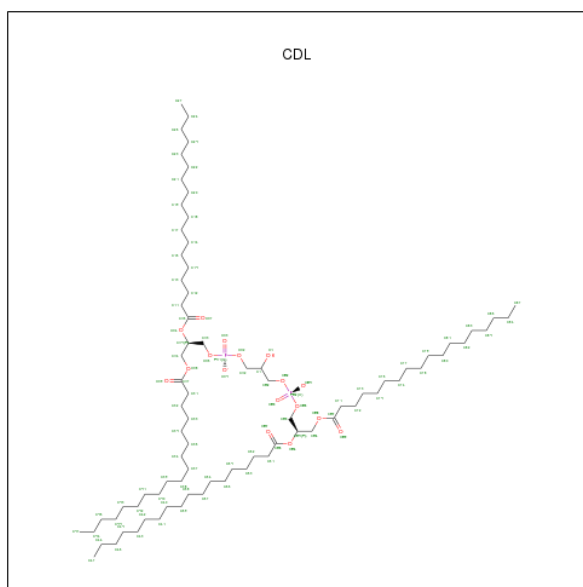
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 18 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



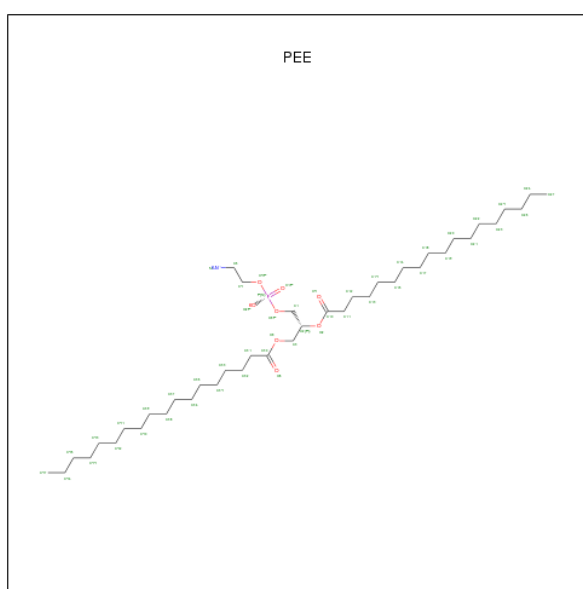
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		
18	P	1	Total	C	O	0	0
			18	14	4		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			39	24	13	2		
19	C	1	Total	C	O	P	0	0
			44	25	17	2		
19	Q	1	Total	C	O	P	0	0
			39	24	13	2		
19	P	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: $C_{41}H_{83}NO_8P$).

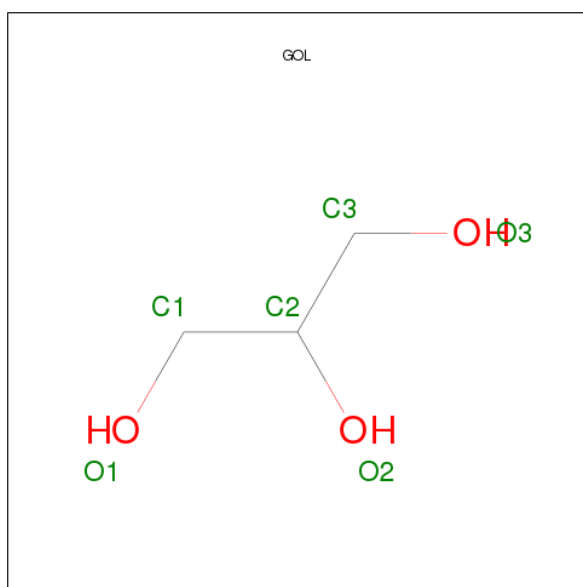


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
20	D	1	Total 51	C 41	N 1	O 8	P 1	0	0	
20	C	1	Total 49	C 39	N 1	O 8	P 1	0	0	
20	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0	
20	P	1	Total 49	C 39	N 1	O 8	P 1	0	0	
20	B	1	Total 8	C 6	O 2				0	0

- Molecule 21 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	7	Total O 8 8	0	0
21	G	3	Total O 3 3	0	0
21	Q	1	Total O 1 1	0	0
21	D	7	Total O 7 7	0	0
21	E	2	Total O 2 2	0	0
21	B	11	Total O 11 11	0	0
21	I	2	Total O 2 2	0	0
21	C	6	Total O 7 7	0	0
21	V	4	Total O 4 4	0	0
21	W	1	Total O 1 1	0	0
21	A	10	Total O 10 10	0	0
21	T	2	Total O 2 2	0	0
21	N	4	Total O 5 5	0	0
21	U	2	Total O 2 2	0	0
21	O	8	Total O 9 9	0	0
21	R	2	Total O 2 2	0	0
21	S	1	Total O 1 1	0	0
21	F	1	Total O 1 1	0	0

- Molecule 22 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			6	3	3		
22	P	1	Total	C	O	0	0
			6	3	3		
22	O	1	Total	C	O	0	0
			6	3	3		
22	E	1	Total	C	O	0	0
			6	3	3		
22	E	1	Total	C	O	0	0
			5	3	2		
22	C	1	Total	C	O	0	0
			6	3	3		
22	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	209	Total	O	0	0
			209	209		
23	B	170	Total	O	0	0
			170	170		
23	C	137	Total	O	0	0
			137	137		
23	D	133	Total	O	0	0
			133	133		
23	E	63	Total	O	0	0
			63	63		

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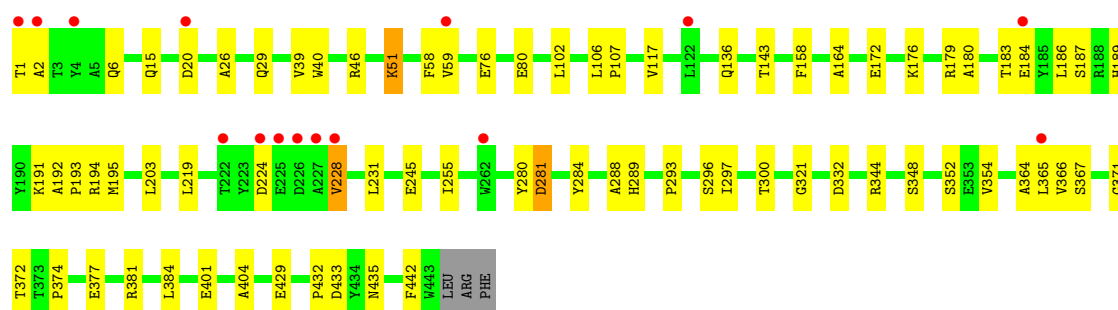
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	F	68	Total 68	O 68	0	0
23	G	31	Total 31	O 31	0	0
23	H	15	Total 15	O 15	0	0
23	I	18	Total 18	O 18	0	0
23	J	7	Total 7	O 7	0	0
23	N	145	Total 145	O 145	0	0
23	O	136	Total 136	O 136	0	0
23	P	135	Total 135	O 135	0	0
23	Q	126	Total 126	O 126	0	0
23	R	77	Total 77	O 77	0	0
23	S	81	Total 81	O 81	0	0
23	T	17	Total 17	O 17	0	0
23	U	16	Total 16	O 16	0	0
23	V	16	Total 16	O 16	0	0
23	W	12	Total 12	O 12	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.

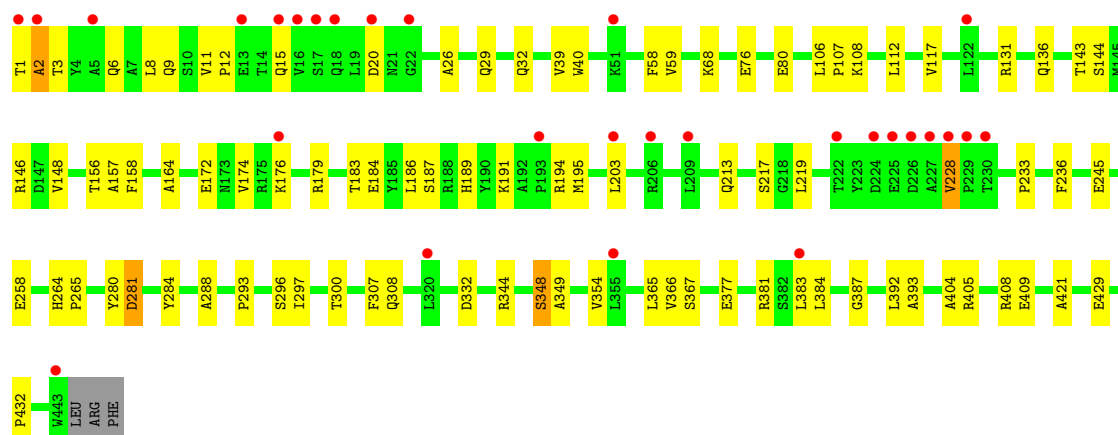
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

Chain A: 



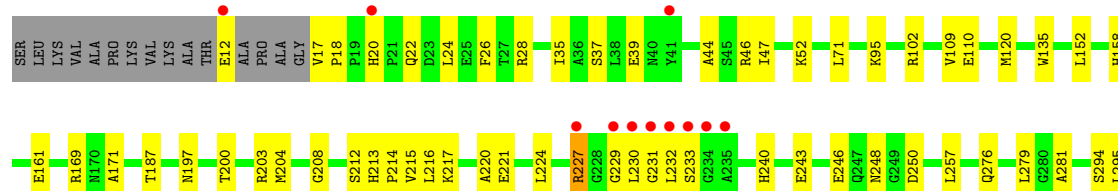
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

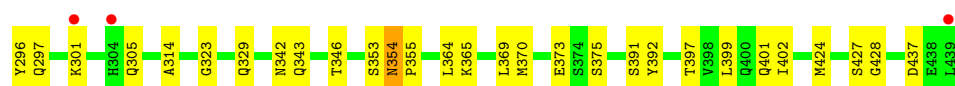
Chain N: 



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

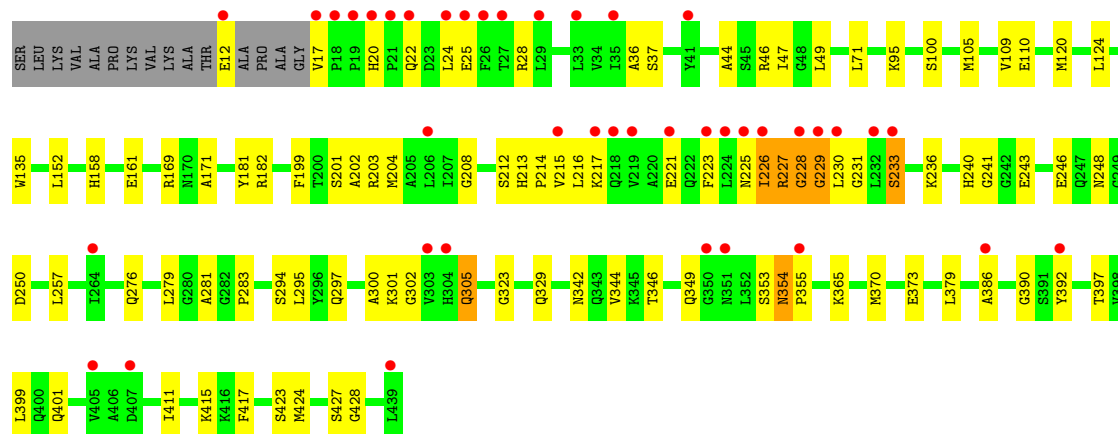
Chain B: 





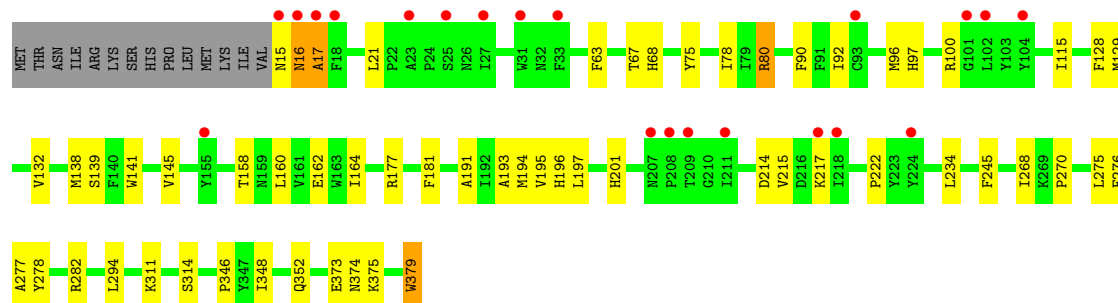
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain O:



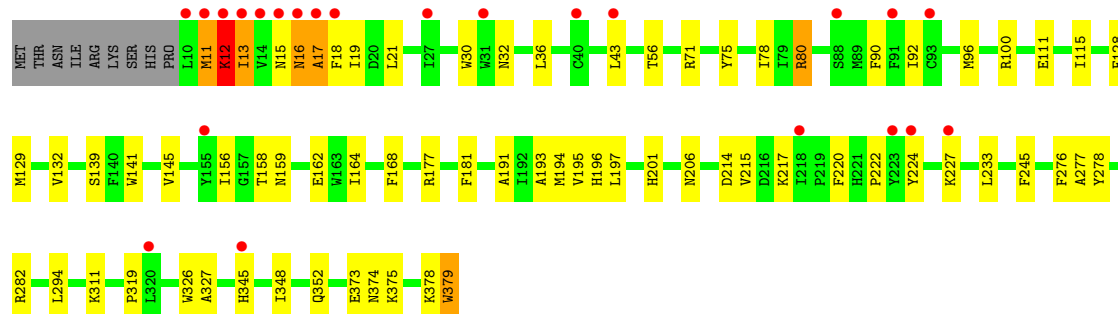
- Molecule 3: Cytochrome b, heme protein, mitochondrial

Chain C:



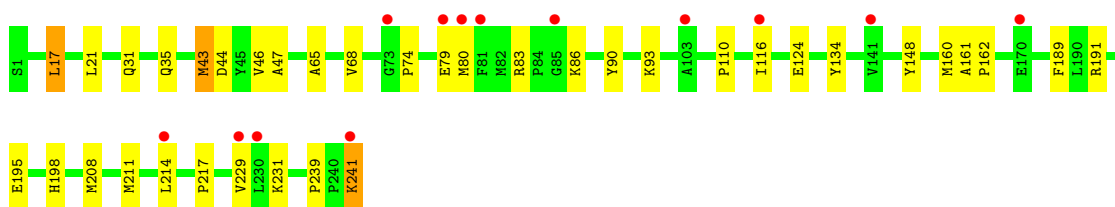
- Molecule 3: Cytochrome b, heme protein, mitochondrial

Chain P:



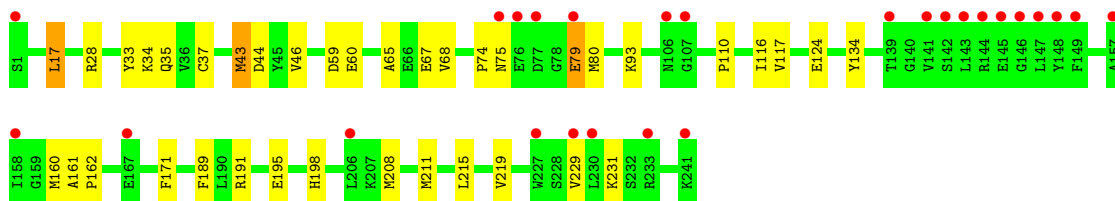
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



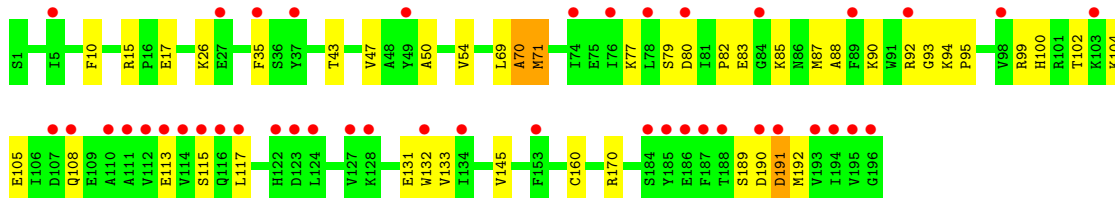
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



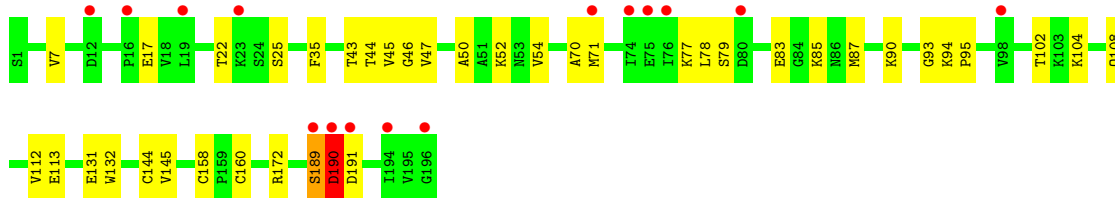
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

Chain E:



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

Chain R:



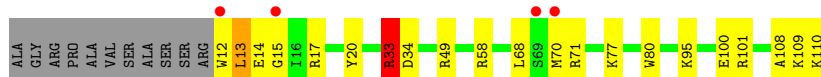
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain F:



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

Chain S:



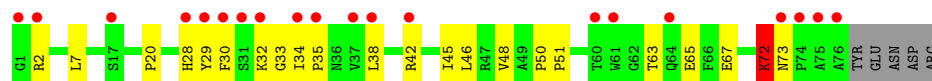
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain G: 



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

Chain T: 



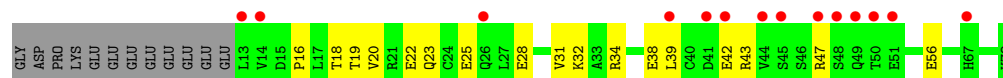
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

Chain H: 



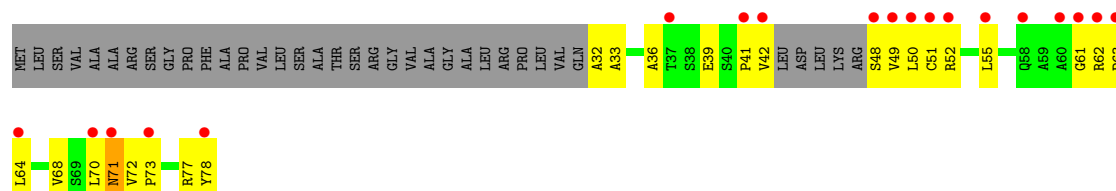
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

Chain U: 



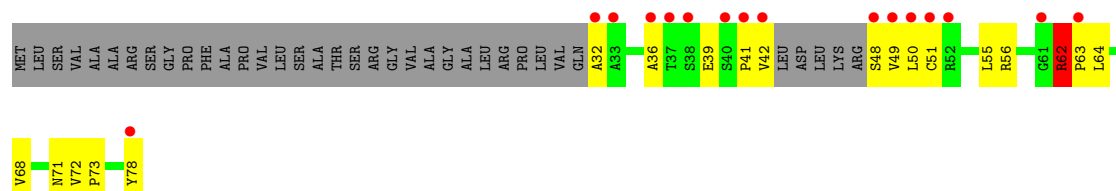
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

Chain I: 



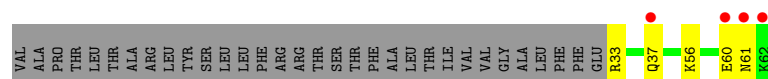
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

Chain V: 



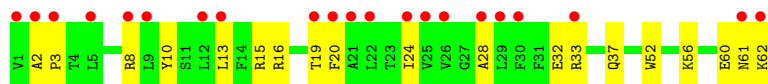
- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

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	128.25Å 168.80Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.10 37.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 91.8 (37.87-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.258 0.221 , 0.253	Depositor DCC
R_{free} test set	15254 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 64.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 308092 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, UNL, 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	0.44	0/3467	0.67	0/4706
1	N	0.38	0/3467	0.64	0/4706
2	B	0.42	0/3235	0.65	0/4387
2	O	0.39	0/3239	0.65	1/4393 (0.0%)
3	C	0.48	0/2992	0.66	0/4097
3	P	0.44	0/3030	0.64	0/4145
4	D	0.44	0/1978	0.64	0/2684
4	Q	0.41	0/1978	0.62	0/2684
5	E	0.35	0/1553	0.70	3/2100 (0.1%)
5	R	0.41	0/1550	0.69	0/2094
6	F	0.45	0/878	0.66	0/1175
6	S	0.44	0/878	0.68	1/1175 (0.1%)
7	G	0.42	0/642	0.63	0/869
7	T	0.39	0/647	0.65	0/876
8	H	0.34	0/544	0.61	0/729
8	U	0.34	0/544	0.56	0/729
9	I	0.60	0/285	0.96	0/384
9	V	0.50	0/285	0.94	1/384 (0.3%)
10	J	0.38	0/252	0.56	0/333
10	W	0.36	0/520	0.59	0/699
All	All	0.42	0/31964	0.66	6/43349 (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
5	E	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	70	ALA	C-N-CA	-6.85	104.57	121.70
2	O	228	GLY	N-CA-C	-6.31	97.33	113.10
5	E	71	MET	C-N-CA	-6.26	106.05	121.70
6	S	33	ARG	NE-CZ-NH2	-6.11	117.24	120.30
9	V	62	ARG	NE-CZ-NH2	5.70	123.15	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	70	ALA	Peptide

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	3398	0	3295	68	0
1	N	3398	0	3295	64	0
2	B	3177	0	3152	88	0
2	O	3180	0	3156	87	0
3	C	2897	0	2943	47	0
3	P	2936	0	2994	74	0
4	D	1919	0	1868	38	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	34	0
5	R	1517	0	1498	38	0
6	F	861	0	854	20	0
6	S	861	0	854	26	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	17	0
8	U	539	0	524	18	0
9	I	285	0	288	41	0
9	V	285	0	288	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	245	0	229	3	0
10	W	507	0	513	22	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	4	0
11	P	18	0	24	0	0
11	S	18	0	24	6	0
12	A	3	0	0	0	0
12	C	3	0	0	0	0
12	G	3	0	0	1	0
12	P	3	0	0	0	0
13	A	5	0	0	0	0
13	B	5	0	0	0	0
13	D	10	0	0	0	0
13	I	5	0	0	1	0
13	O	5	0	0	0	0
13	P	5	0	0	0	0
13	Q	5	0	0	1	0
13	R	10	0	0	0	0
13	T	5	0	0	0	0
14	C	86	0	60	5	0
14	P	86	0	60	3	0
15	D	43	0	30	4	0
15	Q	43	0	30	5	0
16	E	4	0	0	0	0
16	R	4	0	0	0	0
17	C	37	0	42	3	0
17	P	37	0	42	3	0
18	C	18	0	14	4	0
18	P	18	0	14	5	0
19	C	44	0	32	0	0
19	D	39	0	39	1	0
19	P	49	0	42	0	0
19	Q	39	0	39	0	0
20	B	8	0	8	1	0
20	C	49	0	72	0	0
20	D	51	0	82	2	0
20	P	49	0	72	3	0
20	Q	51	0	82	5	0
21	A	10	0	0	0	0
21	B	11	0	0	0	0
21	C	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	D	7	0	0	1	0
21	E	2	0	0	0	0
21	F	1	0	0	0	0
21	G	3	0	0	0	0
21	I	2	0	0	0	0
21	N	5	0	0	0	0
21	O	9	0	0	2	0
21	P	8	0	0	0	0
21	Q	1	0	0	0	0
21	R	2	0	0	0	0
21	S	1	0	0	0	0
21	T	2	0	0	0	0
21	U	2	0	0	0	0
21	V	4	0	0	0	0
21	W	1	0	0	0	0
22	C	12	0	16	0	0
22	E	11	0	13	0	0
22	O	6	0	8	0	0
22	P	12	0	16	2	0
23	A	209	0	0	4	0
23	B	170	0	0	2	0
23	C	137	0	0	6	0
23	D	133	0	0	0	0
23	E	63	0	0	0	0
23	F	68	0	0	4	0
23	G	31	0	0	2	0
23	H	15	0	0	0	0
23	I	18	0	0	4	0
23	J	7	0	0	0	0
23	N	145	0	0	3	0
23	O	136	0	0	6	0
23	P	135	0	0	8	0
23	Q	126	0	0	0	0
23	R	77	0	0	1	0
23	S	81	0	0	2	0
23	T	17	0	0	0	0
23	U	16	0	0	0	0
23	V	16	0	0	0	0
23	W	12	0	0	0	0
All	All	33890	0	31860	708	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 11.

The worst 5 of 708 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:226:ILE:HG13	21:O:4043:UNL:O1	1.38	1.23
9:I:32:ALA:N	9:I:71:ASN:HB2	1.70	1.05
2:B:12:GLU:HG2	2:B:17:VAL:H	1.16	1.04
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.34	1.04
5:R:90:LYS:HE2	5:R:93:GLY:HA2	1.39	1.03

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%)	427 (97%)	12 (3%)	2 (0%)	38	33
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	38	33
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	56	57
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	19	11
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	33	28
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
5	E	194/196 (99%)	179 (92%)	14 (7%)	1 (0%)	38	33
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	22	14
6	F	97/110 (88%)	97 (100%)	0	0	100	100
6	S	97/110 (88%)	95 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	71 (96%)	2 (3%)	1 (1%)	16	9
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	61 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	38/78 (49%)	35 (92%)	1 (3%)	2 (5%)	3	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	8	2
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	5	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	14	6
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	30	23

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	41	PRO
10	J	61	ASN
1	N	2	ALA
2	O	226	ILE
2	O	233	SER

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	363/370 (98%)	356 (98%)	7 (2%)	69	73
1	N	363/370 (98%)	355 (98%)	8 (2%)	64	68
2	B	332/343 (97%)	330 (99%)	2 (1%)	92	95
2	O	332/343 (97%)	329 (99%)	3 (1%)	87	91
3	C	313/327 (96%)	307 (98%)	6 (2%)	69	73
3	P	317/327 (97%)	311 (98%)	6 (2%)	69	73
4	D	206/206 (100%)	203 (98%)	3 (2%)	76	81
4	Q	206/206 (100%)	202 (98%)	4 (2%)	69	73
5	E	168/168 (100%)	167 (99%)	1 (1%)	92	95
5	R	168/168 (100%)	165 (98%)	3 (2%)	71	75
6	F	90/98 (92%)	89 (99%)	1 (1%)	84	88
6	S	90/98 (92%)	88 (98%)	2 (2%)	64	68
7	G	66/71 (93%)	64 (97%)	2 (3%)	53	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	66/71 (93%)	63 (96%)	3 (4%)	38	35
8	H	63/74 (85%)	61 (97%)	2 (3%)	51	52
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	27 (96%)	1 (4%)	47	46
9	V	28/60 (47%)	26 (93%)	2 (7%)	21	16
10	J	23/52 (44%)	23 (100%)	0	100	100
10	W	51/52 (98%)	51 (100%)	0	100	100
All	All	3336/3538 (94%)	3280 (98%)	56 (2%)	73	78

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	20	ASP
1	N	348	SER
7	T	45	ILE
1	N	32	GLN
1	N	184	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	73	ASN
1	N	136	GLN
4	Q	35	GLN
1	N	9	GLN
1	N	32	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

Of 123 ligands modelled in this entry, 74 are unknown - leaving 49 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$
13	PO4	A	2010	-	4,4,4	0.82	0	6,6,6	0.82	0
12	AZI	A	4002	-	2,2,2	1.19	0	0,1,1	0.00	-
11	BHG	A	4004	-	18,18,18	1.31	3 (16%)	23,23,23	0.61	0
13	PO4	B	3009	-	4,4,4	0.81	0	6,6,6	0.82	0
20	PEE	B	4017	-	5,7,50	4.41	2 (40%)	4,7,55	0.43	0
17	SMA	C	2001	-	38,38,38	1.88	6 (15%)	50,52,52	1.74	7 (14%)
18	UQ	C	2002	-	17,18,63	2.89	11 (64%)	21,24,79	0.66	0
19	CDL	C	2004	-	41,43,99	1.16	1 (2%)	50,55,111	1.56	6 (12%)
12	AZI	C	2005	-	2,2,2	0.97	0	0,1,1	0.00	-
20	PEE	C	2007	-	48,48,50	1.08	4 (8%)	53,53,55	0.87	5 (9%)
22	GOL	C	2008	-	5,5,5	1.20	0	5,5,5	0.74	0
11	BHG	C	2011	-	18,18,18	1.77	5 (27%)	23,23,23	0.72	0
22	GOL	C	4008	-	5,5,5	1.14	0	5,5,5	0.62	0
14	HEM	C	501	3	42,50,50	3.24	14 (33%)	27,82,82	1.62	4 (14%)
14	HEM	C	502	3	42,50,50	2.66	13 (30%)	27,82,82	1.67	6 (22%)
19	CDL	D	2003	-	38,38,99	1.17	2 (5%)	47,47,111	1.29	6 (12%)
20	PEE	D	2006	-	50,50,50	1.20	6 (12%)	55,55,55	0.92	5 (9%)
13	PO4	D	4010	-	4,4,4	0.81	0	6,6,6	0.82	0
13	PO4	D	4011	-	4,4,4	0.78	0	6,6,6	0.83	0
15	HEC	D	501	4	50,50,50	3.27	9 (18%)	56,82,82	1.96	7 (12%)
22	GOL	E	4006	-	5,5,5	1.22	0	5,5,5	0.71	0
22	GOL	E	4007	-	3,4,5	2.56	1 (33%)	2,4,5	1.73	1 (50%)
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	F	3012	-	18,18,18	1.82	5 (27%)	23,23,23	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BHG	F	4003	-	18,18,18	1.78	4 (22%)	23,23,23	0.72	0
12	AZI	G	4001	-	2,2,2	1.45	0	0,1,1	0.00	-
13	PO4	I	4015	-	4,4,4	0.80	0	6,6,6	0.83	0
13	PO4	O	2009	-	4,4,4	0.82	0	6,6,6	0.82	0
22	GOL	O	4005	-	5,5,5	1.20	0	5,5,5	0.70	0
17	SMA	P	3001	-	38,38,38	1.84	6 (15%)	50,52,52	1.62	7 (14%)
18	UQ	P	3002	-	17,18,63	2.65	10 (58%)	21,24,79	0.56	0
19	CDL	P	3004	-	46,48,99	1.13	3 (6%)	56,60,111	1.40	6 (10%)
12	AZI	P	3005	-	2,2,2	1.27	0	0,1,1	0.00	-
20	PEE	P	3007	-	48,48,50	1.11	4 (8%)	53,53,55	0.86	4 (7%)
22	GOL	P	3008	-	5,5,5	1.15	0	5,5,5	0.60	0
13	PO4	P	3010	-	4,4,4	0.78	0	6,6,6	0.82	0
11	BHG	P	3011	-	18,18,18	1.76	4 (22%)	23,23,23	0.76	1 (4%)
22	GOL	P	4009	-	5,5,5	1.00	0	5,5,5	0.60	0
14	HEM	P	501	3	42,50,50	2.84	12 (28%)	27,82,82	1.77	5 (18%)
14	HEM	P	502	3	42,50,50	2.91	10 (23%)	27,82,82	1.42	5 (18%)
19	CDL	Q	3003	-	38,38,99	1.22	3 (7%)	47,47,111	1.26	6 (12%)
20	PEE	Q	3006	-	50,50,50	1.18	6 (12%)	55,55,55	0.90	6 (10%)
13	PO4	Q	4012	-	4,4,4	0.89	0	6,6,6	0.82	0
15	HEC	Q	501	4	50,50,50	3.04	8 (16%)	56,82,82	2.28	17 (30%)
13	PO4	R	4013	-	4,4,4	0.86	0	6,6,6	0.82	0
13	PO4	R	4014	-	4,4,4	0.83	0	6,6,6	0.82	0
16	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	S	2012	-	18,18,18	1.81	4 (22%)	23,23,23	0.72	0
13	PO4	T	4016	-	4,4,4	0.78	0	6,6,6	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PO4	A	2010	-	-	0/0/0/0	0/0/0/0
12	AZI	A	4002	-	-	0/0/0/0	0/0/0/0
11	BHG	A	4004	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	B	3009	-	-	0/0/0/0	0/0/0/0
20	PEE	B	4017	-	-	0/3/5/54	0/0/0/0
17	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
18	UQ	C	2002	-	-	0/7/33/87	0/1/1/1
19	CDL	C	2004	-	1/1/9/9	1/52/52/110	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	AZI	C	2005	-	-	0/0/0/0	0/0/0/0
20	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
22	GOL	C	2008	-	-	0/4/4/4	0/0/0/0
11	BHG	C	2011	-	1/1/5/5	0/9/29/29	0/1/1/1
22	GOL	C	4008	-	-	0/4/4/4	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
19	CDL	D	2003	-	-	0/43/43/110	0/0/0/0
20	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
13	PO4	D	4010	-	-	0/0/0/0	0/0/0/0
13	PO4	D	4011	-	-	0/0/0/0	0/0/0/0
15	HEC	D	501	4	-	0/10/54/54	0/0/8/8
22	GOL	E	4006	-	-	0/4/4/4	0/0/0/0
22	GOL	E	4007	-	-	0/2/2/4	0/0/0/0
16	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	BHG	F	3012	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	F	4003	-	1/1/5/5	0/9/29/29	0/1/1/1
12	AZI	G	4001	-	-	0/0/0/0	0/0/0/0
13	PO4	I	4015	-	-	0/0/0/0	0/0/0/0
13	PO4	O	2009	-	-	0/0/0/0	0/0/0/0
22	GOL	O	4005	-	-	0/4/4/4	0/0/0/0
17	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
18	UQ	P	3002	-	-	0/7/33/87	0/1/1/1
19	CDL	P	3004	-	1/1/9/9	1/57/57/110	0/0/0/0
12	AZI	P	3005	-	-	0/0/0/0	0/0/0/0
20	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
22	GOL	P	3008	-	-	0/4/4/4	0/0/0/0
13	PO4	P	3010	-	-	0/0/0/0	0/0/0/0
11	BHG	P	3011	-	1/1/5/5	0/9/29/29	0/1/1/1
22	GOL	P	4009	-	-	0/4/4/4	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	-	-	0/43/43/110	0/0/0/0
20	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
13	PO4	Q	4012	-	-	0/0/0/0	0/0/0/0
15	HEC	Q	501	4	-	0/10/54/54	0/0/8/8
13	PO4	R	4013	-	-	0/0/0/0	0/0/0/0
13	PO4	R	4014	-	-	0/0/0/0	0/0/0/0
16	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	BHG	S	2012	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	T	4016	-	-	0/0/0/0	0/0/0/0

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C3B-CAB	15.07	1.55	1.34
15	Q	501	HEC	C3B-CAB	13.46	1.52	1.34
15	D	501	HEC	C3C-CAC	13.38	1.52	1.34
15	Q	501	HEC	C3C-CAC	12.66	1.51	1.34
14	C	501	HEM	C3C-C2C	-12.51	1.35	1.45

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	CBB-CAB-C3B	-8.16	109.52	127.36
15	D	501	HEC	CBC-CAC-C3C	-8.06	109.75	127.36
17	C	2001	SMA	C9-C2-C3	7.63	129.63	120.42
15	D	501	HEC	CBB-CAB-C3B	-7.16	111.72	127.36
15	Q	501	HEC	CBC-CAC-C3C	-7.04	111.97	127.36

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	C	2004	CDL	CA4
11	C	2011	BHG	C4
11	P	3011	BHG	C4
11	F	3012	BHG	C4
19	P	3004	CDL	CA4

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	2004	CDL	CA6-OA8-CA7-C31
19	P	3004	CDL	CA6-OA8-CA7-C31

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%)	0.17	15 (3%) 43 47	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.51	29 (6%) 18 20	31, 50, 77, 132	1 (0%)
2	B	424/439 (96%)	0.29	14 (3%) 44 49	28, 41, 66, 102	0
2	O	424/439 (96%)	0.59	41 (9%) 8 9	31, 48, 87, 185	0
3	C	365/379 (96%)	0.42	21 (5%) 22 25	24, 34, 48, 108	0
3	P	370/379 (97%)	0.56	23 (6%) 20 22	28, 37, 52, 218	0
4	D	241/241 (100%)	0.41	13 (5%) 25 27	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.65	26 (10%) 6 7	31, 45, 67, 87	0
5	E	196/196 (100%)	1.13	43 (21%) 1 1	32, 57, 105, 117	0
5	R	196/196 (100%)	0.41	15 (7%) 13 15	27, 46, 71, 99	0
6	F	99/110 (90%)	0.50	13 (13%) 4 5	24, 39, 71, 83	0
6	S	99/110 (90%)	0.29	4 (4%) 36 41	28, 40, 67, 88	0
7	G	75/81 (92%)	0.88	11 (14%) 3 3	26, 49, 77, 86	0
7	T	76/81 (93%)	1.65	20 (26%) 1 1	32, 55, 98, 114	0
8	H	66/78 (84%)	1.19	19 (28%) 1 1	40, 56, 73, 78	0
8	U	66/78 (84%)	1.13	14 (21%) 1 1	44, 63, 94, 104	0
9	I	42/78 (53%)	2.18	19 (45%) 1 1	33, 62, 90, 93	0
9	V	42/78 (53%)	2.10	16 (38%) 1 1	36, 78, 94, 100	0
10	J	30/62 (48%)	1.07	4 (13%) 4 4	40, 52, 80, 109	0
10	W	62/62 (100%)	2.29	21 (33%) 1 1	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.59	381 (9%) 8 9	24, 43, 80, 218	2 (0%)

The worst 5 of 381 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	13	ILE	23.4
10	W	1	VAL	21.5
7	T	1	GLY	13.5
7	T	76	ALA	12.4
9	I	50	LEU	12.1

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
13	PO4	R	4014	5/5	0.32	451.00	173,174,174,174	0
21	UNL	B	4039	1/-	0.36	259.00	73,73,73,73	0
21	UNL	D	4083	1/-	0.54	142.33	82,82,82,82	0
21	UNL	P	4046	1/-	0.48	123.00	65,65,65,65	0
21	UNL	N	4029	1/-	1.34	117.47	94,94,94,94	0
21	UNL	C	4068	1/-	0.56	77.00	72,72,72,72	0
21	UNL	N	4022	1/-	0.38	69.50	81,81,81,81	0
21	UNL	R	4069	1/-	0.42	49.18	62,62,62,62	0
21	UNL	B	4025	1/-	1.73	45.59	93,93,93,93	0
21	UNL	B	4026	1/-	1.25	43.74	92,92,92,92	0
21	UNL	I	4072	1/-	2.04	38.33	93,93,93,93	0
11	BHG	F	3012	18/18	0.92	33.87	159,162,164,164	0
21	UNL	A	4075	1/-	0.88	33.18	64,64,64,64	0
21	UNL	V	4078	1/-	1.51	32.00	94,94,94,94	0
21	UNL	A	4087	1/-	0.34	30.78	60,60,60,60	0
21	UNL	C	4023	1/-	0.53	29.94	55,55,55,55	0
21	UNL	A	4035	1/-	0.96	29.77	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	UNL	A	4076	1/-	0.48	28.66	68,68,68,68	0
21	UNL	A	4091	1/-	0.72	27.86	72,72,72,72	0
21	UNL	C	4045	1/-	0.41	27.59	71,71,71,71	0
21	UNL	B	4080	1/-	0.66	25.60	67,67,67,67	0
21	UNL	Q	4044	1/-	1.27	25.49	88,88,88,88	0
21	UNL	B	4057	1/-	0.85	24.81	57,57,57,57	0
21	UNL	C	4063	1/-	0.98	22.67	74,74,74,74	0
21	UNL	B	4030	1/-	0.41	21.83	70,70,70,70	0
21	UNL	N	4019	2/-	0.27	20.35	76,76,76,76	0
21	UNL	I	4033	1/-	0.86	19.47	69,69,69,69	0
21	UNL	O	4084	1/-	0.61	19.28	67,67,67,67	0
21	UNL	F	4028	1/-	0.59	19.13	82,82,82,82	0
21	UNL	A	4032	1/-	0.71	18.59	65,65,65,65	0
21	UNL	B	4079	1/-	0.42	18.09	66,66,66,66	0
21	UNL	U	4056	1/-	1.00	17.02	101,101,101,101	0
21	UNL	G	4064	1/-	0.49	16.73	56,56,56,56	0
11	BHG	F	4003	18/18	0.65	16.38	176,180,181,181	0
21	UNL	C	4018	2/-	0.32	15.93	74,74,74,76	0
21	UNL	P	4089	1/-	0.45	15.86	63,63,63,63	0
21	UNL	D	4067	1/-	0.58	15.51	58,58,58,58	0
21	UNL	E	4050	1/-	0.39	15.29	65,65,65,65	0
21	UNL	G	4053	1/-	0.21	14.51	77,77,77,77	0
11	BHG	S	2012	18/18	0.43	14.46	89,103,106,107	0
11	BHG	C	2011	18/18	0.47	13.47	106,118,123,125	0
21	UNL	P	4058	1/-	0.28	12.06	61,61,61,61	0
21	UNL	T	4065	1/-	0.72	11.68	66,66,66,66	0
12	AZI	P	3005	3/3	0.33	10.27	54,54,59,63	0
22	GOL	E	4007	5/6	0.45	10.16	97,100,101,102	0
22	GOL	O	4005	6/6	0.90	9.16	166,167,167,168	0
21	UNL	O	4071	1/-	0.82	8.84	70,70,70,70	0
21	UNL	V	4090	1/-	0.96	8.67	74,74,74,74	0
11	BHG	P	3011	18/18	0.38	8.52	99,107,109,109	0
12	AZI	A	4002	3/3	0.63	8.03	48,48,58,65	0
21	UNL	D	4036	1/-	0.34	7.74	83,83,83,83	0
13	PO4	R	4013	5/5	0.26	7.73	114,114,116,116	0
22	GOL	P	3008	6/6	0.49	7.12	83,84,85,88	0
21	UNL	U	4049	1/-	0.68	6.18	77,77,77,77	0
21	UNL	A	4048	1/-	0.35	6.04	72,72,72,72	0
12	AZI	C	2005	3/3	0.30	5.71	41,41,55,60	0
21	UNL	D	4027	1/-	0.31	5.02	87,87,87,87	0
21	UNL	P	4040	1/-	0.31	5.01	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
21	UNL	O	4037	1/-	0.78	4.98	62,62,62,62	0
21	UNL	D	4054	1/-	0.49	4.85	76,76,76,76	0
13	PO4	D	4011	5/5	0.31	4.82	130,130,130,131	0
20	PEE	B	4017	8/51	0.40	4.77	85,88,91,92	0
20	PEE	D	2006	51/51	0.32	4.49	85,98,115,118	0
22	GOL	E	4006	6/6	0.25	4.21	67,71,72,75	0
22	GOL	C	2008	6/6	0.29	4.16	60,63,63,70	0
21	UNL	O	4041	1/-	0.31	4.11	71,71,71,71	0
21	UNL	B	4034	1/-	0.68	4.08	87,87,87,87	0
13	PO4	B	3009	5/5	0.12	3.80	97,99,100,101	0
21	UNL	O	4031	1/-	0.46	3.47	86,86,86,86	0
21	UNL	C	4086	1/-	0.21	3.44	50,50,50,50	0
21	UNL	P	4021	2/-	0.20	3.14	71,71,71,73	0
21	UNL	P	4060	1/-	0.34	2.61	88,88,88,88	0
21	UNL	A	4038	1/-	0.59	2.60	85,85,85,85	0
21	UNL	P	4074	1/-	0.15	2.37	59,59,59,59	0
22	GOL	P	4009	6/6	0.34	2.18	67,70,71,72	0
20	PEE	C	2007	49/51	0.25	2.14	33,58,74,74	0
20	PEE	Q	3006	51/51	0.22	2.13	53,65,110,110	0
13	PO4	A	2010	5/5	0.22	2.12	133,133,134,134	0
21	UNL	B	4051	1/-	0.19	2.11	78,78,78,78	0
12	AZI	G	4001	3/3	0.21	2.07	47,47,57,59	0
20	PEE	P	3007	49/51	0.23	2.00	35,58,75,76	0
13	PO4	Q	4012	5/5	0.20	1.95	108,109,110,110	0
21	UNL	G	4070	1/-	0.29	1.65	67,67,67,67	0
19	CDL	P	3004	49/100	0.29	1.57	54,81,117,120	0
13	PO4	I	4015	5/5	0.31	1.34	122,122,123,123	0
21	UNL	N	4073	1/-	0.17	1.21	69,69,69,69	0
21	UNL	B	4052	1/-	0.16	0.93	60,60,60,60	0
18	UQ	C	2002	18/63	0.29	0.92	61,73,76,76	0
19	CDL	C	2004	44/100	0.21	0.92	54,83,104,106	0
17	SMA	C	2001	37/37	0.15	0.64	25,33,44,46	0
19	CDL	D	2003	39/100	0.20	0.61	64,84,106,107	0
18	UQ	P	3002	18/63	0.24	0.36	60,82,85,86	0
22	GOL	C	4008	6/6	0.23	0.29	53,55,60,60	0
15	HEC	D	501	43/43	0.14	0.17	26,33,37,38	0
21	UNL	O	4043	1/-	0.22	0.13	80,80,80,80	0
14	HEM	P	501	43/43	0.15	0.13	22,26,33,40	0
19	CDL	Q	3003	39/100	0.22	0.12	54,90,96,96	0
16	FES	E	501	4/4	0.14	0.11	38,39,40,40	0
14	HEM	C	502	43/43	0.17	0.11	23,26,33,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	BHG	A	4004	18/18	0.13	0.10	29,36,42,44	0
21	UNL	O	4082	1/-	0.16	0.07	73,73,73,73	0
14	HEM	C	501	43/43	0.14	-0.01	21,27,34,38	0
17	SMA	P	3001	37/37	0.14	-0.05	30,39,47,52	0
13	PO4	P	3010	5/5	0.18	-0.30	115,115,115,116	0
15	HEC	Q	501	43/43	0.12	-0.45	29,36,41,45	0
14	HEM	P	502	43/43	0.12	-0.70	23,27,37,39	0
16	FES	R	501	4/4	0.13	-0.76	27,29,30,30	0
13	PO4	T	4016	5/5	0.09	-1.17	107,108,108,108	0
13	PO4	O	2009	5/5	0.09	-1.56	76,79,81,81	0
21	UNL	W	4077	1/-	0.11	-2.44	60,60,60,60	0
21	UNL	T	4066	1/-	0.07	-5.76	70,70,70,70	0
21	UNL	R	4055	1/-	0.13	-	73,73,73,73	0
21	UNL	D	4062	1/-	0.39	-	90,90,90,90	0
13	PO4	D	4010	5/5	0.35	-	169,169,170,170	0
21	UNL	A	4081	1/-	0.48	-	71,71,71,71	0
21	UNL	B	4042	1/-	0.35	-	81,81,81,81	0
21	UNL	O	4020	2/-	0.22	-	96,96,96,97	0
21	UNL	V	4024	1/-	1.25	-	96,96,96,96	0
21	UNL	V	4088	1/-	0.90	-	80,80,80,80	0
21	UNL	D	4059	1/-	0.85	-	57,57,57,57	0
21	UNL	E	4061	1/-	0.16	-	79,79,79,79	0
21	UNL	S	4047	1/-	0.58	-	71,71,71,71	0
21	UNL	A	4085	1/-	0.20	-	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.