



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 04:16 pm GMT

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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

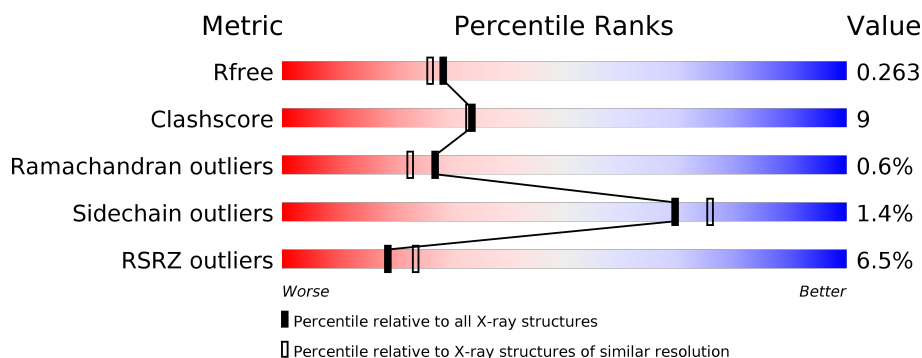
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>..</div> </div> </div>
1	N	446	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
2	B	439	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
2	O	439	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
3	C	379	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
3	P	379	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
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, 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	JZR	A	4002	-	-	-	X
11	JZR	C	2008	-	-	-	X
11	JZR	F	3011	-	-	-	X
11	JZR	F	4001	-	-	-	X
11	JZR	S	2011	-	-	-	X
12	AZI	P	3014	-	-	-	X
13	PEE	G	2005	-	-	-	X
13	PEE	T	3005	-	-	-	X
14	PO4	B	3010	-	X	-	-
14	PO4	O	2010	-	X	-	-
15	GOL	B	2013	-	-	-	X
15	GOL	O	3013	-	-	-	X

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33959 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 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			

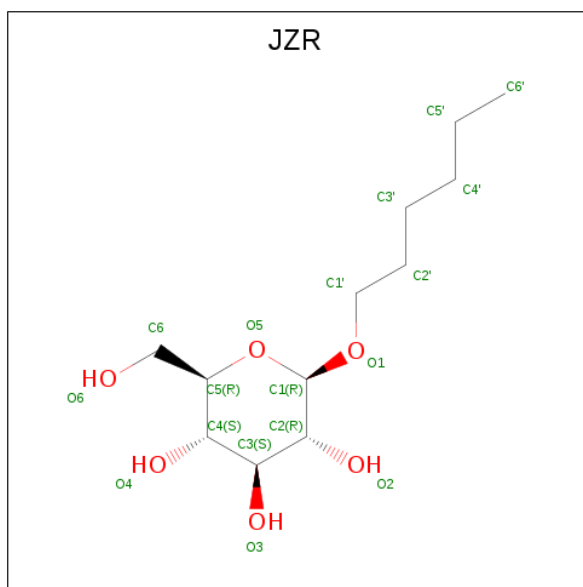
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

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.

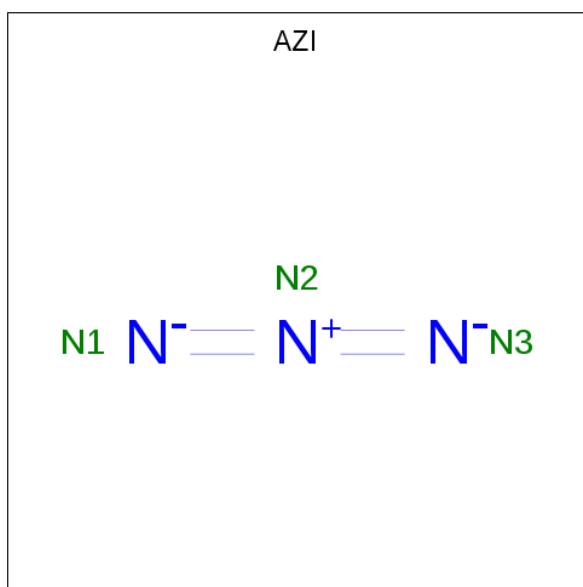
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			507	333	88	86			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: C₁₂H₂₄O₆).



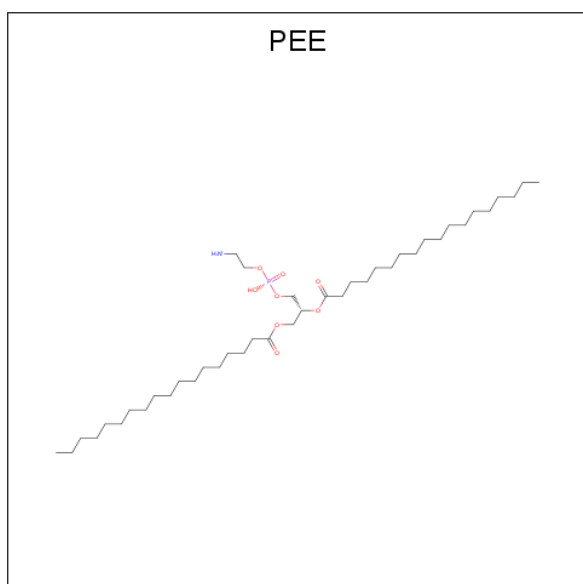
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

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



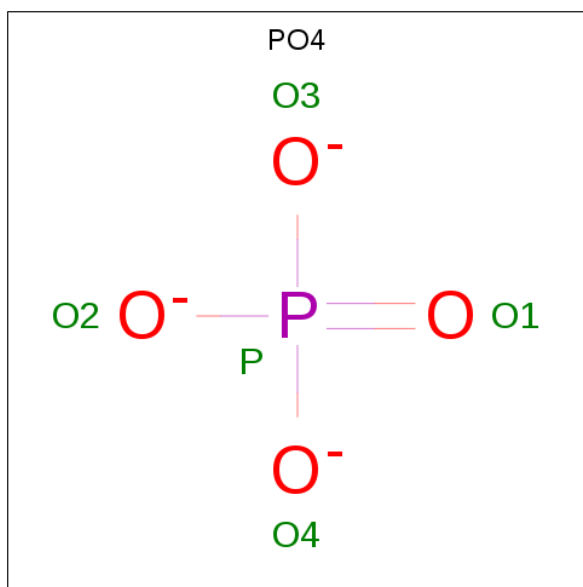
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total N 3 3	0	0
12	C	1	Total N 3 3	0	0
12	D	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0

- Molecule 13 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



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

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



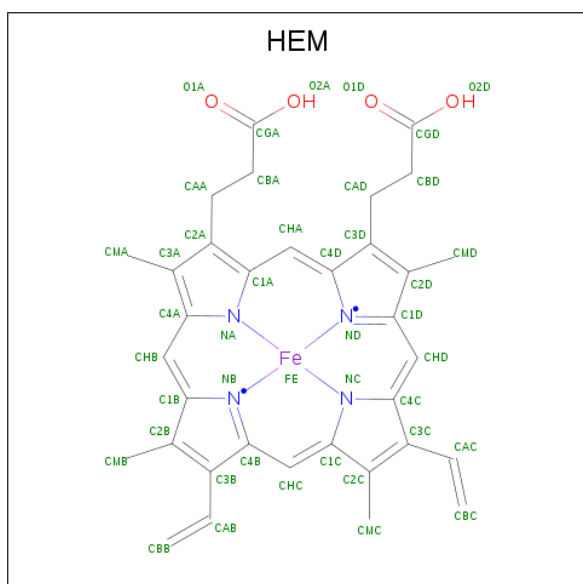
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	O	P	0	0
			5	4	1		
14	O	1	Total	O	P	0	0
			5	4	1		

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



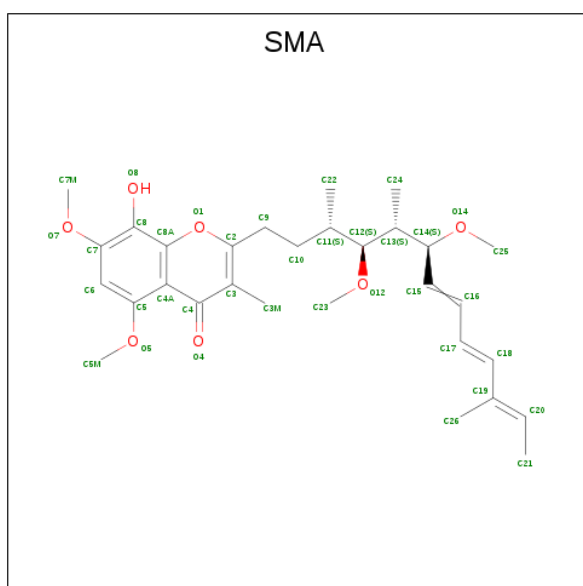
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			6	3	3		
15	C	1	Total	C	O	0	0
			6	3	3		
15	O	1	Total	C	O	0	0
			6	3	3		
15	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



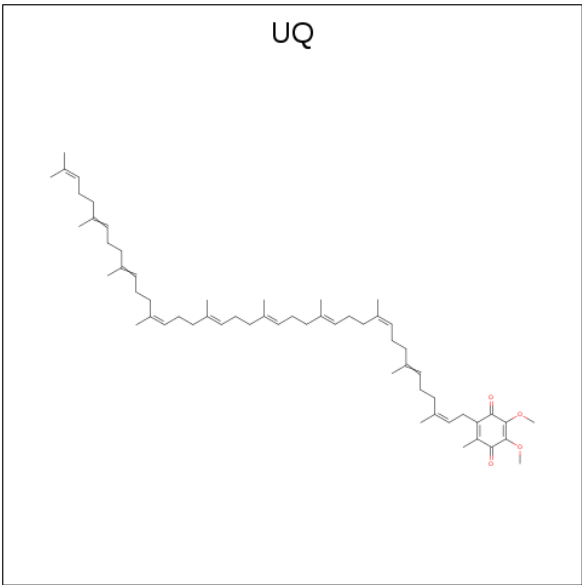
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



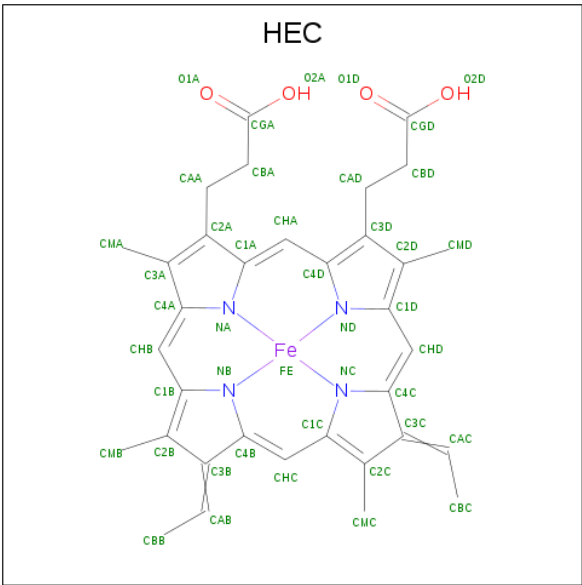
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O		
			37	30	7	0	0
17	P	1	Total	C	O		
			37	30	7	0	0

- Molecule 18 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



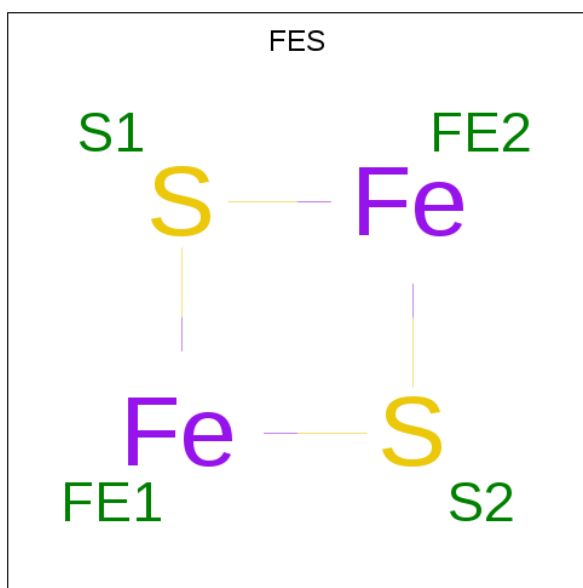
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			14	10	4		
18	P	1	Total	C	O	0	0
			14	10	4		

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



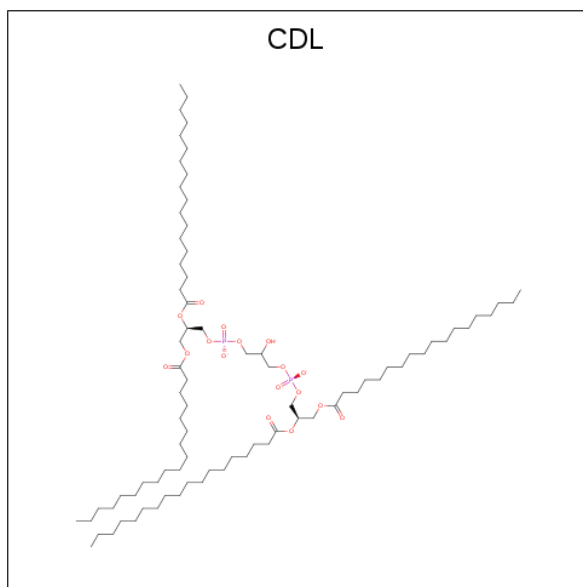
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	G	1	Total	C	O	P	0	0
			50	31	17	2		

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

- 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		
22	I	16	Total	O	0	0
			16	16		
22	J	5	Total	O	0	0
			5	5		
22	N	134	Total	O	0	0
			134	134		
22	O	130	Total	O	0	0
			130	130		
22	P	122	Total	O	0	0
			122	122		
22	Q	109	Total	O	0	0
			109	109		
22	R	64	Total	O	0	0
			64	64		
22	S	73	Total	O	0	0
			73	73		

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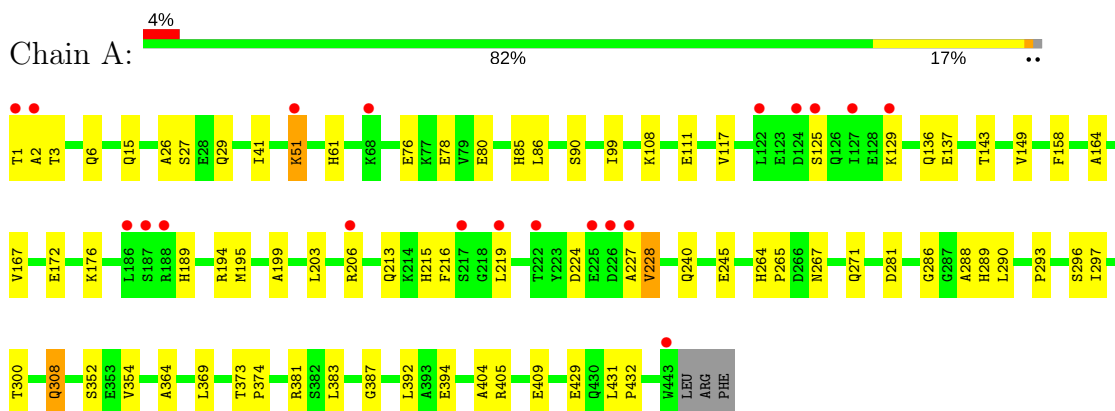
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	T	21	Total 21	O 21	0	0
22	U	16	Total 16	O 16	0	0
22	V	10	Total 10	O 10	0	0
22	W	9	Total 9	O 9	0	0

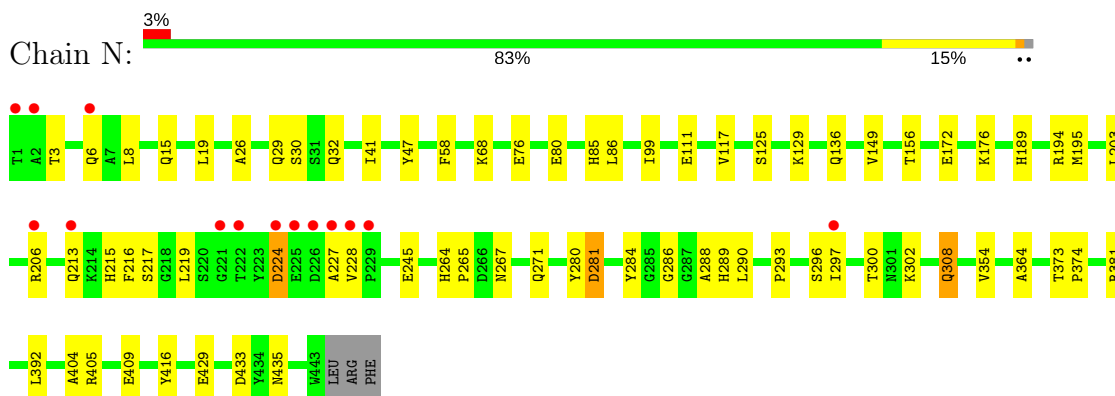
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

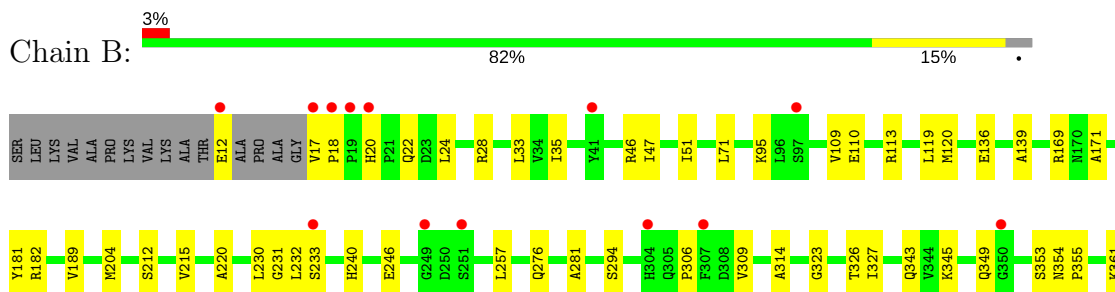
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial



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

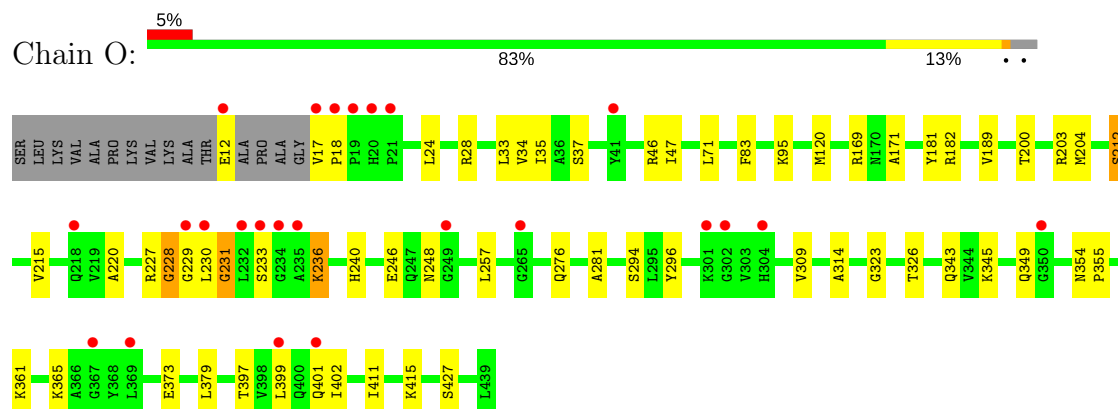


- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

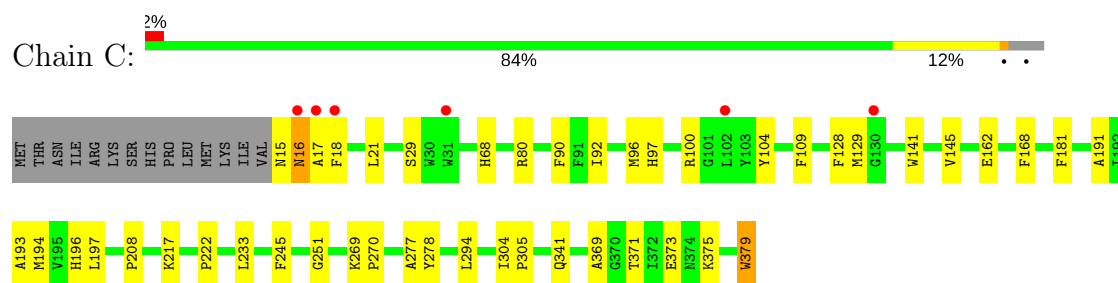




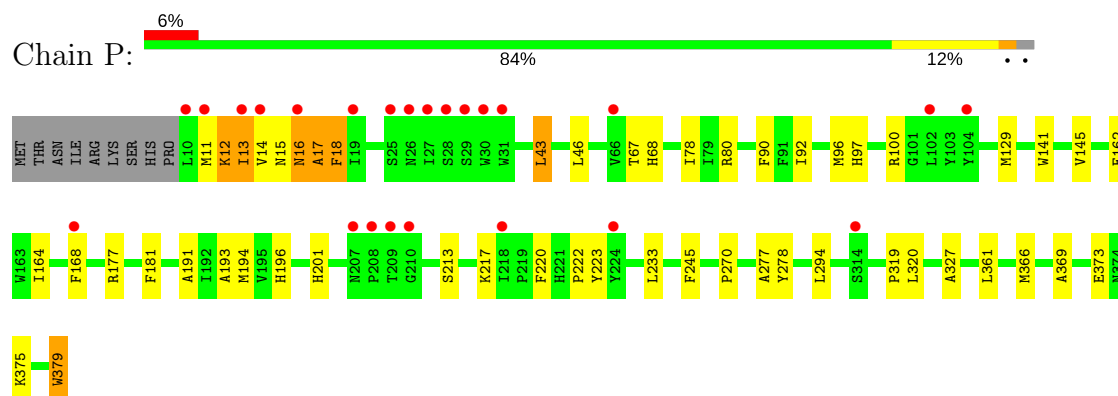
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial



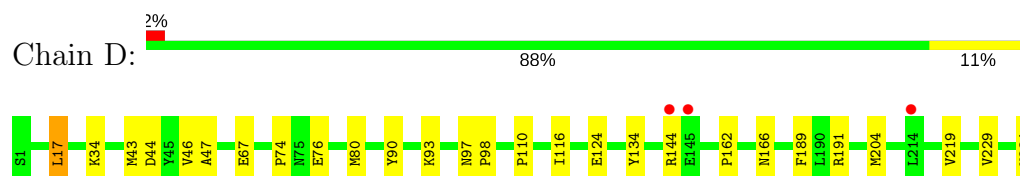
- Molecule 3: Cytochrome b



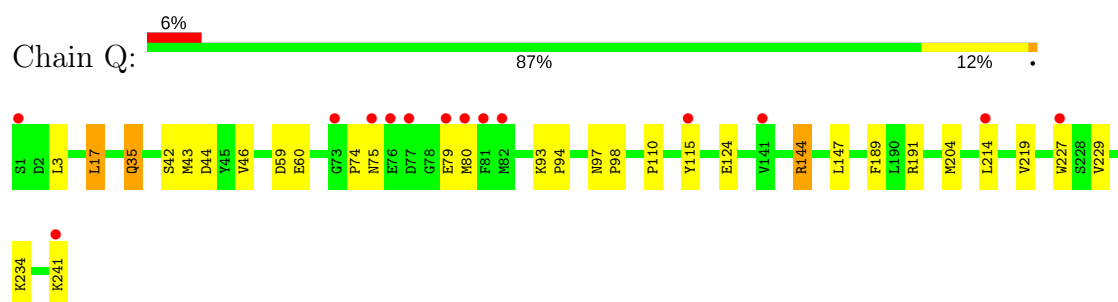
- Molecule 3: Cytochrome b



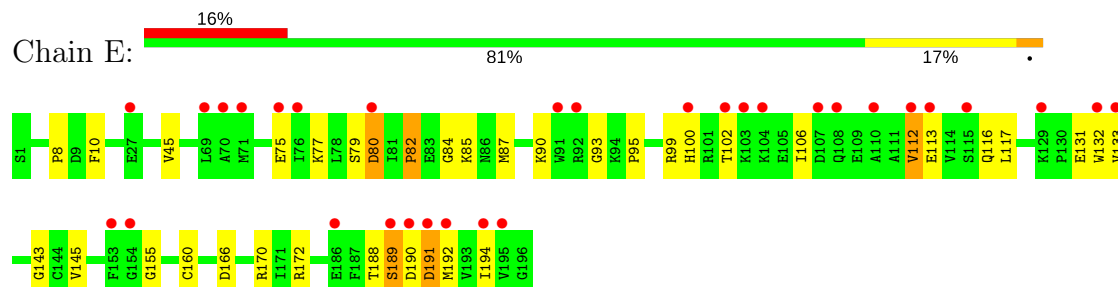
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



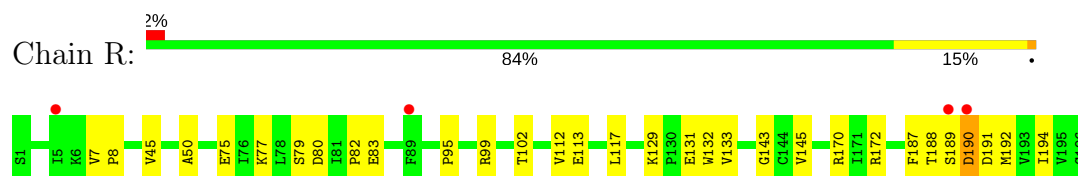
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



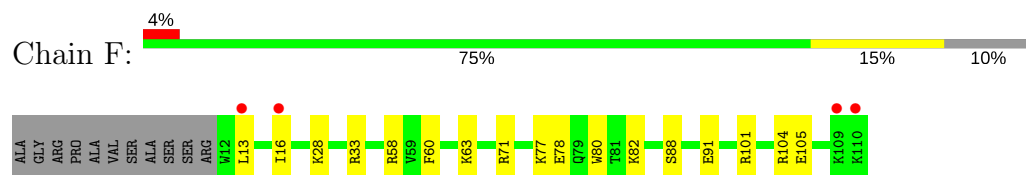
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



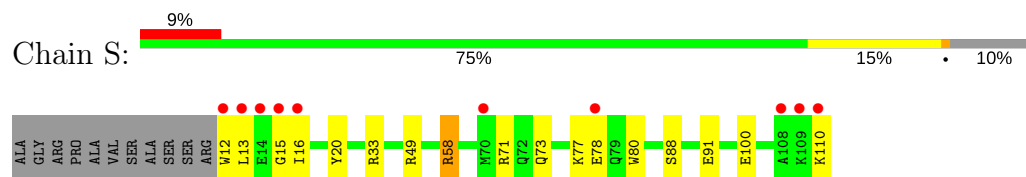
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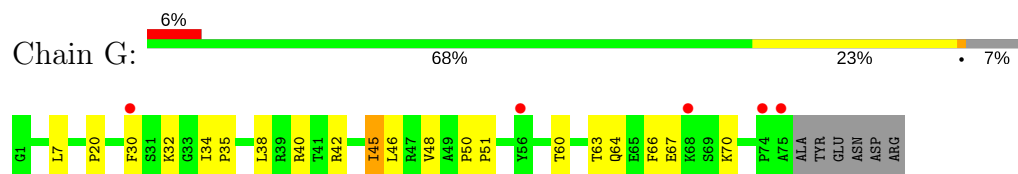
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



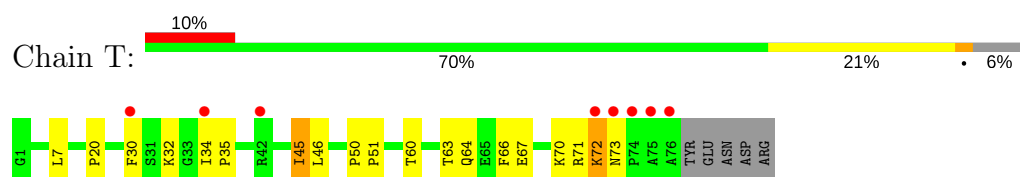
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



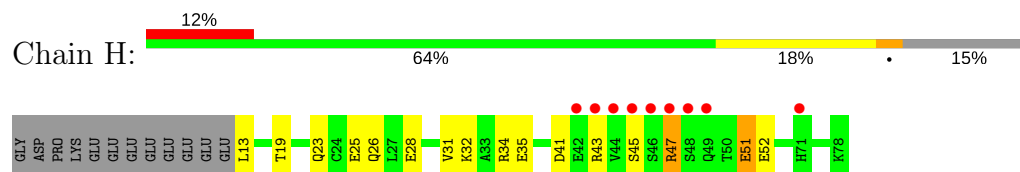
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



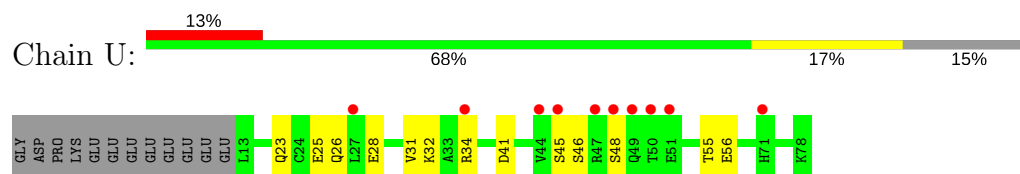
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



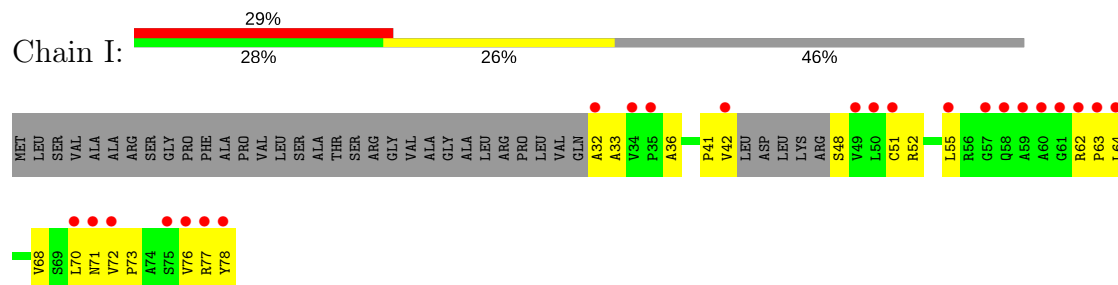
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



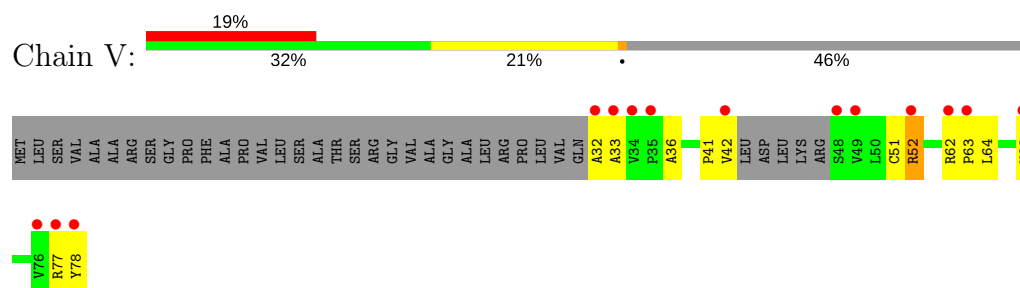
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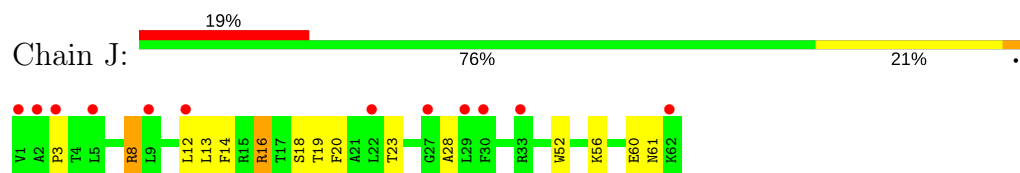
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



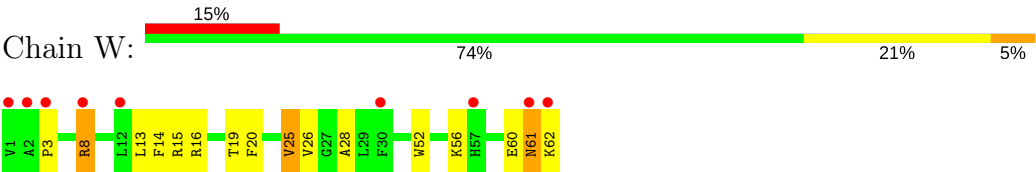
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



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



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



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 0.242 , 0.263	Depositor DCC
R_{free} test set	15323 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, PO4, UQ, FES, HEC, HEM, PEE, JZR, 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	A	3	0	0	0	0
12	C	3	0	0	0	0
12	D	3	0	0	0	0
12	P	3	0	0	0	0
13	A	6	0	5	0	0
13	C	54	0	72	2	0
13	D	51	0	82	1	0
13	G	49	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	5	0	0	0	0
13	P	49	0	72	2	0
13	Q	51	0	82	9	0
13	T	49	0	72	1	0
14	B	5	0	0	0	0
14	O	5	0	0	0	0
15	B	6	0	8	0	0
15	C	6	0	8	0	0
15	O	6	0	8	0	0
15	P	6	0	8	0	0
16	C	86	0	60	5	0
16	P	86	0	60	3	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	D	43	0	30	3	0
19	Q	43	0	30	2	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	G	94	0	76	5	0
21	Q	50	0	44	0	0
21	T	49	0	42	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
22	U	16	0	0	0	0
22	V	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	9	0	0	0	0
All	All	33959	0	32273	593	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 593 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)
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	13:Q:3006:PEE:H30	1.40	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	31	27
1	N	441/446 (99%)	425 (96%)	15 (3%)	1 (0%)	49	51
2	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	49	51
2	O	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	31	27
3	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	21	16
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	12	7
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%)	8	3
5	R	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	31	27
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%)	12	7
8	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
8	U	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	11	5
9	I	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	6	2
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	6	2
10	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	10	5
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	10	5
All	All	3980/4220 (94%)	3851 (97%)	104 (3%)	25 (1%)	27	23

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%)	69	76
1	N	364/370 (98%)	359 (99%)	5 (1%)	69	76
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	332/343 (97%)	330 (99%)	2 (1%)	87	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	312/327 (95%)	307 (98%)	5 (2%)	65	72
3	P	316/327 (97%)	310 (98%)	6 (2%)	60	66
4	D	206/206 (100%)	203 (98%)	3 (2%)	67	73
4	Q	206/206 (100%)	203 (98%)	3 (2%)	67	73
5	E	168/168 (100%)	167 (99%)	1 (1%)	87	91
5	R	168/168 (100%)	166 (99%)	2 (1%)	74	80
6	F	90/98 (92%)	89 (99%)	1 (1%)	76	81
6	S	90/98 (92%)	89 (99%)	1 (1%)	76	81
7	G	66/71 (93%)	65 (98%)	1 (2%)	67	73
7	T	66/71 (93%)	64 (97%)	2 (3%)	44	47
8	H	63/74 (85%)	61 (97%)	2 (3%)	42	44
8	U	63/74 (85%)	62 (98%)	1 (2%)	65	72
9	I	28/60 (47%)	27 (96%)	1 (4%)	38	39
9	V	28/60 (47%)	26 (93%)	2 (7%)	16	13
10	J	51/52 (98%)	49 (96%)	2 (4%)	35	35
10	W	51/52 (98%)	49 (96%)	2 (4%)	35	35
All	All	3364/3538 (95%)	3317 (99%)	47 (1%)	69	76

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 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 ⓘ

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	JZR	A	4002	-	18,18,18	1.88	5 (27%)	23,23,23	0.76	1 (4%)
13	PEE	A	4003	-	5,5,50	1.31	0	5,5,55	0.65	0
12	AZI	A	4005	-	0,2,2	0.00	-	0,1,1	0.00	-
15	GOL	B	2013	-	5,5,5	1.29	0	5,5,5	0.65	0
14	PO4	B	3010	-	4,4,4	1.28	1 (25%)	6,6,6	5.06	5 (83%)
17	SMA	C	2001	-	36,38,38	1.80	8 (22%)	44,52,52	1.99	4 (9%)
18	UQ	C	2002	-	14,14,63	2.23	8 (57%)	18,20,79	0.54	0
13	PEE	C	2007	-	48,48,50	1.19	5 (10%)	51,53,55	0.83	4 (7%)
11	JZR	C	2008	-	18,18,18	1.79	6 (33%)	23,23,23	0.68	0
15	GOL	C	2009	-	5,5,5	1.33	0	5,5,5	0.64	0
13	PEE	C	2012	-	4,4,50	3.09	3 (75%)	6,6,55	0.51	0
12	AZI	C	2014	-	0,2,2	0.00	-	0,1,1	0.00	-
16	HEM	C	501	3	27,50,50	2.34	10 (37%)	17,82,82	2.27	6 (35%)
16	HEM	C	502	3	27,50,50	1.92	8 (29%)	17,82,82	2.14	7 (41%)
13	PEE	D	2006	-	50,50,50	1.26	7 (14%)	53,55,55	0.86	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	AZI	D	4004	-	0,2,2	0.00	-	0,1,1	0.00	-
19	HEC	D	501	4	26,50,50	2.00	6 (23%)	18,82,82	1.45	4 (22%)
20	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	JZR	F	3011	-	18,18,18	1.88	4 (22%)	23,23,23	0.70	0
11	JZR	F	4001	-	18,18,18	1.78	5 (27%)	23,23,23	0.65	0
21	CDL	G	2003	-	49,49,99	1.10	4 (8%)	55,61,111	1.09	4 (7%)
21	CDL	G	2004	-	43,43,99	1.13	2 (4%)	49,55,111	1.22	4 (8%)
13	PEE	G	2005	-	48,48,50	1.28	8 (16%)	51,53,55	0.84	4 (7%)
13	PEE	N	3012	-	4,4,50	2.92	3 (75%)	6,6,55	0.51	0
14	PO4	O	2010	-	4,4,4	1.29	1 (25%)	6,6,6	5.05	5 (83%)
15	GOL	O	3013	-	5,5,5	1.29	0	5,5,5	0.70	0
17	SMA	P	3001	-	36,38,38	1.98	8 (22%)	44,52,52	2.05	4 (9%)
18	UQ	P	3002	-	14,14,63	2.02	8 (57%)	18,20,79	0.40	0
13	PEE	P	3007	-	48,48,50	1.23	5 (10%)	51,53,55	0.81	4 (7%)
11	JZR	P	3008	-	18,18,18	1.80	6 (33%)	23,23,23	0.67	0
15	GOL	P	3009	-	5,5,5	1.35	0	5,5,5	0.62	0
12	AZI	P	3014	-	0,2,2	0.00	-	0,1,1	0.00	-
16	HEM	P	501	3	27,50,50	2.25	8 (29%)	17,82,82	1.58	3 (17%)
16	HEM	P	502	3	27,50,50	2.17	9 (33%)	17,82,82	1.80	3 (17%)
21	CDL	Q	3003	-	49,49,99	1.09	4 (8%)	55,61,111	1.16	4 (7%)
13	PEE	Q	3006	-	50,50,50	1.25	7 (14%)	53,55,55	0.85	5 (9%)
19	HEC	Q	501	4	26,50,50	1.98	5 (19%)	18,82,82	1.21	2 (11%)
20	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	JZR	S	2011	-	18,18,18	1.81	3 (16%)	23,23,23	0.76	0
21	CDL	T	3004	-	48,48,99	1.15	4 (8%)	54,60,111	1.11	2 (3%)
13	PEE	T	3005	-	48,48,50	1.30	8 (16%)	51,53,55	0.84	5 (9%)

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	JZR	A	4002	-	-	0/9/29/29	0/1/1/1
13	PEE	A	4003	-	-	0/4/4/54	0/0/0/0
12	AZI	A	4005	-	-	0/0/0/0	0/0/0/0
15	GOL	B	2013	-	-	0/4/4/4	0/0/0/0
14	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
13	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
11	JZR	C	2008	-	-	0/9/29/29	0/1/1/1
15	GOL	C	2009	-	-	0/4/4/4	0/0/0/0
13	PEE	C	2012	-	-	0/0/0/54	0/0/0/0
12	AZI	C	2014	-	-	0/0/0/0	0/0/0/0
16	HEM	C	501	3	-	0/6/54/54	0/0/8/8
16	HEM	C	502	3	-	0/6/54/54	0/0/8/8
13	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
12	AZI	D	4004	-	-	0/0/0/0	0/0/0/0
19	HEC	D	501	4	-	0/6/54/54	0/0/8/8
20	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	JZR	F	3011	-	-	0/9/29/29	0/1/1/1
11	JZR	F	4001	-	-	0/9/29/29	0/1/1/1
21	CDL	G	2003	-	-	0/58/58/110	0/0/0/0
21	CDL	G	2004	-	-	0/52/52/110	0/0/0/0
13	PEE	G	2005	-	-	0/52/52/54	0/0/0/0
13	PEE	N	3012	-	-	0/0/0/54	0/0/0/0
14	PO4	O	2010	-	-	0/0/0/0	0/0/0/0
15	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
13	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
11	JZR	P	3008	-	-	0/9/29/29	0/1/1/1
15	GOL	P	3009	-	-	0/4/4/4	0/0/0/0
12	AZI	P	3014	-	-	0/0/0/0	0/0/0/0
16	HEM	P	501	3	-	0/6/54/54	0/0/8/8
16	HEM	P	502	3	-	0/6/54/54	0/0/8/8
21	CDL	Q	3003	-	-	0/58/58/110	0/0/0/0
13	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
19	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
20	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	JZR	S	2011	-	-	0/9/29/29	0/1/1/1
21	CDL	T	3004	-	-	0/57/57/110	0/0/0/0
13	PEE	T	3005	-	-	0/52/52/54	0/0/0/0

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	501	HEC	C3C-C2C	-5.96	1.34	1.40
19	D	501	HEC	C3B-C2B	-5.87	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	501	HEM	C3B-CAB	-5.76	1.36	1.47
16	C	501	HEM	C3C-CAC	-5.68	1.36	1.47
16	P	501	HEM	C3C-CAC	-5.16	1.37	1.47

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3010	PO4	O4-P-O1	-6.94	81.24	110.93
14	O	2010	PO4	O4-P-O1	-6.89	81.46	110.93
14	O	2010	PO4	O4-P-O2	-6.81	83.09	107.94
14	B	3010	PO4	O4-P-O2	-6.73	83.37	107.94
17	P	3001	SMA	C9-C10-C11	-6.52	105.94	114.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	4002	JZR	1	0
17	C	2001	SMA	1	0
18	C	2002	UQ	3	0
13	C	2007	PEE	2	0
16	C	501	HEM	2	0
16	C	502	HEM	3	0
13	D	2006	PEE	1	0
19	D	501	HEC	3	0
11	F	3011	JZR	3	0
21	G	2004	CDL	5	0
17	P	3001	SMA	2	0
18	P	3002	UQ	5	0
13	P	3007	PEE	2	0
16	P	501	HEM	1	0
16	P	502	HEM	2	0
13	Q	3006	PEE	9	0
19	Q	501	HEC	2	0
11	S	2011	JZR	8	0
13	T	3005	PEE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.09	20 (4%) 33 39	27, 43, 65, 115	1 (0%)
1	N	442/446 (99%)	0.15	14 (3%) 47 55	28, 43, 63, 128	1 (0%)
2	B	424/439 (96%)	0.14	15 (3%) 44 51	29, 45, 67, 132	0
2	O	424/439 (96%)	0.25	24 (5%) 24 29	33, 47, 73, 162	0
3	C	365/379 (96%)	0.21	6 (1%) 72 76	25, 34, 47, 106	0
3	P	370/379 (97%)	0.28	24 (6%) 19 24	26, 34, 52, 165	0
4	D	241/241 (100%)	-0.00	4 (1%) 70 74	28, 39, 59, 80	0
4	Q	241/241 (100%)	0.06	14 (5%) 23 29	28, 38, 59, 81	0
5	E	196/196 (100%)	0.73	31 (15%) 2 2	29, 54, 96, 117	0
5	R	196/196 (100%)	0.01	4 (2%) 65 69	29, 43, 61, 85	0
6	F	99/110 (90%)	0.23	4 (4%) 38 45	29, 44, 70, 80	0
6	S	99/110 (90%)	0.35	10 (10%) 7 9	28, 39, 79, 109	0
7	G	75/81 (92%)	0.45	5 (6%) 18 22	31, 50, 72, 80	0
7	T	76/81 (93%)	0.93	8 (10%) 6 8	30, 50, 97, 117	0
8	H	66/78 (84%)	0.84	9 (13%) 3 4	40, 55, 87, 101	0
8	U	66/78 (84%)	0.69	10 (15%) 2 3	40, 54, 79, 89	0
9	I	42/78 (53%)	2.49	23 (54%) 0 0	40, 75, 88, 93	0
9	V	42/78 (53%)	1.94	15 (35%) 0 0	45, 72, 92, 97	0
10	J	62/62 (100%)	1.08	12 (19%) 1 1	35, 60, 85, 116	0
10	W	62/62 (100%)	0.91	9 (14%) 2 3	34, 51, 80, 111	0
All	All	4030/4220 (95%)	0.29	261 (6%) 19 24	25, 42, 76, 165	2 (0%)

The worst 5 of 261 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	76	ALA	32.8
10	J	1	VAL	16.0
1	N	1	THR	11.4
2	O	19	PRO	10.0
3	P	13	ILE	9.5

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	GOL	B	2013	6/6	0.08	0.93	145,148,148,149	0
11	JZR	A	4002	18/18	0.28	0.62	130,143,145,145	0
11	JZR	F	4001	18/18	0.30	0.52	168,171,173,173	0
11	JZR	S	2011	18/18	0.31	0.42	73,86,91,91	0
15	GOL	O	3013	6/6	0.36	0.66	112,115,116,116	0
12	AZI	P	3014	3/3	0.41	0.42	54,54,55,61	0
11	JZR	C	2008	18/18	0.46	0.42	109,112,116,116	0
11	JZR	F	3011	18/18	0.48	0.60	114,118,122,122	0
12	AZI	C	2014	3/3	0.52	0.38	53,53,57,59	0
12	AZI	D	4004	3/3	0.53	0.30	69,69,72,73	0
11	JZR	P	3008	18/18	0.57	0.40	100,102,107,109	0
13	PEE	G	2005	49/51	0.62	0.43	105,123,129,129	0
13	PEE	A	4003	6/51	0.68	0.31	110,111,112,113	0
13	PEE	T	3005	49/51	0.71	0.53	96,121,136,136	0
18	UQ	P	3002	14/63	0.71	0.37	90,93,97,97	0
13	PEE	C	2012	5/51	0.73	0.26	116,116,116,116	0
21	CDL	G	2003	50/100	0.74	0.27	62,96,113,113	0
13	PEE	N	3012	5/51	0.77	0.20	94,94,94,96	0
18	UQ	C	2002	14/63	0.77	0.28	74,78,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	AZI	A	4005	3/3	0.79	0.32	72,72,73,74	0
15	GOL	P	3009	6/6	0.80	0.35	59,65,67,68	0
15	GOL	C	2009	6/6	0.85	0.40	56,59,63,67	0
21	CDL	Q	3003	50/100	0.85	0.21	55,78,90,92	0
14	PO4	B	3010	5/5	0.86	0.16	99,100,100,100	0
21	CDL	T	3004	49/100	0.87	0.26	54,69,98,101	0
13	PEE	C	2007	49/51	0.88	0.25	39,53,68,69	0
21	CDL	G	2004	44/100	0.88	0.25	62,79,105,107	0
13	PEE	D	2006	51/51	0.90	0.21	52,66,94,95	0
13	PEE	Q	3006	51/51	0.91	0.18	45,59,83,83	0
14	PO4	O	2010	5/5	0.92	0.11	106,106,107,108	0
17	SMA	P	3001	37/37	0.92	0.15	24,32,37,37	0
13	PEE	P	3007	49/51	0.93	0.22	35,54,62,63	0
17	SMA	C	2001	37/37	0.94	0.13	25,30,32,38	0
19	HEC	D	501	43/43	0.97	0.12	29,33,36,38	0
16	HEM	P	502	43/43	0.97	0.14	24,27,32,37	0
16	HEM	C	502	43/43	0.98	0.13	22,26,31,33	0
19	HEC	Q	501	43/43	0.98	0.10	32,35,36,37	0
20	FES	E	501	4/4	0.98	0.10	34,35,37,37	0
16	HEM	C	501	43/43	0.98	0.14	21,26,33,37	0
16	HEM	P	501	43/43	0.98	0.14	25,29,37,42	0
20	FES	R	501	4/4	0.99	0.09	31,31,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.