



wwPDB X-ray Structure Validation Summary Report

Oct 22, 2014 – 09:48 AM EDT

PDB ID : 3CWB
Title : Chicken Cytochrome BC1 Complex inhibited by an iodinated analogue of the polyketide Crocacin-D
Authors : Huang, L.; Cromartie, T.; Viner, R.; Crowley, P.J.; Berry, E.A.
Deposited on : 2008-04-21
Resolution : 3.51 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>

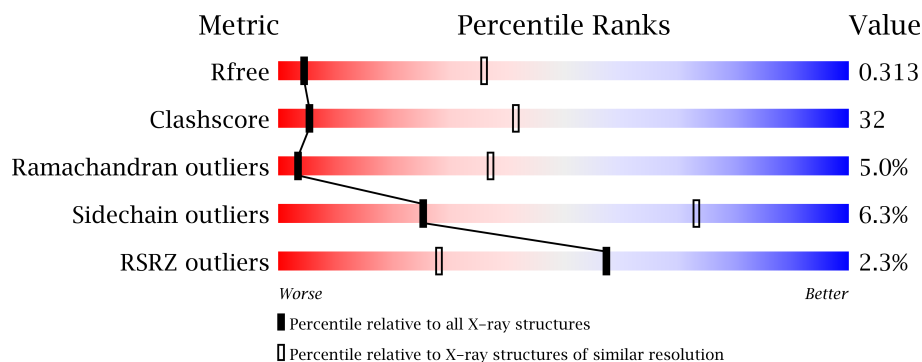
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.51 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.



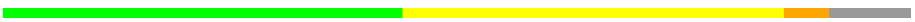





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)

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	441	
2	O	441	
3	C	380	
3	P	380	
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	77	
8	U	77	
9	I	52	
9	V	52	
10	J	61	
10	W	61	

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	BOG	C	3010	-	X
11	BOG	D	2091	-	X
11	BOG	Q	3091	-	X
12	AZI	C	2011	-	X
12	AZI	P	3011	-	X
14	PEE	A	2008	-	X
14	PEE	C	2005	-	X
14	PEE	C	2007	-	X
14	PEE	P	3008	-	X
14	PEE	W	3005	-	X
16	UQ	C	2002	-	X
16	UQ	P	3002	-	X
18	CDL	D	2003	-	X
18	CDL	P	3003	-	X
20	UNL	P	3013	-	X
20	UNL	P	3014	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32696 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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-CRE-DUCTASE COMPLEX CORE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-CRE-DUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1508	948	262	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			
6	S	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

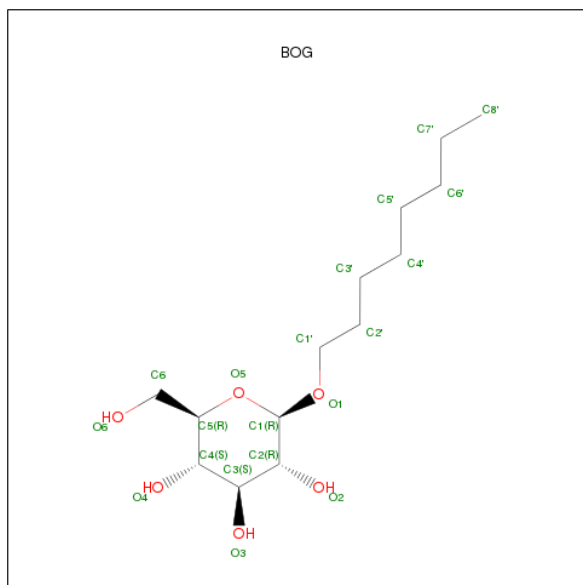
- Molecule 9 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	51	Total	C	N	O	S	0	0	2
			302	181	61	58	2			
9	V	49	Total	C	N	O	S	0	0	3
			292	176	59	55	2			

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

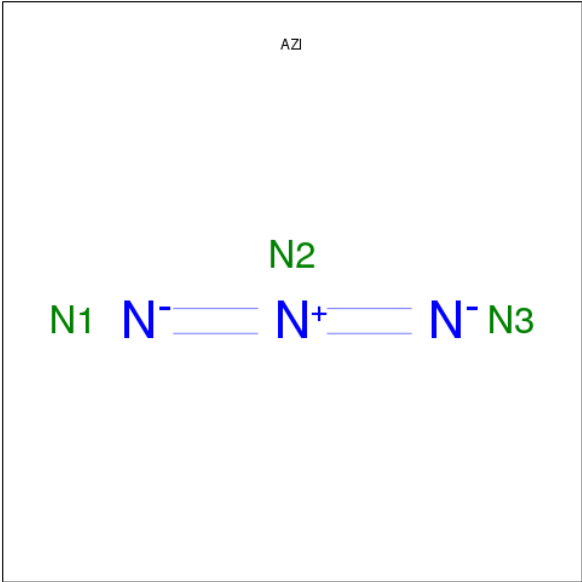
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

- Molecule 11 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



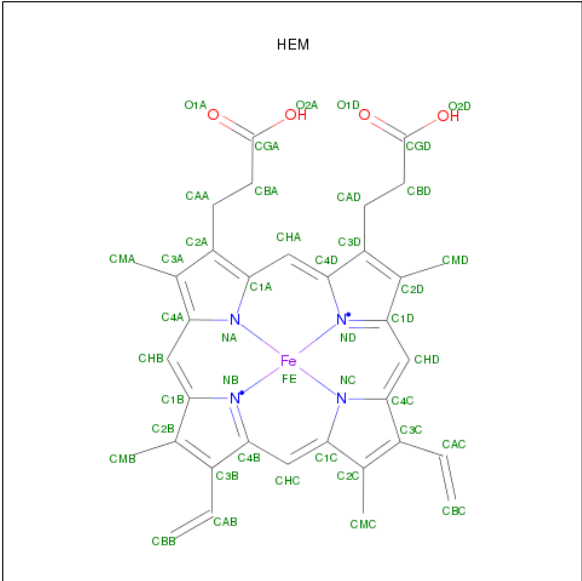
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			12	10	2		
11	D	1	Total	C	O	0	0
			20	14	6		
11	E	1	Total	C	O	0	0
			20	14	6		
11	P	1	Total	C	O	0	0
			19	13	6		
11	Q	1	Total	C	O	0	0
			20	14	6		
11	Q	1	Total	C	O	0	0
			20	14	6		

- 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

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



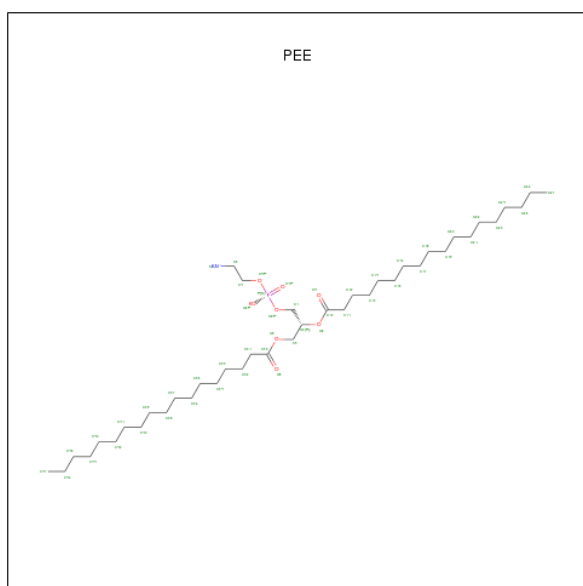
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0

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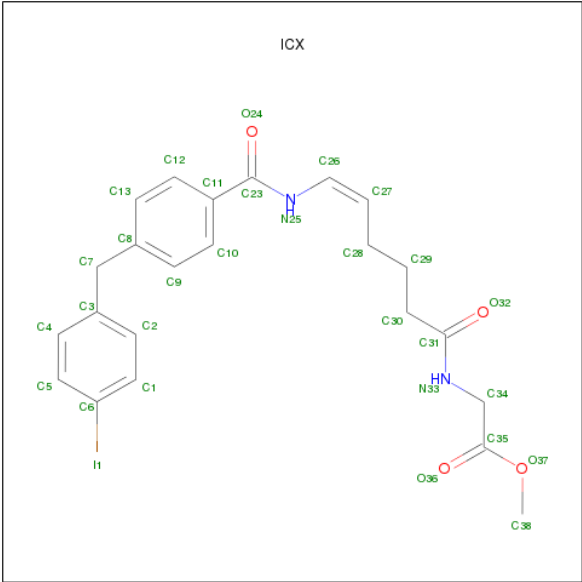
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
13	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
13	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 14 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



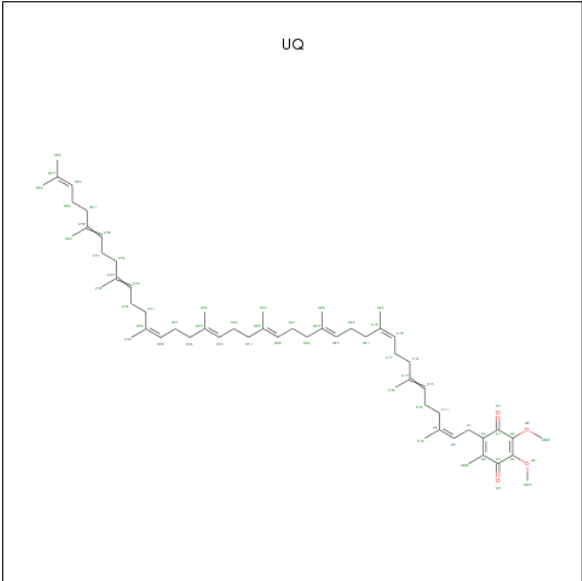
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P		
			21	12	8	1		
14	C	1	Total	C	N	O	P	
			50	40	1	8	1	
14	C	1	Total	C	N	O	P	
			49	39	1	8	1	
14	P	1	Total	C	N	O	P	
			49	39	1	8	1	
14	P	1	Total	O	P			
			5	4	1			
14	W	1	Total	C	N	O	P	
			50	40	1	8	1	

- Molecule 15 is METHYL N-[(5Z)-6-({[4-(4-IODOBENZYL)PHENYL]CARBONYL}AMINO)HEX-5-ENOYL]GLYCINATE (three-letter code: ICX) (formula: $C_{23}H_{25}IN_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	I	N	O	0	0
			30	23	1	2	4		
15	P	1	Total	C	I	N	O	0	0
			30	23	1	2	4		

- Molecule 16 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



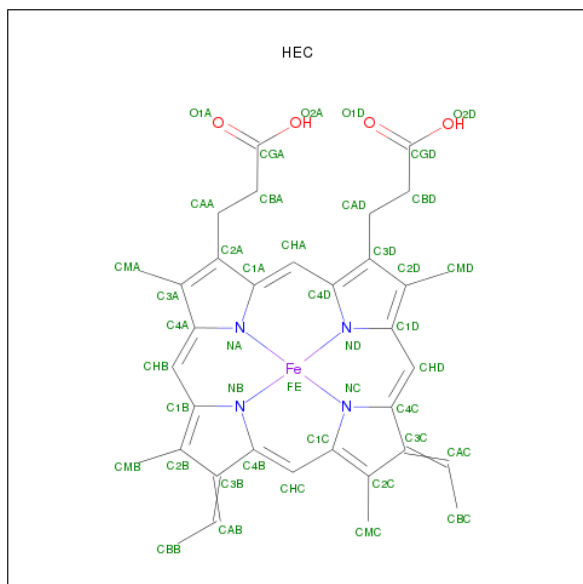
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			19	15	4		

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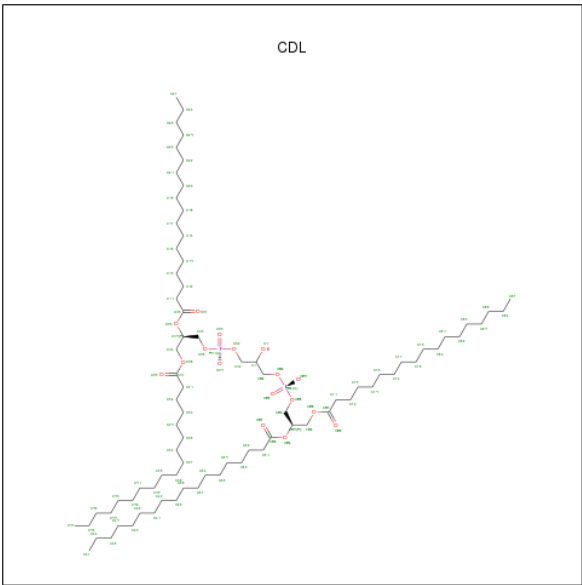
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



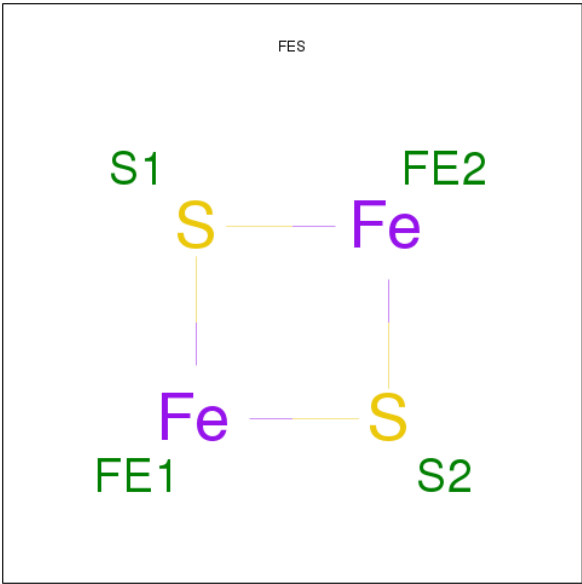
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			42	23	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		
18	P	1	Total	C	O	P	0	0
			42	23	17	2		
18	P	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 20 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	P	2	Total	O	0	0
			2	2		
20	Q	1	Total	O	0	0
			1	1		
20	E	1	Total	O	0	0
			2	2		

- Molecule 21 is water.

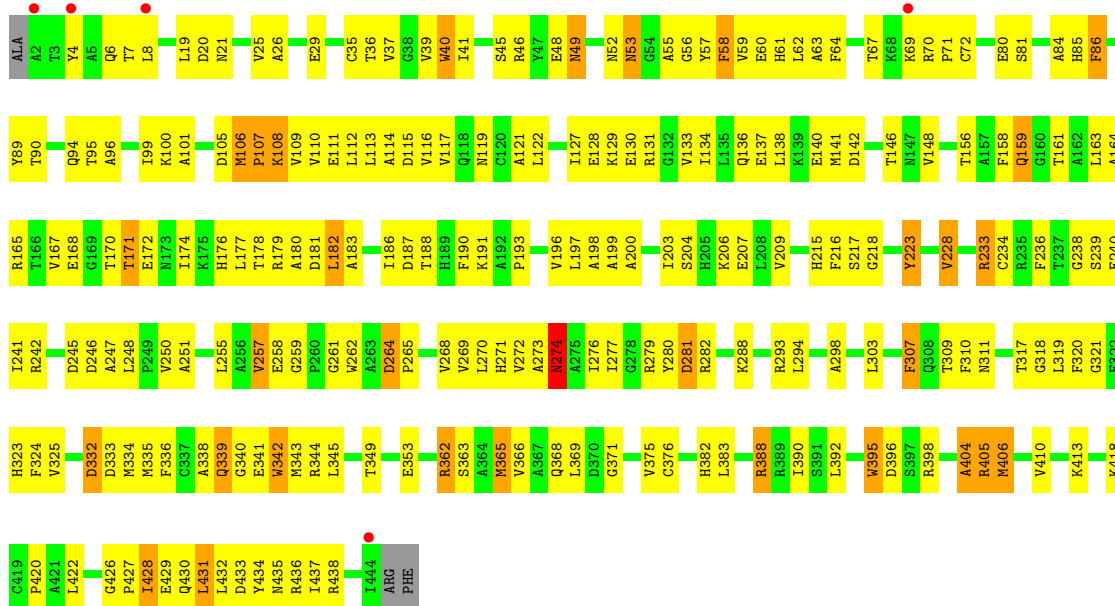
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	C	8	Total	O	0	0
			8	8		
21	P	7	Total	O	0	0
			7	7		
21	U	1	Total	O	0	0
			1	1		

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.

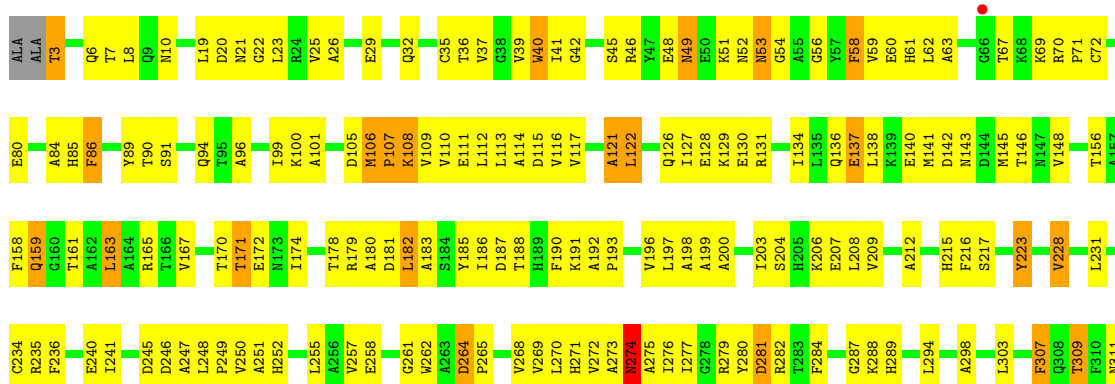
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-CREDUCTASE COMPLEX CORE PROTEIN I

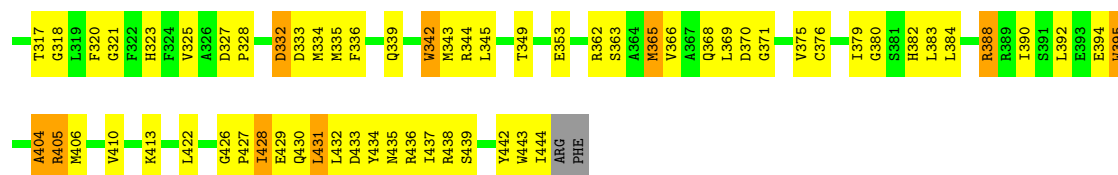
Chain A: 



• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-CREDUCTASE COMPLEX CORE PROTEIN I

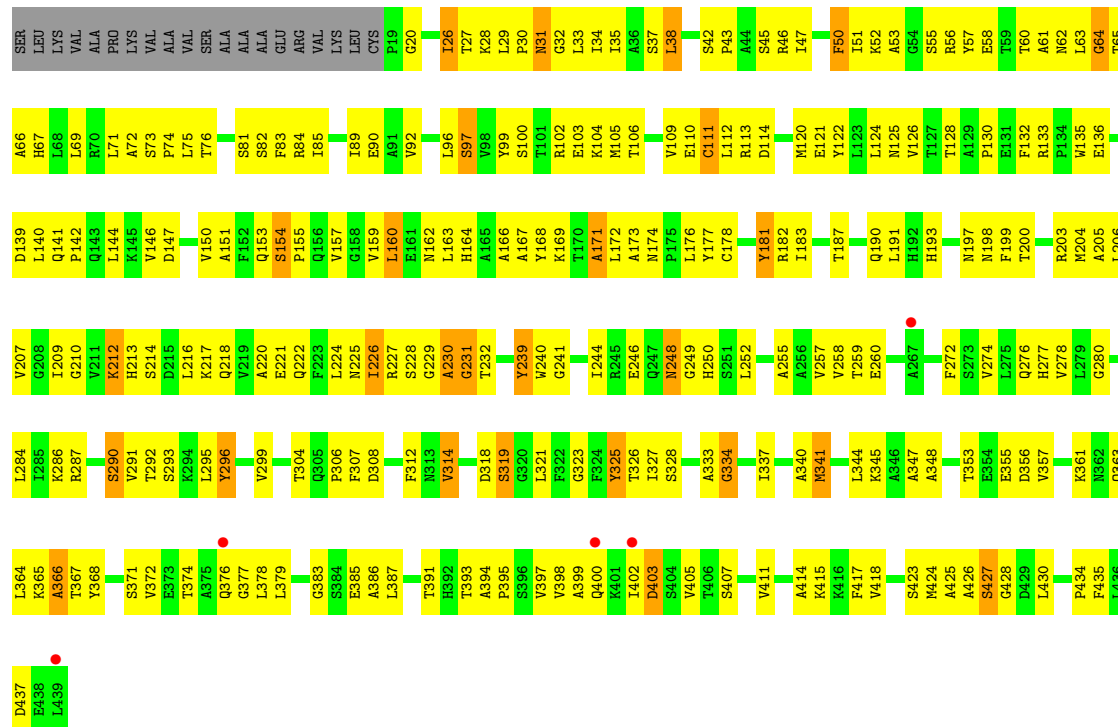
Chain N: 





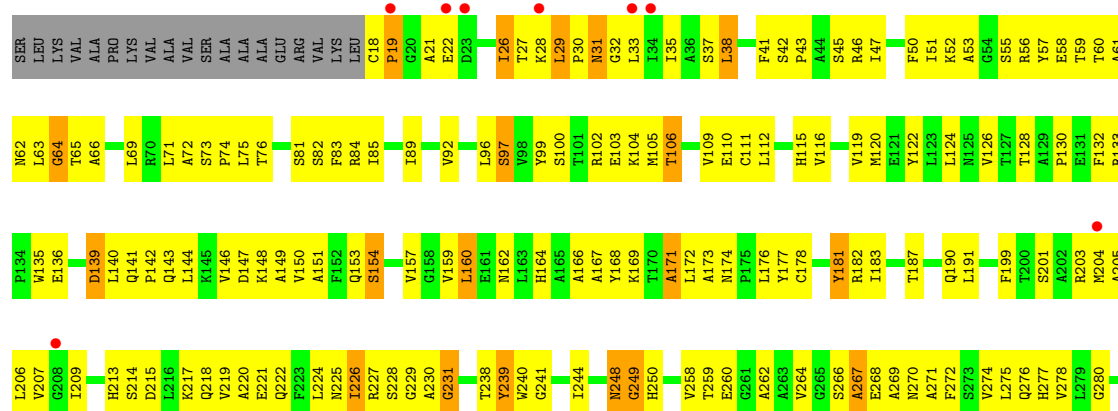
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-CREDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-CREDUCTASE COMPLEX CORE PROTEIN 2

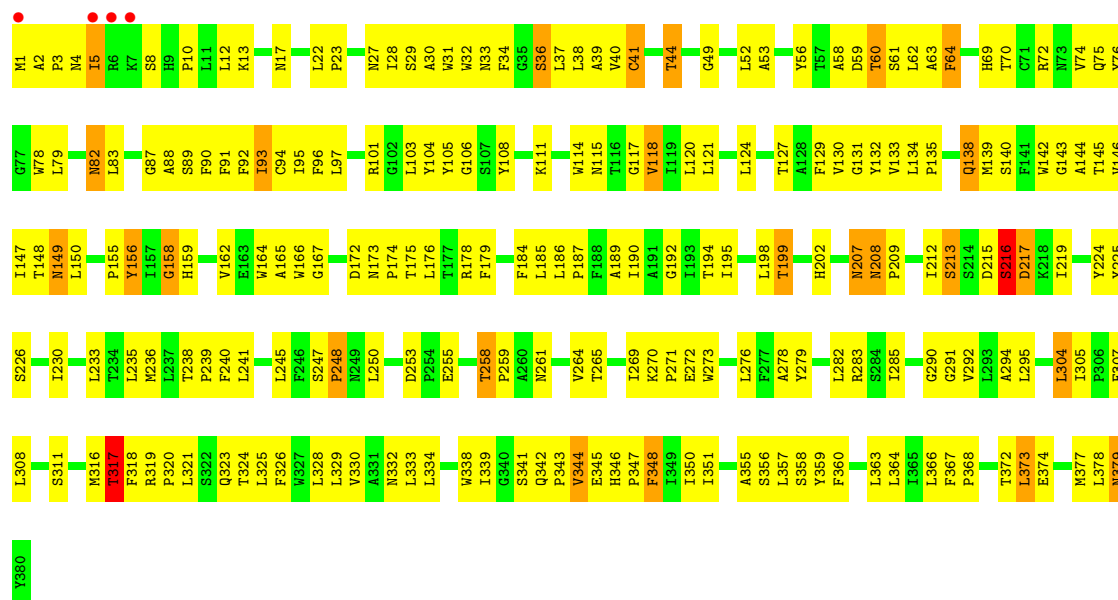
Chain O:





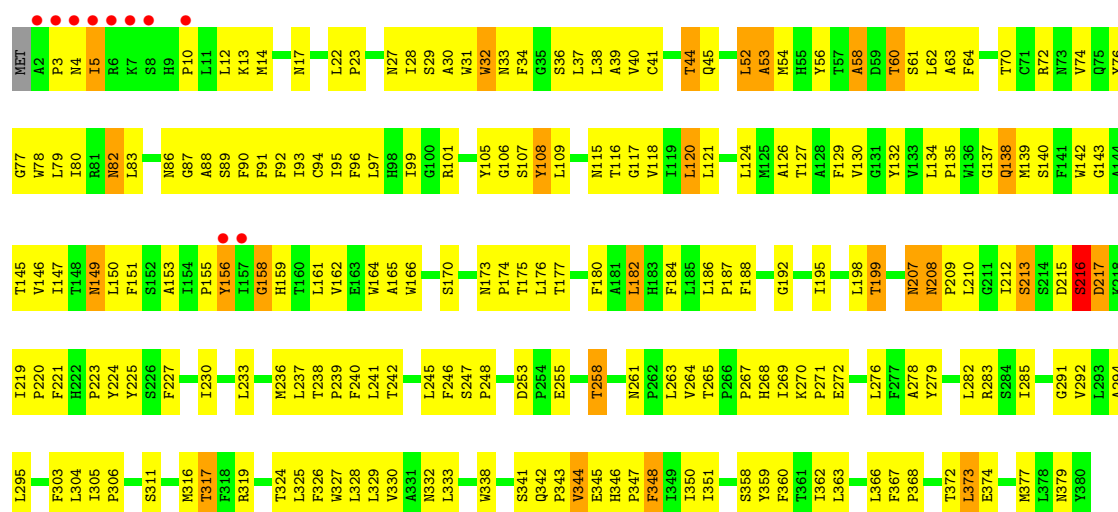
• Molecule 3: Cytochrome b

Chain C:



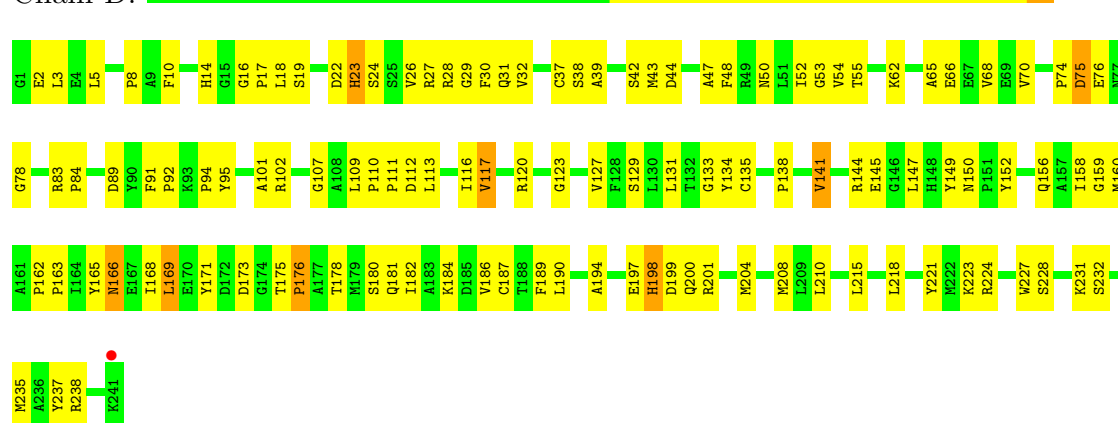
• Molecule 3: Cytochrome b

Chain P:



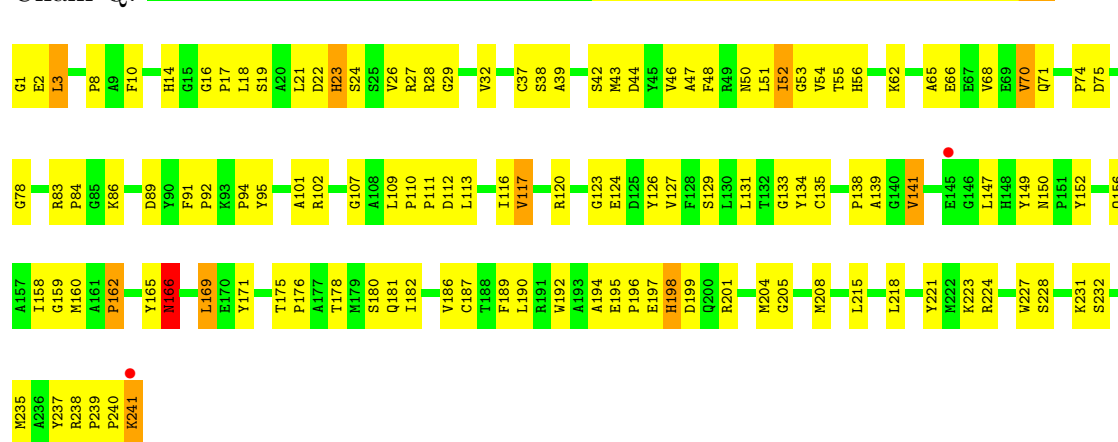
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:



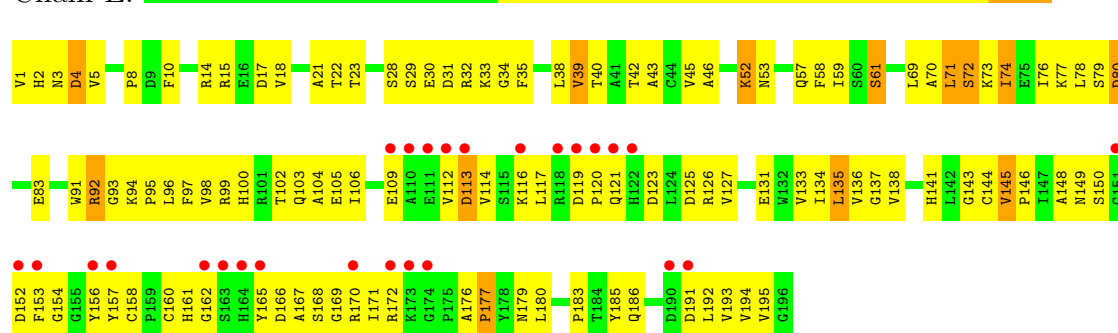
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:



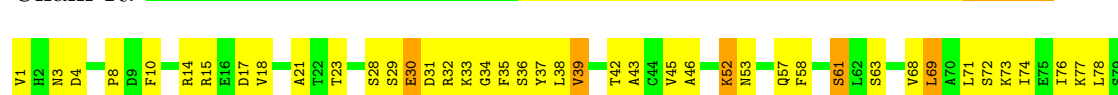
• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN

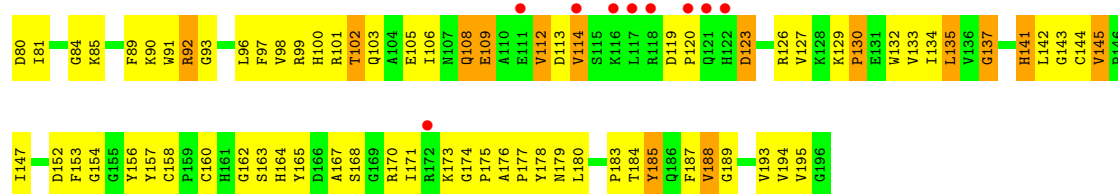
Chain E:



• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN

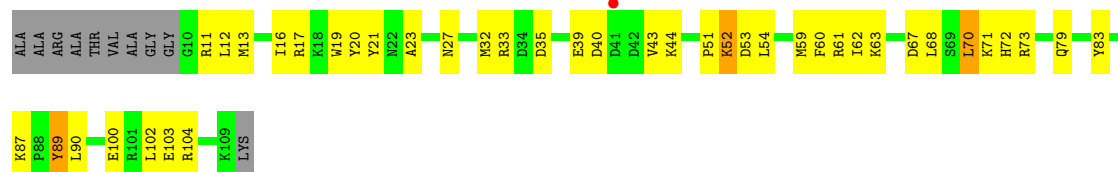
Chain R:





• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

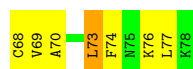
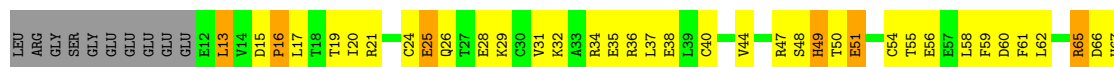
Chain F:





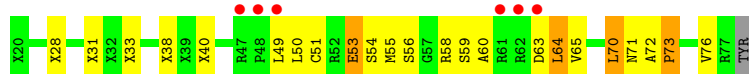
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



- Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence

Chain I:



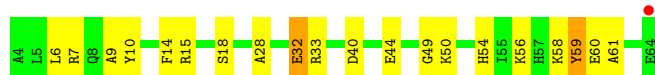
- Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence

Chain V:



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 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	174.78Å 182.66Å 242.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 3.51 44.88 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.8 (21.98-3.51) 98.9 (44.88-3.51)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.285 , 0.319 0.280 , 0.313	Depositor DCC
R_{free} test set	4918 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 24.3	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 96521 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32696	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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, CDL, UQ, ICX, FES, HEC, PEE, UNL, HEM, BOG

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	0.52	0/3511	0.72	0/4757
1	N	0.53	0/3508	0.72	0/4753
2	B	0.47	0/3196	0.66	0/4334
2	O	0.48	0/3202	0.67	0/4343
3	C	0.63	0/3122	0.76	0/4273
3	P	0.53	0/3114	0.72	0/4263
4	D	0.58	0/1956	0.72	0/2658
4	Q	0.47	0/1956	0.67	0/2658
5	E	0.42	0/1547	0.69	1/2103 (0.0%)
5	R	0.47	0/1542	0.73	1/2097 (0.0%)
6	F	0.66	0/901	0.72	0/1207
6	S	0.50	0/901	0.64	0/1207
7	G	0.58	0/698	0.70	0/946
7	T	0.49	0/680	0.65	0/923
8	H	0.53	0/582	0.67	0/779
8	U	0.37	0/561	0.68	1/751 (0.1%)
9	I	0.47	0/218	0.71	0/293
9	V	0.46	0/218	0.69	0/293
10	J	0.52	0/508	0.65	0/682
10	W	0.47	0/489	0.61	0/658
All	All	0.52	0/32410	0.70	3/43978 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	143	GLY	N-CA-C	7.12	130.89	113.10
5	E	143	GLY	N-CA-C	6.33	128.92	113.10
8	U	49	HIS	N-CA-C	-5.70	95.61	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	3440	0	3353	227	0
1	N	3437	0	3349	220	0
2	B	3141	0	3142	275	0
2	O	3147	0	3146	259	0
3	C	3020	0	3070	211	0
3	P	3012	0	3058	216	0
4	D	1898	0	1846	123	0
4	Q	1898	0	1846	135	0
5	E	1513	0	1478	128	0
5	R	1508	0	1466	131	0
6	F	881	0	887	42	0
6	S	881	0	887	48	0
7	G	676	0	659	42	0
7	T	658	0	647	48	0
8	H	574	0	548	37	0
8	U	553	0	535	40	0
9	I	302	0	251	36	0
9	V	292	0	251	29	0
10	J	497	0	490	19	0
10	W	478	0	478	29	0
11	C	12	0	18	0	0
11	D	20	0	28	5	0
11	E	20	0	28	1	0
11	P	19	0	24	1	0
11	Q	40	0	56	0	0
12	C	3	0	0	0	0
12	P	3	0	0	0	0
13	C	86	0	60	19	0
13	P	86	0	60	19	0
14	A	21	0	13	0	0
14	C	99	0	149	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	54	0	72	2	0
14	W	50	0	77	1	0
15	C	30	0	25	2	0
15	P	30	0	25	2	0
16	C	19	0	17	5	0
16	P	19	0	17	6	0
17	D	43	0	30	3	0
17	Q	43	0	30	3	0
18	D	42	0	28	3	0
18	G	40	0	24	1	0
18	P	82	0	52	5	0
19	E	4	0	0	1	0
19	R	4	0	0	0	0
20	E	2	0	0	0	0
20	P	2	0	0	0	0
20	Q	1	0	0	0	0
21	C	8	0	0	2	0
21	P	7	0	0	2	0
21	U	1	0	0	0	0
All	All	32696	0	32220	2098	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 32.

The worst 5 of 2098 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:17:ASN:HD21	7:G:1:GLY:HA3	1.15	1.08
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.37	1.04
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.42	1.01
5:E:73:LYS:O	5:E:74:ILE:HG13	1.60	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	1.00

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%)	345 (78%)	75 (17%)	21 (5%)	4	38
1	N	440/446 (99%)	344 (78%)	75 (17%)	21 (5%)	4	38
2	B	419/441 (95%)	342 (82%)	62 (15%)	15 (4%)	5	49
2	O	420/441 (95%)	333 (79%)	67 (16%)	20 (5%)	4	38
3	C	378/380 (100%)	300 (79%)	62 (16%)	16 (4%)	4	43
3	P	377/380 (99%)	302 (80%)	60 (16%)	15 (4%)	5	45
4	D	239/241 (99%)	195 (82%)	35 (15%)	9 (4%)	5	46
4	Q	239/241 (99%)	190 (80%)	36 (15%)	13 (5%)	3	35
5	E	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	2	28
5	R	194/196 (99%)	146 (75%)	31 (16%)	17 (9%)	1	19
6	F	98/110 (89%)	73 (74%)	22 (22%)	3 (3%)	7	53
6	S	98/110 (89%)	74 (76%)	22 (22%)	2 (2%)	11	63
7	G	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	3	36
7	T	77/81 (95%)	61 (79%)	11 (14%)	5 (6%)	2	29
8	H	68/77 (88%)	49 (72%)	16 (24%)	3 (4%)	4	42
8	U	65/77 (84%)	42 (65%)	17 (26%)	6 (9%)	1	18
9	I	29/52 (56%)	14 (48%)	10 (34%)	5 (17%)	0	4
9	V	29/52 (56%)	18 (62%)	8 (28%)	3 (10%)	1	14
10	J	59/61 (97%)	42 (71%)	15 (25%)	2 (3%)	6	50
10	W	57/61 (93%)	42 (74%)	9 (16%)	6 (10%)	1	14
All	All	4000/4170 (96%)	3120 (78%)	681 (17%)	199 (5%)	3	37

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	159	GLN
2	B	26	ILE
2	B	38	LEU
2	B	171	ALA

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	365/368 (99%)	338 (93%)	27 (7%)	20	66
1	N	365/368 (99%)	336 (92%)	29 (8%)	18	62
2	B	332/347 (96%)	313 (94%)	19 (6%)	29	76
2	O	333/347 (96%)	314 (94%)	19 (6%)	29	76
3	C	329/329 (100%)	306 (93%)	23 (7%)	21	68
3	P	328/329 (100%)	307 (94%)	21 (6%)	25	72
4	D	200/200 (100%)	190 (95%)	10 (5%)	34	80
4	Q	200/200 (100%)	190 (95%)	10 (5%)	34	80
5	E	166/166 (100%)	156 (94%)	10 (6%)	27	74
5	R	165/166 (99%)	153 (93%)	12 (7%)	20	66
6	F	92/96 (96%)	89 (97%)	3 (3%)	50	89
6	S	92/96 (96%)	89 (97%)	3 (3%)	50	89
7	G	71/71 (100%)	64 (90%)	7 (10%)	11	49
7	T	69/71 (97%)	63 (91%)	6 (9%)	15	57
8	H	65/71 (92%)	62 (95%)	3 (5%)	37	82
8	U	63/71 (89%)	59 (94%)	4 (6%)	25	73
9	I	23/26 (88%)	22 (96%)	1 (4%)	40	84
9	V	23/26 (88%)	22 (96%)	1 (4%)	40	84
10	J	49/49 (100%)	47 (96%)	2 (4%)	41	84
10	W	47/49 (96%)	45 (96%)	2 (4%)	40	84
All	All	3377/3446 (98%)	3165 (94%)	212 (6%)	25	73

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	27	PRO
1	N	223	TYR
5	R	185	TYR
7	G	63	THR
1	N	40	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	71	ASN
1	N	274	ASN
6	S	79	GLN
1	N	10	ASN
1	N	118	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 34 ligands modelled in this entry, 4 are unknown - leaving 30 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	$\# Z > 2$
14	PEE	A	2008	-	20,20,50	1.97	7 (35%)	23,25,55	1.14	3 (13%)
15	ICX	C	2001	-	31,31,31	1.29	4 (12%)	39,39,39	0.99	2 (5%)
16	UQ	C	2002	-	19,19,63	2.26	9 (47%)	25,26,79	1.22	2 (8%)
14	PEE	C	2005	-	49,49,50	1.41	10 (20%)	54,54,55	1.07	7 (12%)
14	PEE	C	2007	-	48,48,50	1.39	8 (16%)	53,53,55	1.06	7 (13%)
12	AZI	C	2011	-	2,2,2	1.01	0	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BOG	C	3010	-	10,11,20	1.42	1 (10%)	9,11,25	45.58	2 (22%)
13	HEM	C	501	3	42,50,50	3.77	10 (23%)	27,82,82	2.44	9 (33%)
13	HEM	C	502	3	42,50,50	3.76	13 (30%)	27,82,82	2.09	6 (22%)
18	CDL	D	2003	-	40,41,99	1.23	2 (5%)	50,53,111	1.38	5 (10%)
11	BOG	D	2091	-	20,20,20	1.09	2 (10%)	25,25,25	0.94	1 (4%)
17	HEC	D	501	4	50,50,50	3.43	11 (22%)	56,82,82	3.01	19 (33%)
11	BOG	E	2009	-	20,20,20	1.12	2 (10%)	25,25,25	0.93	2 (8%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
18	CDL	G	2004	-	38,39,99	1.62	5 (13%)	47,51,111	1.49	6 (12%)
11	BOG	P	2010	-	18,18,20	2.40	4 (22%)	21,22,25	0.55	0
15	ICX	P	3001	-	31,31,31	1.36	6 (19%)	39,39,39	0.89	1 (2%)
16	UQ	P	3002	-	19,19,63	2.34	11 (57%)	25,26,79	1.24	3 (12%)
18	CDL	P	3003	-	40,41,99	1.20	2 (5%)	50,53,111	1.41	5 (10%)
18	CDL	P	3004	-	38,39,99	1.45	5 (13%)	47,51,111	1.46	4 (8%)
14	PEE	P	3007	-	48,48,50	1.30	7 (14%)	53,53,55	1.01	6 (11%)
14	PEE	P	3008	-	4,4,50	2.02	3 (75%)	6,6,55	0.73	0
12	AZI	P	3011	-	2,2,2	0.97	0	0,1,1	0.00	-
13	HEM	P	501	3	42,50,50	3.75	13 (30%)	27,82,82	2.31	7 (25%)
13	HEM	P	502	3	42,50,50	2.84	11 (26%)	27,82,82	1.70	6 (22%)
11	BOG	Q	3009	-	20,20,20	1.17	3 (15%)	25,25,25	1.11	1 (4%)
11	BOG	Q	3091	-	20,20,20	1.12	2 (10%)	25,25,25	0.93	1 (4%)
17	HEC	Q	501	4	50,50,50	3.38	11 (22%)	56,82,82	2.79	18 (32%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
14	PEE	W	3005	-	49,49,50	1.50	11 (22%)	54,54,55	1.06	7 (12%)

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
14	PEE	A	2008	-	-	0/24/24/54	0/0/0/0
15	ICX	C	2001	-	-	0/23/24/24	0/2/2/2
16	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
14	PEE	C	2005	-	-	0/53/53/54	0/0/0/0
14	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
12	AZI	C	2011	-	-	0/0/0/0	0/0/0/0
11	BOG	C	3010	-	-	0/9/9/31	0/0/0/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEM	C	501	3	-	0/14/114/114	0/0/8/8
13	HEM	C	502	3	-	0/14/114/114	0/0/8/8
18	CDL	D	2003	-	1/1/9/9	0/51/51/110	0/0/0/0
11	BOG	D	2091	-	-	0/11/31/31	0/1/1/1
17	HEC	D	501	4	-	0/10/54/54	0/0/8/8
11	BOG	E	2009	-	-	0/11/31/31	0/1/1/1
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
18	CDL	G	2004	-	1/1/9/9	0/49/49/110	0/0/0/0
11	BOG	P	2010	-	-	0/6/26/31	0/1/1/1
15	ICX	P	3001	-	-	0/23/24/24	0/2/2/2
16	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
18	CDL	P	3003	-	1/1/9/9	0/51/51/110	0/0/0/0
18	CDL	P	3004	-	1/1/9/9	0/49/49/110	0/0/0/0
14	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
14	PEE	P	3008	-	-	0/0/0/54	0/0/0/0
12	AZI	P	3011	-	-	0/0/0/0	0/0/0/0
13	HEM	P	501	3	-	0/14/114/114	0/0/8/8
13	HEM	P	502	3	-	0/14/114/114	0/0/8/8
11	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
11	BOG	Q	3091	-	-	0/11/31/31	0/1/1/1
17	HEC	Q	501	4	-	0/10/54/54	0/0/8/8
19	FES	R	501	5	-	0/0/4/4	0/1/1/1
14	PEE	W	3005	-	-	0/53/53/54	0/0/0/0

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	C3C-C2C	-17.53	1.31	1.45
13	P	501	HEM	C3B-C2B	-14.57	1.31	1.45
17	D	501	HEC	C3C-CAC	14.54	1.54	1.34
13	C	501	HEM	C3C-C2C	-14.12	1.34	1.45
17	Q	501	HEC	C3C-CAC	13.51	1.53	1.34

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	3010	BOG	O5-C1-O1	-136.68	107.22	123.66
17	D	501	HEC	CBC-CAC-C3C	-13.79	97.23	127.36
17	Q	501	HEC	CBC-CAC-C3C	-13.05	98.84	127.36
17	D	501	HEC	CBB-CAB-C3B	-7.70	110.52	127.36
13	P	501	HEM	CBA-CAA-C2A	-7.27	100.53	112.63

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	D	2003	CDL	CA4
18	G	2004	CDL	CA4
18	P	3004	CDL	CA4
18	P	3003	CDL	CA4

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	443/446 (99%)	-0.02	5 (1%) 77 45	36, 89, 137, 150	0
1	N	442/446 (99%)	-0.05	1 (0%) 93 80	54, 91, 136, 153	0
2	B	421/441 (95%)	0.12	5 (1%) 75 43	60, 113, 170, 193	0
2	O	422/441 (95%)	0.11	10 (2%) 56 27	51, 100, 146, 172	0
3	C	380/380 (100%)	-0.25	4 (1%) 77 45	19, 50, 104, 192	0
3	P	379/380 (99%)	-0.06	10 (2%) 53 25	29, 89, 132, 186	0
4	D	241/241 (100%)	-0.23	1 (0%) 90 71	30, 58, 109, 133	0
4	Q	241/241 (100%)	-0.07	2 (0%) 83 53	65, 105, 150, 165	0
5	E	196/196 (100%)	0.64	26 (13%) 4 3	45, 137, 184, 198	127 (64%)
5	R	196/196 (100%)	0.20	9 (4%) 31 14	53, 101, 166, 184	0
6	F	100/110 (90%)	-0.30	1 (1%) 79 48	31, 61, 87, 102	0
6	S	100/110 (90%)	0.13	1 (1%) 79 48	77, 117, 167, 188	0
7	G	81/81 (100%)	-0.14	0 100 100	43, 77, 129, 156	0
7	T	79/81 (97%)	0.24	4 (5%) 27 12	71, 137, 202, 211	0
8	H	70/77 (90%)	-0.20	0 100 100	51, 94, 117, 153	0
8	U	67/77 (87%)	-0.06	0 100 100	141, 175, 213, 219	0
9	I	31/52 (59%)	0.99	6 (19%) 2 2	109, 158, 223, 229	0
9	V	31/52 (59%)	1.04	6 (19%) 2 2	109, 157, 222, 224	0
10	J	61/61 (100%)	-0.24	1 (1%) 68 36	65, 82, 144, 187	0
10	W	59/61 (96%)	0.09	0 100 100	75, 107, 139, 154	0
All	All	4040/4170 (96%)	0.02	92 (2%) 57 28	19, 93, 168, 229	127 (3%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	2	ALA	7.1
5	E	111	GLU	6.8
5	E	173	LYS	5.9
3	P	8	SER	5.6
7	T	1	GLY	5.5

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. 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
14	PEE	P	3008	5/51	0.87	35.36	213,213,214,214	0
11	BOG	Q	3091	20/20	0.90	10.34	242,249,250,251	0
11	BOG	C	3010	12/20	0.39	7.06	168,168,170,170	0
20	UNL	P	3013	1/-	0.45	6.43	40,40,40,40	0
14	PEE	W	3005	50/51	0.51	6.06	129,146,150,152	0
16	UQ	C	2002	19/63	0.32	5.59	123,126,128,129	0
14	PEE	C	2007	49/51	0.39	5.07	63,76,100,101	0
14	PEE	A	2008	21/51	0.49	4.15	225,229,230,230	0
20	UNL	P	3014	1/-	0.29	3.70	33,33,33,33	0
18	CDL	D	2003	42/100	0.40	3.30	144,158,180,181	0
14	PEE	C	2005	50/51	0.36	3.18	122,134,139,141	0
16	UQ	P	3002	19/63	0.31	3.03	163,166,168,168	0
18	CDL	P	3003	42/100	0.46	2.79	203,214,224,225	0
12	AZI	P	3011	3/3	0.47	2.25	54,54,55,56	0
11	BOG	D	2091	20/20	0.39	2.18	178,180,180,180	0
12	AZI	C	2011	3/3	0.33	2.11	46,46,47,49	0
14	PEE	P	3007	49/51	0.45	1.89	107,122,143,144	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CDL	G	2004	40/100	0.25	1.88	92,97,116,117	0
20	UNL	E	2012	2/-	0.22	1.85	36,36,36,38	0
11	BOG	P	2010	19/20	0.42	1.60	102,248,249,249	0
15	ICX	P	3001	30/30	0.30	1.32	101,117,133,136	0
18	CDL	P	3004	40/100	0.38	1.15	164,168,173,174	0
11	BOG	Q	3009	20/20	0.23	0.53	87,110,112,112	0
13	HEM	P	501	43/43	0.21	0.18	53,59,72,77	0
17	HEC	D	501	43/43	0.17	0.13	25,36,45,53	0
11	BOG	E	2009	20/20	0.16	0.11	71,73,77,77	0
13	HEM	C	501	43/43	0.18	-0.10	30,35,50,57	0
13	HEM	C	502	43/43	0.15	-0.43	25,30,40,43	0
17	HEC	Q	501	43/43	0.19	-0.46	76,84,88,90	0
13	HEM	P	502	43/43	0.18	-0.53	58,62,69,70	0
19	FES	E	501	4/4	0.10	-0.77	105,105,107,107	4
15	ICX	C	2001	30/30	0.15	-1.00	43,56,65,66	0
19	FES	R	501	4/4	0.13	-1.27	60,61,62,63	0
20	UNL	Q	3012	1/-	0.14	-1.35	8,8,8,8	0

6.5 Other polymers ⓘ

There are no such residues in this entry.