



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:02 AM GMT

PDB ID : 3S8F
Title : 1.8 Å structure of ba3 cytochrome c oxidase from *Thermus thermophilus* in lipid environment
Authors : Tiefenbrunn, T.; Liu, W.; Chen, Y.; Katritch, V.; Stout, C.D.; Fee, J.A.; Cherezov, V.
Deposited on : 2011-05-27
Resolution : 1.80 Å(reported)

This is a full wwPDB validation 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>

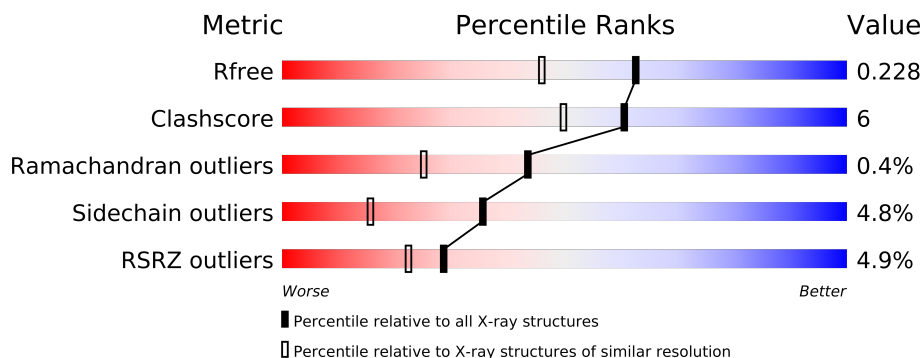
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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	569	
2	B	168	
3	C	34	

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

Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	564	-	X
8	OLC	A	565	-	X
8	OLC	A	566	-	X
8	OLC	A	567	-	X
8	OLC	A	568	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	570	-	X
8	OLC	A	571	-	X
8	OLC	A	572	-	X
8	OLC	A	573	-	X
8	OLC	A	574	-	X
8	OLC	B	169	-	X
8	OLC	B	170	-	X
8	OLC	B	171	-	X
8	OLC	B	172	-	X
8	OLC	C	35	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6567 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	5	0
			4389	2979	699	695	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-5	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1288	837	214	233	4			

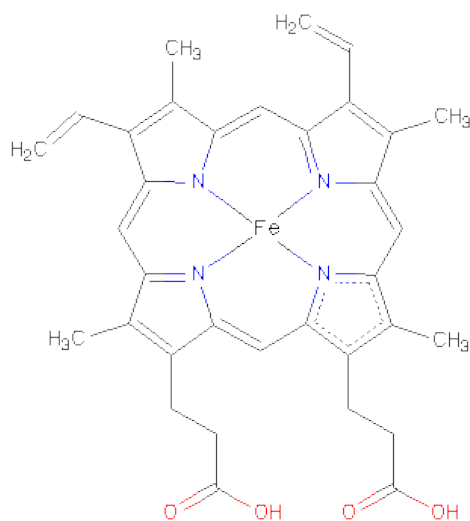
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

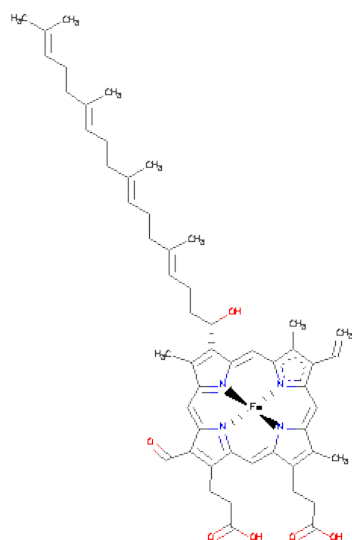
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



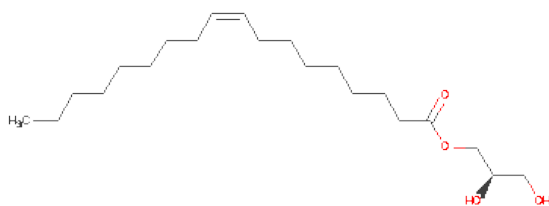
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
6	A	1	65	54	1	4	6	0	0

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

- Molecule 8 is (2R)-2,3-DIHYDROXYPROPYL(9Z)-OCTADEC-9-ENOATE (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			17	13	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			15	11	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			21	19	2		
8	C	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cu 2 2	0	0

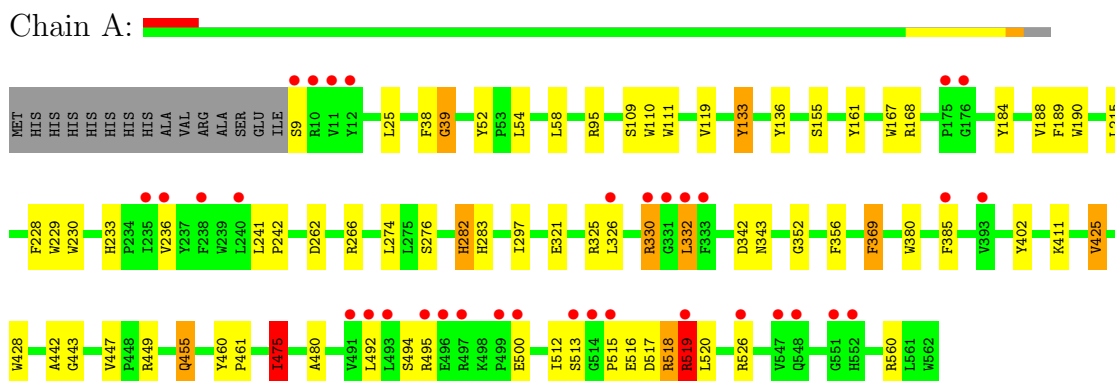
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	117	Total O 117 117	0	0
10	B	71	Total O 71 71	0	0
10	C	5	Total O 5 5	0	0

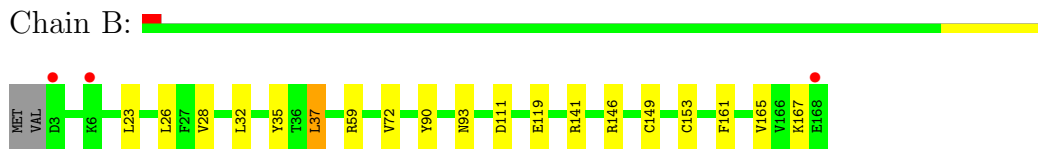
3 Residue-property plots

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: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.59Å 97.82Å 94.95Å 90.00° 128.30° 90.00°	Depositor
Resolution (Å)	37.26 – 1.80 37.26 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.26-1.80) 97.2 (37.26-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.215 0.198 , 0.228	Depositor DCC
R_{free} test set	4656 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 92450 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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: OLC, PER, CUA, HEM, HAS, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.42	29/4562 (0.6%)	1.09	14/6263 (0.2%)
2	B	1.48	8/1330 (0.6%)	1.11	5/1817 (0.3%)
3	C	1.50	4/247 (1.6%)	1.25	3/335 (0.9%)
All	All	1.44	41/6139 (0.7%)	1.11	22/8415 (0.3%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PHE	CE2-CZ	8.17	1.52	1.37
1	A	133	TYR	CD1-CE1	7.43	1.50	1.39
2	B	161	PHE	CE2-CZ	7.36	1.51	1.37
1	A	449	ARG	CZ-NH1	7.29	1.42	1.33
2	B	119	GLU	CB-CG	-7.24	1.38	1.52
1	A	38	PHE	CD2-CE2	6.99	1.53	1.39
1	A	229	TRP	CE3-CZ3	6.59	1.49	1.38
2	B	165	VAL	CB-CG2	6.40	1.66	1.52
1	A	119	VAL	CB-CG2	6.32	1.66	1.52
1	A	480	ALA	CA-CB	6.15	1.65	1.52
2	B	153	CYS	CB-SG	6.12	1.92	1.82
3	C	11	VAL	CB-CG1	6.06	1.65	1.52
2	B	111	ASP	CB-CG	6.05	1.64	1.51
1	A	442	ALA	CA-CB	5.91	1.64	1.52
1	A	136	TYR	CE2-CZ	5.90	1.46	1.38
1	A	39	GLY	N-CA	5.84	1.54	1.46
1	A	352	GLY	CA-C	5.80	1.61	1.51
3	C	8	ALA	CA-CB	-5.74	1.40	1.52
1	A	447	VAL	CB-CG2	5.68	1.64	1.52
1	A	188	VAL	CB-CG1	5.55	1.64	1.52
1	A	52	TYR	CD2-CE2	5.54	1.47	1.39
1	A	110	TRP	CB-CG	5.53	1.60	1.50
1	A	236	VAL	CB-CG2	5.49	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	TRP	CE3-CZ3	5.49	1.47	1.38
1	A	356	PHE	CE1-CZ	5.47	1.47	1.37
3	C	22	PHE	CE1-CZ	5.43	1.47	1.37
1	A	111	TRP	CB-CG	-5.37	1.40	1.50
1	A	461	PRO	N-CA	5.32	1.56	1.47
1	A	228	PHE	CD1-CE1	5.29	1.49	1.39
1	A	460	TYR	CG-CD1	5.28	1.46	1.39
1	A	228	PHE	CE2-CZ	5.25	1.47	1.37
1	A	428	TRP	CG-CD1	5.20	1.44	1.36
2	B	28	VAL	CB-CG2	5.19	1.63	1.52
1	A	276	SER	CB-OG	5.13	1.49	1.42
1	A	380	TRP	CZ3-CH2	5.12	1.48	1.40
1	A	184	TYR	CD1-CE1	5.12	1.47	1.39
1	A	443	GLY	N-CA	5.11	1.53	1.46
2	B	72	VAL	CB-CG1	5.07	1.63	1.52
3	C	21	VAL	CB-CG2	5.05	1.63	1.52
2	B	90	TYR	CD1-CE1	-5.02	1.31	1.39
1	A	385	PHE	CE1-CZ	5.02	1.46	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	ARG	NE-CZ-NH1	-9.75	115.42	120.30
1	A	266	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	266	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	95	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	A	425	VAL	CG1-CB-CG2	7.75	123.30	110.90
1	A	25	LEU	CB-CG-CD1	-7.46	98.31	111.00
2	B	37	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	95	ARG	NE-CZ-NH1	-6.92	116.84	120.30
2	B	146	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	B	23	LEU	CB-CG-CD2	-6.56	99.85	111.00
2	B	149	CYS	CA-CB-SG	-6.40	102.48	114.00
3	C	24	LEU	CB-CG-CD1	6.33	121.75	111.00
3	C	33	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	425	VAL	CA-CB-CG1	6.05	119.98	110.90
3	C	13	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	233	HIS	N-CA-CB	5.78	121.00	110.60
1	A	54	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	332	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	475	ILE	CG1-CB-CG2	5.50	123.49	111.40
1	A	342	ASP	CB-CG-OD1	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	TYR	CA-CB-CG	-5.21	103.51	113.40
1	A	297	ILE	CG1-CB-CG2	-5.20	99.97	111.40

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	4389	0	0	20	0
2	B	1288	0	0	5	0
3	C	241	0	0	0	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
6	A	65	0	62	2	0
7	A	2	0	0	1	0
8	A	222	0	320	16	0
8	B	96	0	153	7	0
8	C	25	0	40	0	0
9	B	2	0	0	0	0
10	A	117	0	0	4	0
10	B	71	0	0	1	1
10	C	5	0	0	0	0
All	All	6567	0	605	41	1

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 6.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:563:PER:O1	7:A:563:PER:O2	1.54	1.23
1:A:330[B]:ARG:CG	1:A:330[B]:ARG:NH1	2.20	1.05
2:B:141:ARG:NH1	8:B:170:OLC:H24A	1.82	0.94
8:A:565:OLC:H12	8:A:572:OLC:H14A	1.48	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:516[A]:GLU:CG	1:A:517:ASP:N	2.41	0.80
2:B:35:TYR:OH	8:B:169:OLC:H24A	1.84	0.76
2:B:93:ASN:O	10:B:201:HOH:O	2.06	0.74
8:A:565:OLC:C12	8:A:572:OLC:H14A	2.22	0.65
8:A:569:OLC:O19	8:A:570:OLC:C8	2.48	0.62
1:A:518:ARG:O	1:A:519:ARG:CB	2.49	0.61
2:B:141:ARG:NH1	8:B:170:OLC:C24	2.62	0.60
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.88	0.60
8:A:564:OLC:O25	8:B:170:OLC:H7A	2.03	0.58
6:A:801:HAS:HMC1	6:A:801:HAS:HBC1	1.87	0.57
8:A:572:OLC:H13A	8:A:572:OLC:C8	2.36	0.56
1:A:161:TYR:CE2	8:A:569:OLC:H21	2.42	0.55
1:A:526:ARG:NH2	10:A:658:HOH:O	2.42	0.52
1:A:475:ILE:CG1	8:A:565:OLC:H13A	2.41	0.50
1:A:516[B]:GLU:OE1	1:A:517:ASP:N	2.44	0.50
10:A:583:HOH:O	8:B:170:OLC:H4A	2.10	0.50
1:A:241:LEU:N	1:A:242:PRO:CD	2.75	0.50
1:A:168:ARG:NH2	8:A:570:OLC:C6	2.76	0.49
1:A:560:ARG:NH1	10:A:579:HOH:O	2.45	0.49
1:A:39:GLY:C	5:A:800:HEM:HMB3	2.33	0.48
1:A:168:ARG:NH2	8:A:570:OLC:H6A	2.28	0.47
1:A:411:LYS:NZ	1:A:492:LEU:O	2.47	0.47
2:B:32:LEU:CD2	8:B:169:OLC:H7A	2.45	0.47
8:A:566:OLC:H13A	8:A:572:OLC:H12	1.97	0.46
8:A:572:OLC:H13A	8:A:572:OLC:H8A	1.97	0.46
1:A:455:GLN:NE2	10:A:580:HOH:O	2.50	0.45
1:A:167:TRP:CH2	8:A:570:OLC:H22	2.51	0.45
8:B:172:OLC:H11A	8:B:172:OLC:H14A	1.90	0.44
1:A:168:ARG:NH2	8:A:570:OLC:H3A	2.34	0.43
1:A:321:GLU:OE1	1:A:325:ARG:NH1	2.52	0.42
8:A:571:OLC:O19	8:A:572:OLC:O23	2.38	0.41
6:A:801:HAS:HAA2	6:A:801:HAS:HHA	1.81	0.41
5:A:800:HEM:HBC2	5:A:800:HEM:CMC	2.51	0.41
1:A:343:ASN:OD1	1:A:402[B]:TYR:CE2	2.74	0.41
8:A:566:OLC:H15	8:A:571:OLC:H12	2.01	0.40
1:A:109:SER:O	1:A:155:SER:OG	2.39	0.40
8:A:574:OLC:H10	8:A:574:OLC:H13	1.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:B:175:HOH:O	10:B:201:HOH:O[2_556]	2.08	0.12

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	556/569 (98%)	536 (96%)	17 (3%)	3 (0%)	38	19
2	B	165/168 (98%)	162 (98%)	3 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	750/771 (97%)	727 (97%)	20 (3%)	3 (0%)	43	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	PRO
1	A	519	ARG
1	A	369	PHE

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	450/463 (97%)	426 (95%)	24 (5%)	32	13
2	B	134/138 (97%)	131 (98%)	3 (2%)	64	48
3	C	24/27 (89%)	21 (88%)	3 (12%)	7	1
All	All	608/628 (97%)	578 (95%)	30 (5%)	35	15

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	282	HIS
1	A	326	LEU
1	A	330[A]	ARG
1	A	330[B]	ARG
1	A	332	LEU
1	A	369	PHE
1	A	425	VAL
1	A	455	GLN
1	A	475	ILE
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	512	ILE
1	A	513	SER
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
2	B	26	LEU
2	B	37	LEU
2	B	167	LYS
3	C	17	LEU
3	C	20	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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$
7	PER	A	563	4,6	1,1,1	1.76	0	0,0,0	0.00	-
8	OLC	A	564	-	24,24,24	0.51	0	25,25,25	0.78	0
8	OLC	A	565	-	24,24,24	0.45	0	25,25,25	0.84	0
8	OLC	A	566	-	22,22,24	0.77	1 (4%)	23,23,25	1.26	2 (8%)
8	OLC	A	567	-	16,17,24	0.54	0	17,18,25	0.73	0
8	OLC	A	568	-	15,16,24	0.67	0	16,17,25	0.76	0
8	OLC	A	569	-	6,7,24	0.28	0	5,7,25	0.85	0
8	OLC	A	570	-	14,14,24	1.14	1 (7%)	15,15,25	1.01	1 (6%)
8	OLC	A	571	-	19,19,24	1.58	1 (5%)	20,20,25	1.57	2 (10%)
8	OLC	A	572	-	24,24,24	0.65	1 (4%)	25,25,25	0.99	2 (8%)
8	OLC	A	573	-	20,20,24	1.54	1 (5%)	21,21,25	1.16	1 (4%)
8	OLC	A	574	-	24,24,24	0.49	0	25,25,25	0.90	0
5	HEM	A	800	1	49,50,50	4.38	25 (51%)	46,82,82	4.93	21 (45%)
6	HAS	A	801	1,7	72,72,72	2.53	27 (37%)	86,109,109	2.84	39 (45%)
8	OLC	B	169	-	24,24,24	0.48	0	25,25,25	0.82	0
8	OLC	B	170	-	24,24,24	0.81	1 (4%)	25,25,25	1.14	2 (8%)
8	OLC	B	171	-	24,24,24	0.49	0	25,25,25	0.52	0
8	OLC	B	172	-	19,20,24	0.53	0	19,20,25	0.57	0
9	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	C	35	-	24,24,24	0.49	0	25,25,25	0.54	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
7	PER	A	563	4,6	-	0/0/0/0	0/0/0/0
8	OLC	A	564	-	-	0/24/24/24	0/0/0/0
8	OLC	A	565	-	-	0/24/24/24	0/0/0/0
8	OLC	A	566	-	-	0/22/22/24	0/0/0/0
8	OLC	A	567	-	-	0/17/17/24	0/0/0/0
8	OLC	A	568	-	-	0/16/16/24	0/0/0/0
8	OLC	A	569	-	-	0/5/6/24	0/0/0/0
8	OLC	A	570	-	-	0/14/14/24	0/0/0/0
8	OLC	A	571	-	-	0/19/19/24	0/0/0/0
8	OLC	A	572	-	-	0/24/24/24	0/0/0/0
8	OLC	A	573	-	-	0/20/20/24	0/0/0/0
8	OLC	A	574	-	-	0/24/24/24	0/0/0/0
5	HEM	A	800	1	-	0/14/114/114	0/0/8/8
6	HAS	A	801	1,7	-	0/36/82/82	0/0/8/8
8	OLC	B	169	-	-	0/24/24/24	0/0/0/0
8	OLC	B	170	-	-	0/24/24/24	0/0/0/0
8	OLC	B	171	-	-	0/24/24/24	0/0/0/0
8	OLC	B	172	-	-	0/19/19/24	0/0/0/0
9	CUA	B	802	2	-	0/0/0/0	0/0/0/0
8	OLC	C	35	-	-	0/24/24/24	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C2B-C1B	-19.79	1.39	1.44
5	A	800	HEM	C2D-C1D	10.00	1.47	1.44
6	A	801	HAS	C4C-NC	8.10	1.48	1.37
5	A	800	HEM	CHB-C1B	7.82	1.46	1.35
5	A	800	HEM	CHC-C1C	7.72	1.51	1.36
5	A	800	HEM	C3D-C4D	7.62	1.46	1.44
6	A	801	HAS	C4D-ND	7.26	1.47	1.37
8	A	571	OLC	C13-C12	-6.53	1.52	1.55
8	A	573	OLC	C14-C13	-6.47	1.52	1.55
6	A	801	HAS	C2D-C1D	6.16	1.50	1.40
6	A	801	HAS	C1D-ND	5.72	1.47	1.36
5	A	800	HEM	CHD-C4C	5.65	1.47	1.36
6	A	801	HAS	C1C-CHC	4.88	1.53	1.39
6	A	801	HAS	C2D-C3D	-4.86	1.32	1.41
5	A	800	HEM	C1A-NA	4.86	1.46	1.36
5	A	800	HEM	C4C-NC	4.57	1.44	1.38
5	A	800	HEM	C3D-C2D	-4.46	1.36	1.43
6	A	801	HAS	C3C-C2C	4.35	1.49	1.41
5	A	800	HEM	C1A-CHA	4.15	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C1C-C2C	-3.95	1.35	1.40
5	A	800	HEM	C2C-C1C	-3.86	1.31	1.43
5	A	800	HEM	C4A-NA	3.86	1.44	1.36
6	A	801	HAS	C3C-CAC	-3.70	1.40	1.48
5	A	800	HEM	CBB-CAB	3.67	1.50	1.28
6	A	801	HAS	FE-NA	3.63	2.08	1.92
5	A	800	HEM	C3C-CAC	3.60	1.51	1.40
5	A	800	HEM	O2A-CGA	3.54	1.43	1.30
8	A	570	OLC	C8-C7	-3.53	1.53	1.55
6	A	801	HAS	C4C-C3C	3.36	1.45	1.41
6	A	801	HAS	C4A-C3A	3.21	1.44	1.40
6	A	801	HAS	C2D-CMD	3.18	1.54	1.46
5	A	800	HEM	C3B-C2B	-3.12	1.38	1.43
6	A	801	HAS	C4D-CHA	2.95	1.47	1.38
6	A	801	HAS	FE-NB	2.88	2.04	1.92
6	A	801	HAS	C4C-CHD	2.86	1.47	1.38
6	A	801	HAS	C4D-C3D	2.85	1.53	1.43
6	A	801	HAS	C4B-C3B	2.72	1.52	1.43
5	A	800	HEM	C3B-C4B	2.67	1.47	1.44
6	A	801	HAS	CBC-CAC	2.66	1.49	1.28
5	A	800	HEM	C4D-ND	-2.65	1.34	1.39
8	A	566	OLC	C16-C15	-2.62	1.54	1.55
6	A	801	HAS	C1D-CHB	2.61	1.47	1.39
5	A	800	HEM	CAA-C2A	-2.59	1.47	1.52
6	A	801	HAS	C1B-NB	-2.55	1.33	1.37
6	A	801	HAS	C4A-NA	-2.53	1.31	1.36
8	B	170	OLC	O20-C1	2.52	1.41	1.33
5	A	800	HEM	C1B-NB	-2.49	1.34	1.39
6	A	801	HAS	C4A-CHD	-2.47	1.33	1.39
5	A	800	HEM	CHC-C4B	-2.45	1.33	1.39
6	A	801	HAS	C4B-NB	-2.44	1.33	1.37
6	A	801	HAS	C3B-C2B	-2.42	1.31	1.40
5	A	800	HEM	C4B-NB	-2.32	1.32	1.37
6	A	801	HAS	CMA-C3A	2.28	1.56	1.51
5	A	800	HEM	CMB-C2B	2.19	1.54	1.47
6	A	801	HAS	C1A-C2A	2.11	1.47	1.43
5	A	800	HEM	CHD-C1D	-2.08	1.34	1.39
5	A	800	HEM	CMD-C2D	2.08	1.53	1.47
8	A	572	OLC	O20-C1	2.02	1.39	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C4C-C3C-C2C	-12.39	98.21	106.87
5	A	800	HEM	CHD-C1D-ND	12.38	134.87	124.58
5	A	800	HEM	C1A-CHA-C4D	-11.14	112.81	127.47
6	A	801	HAS	C2C-C1C-NC	11.06	117.76	109.41
5	A	800	HEM	CHC-C4B-NB	10.94	133.67	124.58
5	A	800	HEM	C4D-ND-C1D	10.31	115.71	105.16
5	A	800	HEM	C4C-NC-C1C	-9.37	95.79	105.53
5	A	800	HEM	C2D-C1D-ND	-9.19	102.07	112.93
5	A	800	HEM	CHA-C4D-ND	8.39	135.84	124.31
5	A	800	HEM	CHC-C1C-NC	-8.18	117.63	124.73
5	A	800	HEM	C3B-C4B-NB	-7.04	108.96	114.00
5	A	800	HEM	C4A-NA-C1A	-5.64	99.33	106.76
6	A	801	HAS	C4C-NC-C1C	-5.62	99.36	106.76
6	A	801	HAS	C4D-CHA-C1A	-5.59	120.12	127.47
5	A	800	HEM	C4A-CHB-C1B	-5.37	120.41	127.47
5	A	800	HEM	C3A-C4A-NA	5.34	113.44	109.41
8	A	571	OLC	C13-C12-C11	-4.97	112.79	117.97
5	A	800	HEM	CHD-C4C-NC	-4.70	120.65	124.73
6	A	801	HAS	C4B-CHC-C1C	-4.69	121.30	127.47
5	A	800	HEM	CHB-C1B-NB	4.47	130.44	124.31
6	A	801	HAS	C3A-C4A-NA	4.42	112.75	109.41
6	A	801	HAS	CHC-C1C-NC	-4.36	117.30	124.58
5	A	800	HEM	O2D-CGD-O1D	-4.18	112.67	123.30
5	A	800	HEM	C1B-NB-C4B	4.14	109.40	105.16
5	A	800	HEM	CBD-CAD-C3D	-3.94	105.78	114.37
6	A	801	HAS	C2B-C1B-NB	3.87	112.33	109.41
6	A	801	HAS	C27-C19-C20	3.84	121.23	115.39
6	A	801	HAS	C4D-ND-C1D	-3.80	101.75	106.76
8	A	573	OLC	C14-C13-C12	-3.52	106.55	114.46
6	A	801	HAS	C2C-C3C-CAC	3.52	134.52	127.33
5	A	800	HEM	O2A-CGA-O1A	-3.48	114.44	123.30
8	B	170	OLC	C21-O20-C1	3.47	127.29	117.13
6	A	801	HAS	C4B-C3B-C2B	-3.41	104.49	106.87
5	A	800	HEM	C4B-CHC-C1C	-3.38	117.66	126.57
6	A	801	HAS	C3C-C2C-C1C	3.36	108.97	107.00
6	A	801	HAS	CBD-CAD-C3D	-3.35	106.09	112.35
6	A	801	HAS	C4D-C3D-C2D	3.35	109.58	106.80
6	A	801	HAS	C2D-C1D-ND	3.30	111.85	108.64
6	A	801	HAS	C3A-C4A-CHD	-3.29	119.75	126.00
8	A	570	OLC	C8-C7-C6	-3.29	107.07	114.46
8	A	571	OLC	C4-C3-C2	-3.26	100.99	113.28
5	A	800	HEM	CMA-C3A-C4A	-3.18	123.74	128.62
6	A	801	HAS	C20-C19-C18	-2.99	115.33	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C2A-C1A-CHA	-2.98	120.36	126.00
8	A	566	OLC	O20-C21-C22	-2.94	91.03	105.69
6	A	801	HAS	CAA-CBA-CGA	-2.82	104.41	113.47
6	A	801	HAS	OMD-CMD-C2D	-2.72	119.45	125.32
6	A	801	HAS	CHA-C1A-NA	2.65	129.00	124.58
6	A	801	HAS	C4A-C3A-C2A	-2.61	105.18	107.00
5	A	800	HEM	O2D-CGD-CBD	2.51	123.08	114.22
8	A	566	OLC	C21-O20-C1	2.50	124.44	117.13
6	A	801	HAS	CAA-C2A-C3A	2.47	136.07	129.00
6	A	801	HAS	CHB-C1D-ND	-2.47	120.46	124.58
8	B	170	OLC	O20-C21-C22	2.45	117.92	105.69
6	A	801	HAS	O2D-CGD-CBD	2.40	122.72	114.22
6	A	801	HAS	C24-C23-C22	-2.32	116.62	121.08
6	A	801	HAS	O2A-CGA-CBA	2.31	122.40	114.22
6	A	801	HAS	C20-C21-C22	2.30	118.18	111.62
6	A	801	HAS	C12-C13-C14	2.27	118.84	112.46
6	A	801	HAS	C4C-CHD-C4A	2.26	130.45	127.47
6	A	801	HAS	C1A-C2A-C3A	-2.26	104.58	106.92
6	A	801	HAS	C3C-C4C-NC	2.25	114.77	111.52
8	A	572	OLC	C21-O20-C1	2.19	123.55	117.13
6	A	801	HAS	C21-C22-C23	-2.19	123.07	127.80
6	A	801	HAS	CMC-C2C-C1C	-2.17	125.28	128.62
6	A	801	HAS	CMA-C3A-C4A	2.16	131.94	128.62
6	A	801	HAS	CAA-C2A-C1A	-2.16	118.99	125.50
6	A	801	HAS	O11-C11-C12	2.14	119.65	110.45
8	A	572	OLC	O20-C21-C22	2.13	116.31	105.69
6	A	801	HAS	O1A-CGA-CBA	-2.12	115.75	123.03

There are no chirality outliers.

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	554/569 (97%)	0.13	34 (6%) 21 15	16, 29, 54, 84	0
2	B	166/168 (98%)	-0.11	3 (1%) 65 60	18, 30, 48, 65	0
3	C	31/34 (91%)	-0.40	1 (3%) 45 37	24, 30, 40, 55	0
All	All	751/771 (97%)	0.06	38 (5%) 28 21	16, 29, 53, 84	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	7.0
1	A	12	TYR	5.7
1	A	495	ARG	5.5
1	A	491	VAL	4.9
1	A	515	PRO	4.4
1	A	499	PRO	4.4
1	A	496	GLU	4.1
2	B	6	LYS	4.1
1	A	330[A]	ARG	4.1
1	A	514	GLY	4.0
1	A	332	LEU	3.7
1	A	492	LEU	3.5
1	A	9	SER	3.5
1	A	11	VAL	3.4
1	A	333	PHE	3.3
1	A	331	GLY	3.1
1	A	235	ILE	3.0
1	A	493	LEU	2.8
1	A	519	ARG	2.6
1	A	236	VAL	2.6
1	A	393	VAL	2.6
2	B	3	ASP	2.5
1	A	176	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	552	HIS	2.4
2	B	168	GLU	2.4
1	A	526	ARG	2.4
3	C	4	LYS	2.4
1	A	240	LEU	2.3
1	A	551	GLY	2.3
1	A	10	ARG	2.2
1	A	385	PHE	2.2
1	A	548	GLN	2.1
1	A	547	VAL	2.1
1	A	238	PHE	2.1
1	A	500	GLU	2.1
1	A	326	LEU	2.0
1	A	175	PRO	2.0
1	A	497	ARG	2.0

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
8	OLC	A	568	17/25	0.29	20.03	59,63,79,80	0
8	OLC	C	35	25/25	0.28	18.27	67,81,92,93	0
8	OLC	A	565	25/25	0.24	13.46	44,65,90,92	0
8	OLC	B	172	21/25	0.23	11.55	60,63,76,79	0
8	OLC	A	571	20/25	0.19	10.58	54,66,71,71	0
8	OLC	A	574	25/25	0.18	9.18	51,58,68,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	OLC	A	572	25/25	0.19	7.63	48,59,64,68	0
8	OLC	B	169	25/25	0.20	6.45	54,65,72,73	0
8	OLC	A	564	25/25	0.23	6.42	45,55,73,76	0
8	OLC	B	171	25/25	0.23	6.37	65,68,73,74	0
8	OLC	A	570	15/25	0.31	5.48	47,64,76,77	0
8	OLC	A	567	18/25	0.17	4.61	47,60,73,74	0
8	OLC	B	170	25/25	0.25	3.46	56,63,72,76	0
8	OLC	A	566	23/25	0.15	2.59	30,45,65,66	0
8	OLC	A	573	21/25	0.20	2.25	56,66,81,82	0
8	OLC	A	569	8/25	0.20	1.71	68,68,70,71	0
6	HAS	A	801	65/65	0.14	0.25	11,20,34,39	0
7	PER	A	563	2/2	0.14	0.01	19,19,19,21	0
5	HEM	A	800	43/43	0.10	-0.56	10,15,19,21	0
4	CU	A	803	1/1	0.10	-0.60	22,22,22,22	0
9	CUA	B	802	2/2	0.09	-1.84	20,20,20,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.