



Full wwPDB X-ray Structure Validation Report i

May 20, 2014 – 02:30 AM EDT

PDB ID : 4NXN
Title : Crystal Structure of the 30S ribosomal subunit from a GidB (RsmG) mutant of *Thermus thermophilus* (HB8), bound with streptomycin
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2013-12-09
Resolution : 3.54 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>

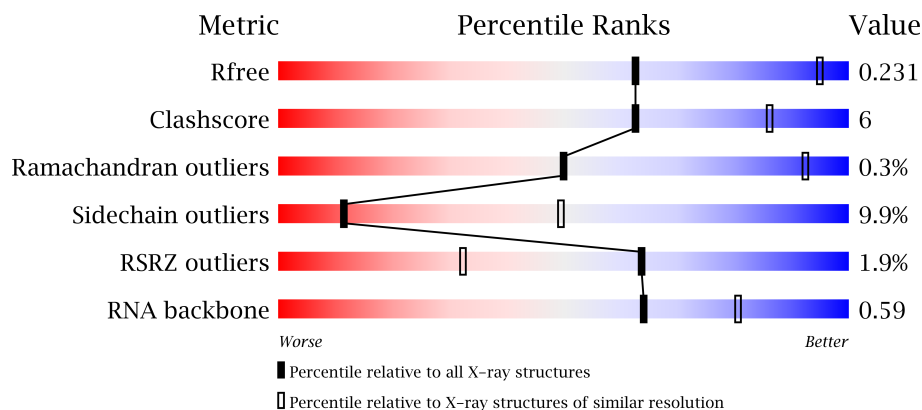
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
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)	:	stable22978

1 Overall quality at a glance

The reported resolution of this entry is 3.54 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.












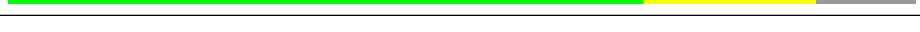
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1270 (3.78-3.30)
Clashscore	79885	1033 (3.70-3.38)
Ramachandran outliers	78287	1067 (3.72-3.36)
Sidechain outliers	78261	1067 (3.72-3.36)
RSRZ outliers	66119	1270 (3.78-3.30)
RNA backbone	1838	1011 (4.30-2.76)

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	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52137 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32506	14476	6011	10507	1512			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	SEE REMARK 999	GB M26923.1
A	1535	A	C	SEE REMARK 999	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

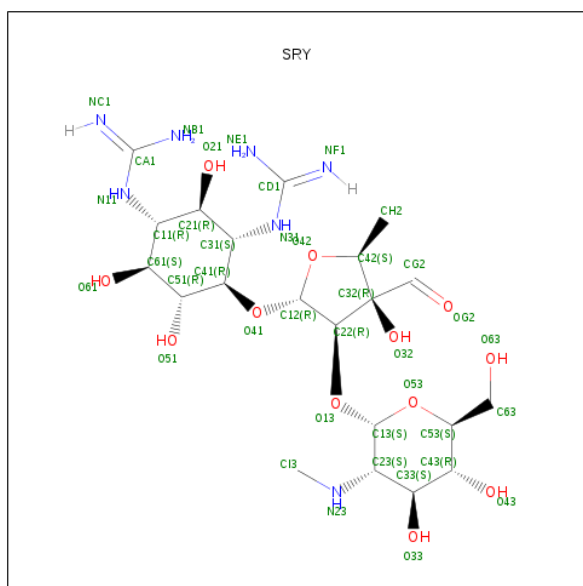
- Molecule 20 is a protein called ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	2	Total	Mg	0	0
			2	2		
23	Q	2	Total	Mg	0	0
			2	2		
23	D	1	Total	Mg	0	0
			1	1		
23	E	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

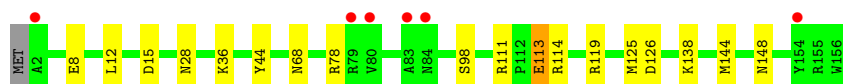
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	3	Total 3	Mg 3	0	0
23	B	1	Total 1	Mg 1	0	0
23	A	227	Total 227	Mg 227	0	0
23	T	1	Total 1	Mg 1	0	0
23	N	1	Total 1	Mg 1	0	0
23	U	1	Total 1	Mg 1	0	0
23	M	1	Total 1	Mg 1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

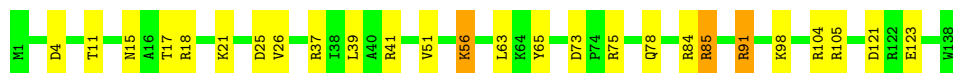
- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	254	Total 254	O 254	0	0
25	D	1	Total 1	O 1	0	0
25	E	4	Total 4	O 4	0	0
25	L	1	Total 1	O 1	0	0



- Molecule 8: ribosomal protein S8

Chain H:



- Molecule 9: ribosomal protein S9

Chain I:



- Molecule 10: ribosomal protein S10

Chain J:



- Molecule 11: ribosomal protein S11

Chain K:



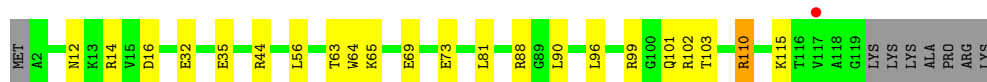
- Molecule 12: ribosomal protein S12

Chain L:



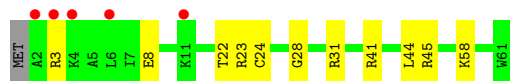
- Molecule 13: ribosomal protein S13

Chain M:



- Molecule 14: ribosomal protein S14

Chain N:



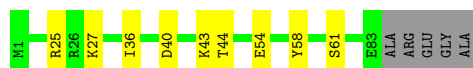
- Molecule 15: ribosomal protein S15

Chain O: 



- Molecule 16: ribosomal protein S16

Chain P: 



- Molecule 17: ribosomal protein S17

Chain Q: 



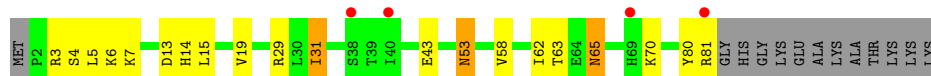
- Molecule 18: ribosomal protein S18

Chain R: 



- Molecule 19: ribosomal protein S19

Chain S: 



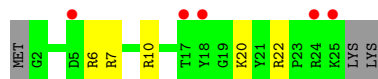
- Molecule 20: ribosomal protein S20

Chain T: 



- Molecule 21: ribosomal protein THX

Chain U: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.06Å 403.06Å 173.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.74 – 3.54 34.74 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.74-3.54) 98.9 (34.74-3.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1555)	Depositor
R, R_{free}	0.193 , 0.231 0.193 , 0.231	Depositor DCC
R_{free} test set	8490 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	124.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 170323 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52137	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, PSU

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	0.45	0/36066	0.79	26/56284 (0.0%)
2	B	0.33	0/1935	0.52	0/2609
3	C	0.25	0/1636	0.46	0/2205
4	D	0.31	0/1733	0.44	0/2318
5	E	0.38	0/1162	0.53	0/1564
6	F	0.26	0/856	0.42	0/1154
7	G	0.26	0/1276	0.43	0/1709
8	H	0.46	0/1136	0.52	0/1527
9	I	0.27	0/1029	0.47	0/1379
10	J	0.25	0/805	0.49	0/1082
11	K	0.32	0/879	0.46	0/1187
12	L	0.34	0/977	0.52	0/1306
13	M	0.26	0/947	0.47	0/1270
14	N	0.26	0/501	0.45	0/664
15	O	0.31	0/740	0.45	0/987
16	P	0.37	0/716	0.50	0/963
17	Q	0.40	0/836	0.55	0/1117
18	R	0.30	0/579	0.46	0/768
19	S	0.23	0/661	0.50	0/890
20	T	0.32	0/765	0.50	0/1007
21	U	0.26	0/212	0.38	0/277
All	All	0.41	0/55447	0.71	26/82267 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
20	T	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	U	C2-N1-C1'	7.82	127.08	117.70
1	A	839	U	N1-C2-O2	7.53	128.07	122.80
1	A	1158	C	N1-C2-O2	7.36	123.32	118.90
1	A	1158	C	C2-N1-C1'	7.16	126.67	118.80
1	A	839	U	N3-C2-O2	-6.66	117.54	122.20
1	A	858	G	C5-C6-O6	6.48	132.49	128.60
1	A	858	G	N1-C6-O6	-6.42	116.05	119.90
1	A	328	C	C2-N1-C1'	5.86	125.25	118.80
1	A	243	A	C8-N9-C4	-5.73	103.51	105.80
1	A	1301	U	P-O3'-C3'	5.65	126.48	119.70
1	A	254	G	O5'-P-OP1	-5.45	100.79	105.70
1	A	1158	C	N3-C2-O2	-5.44	118.09	121.90
1	A	1190	G	P-O3'-C3'	5.36	126.13	119.70
1	A	1305	G	C8-N9-C4	-5.33	104.27	106.40
1	A	839	U	C6-N1-C1'	-5.33	113.74	121.20
1	A	758	G	N1-C2-N3	5.26	127.06	123.90
1	A	428	G	P-O3'-C3'	5.20	125.94	119.70
1	A	1126	U	C5-C6-N1	5.14	125.27	122.70
1	A	329	A	O5'-P-OP1	-5.12	101.09	105.70
1	A	1346	A	P-O3'-C3'	5.08	125.80	119.70
1	A	1067	A	P-O3'-C3'	5.08	125.80	119.70
1	A	1201	A	P-O3'-C3'	5.05	125.75	119.70
1	A	243	A	P-O3'-C3'	5.00	125.71	119.70
1	A	5	U	P-O3'-C3'	5.00	125.70	119.70
1	A	328	C	C6-N1-C2	-5.00	118.30	120.30
1	A	792	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
20	T	93	GLU	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32506	0	32	182	0
2	B	1900	0	0	13	0
3	C	1612	0	0	8	0
4	D	1703	0	0	12	0
5	E	1146	0	0	13	0
6	F	843	0	0	5	0
7	G	1257	0	0	9	0
8	H	1116	0	0	12	0
9	I	1010	0	0	14	0
10	J	792	0	0	4	0
11	K	864	0	0	7	0
12	L	972	0	0	6	0
13	M	937	0	0	6	0
14	N	492	0	0	5	0
15	O	729	0	0	4	0
16	P	700	0	0	3	0
17	Q	823	0	0	5	0
18	R	574	0	0	8	0
19	S	647	0	0	7	0
20	T	763	0	0	6	0
21	U	208	0	0	4	0
22	A	40	0	36	4	0
23	A	227	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	3	0	0	0	0
23	M	1	0	0	0	0
23	N	1	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
23	T	1	0	0	0	0
23	U	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	254	0	0	3	0
25	D	1	0	0	0	0
25	E	4	0	0	0	0
25	L	1	0	0	0	0
All	All	52137	0	68	265	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 6.

All (265) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1126:U:O4	1:A:1147:C:N4	2.14	0.81
1:A:1158:C:N3	1:A:1181:G:N2	2.29	0.80
1:A:279:A:OP2	17:Q:95:TYR:OH	2.04	0.76
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.20	0.74
1:A:1266:G:N2	1:A:1269:A:OP2	2.23	0.72
1:A:201:C:N3	1:A:216:G:N2	2.38	0.71
1:A:1058:G:OP1	3:C:199:LYS:NZ	2.23	0.71
8:H:21:LYS:O	8:H:65:TYR:OH	2.08	0.71
1:A:1347:G:O6	9:I:10:ARG:NH2	2.23	0.71
1:A:80:G:N2	1:A:89:C:N3	2.38	0.70
8:H:17:THR:O	8:H:78:GLN:NE2	2.23	0.70
3:C:156:ARG:NH1	3:C:160:ALA:O	2.24	0.70
1:A:9:G:OP2	5:E:121:LYS:NZ	2.24	0.69
1:A:974:A:OP2	14:N:41:ARG:NH1	2.26	0.69
1:A:1192:C:O2	5:E:25:ARG:NH2	2.26	0.68
12:L:52:LEU:O	12:L:54:LYS:NZ	2.27	0.67
1:A:1147:C:O2'	9:I:5:TYR:OH	2.12	0.66
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.28	0.66
1:A:537:G:OP1	12:L:113:ARG:NH2	2.29	0.66
2:B:20:GLU:OE1	2:B:23:ARG:NH1	2.29	0.65
1:A:835:U:OP1	18:R:64:ARG:NH2	2.30	0.65
1:A:517:G:N1	1:A:533:A:OP2	2.30	0.65
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.30	0.65
1:A:448:A:OP2	1:A:485:G:N2	2.29	0.65
1:A:1505:G:O2'	1:A:1506:U:OP2	2.15	0.65
1:A:564:C:O2'	8:H:91:ARG:NH2	2.30	0.64
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.30	0.64
1:A:103:C:OP1	20:T:17:ARG:NH1	2.30	0.64
1:A:559:A:OP1	5:E:126:ARG:NH1	2.31	0.63
6:F:74:ASP:OD2	6:F:74:ASP:N	2.30	0.63
1:A:964:A:O2'	10:J:55:LYS:NZ	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:102:ASP:OD1	4:D:103:ASN:N	2.32	0.63
1:A:235:C:N4	25:A:1989:HOH:O	2.31	0.62
18:R:20:ALA:O	18:R:55:ARG:NH1	2.32	0.62
1:A:652:U:O4	1:A:752:G:O2'	2.18	0.62
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.32	0.62
1:A:991:U:O4	1:A:1212:U:O2'	2.17	0.62
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.32	0.62
5:E:102:ALA:O	5:E:107:ARG:NH1	2.33	0.61
1:A:427:U:OP1	4:D:13:ARG:NH2	2.34	0.61
2:B:87:ARG:NH2	2:B:220:ASP:OD1	2.33	0.61
9:I:42:ARG:NH2	9:I:75:ASP:OD2	2.34	0.61
1:A:263:A:OP2	20:T:79:ARG:NH1	2.34	0.61
1:A:1050:G:N2	1:A:1208:C:O2	2.34	0.60
1:A:1125:U:OP2	1:A:1145:C:N4	2.34	0.60
1:A:191:G:O2'	20:T:102:GLY:O	2.20	0.60
13:M:65:LYS:NZ	13:M:73:GLU:OE2	2.35	0.60
1:A:191:G:N2	20:T:103:GLY:O	2.35	0.59
7:G:144:MET:O	7:G:148:ASN:ND2	2.35	0.59
1:A:437:U:O2'	4:D:123:HIS:ND1	2.36	0.59
1:A:776:G:N2	1:A:802:A:OP2	2.36	0.59
1:A:984:C:N3	1:A:1221:G:N2	2.51	0.58
1:A:130:A:OP2	1:A:190(E):U:O2'	2.19	0.58
1:A:501:C:OP1	12:L:117:ARG:NH2	2.35	0.58
1:A:1242:C:OP1	21:U:10:ARG:NH1	2.35	0.58
19:S:5:LEU:O	19:S:6:LYS:NZ	2.36	0.58
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.36	0.58
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.36	0.58
14:N:23:ARG:NH1	14:N:28:GLY:O	2.36	0.58
1:A:279:A:OP1	1:A:280:C:O2'	2.21	0.58
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.36	0.58
1:A:512:U:OP1	4:D:46:LYS:NZ	2.37	0.58
18:R:46:GLU:N	18:R:46:GLU:OE1	2.37	0.58
1:A:996:A:N1	1:A:1046:A:O2'	2.36	0.57
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.37	0.57
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.38	0.57
1:A:1226:C:OP2	13:M:103:THR:OG1	2.22	0.57
6:F:36:ARG:NH2	6:F:66:GLU:OE1	2.38	0.57
2:B:84:GLU:OE2	2:B:233:SER:OG	2.23	0.57
1:A:1127:G:O2'	9:I:16:ARG:NH2	2.38	0.57
9:I:60:ASP:OD1	9:I:61:ALA:N	2.37	0.57
1:A:522:C:OP2	12:L:69:TYR:OH	2.22	0.57
1:A:692:U:OP1	11:K:124:LYS:NZ	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:401:C:O2'	1:A:621:A:N3	2.38	0.56
13:M:16:ASP:N	13:M:16:ASP:OD1	2.38	0.56
4:D:8:VAL:O	4:D:11:LEU:N	2.38	0.56
1:A:619:U:N3	4:D:134:ASP:OD2	2.38	0.56
1:A:1347:G:N2	1:A:1374:A:OP2	2.38	0.56
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.39	0.55
1:A:380:G:N2	1:A:383:A:OP2	2.39	0.55
1:A:664:G:OP1	18:R:64:ARG:NH1	2.39	0.55
1:A:788:U:O2'	1:A:1539:C:O2	2.24	0.55
1:A:1101:A:OP2	2:B:96:ARG:NH2	2.39	0.55
1:A:1003(A):G:O6	1:A:1038:C:N4	2.39	0.55
1:A:1150:U:O4	1:A:1151:A:N6	2.40	0.55
1:A:1127:G:N2	1:A:1145:C:O2	2.40	0.55
1:A:921:U:O2'	5:E:19:MET:O	2.25	0.55
9:I:118:LYS:O	9:I:120:ARG:N	2.39	0.55
18:R:59:SER:O	18:R:63:GLN:N	2.40	0.55
1:A:718:G:O6	18:R:74:ARG:NH1	2.40	0.55
1:A:707:C:OP1	11:K:85:ARG:NH1	2.40	0.54
1:A:542:G:OP1	4:D:10:ARG:NH2	2.41	0.54
1:A:28:G:O2'	1:A:296:U:OP1	2.25	0.54
1:A:928:G:O2'	1:A:1533:C:OP1	2.26	0.54
1:A:1376:U:OP1	7:G:98:SER:OG	2.25	0.54
1:A:1095:U:OP1	1:A:1108:G:N2	2.42	0.53
1:A:1183:A:O2'	1:A:1184:G:OP1	2.26	0.53
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.41	0.53
1:A:1037:C:N3	1:A:1038:C:N4	2.57	0.53
1:A:1442:G:N7	1:A:1446:A:N6	2.57	0.53
16:P:58:TYR:O	16:P:61:SER:OG	2.27	0.53
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.42	0.53
1:A:1210:C:O2'	1:A:1213:A:O2'	2.26	0.53
1:A:983:A:O5'	14:N:3:ARG:NH2	2.42	0.52
1:A:782:A:C6	1:A:801:U:C2	2.97	0.52
1:A:110:C:O2'	16:P:25:ARG:O	2.27	0.52
1:A:122:G:C2	1:A:123:C:C2	2.97	0.52
1:A:426:G:OP1	4:D:38:TYR:OH	2.28	0.52
5:E:98:THR:N	5:E:117:ASP:OD1	2.43	0.52
1:A:978:A:O2'	1:A:1322:C:N3	2.43	0.52
1:A:62:U:OP1	1:A:385:C:O2'	2.28	0.51
10:J:36:GLY:N	10:J:73:ASP:O	2.43	0.51
1:A:1422:G:N2	1:A:1478:C:O2	2.43	0.51
1:A:152:A:N6	1:A:170:U:C2	2.78	0.51
1:A:1093:A:N3	1:A:1109:C:O2'	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1074:G:O2'	1:A:1101:A:N1	2.44	0.51
1:A:811:C:O2'	1:A:901:A:N1	2.43	0.51
1:A:527:G:OP2	22:A:1601:SRY:O32	2.14	0.51
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.44	0.51
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.44	0.50
1:A:1145:C:O2'	1:A:1146:A:O5'	2.29	0.50
1:A:765:G:N2	1:A:813:U:OP2	2.45	0.50
1:A:792:A:O2'	1:A:793:U:OP2	2.29	0.50
9:I:104:ARG:NH1	9:I:105:ASP:O	2.44	0.50
3:C:113:ALA:N	3:C:183:ASP:OD1	2.44	0.50
19:S:53:ASN:O	19:S:53:ASN:ND2	2.45	0.50
1:A:563:A:N6	25:A:1936:HOH:O	2.44	0.50
1:A:452:A:O2'	1:A:453:A:O4'	2.30	0.50
1:A:587:G:N2	1:A:754:C:OP2	2.44	0.50
1:A:739:C:O2'	15:O:42:HIS:ND1	2.45	0.50
1:A:452:A:O2'	1:A:453:A:O5'	2.30	0.49
1:A:1393:U:O2'	1:A:1501:C:O2'	2.30	0.49
1:A:781:A:C5	1:A:802:A:C2	3.01	0.49
19:S:65:ASN:OD1	19:S:65:ASN:N	2.42	0.49
1:A:890:G:O2'	1:A:906:G:O6	2.30	0.49
1:A:1080:A:O3'	5:E:16:THR:OG1	2.30	0.49
1:A:254:G:OP1	17:Q:66:SER:OG	2.31	0.49
1:A:78:G:O6	1:A:91:C:N4	2.46	0.49
1:A:689:C:OP1	11:K:44:SER:OG	2.31	0.49
9:I:32:ASP:OD1	9:I:33:PHE:N	2.46	0.49
1:A:123:C:O2'	1:A:290:C:O2	2.31	0.48
5:E:16:THR:OG1	5:E:16:THR:O	2.30	0.48
2:B:25:ASN:O	2:B:27:LYS:N	2.46	0.48
1:A:411:A:N3	1:A:413:G:O2'	2.46	0.48
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.46	0.48
19:S:43:GLU:OE1	19:S:43:GLU:N	2.46	0.48
1:A:581:G:O6	1:A:758:G:C8	2.67	0.48
2:B:17:PHE:CG	2:B:18:GLY:N	2.81	0.48
3:C:3:ASN:OD1	3:C:3:ASN:N	2.45	0.48
1:A:923:A:O2'	1:A:1399:C:OP2	2.32	0.48
1:A:254:G:O2'	17:Q:16:GLN:O	2.32	0.48
1:A:653:A:O5'	8:H:56:LYS:NZ	2.47	0.47
4:D:28:SER:O	4:D:30:LYS:N	2.47	0.47
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.47	0.47
16:P:40:ASP:OD1	16:P:44:THR:OG1	2.32	0.47
1:A:992:U:O2	1:A:993:G:N2	2.48	0.47
8:H:25:ASP:OD1	8:H:25:ASP:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.47
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.32	0.47
2:B:189:ASP:OD1	2:B:189:ASP:N	2.48	0.47
1:A:1120:G:C6	1:A:1121:U:C4	3.02	0.47
1:A:1323:G:OP2	19:S:3:ARG:NH1	2.48	0.47
1:A:1067:A:O2'	1:A:1093:A:O3'	2.33	0.47
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.33	0.47
8:H:41:ARG:NH2	8:H:123:GLU:OE2	2.48	0.47
1:A:1315:U:O2'	1:A:1360:A:O2'	2.32	0.46
1:A:602:A:C2	1:A:637:G:C2	3.03	0.46
1:A:766:A:C8	1:A:814:A:N6	2.84	0.46
13:M:96:LEU:O	13:M:110:ARG:NH1	2.49	0.46
18:R:65:ILE:O	18:R:69:THR:OG1	2.32	0.46
11:K:34:ASP:OD1	11:K:38:ASN:N	2.48	0.46
1:A:1329:A:OP2	21:U:7:ARG:NH2	2.49	0.46
7:G:68:ASN:O	7:G:138:LYS:NZ	2.49	0.46
1:A:27:G:C6	1:A:557:G:C2	3.04	0.46
1:A:483:C:OP2	1:A:484:G:O2'	2.34	0.46
1:A:1284:C:OP2	1:A:1285:A:O2'	2.34	0.46
6:F:11:ASN:OD1	6:F:86:ARG:NH2	2.49	0.46
1:A:738:C:OP2	6:F:92:LYS:NZ	2.48	0.46
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.49	0.46
1:A:103:C:O2'	1:A:172:A:N1	2.49	0.45
1:A:925:G:C2	1:A:927:G:C8	3.04	0.45
2:B:240:GLN:N	2:B:240:GLN:OE1	2.49	0.45
1:A:526:C:O3'	22:A:1601:SRV:HI31	2.16	0.45
1:A:374:A:C6	1:A:375:U:C4	3.04	0.45
10:J:42:THR:OG1	10:J:68:HIS:ND1	2.49	0.45
2:B:60:ASP:OD2	2:B:64:ARG:NH2	2.50	0.45
2:B:198:ASP:OD1	2:B:198:ASP:N	2.49	0.45
19:S:80:TYR:CG	19:S:81:ARG:N	2.84	0.45
1:A:1442:G:C5	1:A:1446:A:N6	2.85	0.45
1:A:922:G:C2	1:A:1396:A:C6	3.05	0.45
5:E:79:GLU:OE1	8:H:104:ARG:NH1	2.50	0.45
1:A:1542:U:H2'	1:A:1543:C:C6	2.51	0.45
1:A:1309:G:OP1	13:M:88:ARG:NH2	2.49	0.45
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.50	0.44
11:K:33:THR:OG1	11:K:37:GLY:O	2.35	0.44
1:A:1320:C:OP2	19:S:70:LYS:NZ	2.50	0.44
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.50	0.44
11:K:27:ASN:OD1	11:K:28:THR:N	2.49	0.44
1:A:1077:G:N2	1:A:1080:A:OP2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:23:ARG:O	2:B:24:TRP:CD1	2.70	0.44
1:A:771:G:N2	1:A:808:C:O2	2.51	0.44
8:H:121:ASP:N	8:H:121:ASP:OD1	2.51	0.44
15:O:4:THR:OG1	15:O:6:GLU:OE2	2.36	0.44
1:A:243:A:C2	1:A:246:A:C8	3.05	0.44
1:A:908:A:C2	1:A:909:A:C5	3.06	0.44
1:A:686:U:O2'	1:A:687:A:C8	2.71	0.43
1:A:807:A:OP1	15:O:48:LYS:NZ	2.50	0.43
1:A:1347:G:O2'	1:A:1348:U:P	2.76	0.43
1:A:686:U:C2	1:A:687:A:N7	2.86	0.43
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.51	0.43
22:A:1601:SRY:O21	22:A:1601:SRY:NE1	2.52	0.43
8:H:73:ASP:OD2	8:H:75:ARG:NE	2.52	0.43
1:A:587:G:O2'	1:A:588:G:OP2	2.37	0.43
1:A:885:G:C2	1:A:913:A:N1	2.86	0.43
1:A:397:A:N7	1:A:547:A:O2'	2.51	0.43
1:A:1426:C:N3	1:A:1474:G:N2	2.67	0.43
1:A:19:C:OP1	5:E:125:SER:OG	2.36	0.43
1:A:335:C:O2'	1:A:1433:A:N3	2.52	0.43
2:B:103:THR:OG1	2:B:176:GLU:OE1	2.36	0.43
4:D:112:VAL:N	4:D:116:GLN:OE1	2.51	0.43
1:A:815:A:N3	1:A:1527:C:O2'	2.52	0.43
1:A:914:A:OP1	22:A:1601:SRY:HI33	2.18	0.43
3:C:77:ILE:O	3:C:83:ARG:N	2.51	0.43
1:A:673:G:O3'	6:F:87:ARG:NH2	2.52	0.43
1:A:1003(A):G:N1	1:A:1038:C:N3	2.67	0.42
1:A:109:A:C6	1:A:327:A:C6	3.08	0.42
1:A:251:G:C6	1:A:266:G:C6	3.07	0.42
1:A:293:G:C4	1:A:305:G:N2	2.87	0.42
13:M:101:GLN:N	13:M:101:GLN:OE1	2.52	0.42
1:A:757:U:O2'	1:A:879:C:O2	2.37	0.42
1:A:886:G:C2	1:A:912:C:O2	2.72	0.42
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.37	0.42
1:A:1347:G:O2'	1:A:1348:U:O5'	2.38	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.42
1:A:908:A:C2	1:A:909:A:C4	3.07	0.42
2:B:25:ASN:O	2:B:28:PHE:N	2.53	0.42
3:C:14:ILE:O	3:C:15:THR:OG1	2.37	0.42
1:A:1196:U:O2'	25:A:2063:HOH:O	2.21	0.42
1:A:1523:G:OP1	11:K:123:LYS:NZ	2.53	0.41
1:A:1374:A:OP1	7:G:36:LYS:NZ	2.54	0.41
1:A:396:G:O2'	1:A:398:C:OP1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:C:N3	1:A:475:G:N2	2.69	0.41
1:A:485:G:O2'	1:A:486:U:P	2.78	0.41
20:T:19:SER:O	20:T:23:ARG:N	2.53	0.41
1:A:1088:G:N2	1:A:1097:C:O2	2.54	0.41
1:A:826:C:O2	8:H:15:ASN:ND2	2.54	0.41
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.54	0.41
1:A:6:G:O6	5:E:95:ALA:N	2.53	0.41
1:A:785:G:N2	1:A:798:G:C4	2.88	0.41
18:R:59:SER:N	18:R:62:GLU:OE1	2.53	0.41
20:T:67:ALA:O	20:T:73:HIS:ND1	2.53	0.41
1:A:144:G:N2	1:A:178:C:N3	2.69	0.41
1:A:9:G:C2	1:A:26:A:N1	2.88	0.41
1:A:607:A:C4	1:A:608:A:C8	3.09	0.41
1:A:892:A:C2	1:A:907:A:C4	3.09	0.41
5:E:147:ASP:N	5:E:147:ASP:OD1	2.54	0.41
1:A:451:A:N6	1:A:481:G:C4	2.89	0.41
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.53	0.41
1:A:1269:A:N1	1:A:1312:G:O2'	2.55	0.40
1:A:108:G:OP2	1:A:326:G:N1	2.54	0.40
1:A:376:G:N3	1:A:389:A:C2	2.89	0.40
5:E:39:GLY:O	5:E:69:VAL:N	2.55	0.40
1:A:1067:A:O2'	1:A:1093:A:O2'	2.39	0.40
1:A:1397:C:O2'	1:A:1398:A:OP1	2.39	0.40
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.54	0.40

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	
2	B	232/256 (91%)	209 (90%)	20 (9%)	3 (1%)	18	73
3	C	204/239 (85%)	178 (87%)	26 (13%)	0	100	100
4	D	206/209 (99%)	193 (94%)	13 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	27	82
10	J	96/105 (91%)	79 (82%)	15 (16%)	2 (2%)	11	63
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	L	121/135 (90%)	111 (92%)	10 (8%)	0	100	100
13	M	116/126 (92%)	106 (91%)	10 (9%)	0	100	100
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
18	R	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	S	78/93 (84%)	68 (87%)	8 (10%)	2 (3%)	8	58
20	T	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
All	All	2336/2541 (92%)	2146 (92%)	182 (8%)	8 (0%)	50	92

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA
19	S	14	HIS
10	J	34	VAL
2	B	229	VAL
10	J	72	VAL

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	
2	B	202/220 (92%)	180 (89%)	22 (11%)	9	44
3	C	160/188 (85%)	136 (85%)	24 (15%)	4	26
4	D	180/181 (99%)	170 (94%)	10 (6%)	30	77
5	E	115/123 (94%)	100 (87%)	15 (13%)	6	33
6	F	90/90 (100%)	83 (92%)	7 (8%)	18	63
7	G	126/127 (99%)	120 (95%)	6 (5%)	35	82
8	H	119/119 (100%)	106 (89%)	13 (11%)	9	44
9	I	98/99 (99%)	87 (89%)	11 (11%)	9	41
10	J	87/92 (95%)	82 (94%)	5 (6%)	29	76
11	K	88/99 (89%)	82 (93%)	6 (7%)	22	70
12	L	103/110 (94%)	88 (85%)	15 (15%)	5	27
13	M	94/101 (93%)	79 (84%)	15 (16%)	3	22
14	N	49/50 (98%)	44 (90%)	5 (10%)	11	48
15	O	79/80 (99%)	72 (91%)	7 (9%)	14	57
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	77
17	Q	94/97 (97%)	87 (93%)	7 (7%)	20	66
18	R	61/77 (79%)	55 (90%)	6 (10%)	12	50
19	S	71/80 (89%)	59 (83%)	12 (17%)	3	19
20	T	76/82 (93%)	71 (93%)	5 (7%)	24	71
21	U	19/22 (86%)	18 (95%)	1 (5%)	32	78
All	All	1983/2111 (94%)	1787 (90%)	196 (10%)	11	49

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	16	HIS
2	B	17	PHE
2	B	24	TRP
2	B	33	TYR
2	B	44	LEU
2	B	48	MET
2	B	60	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	69	LEU
2	B	96	ARG
2	B	111	ARG
2	B	121	LEU
2	B	130	ARG
2	B	144	ARG
2	B	153	ARG
2	B	157	ARG
2	B	158	LEU
2	B	170	GLU
2	B	178	ARG
2	B	198	ASP
2	B	213	LEU
3	C	3	ASN
3	C	10	PHE
3	C	30	ARG
3	C	32	LEU
3	C	34	LEU
3	C	56	ASP
3	C	63	ASN
3	C	79	ARG
3	C	91	LEU
3	C	95	THR
3	C	105	GLU
3	C	107	GLN
3	C	130	VAL
3	C	136	GLN
3	C	142	MET
3	C	147	LYS
3	C	156	ARG
3	C	162	GLN
3	C	166	GLU
3	C	167	TRP
3	C	173	VAL
3	C	177	THR
3	C	188	LEU
3	C	204	LEU
4	D	15	GLU
4	D	34	GLU
4	D	66	ARG
4	D	119	GLN
4	D	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	145	GLU
4	D	151	LYS
4	D	157	LEU
4	D	187	ARG
4	D	194	LEU
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	16	THR
5	E	18	ARG
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	63	ARG
5	E	79	GLU
5	E	89	ILE
5	E	147	ASP
5	E	151	LEU
6	F	10	LEU
6	F	19	LEU
6	F	32	ASN
6	F	43	LEU
6	F	67	MET
6	F	74	ASP
6	F	95	GLU
7	G	8	GLU
7	G	12	LEU
7	G	78	ARG
7	G	113	GLU
7	G	125	MET
7	G	126	ASP
8	H	11	THR
8	H	18	ARG
8	H	26	VAL
8	H	37	ARG
8	H	39	LEU
8	H	51	VAL
8	H	56	LYS
8	H	63	LEU
8	H	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	85	ARG
8	H	91	ARG
8	H	98	LYS
8	H	105	ARG
9	I	3	GLN
9	I	26	VAL
9	I	29	ASN
9	I	59	PHE
9	I	75	ASP
9	I	79	LEU
9	I	86	VAL
9	I	93	ARG
9	I	102	LEU
9	I	121	ARG
9	I	127	LYS
10	J	3	LYS
10	J	57	LYS
10	J	62	HIS
10	J	76	ASN
10	J	80	LYS
11	K	12	ARG
11	K	29	ILE
11	K	33	THR
11	K	48	ILE
11	K	51	LYS
11	K	96	ARG
12	L	18	VAL
12	L	19	ARG
12	L	33	ARG
12	L	43	VAL
12	L	44	THR
12	L	62	SER
12	L	64	TYR
12	L	66	VAL
12	L	67	THR
12	L	96	VAL
12	L	97	ARG
12	L	112	ASP
12	L	113	ARG
12	L	122	THR
12	L	126	LYS
13	M	12	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	14	ARG
13	M	32	GLU
13	M	35	GLU
13	M	44	ARG
13	M	56	LEU
13	M	63	THR
13	M	64	TRP
13	M	69	GLU
13	M	81	LEU
13	M	90	LEU
13	M	99	ARG
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	8	GLU
14	N	22	THR
14	N	24	CYS
14	N	31	ARG
14	N	44	LEU
15	O	5	LYS
15	O	32	LEU
15	O	33	THR
15	O	39	LEU
15	O	45	VAL
15	O	65	ARG
15	O	70	LEU
16	P	27	LYS
16	P	36	ILE
16	P	43	LYS
16	P	54	GLU
17	Q	15	MET
17	Q	34	LYS
17	Q	38	ARG
17	Q	53	LEU
17	Q	60	ILE
17	Q	83	ASP
17	Q	92	ARG
18	R	19	LYS
18	R	21	LYS
18	R	23	LYS
18	R	28	GLU
18	R	47	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	88	LYS
19	S	4	SER
19	S	7	LYS
19	S	13	ASP
19	S	15	LEU
19	S	19	VAL
19	S	29	ARG
19	S	31	ILE
19	S	53	ASN
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
19	S	65	ASN
20	T	9	ASN
20	T	19	SER
20	T	62	LEU
20	T	73	HIS
20	T	84	LEU
21	U	22	ARG

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	258 (17%)	0

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	66	G
1	A	69	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	81	U
1	A	88	A
1	A	91	C
1	A	101	A
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	145	G
1	A	163	C
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	282	A
1	A	289	G
1	A	299	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	460	A
1	A	461	C
1	A	475	G
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	527	G
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	560	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	858	G
1	A	859	A
1	A	872	A
1	A	876	G
1	A	885	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1010	G
1	A	1016	A
1	A	1019	C
1	A	1022	G
1	A	1023	G
1	A	1026	G
1	A	1031	G
1	A	1045	C
1	A	1051	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1126	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1142	G
1	A	1145	C
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1262	C
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1286	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1287	A
1	A	1289	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1306	A
1	A	1319	A
1	A	1320	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1364	U
1	A	1368	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1400	5MC
1	A	1401	G
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1487	G
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1540	PSU

There are no RNA pucker outliers to report.

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

14 non-standard protein/DNA/RNA residues 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
1	2MG	A	1207	1	24,26,27	1.67	6 (25%)	33,38,41	9.76	5 (15%)
1	5MC	A	1400	1	20,22,23	1.74	1 (5%)	26,32,35	1.09	2 (7%)
1	4OC	A	1402	1	21,23,24	1.48	2 (9%)	26,32,35	0.89	1 (3%)
1	5MC	A	1404	1	20,22,23	1.49	1 (5%)	26,32,35	1.13	2 (7%)
1	5MC	A	1407	1	20,22,23	1.69	1 (5%)	26,32,35	1.06	2 (7%)
1	UR3	A	1498	1	20,22,23	1.59	1 (5%)	23,32,35	1.11	2 (8%)
1	MA6	A	1518	1	26,26,27	1.19	2 (7%)	37,38,41	0.99	2 (5%)
1	MA6	A	1519	1	26,26,27	1.25	2 (7%)	37,38,41	0.97	2 (5%)
1	PSU	A	1540	1,23	19,21,22	0.88	0	23,30,33	1.17	2 (8%)
1	PSU	A	1541	1	19,21,22	0.89	0	23,30,33	1.02	2 (8%)
1	PSU	A	516	1,23	19,21,22	0.91	0	23,30,33	0.96	2 (8%)
1	M2G	A	966	1	25,27,28	1.83	5 (20%)	35,40,43	8.59	5 (14%)
1	5MC	A	967	1	20,22,23	1.47	1 (5%)	26,32,35	1.12	2 (7%)
12	0TD	L	92	12	9,9,10	6.86	2 (22%)	9,11,13	1.82	2 (22%)

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
1	2MG	A	1207	1	-	0/10/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/6/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/10/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/6/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/6/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/6/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/13/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519	1	-	0/13/29/30	0/3/3/3
1	PSU	A	1540	1,23	-	1/8/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/8/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/8/25/26	0/2/2/2
1	M2G	A	966	1	-	0/12/29/30	0/3/3/3
1	5MC	A	967	1	-	0/6/25/26	0/2/2/2
12	0TD	L	92	12	-	0/10/12/14	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	O-C	20.29	1.25	1.11
1	A	1400	5MC	C2-N1	6.68	1.45	1.38
1	A	1407	5MC	C2-N1	6.33	1.45	1.38
1	A	1498	UR3	C5-C4	5.92	1.44	1.37
1	A	1402	4OC	C2-N1	5.74	1.44	1.38
1	A	1404	5MC	C2-N1	5.42	1.44	1.38
1	A	967	5MC	C2-N1	5.22	1.44	1.38
1	A	966	M2G	C2-N2	4.82	1.40	1.34
1	A	1207	2MG	C6-N1	4.24	1.42	1.36
1	A	966	M2G	C6-N1	4.20	1.42	1.36
1	A	1207	2MG	C8-N9	4.12	1.42	1.36
1	A	966	M2G	C8-N9	3.95	1.42	1.36
1	A	1519	MA6	C8-N9	3.33	1.41	1.36
1	A	1518	MA6	C8-N9	3.29	1.41	1.36
1	A	966	M2G	C4-N3	2.79	1.40	1.35
12	L	92	0TD	CA-C	2.78	1.55	1.49
1	A	1207	2MG	C2-N2	2.71	1.40	1.33
1	A	1519	MA6	C6-N1	2.44	1.37	1.34
1	A	1207	2MG	C4-N3	2.41	1.39	1.35
1	A	1518	MA6	C6-N1	2.41	1.37	1.34
1	A	1402	4OC	O5'-C5'	-2.14	1.41	1.44
1	A	1207	2MG	C2-N1	2.11	1.41	1.36
1	A	1207	2MG	C5-N7	2.10	1.40	1.38
1	A	966	M2G	C2-N1	2.04	1.40	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-C5-N7	-55.65	126.65	134.14
1	A	966	M2G	C6-C5-N7	-49.94	127.42	134.14
1	A	966	M2G	C6-N1-C2	7.20	123.33	120.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-3.97	94.32	101.29
1	A	1540	PSU	C5-C1'-C2'	-3.83	108.63	115.73
1	A	967	5MC	C2-N3-C4	3.47	118.82	115.50
1	A	1404	5MC	C2-N3-C4	3.39	118.75	115.50
1	A	1400	5MC	C2-N3-C4	3.23	118.59	115.50
1	A	1207	2MG	C6-N1-C2	3.14	121.97	120.20
1	A	966	M2G	N1-C2-N2	-2.87	114.80	118.37
1	A	1207	2MG	C6-C5-C4	2.80	121.58	117.53
1	A	1207	2MG	N3-C4-N9	2.80	131.01	126.91
1	A	516	PSU	C4-N3-C2	-2.78	119.72	125.36
1	A	1407	5MC	C2-N3-C4	2.74	118.13	115.50
12	L	92	0TD	C-CA-N	-2.67	107.59	111.94
1	A	1541	PSU	C4-N3-C2	-2.66	119.97	125.36
1	A	966	M2G	C6-C5-C4	2.62	121.32	117.53
1	A	1540	PSU	C4-N3-C2	-2.61	120.07	125.36
1	A	1519	MA6	C2-N1-C6	2.47	116.86	111.52
1	A	1207	2MG	C4-C5-N7	2.44	111.77	109.41
1	A	1541	PSU	C5-C1'-C2'	-2.38	111.32	115.73
1	A	1498	UR3	C6-C5-C4	2.37	121.56	117.18
1	A	1518	MA6	C2-N1-C6	2.30	116.51	111.52
1	A	1498	UR3	C3'-C2'-C1'	2.22	104.40	100.92
1	A	1400	5MC	CM5-C5-C6	2.20	123.18	118.60
1	A	1404	5MC	CM5-C5-C6	2.19	123.16	118.60
1	A	516	PSU	O4'-C1'-C2'	2.17	108.13	104.43
1	A	1519	MA6	N3-C4-N9	2.16	129.10	125.39
1	A	1407	5MC	N4-C4-N3	-2.11	113.97	116.99
1	A	967	5MC	CM5-C5-C6	2.08	122.93	118.60
1	A	966	M2G	C8-N9-C4	-2.03	105.31	106.96
1	A	1402	4OC	C2-N1-C1'	2.02	121.78	119.03
1	A	1518	MA6	N3-C4-N9	2.00	128.83	125.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1540	PSU	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 244 ligands modelled in this entry, 243 are monoatomic - leaving 1 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	$\# Z > 2$
22	SRY	A	1601	-	42,42,42	2.24	13 (30%)	63,63,63	1.82	12 (19%)

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
22	SRY	A	1601	-	-	0/22/87/87	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	8.06	1.48	1.33
22	A	1601	SRY	CA1-N11	6.59	1.45	1.33
22	A	1601	SRY	O53-C53	-3.68	1.35	1.44
22	A	1601	SRY	C32-C42	-3.45	1.49	1.54
22	A	1601	SRY	C23-N23	-2.98	1.42	1.47
22	A	1601	SRY	O51-C51	-2.69	1.36	1.43
22	A	1601	SRY	O32-C32	-2.57	1.39	1.44
22	A	1601	SRY	C32-C22	-2.36	1.51	1.54
22	A	1601	SRY	C21-C11	-2.36	1.48	1.53
22	A	1601	SRY	CA1-NB1	2.21	1.44	1.34
22	A	1601	SRY	CD1-NE1	2.14	1.44	1.34
22	A	1601	SRY	O43-C43	-2.09	1.37	1.43
22	A	1601	SRY	C32-CG2	-2.01	1.47	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	CI3-N23-C23	-5.47	109.34	113.65
22	A	1601	SRY	C13-O13-C22	-5.41	106.77	116.21
22	A	1601	SRY	C12-O42-C42	-4.75	100.68	108.36
22	A	1601	SRY	O41-C12-C22	4.24	115.47	107.32
22	A	1601	SRY	O41-C12-O42	-4.04	107.67	111.57
22	A	1601	SRY	O13-C13-C23	3.95	116.17	108.07
22	A	1601	SRY	O42-C42-C32	2.82	108.47	104.33
22	A	1601	SRY	C12-O41-C41	-2.73	111.06	118.00
22	A	1601	SRY	C13-O53-C53	-2.65	108.62	113.73
22	A	1601	SRY	C61-C11-N11	-2.34	105.63	110.60
22	A	1601	SRY	C11-N11-CA1	-2.15	120.02	123.97
22	A	1601	SRY	C31-N31-CD1	-2.08	120.14	123.97

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	1511/1522 (99%)	-0.23	29 (1%) 64 32	85, 130, 272, 382	0
2	B	234/256 (91%)	-0.13	0 100 100	98, 143, 227, 240	0
3	C	206/239 (86%)	0.31	11 (5%) 25 11	148, 207, 271, 304	0
4	D	208/209 (99%)	-0.12	1 (0%) 88 65	90, 127, 171, 259	0
5	E	150/162 (92%)	-0.19	0 100 100	77, 106, 136, 201	0
6	F	101/101 (100%)	-0.29	0 100 100	119, 143, 167, 214	0
7	G	155/156 (99%)	0.09	6 (3%) 37 17	135, 180, 230, 263	0
8	H	138/138 (100%)	-0.26	0 100 100	70, 93, 121, 166	0
9	I	127/128 (99%)	0.25	4 (3%) 47 22	136, 204, 249, 303	0
10	J	98/105 (93%)	0.70	7 (7%) 16 7	164, 247, 326, 391	0
11	K	116/129 (89%)	-0.13	0 100 100	96, 124, 170, 203	0
12	L	123/135 (91%)	0.01	1 (0%) 83 53	75, 128, 151, 199	0
13	M	118/126 (93%)	-0.05	1 (0%) 83 53	127, 156, 192, 327	0
14	N	60/61 (98%)	0.61	5 (8%) 11 7	165, 197, 252, 298	0
15	O	87/89 (97%)	-0.19	0 100 100	85, 113, 150, 163	0
16	P	83/88 (94%)	-0.14	0 100 100	104, 124, 153, 198	0
17	Q	99/105 (94%)	-0.22	0 100 100	85, 104, 135, 167	0
18	R	70/88 (79%)	-0.20	0 100 100	96, 124, 170, 215	0
19	S	80/93 (86%)	0.60	4 (5%) 28 12	159, 221, 278, 327	0
20	T	99/106 (93%)	-0.16	0 100 100	103, 119, 155, 199	0
21	U	24/27 (88%)	1.21	5 (20%) 1 2	141, 172, 202, 216	0
All	All	3887/4063 (95%)	-0.08	74 (1%) 64 32	70, 137, 253, 391	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1498	UR3	6.8
1	A	1018	C	6.2
3	C	103	VAL	6.2
1	A	1540	PSU	5.7
1	A	1541	PSU	5.4
3	C	65	ALA	5.4
1	A	793	U	5.1
10	J	37	PRO	5.1
3	C	193	TYR	4.6
1	A	994	A	4.4
10	J	34	VAL	4.1
3	C	66	VAL	4.0
1	A	1129	C	4.0
1	A	81	U	3.8
10	J	90	LEU	3.7
10	J	33	GLN	3.7
1	A	1037	C	3.7
3	C	102	ASN	3.6
1	A	1006	C	3.6
14	N	11	LYS	3.6
1	A	1002	G	3.5
21	U	18	TYR	3.4
1	A	1019	C	3.4
14	N	4	LYS	3.3
3	C	104	GLN	3.3
14	N	3	ARG	3.3
1	A	1257	U	3.3
21	U	24	ARG	3.2
1	A	1144	G	3.2
14	N	2	ALA	3.2
1	A	1539	C	3.1
21	U	25	LYS	3.0
1	A	993	G	3.0
9	I	9	ARG	3.0
9	I	8	GLY	3.0
7	G	79	ARG	2.9
1	A	1036	G	2.9
10	J	75	ILE	2.9
21	U	17	THR	2.7
4	D	35	ARG	2.7
19	S	38	SER	2.7
9	I	128	ARG	2.6
3	C	67	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	74	ILE	2.5
7	G	2	ALA	2.5
10	J	89	ASP	2.5
12	L	19	ARG	2.5
1	A	1026	G	2.4
3	C	68	VAL	2.3
1	A	1050	G	2.3
1	A	202	U	2.3
3	C	101	LEU	2.3
1	A	1216	G	2.3
1	A	1003	G	2.3
21	U	5	ASP	2.2
1	A	1003(A)	G	2.2
1	A	1007	C	2.2
1	A	1207	2MG	2.2
9	I	102	LEU	2.2
19	S	40	ILE	2.2
7	G	80	VAL	2.2
19	S	69	HIS	2.1
1	A	1140	C	2.1
3	C	87	LEU	2.1
1	A	1005	A	2.1
7	G	84	ASN	2.1
1	A	990	C	2.0
14	N	6	LEU	2.0
1	A	1033	G	2.0
7	G	83	ALA	2.0
13	M	117	VAL	2.0
19	S	81	ARG	2.0
7	G	154	TYR	2.0
3	C	156	ARG	2.0

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

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(\AA^2)	Q<0.9
1	MA6	A	1519	24/25	0.17	-	118,122,123,128	0
1	4OC	A	1402	22/23	0.22	-	120,124,130,131	0
12	0TD	L	92	10/11	0.38	-	122,125,128,294	0
1	UR3	A	1498	21/22	0.24	-	120,124,127,129	0
1	M2G	A	966	25/26	0.21	-	123,127,159,162	0
1	5MC	A	967	21/22	0.16	-	119,121,126,126	0
1	5MC	A	1407	21/22	0.15	-	132,139,146,152	0
1	PSU	A	516	20/21	0.10	-	131,135,144,144	0
1	5MC	A	1404	21/22	0.24	-	119,121,132,135	0
1	MA6	A	1518	24/25	0.14	-	122,126,137,140	0
1	5MC	A	1400	21/22	0.18	-	116,122,125,126	0
1	PSU	A	1540	20/21	0.59	-	279,294,305,305	0
1	PSU	A	1541	20/21	0.57	-	288,305,333,335	0
1	2MG	A	1207	24/25	0.32	-	201,210,224,228	0

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(\AA^2)	Q<0.9
23	MG	A	1735	1/1	0.13	-	74,74,74,74	0
23	MG	A	1624	1/1	0.09	-	74,74,74,74	0
23	MG	A	1693	1/1	0.14	-	121,121,121,121	0
23	MG	A	1713	1/1	0.62	-	121,121,121,121	0
23	MG	A	1754	1/1	0.20	-	106,106,106,106	0
23	MG	A	1672	1/1	0.13	-	91,91,91,91	0
23	MG	A	1792	1/1	0.14	-	98,98,98,98	0
23	MG	A	1704	1/1	0.21	-	76,76,76,76	0
23	MG	A	1785	1/1	0.16	-	304,304,304,304	0
23	MG	A	1757	1/1	0.35	-	84,84,84,84	0
23	MG	A	1789	1/1	0.21	-	81,81,81,81	0
23	MG	A	1626	1/1	0.09	-	113,113,113,113	0
23	MG	Q	201	1/1	0.07	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1763	1/1	0.61	-	106,106,106,106	0
23	MG	A	1737	1/1	0.90	-	73,73,73,73	0
23	MG	A	1675	1/1	0.24	-	119,119,119,119	0
23	MG	A	1621	1/1	0.29	-	98,98,98,98	0
23	MG	A	1773	1/1	0.12	-	75,75,75,75	0
23	MG	A	1665	1/1	0.09	-	128,128,128,128	0
23	MG	A	1738	1/1	0.14	-	86,86,86,86	0
23	MG	A	1709	1/1	0.13	-	172,172,172,172	0
23	MG	A	1699	1/1	0.21	-	289,289,289,289	0
23	MG	A	1659	1/1	0.09	-	138,138,138,138	0
23	MG	A	1815	1/1	0.24	-	108,108,108,108	0
23	MG	A	1753	1/1	0.39	-	51,51,51,51	0
23	MG	A	1724	1/1	0.34	-	57,57,57,57	0
23	MG	A	1681	1/1	0.15	-	82,82,82,82	0
23	MG	A	1783	1/1	0.16	-	129,129,129,129	0
23	MG	A	1606	1/1	0.07	-	106,106,106,106	0
23	MG	A	1776	1/1	0.42	-	106,106,106,106	0
23	MG	A	1728	1/1	0.08	-	97,97,97,97	0
23	MG	A	1605	1/1	0.28	-	75,75,75,75	0
23	MG	A	1637	1/1	0.25	-	81,81,81,81	0
23	MG	A	1749	1/1	0.27	-	77,77,77,77	0
23	MG	A	1700	1/1	0.13	-	136,136,136,136	0
23	MG	A	1747	1/1	0.43	-	89,89,89,89	0
23	MG	A	1781	1/1	0.07	-	119,119,119,119	0
23	MG	A	1634	1/1	0.17	-	115,115,115,115	0
23	MG	A	1683	1/1	1.05	-	91,91,91,91	0
23	MG	A	1667	1/1	0.26	-	141,141,141,141	0
23	MG	A	1770	1/1	0.07	-	76,76,76,76	0
23	MG	A	1720	1/1	0.38	-	82,82,82,82	0
23	MG	A	1688	1/1	0.17	-	135,135,135,135	0
23	MG	A	1787	1/1	0.50	-	86,86,86,86	0
23	MG	A	1632	1/1	0.15	-	95,95,95,95	0
23	MG	A	1767	1/1	0.20	-	104,104,104,104	0
23	MG	A	1616	1/1	0.25	-	54,54,54,54	0
22	SRY	A	1601	40/40	0.22	-	86,104,124,135	0
23	MG	A	1643	1/1	0.09	-	81,81,81,81	0
23	MG	N	102	1/1	0.32	-	96,96,96,96	0
23	MG	A	1639	1/1	0.10	-	44,44,44,44	0
23	MG	A	1743	1/1	0.21	-	70,70,70,70	0
23	MG	A	1701	1/1	0.19	-	93,93,93,93	0
23	MG	A	1663	1/1	0.18	-	65,65,65,65	0
23	MG	D	302	1/1	0.12	-	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1614	1/1	0.16	-	66,66,66,66	0
23	MG	A	1730	1/1	0.14	-	148,148,148,148	0
23	MG	A	1692	1/1	0.09	-	143,143,143,143	0
23	MG	A	1646	1/1	0.19	-	111,111,111,111	0
23	MG	A	1612	1/1	0.08	-	101,101,101,101	0
23	MG	A	1800	1/1	0.41	-	131,131,131,131	0
23	MG	A	1679	1/1	0.21	-	121,121,121,121	0
23	MG	A	1630	1/1	0.18	-	79,79,79,79	0
23	MG	A	1677	1/1	0.16	-	126,126,126,126	0
23	MG	A	1654	1/1	0.12	-	115,115,115,115	0
23	MG	A	1641	1/1	0.10	-	101,101,101,101	0
23	MG	A	1826	1/1	0.15	-	119,119,119,119	0
23	MG	A	1694	1/1	0.15	-	144,144,144,144	0
23	MG	A	1674	1/1	0.26	-	68,68,68,68	0
23	MG	A	1687	1/1	0.24	-	76,76,76,76	0
23	MG	H	201	1/1	0.23	-	56,56,56,56	0
23	MG	A	1813	1/1	0.10	-	81,81,81,81	0
23	MG	A	1802	1/1	0.72	-	101,101,101,101	0
23	MG	A	1725	1/1	0.18	-	74,74,74,74	0
23	MG	A	1610	1/1	0.18	-	102,102,102,102	0
23	MG	A	1653	1/1	0.17	-	87,87,87,87	0
23	MG	A	1805	1/1	0.50	-	108,108,108,108	0
23	MG	A	1752	1/1	0.12	-	110,110,110,110	0
23	MG	A	1708	1/1	0.12	-	111,111,111,111	0
23	MG	A	1715	1/1	0.47	-	110,110,110,110	0
23	MG	A	1680	1/1	0.18	-	139,139,139,139	0
23	MG	A	1807	1/1	0.21	-	222,222,222,222	0
23	MG	A	1727	1/1	0.23	-	92,92,92,92	0
23	MG	A	1673	1/1	0.11	-	88,88,88,88	0
23	MG	A	1734	1/1	0.14	-	77,77,77,77	0
23	MG	A	1774	1/1	0.21	-	79,79,79,79	0
23	MG	A	1670	1/1	0.21	-	170,170,170,170	0
23	MG	A	1686	1/1	0.20	-	102,102,102,102	0
23	MG	A	1629	1/1	0.16	-	180,180,180,180	0
23	MG	A	1748	1/1	0.25	-	63,63,63,63	0
23	MG	A	1822	1/1	1.23	-	104,104,104,104	0
23	MG	E	201	1/1	0.07	-	83,83,83,83	0
23	MG	A	1710	1/1	0.07	-	168,168,168,168	0
23	MG	A	1821	1/1	0.09	-	106,106,106,106	0
23	MG	A	1619	1/1	0.09	-	49,49,49,49	0
23	MG	A	1828	1/1	0.26	-	91,91,91,91	0
23	MG	A	1684	1/1	0.13	-	168,168,168,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1645	1/1	0.11	-	164,164,164,164	0
23	MG	A	1761	1/1	0.14	-	89,89,89,89	0
23	MG	A	1742	1/1	0.15	-	97,97,97,97	0
23	MG	A	1810	1/1	0.10	-	433,433,433,433	0
23	MG	Q	202	1/1	0.28	-	55,55,55,55	0
23	MG	A	1750	1/1	0.31	-	77,77,77,77	0
23	MG	P	102	1/1	0.27	-	80,80,80,80	0
23	MG	A	1782	1/1	0.12	-	93,93,93,93	0
23	MG	A	1716	1/1	0.22	-	68,68,68,68	0
23	MG	A	1718	1/1	0.28	-	90,90,90,90	0
23	MG	A	1666	1/1	0.21	-	104,104,104,104	0
23	MG	A	1816	1/1	0.14	-	132,132,132,132	0
23	MG	A	1662	1/1	0.25	-	89,89,89,89	0
23	MG	A	1625	1/1	0.33	-	137,137,137,137	0
23	MG	A	1759	1/1	0.81	-	70,70,70,70	0
23	MG	A	1784	1/1	0.15	-	170,170,170,170	0
23	MG	A	1755	1/1	0.29	-	73,73,73,73	0
23	MG	A	1617	1/1	0.20	-	87,87,87,87	0
23	MG	A	1765	1/1	0.33	-	53,53,53,53	0
23	MG	A	1604	1/1	0.17	-	90,90,90,90	0
23	MG	A	1682	1/1	0.46	-	107,107,107,107	0
23	MG	A	1644	1/1	0.16	-	78,78,78,78	0
23	MG	A	1691	1/1	0.15	-	186,186,186,186	0
23	MG	A	1790	1/1	0.37	-	78,78,78,78	0
23	MG	A	1678	1/1	0.17	-	91,91,91,91	0
23	MG	A	1736	1/1	0.11	-	114,114,114,114	0
23	MG	A	1799	1/1	0.30	-	79,79,79,79	0
23	MG	A	1793	1/1	0.17	-	100,100,100,100	0
23	MG	A	1620	1/1	0.15	-	85,85,85,85	0
23	MG	A	1779	1/1	0.28	-	139,139,139,139	0
23	MG	A	1707	1/1	0.10	-	120,120,120,120	0
23	MG	A	1814	1/1	0.88	-	98,98,98,98	0
23	MG	A	1651	1/1	0.08	-	96,96,96,96	0
23	MG	A	1627	1/1	0.17	-	76,76,76,76	0
23	MG	A	1818	1/1	0.24	-	79,79,79,79	0
23	MG	A	1652	1/1	0.19	-	129,129,129,129	0
23	MG	A	1819	1/1	0.22	-	68,68,68,68	0
23	MG	A	1669	1/1	0.23	-	104,104,104,104	0
23	MG	A	1729	1/1	0.40	-	124,124,124,124	0
23	MG	A	1705	1/1	0.16	-	185,185,185,185	0
23	MG	A	1628	1/1	0.13	-	99,99,99,99	0
23	MG	A	1798	1/1	0.78	-	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1794	1/1	0.64	-	56,56,56,56	0
23	MG	A	1702	1/1	0.12	-	153,153,153,153	0
23	MG	A	1671	1/1	0.41	-	73,73,73,73	0
23	MG	A	1726	1/1	1.05	-	106,106,106,106	0
23	MG	H	203	1/1	0.39	-	76,76,76,76	0
23	MG	A	1636	1/1	0.32	-	76,76,76,76	0
23	MG	A	1746	1/1	0.17	-	100,100,100,100	0
23	MG	A	1739	1/1	0.23	-	55,55,55,55	0
23	MG	A	1655	1/1	0.24	-	116,116,116,116	0
23	MG	A	1613	1/1	0.06	-	102,102,102,102	0
23	MG	A	1695	1/1	0.23	-	273,273,273,273	0
23	MG	A	1712	1/1	0.15	-	83,83,83,83	0
23	MG	A	1656	1/1	0.15	-	76,76,76,76	0
23	MG	A	1668	1/1	0.09	-	105,105,105,105	0
23	MG	A	1603	1/1	0.23	-	90,90,90,90	0
23	MG	A	1731	1/1	0.07	-	90,90,90,90	0
23	MG	A	1795	1/1	0.57	-	108,108,108,108	0
23	MG	A	1685	1/1	0.43	-	72,72,72,72	0
23	MG	A	1721	1/1	0.15	-	100,100,100,100	0
23	MG	A	1780	1/1	0.16	-	84,84,84,84	0
23	MG	A	1633	1/1	0.28	-	130,130,130,130	0
23	MG	A	1649	1/1	0.22	-	67,67,67,67	0
23	MG	A	1772	1/1	0.35	-	107,107,107,107	0
23	MG	A	1623	1/1	0.12	-	58,58,58,58	0
23	MG	A	1664	1/1	0.07	-	135,135,135,135	0
23	MG	A	1764	1/1	0.28	-	146,146,146,146	0
23	MG	P	101	1/1	0.34	-	52,52,52,52	0
23	MG	A	1771	1/1	0.12	-	76,76,76,76	0
24	ZN	N	101	1/1	0.14	-	170,170,170,170	0
23	MG	A	1744	1/1	0.19	-	96,96,96,96	0
23	MG	T	201	1/1	0.33	-	87,87,87,87	0
23	MG	A	1786	1/1	0.19	-	180,180,180,180	0
23	MG	A	1635	1/1	0.13	-	61,61,61,61	0
23	MG	M	201	1/1	0.31	-	91,91,91,91	0
23	MG	A	1732	1/1	0.16	-	73,73,73,73	0
23	MG	A	1607	1/1	0.35	-	91,91,91,91	0
23	MG	A	1777	1/1	0.17	-	83,83,83,83	0
23	MG	A	1801	1/1	0.19	-	70,70,70,70	0
23	MG	A	1808	1/1	0.28	-	205,205,205,205	0
23	MG	A	1676	1/1	0.05	-	157,157,157,157	0
23	MG	A	1788	1/1	0.41	-	99,99,99,99	0
23	MG	A	1660	1/1	0.09	-	123,123,123,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1820	1/1	0.24	-	83,83,83,83	0
23	MG	A	1622	1/1	0.35	-	110,110,110,110	0
23	MG	A	1740	1/1	0.35	-	99,99,99,99	0
23	MG	A	1719	1/1	0.38	-	95,95,95,95	0
23	MG	A	1696	1/1	0.12	-	105,105,105,105	0
23	MG	A	1762	1/1	0.58	-	110,110,110,110	0
23	MG	A	1611	1/1	0.18	-	104,104,104,104	0
23	MG	A	1804	1/1	0.11	-	78,78,78,78	0
23	MG	A	1642	1/1	0.23	-	47,47,47,47	0
23	MG	A	1775	1/1	0.25	-	116,116,116,116	0
23	MG	A	1698	1/1	0.20	-	85,85,85,85	0
23	MG	A	1803	1/1	0.23	-	92,92,92,92	0
23	MG	A	1658	1/1	0.18	-	190,190,190,190	0
23	MG	A	1722	1/1	0.20	-	82,82,82,82	0
23	MG	A	1723	1/1	0.51	-	72,72,72,72	0
23	MG	A	1791	1/1	0.09	-	105,105,105,105	0
23	MG	A	1640	1/1	0.24	-	102,102,102,102	0
23	MG	A	1602	1/1	0.19	-	112,112,112,112	0
23	MG	B	301	1/1	0.59	-	120,120,120,120	0
23	MG	A	1756	1/1	0.08	-	94,94,94,94	0
23	MG	A	1769	1/1	0.38	-	102,102,102,102	0
23	MG	A	1647	1/1	0.14	-	89,89,89,89	0
23	MG	A	1657	1/1	0.24	-	96,96,96,96	0
23	MG	A	1751	1/1	0.96	-	94,94,94,94	0
23	MG	A	1618	1/1	0.33	-	73,73,73,73	0
23	MG	A	1809	1/1	0.22	-	187,187,187,187	0
23	MG	A	1797	1/1	0.19	-	75,75,75,75	0
23	MG	A	1760	1/1	0.34	-	128,128,128,128	0
23	MG	A	1806	1/1	0.21	-	334,334,334,334	0
23	MG	A	1778	1/1	0.26	-	149,149,149,149	0
23	MG	A	1631	1/1	0.14	-	80,80,80,80	0
23	MG	A	1758	1/1	0.10	-	81,81,81,81	0
23	MG	A	1827	1/1	0.12	-	74,74,74,74	0
23	MG	A	1825	1/1	0.15	-	96,96,96,96	0
23	MG	H	202	1/1	0.16	-	57,57,57,57	0
23	MG	A	1817	1/1	0.26	-	63,63,63,63	0
23	MG	A	1812	1/1	0.40	-	68,68,68,68	0
23	MG	A	1714	1/1	0.10	-	110,110,110,110	0
23	MG	A	1609	1/1	0.17	-	72,72,72,72	0
23	MG	A	1661	1/1	0.82	-	91,91,91,91	0
23	MG	A	1768	1/1	0.19	-	79,79,79,79	0
23	MG	A	1717	1/1	0.15	-	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1796	1/1	0.30	-	131,131,131,131	0
23	MG	A	1689	1/1	0.10	-	105,105,105,105	0
23	MG	A	1690	1/1	1.01	-	95,95,95,95	0
23	MG	A	1811	1/1	0.27	-	122,122,122,122	0
23	MG	A	1615	1/1	0.13	-	47,47,47,47	0
23	MG	A	1823	1/1	0.08	-	127,127,127,127	0
23	MG	A	1745	1/1	0.12	-	53,53,53,53	0
24	ZN	D	301	1/1	0.33	-	71,71,71,71	0
23	MG	A	1711	1/1	0.30	-	90,90,90,90	0
23	MG	A	1741	1/1	0.41	-	96,96,96,96	0
23	MG	A	1638	1/1	0.16	-	156,156,156,156	0
23	MG	A	1706	1/1	0.23	-	114,114,114,114	0
23	MG	A	1697	1/1	0.17	-	171,171,171,171	0
23	MG	A	1650	1/1	0.29	-	77,77,77,77	0
23	MG	A	1648	1/1	0.10	-	100,100,100,100	0
23	MG	A	1824	1/1	0.29	-	104,104,104,104	0
23	MG	A	1608	1/1	0.08	-	97,97,97,97	0
23	MG	A	1766	1/1	0.08	-	105,105,105,105	0
23	MG	A	1733	1/1	0.29	-	82,82,82,82	0
23	MG	U	101	1/1	0.25	-	129,129,129,129	0
23	MG	A	1703	1/1	0.15	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.