



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 6, 2017 – 02:03 PM EDT

PDB ID : 5NO2
EMDB ID: : EMD-3661
Title : RsgA-GDPNP bound to the 30S ribosomal subunit (RsgA assembly intermediate)
Authors : Lopez-Alonso, J.P.; Kaminishi, T.; Kikuchi, T.; Hirata, Y.; Iturrioz, I.; Dhimole, N.; Schedlbauer, A.; Hase, Y.; Goto, S.; Kurita, D.; Muto, A.; Zhou, S.; Naoe, C.; Mills, D.J.; Gil-Carton, D.; Takemoto, C.; Himeno, H.; Fucini, P.; Connell, S.R.
Deposited on : unknown
Resolution : 5.16 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

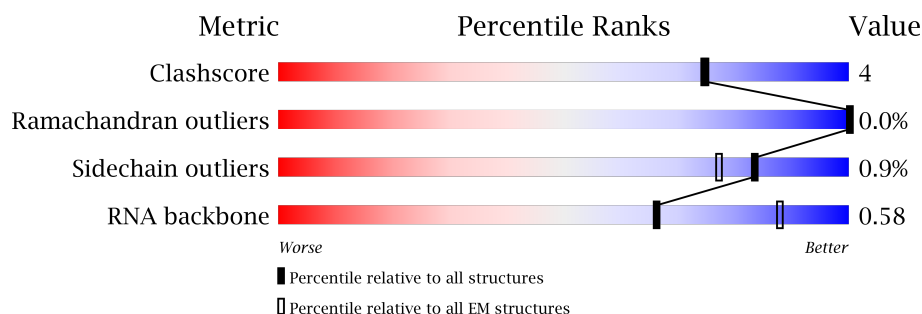
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.16 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1534	74% 24% .
2	D	205	80% 20%
3	E	155	88% 12%
4	F	106	92% 8%
5	G	130	74% 8% 18%
6	H	129	93% 7%
7	I	127	82% 16% .

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Mol	Chain	Length	Quality of chain
8	J	99	 82% 18%
9	K	117	 85% 15%
10	L	14	 71% 29%
11	M	114	 91% 9%
12	N	100	 83% 17%
13	O	88	 95% 5%
14	P	82	 89% 11%
15	Q	80	 89% 11%
16	R	55	 93% 7%
17	S	79	 84% 16%
18	T	86	 86% 14%
19	Z	313	 85% 14% .

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 49225 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 4 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 5 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	107	Total	C	N	O	S	0	0
			841	525	160	153	3		

- Molecule 6 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 7 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 8 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	99	Total	C	N	O	S	0	0
			796	498	152	145	1		

- Molecule 9 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	14	Total	C	N	O	0	0
			114	70	27	17		

- Molecule 11 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 12 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 13 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 14 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 15 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 17 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 19 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	313	Total	C	N	O	S	0	0
			2448	1538	432	468	10		

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	P	1	Total	Mg	0
			1	1	
20	Z	1	Total	Mg	0
			1	1	
20	A	67	Total	Mg	0
			67	67	

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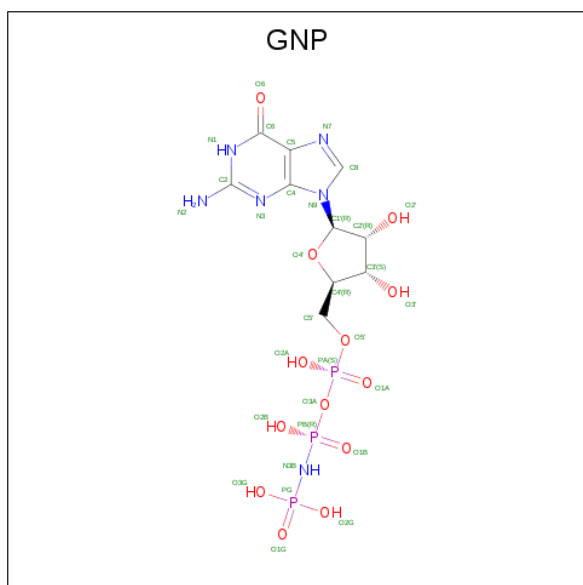
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Mol	Chain	Residues	Atoms		AltConf
20	T	1	Total	Mg	0
			1	1	
20	N	1	Total	Mg	0
			1	1	

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	Z	1	Total	Zn	0
			1	1	

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

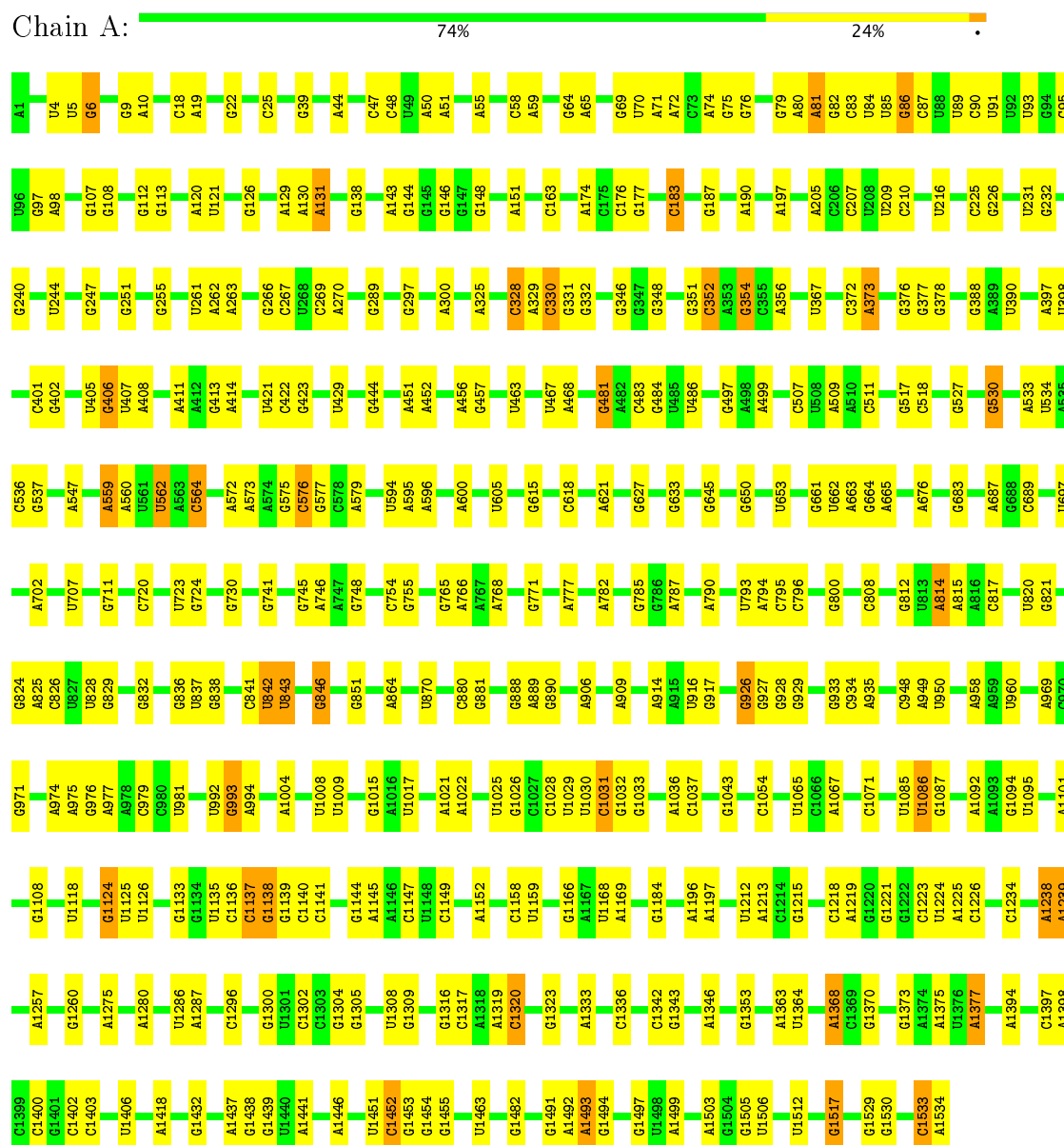


Mol	Chain	Residues	Atoms					AltConf
22	Z	1	Total	C	N	O	P	0
			32	10	6	13	3	

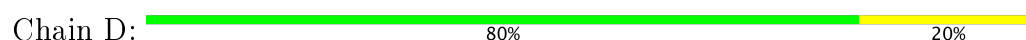
3 Residue-property plots

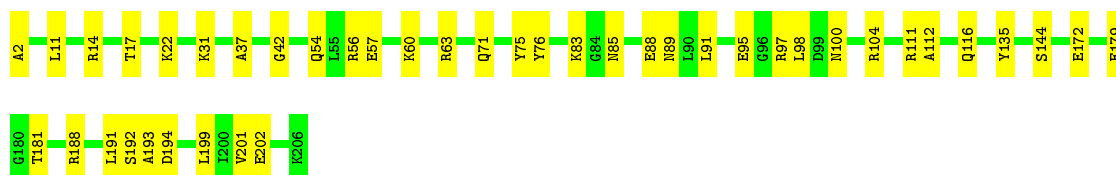
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: 16S ribosomal RNA



- Molecule 2: 30S ribosomal protein S4





- Molecule 3: 30S ribosomal protein S5

Chain E: 88% 12%



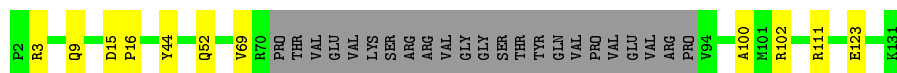
- Molecule 4: 30S ribosomal protein S6

Chain F: 92% 8%



- Molecule 5: 30S ribosomal protein S7

Chain G: 74% 8% 18%



- Molecule 6: 30S ribosomal protein S8

Chain H: 93% 7%



- Molecule 7: 30S ribosomal protein S9

Chain I: 82% 16%



- Molecule 8: 30S ribosomal protein S10

Chain J: 82% 18%



- Molecule 9: 30S ribosomal protein S11

Chain K: 85% 15%



- Molecule 10: 30S ribosomal protein S12

Chain L: 71% 29%



- Molecule 11: 30S ribosomal protein S13

Chain M: 91% 9%



- Molecule 12: 30S ribosomal protein S14

Chain N: 83% 17%



- Molecule 13: 30S ribosomal protein S15

Chain O: 95% 5%



- Molecule 14: 30S ribosomal protein S16

Chain P: 89% 11%



- Molecule 15: 30S ribosomal protein S17

Chain Q: 89% 11%




- Molecule 16: 30S ribosomal protein S18

Chain R: 93% 7%




- Molecule 17: 30S ribosomal protein S19

Chain S:  84% 16%




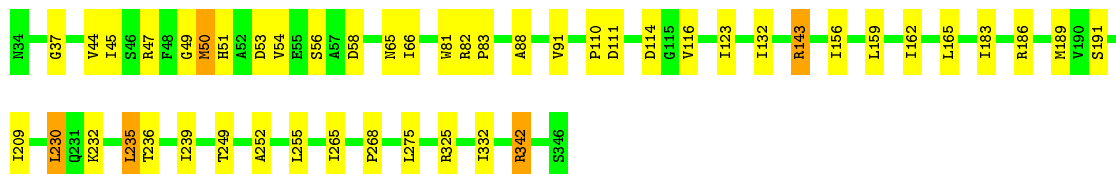
- Molecule 18: 30S ribosomal protein S20

Chain T:  86% 14%



- Molecule 19: Small ribosomal subunit biogenesis GTPase RsgA

Chain Z:  85% 14% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	101000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, G7M, MG, GNP, 2MG, 5MC, UR3, 4OC, 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 >2	RMSZ	# Z >2
1	A	0.19	0/36593	0.80	11/57081 (0.0%)
10	L	0.22	0/114	0.41	0/151
11	M	0.25	0/893	0.50	0/1193
12	N	0.23	0/817	0.44	0/1088
13	O	0.23	0/722	0.47	0/964
14	P	0.24	0/659	0.47	0/884
15	Q	0.24	0/658	0.50	0/881
16	R	0.22	0/463	0.41	0/621
17	S	0.25	0/653	0.49	0/877
18	T	0.24	0/676	0.42	0/895
19	Z	0.26	0/2493	0.56	2/3376 (0.1%)
2	D	0.24	0/1665	0.43	0/2227
3	E	0.26	0/1157	0.51	0/1557
4	F	0.25	0/881	0.48	0/1189
5	G	0.25	0/848	0.47	0/1132
6	H	0.25	0/989	0.48	0/1326
7	I	0.26	0/1034	0.55	0/1375
8	J	0.24	0/806	0.50	0/1089
9	K	0.25	0/893	0.47	0/1205
All	All	0.21	0/53014	0.72	13/79111 (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
19	Z	0	2
8	J	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	C	N1-C2-O2	8.46	123.98	118.90
1	A	1158	C	C2-N1-C1'	8.43	128.07	118.80
19	Z	230	LEU	CA-CB-CG	6.92	131.22	115.30
1	A	754	C	C2-N1-C1'	6.85	126.34	118.80
1	A	1158	C	N3-C2-O2	-6.80	117.14	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	57	VAL	Peptide
19	Z	235	LEU	Peptide
19	Z	342	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32930	0	16591	127	0
2	D	1643	0	1707	24	0
3	E	1144	0	1185	10	0
4	F	862	0	864	4	0
5	G	841	0	886	7	0
6	H	979	0	1031	5	0
7	I	1022	0	1070	18	0
8	J	796	0	836	12	0
9	K	877	0	887	10	0
10	L	114	0	131	3	0
11	M	884	0	941	8	0
12	N	805	0	844	13	0
13	O	714	0	734	2	0
14	P	649	0	666	7	0
15	Q	649	0	691	5	0
16	R	456	0	478	3	0
17	S	638	0	665	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	T	670	0	719	9	0
19	Z	2448	0	2419	27	0
20	A	67	0	0	0	0
20	N	1	0	0	0	0
20	P	1	0	0	0	0
20	T	1	0	0	0	0
20	Z	1	0	0	0	0
21	Z	1	0	0	0	0
22	Z	32	0	13	0	0
All	All	49225	0	33358	249	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 249 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:89:HIS:HB2	3:E:139:ALA:HB2	1.78	0.66
19:Z:252:ALA:HA	19:Z:268:PRO:HG3	1.79	0.65
1:A:376:G:H5''	14:P:5:ARG:HB2	1.81	0.62
8:J:6:ILE:HG22	8:J:102:LEU:HA	1.83	0.61
3:E:76:LEU:HD11	3:E:120:VAL:HG22	1.83	0.61

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 PDB entries followed by that with respect to all EM entries.

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	D	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
3	E	153/155 (99%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
5	G	103/130 (79%)	100 (97%)	3 (3%)	0	100	100
6	H	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
7	I	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
8	J	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
9	K	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
10	L	12/14 (86%)	12 (100%)	0	0	100	100
11	M	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
12	N	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
13	O	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
15	Q	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
16	R	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
17	S	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
18	T	84/86 (98%)	84 (100%)	0	0	100	100
19	Z	311/313 (99%)	294 (94%)	16 (5%)	1 (0%)	44	81
All	All	2018/2079 (97%)	1938 (96%)	79 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	236	THR

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 PDB entries followed by that with respect to all EM entries.

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	D	172/172 (100%)	172 (100%)	0	100	100
3	E	118/118 (100%)	117 (99%)	1 (1%)	85	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	92/92 (100%)	91 (99%)	1 (1%)	78	88
5	G	88/109 (81%)	87 (99%)	1 (1%)	78	88
6	H	104/104 (100%)	104 (100%)	0	100	100
7	I	105/105 (100%)	102 (97%)	3 (3%)	48	73
8	J	87/87 (100%)	87 (100%)	0	100	100
9	K	90/90 (100%)	89 (99%)	1 (1%)	78	88
10	L	12/12 (100%)	11 (92%)	1 (8%)	13	44
11	M	92/92 (100%)	92 (100%)	0	100	100
12	N	83/83 (100%)	82 (99%)	1 (1%)	75	88
13	O	76/76 (100%)	75 (99%)	1 (1%)	73	87
14	P	65/65 (100%)	65 (100%)	0	100	100
15	Q	74/74 (100%)	74 (100%)	0	100	100
16	R	48/48 (100%)	48 (100%)	0	100	100
17	S	70/70 (100%)	68 (97%)	2 (3%)	48	73
18	T	65/65 (100%)	65 (100%)	0	100	100
19	Z	267/267 (100%)	263 (98%)	4 (2%)	70	86
All	All	1708/1729 (99%)	1692 (99%)	16 (1%)	83	91

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	L	5	ASN
12	N	85	ARG
19	Z	50	MET
9	K	128	ARG
19	Z	143	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
7	I	126	GLN
9	K	15	GLN
17	S	57	HIS
7	I	75	GLN
18	T	84	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1530/1534 (99%)	246 (16%)	2 (0%)

5 of 246 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	9	G
1	A	19	A
1	A	22	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	209	U
1	A	1031	C

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

11 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	19,26,27	1.27	2 (10%)	20,38,41	2.26	7 (35%)
1	4OC	A	1402	1	16,23,24	0.63	0	19,32,35	1.10	2 (10%)
1	5MC	A	1407	1	15,22,23	1.42	1 (6%)	17,32,35	0.99	1 (5%)
1	UR3	A	1498	1,20	14,22,23	0.76	0	16,32,35	0.70	0
1	2MG	A	1516	1	19,26,27	1.28	2 (10%)	20,38,41	2.28	7 (35%)
1	MA6	A	1518	1	16,26,27	1.04	1 (6%)	18,38,41	2.45	7 (38%)
1	MA6	A	1519	1	16,26,27	0.99	1 (6%)	18,38,41	2.47	7 (38%)
1	PSU	A	516	1,20	16,21,22	1.28	1 (6%)	20,30,33	3.52	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	A	527	1	19,26,27	1.15	1 (5%)	19,39,42	2.35	6 (31%)
1	2MG	A	966	1	19,26,27	1.28	2 (10%)	20,38,41	2.29	7 (35%)
1	5MC	A	967	1	15,22,23	1.42	1 (6%)	17,32,35	1.00	2 (11%)

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	-	0/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1,20	-	0/3/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	516	1,20	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	0/3/25/26	0/3/3/3
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PSU	C5-C1'	-3.50	1.49	1.52
1	A	1516	2MG	C5-C4	2.98	1.47	1.40
1	A	1207	2MG	C5-C4	3.03	1.47	1.40
1	A	966	2MG	C5-C4	3.03	1.47	1.40
1	A	1519	MA6	C5-C4	3.04	1.47	1.40

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-9.33	121.69	128.40
1	A	516	PSU	C5-C4-N3	-8.52	118.44	125.43
1	A	1519	MA6	N3-C2-N1	-6.12	123.53	128.86
1	A	1518	MA6	N3-C2-N1	-5.66	123.93	128.86
1	A	527	G7M	C5-C6-N1	-4.38	117.25	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 72 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	GNP	Z	402	20	27,34,34	2.65	8 (29%)	26,54,54	1.74	7 (26%)

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	GNP	Z	402	20	-	0/16/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	402	GNP	C4-N9	-7.20	1.38	1.47
22	Z	402	GNP	C5-C6	-6.13	1.41	1.53
22	Z	402	GNP	PB-O3A	-4.93	1.53	1.59
22	Z	402	GNP	C8-N9	-3.05	1.37	1.46
22	Z	402	GNP	PB-O2B	-3.03	1.48	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
22	Z	402	GNP	O3G-PG-O1G	-3.57	104.33	113.41
22	Z	402	GNP	O1B-PB-N3B	-2.39	108.22	111.79
22	Z	402	GNP	PA-O3A-PB	-2.31	124.23	132.38
22	Z	402	GNP	O6-C6-N1	-2.04	119.98	122.70
22	Z	402	GNP	O3G-PG-O2G	2.79	115.50	107.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.