



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 6, 2017 – 05:28 PM EDT

PDB ID : 5NO3
EMDB ID: : EMD-3662
Title : RsgA-GDPNP bound to the 30S ribosomal subunit (RsgA assembly intermediate without uS3)
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

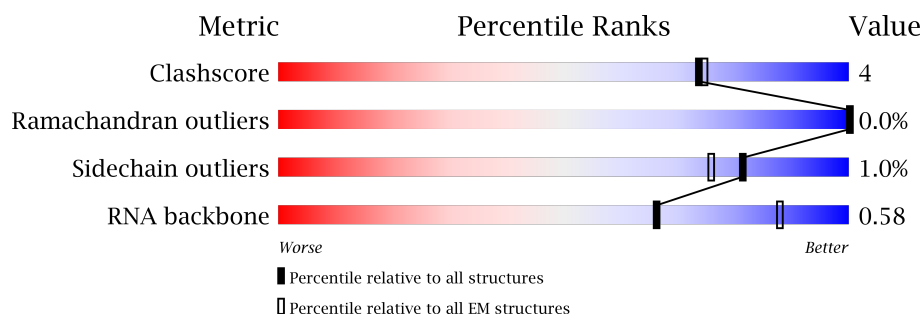
1 Overall quality at a glance

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.






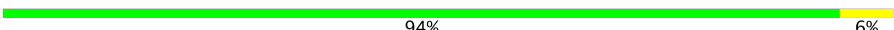

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	72% 26% .
2	B	224	91% 8% .
3	D	205	83% 17%
4	E	155	86% 14%
5	F	106	95% 5%
6	G	130	71% 12% 18%
7	H	129	92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	127	 81% 17% .
9	J	99	 86% 14%
10	K	117	 91% 9%
11	L	14	 71% 29%
12	M	114	 92% 8%
13	N	100	 83% 17%
14	O	88	 94% 6%
15	P	82	 78% 22%
16	Q	80	 89% 11%
17	R	55	 91% 9%
18	S	79	 84% 16%
19	T	86	 92% 8%
20	Z	313	 84% 14% .

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 50979 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 S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

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

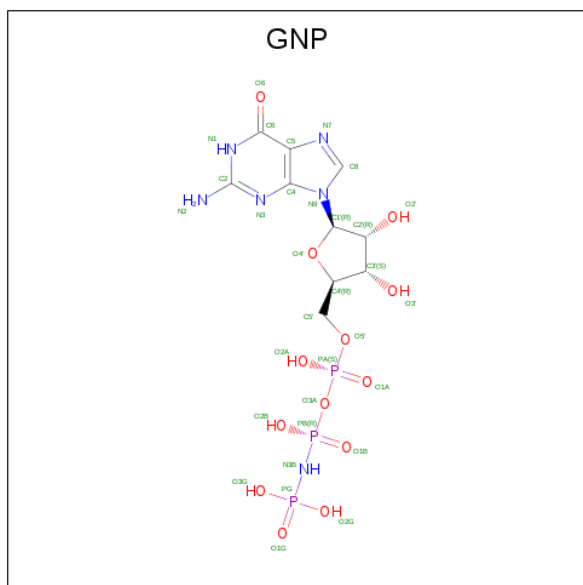
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	P	1	Total	Mg	0
			1	1	
21	Z	1	Total	Mg	0
			1	1	
21	A	67	Total	Mg	0
			67	67	
21	T	1	Total	Mg	0
			1	1	
21	N	1	Total	Mg	0
			1	1	

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	Zn	0
			1	1	
22	Z	1	Total	Zn	0
			1	1	

- Molecule 23 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

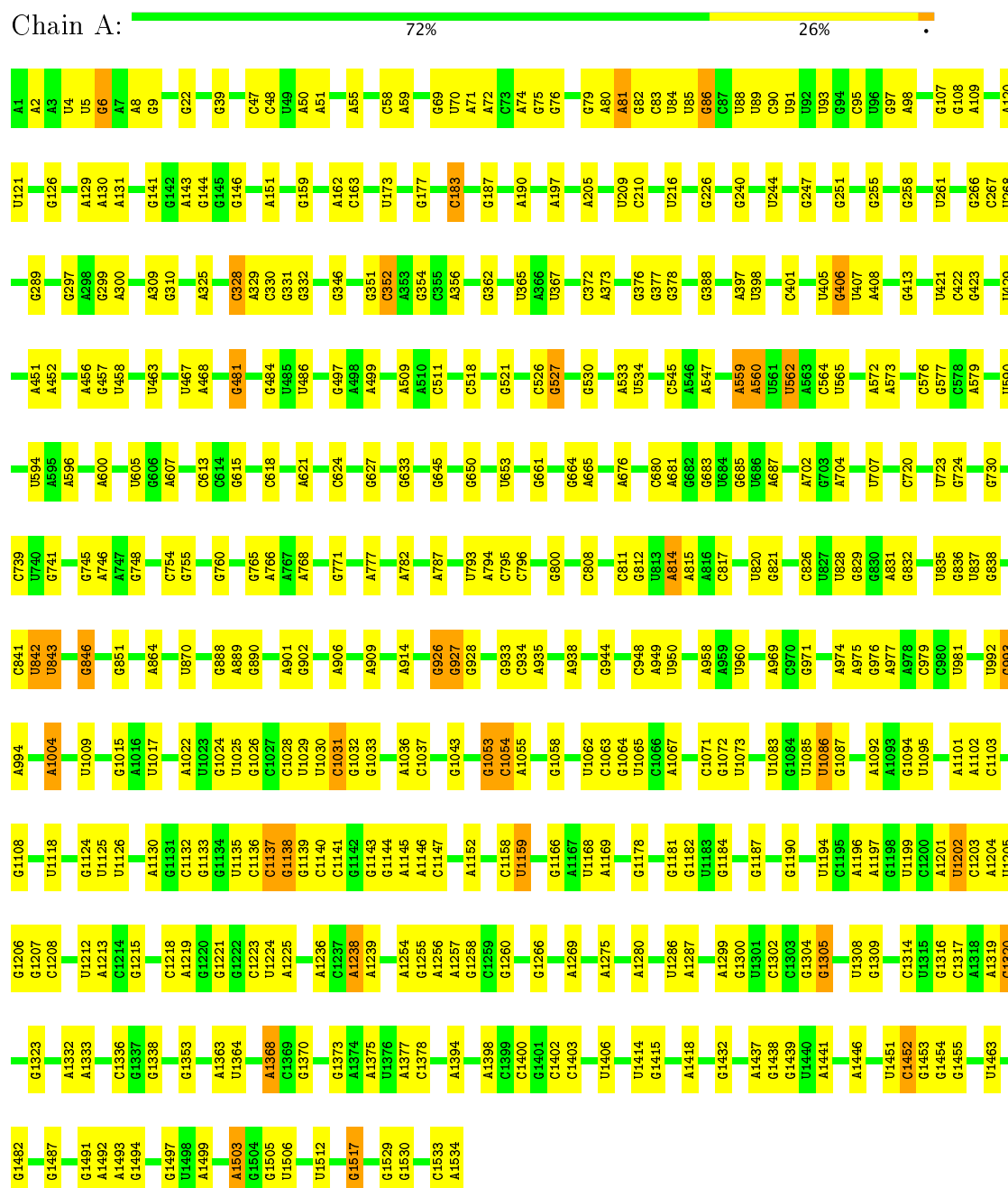


Mol	Chain	Residues	Atoms					AltConf
23	Z	1	Total	C	N	O	P	0
			32	10	6	13	3	

3 Residue-property plots [i](#)

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




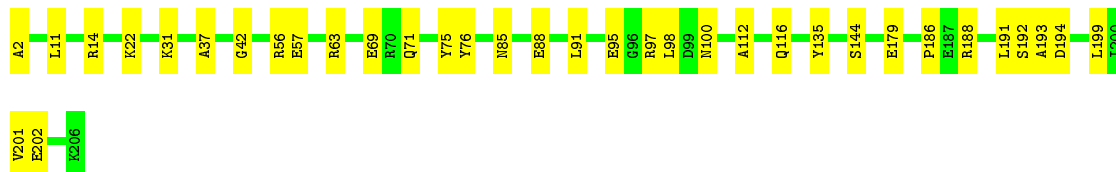
- Molecule 2: 30S ribosomal protein S2

Chain B:  91% 8%




- Molecule 3: 30S ribosomal protein S4

Chain D:  83% 17%



- Molecule 4: 30S ribosomal protein S5

Chain E:  86% 14%



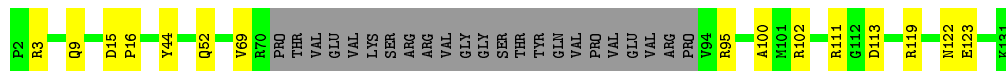
- Molecule 5: 30S ribosomal protein S6

Chain F:  95% 5%



- Molecule 6: 30S ribosomal protein S7

Chain G:  71% 12% 18%




- Molecule 7: 30S ribosomal protein S8

Chain H:  92% 8%

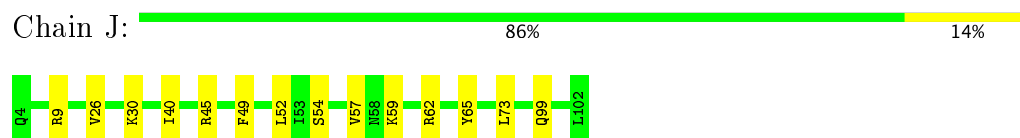


- Molecule 8: 30S ribosomal protein S9

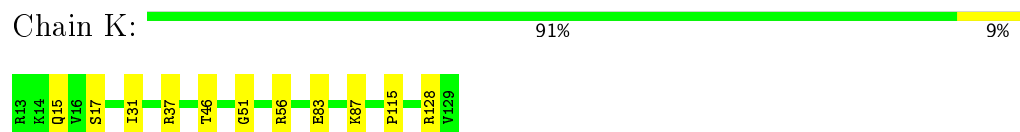
Chain I:  81% 17%



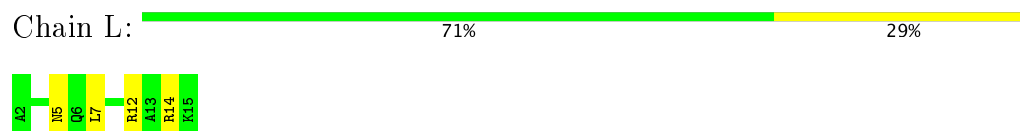
- Molecule 9: 30S ribosomal protein S10



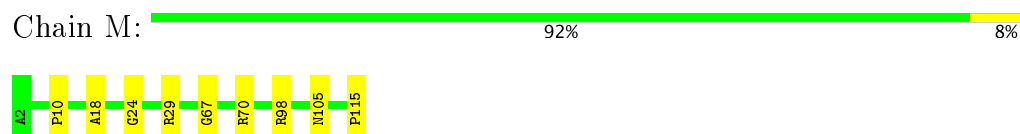
- Molecule 10: 30S ribosomal protein S11



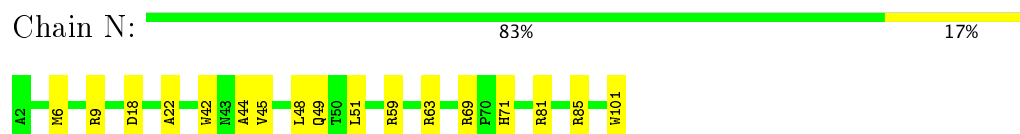
- Molecule 11: 30S ribosomal protein S12



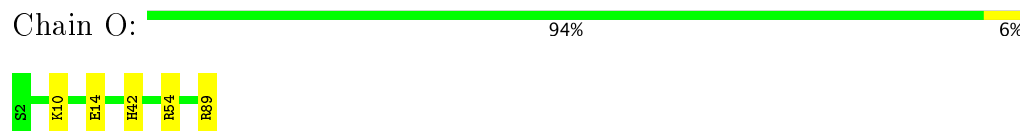
- Molecule 12: 30S ribosomal protein S13



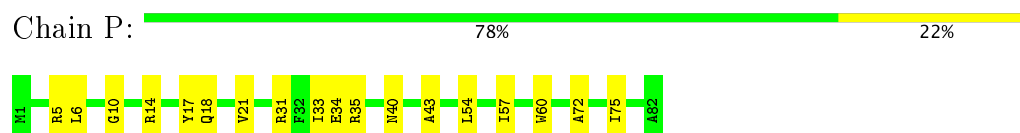
- Molecule 13: 30S ribosomal protein S14




- Molecule 14: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

Chain Q:  89% 11%




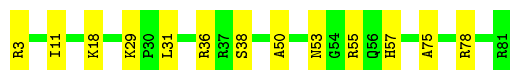
- Molecule 17: 30S ribosomal protein S18

Chain R:  91% 9%



- Molecule 18: 30S ribosomal protein S19

Chain S:  84% 16%




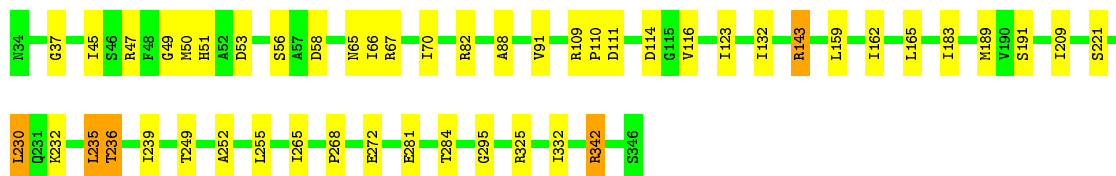
- Molecule 19: 30S ribosomal protein S20

Chain T:  92% 8%



- Molecule 20: Small ribosomal subunit biogenesis GTPase RsgA

Chain Z:  84% 14% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	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	0.79	11/57081 (0.0%)
10	K	0.25	0/893	0.47	0/1205
11	L	0.22	0/114	0.40	0/151
12	M	0.26	0/893	0.50	0/1193
13	N	0.24	0/817	0.43	0/1088
14	O	0.23	0/722	0.45	0/964
15	P	0.25	0/659	0.48	0/884
16	Q	0.24	0/658	0.51	0/881
17	R	0.23	0/463	0.41	0/621
18	S	0.26	0/653	0.48	0/877
19	T	0.24	0/676	0.42	0/895
2	B	0.26	0/1784	0.48	0/2403
20	Z	0.26	0/2493	0.55	2/3376 (0.1%)
3	D	0.24	0/1665	0.42	0/2227
4	E	0.26	0/1157	0.50	0/1557
5	F	0.24	0/881	0.47	0/1189
6	G	0.25	0/848	0.47	0/1132
7	H	0.26	0/989	0.48	0/1326
8	I	0.26	0/1034	0.55	0/1375
9	J	0.25	0/806	0.49	0/1089
All	All	0.21	0/54798	0.72	13/81514 (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
20	Z	0	2
9	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	C2-N1-C1'	8.34	127.97	118.80
1	A	1158	C	N1-C2-O2	8.09	123.75	118.90
20	Z	230	LEU	CA-CB-CG	6.85	131.06	115.30
1	A	754	C	C2-N1-C1'	6.84	126.32	118.80
1	A	1158	C	N3-C2-O2	-6.57	117.30	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	J	57	VAL	Peptide
20	Z	235	LEU	Peptide
20	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	16590	135	0
2	B	1753	0	1780	14	0
3	D	1643	0	1707	22	0
4	E	1144	0	1185	12	0
5	F	862	0	864	3	0
6	G	841	0	886	10	0
7	H	979	0	1031	6	0
8	I	1022	0	1070	18	0
9	J	796	0	836	10	0
10	K	877	0	887	6	0
11	L	114	0	131	2	0
12	M	884	0	941	7	0
13	N	805	0	844	13	0
14	O	714	0	734	3	0
15	P	649	0	666	12	0
16	Q	649	0	691	5	0
17	R	456	0	478	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	638	0	665	9	0
19	T	670	0	719	5	0
20	Z	2448	0	2419	25	0
21	A	67	0	0	0	0
21	N	1	0	0	0	0
21	P	1	0	0	0	0
21	T	1	0	0	0	0
21	Z	1	0	0	0	0
22	B	1	0	0	0	0
22	Z	1	0	0	0	0
23	Z	32	0	13	0	0
All	All	50979	0	35137	263	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 263 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)
1:A:1058:G:H1	1:A:1199:U:H3	1.37	0.73
1:A:1072:G:H21	2:B:106:THR:HG21	1.57	0.69
4:E:89:HIS:HB2	4:E:139:ALA:HB2	1.77	0.66
20:Z:252:ALA:HA	20:Z:268:PRO:HG3	1.79	0.65
3:D:14:ARG:HG3	3:D:56:ARG:HH22	1.63	0.63

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	B	222/224 (99%)	215 (97%)	7 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
4	E	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
5	F	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	G	103/130 (79%)	99 (96%)	4 (4%)	0	100	100
7	H	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
8	I	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
9	J	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
10	K	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
11	L	12/14 (86%)	12 (100%)	0	0	100	100
12	M	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
13	N	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
14	O	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	P	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
16	Q	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
17	R	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
18	S	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
19	T	84/86 (98%)	84 (100%)	0	0	100	100
20	Z	311/313 (99%)	293 (94%)	17 (6%)	1 (0%)	44	81
All	All	2240/2303 (97%)	2155 (96%)	84 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	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	B	186/186 (100%)	184 (99%)	2 (1%)	78	88
3	D	172/172 (100%)	172 (100%)	0	100	100
4	E	118/118 (100%)	117 (99%)	1 (1%)	85	92
5	F	92/92 (100%)	91 (99%)	1 (1%)	78	88
6	G	88/109 (81%)	87 (99%)	1 (1%)	78	88
7	H	104/104 (100%)	104 (100%)	0	100	100
8	I	105/105 (100%)	102 (97%)	3 (3%)	48	73
9	J	87/87 (100%)	87 (100%)	0	100	100
10	K	90/90 (100%)	89 (99%)	1 (1%)	78	88
11	L	12/12 (100%)	11 (92%)	1 (8%)	13	44
12	M	92/92 (100%)	92 (100%)	0	100	100
13	N	83/83 (100%)	82 (99%)	1 (1%)	75	88
14	O	76/76 (100%)	75 (99%)	1 (1%)	73	87
15	P	65/65 (100%)	65 (100%)	0	100	100
16	Q	74/74 (100%)	74 (100%)	0	100	100
17	R	48/48 (100%)	48 (100%)	0	100	100
18	S	70/70 (100%)	68 (97%)	2 (3%)	48	73
19	T	65/65 (100%)	65 (100%)	0	100	100
20	Z	267/267 (100%)	263 (98%)	4 (2%)	70	86
All	All	1894/1915 (99%)	1876 (99%)	18 (1%)	81	90

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	128	ARG
11	L	5	ASN
20	Z	50	MET
8	I	113	ARG
8	I	123	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	15	GLN
12	M	105	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	T	84	ASN
8	I	126	GLN
20	Z	101	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1530/1534 (99%)	255 (16%)	4 (0%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	9	G
1	A	22	G
1	A	39	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	209	U
1	A	1031	C
1	A	1062	U
1	A	1206	G

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	1.35	3 (15%)	20,38,41	2.38	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	A	1402	1	16,23,24	0.64	0	19,32,35	1.14	1 (5%)
1	5MC	A	1407	1	15,22,23	1.40	1 (6%)	17,32,35	0.97	1 (5%)
1	UR3	A	1498	1,21	14,22,23	0.76	0	16,32,35	0.69	0
1	2MG	A	1516	1	19,26,27	1.28	2 (10%)	20,38,41	2.26	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	2.46	7 (38%)
1	PSU	A	516	1,21	16,21,22	1.31	1 (6%)	20,30,33	3.53	6 (30%)
1	G7M	A	527	1	19,26,27	1.14	1 (5%)	19,39,42	2.31	6 (31%)
1	2MG	A	966	1	19,26,27	1.28	2 (10%)	20,38,41	2.32	8 (40%)
1	5MC	A	967	1	15,22,23	1.42	1 (6%)	17,32,35	1.01	1 (5%)

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	1,21	-	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	1,21	-	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 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PSU	C5-C1'	-3.67	1.49	1.52
1	A	1207	2MG	C2-N2	2.54	1.36	1.34
1	A	1519	MA6	C5-C4	3.03	1.47	1.40
1	A	1516	2MG	C5-C4	3.03	1.47	1.40
1	A	966	2MG	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	-9.24	121.75	128.40
1	A	516	PSU	C5-C4-N3	-8.63	118.35	125.43
1	A	1519	MA6	N3-C2-N1	-6.11	123.54	128.86
1	A	1518	MA6	N3-C2-N1	-5.72	123.87	128.86
1	A	527	G7M	C5-C6-N1	-4.36	117.27	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	527	G7M	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 73 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	$\# Z > 2$
23	GNP	Z	402	21	27,34,34	2.65	7 (25%)	26,54,54	1.74	6 (23%)

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
23	GNP	Z	402	21	-	0/16/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	402	GNP	C4-N9	-7.24	1.38	1.47
23	Z	402	GNP	C5-C6	-6.13	1.41	1.53
23	Z	402	GNP	PB-O3A	-4.83	1.53	1.59
23	Z	402	GNP	C8-N9	-3.07	1.37	1.46
23	Z	402	GNP	PB-O2B	-3.01	1.48	1.56

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	402	GNP	O3G-PG-O1G	-3.74	103.90	113.41
23	Z	402	GNP	O1B-PB-N3B	-2.42	108.17	111.79
23	Z	402	GNP	PA-O3A-PB	-2.24	124.48	132.38
23	Z	402	GNP	O3G-PG-O2G	2.86	115.69	107.69
23	Z	402	GNP	O2B-PB-O1B	3.75	117.67	109.87

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.