



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:59 AM GMT

PDB ID : 3CC4  
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-24  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

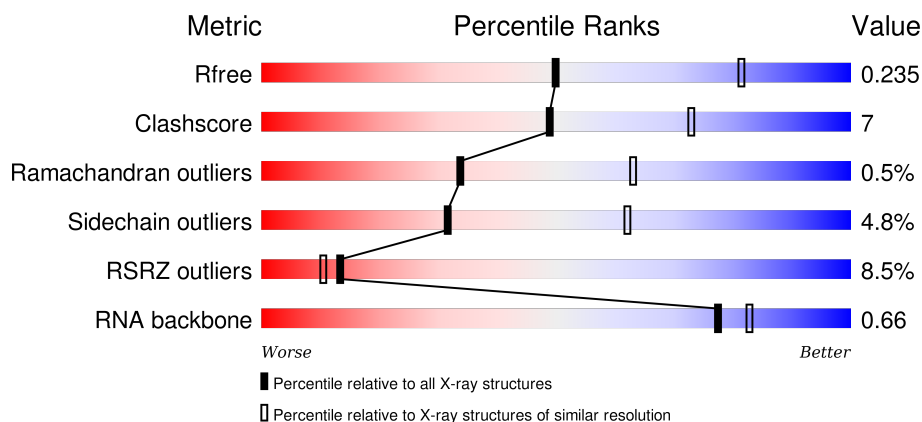
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>41%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8001	-	-	-	X
32	MG	0	8004	-	-	-	X
32	MG	0	8006	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8011	-	-	-	X
32	MG	0	8012	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8016	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8055	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8085	-	-	-	X
32	MG	0	8087	-	-	-	X
32	MG	A	8051	-	-	-	X
33	K	0	8401	-	-	-	X
34	NA	0	8504	-	-	-	X
34	NA	0	8507	-	-	-	X
34	NA	0	8508	-	-	-	X
34	NA	0	8517	-	-	-	X
34	NA	0	8519	-	-	-	X
34	NA	0	8521	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8523	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8533	-	-	-	X
34	NA	0	8534	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8546	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8547	-	-	-	X
34	NA	0	8553	-	-	-	X
34	NA	0	8555	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8557	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8567	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8569	-	-	-	X
34	NA	0	8575	-	-	-	X
34	NA	9	8572	-	-	-	X
34	NA	B	8552	-	-	-	X
34	NA	M	8539	-	-	-	X
36	SR	0	8949	-	-	-	X
36	SR	0	8957	-	-	-	X
36	SR	0	8962	-	-	-	X
36	SR	0	8969	-	-	-	X
36	SR	0	8986	-	-	-	X
36	SR	0	8992	-	-	-	X
36	SR	A	8929	-	-	-	X
36	SR	B	8987	-	-	-	X
37	ANM	0	2924	-	-	-	X

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 99135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	B	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0

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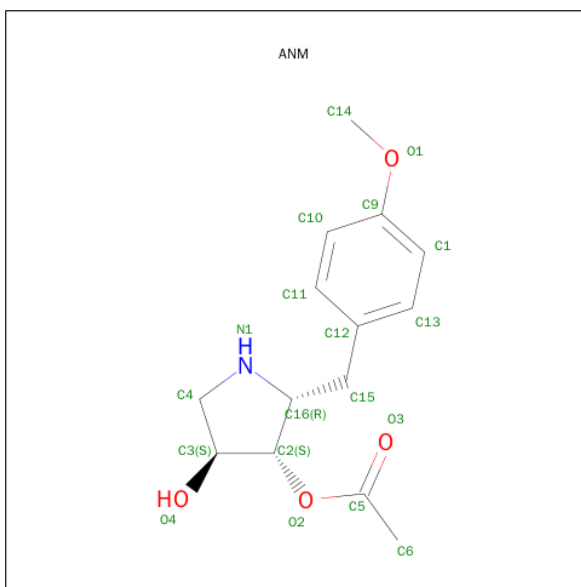
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	92	Total 92	Sr 92	0	0
36	1	2	Total 2	Sr 2	0	0
36	H	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is ANISOMYCIN (three-letter code: ANM) (formula: C<sub>14</sub>H<sub>19</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	0	1	Total	C	N	O	0	0
			19	14	1	4		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5972	Total	O	0	0
			5972	5972		
39	A	110	Total	O	0	0
			110	110		
39	B	140	Total	O	0	0
			140	140		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	163	Total 163	O 163	0	0
39	D	46	Total 46	O 46	0	0
39	E	44	Total 44	O 44	0	0
39	F	26	Total 26	O 26	0	0
39	G	17	Total 17	O 17	0	0
39	H	67	Total 67	O 67	0	0
39	I	6	Total 6	O 6	0	0
39	J	49	Total 49	O 49	0	0
39	K	56	Total 56	O 56	0	0
39	L	85	Total 85	O 85	0	0
39	M	121	Total 121	O 121	0	0
39	N	61	Total 61	O 61	0	0
39	O	44	Total 44	O 44	0	0
39	P	62	Total 62	O 62	0	0
39	Q	48	Total 48	O 48	0	0
39	R	78	Total 78	O 78	0	0
39	S	32	Total 32	O 32	0	0
39	T	39	Total 39	O 39	0	0
39	U	27	Total 27	O 27	0	0
39	V	13	Total 13	O 13	0	0
39	W	65	Total 65	O 65	0	0

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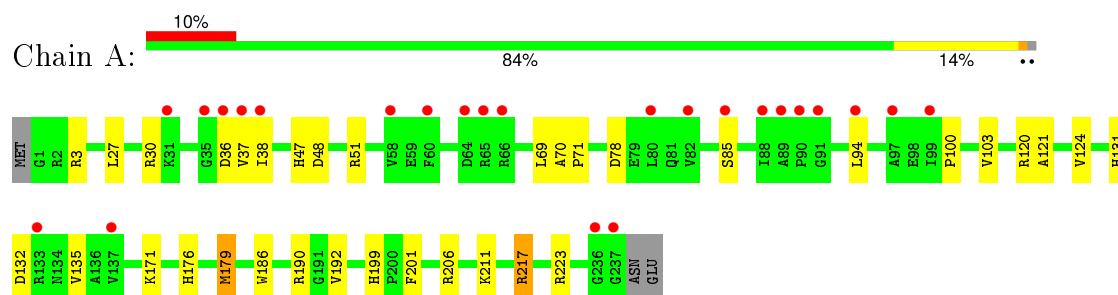
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	23	Total 23	O 23	0	0
39	Y	92	Total 92	O 92	0	0
39	Z	31	Total 31	O 31	0	0
39	1	48	Total 48	O 48	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0
39	9	147	Total 147	O 147	0	0

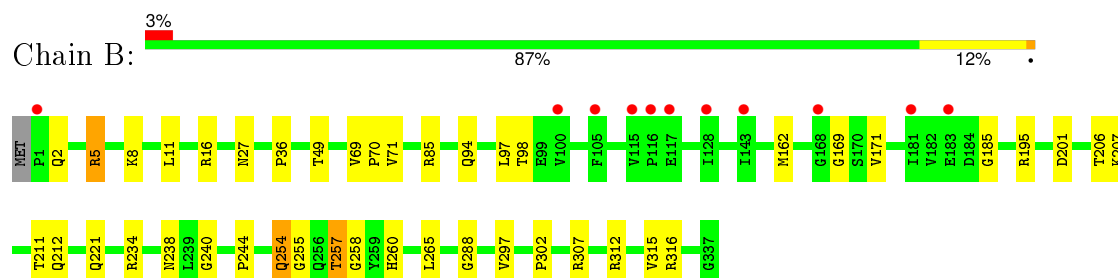
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

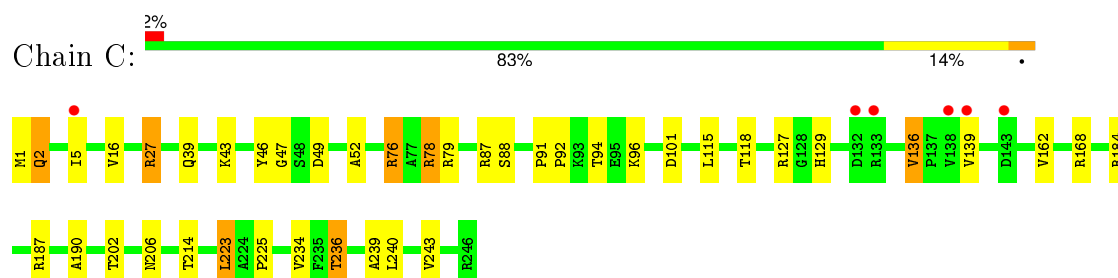
- Molecule 1: 50S ribosomal protein L2P



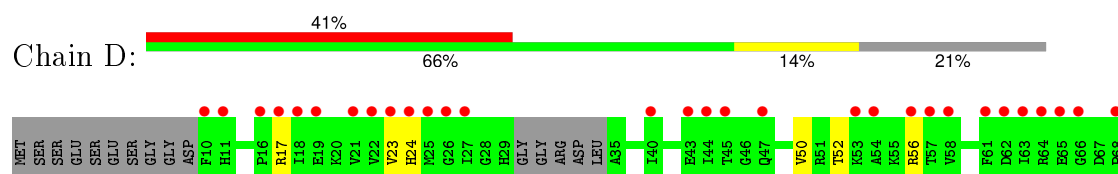
- Molecule 2: 50S ribosomal protein L3P



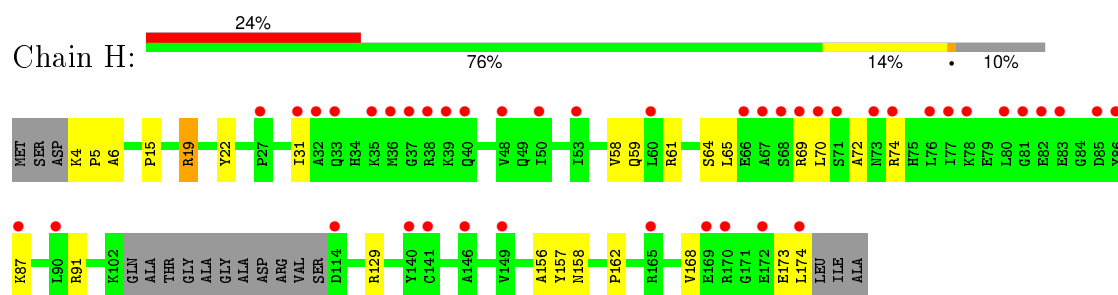
- Molecule 3: 50S ribosomal protein L4P



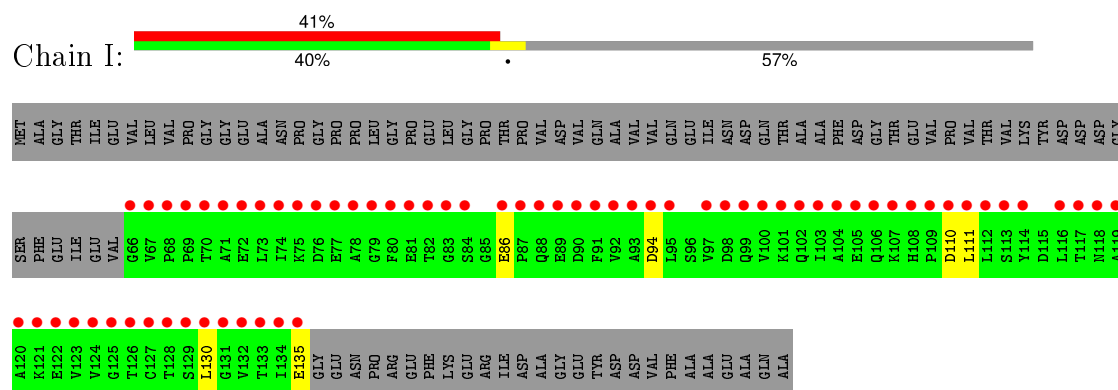
- Molecule 4: 50S ribosomal protein L5P



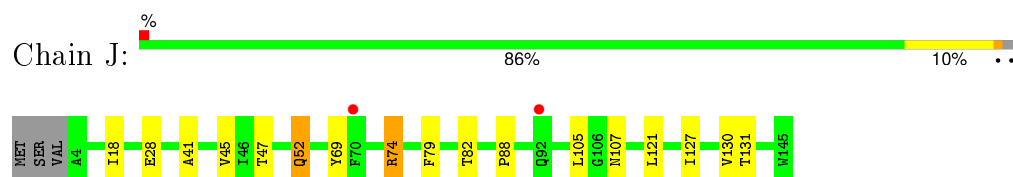




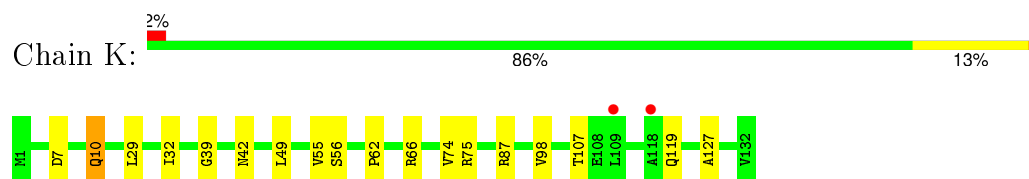
- Molecule 9: 50S ribosomal protein L11P



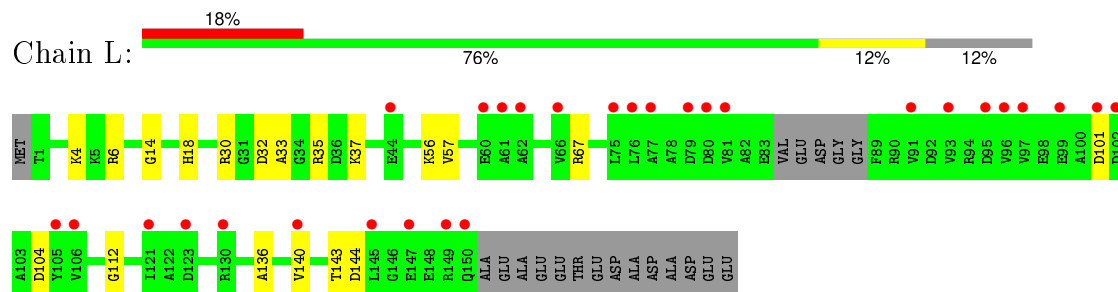
- Molecule 10: 50S ribosomal protein L13P



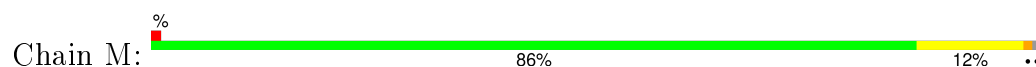
- Molecule 11: 50S ribosomal protein L14P

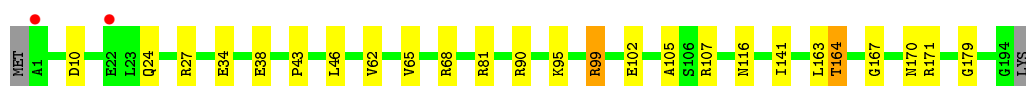


- Molecule 12: 50S ribosomal protein L15P

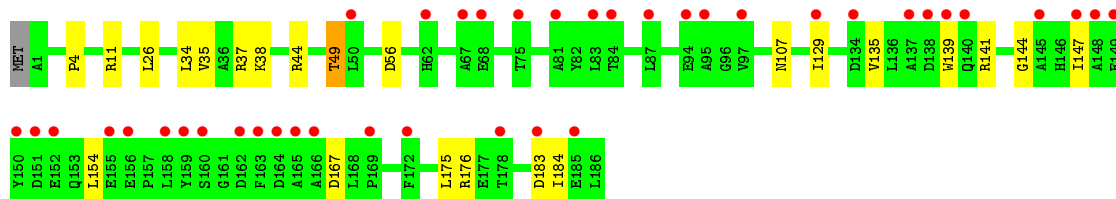
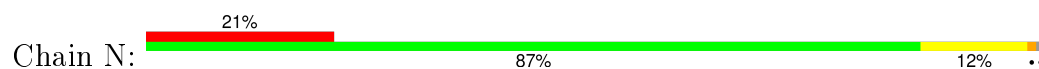


- Molecule 13: 50S ribosomal protein L15e





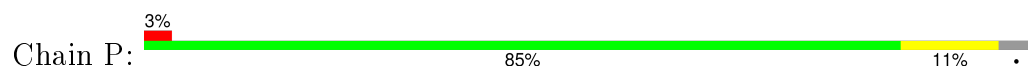
- Molecule 14: 50S ribosomal protein L18P



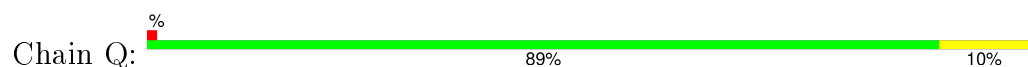
- Molecule 15: 50S ribosomal protein L18e



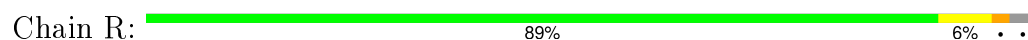
- Molecule 16: 50S ribosomal protein L19e



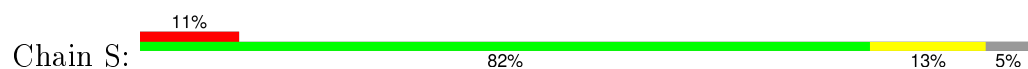
- Molecule 17: 50S ribosomal protein L21e



- Molecule 18: 50S ribosomal protein L22P



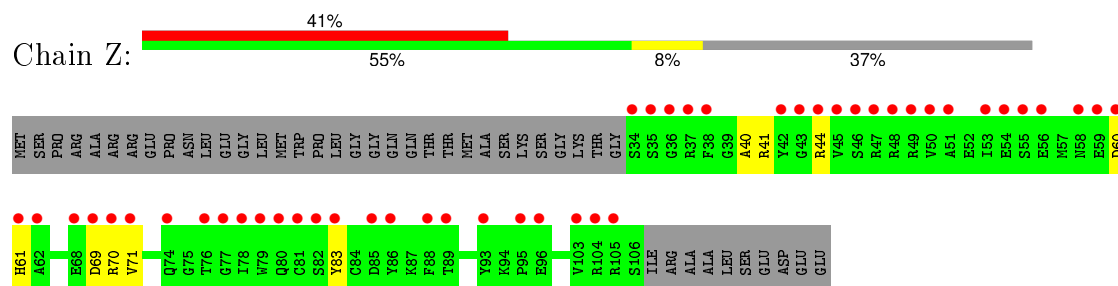
- Molecule 19: 50S ribosomal protein L23P



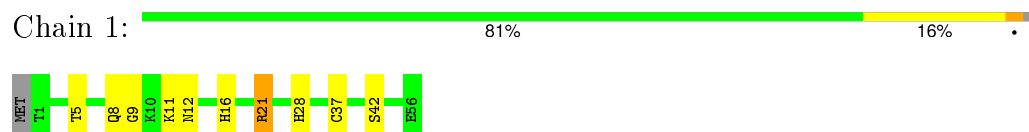
- Molecule 20: 50S ribosomal protein L24P



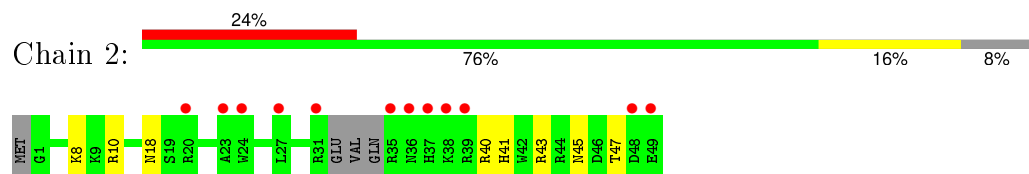
- Molecule 26: 50S ribosomal protein L37Ae



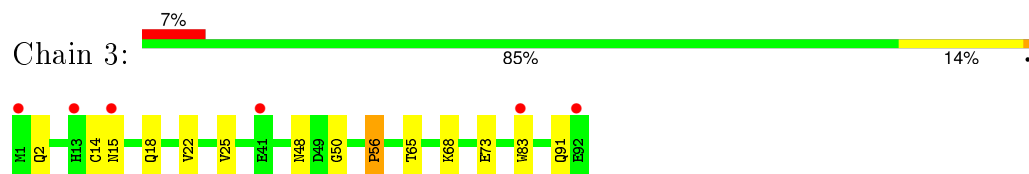
- Molecule 27: 50S ribosomal protein L37e



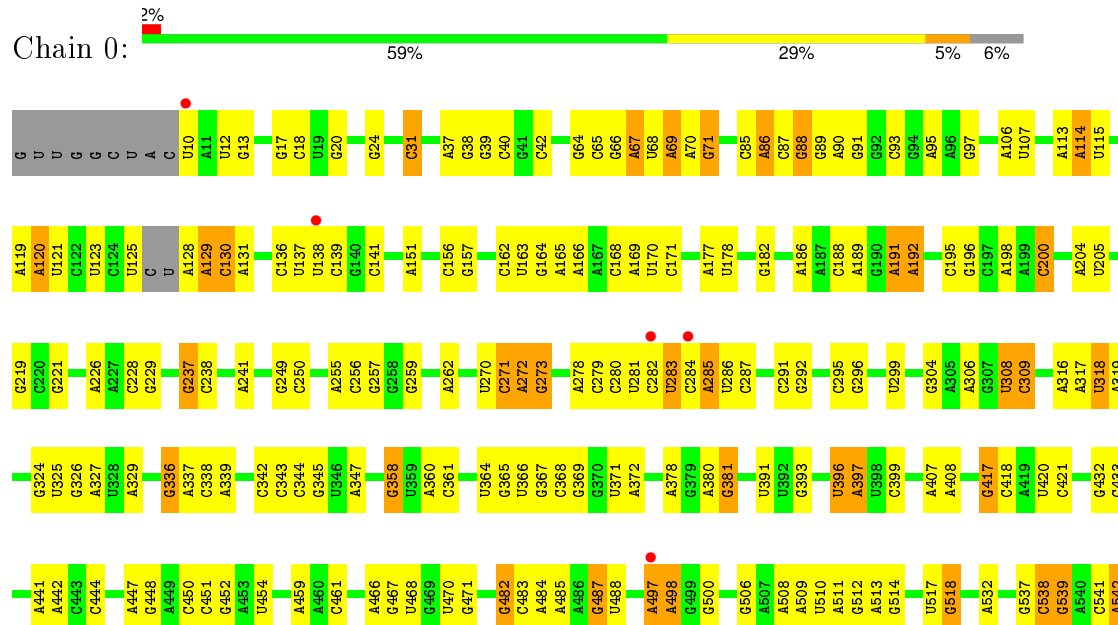
- Molecule 28: 50S ribosomal protein L39e



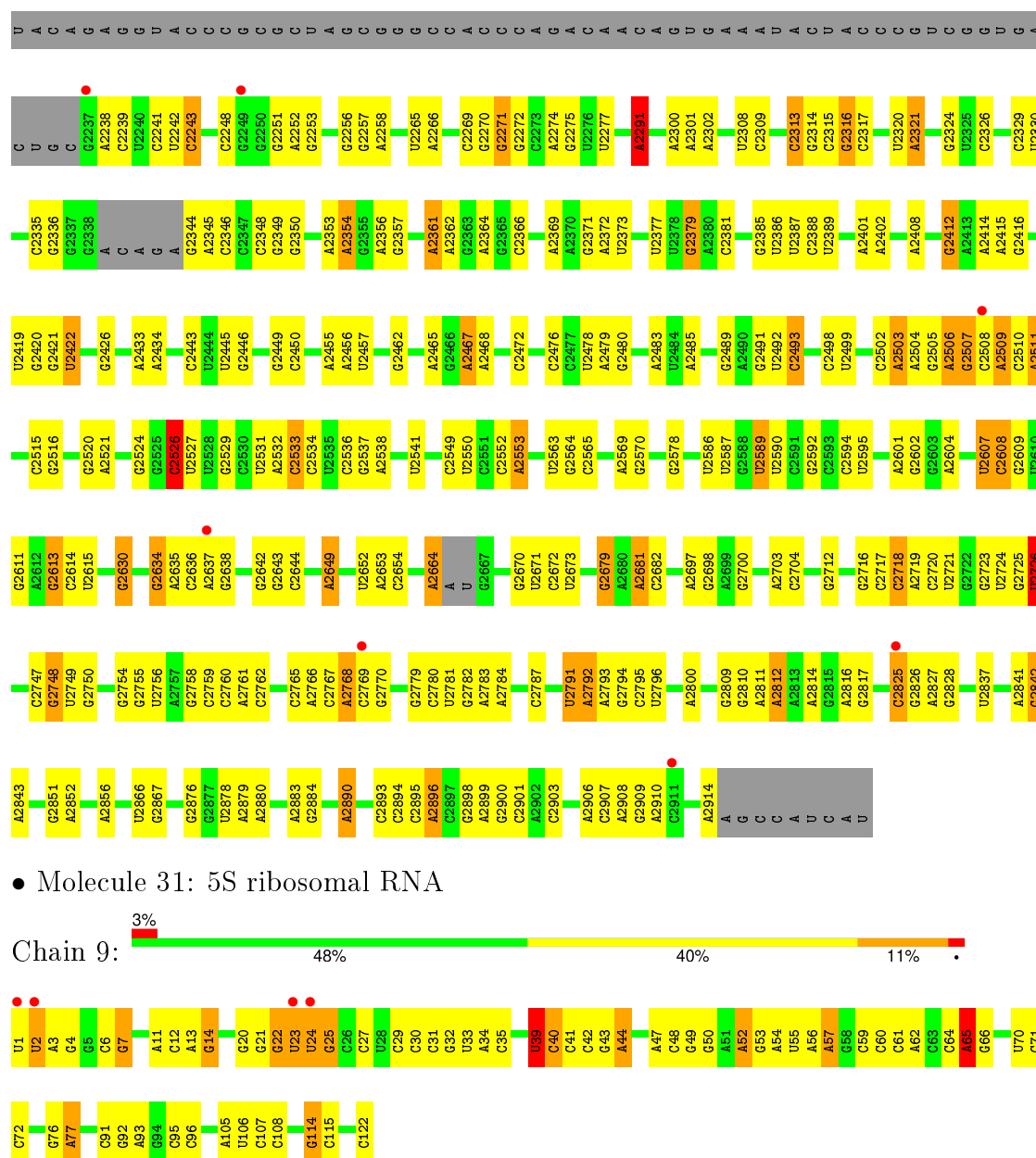
- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S ribosomal RNA



A2089	A1755	U8506	G1391	U1266	U1185	G1087	G	A791	A660	G543
G2090	G1756	A1515	A1392	C1267	C1186	A1088	A	G792	A661	G544
G2091	C1762	U1516	C1396	G1268	A1187		G	A793	A666	G545
G2092	C1763	U1524	C1397	G1269	A1188	U1096	U	U794		A553
A2096	U1766	G1525	A1398	A1278	A1189	A1097	C	A807	G668	
A2100	A1771	A1526	A1399	U1279	A1191	A1098	C	A808	G669	C558
A2101	U1777	U1527	A1406	C1289	A1192	G1099	C	G809	A671	U560
A2102	C1772	A1528	A1407	U1290	A1193		A	A812	G672	G561
A2103	G1773	G1529	G1409	A1294	A1194	C1104	C	G813		G564
C2104	A1778	A1533	A1413	G1295	G1195	U1109	A	G814	G677	
C2105	A1779	C1534	A1414	G1299	G1196	G1110	C	U815	G678	U567
C2106	A1783	G1535	G1415	U1300	A1197		A1005	G816		
G2110	U1784	C1536	G1416	G1300	A1199	U1116	A1006	G817	G681	
G2111	U1784	C1537	G1417	G1301	A1200	A1117	A1007	A818	A682	G581
G2112	U1784	C1537	G1418	U1304	C1201	A1118	C1008	A819	G683	U582
G2134	U1791	U1544	U1419	U1305	G1203	U1120	U1009	G820		
A2135	C1798	C1545	C1421	A1313	C1204	G1121	C1010	C822	A686	G588
G2136	G1799	U1546	C1422	G1314	U1205	U1130	A1014	U823	A687	
A	A1804	A1559	U1422	G1315	U1206	U1131	A1015	U827	A688	U595
C	G1805	U	C1423	G1316	A1207	A1132	U1016	A827	G689	C596
C	G1809	U1561	A1427	A1321	C1208	G1135	C1023	U832	A694	A602
G	A1815	C1562	G1430	G1322	G1210	U1136	G1024	U833	C695	A603
G	C1816	A1573	U1440	A1328	C1212	A1137	G1025	U835		G604
C	G1819	U1587	G1441	G1329	C1213	G1138	U1029	U840	G699	G612
C	G1820	G1588	A1442	G1331	G1214	G1151	G1039	G702	U701	G613
A	A1829	G1589	A1442	G1332	G1215		A1040	G703	G702	U614
U	A1830	G1592	C1451	G1333	G1217	C1157	U1041	C847	G703	
U	C1834	C1593	C1456	U1333	U1218	G1158	U1042	C848	G704	U619
U	U1835	C1594	U1457	C1334	U1219	G1159	U1043	C849	G705	A620
U	A1836	U1596	U1457	G1339	U1220	G1160	C1044	U850	G709	G621
A	G1837	A1597	U1473	U1340	C1229	A1161	G1045	C853	G710	U622
A	U1838	A1598	C1474	A1341	A1230	G1162	G1046	U856	G711	U623
A	U1839	A1603	C1474	A1342	A1231	G1163	C1051	A857	U	U625
A	A1840	G1604	U1478	C1343	A1232	U1164	G1052	U858	G716	A629
A	G1848	G1605	U1481	U1350	A1233	G1165	G1053	G688	G722	A631
A	U1849	A1606	A1482	G1351	U1234	C1168	U1056	G689		A632
A	U1850	A1607	A1482	A1352	U1237	U1169	A1057	G870	G735	A635
A	C1851	A1607	A1482	C1353	C1238	U1170	A1058	G871	A736	G636
A	C1852	G1613	A1485	C1360	G1239	A1171	G1059	U872	A737	G637
A	C1853	G1614	A1485	U1360	U1242	G1172	C1060	C	G738	C638
A	C1854	A1615	G1490	G1363	A1243	A1173	U1066	A875	A738	A639
A	C1855	A1625	U1500	A1372	C1244	U1175	A1067	A876	C741	
A	C1856	G1626	U1503	A1377	U1244	C1176	G1071	G877	G759	G644
A	C1857	G1627	U1504	C1377	A1246	A1177	G1072	C	A761	U645
A	C1858	G1628	A1504	C1384	U1249	U1178	G1072	C	G759	
A	C1859	G1629	A1504	G1385	C1250	U1180	A1078	C	A761	U653
A	C1860	G1630	A1504	G1386	C1251	A1181	A1079	C	A776	A654
A	C1861	G1631	A1504	G1387	C1252	C1182	C1080	A	U777	G655
A	C1862	G1632	A1504	G1387	C1253	C1183	A1081	G		G656
A	C1863	G1633	A1505	G1387	C1253	C1184	A1082	C	A790	G657



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.78Å 299.08Å 573.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.70 85.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.70) 96.9 (85.45-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.202 , 0.244 0.197 , 0.235	Depositor DCC
$R_{free}$ test set	4851 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 667264 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, ANM, 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	0.51	0/1786	0.78	0/2408
2	B	0.53	0/2690	0.78	0/3652
3	C	0.54	0/1885	0.77	0/2552
4	D	0.65	0/1111	0.71	1/1498 (0.1%)
5	E	0.60	0/1382	0.68	0/1880
6	F	0.54	0/901	0.71	0/1224
7	G	0.51	0/241	0.67	0/324
8	H	0.60	0/1302	0.79	0/1743
9	I	0.59	0/526	0.62	0/716
10	J	0.61	0/1136	0.72	0/1530
11	K	0.51	0/1004	0.80	0/1351
12	L	0.49	0/1130	0.76	0/1509
13	M	0.51	0/1582	0.77	0/2116
14	N	0.55	0/1474	0.77	0/1999
15	O	0.47	0/874	0.73	1/1181 (0.1%)
16	P	0.52	0/1147	0.67	0/1528
17	Q	0.49	0/749	0.77	0/1005
18	R	0.54	0/1172	0.74	0/1578
19	S	0.54	0/648	0.67	0/875
20	T	0.46	0/958	0.76	1/1289 (0.1%)
21	U	0.57	0/417	0.71	0/562
22	V	0.44	0/502	0.67	0/675
23	W	0.52	0/1219	0.78	1/1655 (0.1%)
24	X	0.52	0/664	0.72	0/895
25	Y	0.52	0/1146	0.74	0/1536
26	Z	0.69	0/584	0.74	0/781
27	1	0.55	0/438	0.75	0/578
28	2	0.45	0/401	0.70	0/529
29	3	0.59	0/771	0.70	0/1024
30	0	0.37	0/65958	0.68	15/102869 (0.0%)
31	9	0.32	0/2904	0.69	1/4526 (0.0%)
All	All	0.43	0/98702	0.70	20/147588 (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
23	W	0	1
30	0	0	42
31	9	0	2
All	All	0	45

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	4	LEU	CA-CB-CG	7.59	132.77	115.30
30	0	1942	A	C5'-C4'-C3'	6.82	126.92	116.00
30	0	871	G	C5'-C4'-O4'	-6.64	101.13	109.10
30	0	1504	A	N9-C1'-C2'	5.91	121.68	114.00
30	0	2726	U	N1-C1'-C2'	5.85	121.60	114.00

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	221	G	Sidechain
30	0	270	U	Sidechain
30	0	391	U	Sidechain
30	0	396	U	Sidechain
23	W	90	TYR	Sidechain

## 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	1753	0	1766	21	0
2	B	2625	0	2533	29	0
3	C	1860	0	1813	22	0
4	D	1094	0	1085	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	10	0
6	F	890	0	843	8	0
7	G	240	0	231	0	0
8	H	1282	0	1292	18	0
9	I	519	0	500	4	0
10	J	1120	0	1098	14	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	12	0
13	M	1558	0	1573	19	0
14	N	1445	0	1401	16	0
15	O	865	0	873	4	0
16	P	1136	0	1123	11	0
17	Q	735	0	729	6	0
18	R	1149	0	1122	11	0
19	S	641	0	605	5	0
20	T	950	0	924	8	0
21	U	410	0	364	3	0
22	V	499	0	511	4	0
23	W	1196	0	1137	22	0
24	X	654	0	653	11	0
25	Y	1130	0	1133	13	0
26	Z	573	0	532	6	0
27	1	431	0	426	10	0
28	2	396	0	413	5	0
29	3	755	0	729	7	0
30	0	59021	0	29812	846	0
31	9	2599	0	1325	64	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	92	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	19	0	19	5	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5972	0	0	121	0
39	1	48	0	0	0	0
39	2	38	0	0	0	0
39	3	66	0	0	1	0
39	9	147	0	0	5	0
39	A	110	0	0	4	0
39	B	140	0	0	5	0
39	C	163	0	0	2	0
39	D	46	0	0	0	0
39	E	44	0	0	0	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	67	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	I	6	0	0	1	0
39	J	49	0	0	1	0
39	K	56	0	0	0	0
39	L	85	0	0	2	0
39	M	121	0	0	1	0
39	N	61	0	0	1	0
39	O	44	0	0	0	0
39	P	62	0	0	0	0
39	Q	48	0	0	0	0
39	R	78	0	0	0	0
39	S	32	0	0	0	0
39	T	39	0	0	0	0
39	U	27	0	0	0	0
39	V	13	0	0	0	0
39	W	65	0	0	2	0
39	X	23	0	0	1	0
39	Y	92	0	0	3	0
39	Z	31	0	0	1	0
All	All	99135	0	59934	1085	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 7.

The worst 5 of 1085 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)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.22	1.16
31:9:76:G:H3'	31:9:77:A:H5''	1.34	1.02
15:O:3:THR:HG22	30:0:656:G:H5'	1.43	1.00
30:0:871:G:H8	30:0:871:G:H5'	1.27	0.98
30:0:871:G:C8	30:0:871:G:H5'	1.98	0.97

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	21	49
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	30	59
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	13	32
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100	100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	7	16
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	30	59
9	I	68/162 (42%)	60 (88%)	8 (12%)	0	100	100
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	24	51
12	L	141/165 (86%)	134 (95%)	7 (5%)	0	100	100
13	M	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
14	N	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	6	16
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	15	37
24	X	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	64 (90%)	6 (8%)	1 (1%)	14	35
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	17	42
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	34	63

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
14	N	154	LEU
14	N	184	ILE
14	N	183	ASP
1	A	27	LEU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	30	60
2	B	282/283 (100%)	269 (95%)	13 (5%)	33	64
3	C	193/193 (100%)	177 (92%)	16 (8%)	14	31
4	D	117/148 (79%)	107 (92%)	10 (8%)	13	30
5	E	152/156 (97%)	148 (97%)	4 (3%)	54	83
6	F	93/94 (99%)	91 (98%)	2 (2%)	60	86
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	127 (95%)	7 (5%)	29	58
9	I	58/130 (45%)	56 (97%)	2 (3%)	44	75
10	J	118/121 (98%)	110 (93%)	8 (7%)	20	43
11	K	106/106 (100%)	99 (93%)	7 (7%)	21	45
12	L	113/127 (89%)	107 (95%)	6 (5%)	28	57
13	M	158/160 (99%)	150 (95%)	8 (5%)	29	59
14	N	149/150 (99%)	144 (97%)	5 (3%)	44	75
15	O	93/94 (99%)	91 (98%)	2 (2%)	60	86
16	P	113/117 (97%)	109 (96%)	4 (4%)	43	74
17	Q	79/80 (99%)	76 (96%)	3 (4%)	40	71
18	R	117/122 (96%)	114 (97%)	3 (3%)	54	83
19	S	71/74 (96%)	69 (97%)	2 (3%)	51	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	105/106 (99%)	96 (91%)	9 (9%)	13	29
21	U	44/53 (83%)	41 (93%)	3 (7%)	20	43
22	V	51/57 (90%)	49 (96%)	2 (4%)	39	70
23	W	130/130 (100%)	123 (95%)	7 (5%)	27	56
24	X	66/74 (89%)	59 (89%)	7 (11%)	8	19
25	Y	120/196 (61%)	116 (97%)	4 (3%)	45	76
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	60	86
28	2	42/46 (91%)	41 (98%)	1 (2%)	57	85
29	3	79/79 (100%)	75 (95%)	4 (5%)	29	59
All	All	3095/3646 (85%)	2946 (95%)	149 (5%)	31	62

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	79	PHE
12	L	140	VAL
24	X	80	GLU
10	J	130	VAL
11	K	98	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	140	GLN
18	R	22	GLN
27	1	28	HIS
16	P	50	GLN
16	P	118	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	249 (8%)	29 (1%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1692	C
30	0	2761	A
30	0	1377	C
30	0	1856	C

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

5 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	$\# Z  > 2$
30	OMU	0	2587	30	12,22,23	1.00	1 (8%)	19,31,34	3.20	2 (10%)
30	OMG	0	2588	30	17,26,27	1.05	2 (11%)	21,38,41	2.53	3 (14%)
30	UR3	0	2619	30	12,22,23	0.79	0	16,32,35	0.78	0
30	PSU	0	2621	30	13,21,22	1.61	2 (15%)	18,30,33	6.13	3 (16%)
30	1MA	0	628	30,34	14,25,26	1.02	1 (7%)	15,37,40	1.18	1 (6%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.83	1.48	1.52
30	0	2588	OMG	C8-N7	-2.04	1.30	1.34
30	0	2587	OMU	C4-N3	2.33	1.37	1.33
30	0	2621	PSU	C4-N3	2.57	1.37	1.33
30	0	628	1MA	C6-N6	2.84	1.34	1.29

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.46	114.64	128.33
30	0	2588	OMG	C5-C6-N1	-8.77	111.60	123.59
30	0	628	1MA	C2-N3-C4	-3.56	110.89	116.40
30	0	2587	OMU	C5-C4-N3	-3.28	114.70	123.12
30	0	2588	OMG	N3-C2-N1	-2.27	123.99	127.44

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
30	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 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	$\# Z  > 2$
37	ANM	0	2924	33	19,20,20	0.47	0	22,27,27	1.91	6 (27%)

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
37	ANM	0	2924	33	-	0/10/23/23	0/2/2/2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	2924	ANM	C2-O2-C5	-3.73	111.92	117.70
37	0	2924	ANM	C4-C3-C2	-3.51	98.31	103.32
37	0	2924	ANM	C3-C2-C16	-3.07	99.95	104.29
37	0	2924	ANM	C14-O1-C9	-2.59	111.46	117.51
37	0	2924	ANM	O2-C5-O3	-2.04	118.84	122.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	2924	ANM	5	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	0.67	24 (10%) 9 7	24, 49, 88, 107	0
2	B	337/338 (99%)	0.41	11 (3%) 50 50	27, 53, 82, 95	0
3	C	246/246 (100%)	0.32	6 (2%) 62 62	21, 42, 65, 78	0
4	D	140/177 (79%)	2.54	72 (51%) 0 0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.74	16 (9%) 11 8	44, 69, 88, 94	0
6	F	119/120 (99%)	1.37	31 (26%) 1 1	43, 69, 99, 114	0
7	G	29/348 (8%)	1.83	10 (34%) 0 0	77, 95, 103, 106	0
8	H	160/177 (90%)	1.34	43 (26%) 1 1	44, 61, 96, 101	0
9	I	70/162 (43%)	5.22	67 (95%) 0 0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.35	2 (1%) 78 77	35, 50, 71, 91	0
11	K	132/132 (100%)	0.19	2 (1%) 76 76	32, 49, 72, 77	0
12	L	145/165 (87%)	0.99	29 (20%) 1 1	25, 63, 109, 125	0
13	M	194/196 (98%)	0.16	2 (1%) 84 85	28, 40, 56, 63	0
14	N	186/187 (99%)	1.18	40 (21%) 1 1	42, 64, 112, 121	0
15	O	115/116 (99%)	0.54	3 (2%) 59 59	33, 53, 69, 80	0
16	P	143/149 (95%)	0.46	5 (3%) 48 48	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.32	1 (1%) 82 83	34, 45, 62, 73	0
18	R	150/155 (96%)	0.18	0 100 100	30, 43, 63, 71	0
19	S	81/85 (95%)	0.95	9 (11%) 7 5	42, 56, 79, 90	0
20	T	119/120 (99%)	0.70	7 (5%) 26 24	35, 54, 84, 109	0
21	U	53/67 (79%)	0.67	5 (9%) 11 8	40, 56, 78, 84	0
22	V	65/71 (91%)	2.62	28 (43%) 0 0	52, 73, 117, 123	0
23	W	154/154 (100%)	0.58	7 (4%) 37 36	33, 49, 65, 75	0
24	X	82/92 (89%)	0.90	12 (14%) 3 2	43, 60, 85, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	0.21	5 (3%) 48 48	22, 41, 64, 89	0
26	Z	73/116 (62%)	2.55	47 (64%) 0 0	58, 76, 89, 100	0
27	1	56/57 (98%)	0.08	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.06	12 (26%) 1 1	34, 60, 91, 101	0
29	3	92/92 (100%)	0.74	6 (6%) 22 20	36, 59, 72, 86	0
30	0	2749/2923 (94%)	-0.22	62 (2%) 64 64	18, 43, 87, 165	0
31	9	122/122 (100%)	-0.19	4 (3%) 50 50	34, 65, 86, 145	0
All	All	6646/7517 (88%)	0.38	568 (8%) 13 10	18, 50, 99, 165	0

The worst 5 of 568 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	14.9
22	V	1	THR	12.9
22	V	40	PRO	12.1
9	I	74	ILE	11.8
14	N	166	ALA	11.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	OMU	0	2587	21/22	0.98	0.15	-	31,33,35,37	0
30	UR3	0	2619	21/22	0.98	0.17	-	30,34,36,39	0
30	PSU	0	2621	20/21	0.98	0.16	-	22,26,34,34	0
30	1MA	0	628	23/24	0.98	0.18	-	25,28,29,31	0
30	OMG	0	2588	24/25	0.98	0.15	-	27,30,33,35	0

## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8562	1/1	0.78	0.85	129.80	69,69,69,69	0
36	SR	0	8986	1/1	0.51	1.98	59.80	200,200,200,200	0
36	SR	0	8957	1/1	0.28	0.75	35.98	200,200,200,200	0
34	NA	0	8555	1/1	0.77	0.73	32.48	54,54,54,54	0
34	NA	0	8519	1/1	0.88	0.42	30.94	39,39,39,39	0
33	K	0	8401	1/1	0.83	0.41	27.28	81,81,81,81	0
34	NA	0	8547	1/1	0.94	0.42	25.88	54,54,54,54	0
32	MG	0	8041	1/1	0.95	0.33	24.70	24,24,24,24	0
32	MG	0	8047	1/1	0.93	0.44	24.18	49,49,49,49	0
34	NA	0	8565	1/1	0.82	0.54	23.62	62,62,62,62	0
34	NA	0	8542	1/1	0.87	0.42	21.24	42,42,42,42	0
34	NA	0	8553	1/1	0.73	0.42	20.66	79,79,79,79	0
34	NA	0	8567	1/1	0.85	0.43	18.54	78,78,78,78	0
34	NA	0	8517	1/1	0.94	0.32	14.25	30,30,30,30	0
34	NA	0	8535	1/1	0.95	0.25	13.97	52,52,52,52	0
36	SR	0	8969	1/1	0.72	0.39	13.32	150,150,150,150	0
34	NA	9	8572	1/1	0.38	0.43	13.23	76,76,76,76	0
34	NA	0	8507	1/1	0.95	0.29	12.86	45,45,45,45	0
34	NA	0	8546	1/1	0.57	1.03	12.56	95,95,95,95	0
34	NA	0	8563	1/1	0.92	0.38	12.27	60,60,60,60	0
34	NA	B	8552	1/1	0.92	0.34	11.53	56,56,56,56	0
34	NA	0	8522	1/1	0.67	0.53	11.43	78,78,78,78	0
34	NA	0	8521	1/1	0.89	0.29	11.19	61,61,61,61	0
34	NA	0	8523	1/1	0.88	0.26	11.03	48,48,48,48	0
34	NA	0	8568	1/1	0.79	0.39	10.32	47,47,47,47	0
34	NA	0	8527	1/1	0.96	0.26	9.76	52,52,52,52	0
32	MG	0	8028	1/1	0.99	0.26	9.01	22,22,22,22	0
34	NA	0	8559	1/1	0.91	0.23	8.96	75,75,75,75	0
32	MG	0	8016	1/1	0.85	0.33	8.80	49,49,49,49	0
36	SR	B	8987	1/1	0.68	0.68	8.66	200,200,200,200	0
34	NA	0	8560	1/1	0.78	0.47	7.71	69,69,69,69	0
34	NA	0	8504	1/1	0.87	0.28	7.23	26,26,26,26	0
34	NA	0	8556	1/1	0.87	0.50	7.17	44,44,44,44	0
34	NA	0	8530	1/1	0.89	0.28	7.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8009	1/1	0.97	0.26	7.10	21,21,21,21	0
36	SR	0	8992	1/1	0.90	0.24	7.05	123,123,123,123	0
34	NA	0	8534	1/1	0.96	0.28	6.42	32,32,32,32	0
32	MG	0	8014	1/1	0.96	0.22	6.25	30,30,30,30	0
36	SR	0	8962	1/1	0.94	0.25	6.22	167,167,167,167	0
34	NA	0	8508	1/1	0.89	0.23	6.20	37,37,37,37	0
32	MG	0	8011	1/1	0.96	0.29	6.10	23,23,23,23	0
32	MG	A	8051	1/1	0.77	0.50	5.70	81,81,81,81	0
34	NA	0	8528	1/1	0.95	0.20	5.49	45,45,45,45	0
32	MG	0	8085	1/1	0.88	0.28	5.39	80,80,80,80	0
34	NA	0	8558	1/1	0.96	0.26	5.37	44,44,44,44	0
34	NA	0	8575	1/1	0.81	0.35	4.85	94,94,94,94	0
34	NA	0	8569	1/1	0.94	0.26	4.41	53,53,53,53	0
34	NA	0	8564	1/1	0.92	0.19	4.32	65,65,65,65	0
32	MG	0	8006	1/1	0.85	0.21	3.87	30,30,30,30	0
36	SR	0	8949	1/1	0.76	0.20	3.67	110,110,110,110	0
32	MG	0	8062	1/1	0.78	0.23	3.65	34,34,34,34	0
37	ANM	0	2924	19/19	0.95	0.22	3.58	31,37,40,40	0
32	MG	0	8004	1/1	0.97	0.24	3.45	25,25,25,25	0
32	MG	0	8012	1/1	0.94	0.23	3.15	21,21,21,21	0
34	NA	M	8539	1/1	0.74	0.25	3.03	41,41,41,41	0
32	MG	0	8055	1/1	0.86	0.27	2.82	38,38,38,38	0
34	NA	0	8557	1/1	0.72	0.16	2.75	67,67,67,67	0
32	MG	0	8087	1/1	0.96	0.20	2.63	42,42,42,42	0
32	MG	0	8001	1/1	0.96	0.20	2.31	25,25,25,25	0
34	NA	0	8533	1/1	0.77	0.25	2.31	63,63,63,63	0
36	SR	A	8929	1/1	0.91	0.27	2.08	131,131,131,131	0
32	MG	0	8003	1/1	0.97	0.19	1.96	30,30,30,30	0
36	SR	0	8904	1/1	0.99	0.20	1.91	52,52,52,52	0
32	MG	0	8070	1/1	0.94	0.17	1.86	45,45,45,45	0
32	MG	0	8084	1/1	0.95	0.18	1.54	31,31,31,31	0
32	MG	0	8008	1/1	0.91	0.19	1.30	25,25,25,25	0
35	CL	0	8816	1/1	0.96	0.19	0.91	60,60,60,60	0
34	NA	0	8515	1/1	0.95	0.23	0.74	33,33,33,33	0
34	NA	0	8520	1/1	0.89	0.18	0.66	54,54,54,54	0
34	NA	Q	8540	1/1	0.84	0.22	0.65	60,60,60,60	0
35	CL	0	8805	1/1	0.93	0.15	0.43	59,59,59,59	0
32	MG	0	8045	1/1	0.95	0.17	0.23	32,32,32,32	0
32	MG	0	8050	1/1	0.73	0.18	0.05	37,37,37,37	0
36	SR	H	8972	1/1	0.92	0.20	-0.14	130,130,130,130	0
32	MG	0	8043	1/1	0.85	0.15	-0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	J	8538	1/1	0.89	0.20	-0.41	56,56,56,56	0
32	MG	0	8088	1/1	0.82	0.16	-0.62	37,37,37,37	0
36	SR	0	8985	1/1	0.93	0.13	-0.65	110,110,110,110	0
33	K	0	8402	1/1	0.93	0.17	-0.67	64,64,64,64	0
35	CL	O	8808	1/1	0.94	0.17	-0.82	61,61,61,61	0
32	MG	0	8002	1/1	0.98	0.17	-0.83	22,22,22,22	0
32	MG	0	8021	1/1	0.98	0.13	-0.94	32,32,32,32	0
32	MG	0	8053	1/1	0.94	0.16	-1.08	61,61,61,61	0
35	CL	J	8821	1/1	0.95	0.15	-1.19	56,56,56,56	0
32	MG	0	8058	1/1	0.96	0.12	-1.29	23,23,23,23	0
32	MG	0	8025	1/1	0.97	0.13	-1.64	24,24,24,24	0
35	CL	0	8812	1/1	0.98	0.11	-1.67	48,48,48,48	0
32	MG	0	8065	1/1	0.97	0.13	-1.73	33,33,33,33	0
32	MG	0	8044	1/1	0.88	0.12	-1.75	33,33,33,33	0
38	CD	3	8704	1/1	0.99	0.09	-1.82	66,66,66,66	0
38	CD	U	8701	1/1	0.99	0.12	-1.94	58,58,58,58	0
38	CD	Z	8703	1/1	0.93	0.06	-1.94	81,81,81,81	0
35	CL	M	8818	1/1	0.97	0.14	-2.00	37,37,37,37	0
36	SR	3	8932	1/1	0.96	0.13	-2.02	73,73,73,73	0
34	NA	0	8537	1/1	0.95	0.12	-2.19	34,34,34,34	0
32	MG	T	8057	1/1	0.90	0.15	-2.19	57,57,57,57	0
36	SR	0	8975	1/1	0.83	0.11	-2.27	134,134,134,134	0
36	SR	0	8910	1/1	0.85	0.12	-2.32	97,97,97,97	0
35	CL	B	8819	1/1	0.99	0.12	-3.10	46,46,46,46	0
36	SR	0	8943	1/1	0.92	0.08	-3.25	95,95,95,95	0
36	SR	0	8935	1/1	0.97	0.11	-3.44	79,79,79,79	0
35	CL	3	8804	1/1	0.98	0.05	-3.78	54,54,54,54	0
36	SR	0	8902	1/1	0.96	0.15	-3.91	69,69,69,69	0
32	MG	0	8052	1/1	0.98	0.11	-4.04	40,40,40,40	0
38	CD	1	8702	1/1	0.99	0.08	-4.09	57,57,57,57	0
36	SR	0	8936	1/1	0.93	0.13	-4.32	89,89,89,89	0
36	SR	1	8913	1/1	0.96	0.09	-4.97	85,85,85,85	0
35	CL	0	8815	1/1	0.96	0.11	-5.30	57,57,57,57	0
32	MG	0	8075	1/1	0.89	0.08	-5.33	45,45,45,45	0
32	MG	0	8034	1/1	0.92	0.11	-5.71	32,32,32,32	0
36	SR	0	8970	1/1	0.87	0.07	-6.71	131,131,131,131	0
32	MG	0	8013	1/1	0.97	0.08	-7.06	26,26,26,26	0
32	MG	Y	8086	1/1	0.97	0.11	-9.82	39,39,39,39	0
36	SR	0	8966	1/1	0.83	0.08	-	110,110,110,110	0
34	NA	9	8543	1/1	0.80	0.08	-	70,70,70,70	0
36	SR	0	8968	1/1	0.90	0.11	-	143,143,143,143	0
32	MG	0	8056	1/1	0.93	0.20	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8093	1/1	0.95	0.11	-	29,29,29,29	0
36	SR	0	9001	1/1	0.84	0.24	-	169,169,169,169	0
32	MG	0	8005	1/1	0.98	0.30	-	26,26,26,26	0
36	SR	0	8944	1/1	0.70	0.26	-	185,185,185,185	0
34	NA	0	8524	1/1	0.96	0.26	-	45,45,45,45	0
36	SR	A	8977	1/1	0.54	0.18	-	172,172,172,172	0
36	SR	0	8955	1/1	0.16	0.34	-	200,200,200,200	0
32	MG	B	8042	1/1	0.86	0.12	-	50,50,50,50	0
34	NA	0	8511	1/1	0.78	0.32	-	59,59,59,59	0
35	CL	R	8806	1/1	0.99	0.17	-	43,43,43,43	0
32	MG	0	8032	1/1	0.94	0.09	-	40,40,40,40	0
32	MG	0	8020	1/1	0.92	0.20	-	54,54,54,54	0
35	CL	0	8814	1/1	0.96	0.17	-	47,47,47,47	0
36	SR	0	8926	1/1	0.85	0.12	-	115,115,115,115	0
34	NA	0	8549	1/1	0.74	0.42	-	81,81,81,81	0
32	MG	0	8079	1/1	0.80	0.24	-	47,47,47,47	0
35	CL	0	8811	1/1	0.96	0.11	-	53,53,53,53	0
34	NA	0	8551	1/1	0.97	0.23	-	46,46,46,46	0
34	NA	0	8505	1/1	0.85	0.58	-	39,39,39,39	0
36	SR	0	8958	1/1	0.81	0.11	-	108,108,108,108	0
32	MG	0	8081	1/1	0.88	0.24	-	54,54,54,54	0
36	SR	0	8960	1/1	0.74	0.11	-	145,145,145,145	0
36	SR	0	8922	1/1	0.48	0.37	-	159,159,159,159	0
32	MG	0	8072	1/1	0.84	0.28	-	52,52,52,52	0
32	MG	0	8082	1/1	0.97	0.33	-	48,48,48,48	0
36	SR	0	8954	1/1	0.95	0.08	-	105,105,105,105	0
36	SR	0	8921	1/1	0.93	0.12	-	92,92,92,92	0
36	SR	0	8974	1/1	0.80	0.29	-	166,166,166,166	0
32	MG	0	8007	1/1	0.94	0.30	-	26,26,26,26	0
34	NA	0	8574	1/1	0.87	0.43	-	53,53,53,53	0
35	CL	N	8807	1/1	0.96	0.13	-	61,61,61,61	0
36	SR	0	8940	1/1	0.97	0.10	-	85,85,85,85	0
32	MG	0	8019	1/1	0.96	0.30	-	24,24,24,24	0
35	CL	Y	8820	1/1	0.95	0.11	-	38,38,38,38	0
36	SR	0	8947	1/1	0.53	0.48	-	200,200,200,200	0
36	SR	0	8937	1/1	0.96	0.21	-	100,100,100,100	0
36	SR	0	8945	1/1	0.86	0.11	-	99,99,99,99	0
36	SR	R	8912	1/1	0.97	0.16	-	84,84,84,84	0
35	CL	J	8801	1/1	0.95	0.13	-	62,62,62,62	0
36	SR	0	8963	1/1	0.78	0.12	-	133,133,133,133	0
32	MG	0	8073	1/1	0.90	0.14	-	76,76,76,76	0
32	MG	0	8068	1/1	0.93	0.09	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8915	1/1	0.99	0.07	-	117,117,117,117	0
34	NA	S	8510	1/1	0.36	0.43	-	79,79,79,79	0
34	NA	0	8573	1/1	0.68	0.63	-	69,69,69,69	0
34	NA	C	8503	1/1	0.92	0.28	-	37,37,37,37	0
34	NA	0	8506	1/1	0.83	0.25	-	47,47,47,47	0
36	SR	0	8905	1/1	0.99	0.26	-	57,57,57,57	0
36	SR	0	8993	1/1	0.70	0.16	-	168,168,168,168	0
32	MG	0	8067	1/1	0.95	0.28	-	34,34,34,34	0
34	NA	0	8531	1/1	0.78	0.16	-	40,40,40,40	0
36	SR	0	9007	1/1	0.83	0.40	-	200,200,200,200	0
36	SR	0	8920	1/1	0.88	0.11	-	124,124,124,124	0
32	MG	0	8010	1/1	0.93	0.17	-	26,26,26,26	0
36	SR	0	8988	1/1	0.80	0.08	-	163,163,163,163	0
32	MG	0	8029	1/1	0.94	0.18	-	39,39,39,39	0
36	SR	0	8927	1/1	0.95	0.15	-	167,167,167,167	0
36	SR	0	8973	1/1	0.83	0.10	-	137,137,137,137	0
36	SR	0	8941	1/1	0.85	0.19	-	115,115,115,115	0
32	MG	0	8061	1/1	0.94	0.39	-	37,37,37,37	0
36	SR	0	8983	1/1	0.65	0.23	-	164,164,164,164	0
32	MG	0	8076	1/1	0.92	0.22	-	35,35,35,35	0
32	MG	0	8036	1/1	0.93	0.12	-	49,49,49,49	0
32	MG	0	8022	1/1	0.96	0.21	-	29,29,29,29	0
34	NA	0	8536	1/1	0.96	0.12	-	50,50,50,50	0
36	SR	0	8984	1/1	0.66	0.10	-	128,128,128,128	0
34	NA	0	8548	1/1	0.87	0.38	-	57,57,57,57	0
36	SR	0	8959	1/1	0.54	0.26	-	169,169,169,169	0
36	SR	0	9000	1/1	0.83	0.17	-	159,159,159,159	0
36	SR	0	8907	1/1	0.99	0.32	-	76,76,76,76	0
32	MG	0	8024	1/1	0.82	0.57	-	85,85,85,85	0
36	SR	0	8982	1/1	0.76	0.85	-	180,180,180,180	0
32	MG	0	8023	1/1	0.96	0.18	-	22,22,22,22	0
32	MG	0	8071	1/1	0.86	0.27	-	55,55,55,55	0
32	MG	0	8083	1/1	0.91	0.16	-	56,56,56,56	0
36	SR	0	8956	1/1	0.75	0.14	-	142,142,142,142	0
34	NA	0	8561	1/1	0.69	0.83	-	74,74,74,74	0
36	SR	9	8980	1/1	0.77	0.27	-	182,182,182,182	0
34	NA	0	8525	1/1	0.87	0.12	-	69,69,69,69	0
36	SR	0	8917	1/1	0.78	0.18	-	119,119,119,119	0
35	CL	J	8802	1/1	0.97	0.15	-	60,60,60,60	0
32	MG	0	8038	1/1	0.86	0.12	-	58,58,58,58	0
36	SR	0	8938	1/1	0.80	0.08	-	159,159,159,159	0
32	MG	9	8074	1/1	0.95	0.13	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8981	1/1	0.78	0.23	-	167,167,167,167	0
36	SR	0	8903	1/1	0.98	0.20	-	53,53,53,53	0
35	CL	0	8813	1/1	0.97	0.08	-	48,48,48,48	0
36	SR	0	8979	1/1	0.56	0.29	-	194,194,194,194	0
38	CD	O	8705	1/1	0.90	0.06	-	124,124,124,124	0
36	SR	0	8911	1/1	0.89	0.08	-	78,78,78,78	0
32	MG	0	8017	1/1	0.93	0.19	-	56,56,56,56	0
36	SR	0	8906	1/1	0.99	0.21	-	56,56,56,56	0
34	NA	0	8570	1/1	0.94	0.17	-	49,49,49,49	0
36	SR	A	8930	1/1	0.87	0.08	-	116,116,116,116	0
32	MG	0	8027	1/1	0.97	0.14	-	34,34,34,34	0
34	NA	0	8502	1/1	0.87	0.34	-	67,67,67,67	0
36	SR	0	8909	1/1	0.89	0.14	-	94,94,94,94	0
32	MG	0	8077	1/1	0.90	0.16	-	32,32,32,32	0
34	NA	0	8513	1/1	0.97	0.27	-	44,44,44,44	0
34	NA	0	8571	1/1	0.72	0.32	-	83,83,83,83	0
32	MG	0	8018	1/1	0.95	0.24	-	38,38,38,38	0
36	SR	0	8946	1/1	0.95	0.16	-	108,108,108,108	0
36	SR	0	8948	1/1	0.82	0.17	-	102,102,102,102	0
32	MG	0	8037	1/1	0.90	0.22	-	83,83,83,83	0
32	MG	0	8046	1/1	0.96	0.16	-	28,28,28,28	0
36	SR	0	8967	1/1	0.89	0.11	-	133,133,133,133	0
35	CL	0	8803	1/1	0.98	0.07	-	46,46,46,46	0
36	SR	0	8965	1/1	0.91	0.12	-	120,120,120,120	0
34	NA	0	8554	1/1	0.74	0.75	-	65,65,65,65	0
32	MG	0	8015	1/1	0.98	0.19	-	27,27,27,27	0
34	NA	0	8518	1/1	0.86	0.41	-	79,79,79,79	0
36	SR	F	9005	1/1	0.94	0.06	-	136,136,136,136	0
34	NA	0	8529	1/1	0.93	0.09	-	37,37,37,37	0
36	SR	1	8952	1/1	0.97	0.12	-	79,79,79,79	0
36	SR	0	8942	1/1	0.87	0.15	-	121,121,121,121	0
32	MG	0	8048	1/1	0.95	0.28	-	28,28,28,28	0
36	SR	0	8931	1/1	0.95	0.11	-	108,108,108,108	0
35	CL	0	8817	1/1	0.92	0.12	-	53,53,53,53	0
32	MG	0	8049	1/1	0.93	0.37	-	55,55,55,55	0
32	MG	0	8090	1/1	0.96	0.13	-	54,54,54,54	0
36	SR	0	8901	1/1	0.96	0.16	-	58,58,58,58	0
32	MG	0	8039	1/1	0.89	0.33	-	69,69,69,69	0
34	NA	0	8514	1/1	0.90	0.28	-	42,42,42,42	0
32	MG	0	8089	1/1	0.43	0.17	-	48,48,48,48	0
36	SR	0	8991	1/1	0.82	0.23	-	191,191,191,191	0
32	MG	0	8040	1/1	0.74	0.34	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	A	8809	1/1	0.94	0.15	-	57,57,57,57	0
32	MG	0	8064	1/1	0.94	0.27	-	38,38,38,38	0
34	NA	0	8512	1/1	0.72	0.51	-	43,43,43,43	0
34	NA	0	8501	1/1	0.86	0.20	-	39,39,39,39	0
36	SR	0	8976	1/1	0.41	0.45	-	186,186,186,186	0
32	MG	0	8031	1/1	0.81	0.20	-	61,61,61,61	0
36	SR	0	8994	1/1	0.60	0.60	-	190,190,190,190	0
36	SR	0	8919	1/1	0.46	0.24	-	178,178,178,178	0
36	SR	S	8961	1/1	0.67	0.10	-	114,114,114,114	0
35	CL	L	8810	1/1	0.95	0.09	-	49,49,49,49	0
32	MG	0	8091	1/1	0.94	0.07	-	42,42,42,42	0
34	NA	0	8516	1/1	0.94	0.23	-	30,30,30,30	0
36	SR	0	8933	1/1	0.76	0.52	-	138,138,138,138	0
36	SR	0	8951	1/1	0.81	0.07	-	146,146,146,146	0
36	SR	0	8916	1/1	0.71	0.15	-	118,118,118,118	0
36	SR	0	9006	1/1	0.14	1.93	-	200,200,200,200	0
32	MG	0	8092	1/1	0.72	0.14	-	61,61,61,61	0
34	NA	0	8509	1/1	0.88	0.34	-	64,64,64,64	0
36	SR	0	9002	1/1	0.78	0.15	-	184,184,184,184	0
36	SR	0	8971	1/1	0.71	0.17	-	170,170,170,170	0
36	SR	0	8989	1/1	0.66	0.39	-	187,187,187,187	0
36	SR	0	8998	1/1	0.82	0.41	-	173,173,173,173	0
32	MG	0	8063	1/1	0.82	0.28	-	72,72,72,72	0
36	SR	0	8924	1/1	0.64	0.13	-	145,145,145,145	0
32	MG	0	8078	1/1	0.93	0.37	-	51,51,51,51	0
34	NA	0	8526	1/1	0.96	0.09	-	32,32,32,32	0
36	SR	0	8996	1/1	0.50	0.82	-	200,200,200,200	0
32	MG	0	8060	1/1	0.96	0.11	-	42,42,42,42	0
32	MG	0	8030	1/1	0.85	0.37	-	55,55,55,55	0
36	SR	0	8928	1/1	0.83	0.20	-	138,138,138,138	0
36	SR	3	8999	1/1	0.94	0.08	-	95,95,95,95	0
32	MG	0	8026	1/1	0.98	0.14	-	31,31,31,31	0
34	NA	0	8550	1/1	0.94	0.25	-	54,54,54,54	0
32	MG	0	8033	1/1	0.93	0.11	-	45,45,45,45	0
36	SR	0	8997	1/1	0.81	0.63	-	184,184,184,184	0
36	SR	0	8925	1/1	0.98	0.12	-	90,90,90,90	0
36	SR	0	8995	1/1	0.83	0.19	-	136,136,136,136	0
34	NA	0	8566	1/1	0.96	0.29	-	37,37,37,37	0
36	SR	9	8978	1/1	0.09	0.14	-	144,144,144,144	0
36	SR	0	8918	1/1	0.94	0.14	-	79,79,79,79	0
36	SR	0	8908	1/1	0.89	0.18	-	107,107,107,107	0
36	SR	0	8990	1/1	0.77	0.22	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8544	1/1	0.89	0.30	-	64,64,64,64	0
36	SR	0	8953	1/1	0.77	0.24	-	160,160,160,160	0
32	MG	0	8035	1/1	0.95	0.10	-	44,44,44,44	0
32	MG	0	8059	1/1	0.91	0.09	-	36,36,36,36	0
36	SR	0	9008	1/1	0.90	0.14	-	90,90,90,90	0
32	MG	0	8066	1/1	0.88	0.21	-	52,52,52,52	0
34	NA	0	8545	1/1	0.90	0.30	-	37,37,37,37	0
36	SR	0	8939	1/1	0.82	0.18	-	152,152,152,152	0
35	CL	0	8822	1/1	0.95	0.25	-	68,68,68,68	0
36	SR	0	9004	1/1	0.86	0.42	-	200,200,200,200	0
36	SR	0	8923	1/1	0.92	0.19	-	101,101,101,101	0
36	SR	0	8914	1/1	0.80	0.34	-	118,118,118,118	0
32	MG	0	8069	1/1	0.69	0.57	-	47,47,47,47	0
34	NA	R	8532	1/1	0.89	0.18	-	53,53,53,53	0
36	SR	9	9003	1/1	0.60	0.10	-	162,162,162,162	0
34	NA	0	8541	1/1	0.94	0.34	-	53,53,53,53	0
32	MG	0	8080	1/1	0.85	0.29	-	57,57,57,57	0
36	SR	0	8934	1/1	0.64	0.13	-	90,90,90,90	0
32	MG	K	8054	1/1	0.95	0.16	-	39,39,39,39	0
36	SR	0	8964	1/1	0.88	0.08	-	126,126,126,126	0
36	SR	B	8950	1/1	0.88	0.19	-	108,108,108,108	0

## 6.5 Other polymers

There are no such residues in this entry.