



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:14 PM 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 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/ValidationPDFNotes.html>

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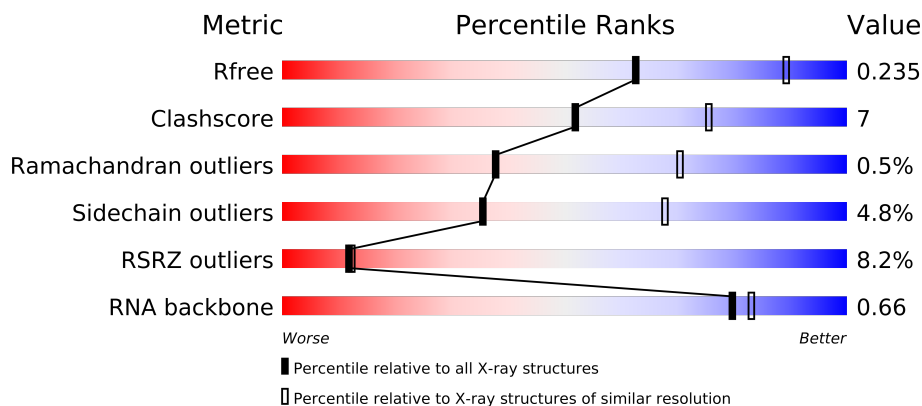
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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

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

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8001	-	X
32	MG	0	8003	-	X
32	MG	0	8004	-	X
32	MG	0	8005	-	X
32	MG	0	8006	-	X
32	MG	0	8007	-	X
32	MG	0	8009	-	X
32	MG	0	8011	-	X
32	MG	0	8012	-	X
32	MG	0	8014	-	X
32	MG	0	8015	-	X
32	MG	0	8016	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8019	-	X
32	MG	0	8020	-	X
32	MG	0	8022	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8024	-	X
32	MG	0	8028	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8037	-	X
32	MG	0	8039	-	X
32	MG	0	8040	-	X
32	MG	0	8041	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8055	-	X
32	MG	0	8056	-	X
32	MG	0	8061	-	X
32	MG	0	8062	-	X
32	MG	0	8064	-	X
32	MG	0	8066	-	X
32	MG	0	8067	-	X
32	MG	0	8069	-	X
32	MG	0	8071	-	X
32	MG	0	8072	-	X
32	MG	0	8073	-	X
32	MG	0	8076	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8080	-	X
32	MG	0	8081	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	0	8087	-	X
32	MG	0	8092	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
34	NA	0	8501	-	X
34	NA	0	8502	-	X
34	NA	0	8504	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8507	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8511	-	X
34	NA	0	8512	-	X
34	NA	0	8513	-	X
34	NA	0	8514	-	X
34	NA	0	8516	-	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	8524	-	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	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8550	-	X
34	NA	0	8551	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	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	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8568	-	X
34	NA	0	8569	-	X
34	NA	0	8570	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
34	NA	9	8572	-	X
34	NA	B	8552	-	X
34	NA	M	8539	-	X
34	NA	S	8510	-	X
35	CL	0	8822	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8907	-	X
36	SR	0	8908	-	X
36	SR	0	8914	-	X
36	SR	0	8919	-	X
36	SR	0	8922	-	X
36	SR	0	8928	-	X
36	SR	0	8933	-	X
36	SR	0	8937	-	X
36	SR	0	8944	-	X
36	SR	0	8947	-	X
36	SR	0	8948	-	X
36	SR	0	8949	-	X
36	SR	0	8953	-	X
36	SR	0	8955	-	X
36	SR	0	8957	-	X
36	SR	0	8959	-	X
36	SR	0	8962	-	X
36	SR	0	8969	-	X
36	SR	0	8971	-	X
36	SR	0	8974	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8989	-	X
36	SR	0	8990	-	X
36	SR	0	8991	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	8998	-	X
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	X
37	ANM	0	2924	-	X

## 2 Entry composition

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

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

- Molecule 1 is a protein called 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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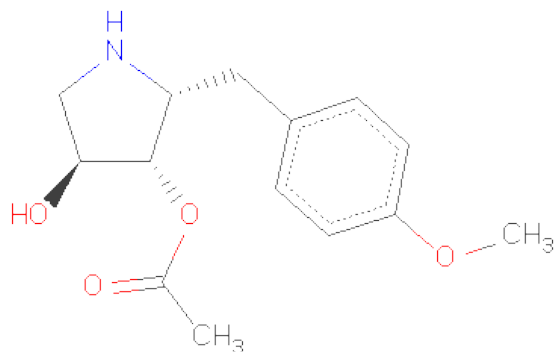
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

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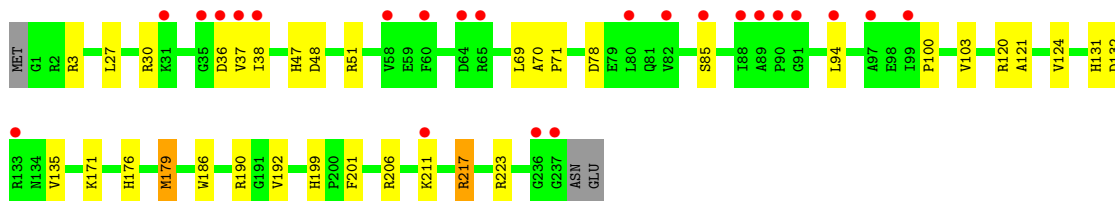
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	23	Total 23	O 23	0	0
39	Y	92	Total 92	O 92	0	0
39	Z	31	Total 31	O 31	0	0
39	1	48	Total 48	O 48	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0
39	9	147	Total 147	O 147	0	0

### 3 Residue-property plots

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

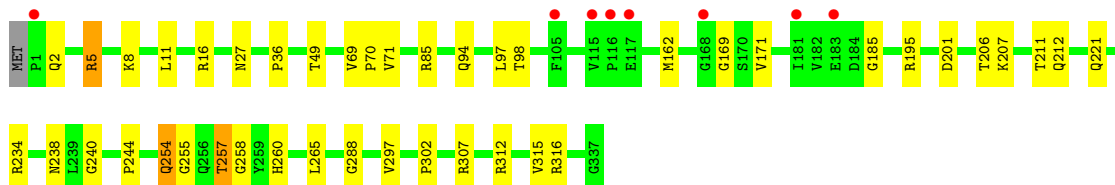
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



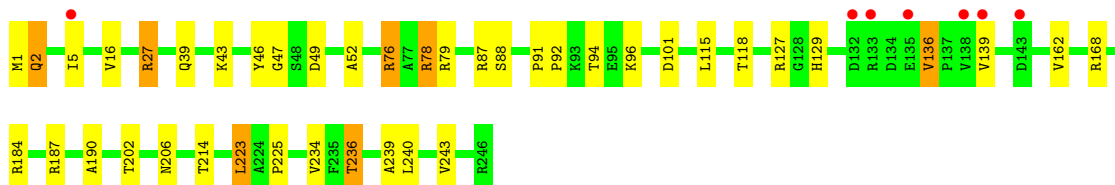
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



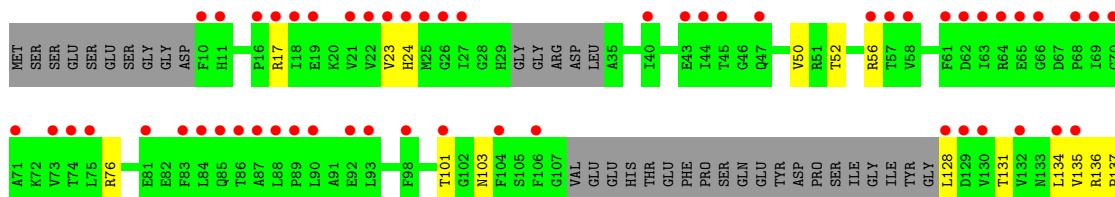
- Molecule 3: 50S ribosomal protein L4P

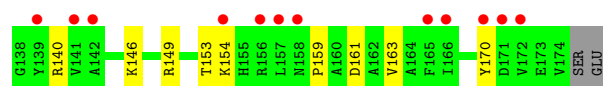
Chain C: 



- Molecule 4: 50S ribosomal protein L5P

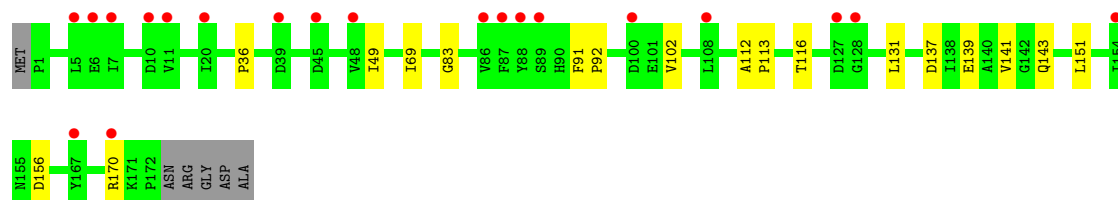
Chain D: 





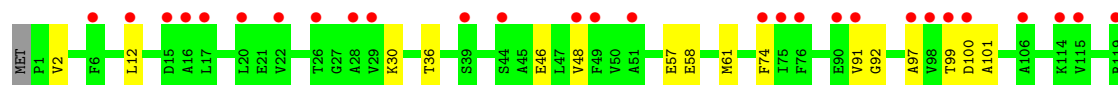
- Molecule 5: 50S ribosomal protein L6P

Chain E:



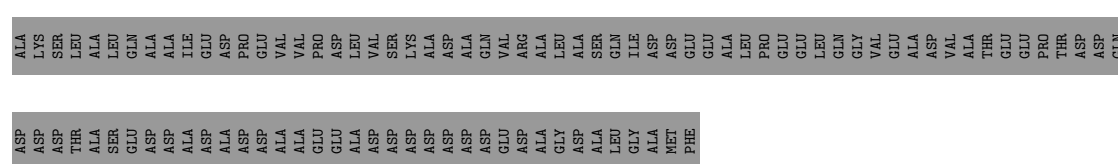
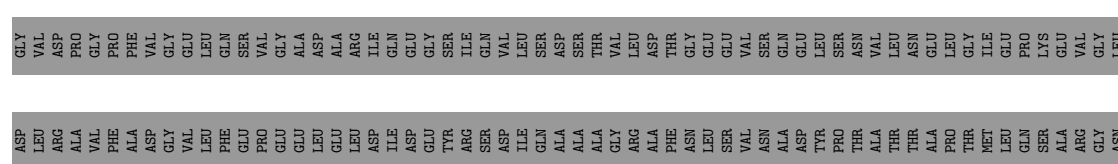
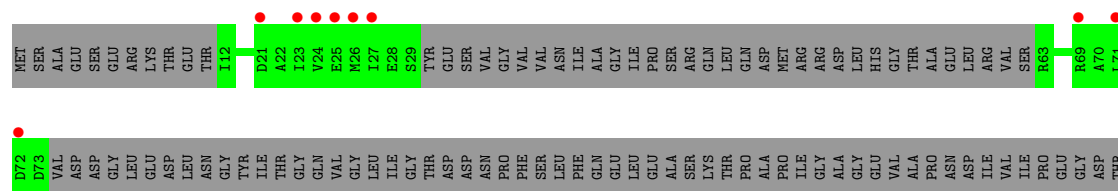
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



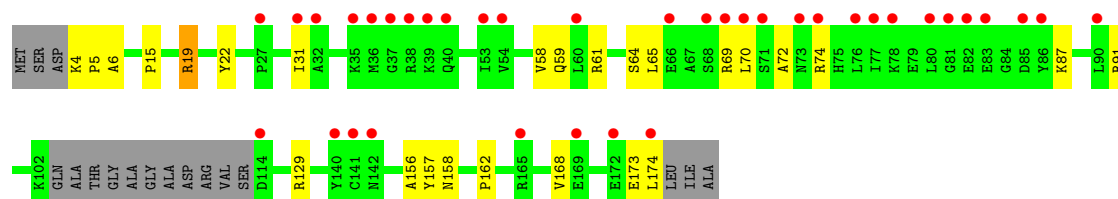
- Molecule 7: 50S ribosomal protein L10E

Chain G:



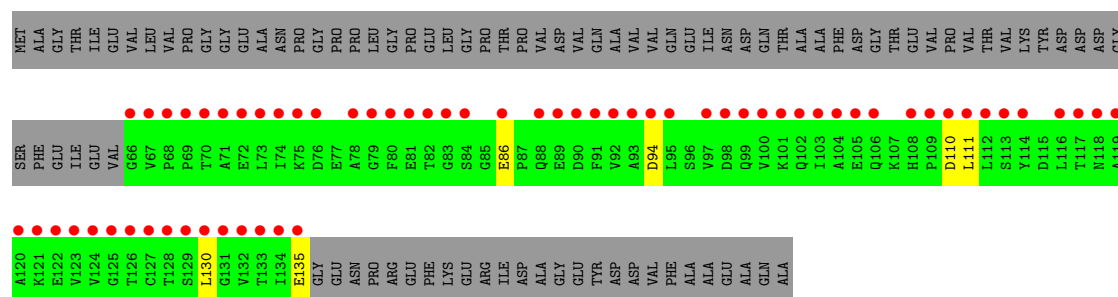
- Molecule 8: 50S ribosomal protein L10e

Chain H:



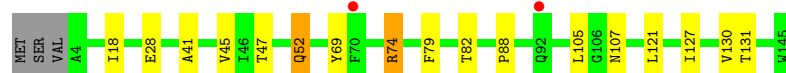
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

Chain J:



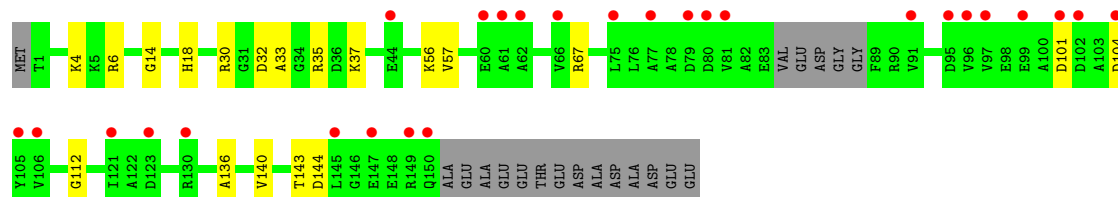
- Molecule 11: 50S ribosomal protein L14P

Chain K:



- Molecule 12: 50S ribosomal protein L15P

Chain L:



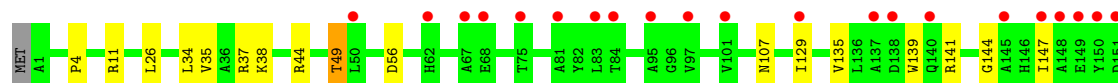
- Molecule 13: 50S ribosomal protein L15e

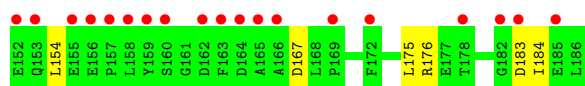
Chain M:



- Molecule 14: 50S ribosomal protein L18P

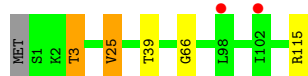
Chain N:





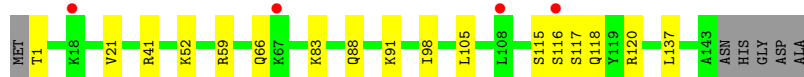
- Molecule 15: 50S ribosomal protein L18e

Chain O:



- Molecule 16: 50S ribosomal protein L19e

Chain P:



- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:



- Molecule 19: 50S ribosomal protein L23P

Chain S:



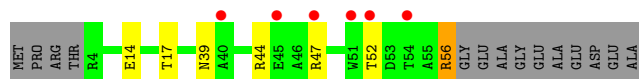
- Molecule 20: 50S ribosomal protein L24P

Chain T:



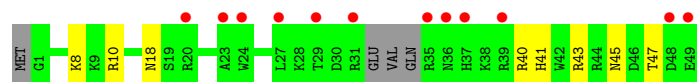
- Molecule 21: 50S ribosomal protein L24e

Chain U:



- Molecule 22: 50S ribosomal protein L29P

Chain 2: 



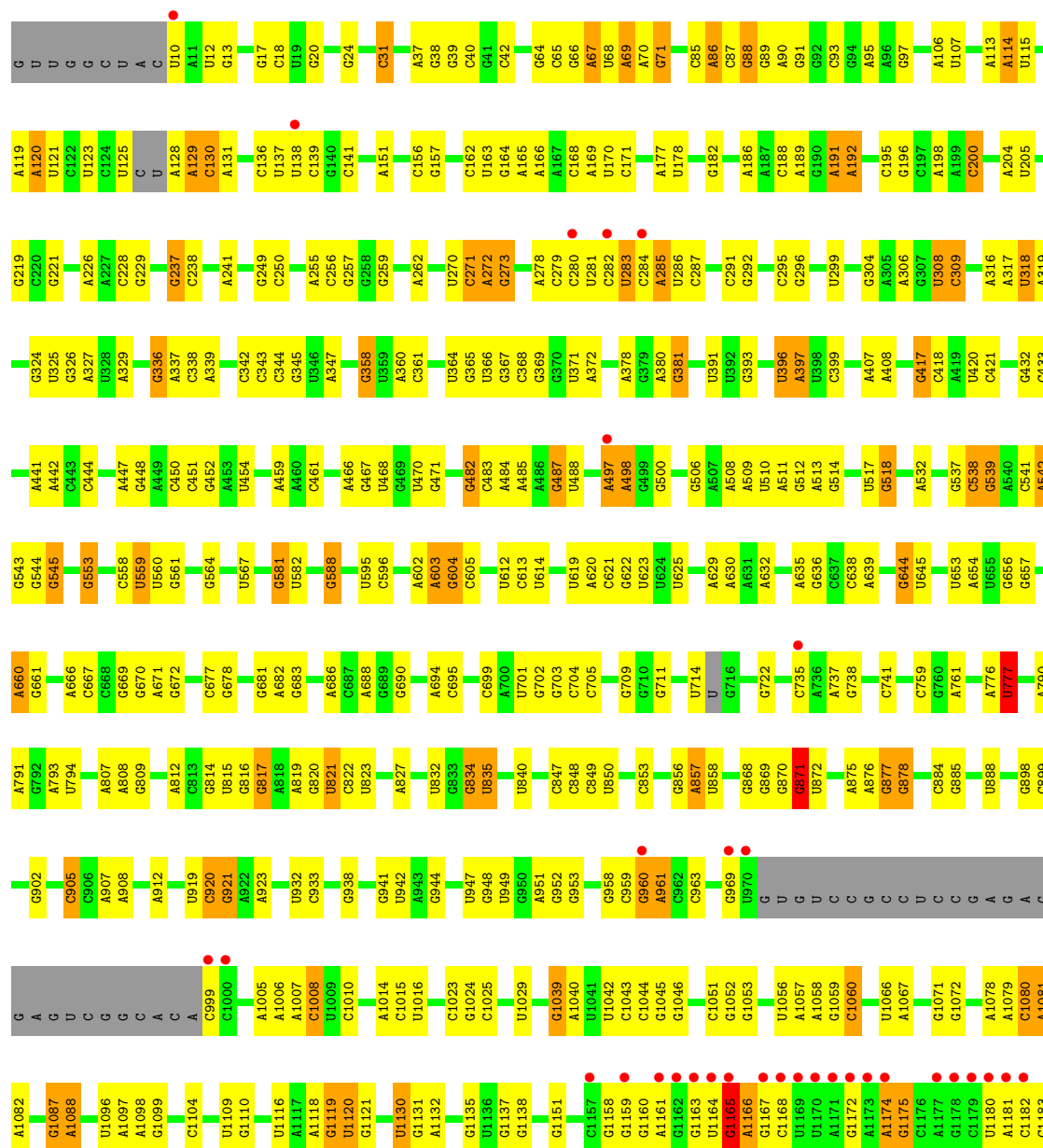
- Molecule 29: 50S ribosomal protein L44E

Chain 3:



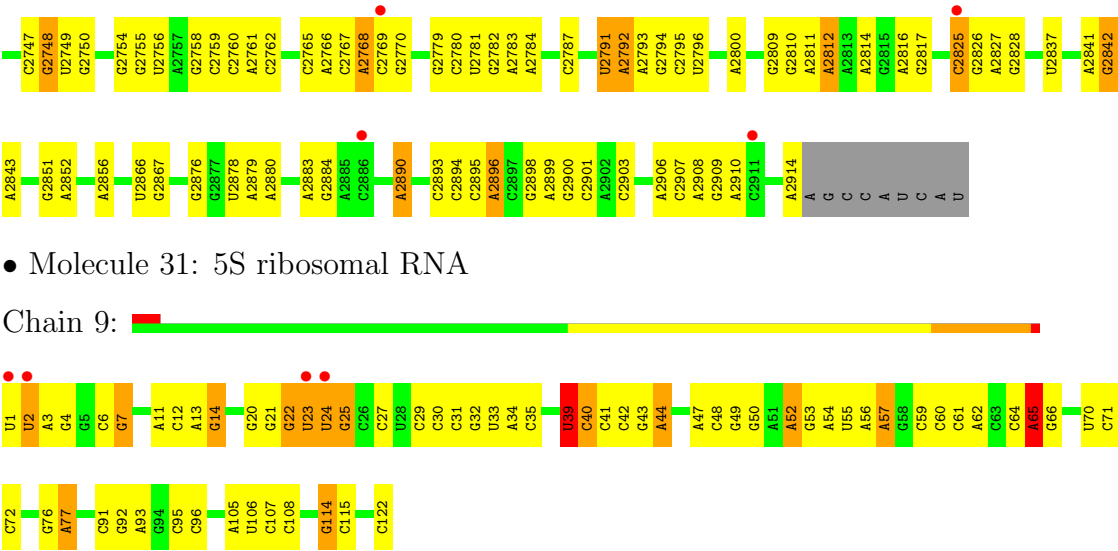
- Molecule 30: 23S ribosomal RNA

Chain 0:



C2611	C2612	C2613	C2614	U2615	C2630	C2515	G2516	G2520	A2521	G2426	A2433	G2524	G2525	C2526	U2527	U2528	G2529	C2530	U2531	A2532	C2533	C2534	A2455	A2456	U2457	A2468	C2472	C2476	G2477	U2478	A2479	G2480	A2483	U2484	A2485	U2586	U2587	C2588	G2589	C2591	C2592	C2593	C2594	U2595	C2601	A2602	C2603	C2720	U2721	C2604	U2607	C2608	U2724	C2725	U2726																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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C2335	G2336	G2337	G2338	A2339	C2340	G2341	A2342	C2343	A2344	C2345	C2346	C2347	C2348	C2349	G2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C2088	A2089	G2090	G2091	G2092	A2096	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416																																																																																																																																																																																																																																												
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A1858	G1863	G1867	G1868	G1877																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										





## 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	4705 reflections (0.99%)	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> )	0.32 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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.

## 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 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	21	0
2	B	2625	0	2533	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1860	0	1813	22	0
4	D	1094	0	1085	11	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	G	17	0	0	0	0
39	H	67	0	0	3	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 1085 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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%)	25	55
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	33	66
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	15	38
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100	100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	8	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	33	66
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%)	27	58
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%)	8	19
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%)	18	43
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%)	16	41
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%)	21	49
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	38	70



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%)	34	66
2	B	282/283 (100%)	269 (95%)	13 (5%)	37	70
3	C	193/193 (100%)	177 (92%)	16 (8%)	16	35
4	D	117/148 (79%)	107 (92%)	10 (8%)	15	34
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	88
6	F	93/94 (99%)	91 (98%)	2 (2%)	64	90
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	127 (95%)	7 (5%)	32	63
9	I	58/130 (45%)	56 (97%)	2 (3%)	49	81
10	J	118/121 (98%)	110 (93%)	8 (7%)	22	48
11	K	106/106 (100%)	99 (93%)	7 (7%)	24	50
12	L	113/127 (89%)	107 (95%)	6 (5%)	32	62
13	M	158/160 (99%)	150 (95%)	8 (5%)	33	64
14	N	149/150 (99%)	144 (97%)	5 (3%)	49	81
15	O	93/94 (99%)	91 (98%)	2 (2%)	64	90
16	P	113/117 (97%)	109 (96%)	4 (4%)	48	80
17	Q	79/80 (99%)	76 (96%)	3 (4%)	44	76
18	R	117/122 (96%)	114 (97%)	3 (3%)	59	88
19	S	71/74 (96%)	69 (97%)	2 (3%)	56	86
20	T	105/106 (99%)	96 (91%)	9 (9%)	15	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	44/53 (83%)	41 (93%)	3 (7%)	22	48
22	V	51/57 (90%)	49 (96%)	2 (4%)	43	76
23	W	130/130 (100%)	123 (95%)	7 (5%)	31	61
24	X	66/74 (89%)	59 (89%)	7 (11%)	10	22
25	Y	120/196 (61%)	116 (97%)	4 (3%)	50	81
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	64	90
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	89
29	3	79/79 (100%)	75 (95%)	4 (5%)	33	64
All	All	3095/3646 (85%)	2946 (95%)	149 (5%)	35	68

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	20,22,23	0.74	1 (5%)	24,31,34	0.82	0
30	OMG	0	2588	30	24,26,27	0.82	0	32,38,41	5.07	3 (9%)
30	UR3	0	2619	30	20,22,23	0.74	0	23,32,35	0.88	0
30	PSU	0	2621	30	19,21,22	1.09	3 (15%)	23,30,33	1.03	1 (4%)
30	1MA	0	628	30	23,25,26	0.84	0	32,37,40	1.01	1 (3%)

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	-	0/8/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMG	0	2588	30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30	-	1/8/25/26	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.70	1.42	1.37
30	0	2587	OMU	P-OP1	2.33	1.49	1.46
30	0	2621	PSU	C6-N1	2.18	1.34	1.32
30	0	2621	PSU	P-OP1	2.14	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.09	130.36	134.14
30	0	2588	OMG	C6-N1-C2	3.20	125.11	119.51
30	0	628	1MA	C2-N3-C4	-3.12	110.89	116.23
30	0	2588	OMG	C2-N3-C4	-2.29	111.87	115.09
30	0	2621	PSU	C5-C4-N3	-2.25	114.76	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	20,20,20	0.46	0	27,27,27	1.78	8 (29%)

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	-	-	0/10/23/23	0/2/2/2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	2924	ANM	O2-C5-C6	5.10	120.72	111.12
37	0	2924	ANM	C2-O2-C5	-3.62	111.92	117.71
37	0	2924	ANM	C4-C3-C2	-3.49	98.31	103.28
37	0	2924	ANM	C2-C16-N1	2.63	105.34	101.08
37	0	2924	ANM	C14-O1-C9	-2.50	111.46	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.60	23 (9%) 8 8	24, 49, 88, 107	0
2	B	337/338 (99%)	0.36	8 (2%) 56 62	27, 53, 82, 95	0
3	C	246/246 (100%)	0.23	7 (2%) 50 56	21, 42, 65, 78	0
4	D	140/177 (79%)	2.44	67 (47%) 1 0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.77	20 (11%) 5 6	44, 69, 88, 94	0
6	F	119/120 (99%)	1.32	28 (23%) 1 1	43, 69, 99, 114	0
7	G	29/348 (8%)	1.81	9 (31%) 1 1	77, 95, 103, 106	0
8	H	160/177 (90%)	1.31	37 (23%) 1 1	44, 61, 96, 101	0
9	I	70/162 (43%)	4.92	64 (91%) 0 0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.35	2 (1%) 72 77	35, 50, 71, 91	0
11	K	132/132 (100%)	0.14	1 (0%) 83 87	32, 49, 72, 77	0
12	L	145/165 (87%)	0.92	27 (18%) 2 2	25, 63, 109, 125	0
13	M	194/196 (98%)	0.09	2 (1%) 79 83	28, 40, 56, 63	0
14	N	186/187 (99%)	1.19	40 (21%) 1 2	42, 64, 112, 121	0
15	O	115/116 (99%)	0.55	2 (1%) 67 73	33, 53, 69, 80	0
16	P	143/149 (95%)	0.46	4 (2%) 50 56	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.31	2 (2%) 60 67	34, 45, 62, 73	0
18	R	150/155 (96%)	0.14	0 100 100	30, 43, 63, 71	0
19	S	81/85 (95%)	0.84	9 (11%) 6 6	42, 56, 79, 90	0
20	T	119/120 (99%)	0.61	6 (5%) 28 30	35, 54, 84, 109	0
21	U	53/67 (79%)	0.62	6 (11%) 6 6	40, 56, 78, 84	0
22	V	65/71 (91%)	2.60	31 (47%) 1 0	52, 73, 117, 123	0
23	W	154/154 (100%)	0.52	4 (2%) 53 59	33, 49, 65, 75	0
24	X	82/92 (89%)	0.88	13 (15%) 3 3	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%)	0.20	6 (4%) 35 39	22, 41, 64, 89	0
26	Z	73/116 (62%)	2.57	42 (57%) 0 0	58, 76, 89, 100	0
27	1	56/57 (98%)	-0.03	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.04	12 (26%) 1 1	34, 60, 91, 101	0
29	3	92/92 (100%)	0.65	7 (7%) 14 14	36, 59, 72, 86	0
30	0	2754/2923 (94%)	0.00	71 (2%) 53 59	18, 43, 87, 165	0
31	9	122/122 (100%)	0.05	4 (3%) 44 49	34, 65, 86, 145	0
All	All	6651/7517 (88%)	0.45	554 (8%) 12 12	18, 50, 99, 165	0

The worst 5 of 554 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	16.2
22	V	40	PRO	13.1
22	V	1	THR	13.0
4	D	63	ILE	11.5
14	N	166	ALA	11.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	UR3	0	2619	21/22	0.16	1.89	30,34,36,39	0
30	1MA	0	628	23/24	0.17	0.05	25,28,29,31	0
30	OMU	0	2587	21/22	0.14	-0.33	31,33,35,37	0
30	PSU	0	2621	20/21	0.14	-1.11	22,26,34,34	0
30	OMG	0	2588	24/25	0.14	-1.24	27,30,33,35	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8955	1/1	0.34	239.00	200,200,200,200	0
36	SR	0	9006	1/1	1.59	208.43	200,200,200,200	0
36	SR	0	8997	1/1	0.61	157.00	184,184,184,184	0
34	NA	0	8562	1/1	0.74	141.94	69,69,69,69	0
34	NA	0	8561	1/1	0.81	83.64	74,74,74,74	0
36	SR	0	8996	1/1	0.79	82.01	200,200,200,200	0
36	SR	0	8979	1/1	0.28	73.00	194,194,194,194	0
36	SR	0	8982	1/1	0.89	72.48	180,180,180,180	0
36	SR	0	8994	1/1	0.73	60.74	190,190,190,190	0
34	NA	0	8548	1/1	0.40	59.03	57,57,57,57	0
32	MG	0	8049	1/1	0.36	48.78	55,55,55,55	0
34	NA	0	8506	1/1	0.27	48.24	47,47,47,47	0
36	SR	0	8986	1/1	1.82	45.27	200,200,200,200	0
34	NA	0	8573	1/1	0.65	42.98	69,69,69,69	0
36	SR	0	8957	1/1	0.85	39.27	200,200,200,200	0
34	NA	0	8511	1/1	0.32	37.79	59,59,59,59	0
32	MG	0	8024	1/1	0.57	37.36	85,85,85,85	0
34	NA	0	8566	1/1	0.37	37.12	37,37,37,37	0
34	NA	0	8505	1/1	0.55	36.58	39,39,39,39	0
34	NA	0	8555	1/1	0.67	36.22	54,54,54,54	0
33	K	0	8401	1/1	0.45	31.99	81,81,81,81	0
34	NA	0	8547	1/1	0.42	27.92	54,54,54,54	0
34	NA	0	8574	1/1	0.39	24.11	53,53,53,53	0
32	MG	0	8072	1/1	0.26	23.80	52,52,52,52	0
34	NA	0	8509	1/1	0.32	23.56	64,64,64,64	0
36	SR	0	8983	1/1	0.23	23.39	164,164,164,164	0
32	MG	0	8041	1/1	0.31	22.17	24,24,24,24	0
34	NA	0	8519	1/1	0.37	22.04	39,39,39,39	0
34	NA	0	8553	1/1	0.38	20.98	79,79,79,79	0
34	NA	0	8542	1/1	0.38	20.10	42,42,42,42	0
32	MG	0	8047	1/1	0.43	19.88	49,49,49,49	0
34	NA	0	8512	1/1	0.49	19.19	43,43,43,43	0
36	SR	0	8974	1/1	0.27	18.22	166,166,166,166	0
34	NA	0	8554	1/1	0.70	18.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8976	1/1	0.49	17.82	186,186,186,186	0
34	NA	0	8549	1/1	0.42	17.80	81,81,81,81	0
32	MG	0	8071	1/1	0.27	17.69	55,55,55,55	0
34	NA	0	8502	1/1	0.31	17.21	67,67,67,67	0
36	SR	0	9007	1/1	0.36	17.15	200,200,200,200	0
36	SR	0	8989	1/1	0.33	17.07	187,187,187,187	0
34	NA	0	8544	1/1	0.27	16.38	64,64,64,64	0
32	MG	0	8048	1/1	0.28	16.10	28,28,28,28	0
32	MG	0	8015	1/1	0.17	15.83	27,27,27,27	0
34	NA	0	8522	1/1	0.52	15.44	78,78,78,78	0
34	NA	9	8572	1/1	0.50	15.43	76,76,76,76	0
32	MG	0	8061	1/1	0.38	15.04	37,37,37,37	0
36	SR	0	8969	1/1	0.38	14.59	150,150,150,150	0
34	NA	0	8545	1/1	0.27	14.45	37,37,37,37	0
32	MG	0	8030	1/1	0.33	14.17	55,55,55,55	0
32	MG	0	8019	1/1	0.28	13.66	24,24,24,24	0
34	NA	0	8565	1/1	0.33	13.41	62,62,62,62	0
36	SR	0	8922	1/1	0.36	13.23	159,159,159,159	0
36	SR	0	8998	1/1	0.36	12.87	173,173,173,173	0
36	SR	0	8914	1/1	0.32	12.70	118,118,118,118	0
32	MG	0	8078	1/1	0.35	12.59	51,51,51,51	0
32	MG	0	8005	1/1	0.30	12.10	26,26,26,26	0
34	NA	0	8524	1/1	0.29	11.95	45,45,45,45	0
34	NA	0	8546	1/1	1.03	11.85	95,95,95,95	0
36	SR	0	8944	1/1	0.24	11.63	185,185,185,185	0
34	NA	0	8507	1/1	0.26	11.34	45,45,45,45	0
34	NA	0	8541	1/1	0.30	11.31	53,53,53,53	0
34	NA	0	8567	1/1	0.39	11.26	78,78,78,78	0
32	MG	0	8007	1/1	0.29	10.95	26,26,26,26	0
34	NA	S	8510	1/1	0.52	10.79	79,79,79,79	0
32	MG	0	8016	1/1	0.34	10.65	49,49,49,49	0
34	NA	0	8568	1/1	0.36	10.65	47,47,47,47	0
32	MG	0	8031	1/1	0.22	10.53	61,61,61,61	0
34	NA	0	8517	1/1	0.26	10.40	30,30,30,30	0
34	NA	0	8521	1/1	0.27	10.34	61,61,61,61	0
34	NA	0	8556	1/1	0.59	10.30	44,44,44,44	0
32	MG	0	8040	1/1	0.31	10.18	83,83,83,83	0
32	MG	0	8028	1/1	0.25	10.15	22,22,22,22	0
34	NA	0	8516	1/1	0.19	10.07	30,30,30,30	0
36	SR	0	8928	1/1	0.21	9.74	138,138,138,138	0
36	SR	9	8980	1/1	0.26	9.70	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	B	8552	1/1	0.31	9.50	56,56,56,56	0
34	NA	0	8535	1/1	0.19	9.46	52,52,52,52	0
32	MG	0	8079	1/1	0.20	9.33	47,47,47,47	0
36	SR	B	8987	1/1	0.67	9.06	200,200,200,200	0
32	MG	0	8018	1/1	0.23	8.89	38,38,38,38	0
34	NA	0	8523	1/1	0.24	8.81	48,48,48,48	0
32	MG	0	8076	1/1	0.23	8.67	35,35,35,35	0
35	CL	0	8822	1/1	0.26	8.48	68,68,68,68	0
34	NA	0	8560	1/1	0.48	8.40	69,69,69,69	0
34	NA	0	8563	1/1	0.31	8.23	60,60,60,60	0
32	MG	0	8039	1/1	0.30	8.22	69,69,69,69	0
34	NA	0	8501	1/1	0.18	8.21	39,39,39,39	0
36	SR	0	8947	1/1	0.49	8.19	200,200,200,200	0
32	MG	0	8014	1/1	0.23	8.00	30,30,30,30	0
36	SR	0	8948	1/1	0.16	7.98	102,102,102,102	0
34	NA	0	8571	1/1	0.33	7.92	83,83,83,83	0
34	NA	0	8559	1/1	0.22	7.67	75,75,75,75	0
32	MG	0	8069	1/1	0.55	7.57	47,47,47,47	0
36	SR	0	8903	1/1	0.19	7.55	53,53,53,53	0
32	MG	0	8081	1/1	0.23	7.44	54,54,54,54	0
32	MG	0	8009	1/1	0.25	7.27	21,21,21,21	0
34	NA	0	8564	1/1	0.21	7.06	65,65,65,65	0
32	MG	A	8051	1/1	0.53	6.98	81,81,81,81	0
36	SR	0	8992	1/1	0.21	6.87	123,123,123,123	0
32	MG	0	8066	1/1	0.20	6.86	52,52,52,52	0
32	MG	0	8064	1/1	0.24	6.71	38,38,38,38	0
36	SR	0	8962	1/1	0.24	6.66	167,167,167,167	0
34	NA	0	8570	1/1	0.20	6.65	49,49,49,49	0
32	MG	0	8085	1/1	0.31	6.52	80,80,80,80	0
36	SR	0	8919	1/1	0.23	6.52	178,178,178,178	0
34	NA	0	8527	1/1	0.22	6.32	52,52,52,52	0
34	NA	0	8550	1/1	0.23	6.18	54,54,54,54	0
32	MG	0	8011	1/1	0.27	5.57	23,23,23,23	0
32	MG	0	8062	1/1	0.23	5.56	34,34,34,34	0
32	MG	0	8067	1/1	0.26	5.50	34,34,34,34	0
32	MG	0	8087	1/1	0.21	5.48	42,42,42,42	0
34	NA	0	8513	1/1	0.24	5.45	44,44,44,44	0
34	NA	0	8530	1/1	0.24	5.44	42,42,42,42	0
36	SR	0	8990	1/1	0.21	5.30	118,118,118,118	0
34	NA	0	8575	1/1	0.34	5.22	94,94,94,94	0
32	MG	0	8092	1/1	0.17	5.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8905	1/1	0.25	5.10	57,57,57,57	0
32	MG	0	8022	1/1	0.20	5.07	29,29,29,29	0
34	NA	0	8504	1/1	0.23	5.06	26,26,26,26	0
34	NA	0	8551	1/1	0.22	5.05	46,46,46,46	0
36	SR	0	8971	1/1	0.17	5.00	170,170,170,170	0
34	NA	0	8534	1/1	0.23	4.77	32,32,32,32	0
36	SR	0	9004	1/1	0.43	4.46	200,200,200,200	0
34	NA	0	8569	1/1	0.24	4.40	53,53,53,53	0
32	MG	0	8037	1/1	0.24	4.21	83,83,83,83	0
34	NA	0	8508	1/1	0.19	4.09	37,37,37,37	0
34	NA	0	8558	1/1	0.23	4.05	44,44,44,44	0
36	SR	0	8949	1/1	0.20	3.95	110,110,110,110	0
34	NA	0	8528	1/1	0.17	3.86	45,45,45,45	0
34	NA	0	8514	1/1	0.24	3.86	42,42,42,42	0
32	MG	0	8006	1/1	0.20	3.86	30,30,30,30	0
32	MG	0	8056	1/1	0.17	3.82	42,42,42,42	0
36	SR	0	8937	1/1	0.18	3.79	100,100,100,100	0
32	MG	0	8017	1/1	0.23	3.74	56,56,56,56	0
36	SR	0	8953	1/1	0.32	3.68	160,160,160,160	0
36	SR	0	8959	1/1	0.20	3.50	169,169,169,169	0
32	MG	0	8004	1/1	0.21	3.19	25,25,25,25	0
36	SR	0	8933	1/1	0.49	3.18	138,138,138,138	0
36	SR	0	8991	1/1	0.22	3.10	191,191,191,191	0
32	MG	0	8073	1/1	0.15	2.97	76,76,76,76	0
37	ANM	0	2924	19/19	0.19	2.87	31,37,40,40	0
32	MG	0	8055	1/1	0.26	2.84	38,38,38,38	0
32	MG	0	8020	1/1	0.19	2.69	54,54,54,54	0
36	SR	0	8908	1/1	0.17	2.65	107,107,107,107	0
32	MG	0	8012	1/1	0.21	2.57	21,21,21,21	0
34	NA	0	8557	1/1	0.14	2.54	67,67,67,67	0
32	MG	0	8001	1/1	0.19	2.53	25,25,25,25	0
36	SR	0	8907	1/1	0.31	2.53	76,76,76,76	0
32	MG	0	8080	1/1	0.25	2.51	57,57,57,57	0
34	NA	M	8539	1/1	0.23	2.45	41,41,41,41	0
34	NA	0	8533	1/1	0.24	2.11	63,63,63,63	0
32	MG	0	8029	1/1	0.16	2.04	39,39,39,39	0
32	MG	0	8082	1/1	0.29	2.03	48,48,48,48	0
32	MG	0	8003	1/1	0.18	2.03	30,30,30,30	0
34	NA	0	8518	1/1	0.36	1.99	79,79,79,79	0
36	SR	0	8923	1/1	0.17	1.97	101,101,101,101	0
32	MG	0	8023	1/1	0.16	1.93	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8008	1/1	0.19	1.92	25,25,25,25	0
36	SR	0	8995	1/1	0.18	1.83	136,136,136,136	0
36	SR	0	8925	1/1	0.12	1.80	90,90,90,90	0
35	CL	0	8805	1/1	0.16	1.80	59,59,59,59	0
36	SR	0	8941	1/1	0.17	1.75	115,115,115,115	0
36	SR	B	8950	1/1	0.18	1.75	108,108,108,108	0
32	MG	0	8088	1/1	0.17	1.63	37,37,37,37	0
36	SR	0	8917	1/1	0.17	1.49	119,119,119,119	0
36	SR	0	8981	1/1	0.23	1.48	167,167,167,167	0
36	SR	A	8929	1/1	0.24	1.40	131,131,131,131	0
32	MG	0	8070	1/1	0.16	1.38	45,45,45,45	0
36	SR	0	8904	1/1	0.18	1.30	52,52,52,52	0
36	SR	0	8901	1/1	0.16	1.27	58,58,58,58	0
36	SR	0	8916	1/1	0.15	1.24	118,118,118,118	0
32	MG	0	8084	1/1	0.17	1.02	31,31,31,31	0
34	NA	0	8520	1/1	0.18	0.81	54,54,54,54	0
36	SR	0	9002	1/1	0.15	0.74	184,184,184,184	0
35	CL	0	8816	1/1	0.18	0.72	60,60,60,60	0
32	MG	0	8045	1/1	0.17	0.70	32,32,32,32	0
32	MG	0	8043	1/1	0.17	0.66	49,49,49,49	0
36	SR	0	8942	1/1	0.15	0.61	121,121,121,121	0
32	MG	0	8010	1/1	0.17	0.48	26,26,26,26	0
32	MG	0	8027	1/1	0.14	0.37	34,34,34,34	0
32	MG	0	8046	1/1	0.16	0.34	28,28,28,28	0
34	NA	Q	8540	1/1	0.21	0.33	60,60,60,60	0
36	SR	0	8906	1/1	0.20	0.26	56,56,56,56	0
34	NA	R	8532	1/1	0.18	0.22	53,53,53,53	0
36	SR	0	8939	1/1	0.16	0.22	152,152,152,152	0
36	SR	0	8985	1/1	0.14	0.22	110,110,110,110	0
36	SR	0	9000	1/1	0.15	0.20	159,159,159,159	0
34	NA	C	8503	1/1	0.20	0.11	37,37,37,37	0
34	NA	0	8515	1/1	0.19	0.10	33,33,33,33	0
32	MG	K	8054	1/1	0.16	0.07	39,39,39,39	0
36	SR	0	8918	1/1	0.14	0.06	79,79,79,79	0
32	MG	0	8050	1/1	0.17	0.02	37,37,37,37	0
36	SR	H	8972	1/1	0.21	-0.04	130,130,130,130	0
36	SR	R	8912	1/1	0.15	-0.11	84,84,84,84	0
36	SR	0	8993	1/1	0.18	-0.36	168,168,168,168	0
34	NA	0	8531	1/1	0.15	-0.40	40,40,40,40	0
36	SR	0	8967	1/1	0.12	-0.40	133,133,133,133	0
36	SR	0	8909	1/1	0.14	-0.41	94,94,94,94	0
32	MG	0	8002	1/1	0.16	-0.47	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	J	8538	1/1	0.18	-0.49	56,56,56,56	0
35	CL	O	8808	1/1	0.19	-0.57	61,61,61,61	0
36	SR	0	8927	1/1	0.13	-0.64	167,167,167,167	0
32	MG	B	8042	1/1	0.13	-0.68	50,50,50,50	0
32	MG	0	8077	1/1	0.15	-0.70	32,32,32,32	0
32	MG	0	8065	1/1	0.13	-0.71	33,33,33,33	0
36	SR	A	8977	1/1	0.17	-0.83	172,172,172,172	0
35	CL	J	8801	1/1	0.14	-0.84	62,62,62,62	0
36	SR	0	8956	1/1	0.14	-0.88	142,142,142,142	0
32	MG	0	8053	1/1	0.14	-0.96	61,61,61,61	0
32	MG	0	8058	1/1	0.12	-1.12	23,23,23,23	0
36	SR	9	8978	1/1	0.14	-1.12	144,144,144,144	0
34	NA	0	8536	1/1	0.11	-1.14	50,50,50,50	0
35	CL	J	8802	1/1	0.12	-1.23	60,60,60,60	0
32	MG	0	8021	1/1	0.12	-1.28	32,32,32,32	0
35	CL	J	8821	1/1	0.13	-1.28	56,56,56,56	0
35	CL	R	8806	1/1	0.14	-1.39	43,43,43,43	0
36	SR	0	8910	1/1	0.12	-1.41	97,97,97,97	0
35	CL	Y	8820	1/1	0.10	-1.43	38,38,38,38	0
32	MG	9	8074	1/1	0.12	-1.44	67,67,67,67	0
35	CL	A	8809	1/1	0.17	-1.50	57,57,57,57	0
32	MG	0	8025	1/1	0.12	-1.55	24,24,24,24	0
35	CL	0	8812	1/1	0.11	-1.56	48,48,48,48	0
36	SR	0	8960	1/1	0.11	-1.60	145,145,145,145	0
36	SR	0	8975	1/1	0.11	-1.67	134,134,134,134	0
34	NA	0	8537	1/1	0.12	-1.67	34,34,34,34	0
34	NA	0	8525	1/1	0.10	-1.72	69,69,69,69	0
32	MG	0	8083	1/1	0.13	-1.76	56,56,56,56	0
38	CD	3	8704	1/1	0.09	-1.76	66,66,66,66	0
38	CD	U	8701	1/1	0.12	-1.77	58,58,58,58	0
36	SR	F	9005	1/1	0.06	-1.77	136,136,136,136	0
36	SR	0	8938	1/1	0.10	-1.78	159,159,159,159	0
36	SR	3	8999	1/1	0.09	-1.84	95,95,95,95	0
36	SR	0	8926	1/1	0.12	-1.86	115,115,115,115	0
36	SR	0	8902	1/1	0.15	-1.86	69,69,69,69	0
36	SR	0	8968	1/1	0.09	-1.88	143,143,143,143	0
35	CL	0	8817	1/1	0.13	-1.90	53,53,53,53	0
38	CD	Z	8703	1/1	0.06	-2.00	81,81,81,81	0
35	CL	0	8814	1/1	0.15	-2.06	47,47,47,47	0
36	SR	3	8932	1/1	0.11	-2.07	73,73,73,73	0
32	MG	0	8090	1/1	0.12	-2.10	54,54,54,54	0
36	SR	0	8946	1/1	0.14	-2.10	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8044	1/1	0.11	-2.12	33,33,33,33	0
32	MG	0	8036	1/1	0.10	-2.15	49,49,49,49	0
36	SR	S	8961	1/1	0.10	-2.16	114,114,114,114	0
35	CL	N	8807	1/1	0.13	-2.19	61,61,61,61	0
34	NA	0	8529	1/1	0.07	-2.22	37,37,37,37	0
35	CL	M	8818	1/1	0.13	-2.25	37,37,37,37	0
34	NA	9	8543	1/1	0.08	-2.27	70,70,70,70	0
32	MG	T	8057	1/1	0.13	-2.31	57,57,57,57	0
36	SR	A	8930	1/1	0.08	-2.36	116,116,116,116	0
33	K	0	8402	1/1	0.13	-2.40	64,64,64,64	0
32	MG	0	8032	1/1	0.09	-2.44	40,40,40,40	0
32	MG	0	8026	1/1	0.12	-2.55	31,31,31,31	0
36	SR	0	8936	1/1	0.12	-2.66	89,89,89,89	0
32	MG	0	8035	1/1	0.09	-2.70	44,44,44,44	0
32	MG	0	8060	1/1	0.09	-2.74	42,42,42,42	0
36	SR	9	9003	1/1	0.10	-2.87	162,162,162,162	0
36	SR	0	8924	1/1	0.13	-2.99	145,145,145,145	0
36	SR	0	8943	1/1	0.08	-3.01	95,95,95,95	0
36	SR	0	8911	1/1	0.07	-3.06	78,78,78,78	0
36	SR	0	8940	1/1	0.09	-3.11	85,85,85,85	0
36	SR	0	8965	1/1	0.12	-3.21	120,120,120,120	0
35	CL	0	8815	1/1	0.11	-3.41	57,57,57,57	0
36	SR	0	8954	1/1	0.08	-3.47	105,105,105,105	0
35	CL	0	8811	1/1	0.09	-3.52	53,53,53,53	0
36	SR	0	8958	1/1	0.11	-3.60	108,108,108,108	0
36	SR	0	8964	1/1	0.07	-3.61	126,126,126,126	0
35	CL	3	8804	1/1	0.09	-3.68	54,54,54,54	0
32	MG	Y	8086	1/1	0.12	-3.71	39,39,39,39	0
36	SR	0	8966	1/1	0.09	-3.78	110,110,110,110	0
36	SR	0	8984	1/1	0.10	-3.78	128,128,128,128	0
36	SR	0	8935	1/1	0.10	-3.87	79,79,79,79	0
32	MG	0	8089	1/1	0.16	-3.89	48,48,48,48	0
36	SR	0	8988	1/1	0.07	-3.92	163,163,163,163	0
35	CL	B	8819	1/1	0.09	-3.93	46,46,46,46	0
38	CD	O	8705	1/1	0.06	-4.00	124,124,124,124	0
36	SR	0	8945	1/1	0.10	-4.11	99,99,99,99	0
36	SR	0	8934	1/1	0.13	-4.21	90,90,90,90	0
36	SR	0	9008	1/1	0.13	-4.64	90,90,90,90	0
32	MG	0	8068	1/1	0.07	-4.67	47,47,47,47	0
32	MG	0	8093	1/1	0.12	-4.69	29,29,29,29	0
34	NA	0	8526	1/1	0.07	-4.77	32,32,32,32	0
36	SR	0	8915	1/1	0.06	-4.79	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8963	1/1	0.12	-4.82	133,133,133,133	0
32	MG	0	8059	1/1	0.08	-4.84	36,36,36,36	0
36	SR	0	8951	1/1	0.07	-4.89	146,146,146,146	0
32	MG	0	8052	1/1	0.10	-4.93	40,40,40,40	0
38	CD	1	8702	1/1	0.08	-5.04	57,57,57,57	0
32	MG	0	8075	1/1	0.09	-5.19	45,45,45,45	0
36	SR	0	8931	1/1	0.10	-5.29	108,108,108,108	0
36	SR	1	8952	1/1	0.12	-5.70	79,79,79,79	0
35	CL	0	8803	1/1	0.06	-5.90	46,46,46,46	0
36	SR	1	8913	1/1	0.08	-5.94	85,85,85,85	0
36	SR	0	8973	1/1	0.09	-6.29	137,137,137,137	0
36	SR	0	8921	1/1	0.11	-6.32	92,92,92,92	0
36	SR	0	8920	1/1	0.11	-6.44	124,124,124,124	0
36	SR	0	8970	1/1	0.07	-6.49	131,131,131,131	0
32	MG	0	8034	1/1	0.10	-6.63	32,32,32,32	0
35	CL	L	8810	1/1	0.09	-6.63	49,49,49,49	0
32	MG	0	8013	1/1	0.08	-6.99	26,26,26,26	0
35	CL	0	8813	1/1	0.06	-11.76	48,48,48,48	0
32	MG	0	8033	1/1	0.11	-13.44	45,45,45,45	0
32	MG	0	8038	1/1	0.11	-15.36	58,58,58,58	0
32	MG	0	8091	1/1	0.05	-32.60	42,42,42,42	0
36	SR	0	9001	1/1	0.20	-	169,169,169,169	0
32	MG	0	8063	1/1	0.30	-	72,72,72,72	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.