



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:33 AM GMT

PDB ID : 3I56
Title : Co-crystal structure of Triacetyloleandomycin Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 2.90 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

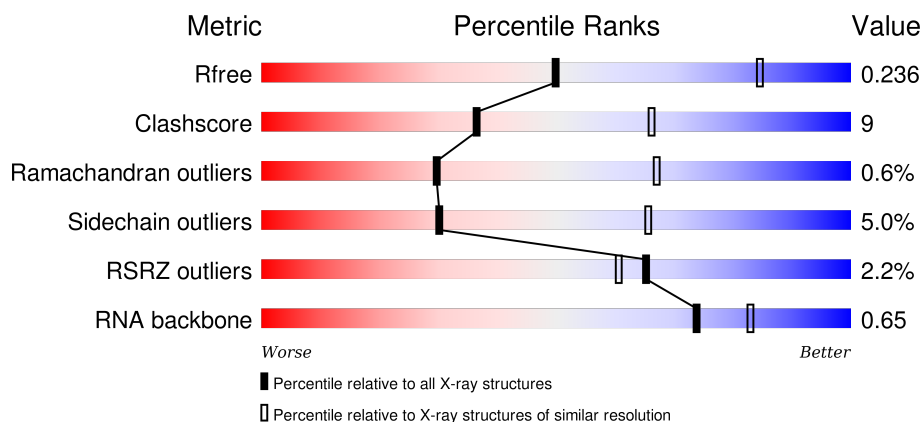
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
3	C	246	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
4	D	177	<div> <div>18%</div> <div>64%</div> <div>14%</div> <div>..</div> <div>21%</div> </div>



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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	174	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	194	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	66	
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	8002	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8010	-	-	-	X
32	MG	0	8011	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8034	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8044	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8052	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8070	-	-	-	X
32	MG	9	8040	-	-	-	X
32	MG	A	8051	-	-	-	X
32	MG	K	8054	-	-	-	X
32	MG	Y	8086	-	-	-	X
33	CL	0	8805	-	-	-	X
33	CL	0	8815	-	-	-	X
33	CL	K	8812	-	-	X	-
34	SR	0	8902	-	-	-	X
34	SR	0	8904	-	-	-	X
34	SR	0	8908	-	-	-	X
34	SR	0	8921	-	-	-	X
34	SR	0	8943	-	-	-	X
34	SR	0	8947	-	-	-	X
34	SR	0	8949	-	-	-	X
34	SR	0	8962	-	-	-	X
34	SR	0	8969	-	-	-	X
34	SR	0	8985	-	-	-	X
34	SR	1	8913	-	-	-	X
34	SR	A	8929	-	-	-	X
34	SR	B	8987	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8502	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8519	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8548	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	B	8552	-	-	-	X
35	NA	R	8533	-	-	-	X
35	NA	R	8575	-	-	-	X
37	K	0	8401	-	-	-	X
38	TAO	0	2924	X	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99181 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
			1283	798	240	239	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
			1559	943	333	282	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			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	EXPRESSION TAG	UNP P60619
Z	2	SER	-	EXPRESSION TAG	UNP P60619
Z	3	PRO	-	EXPRESSION TAG	UNP P60619
Z	4	ARG	-	EXPRESSION TAG	UNP P60619
Z	5	ALA	-	EXPRESSION TAG	UNP P60619
Z	6	ARG	-	EXPRESSION TAG	UNP P60619

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	7	ARG	-	EXPRESSION TAG	UNP P60619
Z	8	GLU	-	EXPRESSION TAG	UNP P60619
Z	9	PRO	-	EXPRESSION TAG	UNP P60619
Z	10	ASN	-	EXPRESSION TAG	UNP P60619
Z	11	LEU	-	EXPRESSION TAG	UNP P60619
Z	12	GLU	-	EXPRESSION TAG	UNP P60619
Z	13	GLY	-	EXPRESSION TAG	UNP P60619
Z	14	LEU	-	EXPRESSION TAG	UNP P60619
Z	15	MET	-	EXPRESSION TAG	UNP P60619
Z	16	TRP	-	EXPRESSION TAG	UNP P60619
Z	17	PRO	-	EXPRESSION TAG	UNP P60619
Z	18	LEU	-	EXPRESSION TAG	UNP P60619
Z	19	GLY	-	EXPRESSION TAG	UNP P60619
Z	20	GLY	-	EXPRESSION TAG	UNP P60619
Z	21	GLN	-	EXPRESSION TAG	UNP P60619
Z	22	GLN	-	EXPRESSION TAG	UNP P60619
Z	23	THR	-	EXPRESSION TAG	UNP P60619
Z	24	THR	-	EXPRESSION TAG	UNP P60619

- 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
			59020	26349	10873	19053	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	82	Total	Mg	0	0
			82	82		
32	9	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	C	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	7	Total	Cl	0	0
			7	7		
33	J	3	Total	Cl	0	0
			3	3		
33	Q	1	Total	Cl	0	0
			1	1		
33	K	1	Total	Cl	0	0
			1	1		
33	B	1	Total	Cl	0	0
			1	1		
33	A	1	Total	Cl	0	0
			1	1		
33	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	2	Total 2	Cl 2	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	91	Total 91	Sr 91	0	0
34	9	2	Total 2	Sr 2	0	0
34	1	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	3	Total 3	Sr 3	0	0
34	A	3	Total 3	Sr 3	0	0
34	T	1	Total 1	Sr 1	0	0
34	R	1	Total 1	Sr 1	0	0
34	Y	1	Total 1	Sr 1	0	0
34	S	1	Total 1	Sr 1	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	60	Total Na 60 60	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	3	Total Na 3 3	0	0
35	2	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

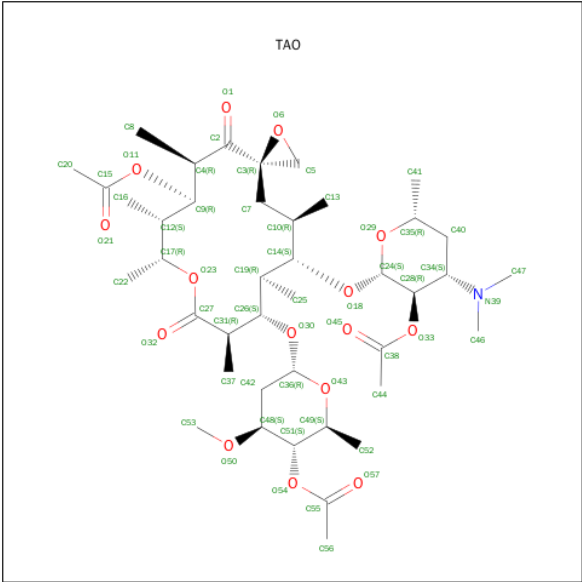
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is TROLEANDOMYCIN (three-letter code: TAO) (formula: C₄₁H₆₇NO₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	0	1	Total	C	N	O	0	0
			57	41	1	15		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	106	Total	O	0	0
			106	106		
39	B	135	Total	O	0	0
			135	135		
39	C	168	Total	O	0	0
			168	168		
39	D	45	Total	O	0	0
			45	45		
39	E	40	Total	O	0	0
			40	40		
39	F	23	Total	O	0	0
			23	23		
39	G	18	Total	O	0	0
			18	18		
39	H	71	Total	O	0	0
			71	71		
39	I	7	Total	O	0	0
			7	7		
39	J	46	Total	O	0	0
			46	46		
39	K	52	Total	O	0	0
			52	52		

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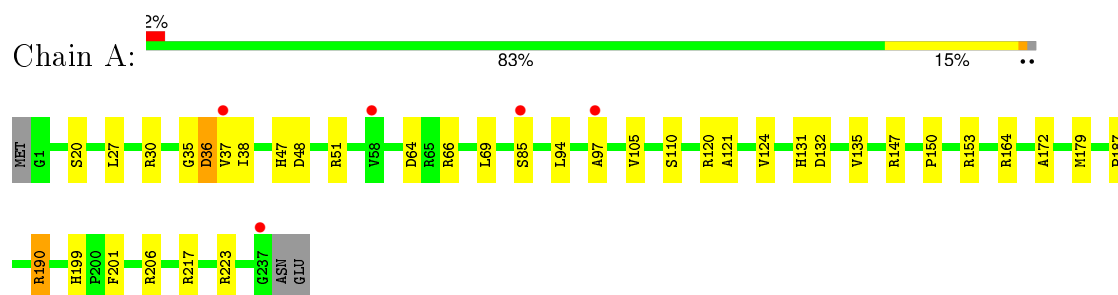
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	L	87	Total 87	O 87	0	0
39	M	123	Total 123	O 123	0	0
39	N	66	Total 66	O 66	0	0
39	O	44	Total 44	O 44	0	0
39	P	55	Total 55	O 55	0	0
39	Q	42	Total 42	O 42	0	0
39	R	78	Total 78	O 78	0	0
39	S	28	Total 28	O 28	0	0
39	T	35	Total 35	O 35	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	66	Total 66	O 66	0	0
39	X	22	Total 22	O 22	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	27	Total 27	O 27	0	0
39	1	49	Total 49	O 49	0	0
39	2	34	Total 34	O 34	0	0
39	3	62	Total 62	O 62	0	0
39	0	6021	Total 6021	O 6021	0	0
39	9	142	Total 142	O 142	0	0

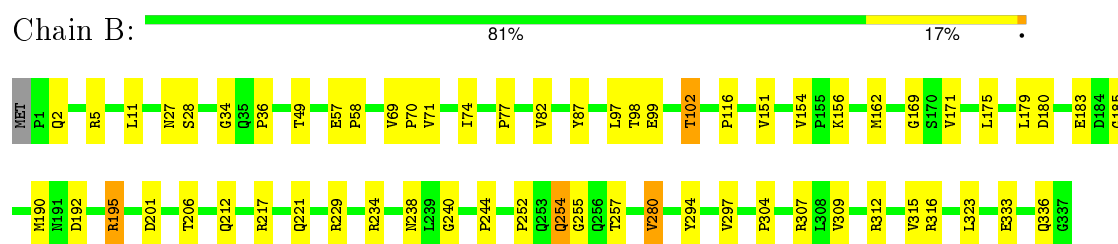
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

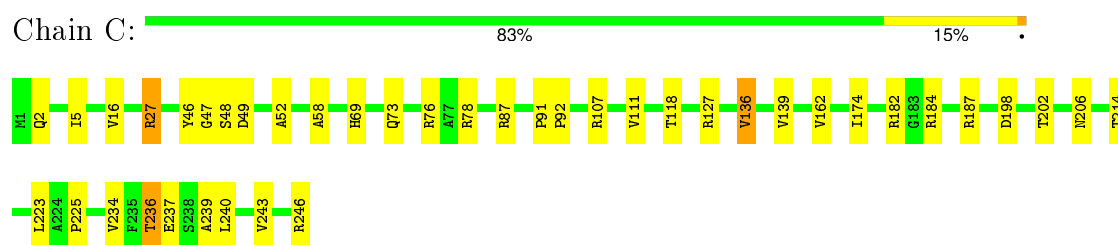
- Molecule 1: 50S ribosomal protein L2P



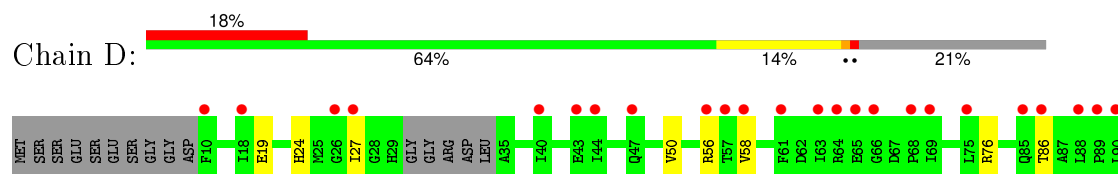
- Molecule 2: 50S ribosomal protein L3P

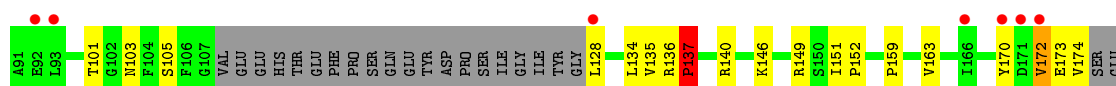


- Molecule 3: 50S ribosomal protein L4P

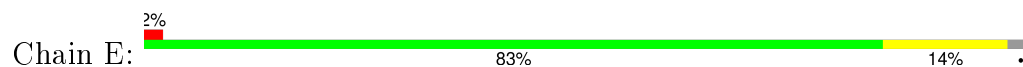


- Molecule 4: 50S ribosomal protein L5P

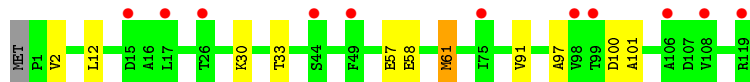
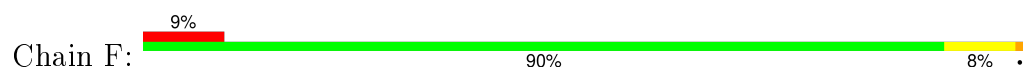




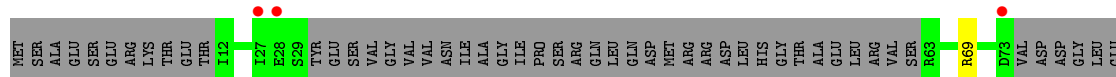
- Molecule 5: 50S ribosomal protein L6P



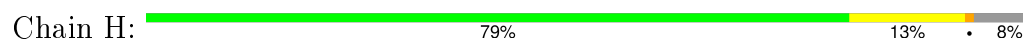
- Molecule 6: 50S ribosomal protein L7Ae



- Molecule 7: 50S ribosomal protein L10E



- Molecule 8: 50S ribosomal protein L10e




- Molecule 9: 50S ribosomal protein L11P

Chain O:  91% 8%




- Molecule 16: 50S ribosomal protein L19e

Chain P:  83% 13%




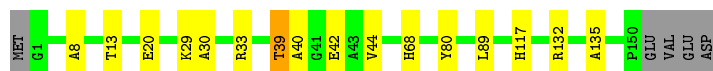
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  88% 11%




- Molecule 18: 50S ribosomal protein L22P

Chain R:  86% 10%




- Molecule 19: 50S ribosomal protein L23P

Chain S:  76% 19% 5%



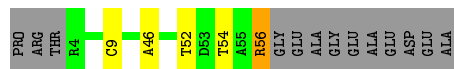
- Molecule 20: 50S ribosomal protein L24P

Chain T:  81% 17% 2%




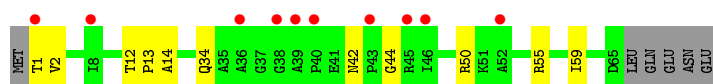
- Molecule 21: 50S ribosomal protein L24e

Chain U:  73% 6% 20%



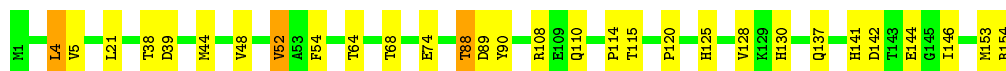
- Molecule 22: 50S ribosomal protein L29P

Chain V:  76% 15% 8%



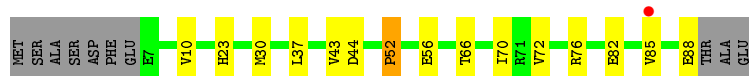
- Molecule 23: 50S ribosomal protein L30P

Chain W: 81% 18%



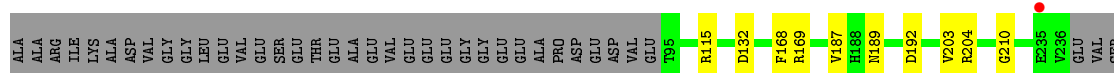
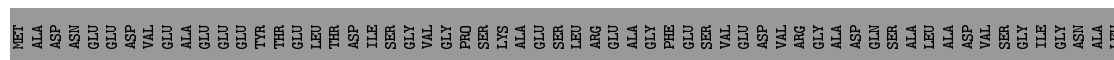
- Molecule 24: 50S ribosomal protein L31e

Chain X: 73% 15% 11%



- Molecule 25: 50S ribosomal protein L32e

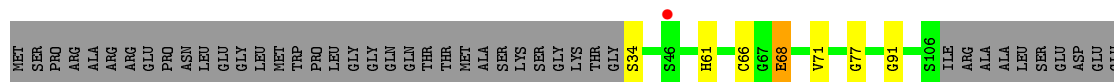
Chain Y: 55% 41%



GLU

- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 57% 5% 37%



- Molecule 27: 50S ribosomal protein L37e

Chain 1: 77% 19%



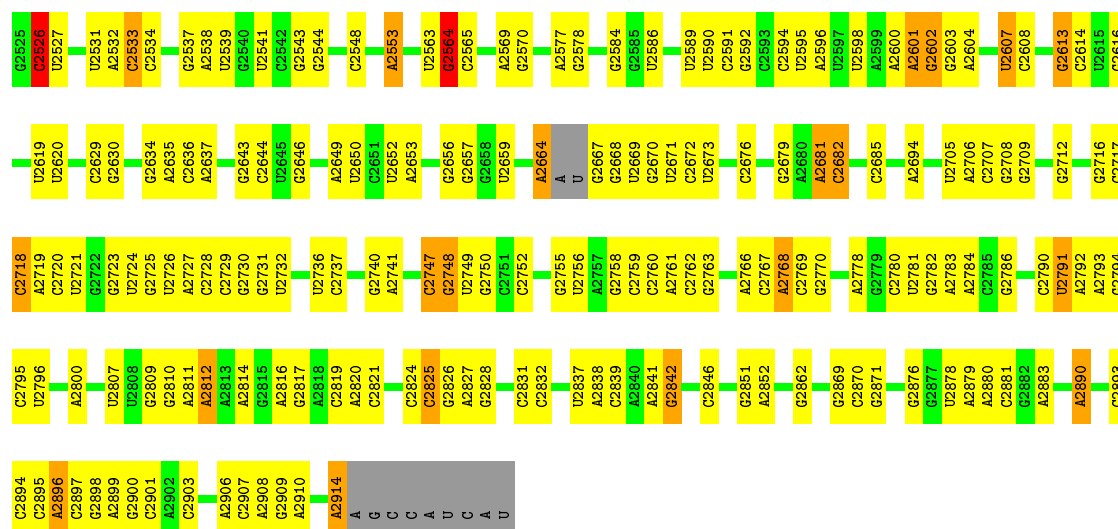
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 66% 26% 8%

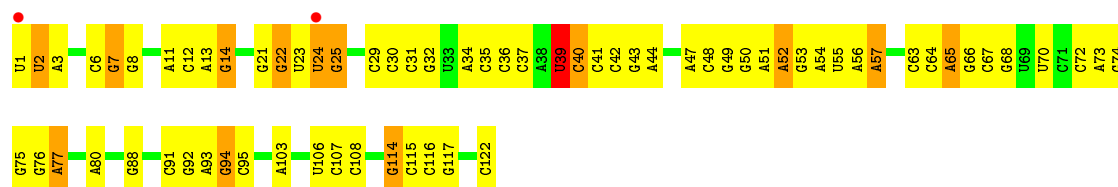
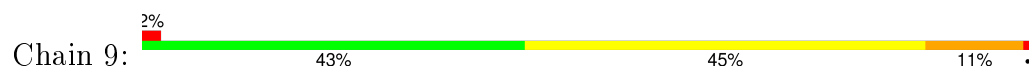


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C2440	G2113	G2251	C	G2114	A2353	G2252	G	G2115	A2354	A2352	G	G2116	C2031	A2030	G2117	C	G2118	A1941	C1940	G1834	A1759	U1668	G1595	A1504	A1413	C1320	C1228	G1158
G2441	C2114	A2354	G	C2115	C2032	G2253	C	C2116	A1942	A1943	C	C2117	C2033	C2031	G2119	U	G2120	A1944	G1943	U1838	G1760	G1669	U1596	U1505	A1414	C1321	C1229	G1159
C2442	U2116	G2255	C	U2117	G2034	G2256	C	U2118	A1945	A1946	G	U2119	U2035	C2032	G2121	G	U2120	A1947	G1944	A1839	C1762	G1670	A1597	A1506	G1415	C1322	C1230	G1160
U2443	G2120	G2257	A	U2121	U2036	G2258	G	U2122	G1948	G1949	C	U2123	U2037	C2033	G2122	C	U2124	G1949	G1950	A1840	C1763	G1671	U1599	U1507	G1416	C1323	C1231	G1161
U2444	G2121	A2355	G	U2123	U2038	G2259	C	U2124	G1950	G1951	C	U2125	U2039	C2034	G2124	G	U2126	G1951	G1952	A1841	U1766	C1602	G1600	U1508	G1417	C1324	C1232	G1162
U2445	A2135	G2260	G	A2136	A2039	G2261	C	A2137	G1952	G1953	C	A2138	C2040	C2035	G2125	C	A2139	G1954	G1955	A1842	C1767	A1603	G1601	U1509	G1418	C1325	C1233	G1163
U2446	G2136	A2356	C	G2137	C2041	A2357	C	G2138	G1956	G1957	C	G2139	U2042	C2036	G2136	C	G2140	G1958	G1959	A1843	U1768	G1604	G1602	U1510	G1419	C1326	C1234	U1164
C2450	A	G2262	A	A	U2043	U2263	C	A	A	A	C	A	U2044	C2043	G2137	C	A	A	A	A1844	C1772	A1605	G1603	U1511	G1420	C1327	C1235	G1165
G2451	C	A2358	C	C	G2045	A2359	C	C	A	A	C	C	G2046	U2045	G2138	C	C	A	A	A1845	C1773	A1606	G1604	U1512	G1421	C1328	C1236	G1166
G2452	G	A2359	C	G	C2047	G2264	C	G	A	A	C	C	G2048	C2046	G2139	C	C	A	A	A1846	C1774	A1607	G1605	U1513	G1422	C1329	C1237	G1167
G2453	C	A2360	C	C	U2048	A2361	C	C	A	A	C	C	G2049	U2047	G2140	C	C	A	A	A1847	C1775	A1608	G1606	U1514	G1423	C1330	C1238	G1168
G2454	C	A2361	C	C	C2049	A2362	C	C	A	A	C	C	G2050	C2048	G2141	C	C	A	A	A1848	C1776	A1609	G1607	U1515	G1424	C1331	C1239	G1169
G2455	C	A2362	C	C	U2050	A2363	C	C	A	A	C	C	G2051	U2049	G2142	C	C	A	A	A1849	C1777	A1610	G1608	U1516	G1425	C1332	C1240	G1170
G2456	C	A2363	C	C	U2051	A2364	C	C	A	A	C	C	G2052	U2050	G2143	C	C	A	A	A1850	C1778	A1611	G1609	U1517	G1426	C1333	C1241	G1171
G2457	C	A2364	C	C	U2052	A2365	C	C	A	A	C	C	G2053	U2051	G2144	C	C	A	A	A1851	C1779	A1612	G1610	U1518	G1427	C1334	C1242	G1172
G2458	C	A2365	C	C	U2053	A2366	C	C	A	A	C	C	G2054	U2052	G2145	C	C	A	A	A1852	C1780	A1613	G1611	U1519	G1428	C1335	C1243	G1173
G2459	C	A2366	C	C	U2054	A2367	C	C	A	A	C	C	G2055	U2053	G2146	C	C	A	A	A1853	C1781	A1614	G1612	U1520	G1429	C1336	C1244	G1174
G2460	C	A2367	C	C	U2055	A2368	C	C	A	A	C	C	G2056	U2054	G2147	C	C	A	A	A1854	C1782	A1615	G1613	U1521	G1430	C1337	C1245	G1175
G2461	C	A2368	C	C	U2056	A2369	C	C	A	A	C	C	G2057	U2055	G2148	C	C	A	A	A1855	C1783	A1616	G1614	U1522	G1431	C1338	C1246	G1176
G2462	C	A2369	C	C	U2057	A2370	C	C	A	A	C	C	G2058	U2056	G2149	C	C	A	A	A1856	C1784	A1617	G1615	U1523	G1432	C1339	C1247	G1177
A2463	C	A2370	C	C	U2058	A2371	C	C	A	A	C	C	G2059	U2057	G2150	C	C	A	A	A1857	C1785	A1618	G1616	U1524	G1433	C1340	C1248	G1178
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A2466	C	A2373	C	C	U2061	A2374	C	C	A	A	C	C	G2062	U2060	G2153	C	C	A	A	A1860	C1788	A1621	G1619	U1527	G1436	C1343	C1251	G1181
A2467	C	A2374	C	C	U2062	A2375	C	C	A	A	C	C	G2063	U2061	G2154	C	C	A	A	A1861	C1789	A1622	G1620	U1528	G1437	C1344	C1252	G1182
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C2472	C	A2376	C	C	U2064	A2377	C	C	A	A	C	C	G2065	U2063	G2156	C	C	A	A	A1863	C1791	A1624	G1622	U1530	G1439	C1346	C1254	G1184
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U2474	C	A2378	C	C	U2066	A2379	C	C	A	A	C	C	G2067	U2065	G2158	C	C	A	A	A1865	C1793	A1626	G1624	U1532	G1441	C1348	C1256	G1186
A2475	C	A2379	C	C	U2067	A2380	C	C	A	A	C	C	G2068	U2066	G2159	C	C	A	A	A1866	C1794	A1627	G1625	U1533	G1442	C1349	C1257	G1187
G2480	C	A2380	C	C	U2068	A2381	C	C	A	A	C	C	G2069	U2067	G2160	C	C	A	A	A1867	C1795	A1628	G1626	U1534	G1443	C1350	C1258	G1188
C2476	C	A2381	C	C	U2069	A2382	C	C	A	A	C	C	G2070	U2068	G2161	C	C	A	A	A1868	C1796	A1629	G1627	U1535	G1444	C1351	C1259	G1189
C2477	C	A2382	C	C	U2070	A2383	C	C	A	A	C	C	G2071	U2069	G2162	C	C	A	A	A1869	C1797	A1630	G1628	U1536	G1445	C1352	C1260	G1190
U2478	C	A2383	C	C	U2071	A2384	C	C	A	A	C	C	G2072	U2070	G2163	C	C	A	A	A1870	C1798	A1631	G1629	U1537	G1446	C1353	C1261	G1191
U2479	C	A2384	C	C	U2072	A2385	C	C	A	A	C	C	G2073	U2071	G2164	C	C	A	A	A1871	C1799	A1632	G1630	U1538	G1447	C1354	C1262	G1192
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C2483	C	A2386	C	C	U2074	A2387	C	C	A	A	C	C	G2075	U2073	G2166	C	C	A	A	A1873	C1801	A1634	G1632	U1540	G1449	C1356	C1264	G1194
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A2487	C	A2390	C	C	U2078	A2391	C	C	A	A	C	C	G2079	U2077	G2170	C	C	A	A	A1877	C1805	A1638	G1636	U1544	G1453	C1360	C1268	G1198
A2488	C	A2391	C	C	U2079	A2392	C	C	A	A	C	C	G2080	U2078	G2171	C	C	A	A	A1878	C1806	A1639	G1637	U1545	G1454	C1361	C1269	G1199
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A2490	C	A2393	C	C	U2081	A2394	C	C	A	A	C	C	G2082	U2080	G2173	C	C	A	A	A1880	C1808	A1641	G1639	U1547	G1456	C1363	C1271	G1201
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A2493	C	A2396	C	C	U2084	A2397	C	C	A	A	C	C	G2085	U2083	G2176	C	C	A	A	A1883	C1811	A1644	G1642	U1550	G1459	C1366	C1274	G1204
C2500	C	A2397	C	C	U2085	A2398	C	C	A	A	C	C	G2086	U2084	G2177	C	C	A	A	A1884	C1812	A1645	G1643	U1551	G1460	C1367	C1275	G1205
C2501	C	A2398	C	C	U2086	A2399	C	C	A	A	C	C	G2087	U2085	G2178	C	C	A	A	A1885	C1813	A1646	G1644	U1552	G1461	C1368	C1276	G1206
C2502	C	A2399	C	C	U2087	A2400	C	C	A	A	C	C	G2088	U2086	G2179	C	C	A	A	A1886	C1814	A1647	G1645	U1553	G1462	C1369	C1277	G1207
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A2505	C	A2402	C	C	U2090	A2403	C	C	A	A	C	C	G2091	U2089	G2182	C	C	A	A	A1889	C1817	A1650	G1648	U1556	G1465	C1372	C1280	G1210
A2506	C	A2403	C	C	U2091	A2404	C	C	A	A	C	C	G2092	U2090	G2183	C	C	A	A	A1890	C1818	A1651	G1649	U1557	G1466	C1373	C1281	G1211
A2507	C	A2404	C	C	U2092	A2405	C	C	A	A	C	C	G2093	U2091	G2184	C	C	A	A	A1891	C1819	A1652	G1650	U1558	G1467	C1374	C1282	G1212
A2508	C	A2405	C	C	U2093	A2																						



• Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.43Å 300.77Å 575.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 85.79 – 2.41	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.00-2.90) 90.7 (85.79-2.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.243 0.189 , 0.236	Depositor DCC
R_{free} test set	3941 reflections (1.17%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 667226 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99181	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, TAO, 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	0.49	0/1786	0.76	0/2408
2	B	0.53	0/2690	0.76	0/3652
3	C	0.54	0/1885	0.76	0/2552
4	D	0.63	0/1111	0.74	2/1498 (0.1%)
5	E	0.59	0/1382	0.70	0/1880
6	F	0.53	0/901	0.72	0/1224
7	G	0.51	0/241	0.63	0/324
8	H	0.59	0/1303	0.77	0/1743
9	I	0.59	0/526	0.68	0/716
10	J	0.61	0/1136	0.74	0/1530
11	K	0.50	0/1004	0.78	0/1351
12	L	0.50	0/1130	0.76	0/1509
13	M	0.50	0/1583	0.74	0/2116
14	N	0.54	0/1474	0.79	0/1999
15	O	0.49	0/874	0.72	1/1181 (0.1%)
16	P	0.54	0/1147	0.65	0/1528
17	Q	0.51	0/749	0.77	0/1005
18	R	0.57	0/1172	0.73	0/1578
19	S	0.52	0/648	0.66	0/875
20	T	0.49	0/958	0.75	1/1289 (0.1%)
21	U	0.56	0/417	0.69	0/562
22	V	0.44	0/502	0.71	0/675
23	W	0.52	0/1219	0.76	1/1655 (0.1%)
24	X	0.53	0/664	0.76	0/895
25	Y	0.49	0/1146	0.74	0/1536
26	Z	0.62	0/584	0.77	0/781
27	1	0.55	0/438	0.74	0/578
28	2	0.45	0/401	0.69	0/529
29	3	0.55	0/771	0.68	0/1024
30	0	0.41	0/65957	0.69	12/102867 (0.0%)
31	9	0.36	0/2904	0.69	1/4526 (0.0%)
All	All	0.45	0/98703	0.70	18/147586 (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	35
31	9	0	2
All	All	0	38

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
30	0	2291	A	N9-C1'-C2'	6.13	121.97	114.00
30	0	871	G	C5'-C4'-O4'	-6.06	101.83	109.10
30	0	1942	A	C5'-C4'-C3'	5.87	125.38	116.00
31	9	39	U	N1-C1'-C2'	5.60	121.29	114.00

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	482	G	Sidechain
30	0	49	A	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	22	0
2	B	2625	0	2533	35	0
3	C	1860	0	1813	28	0
4	D	1094	0	1085	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	14	0
6	F	890	0	843	5	0
7	G	240	0	231	0	0
8	H	1283	0	1292	17	0
9	I	519	0	500	6	0
10	J	1120	0	1098	15	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	11	0
13	M	1559	0	1573	18	0
14	N	1445	0	1401	13	0
15	O	865	0	873	7	0
16	P	1136	0	1123	12	0
17	Q	735	0	729	9	0
18	R	1149	0	1122	11	0
19	S	641	0	605	8	0
20	T	950	0	924	10	0
21	U	410	0	364	4	0
22	V	499	0	511	7	0
23	W	1196	0	1137	20	0
24	X	654	0	653	7	0
25	Y	1130	0	1133	10	0
26	Z	573	0	531	5	0
27	1	431	0	426	14	0
28	2	396	0	413	10	0
29	3	755	0	728	9	0
30	0	59020	0	29812	1178	0
31	9	2599	0	1325	71	0
32	0	82	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	C	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	7	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	0	0
33	K	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	2	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	91	0	0	0	0
34	1	2	0	0	0	0
34	3	3	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	60	0	0	0	0
35	2	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	3	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	57	0	67	14	0
39	0	6021	0	0	144	0
39	1	49	0	0	0	0
39	2	34	0	0	0	0
39	3	62	0	0	0	0
39	9	142	0	0	3	0
39	A	106	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	135	0	0	4	0
39	C	168	0	0	2	0
39	D	45	0	0	0	0
39	E	40	0	0	1	0
39	F	23	0	0	0	0
39	G	18	0	0	0	0
39	H	71	0	0	1	0
39	I	7	0	0	0	0
39	J	46	0	0	1	0
39	K	52	0	0	0	0
39	L	87	0	0	2	0
39	M	123	0	0	0	0
39	N	66	0	0	2	0
39	O	44	0	0	1	0
39	P	55	0	0	0	0
39	Q	42	0	0	0	0
39	R	78	0	0	2	0
39	S	28	0	0	0	0
39	T	35	0	0	1	0
39	U	26	0	0	0	0
39	V	11	0	0	0	0
39	W	66	0	0	1	0
39	X	22	0	0	0	0
39	Y	94	0	0	3	0
39	Z	27	0	0	0	0
All	All	99181	0	59980	1428	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 9.

The worst 5 of 1428 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'	1.25	1.16
30:0:871:G:H8	30:0:871:G:H5'	1.06	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.90	1.06
30:0:2717:C:H2'	30:0:2718:C:H5''	1.42	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.42	1.01

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%)	219 (93%)	14 (6%)	2 (1%)	21	57
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	21	57
3	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
4	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	8	31
5	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
6	F	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	7	26
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/174 (90%)	146 (94%)	9 (6%)	1 (1%)	30	67
9	I	68/162 (42%)	62 (91%)	6 (9%)	0	100	100
10	J	140/145 (97%)	133 (95%)	6 (4%)	1 (1%)	26	63
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	131 (93%)	10 (7%)	0	100	100
13	M	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	6	25
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	17	51
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	26	63
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	111 (95%)	4 (3%)	2 (2%)	11	38
21	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	7	27
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	3705/4466 (83%)	3492 (94%)	189 (5%)	24 (1%)	30	67

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
10	J	5	GLU
14	N	154	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%)	165 (92%)	14 (8%)	16	41
2	B	282/283 (100%)	265 (94%)	17 (6%)	24	57
3	C	193/193 (100%)	175 (91%)	18 (9%)	11	32
4	D	117/148 (79%)	107 (92%)	10 (8%)	13	37
5	E	152/156 (97%)	147 (97%)	5 (3%)	45	80
6	F	93/94 (99%)	91 (98%)	2 (2%)	60	88
7	G	27/282 (10%)	26 (96%)	1 (4%)	41	77
8	H	134/143 (94%)	128 (96%)	6 (4%)	34	70
9	I	58/130 (45%)	57 (98%)	1 (2%)	68	91
10	J	118/121 (98%)	109 (92%)	9 (8%)	16	43
11	K	106/106 (100%)	101 (95%)	5 (5%)	32	68
12	L	113/127 (89%)	107 (95%)	6 (5%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/158 (100%)	153 (97%)	5 (3%)	46	81
14	N	149/150 (99%)	143 (96%)	6 (4%)	38	74
15	O	93/94 (99%)	91 (98%)	2 (2%)	60	88
16	P	113/117 (97%)	108 (96%)	5 (4%)	35	70
17	Q	79/80 (99%)	75 (95%)	4 (5%)	29	65
18	R	117/122 (96%)	115 (98%)	2 (2%)	68	91
19	S	71/74 (96%)	68 (96%)	3 (4%)	36	73
20	T	105/106 (99%)	96 (91%)	9 (9%)	13	36
21	U	44/52 (85%)	43 (98%)	1 (2%)	58	87
22	V	51/57 (90%)	49 (96%)	2 (4%)	39	75
23	W	130/130 (100%)	124 (95%)	6 (5%)	33	69
24	X	66/74 (89%)	60 (91%)	6 (9%)	12	34
25	Y	120/196 (61%)	118 (98%)	2 (2%)	68	91
26	Z	60/94 (64%)	59 (98%)	1 (2%)	68	91
27	1	46/47 (98%)	45 (98%)	1 (2%)	60	88
28	2	42/46 (91%)	41 (98%)	1 (2%)	57	86
29	3	79/79 (100%)	74 (94%)	5 (6%)	22	54
All	All	3095/3641 (85%)	2940 (95%)	155 (5%)	30	65

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	87	LYS
11	K	107	THR
24	X	82	GLU
8	H	169	GLU
10	J	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	50	GLN
18	R	98	ASN
28	2	18	ASN
16	P	57	ASN

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Mol	Chain	Res	Type
17	Q	16	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	235 (8%)	22 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	251 (8%)	23 (0%)

5 of 251 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 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1237	U
30	0	1352	A
30	0	2791	U
30	0	1246	A
30	0	1377	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	30,35	12,22,23	1.04	1 (8%)	19,31,34	3.14	2 (10%)
30	OMG	0	2588	30	17,26,27	1.06	1 (5%)	21,38,41	2.56	3 (14%)
30	UR3	0	2619	30	12,22,23	0.76	0	16,32,35	0.78	0
30	PSU	0	2621	30	13,21,22	1.59	2 (15%)	18,30,33	6.06	3 (16%)
30	1MA	0	628	30	14,25,26	0.98	1 (7%)	15,37,40	1.12	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	30,35	-	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	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.78	1.48	1.52
30	0	2621	PSU	C4-N3	2.37	1.37	1.33
30	0	2587	OMU	C4-N3	2.47	1.37	1.33
30	0	628	1MA	C6-N6	2.77	1.34	1.29
30	0	2588	OMG	C6-N1	3.27	1.39	1.33

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	-21.15	114.84	128.33
30	0	2588	OMG	C5-C6-N1	-8.86	111.48	123.59
30	0	628	1MA	C2-N3-C4	-3.64	110.76	116.40
30	0	2587	OMU	C5-C4-N3	-3.21	114.89	123.12
30	0	2588	OMG	N3-C2-N1	-2.29	123.96	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	2619	UR3	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	$\# Z > 2$
38	TAO	0	2924	-	58,60,60	0.63	0	77,89,89	1.79	14 (18%)

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
38	TAO	0	2924	-	2/2/24/24	0/77/113/113	0/3/4/4

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	C17-O23-C27	-4.57	110.42	117.44
38	0	2924	TAO	C51-O54-C55	-4.24	111.12	117.70
38	0	2924	TAO	C3-C7-C10	-3.52	111.11	117.67
38	0	2924	TAO	C9-O11-C15	-3.33	112.53	117.70
38	0	2924	TAO	C24-O18-C14	-3.27	109.47	118.01

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
38	0	2924	TAO	C10
38	0	2924	TAO	C9

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	TAO	14	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	-0.32	5 (2%) 67 62	19, 43, 83, 105	0
2	B	337/338 (99%)	-0.46	0 100 100	17, 47, 75, 90	0
3	C	246/246 (100%)	-0.38	0 100 100	12, 41, 66, 78	0
4	D	140/177 (79%)	1.00	31 (22%) 1 0	51, 92, 120, 131	0
5	E	172/178 (96%)	-0.18	4 (2%) 64 59	39, 62, 89, 96	0
6	F	119/120 (99%)	0.41	11 (9%) 11 7	43, 70, 104, 120	0
7	G	29/348 (8%)	0.83	3 (10%) 9 5	62, 88, 97, 98	0
8	H	160/174 (91%)	-0.35	0 100 100	24, 48, 85, 99	0
9	I	70/162 (43%)	3.23	51 (72%) 0 0	124, 138, 160, 161	0
10	J	142/145 (97%)	-0.51	1 (0%) 89 88	25, 43, 65, 80	0
11	K	132/132 (100%)	-0.54	0 100 100	25, 43, 68, 75	0
12	L	145/165 (87%)	0.07	6 (4%) 41 34	13, 60, 107, 118	0
13	M	194/194 (100%)	-0.60	0 100 100	22, 36, 55, 62	0
14	N	186/187 (99%)	0.09	8 (4%) 39 32	32, 58, 111, 119	0
15	O	115/116 (99%)	-0.37	0 100 100	30, 49, 66, 74	0
16	P	143/149 (95%)	-0.41	0 100 100	30, 49, 64, 67	0
17	Q	95/96 (98%)	-0.59	1 (1%) 82 80	25, 36, 51, 71	0
18	R	150/155 (96%)	-0.63	0 100 100	21, 37, 61, 73	0
19	S	81/85 (95%)	-0.06	1 (1%) 81 78	35, 57, 74, 82	0
20	T	119/120 (99%)	-0.16	2 (1%) 73 70	32, 53, 80, 100	0
21	U	53/66 (80%)	-0.50	0 100 100	30, 49, 70, 74	0
22	V	65/71 (91%)	0.92	10 (15%) 3 1	49, 72, 108, 116	0
23	W	154/154 (100%)	-0.65	0 100 100	26, 40, 59, 70	0
24	X	82/92 (89%)	-0.21	1 (1%) 81 78	36, 49, 73, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.51	1 (0%) 89 88	18, 39, 64, 81	0
26	Z	73/116 (62%)	-0.31	1 (1%) 78 76	34, 54, 77, 93	0
27	1	56/57 (98%)	-0.62	0 100 100	16, 26, 35, 43	0
28	2	46/50 (92%)	-0.15	0 100 100	29, 56, 81, 98	0
29	3	92/92 (100%)	-0.40	0 100 100	27, 47, 62, 73	0
30	0	2749/2923 (94%)	-0.60	6 (0%) 95 95	11, 36, 81, 154	0
31	9	122/122 (100%)	-0.71	2 (1%) 74 72	22, 51, 78, 129	0
All	All	6646/7511 (88%)	-0.37	145 (2%) 65 60	11, 44, 93, 161	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	112	LEU	9.3
9	I	97	VAL	9.0
9	I	72	GLU	8.2
22	V	40	PRO	7.6
9	I	109	PRO	7.6

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.98	0.14	-	13,18,20,21	0
30	OMU	0	2587	21/22	0.98	0.11	-	22,25,29,32	0
30	PSU	0	2621	20/21	0.98	0.13	-	18,19,25,25	0
30	OMG	0	2588	24/25	0.98	0.13	-	20,23,24,28	0
30	UR3	0	2619	21/22	0.98	0.12	-	21,24,26,29	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8565	1/1	0.67	1.07	71.39	79,79,79,79	0
35	NA	0	8507	1/1	0.80	0.58	52.70	68,68,68,68	0
35	NA	0	8564	1/1	0.86	0.94	45.78	91,91,91,91	0
32	MG	9	8040	1/1	0.92	0.64	44.60	71,71,71,71	0
35	NA	0	8519	1/1	0.62	0.37	39.27	76,76,76,76	0
35	NA	0	8559	1/1	0.82	0.34	36.42	94,94,94,94	0
35	NA	9	8572	1/1	0.76	0.68	34.63	103,103,103,103	0
35	NA	0	8522	1/1	0.87	0.84	28.96	73,73,73,73	0
34	SR	0	8943	1/1	0.78	0.38	26.41	179,179,179,179	0
38	TAO	0	2924	57/57	0.80	0.35	25.75	83,95,107,109	0
35	NA	0	8557	1/1	0.45	0.24	23.53	89,89,89,89	0
37	K	0	8401	1/1	0.82	0.41	22.37	150,150,150,150	0
32	MG	0	8034	1/1	0.65	0.50	22.06	60,60,60,60	0
35	NA	0	8560	1/1	0.65	0.45	19.63	104,104,104,104	0
35	NA	0	8553	1/1	0.88	0.41	17.88	59,59,59,59	0
35	NA	0	8523	1/1	0.98	0.29	15.80	46,46,46,46	0
32	MG	0	8010	1/1	0.99	0.29	14.64	3,3,3,3	0
32	MG	0	8062	1/1	0.96	0.32	13.32	64,64,64,64	0
35	NA	0	8568	1/1	0.73	0.44	13.16	46,46,46,46	0
35	NA	0	8562	1/1	0.94	0.28	12.74	45,45,45,45	0
34	SR	1	8913	1/1	0.95	0.35	12.72	179,179,179,179	0
35	NA	R	8575	1/1	0.97	0.40	12.48	65,65,65,65	0
34	SR	0	8904	1/1	0.86	0.34	12.43	200,200,200,200	0
34	SR	0	8949	1/1	0.58	0.20	12.06	132,132,132,132	0
35	NA	0	8502	1/1	0.72	0.29	11.82	54,54,54,54	0
35	NA	0	8530	1/1	0.89	0.36	11.67	46,46,46,46	0
34	SR	0	8969	1/1	0.84	0.25	11.25	181,181,181,181	0
32	MG	0	8041	1/1	0.96	0.24	10.76	28,28,28,28	0
35	NA	B	8552	1/1	0.97	0.23	10.46	56,56,56,56	0
33	CL	0	8815	1/1	0.95	0.22	9.46	72,72,72,72	0
35	NA	0	8548	1/1	0.19	0.23	9.12	59,59,59,59	0
35	NA	0	8542	1/1	0.97	0.30	9.02	36,36,36,36	0
35	NA	0	8555	1/1	0.82	0.37	9.00	38,38,38,38	0
34	SR	A	8929	1/1	0.44	0.46	8.34	174,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8052	1/1	0.79	0.23	7.95	59,59,59,59	0
32	MG	0	8044	1/1	0.98	0.27	7.82	38,38,38,38	0
34	SR	0	8908	1/1	0.23	0.26	7.73	200,200,200,200	0
32	MG	K	8054	1/1	0.91	0.27	7.70	62,62,62,62	0
35	NA	0	8556	1/1	0.90	0.32	6.81	41,41,41,41	0
34	SR	0	8962	1/1	0.73	0.26	6.71	197,197,197,197	0
35	NA	0	8571	1/1	0.75	0.21	6.53	73,73,73,73	0
32	MG	0	8009	1/1	0.98	0.22	6.43	15,15,15,15	0
35	NA	0	8547	1/1	0.89	0.21	5.79	49,49,49,49	0
33	CL	0	8805	1/1	0.94	0.18	5.57	62,62,62,62	0
35	NA	0	8527	1/1	0.97	0.21	5.52	44,44,44,44	0
32	MG	0	8028	1/1	0.94	0.18	5.49	16,16,16,16	0
32	MG	A	8051	1/1	0.95	0.46	5.22	117,117,117,117	0
34	SR	0	8985	1/1	0.96	0.14	5.14	128,128,128,128	0
32	MG	0	8047	1/1	0.95	0.25	4.92	34,34,34,34	0
32	MG	0	8011	1/1	0.99	0.23	4.86	1,1,1,1	0
35	NA	0	8563	1/1	0.97	0.21	4.48	61,61,61,61	0
34	SR	0	8902	1/1	0.92	0.18	4.19	107,107,107,107	0
32	MG	0	8070	1/1	0.98	0.18	4.17	31,31,31,31	0
32	MG	0	8002	1/1	0.88	0.16	3.62	14,14,14,14	0
32	MG	Y	8086	1/1	0.98	0.19	3.36	69,69,69,69	0
34	SR	B	8987	1/1	0.42	0.29	3.36	199,199,199,199	0
34	SR	0	8947	1/1	0.78	0.32	2.60	200,200,200,200	0
35	NA	R	8533	1/1	0.96	0.20	2.37	51,51,51,51	0
32	MG	0	8001	1/1	0.99	0.16	2.20	2,2,2,2	0
34	SR	0	8921	1/1	0.85	0.14	2.14	155,155,155,155	0
35	NA	0	8517	1/1	0.99	0.15	1.95	14,14,14,14	0
32	MG	0	8004	1/1	0.91	0.18	1.94	23,23,23,23	0
37	K	0	8402	1/1	0.95	0.17	1.48	78,78,78,78	0
33	CL	0	8816	1/1	0.96	0.18	1.46	60,60,60,60	0
32	MG	A	8050	1/1	0.88	0.16	1.44	18,18,18,18	0
32	MG	B	8043	1/1	0.85	0.13	1.37	37,37,37,37	0
32	MG	0	8014	1/1	0.99	0.12	1.21	15,15,15,15	0
35	NA	J	8538	1/1	0.45	0.22	0.66	49,49,49,49	0
34	SR	0	8948	1/1	0.87	0.11	0.61	94,94,94,94	0
35	NA	0	8537	1/1	0.95	0.14	0.30	22,22,22,22	0
34	SR	0	8992	1/1	0.83	0.13	0.24	151,151,151,151	0
32	MG	C	8012	1/1	0.98	0.15	0.12	10,10,10,10	0
34	SR	H	8972	1/1	0.85	0.14	-0.00	131,131,131,131	0
36	CD	1	8702	1/1	0.98	0.12	-0.21	58,58,58,58	0
32	MG	0	8003	1/1	0.97	0.12	-0.23	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8534	1/1	0.95	0.14	-0.32	15,15,15,15	0
32	MG	0	8088	1/1	0.96	0.12	-0.36	33,33,33,33	0
34	SR	0	8936	1/1	0.91	0.11	-0.37	100,100,100,100	0
32	MG	0	8053	1/1	0.71	0.11	-0.40	78,78,78,78	0
36	CD	U	8701	1/1	0.99	0.11	-0.42	58,58,58,58	0
33	CL	O	8808	1/1	0.95	0.13	-0.54	68,68,68,68	0
35	NA	0	8569	1/1	0.96	0.12	-0.60	40,40,40,40	0
35	NA	R	8532	1/1	0.78	0.12	-0.62	39,39,39,39	0
35	NA	0	8504	1/1	0.97	0.13	-0.69	18,18,18,18	0
35	NA	Q	8540	1/1	0.81	0.11	-0.74	34,34,34,34	0
35	NA	M	8539	1/1	0.86	0.10	-0.85	19,19,19,19	0
33	CL	J	8821	1/1	0.93	0.10	-0.88	61,61,61,61	0
36	CD	Z	8703	1/1	1.00	0.12	-0.90	55,55,55,55	0
32	MG	0	8025	1/1	0.97	0.10	-0.92	10,10,10,10	0
34	SR	0	8910	1/1	0.72	0.10	-1.12	92,92,92,92	0
36	CD	3	8704	1/1	0.99	0.10	-1.26	56,56,56,56	0
32	MG	0	8058	1/1	0.99	0.08	-1.44	1,1,1,1	0
35	NA	0	8528	1/1	0.84	0.09	-1.45	49,49,49,49	0
32	MG	0	8065	1/1	0.97	0.09	-1.79	16,16,16,16	0
33	CL	3	8804	1/1	0.96	0.11	-2.02	59,59,59,59	0
33	CL	K	8812	1/1	0.96	0.07	-2.04	39,39,39,39	0
32	MG	0	8008	1/1	0.96	0.09	-2.08	8,8,8,8	0
33	CL	M	8818	1/1	0.98	0.06	-2.17	36,36,36,36	0
35	NA	2	8515	1/1	0.99	0.09	-2.22	19,19,19,19	0
33	CL	L	8810	1/1	0.87	0.08	-2.32	69,69,69,69	0
34	SR	0	8975	1/1	0.97	0.06	-2.59	131,131,131,131	0
33	CL	B	8819	1/1	0.98	0.10	-3.15	42,42,42,42	0
32	MG	0	8013	1/1	0.98	0.09	-3.62	11,11,11,11	0
32	MG	T	8057	1/1	0.92	0.05	-3.77	60,60,60,60	0
32	MG	0	8006	1/1	0.95	0.06	-3.80	7,7,7,7	0
35	NA	0	8521	1/1	0.87	0.08	-4.60	28,28,28,28	0
32	MG	0	8075	1/1	0.91	0.06	-8.00	32,32,32,32	0
34	SR	0	8967	1/1	0.92	0.24	-	191,191,191,191	0
32	MG	0	8046	1/1	0.95	0.12	-	25,25,25,25	0
33	CL	0	8803	1/1	0.94	0.14	-	50,50,50,50	0
36	CD	O	8705	1/1	0.98	0.09	-	91,91,91,91	0
35	NA	0	8535	1/1	0.45	0.39	-	68,68,68,68	0
34	SR	9	9003	1/1	0.80	0.23	-	195,195,195,195	0
33	CL	N	8807	1/1	0.97	0.14	-	45,45,45,45	0
32	MG	0	8090	1/1	0.97	0.16	-	50,50,50,50	0
35	NA	0	8573	1/1	0.92	0.26	-	65,65,65,65	0
32	MG	0	8072	1/1	0.93	0.21	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8005	1/1	0.87	0.21	-	26,26,26,26	0
35	NA	C	8554	1/1	0.99	0.51	-	52,52,52,52	0
32	MG	0	8037	1/1	0.58	0.94	-	88,88,88,88	0
34	SR	A	8930	1/1	0.08	2.72	-	200,200,200,200	0
33	CL	J	8801	1/1	0.93	0.09	-	58,58,58,58	0
32	MG	0	8068	1/1	0.90	0.13	-	54,54,54,54	0
34	SR	3	8999	1/1	0.45	0.23	-	200,200,200,200	0
34	SR	0	8965	1/1	0.27	0.09	-	143,143,143,143	0
32	MG	0	8084	1/1	0.97	0.16	-	37,37,37,37	0
34	SR	0	8958	1/1	0.67	0.10	-	147,147,147,147	0
34	SR	0	8963	1/1	0.94	0.20	-	182,182,182,182	0
34	SR	0	8966	1/1	0.27	0.27	-	178,178,178,178	0
34	SR	0	8976	1/1	0.97	0.20	-	195,195,195,195	0
32	MG	0	8093	1/1	0.92	0.05	-	13,13,13,13	0
32	MG	0	8029	1/1	0.89	0.23	-	111,111,111,111	0
34	SR	0	8986	1/1	0.80	1.33	-	200,200,200,200	0
34	SR	0	8970	1/1	0.51	0.46	-	200,200,200,200	0
32	MG	0	8059	1/1	0.83	0.11	-	33,33,33,33	0
35	NA	0	8541	1/1	0.93	0.73	-	86,86,86,86	0
34	SR	0	8956	1/1	0.64	0.10	-	147,147,147,147	0
32	MG	0	8076	1/1	0.99	0.05	-	9,9,9,9	0
34	SR	0	8903	1/1	0.23	0.12	-	168,168,168,168	0
34	SR	Y	9002	1/1	0.58	0.40	-	200,200,200,200	0
34	SR	0	8945	1/1	0.70	0.09	-	131,131,131,131	0
32	MG	2	8060	1/1	0.70	0.28	-	67,67,67,67	0
32	MG	0	8035	1/1	0.88	0.21	-	65,65,65,65	0
34	SR	3	8953	1/1	0.88	0.21	-	200,200,200,200	0
32	MG	0	8018	1/1	0.95	0.26	-	53,53,53,53	0
34	SR	S	8961	1/1	0.94	0.21	-	165,165,165,165	0
32	MG	0	8036	1/1	0.77	0.08	-	46,46,46,46	0
35	NA	0	8512	1/1	0.95	0.30	-	32,32,32,32	0
34	SR	0	8968	1/1	0.55	0.14	-	170,170,170,170	0
32	MG	0	8085	1/1	0.96	0.14	-	51,51,51,51	0
34	SR	0	8909	1/1	0.70	0.25	-	189,189,189,189	0
34	SR	0	8938	1/1	-0.47	0.70	-	200,200,200,200	0
34	SR	0	8919	1/1	0.59	0.40	-	188,188,188,188	0
34	SR	0	8982	1/1	0.57	1.21	-	200,200,200,200	0
33	CL	0	8813	1/1	0.98	0.06	-	43,43,43,43	0
34	SR	0	8925	1/1	0.57	0.18	-	178,178,178,178	0
32	MG	0	8031	1/1	0.94	0.10	-	69,69,69,69	0
32	MG	0	8066	1/1	0.96	0.40	-	87,87,87,87	0
33	CL	A	8809	1/1	0.98	0.12	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8928	1/1	-0.11	1.41	-	200,200,200,200	0
34	SR	0	8926	1/1	0.40	0.39	-	199,199,199,199	0
32	MG	0	8082	1/1	0.85	0.33	-	39,39,39,39	0
32	MG	0	8020	1/1	0.82	0.11	-	36,36,36,36	0
32	MG	0	8032	1/1	0.90	0.09	-	47,47,47,47	0
34	SR	0	8934	1/1	0.57	0.75	-	168,168,168,168	0
34	SR	1	8952	1/1	0.48	0.68	-	200,200,200,200	0
32	MG	0	8039	1/1	0.77	0.31	-	56,56,56,56	0
34	SR	0	9004	1/1	0.51	0.53	-	200,200,200,200	0
34	SR	0	8905	1/1	0.90	0.21	-	161,161,161,161	0
35	NA	0	8511	1/1	0.44	0.20	-	56,56,56,56	0
33	CL	0	8817	1/1	0.98	0.07	-	57,57,57,57	0
35	NA	0	8531	1/1	0.84	0.22	-	47,47,47,47	0
34	SR	0	8989	1/1	0.82	0.69	-	200,200,200,200	0
35	NA	0	8536	1/1	0.94	0.16	-	46,46,46,46	0
34	SR	0	8906	1/1	0.83	0.40	-	191,191,191,191	0
32	MG	0	8061	1/1	0.98	0.17	-	23,23,23,23	0
35	NA	0	8514	1/1	0.98	0.40	-	40,40,40,40	0
32	MG	0	8091	1/1	0.09	0.29	-	79,79,79,79	0
35	NA	0	8544	1/1	0.96	0.19	-	49,49,49,49	0
32	MG	9	8074	1/1	0.90	0.08	-	45,45,45,45	0
32	MG	0	8024	1/1	0.97	0.27	-	43,43,43,43	0
35	NA	0	8526	1/1	0.85	0.09	-	51,51,51,51	0
32	MG	0	8021	1/1	0.94	0.07	-	16,16,16,16	0
35	NA	0	8549	1/1	0.77	0.43	-	60,60,60,60	0
34	SR	0	8917	1/1	0.82	0.62	-	199,199,199,199	0
35	NA	0	8561	1/1	0.81	0.46	-	52,52,52,52	0
32	MG	0	8019	1/1	0.92	0.25	-	1,1,1,1	0
35	NA	0	8545	1/1	0.95	0.18	-	41,41,41,41	0
35	NA	0	8513	1/1	0.97	0.14	-	34,34,34,34	0
33	CL	R	8806	1/1	0.97	0.07	-	32,32,32,32	0
35	NA	0	8570	1/1	0.65	0.53	-	81,81,81,81	0
32	MG	0	8023	1/1	0.94	0.13	-	14,14,14,14	0
35	NA	S	8510	1/1	0.77	0.18	-	35,35,35,35	0
32	MG	0	8055	1/1	0.88	0.15	-	49,49,49,49	0
34	SR	0	8983	1/1	0.84	0.35	-	170,170,170,170	0
34	SR	0	8901	1/1	0.53	0.12	-	73,73,73,73	0
34	SR	0	8991	1/1	0.38	0.10	-	162,162,162,162	0
33	CL	Q	8811	1/1	0.98	0.04	-	51,51,51,51	0
32	MG	0	8015	1/1	0.99	0.15	-	5,5,5,5	0
34	SR	9	8980	1/1	0.10	0.39	-	200,200,200,200	0
34	SR	0	8940	1/1	0.85	0.28	-	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8916	1/1	0.75	0.34	-	178,178,178,178	0
35	NA	C	8558	1/1	0.61	0.45	-	33,33,33,33	0
34	SR	0	8918	1/1	0.94	0.12	-	122,122,122,122	0
32	MG	0	8073	1/1	0.95	0.10	-	47,47,47,47	0
32	MG	0	8092	1/1	0.86	0.06	-	61,61,61,61	0
32	MG	0	8045	1/1	0.95	0.11	-	13,13,13,13	0
34	SR	0	8990	1/1	0.84	0.08	-	91,91,91,91	0
35	NA	0	8567	1/1	0.76	0.46	-	63,63,63,63	0
34	SR	0	8964	1/1	0.62	0.41	-	188,188,188,188	0
34	SR	0	9000	1/1	0.15	1.21	-	200,200,200,200	0
34	SR	0	9008	1/1	0.87	0.08	-	135,135,135,135	0
32	MG	0	8069	1/1	0.89	0.34	-	38,38,38,38	0
32	MG	B	8042	1/1	0.94	0.14	-	41,41,41,41	0
34	SR	0	8937	1/1	0.93	0.28	-	155,155,155,155	0
32	MG	0	8048	1/1	0.99	0.27	-	44,44,44,44	0
32	MG	0	8087	1/1	0.97	0.09	-	14,14,14,14	0
34	SR	0	9007	1/1	0.84	0.41	-	200,200,200,200	0
35	NA	C	8503	1/1	0.93	0.17	-	31,31,31,31	0
34	SR	0	8998	1/1	0.71	0.37	-	196,196,196,196	0
34	SR	0	8959	1/1	-0.06	0.67	-	195,195,195,195	0
34	SR	0	8981	1/1	0.84	0.50	-	200,200,200,200	0
34	SR	0	8957	1/1	0.84	0.75	-	200,200,200,200	0
34	SR	0	8955	1/1	0.83	0.13	-	184,184,184,184	0
35	NA	0	8509	1/1	0.22	0.33	-	53,53,53,53	0
34	SR	0	8954	1/1	0.70	0.87	-	198,198,198,198	0
32	MG	0	8067	1/1	0.94	0.37	-	51,51,51,51	0
32	MG	0	8016	1/1	0.99	0.22	-	2,2,2,2	0
34	SR	0	9005	1/1	0.83	0.24	-	190,190,190,190	0
32	MG	0	8056	1/1	0.88	0.19	-	37,37,37,37	0
32	MG	0	8033	1/1	0.91	0.12	-	78,78,78,78	0
34	SR	0	8942	1/1	0.74	0.33	-	162,162,162,162	0
34	SR	0	8922	1/1	0.45	0.55	-	155,155,155,155	0
32	MG	0	8083	1/1	0.77	0.09	-	41,41,41,41	0
34	SR	T	8939	1/1	0.58	0.64	-	200,200,200,200	0
32	MG	0	8049	1/1	0.86	0.32	-	43,43,43,43	0
34	SR	0	8946	1/1	0.70	0.39	-	190,190,190,190	0
32	MG	0	8038	1/1	0.96	0.07	-	52,52,52,52	0
32	MG	0	8089	1/1	0.94	0.27	-	56,56,56,56	0
35	NA	0	8525	1/1	0.12	1.04	-	107,107,107,107	0
34	SR	0	8995	1/1	0.56	0.38	-	164,164,164,164	0
32	MG	0	8080	1/1	0.97	0.16	-	39,39,39,39	0
33	CL	0	8822	1/1	0.89	0.10	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8064	1/1	0.96	0.14	-	29,29,29,29	0
32	MG	0	8081	1/1	0.84	0.49	-	94,94,94,94	0
34	SR	0	8941	1/1	0.94	0.20	-	180,180,180,180	0
34	SR	0	8951	1/1	0.96	0.14	-	164,164,164,164	0
35	NA	0	8546	1/1	0.83	0.68	-	106,106,106,106	0
34	SR	0	8923	1/1	0.72	0.59	-	165,165,165,165	0
34	SR	0	8979	1/1	0.71	0.09	-	180,180,180,180	0
34	SR	0	8933	1/1	0.47	0.14	-	137,137,137,137	0
35	NA	H	8518	1/1	0.99	0.13	-	48,48,48,48	0
34	SR	0	8978	1/1	0.81	0.78	-	200,200,200,200	0
35	NA	0	8501	1/1	0.87	0.25	-	29,29,29,29	0
32	MG	0	8078	1/1	0.94	0.17	-	28,28,28,28	0
32	MG	0	8007	1/1	0.96	0.17	-	3,3,3,3	0
34	SR	3	8932	1/1	0.71	0.11	-	133,133,133,133	0
35	NA	0	8550	1/1	0.90	0.12	-	25,25,25,25	0
32	MG	0	8027	1/1	0.80	0.16	-	37,37,37,37	0
32	MG	0	8022	1/1	0.96	0.13	-	20,20,20,20	0
34	SR	0	9001	1/1	0.80	0.70	-	187,187,187,187	0
34	SR	0	8911	1/1	0.35	0.39	-	200,200,200,200	0
34	SR	0	8915	1/1	0.86	0.14	-	200,200,200,200	0
32	MG	0	8030	1/1	0.94	0.30	-	45,45,45,45	0
35	NA	0	8508	1/1	0.90	0.75	-	41,41,41,41	0
35	NA	0	8520	1/1	0.85	0.11	-	44,44,44,44	0
34	SR	0	8960	1/1	0.68	0.35	-	200,200,200,200	0
34	SR	A	8993	1/1	0.03	0.21	-	200,200,200,200	0
34	SR	0	8977	1/1	0.72	0.12	-	194,194,194,194	0
32	MG	0	8071	1/1	0.88	0.44	-	136,136,136,136	0
34	SR	0	8931	1/1	0.66	0.16	-	193,193,193,193	0
34	SR	0	8996	1/1	0.86	0.62	-	200,200,200,200	0
34	SR	0	8994	1/1	0.85	0.23	-	192,192,192,192	0
34	SR	0	8927	1/1	0.67	0.23	-	184,184,184,184	0
33	CL	Y	8820	1/1	0.93	0.09	-	33,33,33,33	0
34	SR	B	8950	1/1	0.53	0.62	-	196,196,196,196	0
32	MG	0	8063	1/1	0.89	0.12	-	47,47,47,47	0
33	CL	L	8814	1/1	0.92	0.19	-	51,51,51,51	0
35	NA	0	8551	1/1	0.93	0.13	-	36,36,36,36	0
34	SR	0	8935	1/1	0.32	0.11	-	159,159,159,159	0
34	SR	0	8944	1/1	0.86	0.21	-	200,200,200,200	0
34	SR	0	8971	1/1	0.82	0.10	-	195,195,195,195	0
35	NA	0	8574	1/1	0.89	0.28	-	52,52,52,52	0
35	NA	0	8516	1/1	0.94	0.12	-	18,18,18,18	0
34	SR	0	8973	1/1	0.68	0.14	-	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8997	1/1	0.40	1.19	-	200,200,200,200	0
34	SR	0	8984	1/1	0.36	0.08	-	170,170,170,170	0
35	NA	9	8543	1/1	0.95	0.09	-	22,22,22,22	0
33	CL	J	8802	1/1	0.84	0.07	-	66,66,66,66	0
34	SR	0	8907	1/1	0.26	0.22	-	180,180,180,180	0
32	MG	0	8079	1/1	0.90	0.15	-	51,51,51,51	0
34	SR	0	9006	1/1	0.18	0.41	-	192,192,192,192	0
34	SR	R	8912	1/1	0.88	0.11	-	157,157,157,157	0
35	NA	0	8506	1/1	0.90	0.31	-	50,50,50,50	0
34	SR	0	8988	1/1	0.67	0.19	-	177,177,177,177	0
35	NA	0	8505	1/1	0.74	0.52	-	31,31,31,31	0
32	MG	0	8026	1/1	0.93	0.11	-	22,22,22,22	0
32	MG	0	8017	1/1	0.98	0.07	-	31,31,31,31	0
34	SR	0	8924	1/1	0.74	0.12	-	184,184,184,184	0
34	SR	0	8920	1/1	0.28	0.55	-	200,200,200,200	0
34	SR	0	8974	1/1	0.93	0.20	-	165,165,165,165	0
32	MG	0	8077	1/1	0.96	0.09	-	36,36,36,36	0
34	SR	0	8914	1/1	0.92	0.49	-	198,198,198,198	0
35	NA	0	8529	1/1	0.74	0.08	-	33,33,33,33	0
35	NA	0	8524	1/1	0.87	0.19	-	43,43,43,43	0
35	NA	0	8566	1/1	0.94	0.15	-	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.