



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:42 PM GMT

PDB ID : 1VQN
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

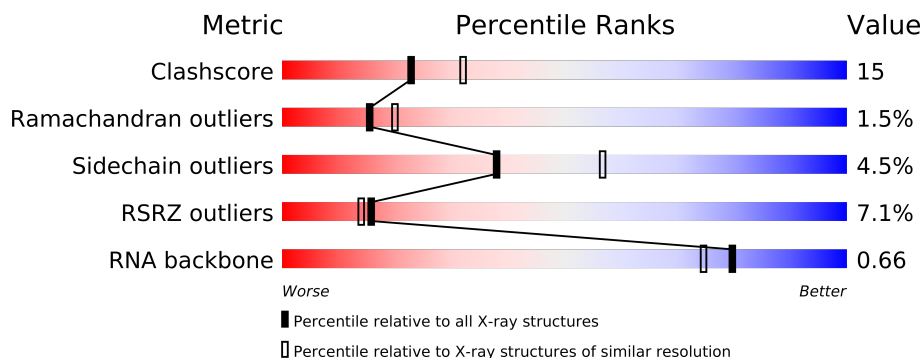
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

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. 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	0	2922	
2	9	122	
3	4	4	
4	5	6	
5	A	240	
6	B	338	
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	

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Mol	Chain	Length	Quality of chain
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	
32	3	92	
33	I	162	

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

Mol	Type	Chain	Res	Geometry	Electron density
34	MG	0	8001	-	X
34	MG	0	8008	-	X
34	MG	0	8012	-	X
34	MG	0	8013	-	X
34	MG	0	8014	-	X
34	MG	0	8021	-	X
34	MG	0	8022	-	X
34	MG	0	8024	-	X
34	MG	0	8025	-	X
34	MG	0	8027	-	X
34	MG	0	8029	-	X
34	MG	0	8038	-	X
34	MG	0	8039	-	X
34	MG	0	8045	-	X
34	MG	0	8047	-	X
34	MG	0	8050	-	X
34	MG	0	8051	-	X
34	MG	0	8052	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	MG	0	8054	-	X
34	MG	0	8055	-	X
34	MG	0	8056	-	X
34	MG	0	8059	-	X
34	MG	0	8061	-	X
34	MG	0	8065	-	X
34	MG	0	8072	-	X
34	MG	0	8082	-	X
34	MG	0	8084	-	X
34	MG	0	8085	-	X
34	MG	0	8089	-	X
34	MG	0	8090	-	X
34	MG	0	8091	-	X
34	MG	0	8092	-	X
34	MG	0	8094	-	X
34	MG	0	8099	-	X
34	MG	0	8101	-	X
34	MG	0	8103	-	X
34	MG	0	8108	-	X
34	MG	0	8114	-	X
34	MG	5	8118	-	X
34	MG	9	8095	-	X
34	MG	K	8069	-	X
35	K	0	9001	-	X
36	NA	0	9102	-	X
36	NA	0	9106	-	X
36	NA	0	9107	-	X
36	NA	0	9110	-	X
36	NA	0	9111	-	X
36	NA	0	9114	-	X
36	NA	0	9115	-	X
36	NA	0	9116	-	X
36	NA	0	9118	-	X
36	NA	0	9120	-	X
36	NA	0	9122	-	X
36	NA	0	9125	-	X
36	NA	0	9131	-	X
36	NA	0	9132	-	X
36	NA	0	9135	-	X
36	NA	0	9149	-	X
36	NA	0	9150	-	X
36	NA	0	9152	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	NA	0	9156	-	X
36	NA	0	9157	-	X
36	NA	0	9158	-	X
36	NA	0	9159	-	X
36	NA	0	9160	-	X
36	NA	0	9161	-	X
36	NA	0	9162	-	X
36	NA	0	9164	-	X
36	NA	0	9165	-	X
36	NA	0	9168	-	X
36	NA	0	9169	-	X
36	NA	0	9170	-	X
36	NA	0	9171	-	X
36	NA	0	9172	-	X
36	NA	0	9173	-	X
36	NA	0	9174	-	X
36	NA	0	9175	-	X
36	NA	0	9177	-	X
36	NA	0	9178	-	X
36	NA	0	9179	-	X
36	NA	0	9181	-	X
36	NA	0	9182	-	X
36	NA	0	9184	-	X
36	NA	0	9185	-	X
36	NA	9	9183	-	X
36	NA	R	9186	-	X
36	NA	S	9112	-	X
37	CL	0	9316	-	X
37	CL	0	9322	-	X
37	CL	B	9319	-	X
38	SR	0	9405	-	X
38	SR	0	9432	-	X
38	SR	0	9434	-	X
38	SR	0	9482	-	X
38	SR	0	9484	-	X
38	SR	0	9500	-	X
38	SR	0	9501	-	X
38	SR	0	9529	-	X
38	SR	0	9539	-	X
38	SR	0	9547	-	X
38	SR	0	9626	-	X
38	SR	B	9521	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99077 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 RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

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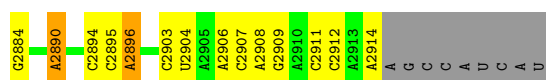
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

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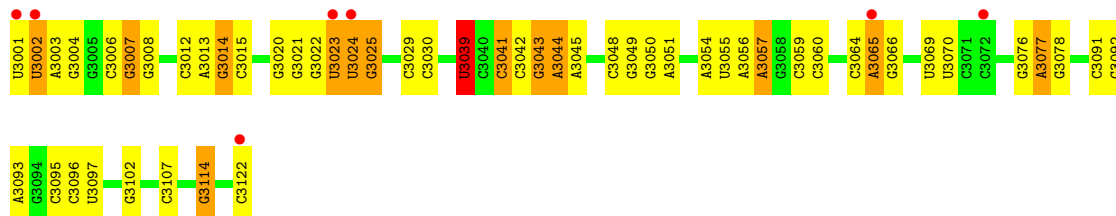
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40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0





- Molecule 2: 5S ribosomal RNA

Chain 9:



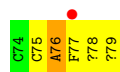
- Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'

Chain 4:



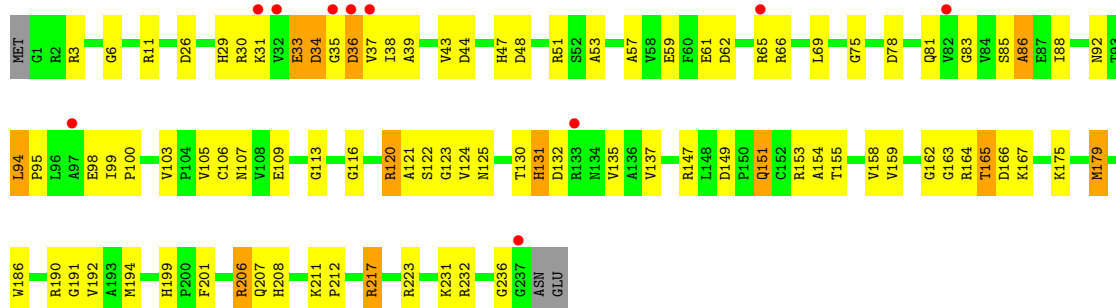
- Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

Chain 5:



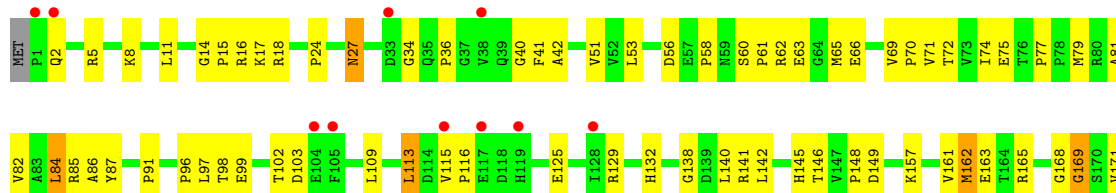
- Molecule 5: 50S ribosomal protein L2P

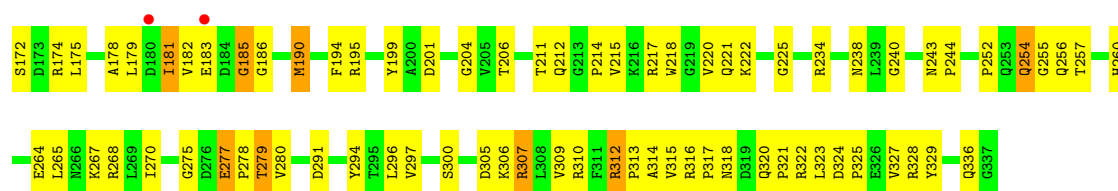
Chain A:



- Molecule 6: 50S ribosomal protein L3P

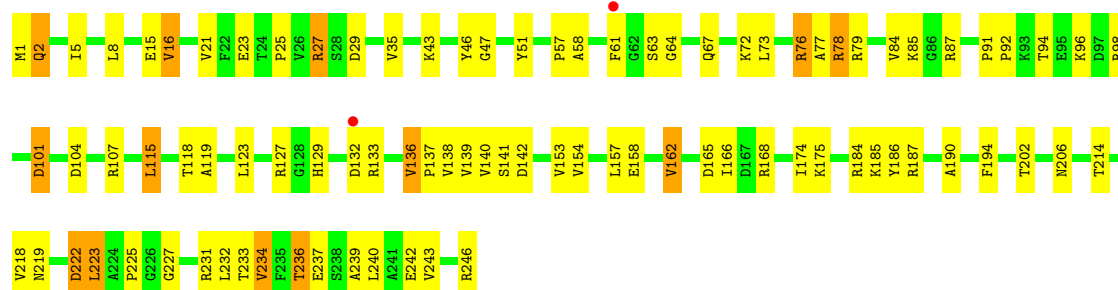
Chain B:





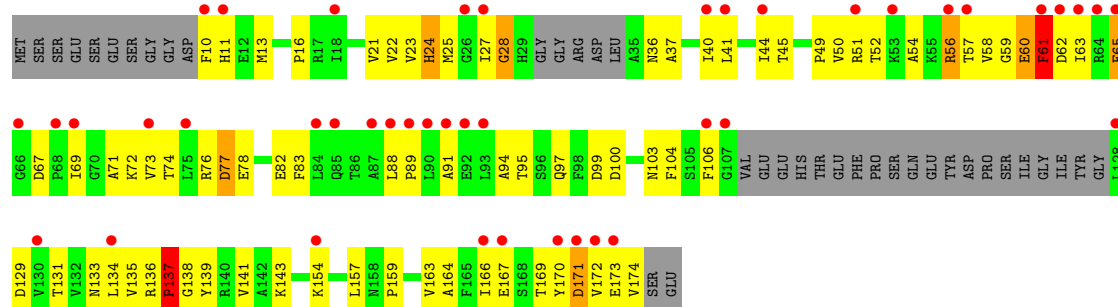
• Molecule 7: 50S ribosomal protein L4E

Chain C:



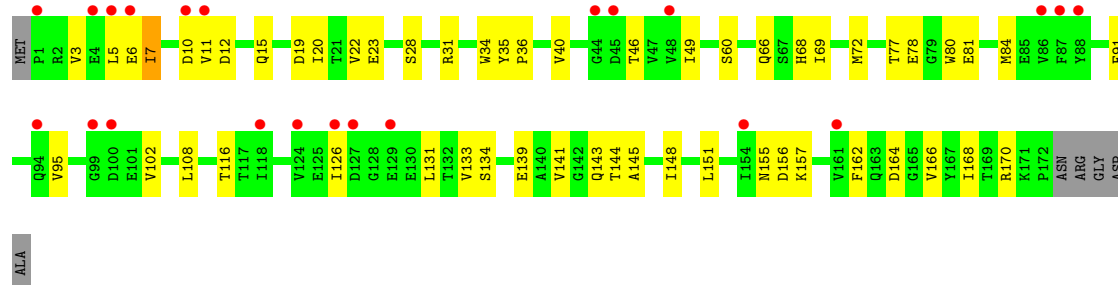
• Molecule 8: 50S ribosomal protein L5P

Chain D:



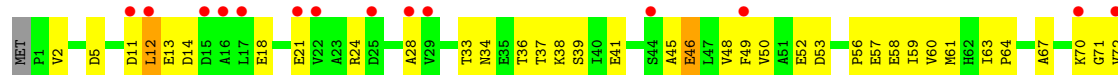
• Molecule 9: 50S ribosomal protein L6P

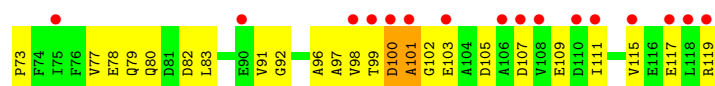
Chain E:



• Molecule 10: 50S ribosomal protein L7AE

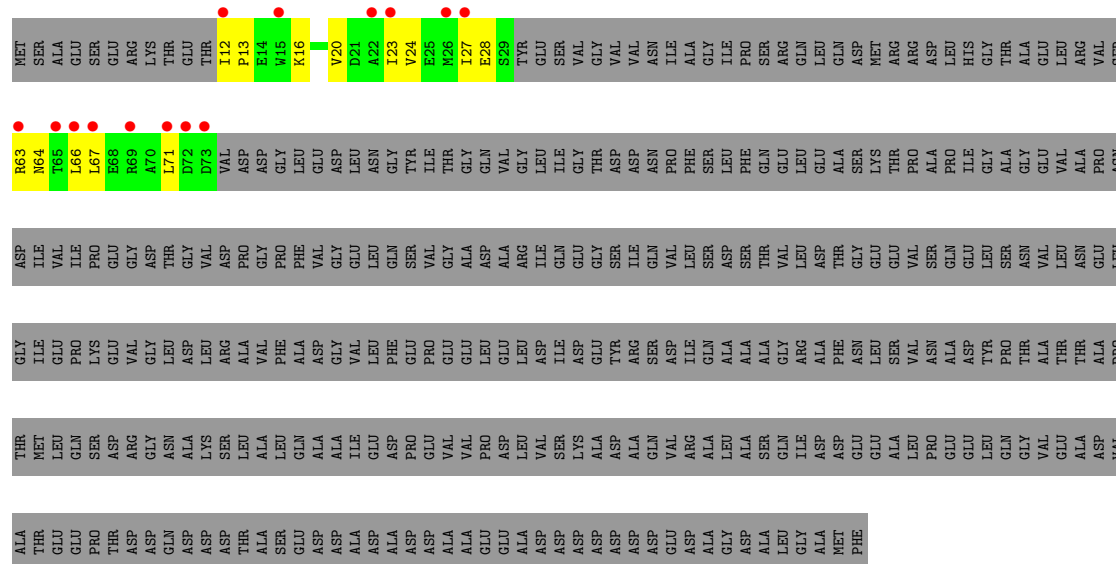
Chain F:





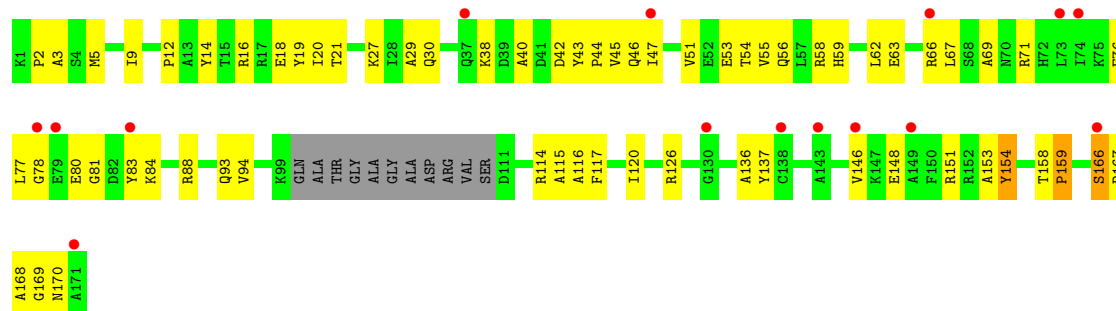
• Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



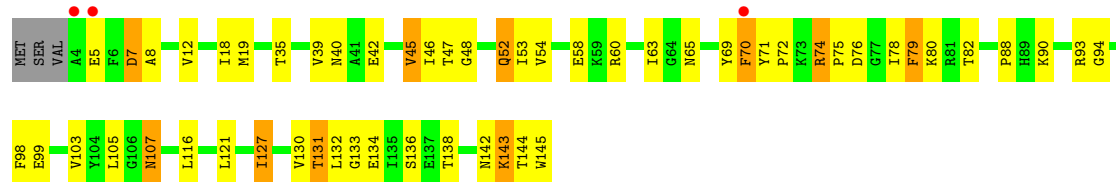
• Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain H:



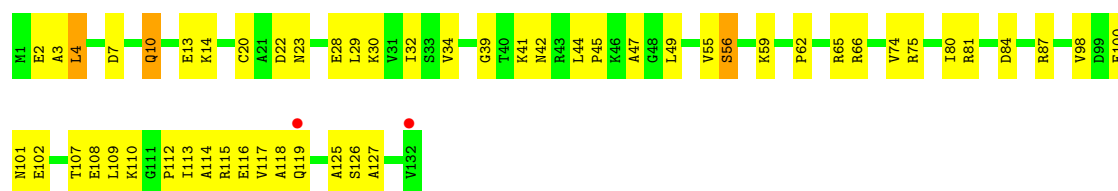
• Molecule 13: 50S ribosomal protein L13P

Chain J:



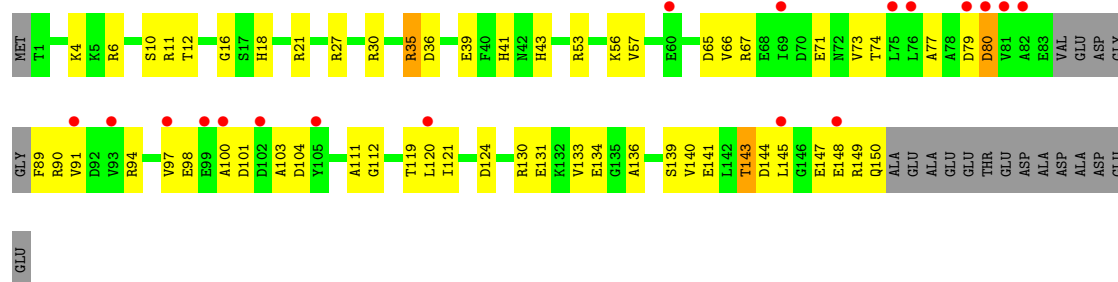
• Molecule 14: 50S ribosomal protein L14P

Chain K:



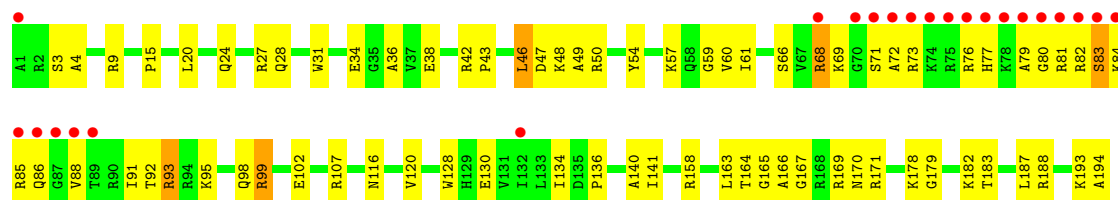
- Molecule 15: 50S ribosomal protein L15P

Chain L:



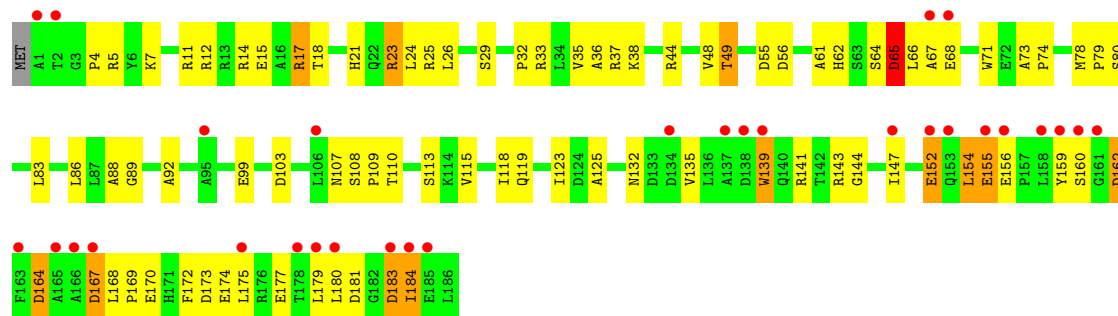
- Molecule 16: 50S Ribosomal Protein L15E

Chain M:



- Molecule 17: 50S ribosomal protein L18P

Chain N:



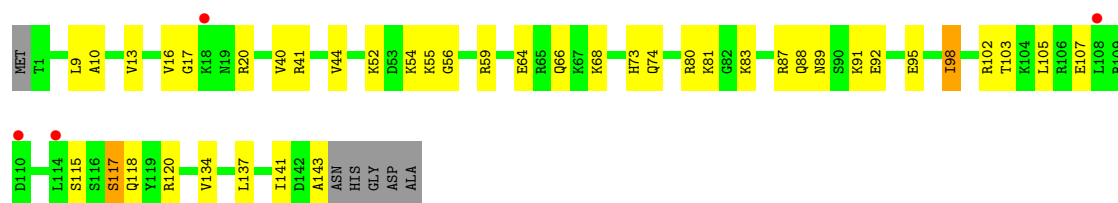
- Molecule 18: 50S ribosomal protein L18e

Chain O:



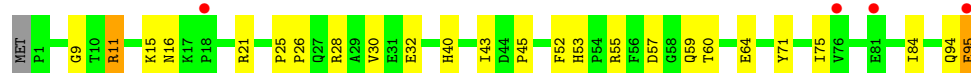
- Molecule 19: 50S ribosomal protein L19E

Chain P:



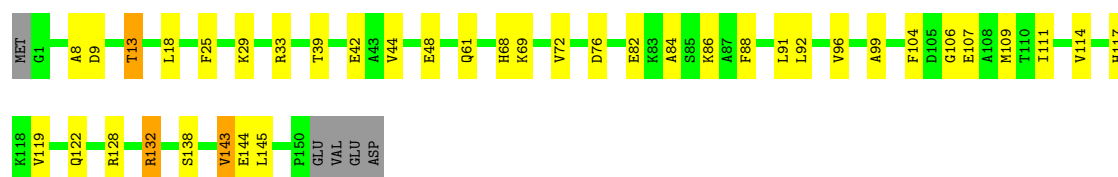
- Molecule 20: 50S ribosomal protein L21e

Chain Q:



- Molecule 21: 50S ribosomal protein L22P

Chain R:



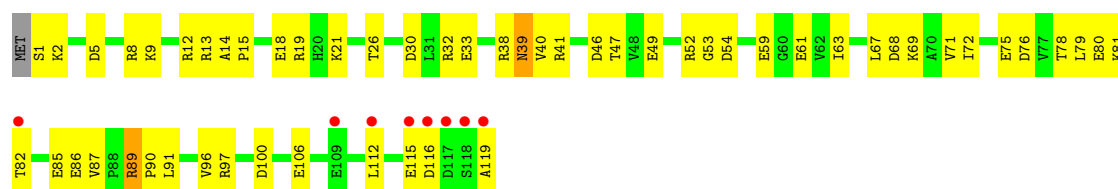
- Molecule 22: 50S ribosomal protein L23P

Chain S:



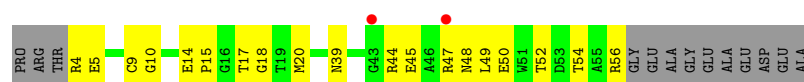
- Molecule 23: 50S ribosomal protein L24P

Chain T:



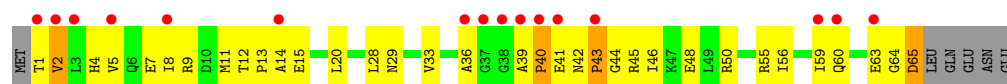
- Molecule 24: 50S ribosomal protein L24E

Chain U:



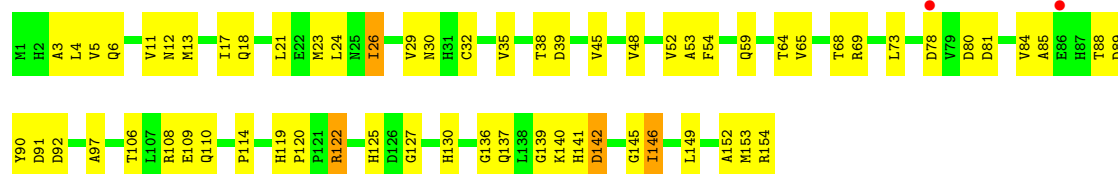
- Molecule 25: 50S ribosomal protein L29P

Chain V:



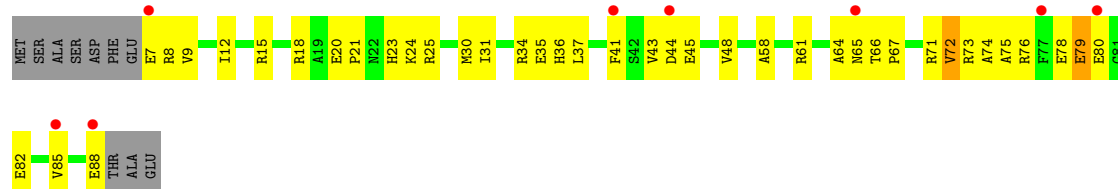
- Molecule 26: 50S ribosomal protein L30P

Chain W:



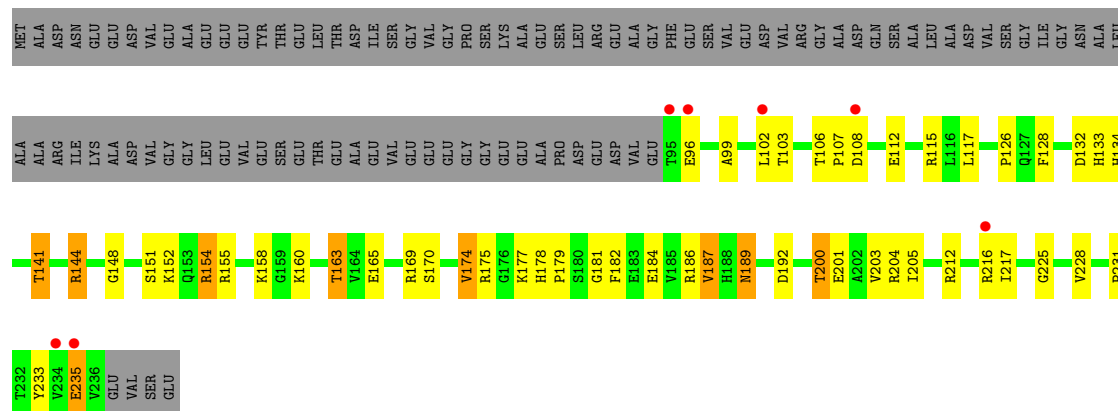
- Molecule 27: 50S ribosomal protein L31e

Chain X:



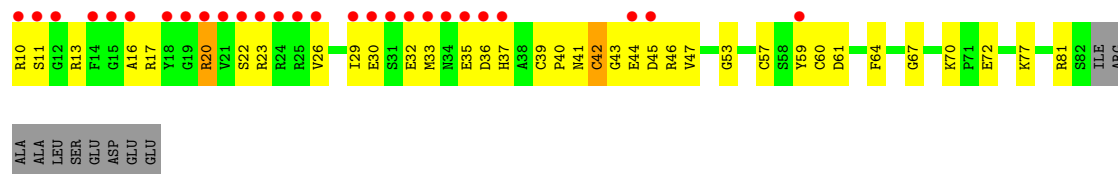
- Molecule 28: 50S ribosomal protein L32E

Chain Y:



- Molecule 29: 50S ribosomal protein L37Ae

Chain Z:



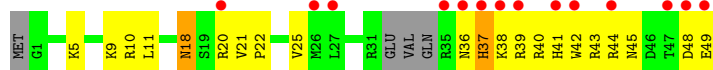
- Molecule 30: 50S ribosomal protein L37e

Chain 1:



- Molecule 31: 50S ribosomal protein L39e

Chain 2:



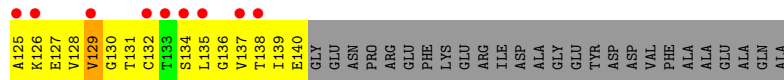
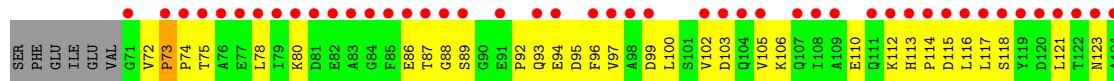
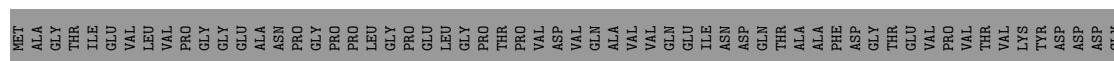
- Molecule 32: 50S ribosomal protein L44E

Chain 3:



- Molecule 33: 50S RIBOSOMAL PROTEIN L11P

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 697789 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ACA, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, 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	0	0.38	0/65959	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (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
1	0	0	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	22	U	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	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	0	59021	0	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	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 15.

The worst 5 of 2220 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:O:1160:G:H5'	1:O:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04

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	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	18	24
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	15	20
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	27	39
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	8	8
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	8	8
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	7	6
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	27	39
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	16	22
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	38	53
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	3	2
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	14	17
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	4	2
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	4	3
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	9	9
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	21	29
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	7	6
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	15	20

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER

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	
5	A	179/182 (98%)	165 (92%)	14 (8%)	18	27
6	B	282/283 (100%)	267 (95%)	15 (5%)	32	48
7	C	193/193 (100%)	173 (90%)	20 (10%)	10	14
8	D	117/148 (79%)	112 (96%)	5 (4%)	40	59
9	E	152/156 (97%)	146 (96%)	6 (4%)	43	64
10	F	93/94 (99%)	91 (98%)	2 (2%)	64	83
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	44	65
13	J	118/121 (98%)	108 (92%)	10 (8%)	15	23
14	K	106/106 (100%)	101 (95%)	5 (5%)	36	54
15	L	113/127 (89%)	110 (97%)	3 (3%)	57	78
16	M	158/158 (100%)	153 (97%)	5 (3%)	51	72
17	N	149/150 (99%)	142 (95%)	7 (5%)	36	54
18	O	93/94 (99%)	92 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	P	113/117 (97%)	110 (97%)	3 (3%)	57	78
20	Q	79/80 (99%)	75 (95%)	4 (5%)	33	50
21	R	117/122 (96%)	114 (97%)	3 (3%)	59	79
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	44	65
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	68	86
26	W	130/130 (100%)	124 (95%)	6 (5%)	37	55
27	X	66/74 (89%)	63 (96%)	3 (4%)	38	57
28	Y	120/196 (61%)	109 (91%)	11 (9%)	13	19
29	Z	60/68 (88%)	59 (98%)	1 (2%)	73	89
30	1	46/47 (98%)	45 (98%)	1 (2%)	64	83
31	2	42/46 (91%)	41 (98%)	1 (2%)	61	81
32	3	79/79 (100%)	77 (98%)	2 (2%)	60	80
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	38	57

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	H	18	GLU
14	K	4	LEU
28	Y	174	VAL
12	H	88	ARG
13	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
19	P	50	GLN
21	R	61	GLN
31	2	16	ASN
19	P	66	GLN
19	P	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	33 (1%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1730	G
1	0	2761	A
1	0	1684	A
1	0	1685	A

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	20,22,23	0.77	1 (5%)	24,31,34	0.69	0
1	OMG	0	2588	1,3	24,26,27	0.89	1 (4%)	32,38,41	5.45	3 (9%)
1	UR3	0	2619	1,38	20,22,23	0.82	0	23,32,35	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	0	2621	1	19,21,22	1.28	3 (15%)	23,30,33	1.06	1 (4%)
1	1MA	0	628	1,36	23,25,26	0.85	0	32,37,40	1.01	1 (3%)
3	PPU	4	76	1,3	24,26,41	0.76	1 (4%)	33,38,60	0.95	1 (3%)
3	HFA	4	77	3	11,11,12	5.54	2 (18%)	10,13,15	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1,38	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1,36	-	1/8/25/26	0/1/3/3
3	PPU	4	76	1,3	-	0/12/29/44	0/1/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	77	HFA	O-C	18.00	1.23	1.11
3	4	77	HFA	OA-CA	3.30	1.48	1.42
1	0	2621	PSU	C2-N1	3.07	1.43	1.37
1	0	2621	PSU	C6-N1	2.92	1.35	1.32
1	0	2587	OMU	P-OP1	2.45	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-30.23	130.07	134.14
3	4	76	PPU	C2-N1-C6	3.39	118.88	111.53
1	0	2588	OMG	C6-N1-C2	3.22	125.14	119.51
1	0	628	1MA	C2-N3-C4	-3.16	110.83	116.23
1	0	2621	PSU	C5-C4-N3	-2.31	114.65	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	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 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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	0	2754/2922 (94%)	-0.15	90 (3%) 44 42	24, 49, 93, 153	0
2	9	122/122 (100%)	0.27	7 (5%) 23 21	41, 69, 93, 152	0
3	4	4/4 (100%)	-0.20	0 100 100	43, 45, 46, 52	0
4	5	6/6 (100%)	0.27	1 (16%) 2 2	55, 58, 75, 87	0
5	A	237/240 (98%)	0.29	10 (4%) 35 32	31, 54, 86, 106	0
6	B	337/338 (99%)	0.15	12 (3%) 41 39	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.03	2 (0%) 83 82	27, 49, 70, 87	0
8	D	140/177 (79%)	1.56	43 (30%) 1 1	64, 96, 125, 132	0
9	E	172/178 (96%)	0.73	22 (12%) 4 4	44, 66, 86, 92	0
10	F	119/120 (99%)	1.02	30 (25%) 1 1	49, 74, 100, 112	0
11	G	29/348 (8%)	2.15	14 (48%) 1 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.60	15 (9%) 9 8	47, 65, 96, 103	0
13	J	142/145 (97%)	0.06	3 (2%) 60 58	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.16	2 (1%) 70 69	37, 48, 71, 84	0
15	L	145/165 (87%)	0.59	18 (12%) 5 4	29, 69, 112, 121	0
16	M	194/194 (100%)	0.51	23 (11%) 5 4	37, 48, 85, 93	0
17	N	186/187 (99%)	0.87	30 (16%) 2 2	49, 68, 112, 119	0
18	O	115/116 (99%)	0.21	3 (2%) 53 51	40, 59, 73, 81	0
19	P	143/149 (95%)	0.26	4 (2%) 50 48	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.09	4 (4%) 35 32	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.12	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.30	2 (2%) 54 52	43, 61, 84, 97	0
23	T	119/120 (99%)	0.61	8 (6%) 17 16	41, 59, 85, 110	0
24	U	53/66 (80%)	0.22	2 (3%) 38 36	42, 56, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.57	16 (24%) 1 1	56, 78, 115, 120	0
26	W	154/154 (100%)	0.03	2 (1%) 74 73	40, 53, 74, 82	0
27	X	82/92 (89%)	0.51	8 (9%) 8 7	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.12	7 (4%) 28 26	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.74	27 (36%) 1 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.39	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.26	14 (30%) 1 1	41, 68, 96, 102	0
32	3	92/92 (100%)	0.32	5 (5%) 25 23	41, 61, 73, 86	0
33	I	70/162 (43%)	4.52	55 (78%) 0 0	111, 125, 142, 144	0
All	All	6661/7484 (89%)	0.23	479 (7%) 16 13	24, 54, 99, 153	0

The worst 5 of 479 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	V	1	THR	13.7
33	I	71	GLY	11.5
33	I	79	ILE	11.4
29	Z	11	SER	10.6
16	M	70	GLY	10.5

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.15	1.10	39,42,45,48	0
3	HFA	4	77	11/12	0.19	0.63	42,44,47,48	0
1	OMU	0	2587	21/22	0.12	0.02	32,37,40,40	0
1	OMG	0	2588	24/25	0.12	-0.33	31,34,39,41	0
3	PPU	4	76	24/38	0.13	-0.47	41,44,45,49	0
1	PSU	0	2621	20/21	0.13	-0.61	36,38,43,43	0
1	1MA	0	628	23/24	0.12	-1.49	32,35,37,38	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	MG	0	8094	1/1	0.42	210.72	72,72,72,72	0
36	NA	0	9152	1/1	0.95	161.75	83,83,83,83	0
34	MG	0	8059	1/1	0.48	89.53	84,84,84,84	0
34	MG	0	8072	1/1	0.61	75.87	89,89,89,89	0
36	NA	0	9125	1/1	0.71	67.06	92,92,92,92	0
36	NA	0	9106	1/1	0.47	60.43	44,44,44,44	0
36	NA	0	9161	1/1	0.77	57.95	68,68,68,68	0
36	NA	0	9149	1/1	0.37	55.43	49,49,49,49	0
36	NA	0	9164	1/1	0.54	50.24	61,61,61,61	0
34	MG	0	8022	1/1	1.03	44.40	112,112,112,112	0
36	NA	0	9175	1/1	0.39	41.81	55,55,55,55	0
34	MG	0	8024	1/1	0.47	40.71	86,86,86,86	0
38	SR	0	9500	1/1	1.45	39.64	200,200,200,200	0
36	NA	0	9135	1/1	0.38	39.60	55,55,55,55	0
34	MG	0	8090	1/1	0.30	38.95	68,68,68,68	0
36	NA	0	9179	1/1	0.62	38.78	121,121,121,121	0
36	NA	0	9111	1/1	0.31	38.27	63,63,63,63	0
34	MG	0	8114	1/1	0.51	35.90	83,83,83,83	0
36	NA	0	9184	1/1	0.42	35.48	87,87,87,87	0
36	NA	0	9185	1/1	0.56	31.98	54,54,54,54	0
36	NA	0	9158	1/1	0.46	30.65	66,66,66,66	0
37	CL	0	9322	1/1	0.39	30.13	61,61,61,61	0
34	MG	0	8047	1/1	0.48	29.61	107,107,107,107	0
36	NA	0	9116	1/1	0.39	27.75	52,52,52,52	0
34	MG	0	8092	1/1	0.26	25.22	77,77,77,77	0
34	MG	0	8025	1/1	0.40	23.29	27,27,27,27	0
36	NA	0	9107	1/1	0.39	22.62	71,71,71,71	0
34	MG	0	8052	1/1	0.24	21.16	99,99,99,99	0
38	SR	0	9547	1/1	0.35	18.22	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	NA	9	9183	1/1	0.45	16.87	75,75,75,75	0
38	SR	B	9521	1/1	0.60	16.85	200,200,200,200	0
36	NA	0	9178	1/1	0.41	16.37	54,54,54,54	0
38	SR	0	9539	1/1	0.38	16.12	157,157,157,157	0
34	MG	0	8013	1/1	0.32	15.75	25,25,25,25	0
34	MG	0	8082	1/1	0.17	15.00	82,82,82,82	0
36	NA	0	9182	1/1	0.39	14.44	90,90,90,90	0
36	NA	R	9186	1/1	0.40	14.03	80,80,80,80	0
36	NA	0	9110	1/1	0.27	13.79	46,46,46,46	0
36	NA	0	9171	1/1	0.27	13.08	61,61,61,61	0
34	MG	0	8014	1/1	0.30	12.99	73,73,73,73	0
35	K	0	9001	1/1	0.33	12.99	74,74,74,74	0
38	SR	0	9626	1/1	0.26	12.49	154,154,154,154	0
36	NA	0	9173	1/1	0.36	11.94	69,69,69,69	0
34	MG	0	8089	1/1	0.23	11.87	61,61,61,61	0
38	SR	0	9482	1/1	0.34	11.42	135,135,135,135	0
34	MG	0	8084	1/1	0.34	11.29	89,89,89,89	0
34	MG	5	8118	1/1	0.34	11.27	45,45,45,45	0
36	NA	0	9157	1/1	0.18	11.18	47,47,47,47	0
36	NA	0	9170	1/1	0.27	10.86	77,77,77,77	0
34	MG	9	8095	1/1	0.33	10.80	55,55,55,55	0
36	NA	0	9177	1/1	0.30	10.48	77,77,77,77	0
36	NA	0	9174	1/1	0.38	10.41	65,65,65,65	0
36	NA	0	9159	1/1	0.42	10.37	58,58,58,58	0
34	MG	0	8039	1/1	0.20	10.18	49,49,49,49	0
38	SR	0	9529	1/1	0.27	9.80	131,131,131,131	0
34	MG	0	8038	1/1	0.23	9.74	25,25,25,25	0
36	NA	0	9120	1/1	0.24	9.71	61,61,61,61	0
36	NA	0	9118	1/1	0.19	9.14	66,66,66,66	0
38	SR	0	9484	1/1	0.15	8.56	149,149,149,149	0
34	MG	0	8108	1/1	0.19	8.52	103,103,103,103	0
36	NA	0	9168	1/1	0.17	8.50	69,69,69,69	0
34	MG	0	8061	1/1	0.18	8.42	87,87,87,87	0
34	MG	0	8085	1/1	0.18	8.25	63,63,63,63	0
38	SR	0	9405	1/1	0.16	7.87	59,59,59,59	0
34	MG	0	8101	1/1	0.23	7.86	80,80,80,80	0
34	MG	0	8012	1/1	0.22	6.96	39,39,39,39	0
34	MG	0	8051	1/1	0.19	6.91	36,36,36,36	0
36	NA	0	9172	1/1	0.31	6.33	76,76,76,76	0
36	NA	S	9112	1/1	0.27	6.31	80,80,80,80	0
36	NA	0	9131	1/1	0.17	6.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8027	1/1	0.22	6.21	36,36,36,36	0
36	NA	0	9102	1/1	0.19	6.01	63,63,63,63	0
34	MG	0	8099	1/1	0.15	5.91	75,75,75,75	0
36	NA	0	9150	1/1	0.17	5.60	47,47,47,47	0
34	MG	0	8056	1/1	0.23	5.49	44,44,44,44	0
34	MG	0	8050	1/1	0.21	5.33	89,89,89,89	0
36	NA	0	9132	1/1	0.22	5.14	68,68,68,68	0
36	NA	0	9169	1/1	0.37	5.12	116,116,116,116	0
36	NA	0	9165	1/1	0.35	4.95	45,45,45,45	0
36	NA	0	9115	1/1	0.19	4.91	41,41,41,41	0
36	NA	0	9160	1/1	0.20	4.81	46,46,46,46	0
34	MG	0	8054	1/1	0.15	4.81	63,63,63,63	0
34	MG	0	8008	1/1	0.18	4.63	16,16,16,16	0
36	NA	0	9122	1/1	0.41	4.58	90,90,90,90	0
34	MG	0	8065	1/1	0.34	4.42	107,107,107,107	0
34	MG	0	8029	1/1	0.20	3.98	35,35,35,35	0
34	MG	0	8091	1/1	0.15	3.78	64,64,64,64	0
34	MG	K	8069	1/1	0.15	3.77	25,25,25,25	0
34	MG	0	8001	1/1	0.18	3.69	22,22,22,22	0
37	CL	0	9316	1/1	0.26	3.52	78,78,78,78	0
36	NA	0	9114	1/1	0.21	3.35	65,65,65,65	0
34	MG	0	8021	1/1	0.18	3.29	56,56,56,56	0
34	MG	0	8055	1/1	0.27	3.14	97,97,97,97	0
38	SR	0	9501	1/1	0.19	2.97	159,159,159,159	0
36	NA	0	9162	1/1	0.17	2.76	52,52,52,52	0
38	SR	0	9432	1/1	0.12	2.67	68,68,68,68	0
36	NA	0	9181	1/1	0.17	2.54	54,54,54,54	0
36	NA	0	9156	1/1	0.16	2.44	57,57,57,57	0
38	SR	0	9434	1/1	0.15	2.38	64,64,64,64	0
37	CL	B	9319	1/1	0.17	2.28	54,54,54,54	0
34	MG	0	8045	1/1	0.25	2.20	72,72,72,72	0
34	MG	0	8103	1/1	0.14	2.16	67,67,67,67	0
34	MG	0	8057	1/1	0.23	2.00	77,77,77,77	0
38	SR	0	9420	1/1	0.15	1.72	70,70,70,70	0
36	NA	0	9141	1/1	0.13	1.60	73,73,73,73	0
38	SR	0	9515	1/1	0.15	1.58	100,100,100,100	0
34	MG	0	8058	1/1	0.20	1.55	41,41,41,41	0
34	MG	0	8080	1/1	0.15	1.52	57,57,57,57	0
37	CL	J	9301	1/1	0.22	1.35	60,60,60,60	0
38	SR	0	9425	1/1	0.14	1.33	56,56,56,56	0
34	MG	0	8107	1/1	0.18	1.31	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9128	1/1	0.13	1.19	49,49,49,49	0
38	SR	0	9433	1/1	0.11	1.18	75,75,75,75	0
36	NA	0	9129	1/1	0.12	1.15	72,72,72,72	0
38	SR	S	9470	1/1	0.14	1.12	101,101,101,101	0
36	NA	0	9154	1/1	0.16	1.10	54,54,54,54	0
38	SR	0	9495	1/1	0.13	1.06	111,111,111,111	0
34	MG	0	8026	1/1	0.13	1.02	30,30,30,30	0
38	SR	0	9410	1/1	0.14	0.94	41,41,41,41	0
36	NA	0	9124	1/1	0.17	0.94	50,50,50,50	0
34	MG	0	8074	1/1	0.17	0.81	27,27,27,27	0
38	SR	0	9509	1/1	0.15	0.80	95,95,95,95	0
38	SR	0	9537	1/1	0.19	0.75	157,157,157,157	0
34	MG	0	8020	1/1	0.16	0.74	36,36,36,36	0
38	SR	R	9418	1/1	0.14	0.72	57,57,57,57	0
34	MG	0	8104	1/1	0.14	0.70	57,57,57,57	0
36	NA	0	9155	1/1	0.20	0.64	60,60,60,60	0
38	SR	0	9407	1/1	0.12	0.56	47,47,47,47	0
37	CL	A	9309	1/1	0.20	0.52	66,66,66,66	0
38	SR	0	9534	1/1	0.14	0.49	111,111,111,111	0
34	MG	0	8040	1/1	0.21	0.43	92,92,92,92	0
38	SR	F	9595	1/1	0.17	0.40	109,109,109,109	0
34	MG	0	8017	1/1	0.12	0.35	31,31,31,31	0
38	SR	0	9411	1/1	0.13	0.25	43,43,43,43	0
35	K	0	9002	1/1	0.18	0.13	88,88,88,88	0
34	MG	0	8102	1/1	0.11	0.11	68,68,68,68	0
38	SR	0	9451	1/1	0.12	0.11	60,60,60,60	0
38	SR	9	9588	1/1	0.13	0.10	143,143,143,143	0
38	SR	0	9406	1/1	0.12	0.00	35,35,35,35	0
34	MG	0	8079	1/1	0.12	-0.01	33,33,33,33	0
34	MG	0	8070	1/1	0.13	-0.05	24,24,24,24	0
34	MG	Y	8109	1/1	0.14	-0.10	45,45,45,45	0
34	MG	0	8060	1/1	0.12	-0.13	82,82,82,82	0
34	MG	0	8097	1/1	0.12	-0.18	57,57,57,57	0
38	SR	0	9475	1/1	0.11	-0.23	83,83,83,83	0
38	SR	H	9486	1/1	0.14	-0.24	125,125,125,125	0
36	NA	0	9126	1/1	0.12	-0.34	63,63,63,63	0
34	MG	0	8117	1/1	0.12	-0.34	46,46,46,46	0
34	MG	0	8042	1/1	0.11	-0.35	48,48,48,48	0
38	SR	0	9452	1/1	0.13	-0.38	106,106,106,106	0
34	MG	2	8076	1/1	0.11	-0.44	64,64,64,64	0
36	NA	C	9104	1/1	0.15	-0.45	33,33,33,33	0
37	CL	0	9311	1/1	0.14	-0.48	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	M	9147	1/1	0.14	-0.52	42,42,42,42	0
36	NA	O	9143	1/1	0.14	-0.56	40,40,40,40	0
36	NA	O	9139	1/1	0.12	-0.57	43,43,43,43	0
38	SR	O	9490	1/1	0.11	-0.64	116,116,116,116	0
36	NA	O	9130	1/1	0.12	-0.64	50,50,50,50	0
38	SR	O	9427	1/1	0.12	-0.66	56,56,56,56	0
36	NA	O	9140	1/1	0.15	-0.69	57,57,57,57	0
38	SR	O	9477	1/1	0.11	-0.70	86,86,86,86	0
34	MG	O	8116	1/1	0.10	-0.87	64,64,64,64	0
34	MG	O	8088	1/1	0.09	-0.89	28,28,28,28	0
38	SR	O	9424	1/1	0.14	-0.89	49,49,49,49	0
39	CD	Z	9203	1/1	0.14	-0.89	84,84,84,84	0
36	NA	J	9146	1/1	0.11	-0.92	55,55,55,55	0
38	SR	O	9504	1/1	0.12	-0.93	108,108,108,108	0
37	CL	M	9318	1/1	0.15	-0.93	41,41,41,41	0
36	NA	D	9151	1/1	0.22	-0.97	68,68,68,68	0
38	SR	A	9497	1/1	0.08	-1.01	96,96,96,96	0
38	SR	O	9455	1/1	0.08	-1.05	88,88,88,88	0
38	SR	A	9437	1/1	0.10	-1.11	70,70,70,70	0
38	SR	O	9545	1/1	0.04	-1.17	85,85,85,85	0
34	MG	A	8066	1/1	0.11	-1.17	57,57,57,57	0
34	MG	O	8083	1/1	0.11	-1.19	53,53,53,53	0
36	NA	O	9117	1/1	0.08	-1.32	51,51,51,51	0
36	NA	O	9166	1/1	0.08	-1.34	74,74,74,74	0
38	SR	O	9414	1/1	0.10	-1.35	57,57,57,57	0
34	MG	O	8015	1/1	0.10	-1.42	35,35,35,35	0
38	SR	O	9417	1/1	0.08	-1.43	63,63,63,63	0
34	MG	O	8031	1/1	0.10	-1.43	49,49,49,49	0
37	CL	O	9308	1/1	0.10	-1.44	67,67,67,67	0
37	CL	J	9321	1/1	0.07	-1.45	66,66,66,66	0
38	SR	O	9590	1/1	0.11	-1.49	131,131,131,131	0
37	CL	L	9310	1/1	0.13	-1.52	58,58,58,58	0
39	CD	U	9201	1/1	0.09	-1.53	53,53,53,53	0
34	MG	O	8028	1/1	0.12	-1.56	37,37,37,37	0
37	CL	O	9305	1/1	0.10	-1.56	61,61,61,61	0
34	MG	O	8041	1/1	0.10	-1.58	55,55,55,55	0
38	SR	O	9431	1/1	0.12	-1.62	65,65,65,65	0
34	MG	O	8002	1/1	0.10	-1.63	34,34,34,34	0
34	MG	O	8068	1/1	0.12	-1.63	48,48,48,48	0
38	SR	O	9421	1/1	0.10	-1.67	78,78,78,78	0
36	NA	O	9136	1/1	0.11	-1.68	34,34,34,34	0
38	SR	O	9413	1/1	0.10	-1.72	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9113	1/1	0.10	-1.74	60,60,60,60	0
37	CL	0	9312	1/1	0.08	-1.76	57,57,57,57	0
38	SR	0	9450	1/1	0.06	-1.78	72,72,72,72	0
36	NA	0	9127	1/1	0.10	-1.79	60,60,60,60	0
38	SR	0	9488	1/1	0.10	-1.79	86,86,86,86	0
36	NA	Q	9148	1/1	0.08	-1.79	49,49,49,49	0
34	MG	T	8073	1/1	0.09	-1.79	43,43,43,43	0
34	MG	0	8037	1/1	0.09	-1.92	46,46,46,46	0
36	NA	0	9138	1/1	0.06	-1.96	62,62,62,62	0
39	CD	3	9204	1/1	0.03	-1.96	64,64,64,64	0
34	MG	0	8004	1/1	0.09	-2.00	35,35,35,35	0
34	MG	0	8115	1/1	0.07	-2.11	59,59,59,59	0
36	NA	0	9134	1/1	0.07	-2.13	47,47,47,47	0
38	SR	9	9481	1/1	0.09	-2.18	89,89,89,89	0
38	SR	0	9461	1/1	0.06	-2.19	82,82,82,82	0
38	SR	0	9428	1/1	0.07	-2.21	55,55,55,55	0
37	CL	0	9314	1/1	0.07	-2.21	51,51,51,51	0
38	SR	0	9508	1/1	0.09	-2.22	97,97,97,97	0
34	MG	0	8003	1/1	0.13	-2.23	35,35,35,35	0
38	SR	0	9517	1/1	0.05	-2.25	110,110,110,110	0
38	SR	0	9412	1/1	0.12	-2.26	45,45,45,45	0
38	SR	0	9459	1/1	0.09	-2.28	103,103,103,103	0
36	NA	R	9137	1/1	0.06	-2.30	36,36,36,36	0
34	MG	0	8067	1/1	0.11	-2.38	40,40,40,40	0
38	SR	0	9468	1/1	0.05	-2.52	128,128,128,128	0
37	CL	J	9302	1/1	0.06	-2.52	53,53,53,53	0
38	SR	3	9439	1/1	0.05	-2.54	72,72,72,72	0
38	SR	0	9443	1/1	0.09	-2.56	63,63,63,63	0
38	SR	0	9456	1/1	0.09	-2.60	67,67,67,67	0
34	MG	0	8093	1/1	0.12	-2.60	49,49,49,49	0
38	SR	A	9436	1/1	0.06	-2.67	60,60,60,60	0
38	SR	0	9447	1/1	0.07	-2.71	73,73,73,73	0
34	MG	0	8032	1/1	0.10	-2.75	48,48,48,48	0
39	CD	O	9205	1/1	0.04	-2.79	132,132,132,132	0
38	SR	0	9474	1/1	0.07	-2.83	73,73,73,73	0
38	SR	0	9465	1/1	0.09	-2.84	107,107,107,107	0
34	MG	0	8036	1/1	0.10	-2.85	65,65,65,65	0
36	NA	0	9167	1/1	0.10	-2.86	65,65,65,65	0
37	CL	R	9306	1/1	0.08	-2.87	45,45,45,45	0
38	SR	1	9460	1/1	0.09	-2.90	52,52,52,52	0
34	MG	0	8113	1/1	0.13	-2.90	52,52,52,52	0
37	CL	N	9307	1/1	0.12	-2.93	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9108	1/1	0.07	-2.94	34,34,34,34	0
38	SR	0	9408	1/1	0.11	-2.95	36,36,36,36	0
37	CL	3	9304	1/1	0.06	-2.97	61,61,61,61	0
38	SR	0	9448	1/1	0.06	-2.98	63,63,63,63	0
36	NA	0	9163	1/1	0.14	-3.14	73,73,73,73	0
38	SR	0	9426	1/1	0.07	-3.19	71,71,71,71	0
38	SR	1	9419	1/1	0.07	-3.25	40,40,40,40	0
38	SR	0	9568	1/1	0.07	-3.33	80,80,80,80	0
38	SR	0	9430	1/1	0.08	-3.34	49,49,49,49	0
38	SR	0	9560	1/1	0.07	-3.34	101,101,101,101	0
38	SR	0	9467	1/1	0.09	-3.35	86,86,86,86	0
38	SR	0	9566	1/1	0.04	-3.36	80,80,80,80	0
38	SR	0	9449	1/1	0.08	-3.41	67,67,67,67	0
38	SR	0	9435	1/1	0.07	-3.50	76,76,76,76	0
38	SR	0	9445	1/1	0.07	-3.57	57,57,57,57	0
38	SR	0	9422	1/1	0.10	-3.65	58,58,58,58	0
39	CD	1	9202	1/1	0.04	-3.66	54,54,54,54	0
38	SR	0	9446	1/1	0.06	-3.69	88,88,88,88	0
38	SR	L	9409	1/1	0.06	-3.70	37,37,37,37	0
34	MG	0	8096	1/1	0.04	-3.83	41,41,41,41	0
37	CL	0	9303	1/1	0.10	-3.91	53,53,53,53	0
38	SR	0	9466	1/1	0.06	-4.00	96,96,96,96	0
38	SR	0	9585	1/1	0.07	-4.05	94,94,94,94	0
34	MG	0	8112	1/1	0.06	-4.19	46,46,46,46	0
38	SR	0	9532	1/1	0.04	-4.20	120,120,120,120	0
38	SR	0	9429	1/1	0.10	-4.26	72,72,72,72	0
38	SR	0	9444	1/1	0.05	-4.42	55,55,55,55	0
34	MG	0	8046	1/1	0.05	-4.45	39,39,39,39	0
37	CL	0	9315	1/1	0.09	-4.58	52,52,52,52	0
36	NA	0	9101	1/1	0.11	-4.62	46,46,46,46	0
38	SR	0	9581	1/1	0.08	-4.63	130,130,130,130	0
34	MG	0	8030	1/1	0.07	-4.65	37,37,37,37	0
34	MG	0	8106	1/1	0.08	-4.66	51,51,51,51	0
38	SR	0	9457	1/1	0.07	-4.71	51,51,51,51	0
38	SR	0	9489	1/1	0.07	-4.76	94,94,94,94	0
38	SR	0	9530	1/1	0.10	-4.90	72,72,72,72	0
37	CL	Y	9320	1/1	0.06	-5.00	47,47,47,47	0
36	NA	0	9105	1/1	0.08	-5.14	44,44,44,44	0
38	SR	0	9462	1/1	0.10	-5.17	74,74,74,74	0
37	CL	0	9313	1/1	0.08	-5.26	59,59,59,59	0
34	MG	0	8009	1/1	0.08	-5.26	21,21,21,21	0
38	SR	0	9478	1/1	0.06	-5.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	SR	0	9473	1/1	0.02	-5.40	82,82,82,82	0
38	SR	0	9469	1/1	0.04	-5.49	85,85,85,85	0
38	SR	0	9442	1/1	0.09	-5.53	66,66,66,66	0
38	SR	0	9416	1/1	0.06	-5.64	43,43,43,43	0
34	MG	0	8044	1/1	0.05	-5.71	35,35,35,35	0
38	SR	9	9503	1/1	0.06	-5.87	122,122,122,122	0
38	SR	0	9423	1/1	0.04	-5.97	64,64,64,64	0
38	SR	0	9629	1/1	0.07	-6.12	75,75,75,75	0
34	MG	0	8098	1/1	0.06	-6.26	45,45,45,45	0
38	SR	0	9505	1/1	0.06	-6.29	106,106,106,106	0
38	SR	0	9601	1/1	0.06	-6.30	119,119,119,119	0
34	MG	0	8110	1/1	0.09	-6.35	45,45,45,45	0
34	MG	0	8019	1/1	0.05	-6.56	51,51,51,51	0
38	SR	0	9483	1/1	0.06	-6.60	77,77,77,77	0
38	SR	0	9415	1/1	0.08	-6.76	56,56,56,56	0
38	SR	0	9453	1/1	0.05	-6.98	72,72,72,72	0
34	MG	0	8043	1/1	0.06	-7.21	52,52,52,52	0
36	NA	0	9123	1/1	0.07	-7.50	52,52,52,52	0
38	SR	0	9506	1/1	0.04	-7.73	68,68,68,68	0
34	MG	0	8063	1/1	0.09	-7.85	65,65,65,65	0
38	SR	0	9438	1/1	0.08	-7.89	70,70,70,70	0
38	SR	B	9458	1/1	0.03	-7.98	82,82,82,82	0
38	SR	0	9464	1/1	0.04	-7.99	81,81,81,81	0
34	MG	0	8005	1/1	0.06	-8.04	29,29,29,29	0
34	MG	0	8075	1/1	0.07	-8.76	47,47,47,47	0
38	SR	0	9441	1/1	0.06	-8.99	68,68,68,68	0
38	SR	0	9440	1/1	0.04	-10.75	72,72,72,72	0
38	SR	0	9454	1/1	0.07	-11.62	82,82,82,82	0
38	SR	0	9498	1/1	0.04	-11.94	63,63,63,63	0
37	CL	0	9317	1/1	0.07	-12.26	52,52,52,52	0
38	SR	0	9570	1/1	0.06	-14.00	111,111,111,111	0
38	SR	0	9522	1/1	0.03	-16.14	114,114,114,114	0
38	SR	0	9480	1/1	0.04	-24.60	93,93,93,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.