



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 08:08 PM GMT

PDB ID : 1VQK
Title : The structure of CCDA-PHE-CAP-BIO bound to the a site of the ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.30 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>

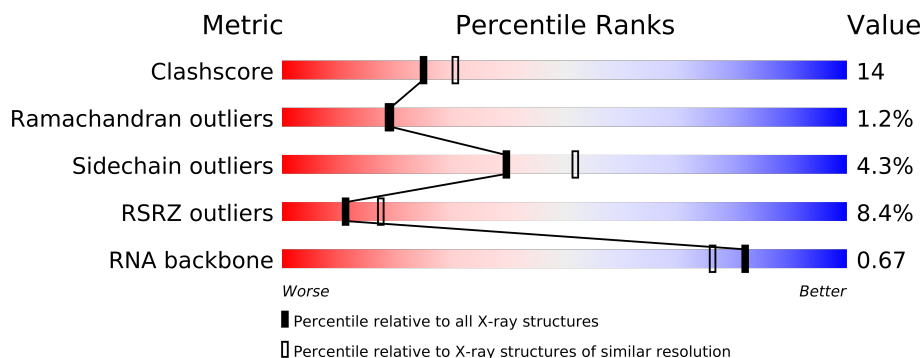
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)
RNA backbone	1838	1081 (3.00-1.60)

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	5	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	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
33	MG	0	8001	-	X
33	MG	0	8008	-	X
33	MG	0	8012	-	X
33	MG	0	8013	-	X
33	MG	0	8017	-	X
33	MG	0	8020	-	X
33	MG	0	8021	-	X
33	MG	0	8022	-	X
33	MG	0	8024	-	X
33	MG	0	8025	-	X
33	MG	0	8026	-	X
33	MG	0	8029	-	X
33	MG	0	8038	-	X
33	MG	0	8040	-	X
33	MG	0	8047	-	X
33	MG	0	8050	-	X
33	MG	0	8051	-	X
33	MG	0	8052	-	X
33	MG	0	8057	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8058	-	X
33	MG	0	8059	-	X
33	MG	0	8061	-	X
33	MG	0	8065	-	X
33	MG	0	8070	-	X
33	MG	0	8072	-	X
33	MG	0	8076	-	X
33	MG	0	8080	-	X
33	MG	0	8082	-	X
33	MG	0	8084	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
33	MG	0	8092	-	X
33	MG	0	8094	-	X
33	MG	0	8099	-	X
33	MG	0	8102	-	X
33	MG	0	8103	-	X
33	MG	0	8107	-	X
33	MG	0	8108	-	X
33	MG	0	8114	-	X
33	MG	9	8095	-	X
33	MG	B	8055	-	X
33	MG	K	8069	-	X
34	K	0	9001	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X
35	NA	0	9110	-	X
35	NA	0	9111	-	X
35	NA	0	9115	-	X
35	NA	0	9116	-	X
35	NA	0	9118	-	X
35	NA	0	9120	-	X
35	NA	0	9122	-	X
35	NA	0	9125	-	X
35	NA	0	9127	-	X
35	NA	0	9129	-	X
35	NA	0	9132	-	X
35	NA	0	9135	-	X
35	NA	0	9140	-	X
35	NA	0	9149	-	X
35	NA	0	9150	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9152	-	X
35	NA	0	9154	-	X
35	NA	0	9156	-	X
35	NA	0	9157	-	X
35	NA	0	9160	-	X
35	NA	0	9161	-	X
35	NA	0	9162	-	X
35	NA	0	9163	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9168	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	X
35	NA	0	9173	-	X
35	NA	0	9174	-	X
35	NA	0	9175	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	3	9169	-	X
35	NA	9	9183	-	X
35	NA	R	9186	-	X
36	CL	0	9316	-	X
36	CL	0	9322	-	X
37	SR	0	9405	-	X
37	SR	0	9406	-	X
37	SR	0	9408	-	X
37	SR	0	9432	-	X
37	SR	0	9434	-	X
37	SR	0	9452	-	X
37	SR	0	9477	-	X
37	SR	0	9482	-	X
37	SR	0	9484	-	X
37	SR	0	9500	-	X
37	SR	0	9501	-	X
37	SR	0	9515	-	X
37	SR	0	9539	-	X
37	SR	0	9547	-	X
37	SR	0	9601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	O	9626	-	X
37	SR	B	9521	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99036 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*(DA)*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			73	40	12	19	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	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 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	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 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	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 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	3	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	3	Total 3	Na 3	0	0
35	9	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	J	3	Total 3	Cl 3	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5769	Total 5769	O 5769	0	0
39	9	140	Total 140	O 140	0	0
39	A	121	Total 121	O 121	0	0

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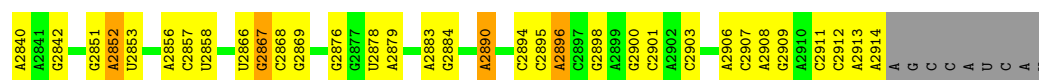
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	B	144	Total 144	O 144	0	0
39	C	177	Total 177	O 177	0	0
39	D	48	Total 48	O 48	0	0
39	E	44	Total 44	O 44	0	0
39	F	27	Total 27	O 27	0	0
39	G	17	Total 17	O 17	0	0
39	H	69	Total 69	O 69	0	0
39	J	52	Total 52	O 52	0	0
39	K	57	Total 57	O 57	0	0
39	L	81	Total 81	O 81	0	0
39	M	130	Total 130	O 130	0	0
39	N	61	Total 61	O 61	0	0
39	O	40	Total 40	O 40	0	0
39	P	64	Total 64	O 64	0	0
39	Q	49	Total 49	O 49	0	0
39	R	82	Total 82	O 82	0	0
39	S	32	Total 32	O 32	0	0
39	T	37	Total 37	O 37	0	0
39	U	29	Total 29	O 29	0	0
39	V	14	Total 14	O 14	0	0
39	W	69	Total 69	O 69	0	0

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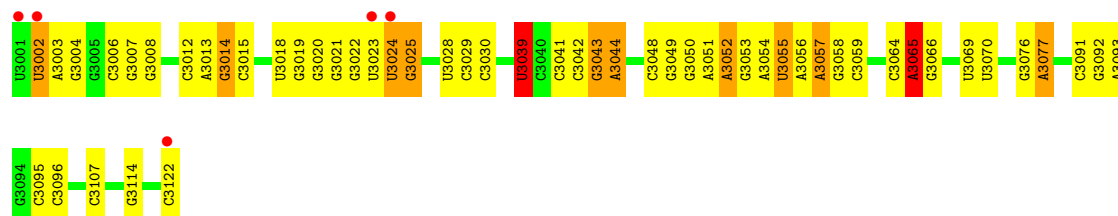
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	24	Total 24	O 24	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	31	Total 31	O 31	0	0
39	1	50	Total 50	O 50	0	0
39	2	40	Total 40	O 40	0	0
39	3	67	Total 67	O 67	0	0
39	I	7	Total 7	O 7	0	0

U2749	A2511	G2412	G2272	G	G2134	U1996	U1879	U1766	U1654	C1477	G1299	G1190
G2750	A2521	A2413	A2291	G	A2135	U2003	C1882	A1767	G1655	U1478	G1311	A1191
G2754	G2524	A2414	A2302	C	A	U2004	G1902	C1768	A1656	C1495	G1314	A1192
U2755	G2525	G2415	C2309	C	G	C2006	U1903	C1769	A1659	G1496	U1314	A1193
U2761	C2526	G2417	C	U	G	A2007	A1919	A1778	G1660	A1501	A1328	G1194
C2762	U2531	G2418	C	G	G	U2008	C1920	A1779	C1666	A1502	A1331	G1195
U2765	A2532	G2419	C	G	G	A2011	U1921	C1786	U1667	A1503	A1332	G1196
C2765	C2533	G2421	A	U	U	G2012	A1922	A1787	U1668	A1504	U1333	G1197
A2768	G2534	G2422	G	G	G	G2013	G1926	U1788	U1668	U1505	C1334	A1200
C2769	U2535	G2426	U	C	C	G2014	G1927	G1789	G1681	U1506	C1335	C1201
G2770	C2536	C2427	C	C	C	A2015	A1927	G1789	A1682	G1523	G1360	G1202
U2771	G2537	U2435	A	G	G	U2016	G1928	G1794	G1683	U1524	G1360	G1203
C2779	A2538	U2435	C	A	A	U2017	G1929	G1795	G1684	U1525	G1360	C1204
G2780	U2541	C2443	A	U	U	U2032	U1937	A1796	G1685	A1526	A1342	U1205
U2781	U2545	G2452	U	G	G	G2033	U1938	A1797	C1686	A1527	C1343	U1206
G2782	C2548	G2453	G	U	U	U2034	U1939	C1798	C1687	A1528	U1360	A1207
A2784	U2552	U2457	A	G	G	C2035	G1940	G1799	C1692	G1529	U1360	C1208
C2785	A2553	G2462	A	A	A	U2042	A1941	G1809	C1700	G1552	A1352	C1209
G2786	U2553	G2462	U	C	C	G2043	C1942	G1818	A1701	G1555	C1353	G1210
U2791	U2563	A2465	C	U	U	U2044	G1946	G1819	U1702	G1555	G1212	C1211
A2792	G2564	G2466	G	A	A	G2053	G1947	G1820	A1710	A1559	G1216	G1217
G2794	C2565	G2467	A	G	G	A2054	G1948	A1821	U	U1561	U1218	U1219
C2795	G2679	A2467	C	U	U	C2061	G1949	A1822	C1714	C1562	A1372	G1226
U2796	A2680	A2468	C	G	G	U2062	G1950	A1829	C1715	G1563	G1377	G1229
A2800	A2681	C2472	G	A	A	U2063	G1951	G1834	A1716	C1564	C1378	A1230
U2807	C2682	C2472	U	G	G	U2064	U	U1835	A1717	A1573	C1384	A1231
U2808	A2694	C2476	C	A	A	U2067	A	U1836	G1718	C1574	A1406	A1232
G2809	U2586	G2480	G	G	G	A2067	C	G1837	U1722	G1592	A1407	A1233
C2810	C2588	G2481	U	A	C	G2068	U	U1838	G1723	C1593	U1234	U1234
A2811	U2589	G2482	G	A	A	G2072	A	U1839	U1724	C1594	G1408	G1235
A2812	U2590	A2483	A	C	C	G2073	U	A1840	C1725	C1594	U1409	U1237
G2813	C2701	C2487	U	U	U	A2074	G	A1845	G1730	G1595	U1419	C1238
A2814	G2592	C2487	C	C	C	A2081	C	U1846	C1731	U1596	U1419	C1239
G2815	U2599	A2490	C	A	A	A2089	C	A1847	A1732	A1598	U1422	A1242
A2816	A2600	G2491	A	C	C	G2090	U1964	G1848	A1736	A1603	C1423	A1243
G2817	G2602	C2493	G	G	A	G2091	C1965	G1849	G1604	G1604	C1426	G1243
C2819	G2715	U2499	C	G	G	U2096	U1966	C1853	G1739	G1605	U1435	U1244
A2820	C2717	U2499	C	U	U	A2096	U1967	C1856	U1741	A1615	G1430	A1245
G2821	C2718	C2500	C	A	A	A2096	G1971	C1856	G1744	U1625	A1435	A1246
C2824	A2719	G2501	C	C	C	A2100	U1972	G1861	G1745	A1626	U1461	A1252
C2825	G2611	C2502	C	C	C	A2101	A1973	G1862	U1748	G1627	C1461	C1253
G2826	G2613	G2503	G	G	G	A2102	U1979	G1867	G1752	A1630	C1462	C1268
A2827	G2618	A2504	C	C	C	A2103	U1980	G1868	G1752	A1630	A1463	U1278
G2828	G2618	G2505	C	C	C	G2110	A1981	G1873	G1752	C1633	U1279	U1279
C2831	C2626	G2507	U	U	U	A2112	U1992	G1877	A1755	G1834	A1470	C1289
U2837	G2627	A2401	A	A	A	G2113	C1993	G1877	G1756	A1641	C1474	U1298
	G2632	C2510	C	C	C	U2133	G1995	G1878	A1759	A1642		



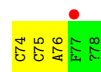
• Molecule 2: 5S ribosomal RNA

Chain 9:



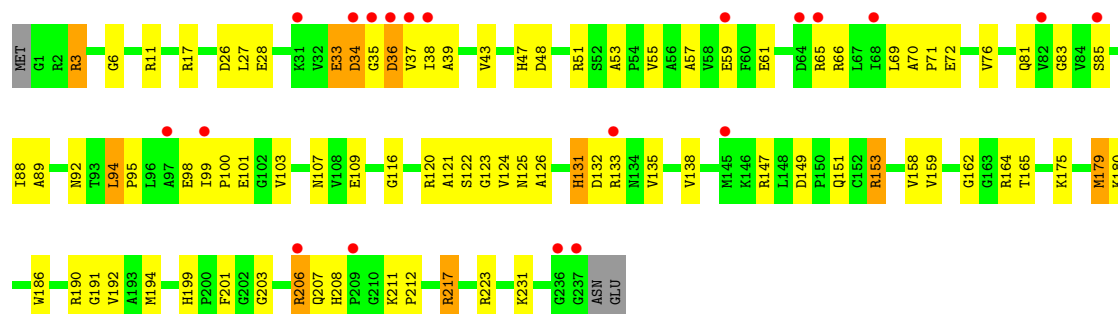
• Molecule 3: 5'-R(*CP*CP*(DA)*(PHE)*(ACA))-3'

Chain 4:



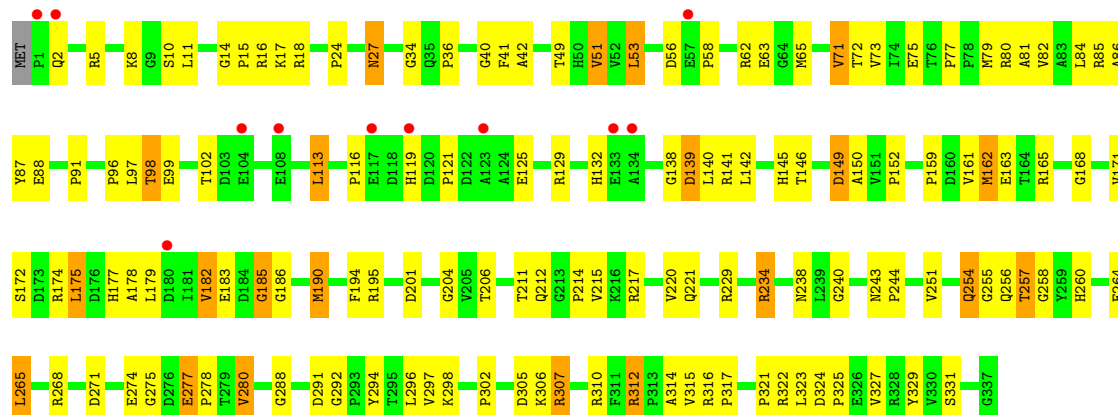
• Molecule 4: 50S ribosomal protein L2P

Chain A:



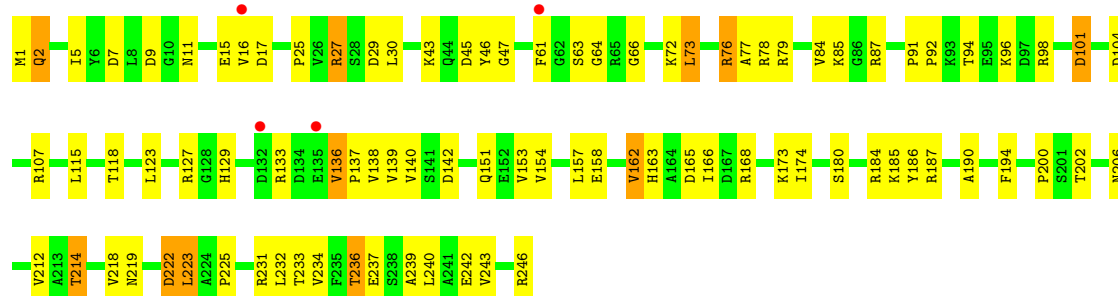
• Molecule 5: 50S ribosomal protein L3P

Chain B:



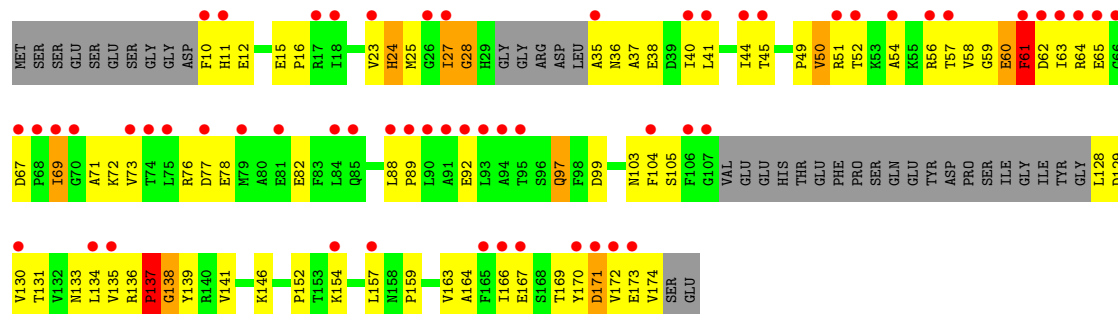
• Molecule 6: 50S ribosomal protein L4E

Chain C:



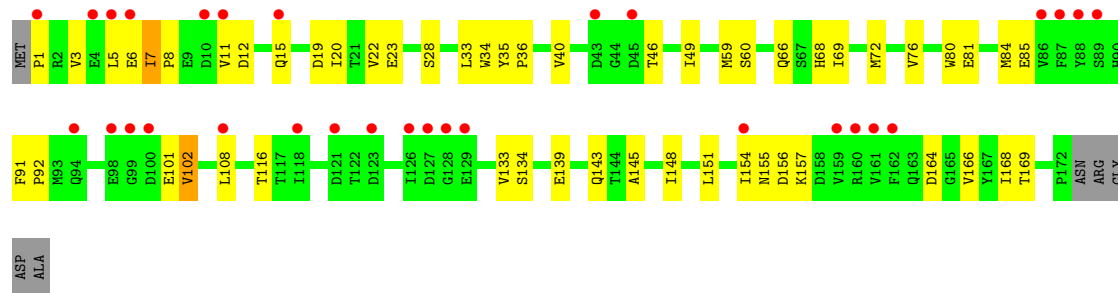
• Molecule 7: 50S ribosomal protein L5P

Chain D:



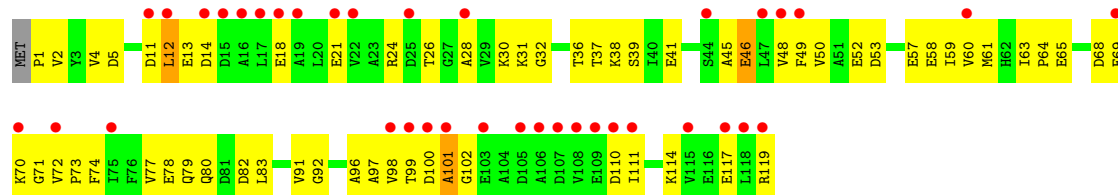
• Molecule 8: 50S ribosomal protein L6P

Chain E:



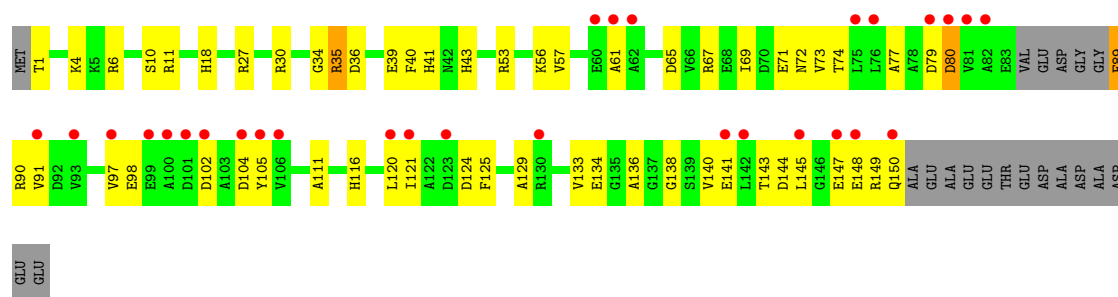
• Molecule 9: 50S ribosomal protein L7AE

Chain F:



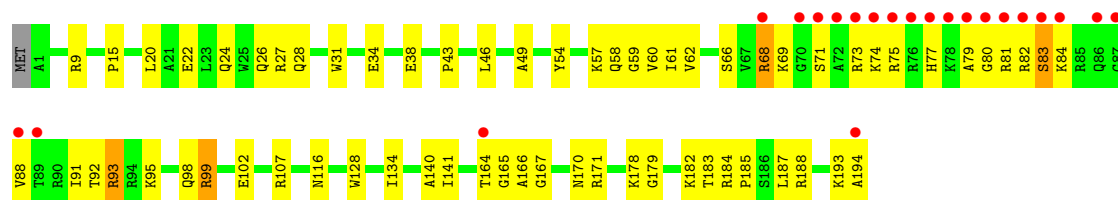
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



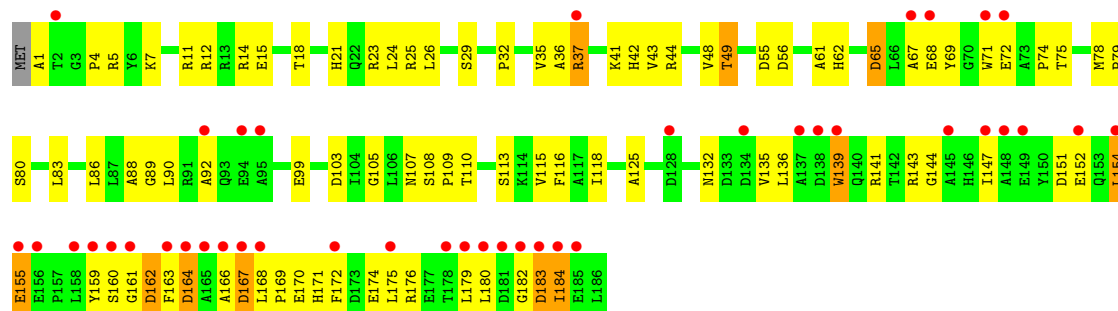
- Molecule 15: 50S Ribosomal Protein L15E

Chain M:



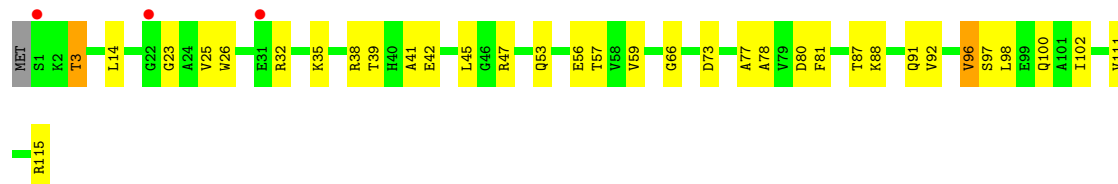
- Molecule 16: 50S ribosomal protein L18P

Chain N:



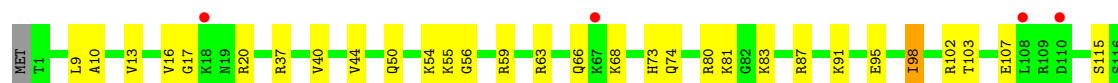
- Molecule 17: 50S ribosomal protein L18e

Chain O:



- Molecule 18: 50S ribosomal protein L19E

Chain P:





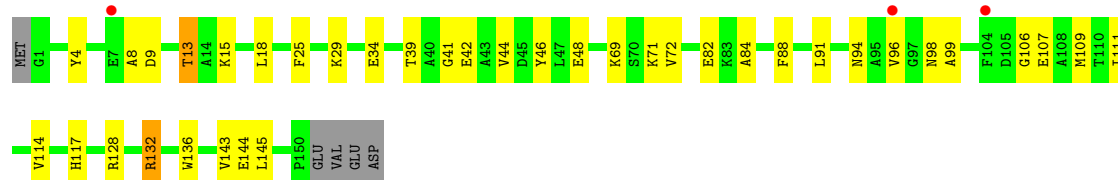
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



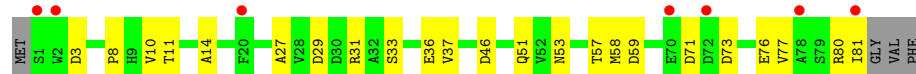
- Molecule 20: 50S ribosomal protein L22P

Chain R:



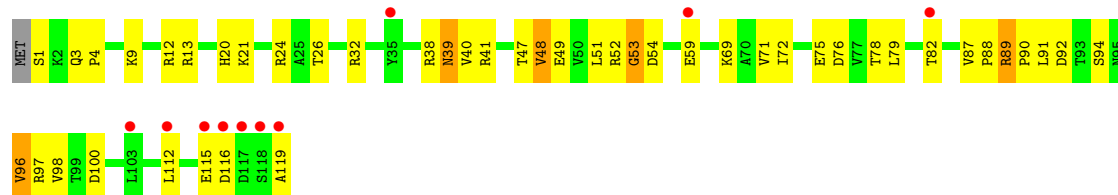
- Molecule 21: 50S ribosomal protein L23P

Chain S:



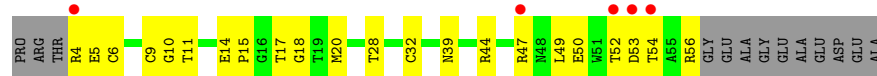
- Molecule 22: 50S ribosomal protein L24P

Chain T:



- Molecule 23: 50S ribosomal protein L24E

Chain U:



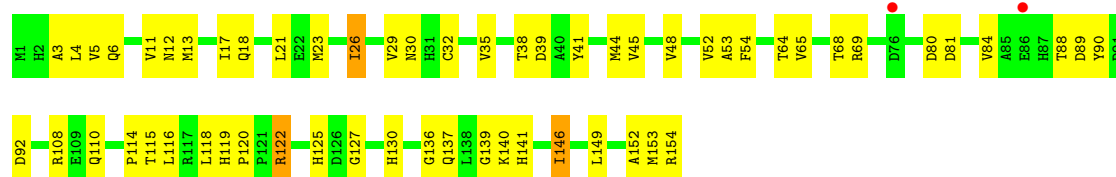
- Molecule 24: 50S ribosomal protein L29P

Chain V:



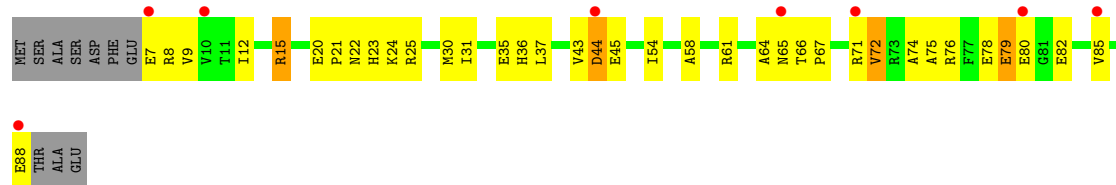
- Molecule 25: 50S ribosomal protein L30P

Chain W:



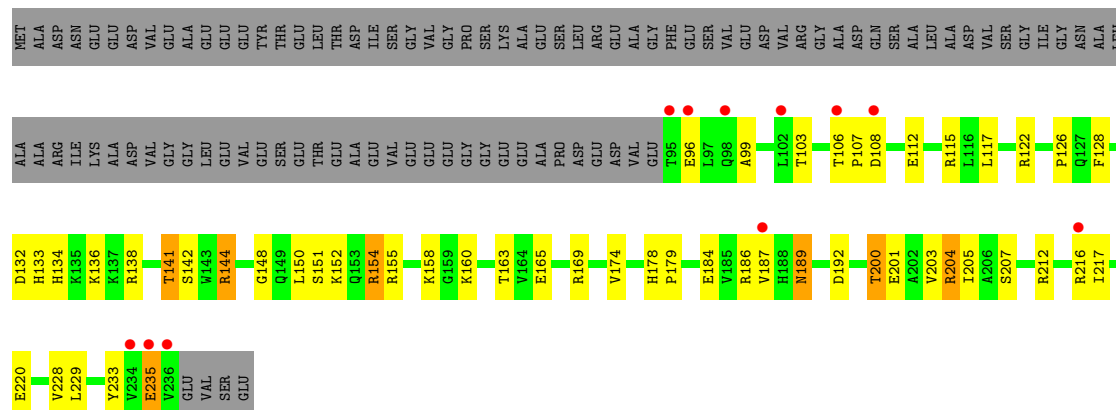
- Molecule 26: 50S ribosomal protein L31e

Chain X:



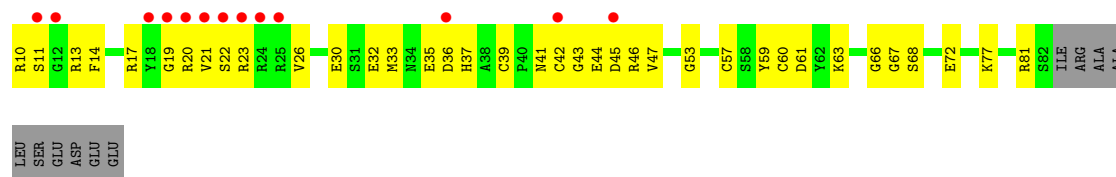
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



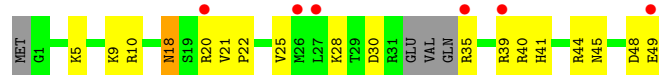
- Molecule 29: 50S ribosomal protein L37e

Chain 1:



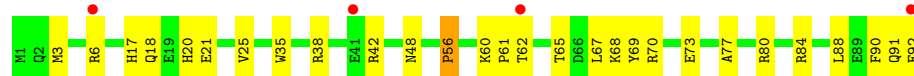
- Molecule 30: 50S ribosomal protein L39e

Chain 2: 



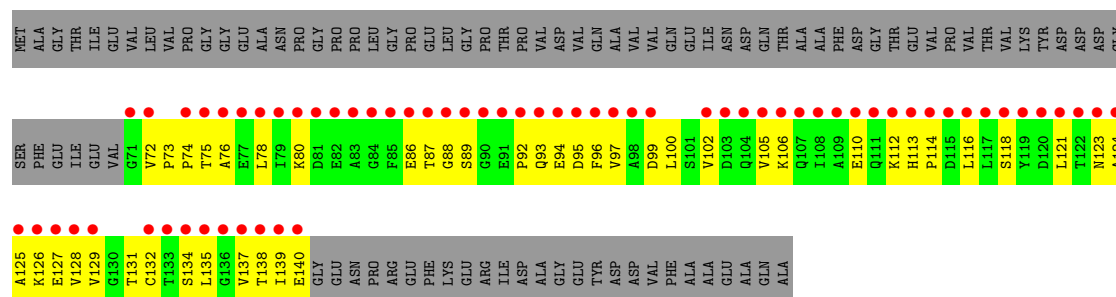
- Molecule 31: 50S ribosomal protein L44E

Chain 3: 



- Molecule 32: 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	211.87Å 298.57Å 575.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 89.6 (49.73-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.250 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 797435 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99036	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: MG, OMG, CL, SR, NA, K, ACA, CD, OMU, UR3, 1MA, 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	0.37	0/65959	0.70	26/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.52	0/75	0.73	0/110
4	A	0.34	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.66	0/3652
6	C	0.38	0/1884	0.64	1/2551 (0.0%)
7	D	0.29	0/1111	0.54	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.31	0/901	0.54	0/1224
10	G	0.27	0/241	0.47	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.33	0/874	0.59	1/1181 (0.1%)
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.35	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.31	0/958	0.63	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.27	0/502	0.53	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.34	0/589	0.61	0/787
29	1	0.43	0/438	0.66	0/578
30	2	0.35	0/401	0.60	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98767	0.67	30/147687 (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	1	39
2	9	0	2
All	All	1	41

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.69	130.83	109.50
2	9	3039	U	N1-C1'-C2'	7.45	123.68	114.00
1	0	1942	A	C5'-C4'-C3'	7.27	127.63	116.00
1	0	1819	G	C5'-C4'-C3'	6.86	126.98	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	24	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	469	G	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	29813	722	0
2	9	2600	0	1326	50	0
3	4	73	0	44	2	0
4	A	1753	0	1766	101	0
5	B	2625	0	2532	145	0
6	C	1859	0	1816	106	0
7	D	1094	0	1085	79	0
8	E	1357	0	1266	45	0
9	F	890	0	843	57	0
10	G	240	0	231	11	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1560	0	1568	63	0
16	N	1445	0	1401	97	0
17	O	865	0	873	40	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	18	0
20	R	1149	0	1122	37	0
21	S	641	0	605	16	0
22	T	950	0	923	47	0
23	U	410	0	364	26	0
24	V	499	0	511	38	0
25	W	1196	0	1137	82	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	28	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	26	0
32	I	519	0	500	51	0
33	0	87	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	64	0	0	0	0
35	3	1	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	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	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5769	0	0	106	0
39	1	50	0	0	2	0
39	2	40	0	0	3	0
39	3	67	0	0	4	0
39	9	140	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	A	121	0	0	11	0
39	B	144	0	0	18	0
39	C	177	0	0	18	0
39	D	48	0	0	10	0
39	E	44	0	0	1	0
39	F	27	0	0	4	0
39	G	17	0	0	1	0
39	H	69	0	0	7	0
39	I	7	0	0	1	0
39	J	52	0	0	4	0
39	K	57	0	0	6	0
39	L	81	0	0	14	0
39	M	130	0	0	3	0
39	N	61	0	0	9	0
39	O	40	0	0	5	0
39	P	64	0	0	2	0
39	Q	49	0	0	5	0
39	R	82	0	0	3	0
39	S	32	0	0	1	0
39	T	37	0	0	3	0
39	U	29	0	0	3	0
39	V	14	0	0	2	0
39	W	69	0	0	5	0
39	X	24	0	0	6	0
39	Y	96	0	0	9	0
39	Z	31	0	0	2	0
All	All	99036	0	59943	2083	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 14.

The worst 5 of 2083 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.29	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.07
1:O:656:G:H5'	17:O:3:THR:HG22	1.38	1.05
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	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	
4	A	235/240 (98%)	209 (89%)	23 (10%)	3 (1%)	18	17
5	B	335/338 (99%)	314 (94%)	17 (5%)	4 (1%)	19	19
6	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
7	D	134/177 (76%)	105 (78%)	17 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	100 (86%)	15 (13%)	2 (2%)	14	11
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	18	17
12	J	140/145 (97%)	131 (94%)	6 (4%)	3 (2%)	11	8
13	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	30	34
15	M	192/195 (98%)	182 (95%)	8 (4%)	2 (1%)	22	23
16	N	184/187 (98%)	163 (89%)	12 (6%)	9 (5%)	3	1
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	18	17
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	25	26
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	14	12
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	4	2
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	1 (1%)	1 (1%)	21	21
32	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	15	13
All	All	3705/4431 (84%)	3430 (93%)	229 (6%)	46 (1%)	19	19

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	37	VAL
5	B	139	ASP
7	D	137	PRO
9	F	101	ALA

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	
4	A	179/182 (98%)	169 (94%)	10 (6%)	30	38
5	B	282/283 (100%)	261 (93%)	21 (7%)	20	24
6	C	193/193 (100%)	178 (92%)	15 (8%)	18	22
7	D	117/148 (79%)	112 (96%)	5 (4%)	40	52
8	E	152/156 (97%)	145 (95%)	7 (5%)	37	48
9	F	93/94 (99%)	91 (98%)	2 (2%)	64	81
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	38	50
12	J	118/121 (98%)	109 (92%)	9 (8%)	19	22
13	K	106/106 (100%)	103 (97%)	3 (3%)	56	73
14	L	113/127 (89%)	109 (96%)	4 (4%)	48	63
15	M	158/159 (99%)	153 (97%)	5 (3%)	51	67
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	64
17	O	93/94 (99%)	91 (98%)	2 (2%)	64	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	113/117 (97%)	112 (99%)	1 (1%)	87	95
19	Q	79/80 (99%)	75 (95%)	4 (5%)	33	43
20	R	117/122 (96%)	114 (97%)	3 (3%)	59	76
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	73
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	59
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	84
25	W	130/130 (100%)	126 (97%)	4 (3%)	52	68
26	X	66/74 (89%)	60 (91%)	6 (9%)	14	15
27	Y	120/196 (61%)	110 (92%)	10 (8%)	16	19
28	Z	60/68 (88%)	59 (98%)	1 (2%)	73	87
29	1	46/47 (98%)	45 (98%)	1 (2%)	64	81
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	79
31	3	79/79 (100%)	78 (99%)	1 (1%)	80	91
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	40	52

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	1	LYS
12	J	131	THR
27	Y	154	ARG
11	H	18	GLU
12	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	170	ASN
18	P	89	ASN
30	2	41	HIS
16	N	93	GLN
17	O	100	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	238 (8%)	33 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	254 (8%)	35 (1%)

5 of 254 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 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1692	C
1	0	2852	A
1	0	1563	G
1	0	1684	A

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	$\# Z > 2$
1	OMU	0	2587	1	20,22,23	0.74	1 (5%)	24,31,34	0.78	0
1	OMG	0	2588	1,3	24,26,27	0.80	0	32,38,41	5.21	3 (9%)
1	UR3	0	2619	1	20,22,23	0.82	0	23,32,35	0.78	0
1	PSU	0	2621	1	19,21,22	1.19	2 (10%)	23,30,33	1.07	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	0	628	1,35	23,25,26	0.80	0	32,37,40	0.96	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	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	1,35	-	1/8/25/26	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.23	1.43	1.37
1	0	2621	PSU	C6-N1	2.52	1.34	1.32
1	0	2587	OMU	P-OP1	2.31	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	-28.90	130.25	134.14
1	0	2588	OMG	C6-N1-C2	3.18	125.08	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
1	0	2588	OMG	C2-N3-C4	-2.22	111.98	115.09

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 311 ligands modelled in this entry, 311 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%)	-0.06	94 (3%) 43 53	22, 45, 89, 149	0
2	9	122/122 (100%)	0.21	5 (4%) 35 46	38, 63, 87, 149	0
3	4	5/5 (100%)	1.39	1 (20%) 2 3	61, 64, 72, 74	0
4	A	237/240 (98%)	0.50	20 (8%) 11 17	28, 50, 82, 104	0
5	B	337/338 (99%)	0.28	11 (3%) 44 54	28, 50, 75, 86	0
6	C	246/246 (100%)	0.10	4 (1%) 68 77	25, 46, 68, 80	0
7	D	140/177 (79%)	2.05	58 (41%) 1 1	58, 88, 120, 130	0
8	E	172/178 (96%)	0.96	30 (17%) 2 4	40, 62, 80, 86	0
9	F	119/120 (99%)	1.40	37 (31%) 1 1	44, 71, 100, 110	0
10	G	29/348 (8%)	2.51	18 (62%) 0 0	71, 89, 99, 100	0
11	H	160/171 (93%)	0.82	24 (15%) 3 5	43, 61, 93, 101	0
12	J	142/145 (97%)	0.17	4 (2%) 50 60	36, 47, 67, 89	0
13	K	132/132 (100%)	-0.08	1 (0%) 83 90	33, 46, 67, 72	0
14	L	145/165 (87%)	0.91	29 (20%) 2 3	27, 64, 110, 120	0
15	M	194/195 (99%)	0.58	22 (11%) 6 9	31, 44, 77, 87	0
16	N	186/187 (99%)	1.15	42 (22%) 1 2	43, 63, 108, 113	0
17	O	115/116 (99%)	0.19	3 (2%) 53 63	39, 53, 67, 75	0
18	P	143/149 (95%)	0.26	5 (3%) 42 52	38, 51, 65, 76	0
19	Q	95/96 (98%)	0.22	6 (6%) 19 28	38, 47, 61, 76	0
20	R	150/155 (96%)	0.02	3 (2%) 62 72	29, 43, 61, 71	0
21	S	81/85 (95%)	0.45	7 (8%) 11 17	42, 58, 80, 95	0
22	T	119/120 (99%)	0.68	10 (8%) 11 17	40, 54, 81, 110	0
23	U	53/66 (80%)	0.32	5 (9%) 9 14	40, 50, 68, 79	0
24	V	65/71 (91%)	2.01	20 (30%) 1 1	52, 76, 110, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.14	2 (1%) 74 82	37, 49, 69, 78	0
26	X	82/92 (89%)	0.73	8 (9%) 8 13	40, 53, 82, 101	0
27	Y	142/241 (58%)	0.26	11 (7%) 13 20	29, 42, 63, 85	0
28	Z	73/83 (87%)	0.91	13 (17%) 2 3	48, 70, 85, 92	0
29	1	56/57 (98%)	-0.36	0 100 100	26, 32, 39, 49	0
30	2	46/50 (92%)	0.63	6 (13%) 4 7	33, 51, 67, 80	0
31	3	92/92 (100%)	0.38	4 (4%) 34 44	33, 55, 70, 83	0
32	I	70/162 (43%)	5.95	65 (92%) 0 0	111, 123, 141, 143	0
All	All	6656/7480 (88%)	0.36	568 (8%) 11 17	22, 50, 95, 149	0

The worst 5 of 568 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.8
24	V	1	THR	15.1
24	V	39	ALA	14.7
24	V	40	PRO	14.6
7	D	63	ILE	13.9

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	OMU	0	2587	21/22	0.11	-0.02	35,37,38,39	0
1	1MA	0	628	23/24	0.12	-0.64	31,33,36,39	0
1	UR3	0	2619	21/22	0.14	-0.66	42,46,49,51	0
1	PSU	0	2621	20/21	0.11	-1.01	33,36,44,45	0
1	OMG	0	2588	24/25	0.11	-1.24	32,34,38,40	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
37	SR	0	9601	1/1	1.05	373.00	200,200,200,200	0
37	SR	0	9501	1/1	0.31	77.00	200,200,200,200	0
33	MG	0	8047	1/1	0.47	74.60	94,94,94,94	0
33	MG	0	8092	1/1	1.40	68.87	83,83,83,83	0
35	NA	0	9179	1/1	0.99	66.42	84,84,84,84	0
37	SR	0	9500	1/1	1.60	64.81	200,200,200,200	0
33	MG	0	8085	1/1	0.39	63.89	102,102,102,102	0
33	MG	0	8094	1/1	0.34	62.81	82,82,82,82	0
35	NA	0	9125	1/1	0.90	55.04	106,106,106,106	0
37	SR	0	9539	1/1	0.46	54.19	167,167,167,167	0
35	NA	0	9164	1/1	0.49	53.98	67,67,67,67	0
33	MG	0	8059	1/1	0.32	52.14	60,60,60,60	0
35	NA	0	9106	1/1	0.28	47.88	37,37,37,37	0
35	NA	0	9111	1/1	0.20	42.21	57,57,57,57	0
35	NA	0	9129	1/1	0.39	41.76	88,88,88,88	0
35	NA	0	9184	1/1	0.46	40.47	86,86,86,86	0
33	MG	0	8025	1/1	0.31	35.75	23,23,23,23	0
35	NA	0	9161	1/1	0.41	32.88	57,57,57,57	0
33	MG	0	8026	1/1	0.16	32.83	26,26,26,26	0
35	NA	0	9122	1/1	0.54	32.34	98,98,98,98	0
35	NA	0	9152	1/1	0.32	26.93	67,67,67,67	0
33	MG	0	8024	1/1	1.07	25.31	90,90,90,90	0
33	MG	0	8082	1/1	0.39	24.74	103,103,103,103	0
37	SR	B	9521	1/1	0.73	23.37	200,200,200,200	0
33	MG	0	8084	1/1	0.42	22.58	109,109,109,109	0
35	NA	0	9107	1/1	0.32	21.71	58,58,58,58	0
35	NA	0	9185	1/1	0.47	21.69	54,54,54,54	0
35	NA	0	9168	1/1	0.23	19.84	72,72,72,72	0
35	NA	0	9162	1/1	0.32	19.80	51,51,51,51	0
35	NA	0	9150	1/1	0.24	18.27	54,54,54,54	0
37	SR	0	9547	1/1	0.41	17.97	200,200,200,200	0
35	NA	0	9116	1/1	0.31	17.46	45,45,45,45	0
33	MG	0	8108	1/1	0.24	17.45	115,115,115,115	0
33	MG	0	8072	1/1	0.20	17.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9154	1/1	0.25	16.87	51,51,51,51	0
35	NA	0	9115	1/1	0.26	15.45	43,43,43,43	0
33	MG	0	8052	1/1	0.32	15.30	72,72,72,72	0
35	NA	0	9177	1/1	0.34	14.33	70,70,70,70	0
35	NA	9	9183	1/1	0.30	14.05	72,72,72,72	0
37	SR	0	9484	1/1	0.15	14.00	150,150,150,150	0
35	NA	0	9173	1/1	0.31	12.94	66,66,66,66	0
33	MG	0	8038	1/1	0.24	12.93	13,13,13,13	0
35	NA	0	9132	1/1	0.31	12.42	61,61,61,61	0
33	MG	0	8022	1/1	0.54	12.30	113,113,113,113	0
33	MG	0	8051	1/1	0.26	11.67	22,22,22,22	0
33	MG	0	8013	1/1	0.35	11.51	16,16,16,16	0
33	MG	0	8021	1/1	0.22	11.47	51,51,51,51	0
33	MG	0	8057	1/1	0.55	11.43	79,79,79,79	0
35	NA	0	9157	1/1	0.17	11.27	41,41,41,41	0
35	NA	0	9156	1/1	0.25	11.15	55,55,55,55	0
35	NA	0	9120	1/1	0.23	10.88	61,61,61,61	0
33	MG	0	8103	1/1	0.23	10.74	79,79,79,79	0
35	NA	0	9172	1/1	0.34	10.71	68,68,68,68	0
33	MG	0	8058	1/1	0.48	10.49	85,85,85,85	0
35	NA	0	9163	1/1	0.30	10.18	77,77,77,77	0
37	SR	0	9626	1/1	0.26	9.98	140,140,140,140	0
33	MG	0	8012	1/1	0.25	9.29	37,37,37,37	0
35	NA	0	9149	1/1	0.20	9.11	41,41,41,41	0
35	NA	0	9171	1/1	0.21	8.99	63,63,63,63	0
37	SR	0	9482	1/1	0.20	8.94	118,118,118,118	0
34	K	0	9001	1/1	0.44	8.81	95,95,95,95	0
35	NA	0	9170	1/1	0.27	8.42	75,75,75,75	0
33	MG	0	8114	1/1	0.17	8.42	83,83,83,83	0
35	NA	0	9174	1/1	0.19	8.41	67,67,67,67	0
33	MG	B	8055	1/1	0.26	8.41	104,104,104,104	0
35	NA	3	9169	1/1	0.45	7.74	102,102,102,102	0
33	MG	0	8001	1/1	0.20	7.35	17,17,17,17	0
36	CL	0	9322	1/1	0.18	7.06	54,54,54,54	0
33	MG	0	8008	1/1	0.20	6.82	14,14,14,14	0
33	MG	0	8050	1/1	0.21	6.43	94,94,94,94	0
35	NA	0	9140	1/1	0.25	6.39	61,61,61,61	0
35	NA	0	9160	1/1	0.17	6.32	42,42,42,42	0
35	NA	0	9118	1/1	0.19	6.14	41,41,41,41	0
33	MG	9	8095	1/1	0.21	5.36	44,44,44,44	0
37	SR	0	9405	1/1	0.14	5.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	K	8069	1/1	0.18	5.18	23,23,23,23	0
33	MG	0	8070	1/1	0.15	5.03	21,21,21,21	0
37	SR	0	9406	1/1	0.15	4.95	33,33,33,33	0
35	NA	0	9135	1/1	0.16	4.53	46,46,46,46	0
33	MG	0	8029	1/1	0.21	4.36	27,27,27,27	0
33	MG	0	8089	1/1	0.15	4.35	61,61,61,61	0
33	MG	0	8040	1/1	0.36	4.23	94,94,94,94	0
37	SR	0	9434	1/1	0.14	4.19	58,58,58,58	0
35	NA	0	9102	1/1	0.14	4.07	58,58,58,58	0
33	MG	0	8102	1/1	0.14	3.98	70,70,70,70	0
35	NA	0	9165	1/1	0.32	3.76	41,41,41,41	0
36	CL	0	9316	1/1	0.22	3.64	74,74,74,74	0
35	NA	0	9178	1/1	0.18	3.64	54,54,54,54	0
33	MG	0	8076	1/1	0.14	3.50	55,55,55,55	0
35	NA	0	9175	1/1	0.16	3.48	52,52,52,52	0
37	SR	0	9452	1/1	0.16	3.39	114,114,114,114	0
33	MG	0	8017	1/1	0.15	3.38	20,20,20,20	0
35	NA	0	9110	1/1	0.17	3.17	49,49,49,49	0
35	NA	R	9186	1/1	0.19	3.07	64,64,64,64	0
33	MG	0	8099	1/1	0.15	2.97	77,77,77,77	0
35	NA	0	9127	1/1	0.16	2.90	65,65,65,65	0
33	MG	0	8061	1/1	0.13	2.88	81,81,81,81	0
37	SR	0	9432	1/1	0.11	2.79	63,63,63,63	0
37	SR	0	9515	1/1	0.18	2.67	100,100,100,100	0
33	MG	0	8107	1/1	0.20	2.47	68,68,68,68	0
33	MG	0	8065	1/1	0.27	2.37	92,92,92,92	0
37	SR	0	9408	1/1	0.14	2.34	38,38,38,38	0
33	MG	0	8080	1/1	0.20	2.29	48,48,48,48	0
33	MG	0	8020	1/1	0.18	2.17	30,30,30,30	0
37	SR	0	9477	1/1	0.12	2.14	82,82,82,82	0
33	MG	0	8027	1/1	0.16	1.95	30,30,30,30	0
37	SR	9	9588	1/1	0.15	1.86	122,122,122,122	0
37	SR	0	9411	1/1	0.14	1.82	42,42,42,42	0
33	MG	0	8056	1/1	0.19	1.81	47,47,47,47	0
33	MG	A	8066	1/1	0.18	1.75	53,53,53,53	0
35	NA	0	9181	1/1	0.13	1.74	48,48,48,48	0
37	SR	0	9407	1/1	0.12	1.71	42,42,42,42	0
35	NA	0	9159	1/1	0.15	1.68	56,56,56,56	0
33	MG	0	8104	1/1	0.28	1.53	83,83,83,83	0
33	MG	0	8014	1/1	0.27	1.52	78,78,78,78	0
37	SR	0	9475	1/1	0.12	1.48	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	S	9470	1/1	0.13	1.33	95,95,95,95	0
33	MG	0	8054	1/1	0.12	1.28	58,58,58,58	0
33	MG	0	8045	1/1	0.17	1.28	75,75,75,75	0
33	MG	0	8079	1/1	0.12	1.20	30,30,30,30	0
37	SR	H	9486	1/1	0.17	1.19	121,121,121,121	0
33	MG	0	8090	1/1	0.27	1.18	81,81,81,81	0
35	NA	0	9126	1/1	0.13	1.15	55,55,55,55	0
34	K	0	9002	1/1	0.23	1.14	86,86,86,86	0
33	MG	0	8003	1/1	0.17	1.10	29,29,29,29	0
35	NA	0	9155	1/1	0.21	1.05	54,54,54,54	0
37	SR	0	9420	1/1	0.14	1.01	60,60,60,60	0
33	MG	0	8074	1/1	0.19	1.00	20,20,20,20	0
33	MG	0	8043	1/1	0.11	0.88	47,47,47,47	0
35	NA	S	9112	1/1	0.17	0.64	74,74,74,74	0
36	CL	R	9306	1/1	0.12	0.60	46,46,46,46	0
36	CL	B	9319	1/1	0.13	0.48	59,59,59,59	0
33	MG	0	8097	1/1	0.12	0.31	55,55,55,55	0
33	MG	0	8031	1/1	0.12	0.24	48,48,48,48	0
37	SR	0	9410	1/1	0.13	0.20	34,34,34,34	0
36	CL	A	9309	1/1	0.17	0.19	64,64,64,64	0
33	MG	0	8096	1/1	0.13	0.14	44,44,44,44	0
35	NA	0	9141	1/1	0.10	0.09	61,61,61,61	0
37	SR	0	9415	1/1	0.10	0.08	50,50,50,50	0
35	NA	0	9124	1/1	0.12	0.05	51,51,51,51	0
35	NA	0	9139	1/1	0.17	0.04	57,57,57,57	0
37	SR	0	9433	1/1	0.10	0.02	73,73,73,73	0
35	NA	0	9114	1/1	0.14	0.01	51,51,51,51	0
35	NA	C	9104	1/1	0.14	-0.10	27,27,27,27	0
37	SR	0	9537	1/1	0.14	-0.11	152,152,152,152	0
37	SR	F	9595	1/1	0.15	-0.12	95,95,95,95	0
33	MG	0	8002	1/1	0.12	-0.12	22,22,22,22	0
37	SR	0	9474	1/1	0.09	-0.14	96,96,96,96	0
36	CL	0	9303	1/1	0.13	-0.14	49,49,49,49	0
35	NA	0	9128	1/1	0.10	-0.18	40,40,40,40	0
35	NA	0	9182	1/1	0.11	-0.20	84,84,84,84	0
37	SR	R	9418	1/1	0.13	-0.25	53,53,53,53	0
33	MG	0	8041	1/1	0.12	-0.30	47,47,47,47	0
37	SR	0	9417	1/1	0.12	-0.32	53,53,53,53	0
37	SR	A	9437	1/1	0.12	-0.37	64,64,64,64	0
35	NA	0	9131	1/1	0.12	-0.38	47,47,47,47	0
37	SR	0	9505	1/1	0.12	-0.43	104,104,104,104	0
35	NA	0	9117	1/1	0.11	-0.44	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9509	1/1	0.12	-0.61	83,83,83,83	0
37	SR	0	9488	1/1	0.10	-0.65	78,78,78,78	0
37	SR	A	9497	1/1	0.10	-0.76	85,85,85,85	0
37	SR	1	9419	1/1	0.10	-0.80	38,38,38,38	0
33	MG	0	8093	1/1	0.13	-0.80	42,42,42,42	0
37	SR	0	9534	1/1	0.11	-0.81	106,106,106,106	0
37	SR	0	9414	1/1	0.11	-0.82	53,53,53,53	0
36	CL	J	9302	1/1	0.08	-0.87	55,55,55,55	0
37	SR	0	9421	1/1	0.09	-0.89	65,65,65,65	0
35	NA	J	9146	1/1	0.10	-0.90	62,62,62,62	0
37	SR	0	9413	1/1	0.10	-0.92	44,44,44,44	0
33	MG	0	8004	1/1	0.10	-0.92	27,27,27,27	0
37	SR	0	9430	1/1	0.12	-0.93	41,41,41,41	0
36	CL	M	9318	1/1	0.13	-0.95	37,37,37,37	0
33	MG	0	8015	1/1	0.10	-0.96	29,29,29,29	0
37	SR	0	9424	1/1	0.14	-0.97	43,43,43,43	0
37	SR	0	9504	1/1	0.10	-1.00	92,92,92,92	0
38	CD	U	9201	1/1	0.09	-1.00	56,56,56,56	0
37	SR	0	9462	1/1	0.12	-1.00	66,66,66,66	0
35	NA	0	9158	1/1	0.11	-1.04	62,62,62,62	0
33	MG	0	8068	1/1	0.13	-1.17	47,47,47,47	0
35	NA	D	9151	1/1	0.19	-1.18	63,63,63,63	0
37	SR	0	9447	1/1	0.10	-1.20	66,66,66,66	0
36	CL	J	9321	1/1	0.07	-1.20	58,58,58,58	0
37	SR	0	9490	1/1	0.10	-1.22	105,105,105,105	0
35	NA	R	9137	1/1	0.09	-1.28	32,32,32,32	0
38	CD	Z	9203	1/1	0.07	-1.33	75,75,75,75	0
37	SR	0	9530	1/1	0.12	-1.37	94,94,94,94	0
33	MG	0	8088	1/1	0.06	-1.37	43,43,43,43	0
35	NA	0	9166	1/1	0.09	-1.38	65,65,65,65	0
33	MG	T	8073	1/1	0.13	-1.45	42,42,42,42	0
35	NA	Q	9148	1/1	0.10	-1.51	50,50,50,50	0
37	SR	0	9545	1/1	0.04	-1.55	67,67,67,67	0
35	NA	0	9134	1/1	0.07	-1.56	47,47,47,47	0
36	CL	J	9301	1/1	0.08	-1.57	55,55,55,55	0
35	NA	0	9108	1/1	0.08	-1.63	34,34,34,34	0
37	SR	0	9590	1/1	0.07	-1.64	142,142,142,142	0
37	SR	0	9450	1/1	0.06	-1.65	64,64,64,64	0
35	NA	R	9138	1/1	0.06	-1.65	52,52,52,52	0
35	NA	M	9147	1/1	0.07	-1.65	38,38,38,38	0
33	MG	0	8046	1/1	0.07	-1.66	40,40,40,40	0
37	SR	0	9423	1/1	0.09	-1.66	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	CD	3	9204	1/1	0.05	-1.67	58,58,58,58	0
37	SR	0	9451	1/1	0.07	-1.69	63,63,63,63	0
36	CL	0	9311	1/1	0.08	-1.71	56,56,56,56	0
35	NA	0	9113	1/1	0.11	-1.73	64,64,64,64	0
37	SR	0	9566	1/1	0.05	-1.76	75,75,75,75	0
36	CL	O	9308	1/1	0.08	-1.84	67,67,67,67	0
37	SR	1	9460	1/1	0.10	-1.84	49,49,49,49	0
35	NA	0	9136	1/1	0.10	-1.84	31,31,31,31	0
35	NA	0	9105	1/1	0.10	-1.91	41,41,41,41	0
33	MG	0	8117	1/1	0.09	-1.92	39,39,39,39	0
33	MG	0	8060	1/1	0.09	-1.93	81,81,81,81	0
33	MG	0	8101	1/1	0.10	-2.02	51,51,51,51	0
37	SR	0	9431	1/1	0.12	-2.04	55,55,55,55	0
37	SR	0	9425	1/1	0.07	-2.14	71,71,71,71	0
33	MG	0	8067	1/1	0.11	-2.15	36,36,36,36	0
37	SR	3	9439	1/1	0.05	-2.18	63,63,63,63	0
37	SR	0	9422	1/1	0.10	-2.32	53,53,53,53	0
36	CL	N	9307	1/1	0.08	-2.38	54,54,54,54	0
33	MG	Y	8109	1/1	0.10	-2.39	38,38,38,38	0
37	SR	0	9568	1/1	0.08	-2.40	75,75,75,75	0
37	SR	0	9446	1/1	0.08	-2.41	80,80,80,80	0
37	SR	0	9468	1/1	0.05	-2.42	115,115,115,115	0
36	CL	0	9317	1/1	0.09	-2.47	49,49,49,49	0
33	MG	0	8115	1/1	0.10	-2.50	53,53,53,53	0
35	NA	0	9130	1/1	0.07	-2.60	45,45,45,45	0
37	SR	0	9427	1/1	0.10	-2.66	53,53,53,53	0
37	SR	0	9467	1/1	0.09	-2.66	74,74,74,74	0
37	SR	0	9444	1/1	0.07	-2.67	47,47,47,47	0
37	SR	0	9517	1/1	0.05	-2.67	96,96,96,96	0
37	SR	0	9506	1/1	0.07	-2.68	86,86,86,86	0
37	SR	L	9409	1/1	0.09	-2.69	36,36,36,36	0
36	CL	L	9310	1/1	0.09	-2.72	56,56,56,56	0
37	SR	A	9436	1/1	0.05	-2.74	57,57,57,57	0
37	SR	0	9429	1/1	0.10	-2.75	63,63,63,63	0
37	SR	0	9473	1/1	0.04	-2.85	69,69,69,69	0
37	SR	0	9459	1/1	0.07	-2.86	96,96,96,96	0
36	CL	0	9312	1/1	0.06	-2.88	45,45,45,45	0
36	CL	0	9313	1/1	0.08	-2.89	51,51,51,51	0
35	NA	0	9123	1/1	0.09	-2.89	37,37,37,37	0
36	CL	Y	9320	1/1	0.07	-2.91	42,42,42,42	0
37	SR	0	9455	1/1	0.08	-2.94	61,61,61,61	0
37	SR	0	9443	1/1	0.09	-2.96	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9461	1/1	0.03	-3.00	73,73,73,73	0
33	MG	0	8042	1/1	0.06	-3.05	53,53,53,53	0
33	MG	0	8098	1/1	0.07	-3.08	43,43,43,43	0
37	SR	0	9426	1/1	0.07	-3.09	66,66,66,66	0
37	SR	0	9457	1/1	0.08	-3.11	47,47,47,47	0
37	SR	0	9508	1/1	0.08	-3.12	83,83,83,83	0
36	CL	0	9314	1/1	0.06	-3.13	47,47,47,47	0
37	SR	0	9581	1/1	0.07	-3.16	134,134,134,134	0
33	MG	0	8032	1/1	0.08	-3.18	36,36,36,36	0
35	NA	0	9143	1/1	0.07	-3.19	38,38,38,38	0
37	SR	0	9442	1/1	0.09	-3.31	59,59,59,59	0
33	MG	0	8110	1/1	0.10	-3.63	46,46,46,46	0
37	SR	9	9481	1/1	0.05	-3.63	83,83,83,83	0
33	MG	0	8036	1/1	0.08	-3.64	63,63,63,63	0
37	SR	0	9412	1/1	0.10	-3.64	43,43,43,43	0
33	MG	0	8028	1/1	0.10	-3.65	34,34,34,34	0
37	SR	0	9438	1/1	0.07	-3.67	63,63,63,63	0
38	CD	1	9202	1/1	0.03	-3.71	51,51,51,51	0
35	NA	0	9101	1/1	0.12	-3.76	43,43,43,43	0
33	MG	0	8005	1/1	0.08	-3.80	29,29,29,29	0
33	MG	0	8113	1/1	0.08	-3.81	45,45,45,45	0
33	MG	0	8116	1/1	0.06	-3.86	51,51,51,51	0
37	SR	0	9560	1/1	0.07	-3.95	97,97,97,97	0
37	SR	0	9465	1/1	0.07	-3.95	96,96,96,96	0
33	MG	0	8106	1/1	0.04	-3.97	37,37,37,37	0
37	SR	0	9445	1/1	0.08	-4.02	62,62,62,62	0
37	SR	0	9478	1/1	0.07	-4.13	70,70,70,70	0
33	MG	0	8063	1/1	0.07	-4.23	74,74,74,74	0
37	SR	0	9469	1/1	0.03	-4.27	85,85,85,85	0
36	CL	3	9304	1/1	0.08	-4.31	59,59,59,59	0
37	SR	0	9529	1/1	0.09	-4.41	116,116,116,116	0
37	SR	0	9448	1/1	0.06	-4.42	62,62,62,62	0
37	SR	0	9480	1/1	0.04	-4.58	86,86,86,86	0
37	SR	0	9466	1/1	0.03	-4.70	87,87,87,87	0
37	SR	0	9489	1/1	0.05	-4.74	87,87,87,87	0
37	SR	0	9435	1/1	0.07	-4.87	68,68,68,68	0
33	MG	0	8044	1/1	0.04	-4.92	42,42,42,42	0
38	CD	O	9205	1/1	0.04	-4.94	85,85,85,85	0
37	SR	0	9449	1/1	0.07	-4.98	59,59,59,59	0
37	SR	0	9441	1/1	0.07	-5.02	54,54,54,54	0
37	SR	0	9428	1/1	0.05	-5.21	43,43,43,43	0
37	SR	0	9483	1/1	0.06	-5.50	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9532	1/1	0.05	-5.55	100,100,100,100	0
33	MG	0	8091	1/1	0.06	-5.58	56,56,56,56	0
37	SR	0	9498	1/1	0.04	-5.60	63,63,63,63	0
37	SR	0	9629	1/1	0.07	-5.85	69,69,69,69	0
37	SR	0	9453	1/1	0.07	-5.93	68,68,68,68	0
36	CL	0	9305	1/1	0.05	-6.09	52,52,52,52	0
33	MG	0	8075	1/1	0.04	-6.12	37,37,37,37	0
33	MG	0	8037	1/1	0.06	-6.18	40,40,40,40	0
36	CL	0	9315	1/1	0.08	-6.21	54,54,54,54	0
33	MG	0	8009	1/1	0.06	-6.27	31,31,31,31	0
33	MG	0	8112	1/1	0.03	-6.36	44,44,44,44	0
33	MG	0	8019	1/1	0.04	-6.46	53,53,53,53	0
37	SR	0	9416	1/1	0.07	-6.61	45,45,45,45	0
37	SR	0	9495	1/1	0.10	-6.72	88,88,88,88	0
37	SR	0	9454	1/1	0.06	-6.86	73,73,73,73	0
37	SR	0	9464	1/1	0.04	-7.30	80,80,80,80	0
37	SR	B	9458	1/1	0.06	-8.05	73,73,73,73	0
37	SR	0	9456	1/1	0.06	-8.13	67,67,67,67	0
33	MG	0	8039	1/1	0.05	-8.37	56,56,56,56	0
37	SR	0	9585	1/1	0.07	-9.31	86,86,86,86	0
35	NA	0	9167	1/1	0.06	-9.43	50,50,50,50	0
33	MG	0	8030	1/1	0.04	-10.22	34,34,34,34	0
37	SR	0	9440	1/1	0.04	-10.40	63,63,63,63	0
37	SR	9	9503	1/1	0.03	-12.62	109,109,109,109	0
33	MG	0	8083	1/1	0.06	-14.21	51,51,51,51	0
37	SR	0	9570	1/1	0.05	-35.36	96,96,96,96	0
37	SR	0	9522	1/1	0.06	-69.49	104,104,104,104	0

6.5 Other polymers ⓘ

There are no such residues in this entry.