



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:24 PM UTC

PDB ID : 1QVG / pdb_00001qvg
Title : Structure of CCA oligonucleotide bound to the tRNA binding sites of the large ribosomal subunit of *Haloarcula marismortui*
Authors : Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-27
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

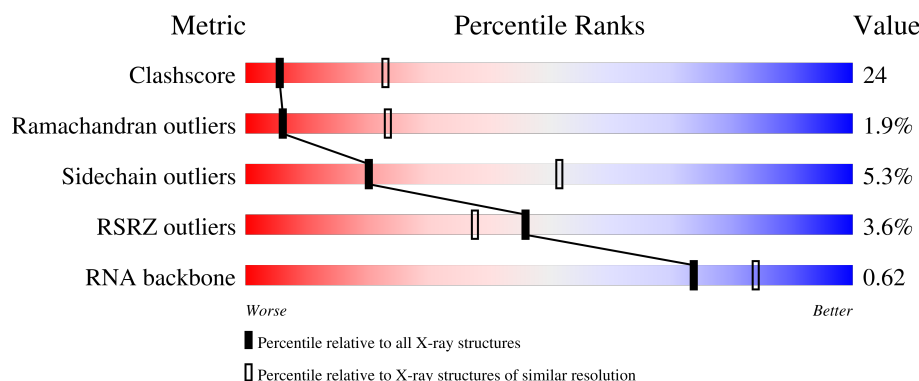
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	45% 41% 7% 6%
2	9	122	4% 44% 39% 13%
3	3	3	33% 33% 67%
3	4	3	33% 33% 67%
3	5	3	67% 33%

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Mol	Chain	Length	Quality of chain
4	A	239	
5	B	337	
6	C	246	
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	
15	L	194	
16	M	186	
17	N	115	
18	O	148	
19	P	95	
20	Q	154	
21	R	84	
22	S	119	
23	T	66	
24	U	70	
25	V	154	
26	W	91	
27	X	240	
28	Y	73	

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Mol	Chain	Length	Quality of chain
29	Z	56	
30	1	48	
31	2	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8329	-	-	-	X
34	NA	0	8384	-	-	-	X
34	NA	Q	8386	-	-	-	X
35	CL	I	8502	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	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 Oligonucleotide CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			
3	4	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			
3	5	3	Total	C	N	O	P	0	0	0
			59	28	11	18	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
			1754	1072	352	325	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
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P20279
B	310	ARG	PHE	conflict	UNP P20279

- 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
			1858	1131	344	382	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
			885	552	141	191	1			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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 L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	O	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	conflict	UNP P14119

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	P	95	Total	C	N	O	0	0	0
			734	450	141	143			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	S	119	Total	C	N	O	0	0	0
			949	568	180	201			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	V	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	W	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	X	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Z	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	deletion	UNP P22452

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	107	Total	Mg	0	0
			107	107		
32	9	1	Total	Mg	0	0
			1	1		
32	A	3	Total	Mg	0	0
			3	3		
32	B	1	Total	Mg	0	0
			1	1		
32	J	1	Total	Mg	0	0
			1	1		
32	S	1	Total	Mg	0	0
			1	1		
32	X	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	73	Total	Na	0	0
			73	73		
34	9	2	Total	Na	0	0
			2	2		
34	A	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	I	1	Total 1	Na 1	0	0
34	K	1	Total 1	Na 1	0	0
34	L	1	Total 1	Na 1	0	0
34	P	1	Total 1	Na 1	0	0
34	Q	3	Total 3	Na 3	0	0
34	R	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	9	Total 9	Cl 9	0	0
35	A	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	I	3	Total 3	Cl 3	0	0
35	J	1	Total 1	Cl 1	0	0
35	K	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	X	1	Total 1	Cl 1	0	0
35	2	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	N	1	Total Cd 1 1	0	0
36	T	1	Total Cd 1 1	0	0
36	Y	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	5766	Total O 5766 5766	0	0
37	9	148	Total O 148 148	0	0
37	4	1	Total O 1 1	0	0
37	5	2	Total O 2 2	0	0
37	A	115	Total O 115 115	0	0
37	B	146	Total O 146 146	0	0
37	C	166	Total O 166 166	0	0
37	D	48	Total O 48 48	0	0
37	E	43	Total O 43 43	0	0
37	F	25	Total O 25 25	0	0
37	G	20	Total O 20 20	0	0
37	H	77	Total O 77 77	0	0
37	I	56	Total O 56 56	0	0
37	J	56	Total O 56 56	0	0
37	K	80	Total O 80 80	0	0

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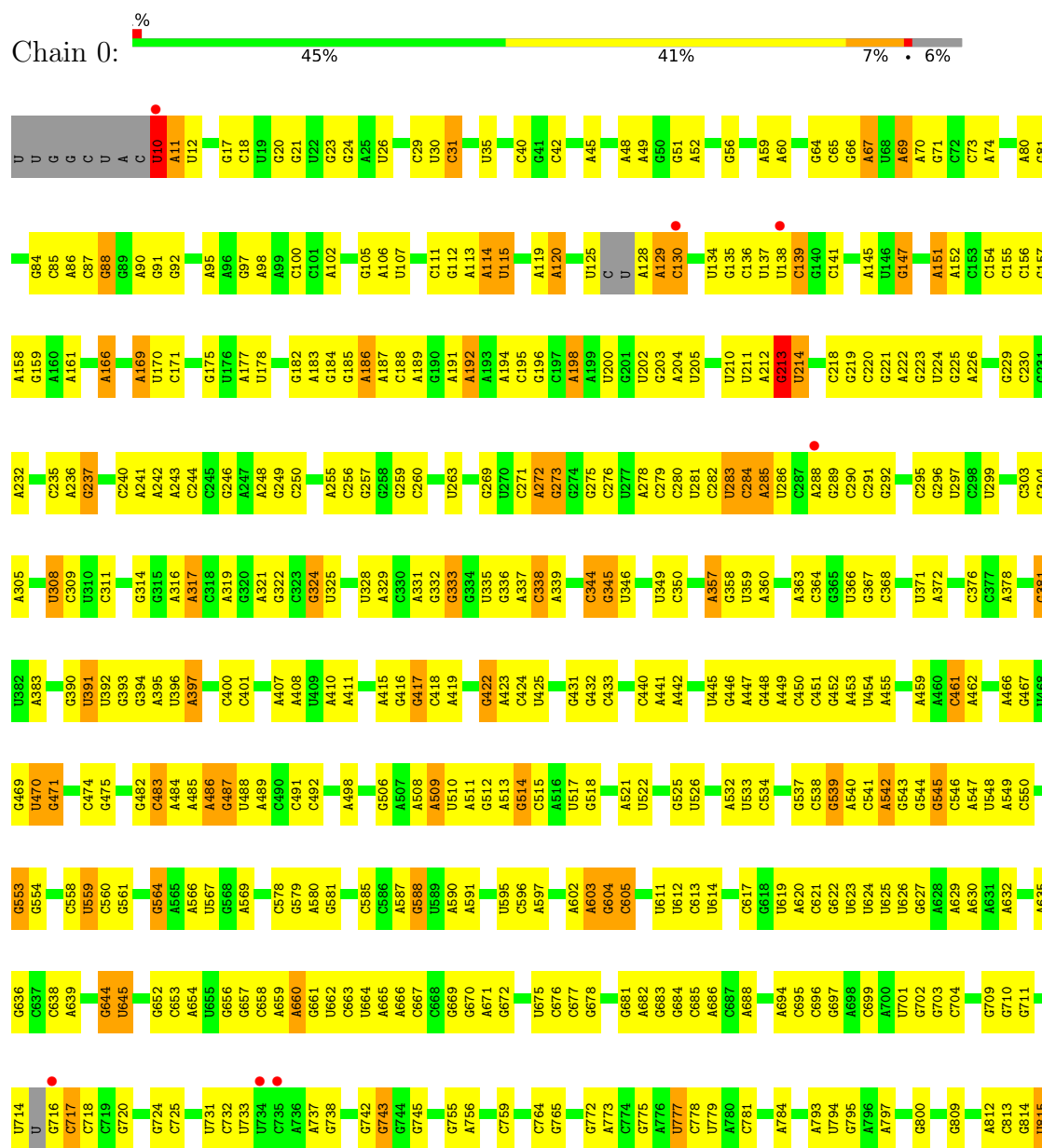
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	129	Total 129	O 129	0	0
37	M	56	Total 56	O 56	0	0
37	N	43	Total 43	O 43	0	0
37	O	58	Total 58	O 58	0	0
37	P	57	Total 57	O 57	0	0
37	Q	85	Total 85	O 85	0	0
37	R	31	Total 31	O 31	0	0
37	S	38	Total 38	O 38	0	0
37	T	30	Total 30	O 30	0	0
37	U	12	Total 12	O 12	0	0
37	V	69	Total 69	O 69	0	0
37	W	27	Total 27	O 27	0	0
37	X	97	Total 97	O 97	0	0
37	Y	35	Total 35	O 35	0	0
37	Z	54	Total 54	O 54	0	0
37	1	42	Total 42	O 42	0	0
37	2	56	Total 56	O 56	0	0

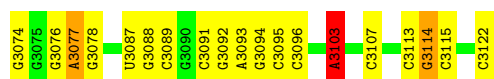
3 Residue-property plots

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

- Molecule 1: 23S ribosomal rna







• Molecule 3: Oligonucleotide CCA



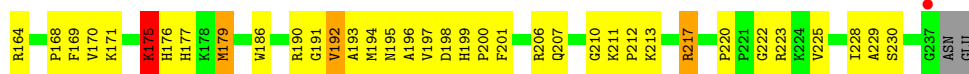
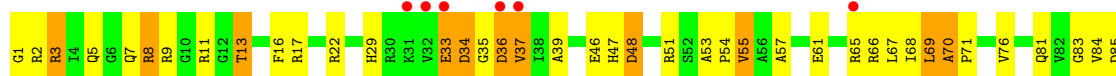
• Molecule 3: Oligonucleotide CCA



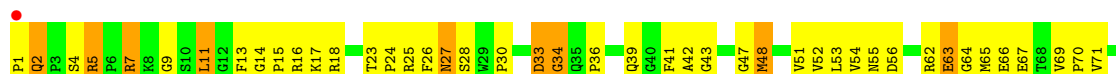
• Molecule 3: Oligonucleotide CCA



• Molecule 4: 50S ribosomal protein L2P

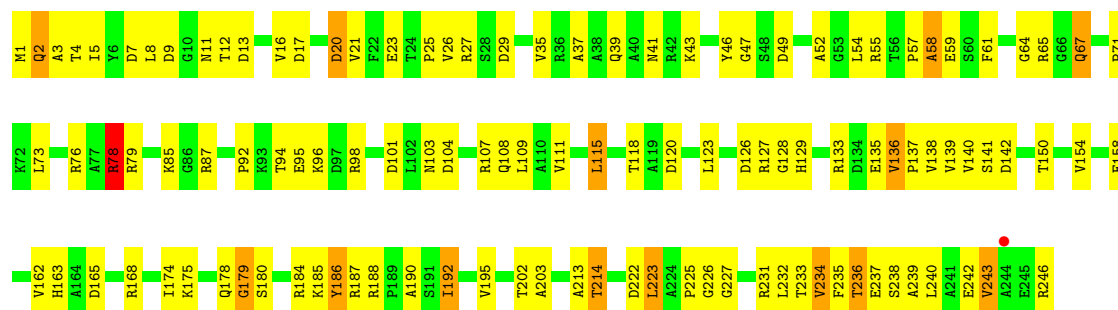


• Molecule 5: 50S ribosomal protein L3P

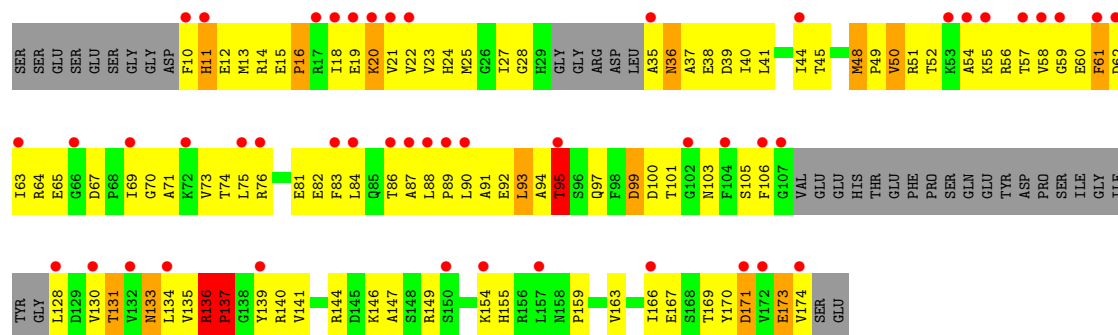




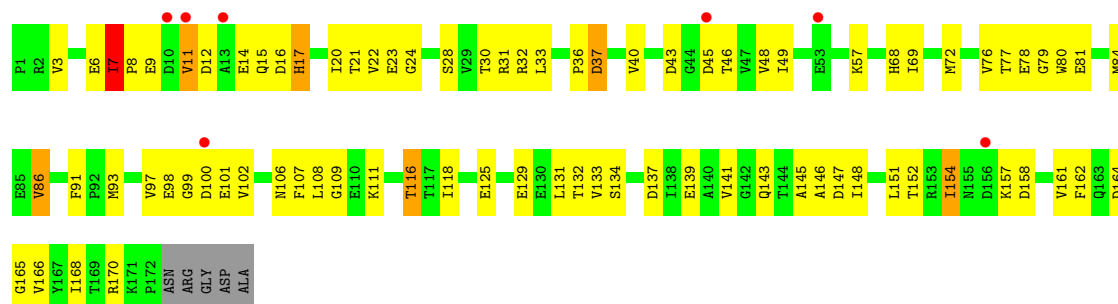
• Molecule 6: 50S ribosomal protein L4E



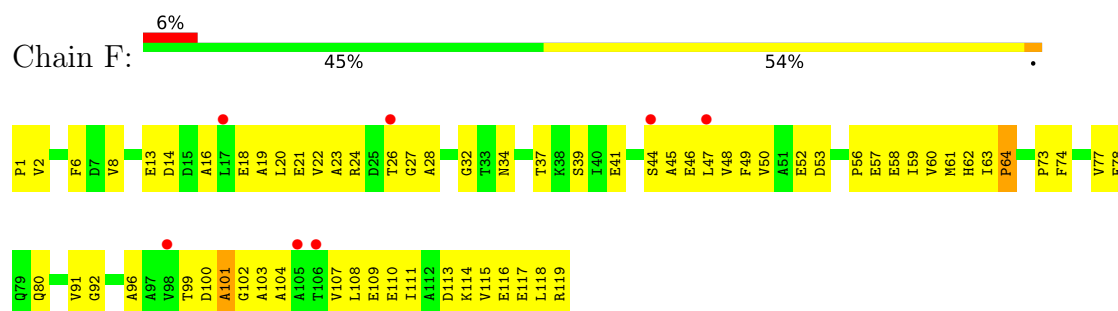
• Molecule 7: 50S ribosomal protein L5P



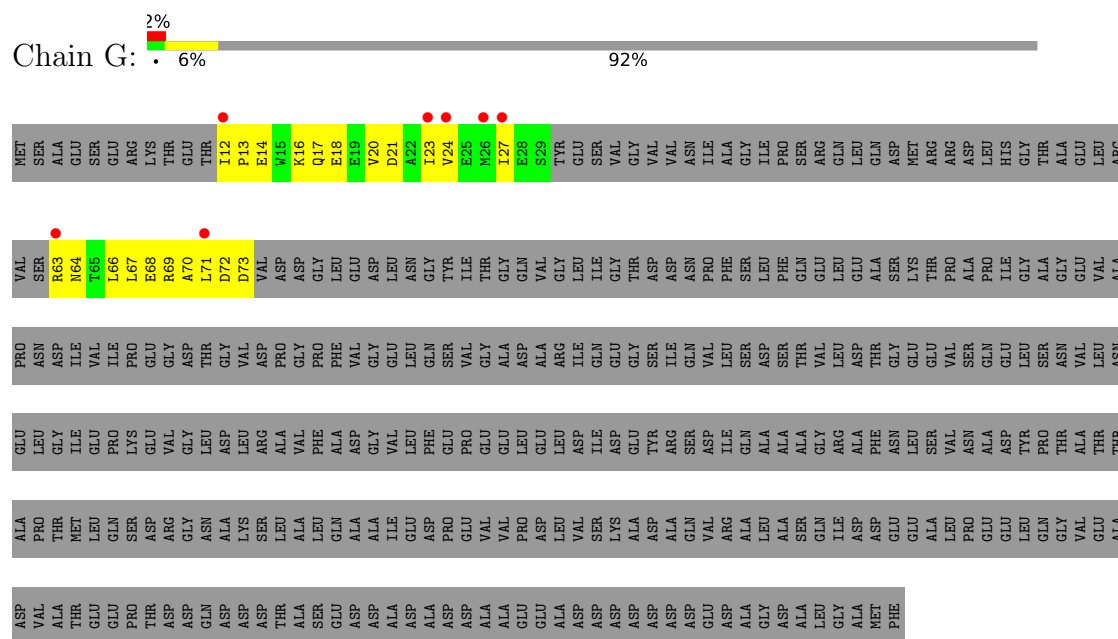
• Molecule 8: 50S ribosomal protein L6P



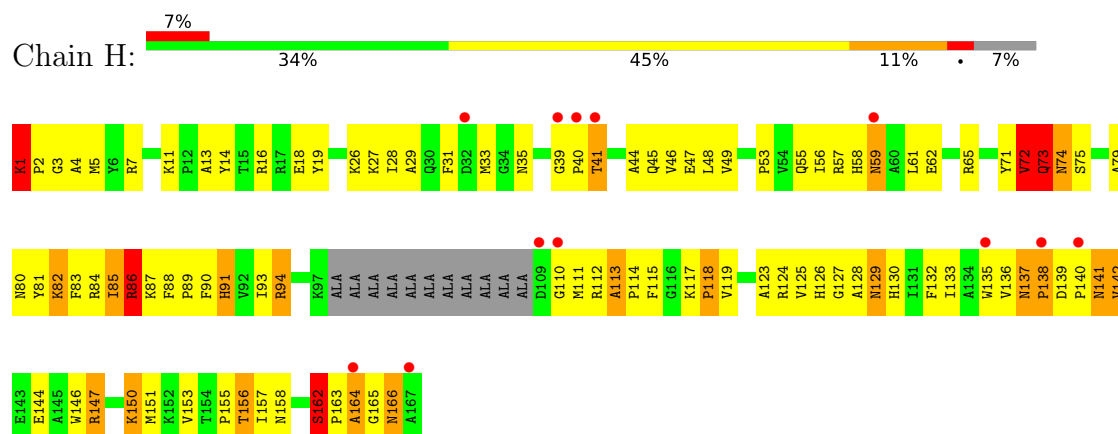
- Molecule 9: 50S ribosomal protein L7Ae



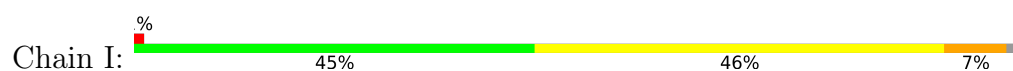
- Molecule 10: 50S RIBOSOMAL PROTEIN L10E

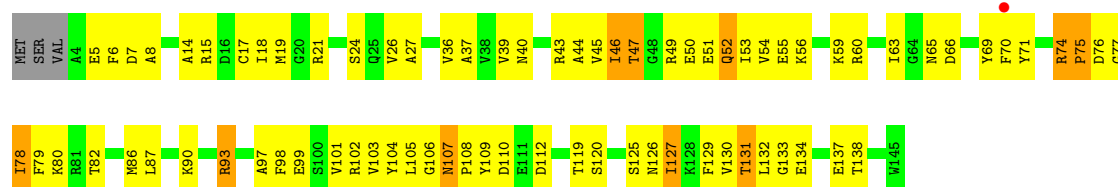


- Molecule 11: L10 Ribosomal Protein

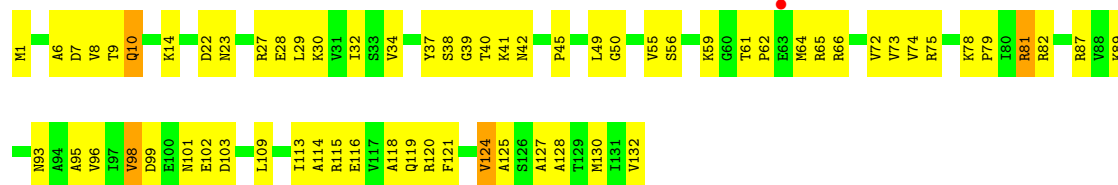


- Molecule 12: 50S ribosomal protein L13P

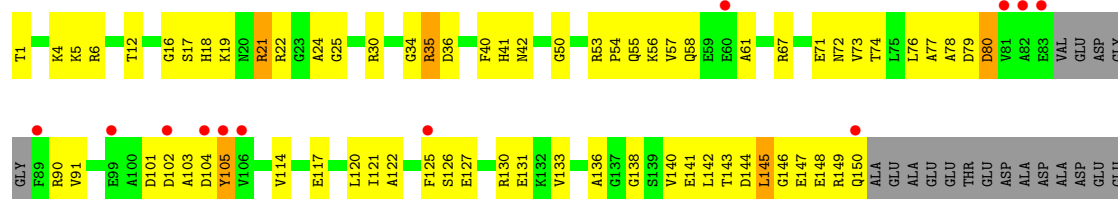




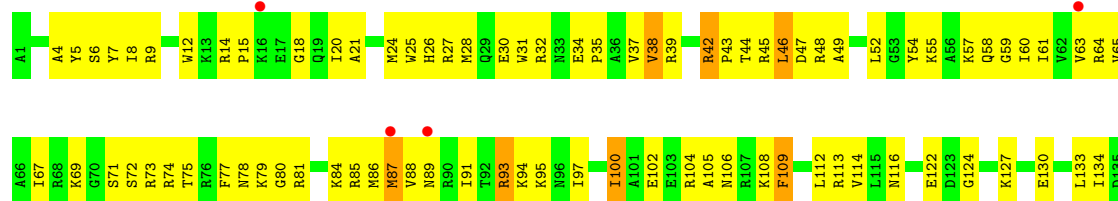
• Molecule 13: 50S ribosomal protein L14P



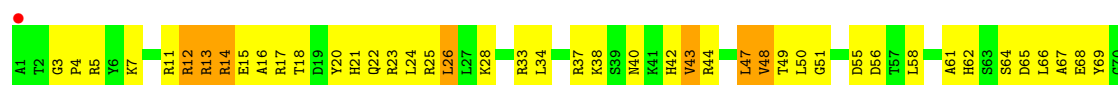
• Molecule 14: 50S ribosomal protein L15P

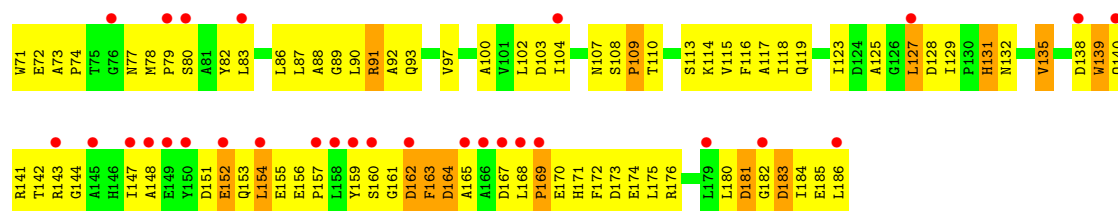


• Molecule 15: L15 Ribosomal Protein



• Molecule 16: 50S ribosomal protein L18P

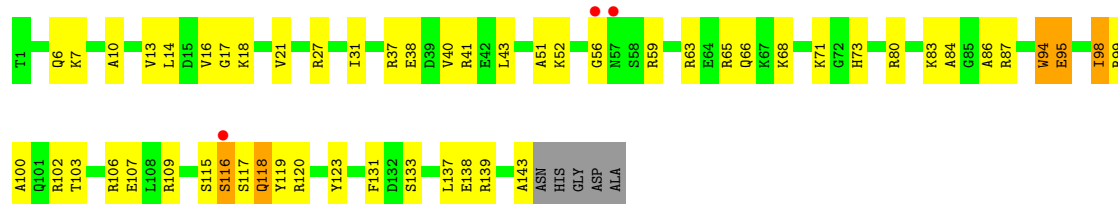




• Molecule 17: 50S ribosomal protein L18e



• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e

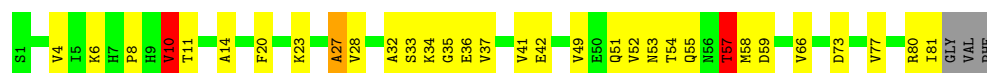


• Molecule 20: 50S ribosomal protein L22P



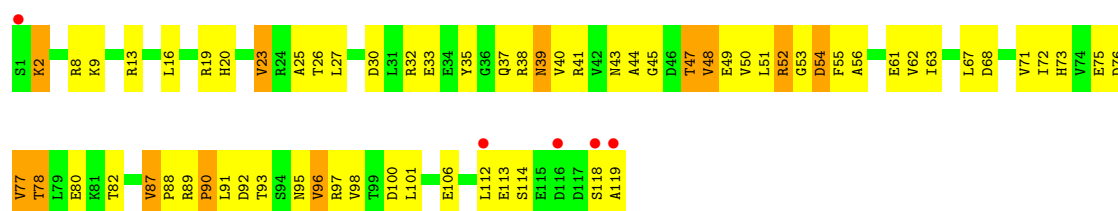
• Molecule 21: 50S ribosomal protein L23P

Chain R:  58% 35% ..



• Molecule 22: 50S ribosomal protein L24P

Chain S:  4% 45% 45% 10%



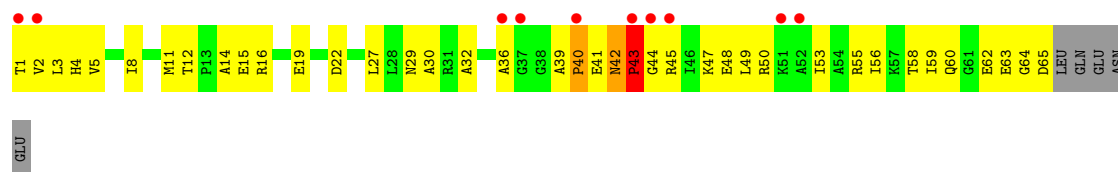
• Molecule 23: 50S ribosomal protein L24E

Chain T:  2% 38% 42% 20%



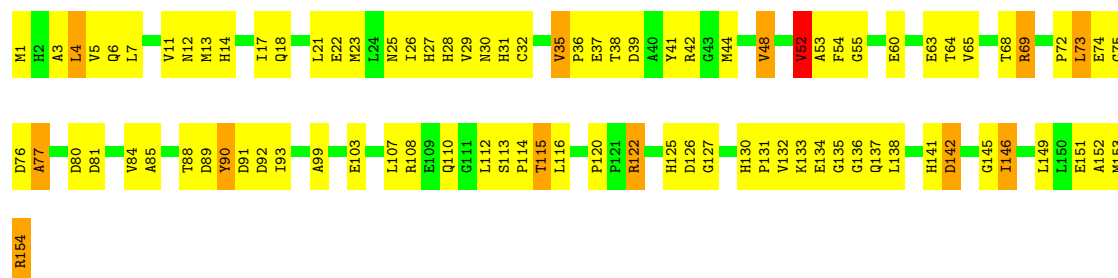
• Molecule 24: 50S ribosomal protein L29P

Chain U:  14% 37% 51% 7%



• Molecule 25: 50S ribosomal protein L30P

Chain V:  41% 51% 8%

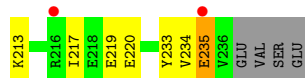
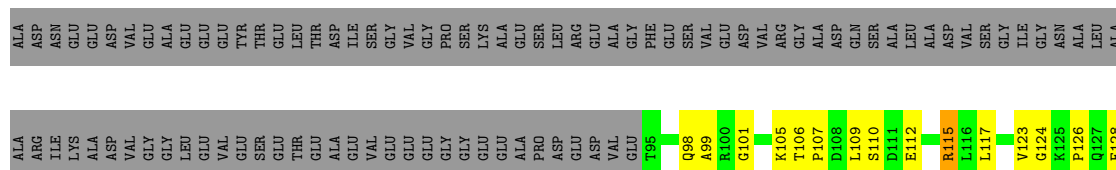
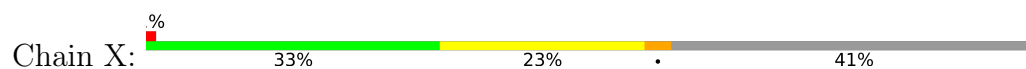


• Molecule 26: 50S ribosomal protein L31e

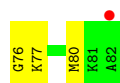
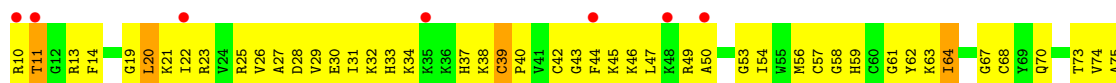
Chain W:  2% 38% 44% 7% 10%



• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: L37Ae 50S ribosomal protein



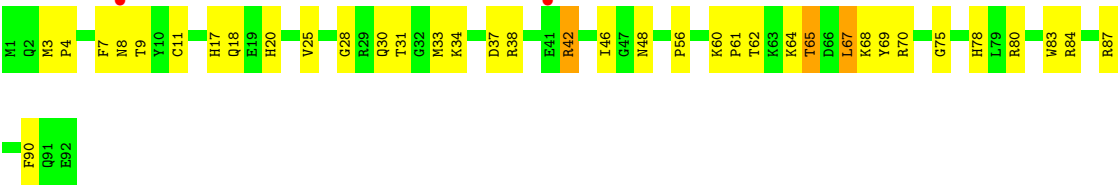
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.52Å 300.61Å 573.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 89.6 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.258 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	98494	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CD, MG, K, CL

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	0.55	0/66076	0.74	42/103052 (0.0%)
2	9	0.53	0/2905	0.76	7/4528 (0.2%)
3	3	0.54	0/65	0.84	0/99
3	4	0.73	0/65	0.77	0/99
3	5	0.47	0/65	0.79	0/99
4	A	0.68	0/1787	1.09	12/2409 (0.5%)
5	B	0.73	0/2689	1.13	24/3652 (0.7%)
6	C	0.80	0/1883	1.12	7/2551 (0.3%)
7	D	0.54	0/1111	0.98	5/1498 (0.3%)
8	E	0.72	0/1382	1.00	5/1880 (0.3%)
9	F	0.60	0/896	0.97	2/1219 (0.2%)
10	G	0.60	0/241	0.84	1/324 (0.3%)
11	H	0.80	1/1246 (0.1%)	1.40	22/1686 (1.3%)
12	I	0.79	0/1135	1.07	5/1530 (0.3%)
13	J	0.71	0/1003	1.12	4/1351 (0.3%)
14	K	0.62	0/1126	1.05	3/1504 (0.2%)
15	L	0.75	0/1633	1.13	10/2180 (0.5%)
16	M	0.59	0/1473	1.16	13/1999 (0.7%)
17	N	0.74	0/873	1.07	6/1181 (0.5%)
18	O	0.66	0/1143	0.98	3/1521 (0.2%)
19	P	0.74	0/748	1.18	6/1005 (0.6%)
20	Q	0.77	0/1172	1.07	5/1578 (0.3%)
21	R	0.57	0/648	0.91	3/875 (0.3%)
22	S	0.62	0/957	1.04	8/1289 (0.6%)
23	T	0.69	0/417	1.05	0/562
24	U	0.52	0/502	1.05	2/675 (0.3%)
25	V	0.83	0/1218	1.10	4/1655 (0.2%)
26	W	0.81	0/664	1.13	7/895 (0.8%)
27	X	0.74	0/1146	1.06	2/1536 (0.1%)
28	Y	0.66	0/575	1.04	1/763 (0.1%)
29	Z	0.70	0/437	1.04	3/578 (0.5%)
30	1	0.62	0/398	0.82	0/527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	2	0.68	0/771	1.00	1/1024 (0.1%)
All	All	0.60	1/98450 (0.0%)	0.84	213/147324 (0.1%)

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	105
2	9	0	4
25	V	0	1
All	All	0	110

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	41	THR	CA-CB	5.49	1.60	1.53

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	74	ASN	N-CA-C	-15.73	91.57	114.39
1	0	1563	G	C2'-C3'-O3'	14.45	131.17	109.50
11	H	141	ASN	N-CA-C	-12.69	97.78	113.38
15	L	141	ILE	N-CA-C	-10.95	102.01	112.96
1	0	1979	G	C2'-C3'-O3'	10.69	125.53	109.50

There are no chirality outliers.

5 of 110 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	147	G	Sidechain
1	0	171	C	Sidechain
1	0	26	U	Sidechain
1	0	48	A	Sidechain
1	0	49	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29802	1343	0
2	9	2600	0	1326	87	0
3	3	59	0	35	1	0
3	4	59	0	35	3	0
3	5	59	0	35	0	0
4	A	1754	0	1763	128	0
5	B	2624	0	2533	215	0
6	C	1858	0	1816	136	0
7	D	1094	0	1085	149	0
8	E	1357	0	1266	90	0
9	F	885	0	854	73	0
10	G	240	0	231	30	0
11	H	1215	0	1215	178	0
12	I	1119	0	1098	86	0
13	J	993	0	1027	80	0
14	K	1114	0	1072	73	0
15	L	1605	0	1676	176	0
16	M	1444	0	1401	166	0
17	N	864	0	873	47	0
18	O	1133	0	1127	64	0
19	P	734	0	728	38	0
20	Q	1149	0	1122	81	0
21	R	641	0	605	33	0
22	S	949	0	923	80	0
23	T	410	0	364	41	0
24	U	499	0	511	39	0
25	V	1195	0	1137	118	0
26	W	654	0	653	55	0
27	X	1130	0	1133	80	0
28	Y	563	0	597	58	0
29	Z	430	0	426	35	0
30	1	393	0	406	44	0
31	2	755	0	728	37	0
32	0	107	0	0	0	0
32	2	1	0	0	0	0
32	9	1	0	0	0	0
32	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	1	0	0	0	0
32	J	1	0	0	0	0
32	S	1	0	0	0	0
32	X	1	0	0	0	0
33	0	2	0	0	0	0
34	0	73	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	I	1	0	0	0	0
34	K	1	0	0	0	0
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	3	0	0	0	0
34	R	1	0	0	0	0
35	0	9	0	0	1	0
35	2	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	2	0
35	J	1	0	0	1	0
35	K	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	Q	1	0	0	0	0
35	X	1	0	0	0	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5766	0	0	297	0
37	1	42	0	0	4	0
37	2	56	0	0	10	0
37	4	1	0	0	0	0
37	5	2	0	0	0	0
37	9	148	0	0	15	0
37	A	115	0	0	23	0
37	B	146	0	0	27	0
37	C	166	0	0	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	48	0	0	24	0
37	E	43	0	0	15	0
37	F	25	0	0	10	0
37	G	20	0	0	7	0
37	H	77	0	0	28	0
37	I	56	0	0	11	0
37	J	56	0	0	12	0
37	K	80	0	0	18	0
37	L	129	0	0	22	0
37	M	56	0	0	27	0
37	N	43	0	0	13	0
37	O	58	0	0	5	0
37	P	57	0	0	8	0
37	Q	85	0	0	11	0
37	R	31	0	0	9	0
37	S	38	0	0	7	0
37	T	30	0	0	9	0
37	U	12	0	0	2	0
37	V	69	0	0	14	0
37	W	27	0	0	7	0
37	X	97	0	0	21	0
37	Y	35	0	0	7	0
37	Z	54	0	0	6	0
All	All	98494	0	59603	3529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 3529 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:86:ARG:NH1	11:H:133:ILE:HG13	1.55	1.20
20:Q:99:ALA:HB1	20:Q:109:MET:HE1	1.21	1.14
7:D:25:MET:HE2	7:D:41:LEU:HG	1.29	1.14
24:U:12:THR:HG22	24:U:15:GLU:HG3	1.32	1.11
12:I:19:MET:HE3	12:I:132:LEU:HD11	1.29	1.07

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	235/239 (98%)	204 (87%)	27 (12%)	4 (2%)	7	26
5	B	335/337 (99%)	295 (88%)	31 (9%)	9 (3%)	4	16
6	C	244/246 (99%)	221 (91%)	21 (9%)	2 (1%)	16	44
7	D	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	0	1
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	21	51
9	F	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	4	17
10	G	25/348 (7%)	21 (84%)	3 (12%)	1 (4%)	2	9
11	H	152/167 (91%)	131 (86%)	16 (10%)	5 (3%)	3	13
12	I	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	3	15
13	J	130/132 (98%)	111 (85%)	18 (14%)	1 (1%)	16	44
14	K	141/164 (86%)	118 (84%)	20 (14%)	3 (2%)	5	21
15	L	192/194 (99%)	165 (86%)	24 (12%)	3 (2%)	7	27
16	M	184/186 (99%)	161 (88%)	15 (8%)	8 (4%)	2	8
17	N	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	6	25
18	O	141/148 (95%)	132 (94%)	8 (6%)	1 (1%)	18	48
19	P	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	11	36
20	Q	148/154 (96%)	136 (92%)	12 (8%)	0	100	100
21	R	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	9	32
22	S	117/119 (98%)	99 (85%)	17 (14%)	1 (1%)	14	41
23	T	51/66 (77%)	45 (88%)	5 (10%)	1 (2%)	6	22
24	U	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	13
25	V	152/154 (99%)	139 (91%)	12 (8%)	1 (1%)	18	48
26	W	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	4	17
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	57 (80%)	13 (18%)	1 (1%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
30	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
31	2	90/92 (98%)	84 (93%)	6 (7%)	0	100	100
All	All	3633/4235 (86%)	3220 (89%)	344 (10%)	69 (2%)	6	23

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP
7	D	16	PRO
7	D	93	LEU
7	D	95	THR
7	D	137	PRO

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	179/181 (99%)	166 (93%)	13 (7%)	13	38
5	B	282/282 (100%)	262 (93%)	20 (7%)	13	40
6	C	193/193 (100%)	178 (92%)	15 (8%)	11	35
7	D	117/147 (80%)	108 (92%)	9 (8%)	12	35
8	E	152/155 (98%)	146 (96%)	6 (4%)	28	63
9	F	92/92 (100%)	92 (100%)	0	100	100
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	108 (88%)	14 (12%)	5	18
12	I	118/121 (98%)	110 (93%)	8 (7%)	14	42
13	J	106/106 (100%)	103 (97%)	3 (3%)	38	72
14	K	112/126 (89%)	109 (97%)	3 (3%)	39	73
15	L	166/166 (100%)	159 (96%)	7 (4%)	26	60
16	M	149/149 (100%)	140 (94%)	9 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	93/93 (100%)	87 (94%)	6 (6%)	15	44
18	O	113/116 (97%)	110 (97%)	3 (3%)	39	73
19	P	79/79 (100%)	75 (95%)	4 (5%)	21	53
20	Q	117/121 (97%)	113 (97%)	4 (3%)	32	66
21	R	71/73 (97%)	68 (96%)	3 (4%)	26	60
22	S	105/105 (100%)	101 (96%)	4 (4%)	29	64
23	T	44/52 (85%)	43 (98%)	1 (2%)	44	76
24	U	51/56 (91%)	50 (98%)	1 (2%)	48	78
25	V	130/130 (100%)	121 (93%)	9 (7%)	14	41
26	W	66/73 (90%)	61 (92%)	5 (8%)	12	36
27	X	120/195 (62%)	112 (93%)	8 (7%)	15	43
28	Y	56/56 (100%)	54 (96%)	2 (4%)	31	65
29	Z	46/46 (100%)	46 (100%)	0	100	100
30	1	42/44 (96%)	41 (98%)	1 (2%)	43	75
31	2	79/79 (100%)	76 (96%)	3 (4%)	29	64
All	All	3027/3441 (88%)	2866 (95%)	161 (5%)	20	52

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	O	98	ILE
26	W	27	ASP
19	P	95	GLU
22	S	96	VAL
27	X	172	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
19	P	40	HIS
22	S	73	HIS
30	1	18	ASN
19	P	67	GLN
20	Q	123	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	277 (10%)	55 (2%)
2	9	121/122 (99%)	20 (16%)	7 (5%)
3	3	2/3 (66%)	1 (50%)	0
3	4	2/3 (66%)	0	0
3	5	2/3 (66%)	1 (50%)	0
All	All	2873/3053 (94%)	299 (10%)	62 (2%)

5 of 299 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1380	U
2	9	3002	U
1	0	1752	G
1	0	2850	C
2	9	3065	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 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.

No monomer is involved in short contacts.

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%)	-0.27	40 (1%) 72 64	23, 53, 103, 166	0
2	9	122/122 (100%)	0.11	5 (4%) 41 33	36, 67, 104, 164	0
3	3	3/3 (100%)	1.03	1 (33%) 1 1	68, 68, 83, 120	0
3	4	3/3 (100%)	1.77	1 (33%) 1 1	88, 88, 89, 103	0
3	5	3/3 (100%)	0.14	0 100 100	57, 57, 58, 64	0
4	A	237/239 (99%)	0.33	7 (2%) 52 43	33, 66, 100, 126	0
5	B	337/337 (100%)	0.21	1 (0%) 90 87	27, 60, 86, 95	0
6	C	246/246 (100%)	0.16	1 (0%) 88 85	27, 57, 81, 88	0
7	D	140/176 (79%)	1.64	48 (34%) 1 1	65, 111, 129, 137	0
8	E	172/177 (97%)	0.43	7 (4%) 41 33	43, 69, 95, 101	0
9	F	119/119 (100%)	0.81	7 (5%) 28 22	65, 88, 112, 117	0
10	G	29/348 (8%)	1.19	7 (24%) 2 2	72, 95, 107, 111	0
11	H	156/167 (93%)	0.39	12 (7%) 19 16	31, 56, 83, 92	0
12	I	142/145 (97%)	0.06	1 (0%) 84 79	37, 50, 75, 87	0
13	J	132/132 (100%)	0.30	1 (0%) 82 77	41, 60, 83, 90	0
14	K	145/164 (88%)	0.70	12 (8%) 17 14	31, 77, 121, 127	0
15	L	194/194 (100%)	0.30	7 (3%) 46 38	37, 56, 80, 88	0
16	M	186/186 (100%)	1.03	30 (16%) 4 4	43, 78, 123, 135	0
17	N	115/115 (100%)	0.34	1 (0%) 81 75	47, 65, 83, 86	0
18	O	143/148 (96%)	0.58	3 (2%) 63 54	39, 65, 85, 94	0
19	P	95/95 (100%)	0.01	0 100 100	35, 49, 67, 86	0
20	Q	150/154 (97%)	-0.20	0 100 100	35, 47, 69, 80	0
21	R	81/84 (96%)	0.46	0 100 100	56, 80, 96, 103	0
22	S	119/119 (100%)	0.56	5 (4%) 40 32	52, 71, 101, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
23	T	53/66 (80%)	0.29	1 (1%) 66 58	48, 62, 79, 91	0
24	U	65/70 (92%)	1.03	10 (15%) 5 4	67, 93, 127, 133	0
25	V	154/154 (100%)	-0.10	0 100 100	32, 49, 70, 80	0
26	W	82/91 (90%)	0.39	2 (2%) 59 50	46, 63, 84, 101	0
27	X	142/240 (59%)	0.01	2 (1%) 73 65	28, 52, 77, 93	0
28	Y	73/73 (100%)	0.85	8 (10%) 10 9	55, 72, 90, 96	0
29	Z	56/56 (100%)	-0.41	0 100 100	29, 42, 50, 53	0
30	1	46/48 (95%)	1.42	13 (28%) 1 1	42, 77, 136, 138	0
31	2	92/92 (100%)	0.55	2 (2%) 62 53	44, 67, 80, 91	0
All	All	6586/7288 (90%)	0.12	235 (3%) 46 38	23, 60, 108, 166	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	U	1	THR	7.2
7	D	88	LEU	6.7
2	9	3001	U	5.6
30	1	42	TRP	5.3
7	D	10	PHE	5.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	0	8329	1/1	0.50	0.41	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	9	8351	1/1	0.53	0.24	89,89,89,89	0
34	NA	R	8312	1/1	0.61	0.17	60,60,60,60	0
32	MG	0	8092	1/1	0.77	0.17	109,109,109,109	0
34	NA	0	8384	1/1	0.77	0.43	132,132,132,132	0
34	NA	Q	8386	1/1	0.78	0.48	84,84,84,84	0
32	MG	9	8095	1/1	0.79	0.12	73,73,73,73	0
34	NA	0	8341	1/1	0.81	0.07	42,42,42,42	0
34	NA	0	8372	1/1	0.81	0.43	71,71,71,71	0
35	CL	N	8508	1/1	0.82	0.22	101,101,101,101	0
34	NA	0	8381	1/1	0.84	0.09	47,47,47,47	0
34	NA	0	8382	1/1	0.84	0.15	64,64,64,64	0
34	NA	9	8383	1/1	0.84	0.10	62,62,62,62	0
34	NA	0	8326	1/1	0.85	0.17	52,52,52,52	0
34	NA	0	8369	1/1	0.85	0.22	68,68,68,68	0
34	NA	Q	8337	1/1	0.85	0.08	43,43,43,43	0
34	NA	0	8302	1/1	0.86	0.07	40,40,40,40	0
34	NA	0	8324	1/1	0.86	0.17	62,62,62,62	0
34	NA	0	8350	1/1	0.86	0.23	61,61,61,61	0
34	NA	0	8352	1/1	0.86	0.30	61,61,61,61	0
35	CL	0	8505	1/1	0.86	0.18	87,87,87,87	0
32	MG	0	8049	1/1	0.86	0.10	64,64,64,64	0
34	NA	0	8365	1/1	0.87	0.15	58,58,58,58	0
34	NA	0	8368	1/1	0.87	0.12	51,51,51,51	0
32	MG	0	8104	1/1	0.87	0.09	58,58,58,58	0
32	MG	0	8087	1/1	0.87	0.08	83,83,83,83	0
32	MG	0	8011	1/1	0.87	0.25	1,1,1,1	0
34	NA	0	8317	1/1	0.87	0.09	75,75,75,75	0
32	MG	0	8101	1/1	0.87	0.15	68,68,68,68	0
35	CL	0	8511	1/1	0.88	0.18	90,90,90,90	0
32	MG	J	8069	1/1	0.88	0.11	114,114,114,114	0
34	NA	0	8363	1/1	0.89	0.16	47,47,47,47	0
35	CL	0	8503	1/1	0.89	0.15	67,67,67,67	0
34	NA	0	8316	1/1	0.89	0.15	39,39,39,39	0
32	MG	0	8076	1/1	0.89	0.09	83,83,83,83	0
34	NA	0	8359	1/1	0.89	0.28	66,66,66,66	0
34	NA	0	8362	1/1	0.90	0.23	73,73,73,73	0
34	NA	0	8371	1/1	0.90	0.18	58,58,58,58	0
32	MG	0	8103	1/1	0.90	0.18	88,88,88,88	0
34	NA	0	8360	1/1	0.91	0.24	47,47,47,47	0
32	MG	0	8046	1/1	0.91	0.07	61,61,61,61	0
34	NA	0	8303	1/1	0.91	0.19	54,54,54,54	0
34	NA	0	8364	1/1	0.91	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8307	1/1	0.91	0.08	40,40,40,40	0
34	NA	0	8357	1/1	0.91	0.11	63,63,63,63	0
35	CL	M	8507	1/1	0.91	0.08	66,66,66,66	0
32	MG	0	8067	1/1	0.91	0.07	78,78,78,78	0
34	NA	P	8348	1/1	0.92	0.06	47,47,47,47	0
34	NA	0	8308	1/1	0.92	0.09	54,54,54,54	0
34	NA	0	8373	1/1	0.92	0.10	53,53,53,53	0
34	NA	0	8325	1/1	0.92	0.16	45,45,45,45	0
32	MG	0	8050	1/1	0.92	0.07	50,50,50,50	0
32	MG	0	8099	1/1	0.92	0.13	73,73,73,73	0
34	NA	0	8332	1/1	0.92	0.07	30,30,30,30	0
35	CL	0	8515	1/1	0.92	0.13	96,96,96,96	0
35	CL	0	8517	1/1	0.92	0.09	64,64,64,64	0
35	CL	K	8510	1/1	0.92	0.13	71,71,71,71	0
34	NA	0	8322	1/1	0.92	0.28	65,65,65,65	0
34	NA	K	8380	1/1	0.92	0.16	77,77,77,77	0
34	NA	0	8356	1/1	0.93	0.23	77,77,77,77	0
34	NA	0	8374	1/1	0.93	0.24	74,74,74,74	0
32	MG	0	8113	1/1	0.93	0.07	39,39,39,39	0
34	NA	0	8370	1/1	0.93	0.28	60,60,60,60	0
35	CL	I	8502	1/1	0.93	0.06	54,54,54,54	0
34	NA	0	8306	1/1	0.93	0.15	57,57,57,57	0
34	NA	0	8385	1/1	0.93	0.23	44,44,44,44	0
32	MG	0	8024	1/1	0.93	0.31	146,146,146,146	0
35	CL	X	8520	1/1	0.93	0.08	43,43,43,43	0
34	NA	0	8305	1/1	0.94	0.07	39,39,39,39	0
32	MG	0	8082	1/1	0.94	0.10	77,77,77,77	0
35	CL	0	8522	1/1	0.94	0.23	68,68,68,68	0
35	CL	A	8509	1/1	0.94	0.14	78,78,78,78	0
35	CL	I	8501	1/1	0.94	0.08	64,64,64,64	0
32	MG	0	8044	1/1	0.94	0.11	54,54,54,54	0
32	MG	0	8047	1/1	0.94	0.08	48,48,48,48	0
34	NA	0	8333	1/1	0.94	0.07	34,34,34,34	0
34	NA	0	8339	1/1	0.94	0.08	34,34,34,34	0
34	NA	0	8379	1/1	0.94	0.08	34,34,34,34	0
34	NA	0	8310	1/1	0.95	0.14	20,20,20,20	0
34	NA	0	8314	1/1	0.95	0.11	26,26,26,26	0
32	MG	0	8051	1/1	0.95	0.07	86,86,86,86	0
32	MG	0	8084	1/1	0.95	0.13	101,101,101,101	0
34	NA	0	8358	1/1	0.95	0.18	102,102,102,102	0
34	NA	0	8320	1/1	0.95	0.07	44,44,44,44	0
34	NA	L	8347	1/1	0.95	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8085	1/1	0.95	0.07	82,82,82,82	0
34	NA	0	8361	1/1	0.95	0.14	47,47,47,47	0
32	MG	0	8057	1/1	0.95	0.08	51,51,51,51	0
32	MG	0	8090	1/1	0.95	0.11	65,65,65,65	0
32	MG	0	8091	1/1	0.95	0.07	73,73,73,73	0
34	NA	0	8328	1/1	0.95	0.10	51,51,51,51	0
34	NA	0	8367	1/1	0.95	0.08	54,54,54,54	0
35	CL	0	8513	1/1	0.95	0.07	62,62,62,62	0
35	CL	0	8514	1/1	0.95	0.12	80,80,80,80	0
32	MG	0	8059	1/1	0.95	0.08	84,84,84,84	0
34	NA	0	8330	1/1	0.95	0.06	45,45,45,45	0
32	MG	0	8097	1/1	0.95	0.17	37,37,37,37	0
32	MG	0	8041	1/1	0.95	0.08	53,53,53,53	0
35	CL	B	8519	1/1	0.95	0.17	58,58,58,58	0
34	NA	0	8334	1/1	0.95	0.09	36,36,36,36	0
32	MG	0	8100	1/1	0.95	0.10	74,74,74,74	0
32	MG	0	8045	1/1	0.95	0.07	67,67,67,67	0
34	NA	0	8378	1/1	0.95	0.38	45,45,45,45	0
34	NA	0	8342	1/1	0.95	0.07	36,36,36,36	0
34	NA	0	8343	1/1	0.95	0.05	33,33,33,33	0
34	NA	0	8335	1/1	0.96	0.17	54,54,54,54	0
34	NA	0	8375	1/1	0.96	0.13	55,55,55,55	0
34	NA	0	8323	1/1	0.96	0.12	46,46,46,46	0
34	NA	0	8340	1/1	0.96	0.10	36,36,36,36	0
32	MG	0	8116	1/1	0.96	0.04	40,40,40,40	0
34	NA	0	8311	1/1	0.96	0.10	44,44,44,44	0
32	MG	0	8088	1/1	0.96	0.08	34,34,34,34	0
34	NA	0	8366	1/1	0.96	0.05	48,48,48,48	0
32	MG	A	8066	1/1	0.96	0.06	44,44,44,44	0
32	MG	A	8105	1/1	0.96	0.09	29,29,29,29	0
34	NA	A	8345	1/1	0.96	0.06	58,58,58,58	0
34	NA	C	8304	1/1	0.96	0.05	59,59,59,59	0
34	NA	0	8355	1/1	0.96	0.12	59,59,59,59	0
35	CL	I	8521	1/1	0.96	0.07	54,54,54,54	0
34	NA	0	8318	1/1	0.96	0.09	20,20,20,20	0
32	MG	0	8098	1/1	0.96	0.13	18,18,18,18	0
34	NA	0	8321	1/1	0.96	0.09	45,45,45,45	0
33	K	0	8201	1/1	0.96	0.17	74,74,74,74	0
35	CL	2	8504	1/1	0.96	0.08	77,77,77,77	0
36	CD	N	8405	1/1	0.96	0.05	90,90,90,90	0
32	MG	0	8108	1/1	0.97	0.07	61,61,61,61	0
34	NA	Q	8338	1/1	0.97	0.09	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8111	1/1	0.97	0.04	57,57,57,57	0
34	NA	0	8353	1/1	0.97	0.06	40,40,40,40	0
34	NA	0	8354	1/1	0.97	0.14	44,44,44,44	0
32	MG	0	8028	1/1	0.97	0.05	93,93,93,93	0
34	NA	0	8327	1/1	0.97	0.05	37,37,37,37	0
34	NA	0	8376	1/1	0.97	0.10	33,33,33,33	0
34	NA	0	8377	1/1	0.97	0.18	66,66,66,66	0
32	MG	0	8093	1/1	0.97	0.04	37,37,37,37	0
35	CL	0	8516	1/1	0.97	0.17	65,65,65,65	0
32	MG	0	8094	1/1	0.97	0.07	56,56,56,56	0
34	NA	0	8313	1/1	0.97	0.06	77,77,77,77	0
32	MG	0	8062	1/1	0.97	0.05	67,67,67,67	0
34	NA	0	8315	1/1	0.97	0.08	41,41,41,41	0
32	MG	0	8063	1/1	0.97	0.07	143,143,143,143	0
32	MG	0	8055	1/1	0.97	0.04	54,54,54,54	0
34	NA	0	8336	1/1	0.97	0.06	50,50,50,50	0
35	CL	J	8512	1/1	0.97	0.08	40,40,40,40	0
32	MG	0	8071	1/1	0.97	0.06	104,104,104,104	0
35	CL	L	8518	1/1	0.97	0.08	52,52,52,52	0
34	NA	0	8301	1/1	0.97	0.04	30,30,30,30	0
34	NA	H	8309	1/1	0.97	0.08	29,29,29,29	0
32	MG	0	8089	1/1	0.97	0.04	60,60,60,60	0
32	MG	0	8075	1/1	0.97	0.03	54,54,54,54	0
32	MG	0	8042	1/1	0.97	0.06	32,32,32,32	0
32	MG	0	8102	1/1	0.98	0.06	61,61,61,61	0
32	MG	0	8117	1/1	0.98	0.05	28,28,28,28	0
32	MG	0	8048	1/1	0.98	0.04	35,35,35,35	0
34	NA	0	8344	1/1	0.98	0.04	21,21,21,21	0
34	NA	0	8349	1/1	0.98	0.10	51,51,51,51	0
32	MG	0	8074	1/1	0.98	0.04	29,29,29,29	0
32	MG	0	8106	1/1	0.98	0.04	58,58,58,58	0
32	MG	0	8054	1/1	0.98	0.09	17,17,17,17	0
32	MG	S	8073	1/1	0.98	0.04	64,64,64,64	0
32	MG	X	8109	1/1	0.98	0.04	34,34,34,34	0
34	NA	0	8331	1/1	0.98	0.16	50,50,50,50	0
32	MG	0	8110	1/1	0.98	0.05	34,34,34,34	0
33	K	0	8202	1/1	0.98	0.08	79,79,79,79	0
32	MG	0	8012	1/1	0.98	0.07	18,18,18,18	0
34	NA	0	8319	1/1	0.98	0.04	37,37,37,37	0
35	CL	Q	8506	1/1	0.98	0.06	52,52,52,52	0
32	MG	0	8112	1/1	0.98	0.08	52,52,52,52	0
32	MG	0	8039	1/1	0.98	0.04	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8115	1/1	0.98	0.06	27,27,27,27	0
32	MG	0	8008	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8025	1/1	0.99	0.03	24,24,24,24	0
32	MG	0	8027	1/1	0.99	0.05	69,69,69,69	0
32	MG	0	8009	1/1	0.99	0.03	53,53,53,53	0
32	MG	0	8052	1/1	0.99	0.08	42,42,42,42	0
32	MG	0	8053	1/1	0.99	0.04	47,47,47,47	0
34	NA	I	8346	1/1	0.99	0.02	39,39,39,39	0
32	MG	0	8029	1/1	0.99	0.03	38,38,38,38	0
32	MG	0	8096	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8030	1/1	0.99	0.04	25,25,25,25	0
32	MG	0	8032	1/1	0.99	0.06	26,26,26,26	0
32	MG	0	8058	1/1	0.99	0.04	63,63,63,63	0
32	MG	0	8034	1/1	0.99	0.06	16,16,16,16	0
32	MG	0	8060	1/1	0.99	0.03	34,34,34,34	0
32	MG	0	8061	1/1	0.99	0.02	23,23,23,23	0
32	MG	0	8035	1/1	0.99	0.04	50,50,50,50	0
32	MG	0	8037	1/1	0.99	0.03	32,32,32,32	0
32	MG	0	8064	1/1	0.99	0.12	22,22,22,22	0
32	MG	0	8107	1/1	0.99	0.03	52,52,52,52	0
32	MG	0	8004	1/1	0.99	0.03	44,44,44,44	0
32	MG	0	8068	1/1	0.99	0.03	52,52,52,52	0
32	MG	0	8070	1/1	0.99	0.07	41,41,41,41	0
32	MG	0	8040	1/1	0.99	0.03	53,53,53,53	0
32	MG	0	8072	1/1	0.99	0.07	38,38,38,38	0
32	MG	0	8006	1/1	0.99	0.03	46,46,46,46	0
32	MG	0	8013	1/1	0.99	0.04	64,64,64,64	0
32	MG	0	8043	1/1	0.99	0.07	58,58,58,58	0
32	MG	0	8079	1/1	0.99	0.03	50,50,50,50	0
32	MG	0	8081	1/1	0.99	0.04	34,34,34,34	0
32	MG	0	8014	1/1	0.99	0.05	16,16,16,16	0
32	MG	B	8056	1/1	0.99	0.03	65,65,65,65	0
32	MG	0	8083	1/1	0.99	0.07	36,36,36,36	0
32	MG	0	8016	1/1	0.99	0.03	50,50,50,50	0
32	MG	0	8018	1/1	0.99	0.03	75,75,75,75	0
32	MG	2	8078	1/1	0.99	0.02	31,31,31,31	0
32	MG	0	8086	1/1	0.99	0.08	61,61,61,61	0
32	MG	0	8023	1/1	0.99	0.03	20,20,20,20	0
36	CD	2	8404	1/1	0.99	0.03	76,76,76,76	0
32	MG	A	8065	1/1	1.00	0.02	56,56,56,56	0
32	MG	0	8021	1/1	1.00	0.03	19,19,19,19	0
32	MG	0	8077	1/1	1.00	0.02	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8038	1/1	1.00	0.01	23,23,23,23	0
32	MG	0	8080	1/1	1.00	0.02	39,39,39,39	0
32	MG	0	8022	1/1	1.00	0.06	27,27,27,27	0
32	MG	0	8005	1/1	1.00	0.05	55,55,55,55	0
32	MG	0	8002	1/1	1.00	0.03	23,23,23,23	0
32	MG	0	8007	1/1	1.00	0.03	14,14,14,14	0
32	MG	0	8026	1/1	1.00	0.02	25,25,25,25	0
32	MG	0	8003	1/1	1.00	0.03	26,26,26,26	0
32	MG	0	8015	1/1	1.00	0.02	61,61,61,61	0
32	MG	0	8001	1/1	1.00	0.02	40,40,40,40	0
32	MG	0	8017	1/1	1.00	0.04	33,33,33,33	0
32	MG	0	8031	1/1	1.00	0.06	19,19,19,19	0
32	MG	0	8010	1/1	1.00	0.04	19,19,19,19	0
32	MG	0	8033	1/1	1.00	0.01	15,15,15,15	0
32	MG	0	8019	1/1	1.00	0.05	24,24,24,24	0
32	MG	0	8020	1/1	1.00	0.02	25,25,25,25	0
36	CD	T	8401	1/1	1.00	0.02	78,78,78,78	0
36	CD	Y	8403	1/1	1.00	0.02	82,82,82,82	0
36	CD	Z	8402	1/1	1.00	0.03	75,75,75,75	0
32	MG	0	8036	1/1	1.00	0.03	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.