



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:06 AM GMT

PDB ID : 2OTJ
Title : 13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

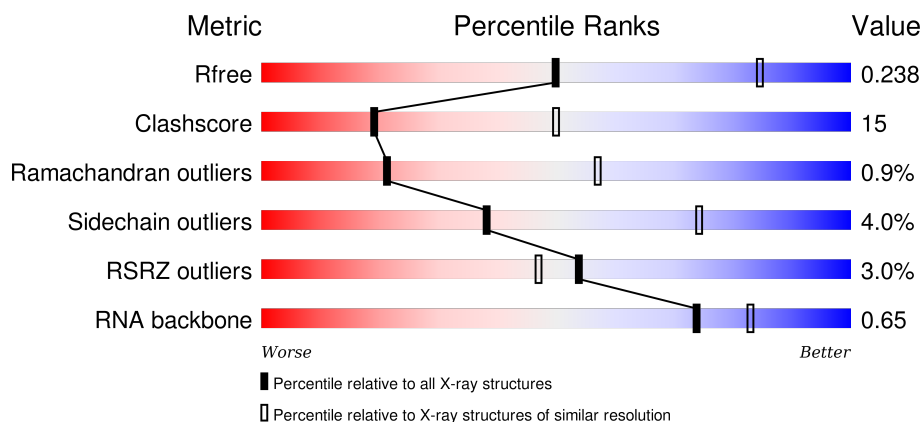
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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








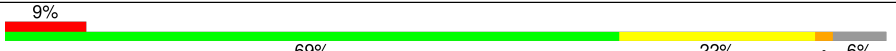
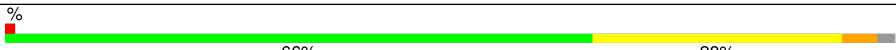

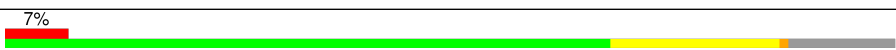

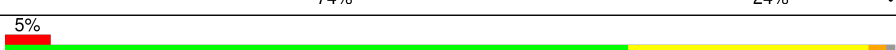
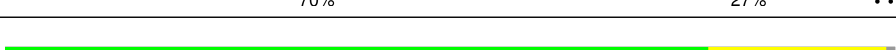

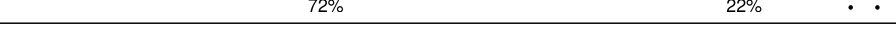
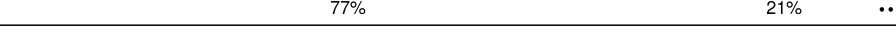
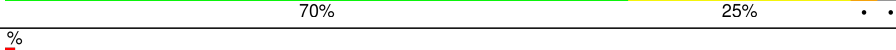





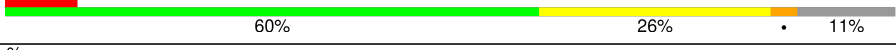
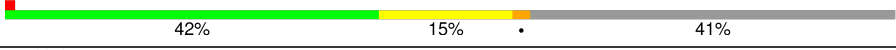


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>49%</div> <div>39%</div> <div>6%</div> <div>6%</div> </div>
2	9	122	<div>2%</div> <div>38%</div> <div>48%</div> <div>13%</div> <div>.</div>
3	A	240	<div>3%</div> <div>68%</div> <div>27%</div> <div>.</div> <div>.</div>
4	B	338	<div>62%</div> <div>34%</div> <div>.</div>



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	3	92	
31	I	161	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	13T	0	9000	-	-	X	X
33	MG	0	8013	-	-	-	X
33	MG	0	8062	-	-	-	X
33	MG	0	8102	-	-	-	X
33	MG	0	8114	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8515	-	-	-	X
35	NA	0	8520	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8531	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8539	-	-	-	X
35	NA	0	8540	-	-	-	X
35	NA	0	8542	-	-	X	-
35	NA	0	8543	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8579	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	J	8801	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99043 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
			59021	26350	10878	19048	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

- 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 protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	-	INSERTION	UNP P60617
H	166	SER	-	INSERTION	UNP P60617
H	167	PRO	-	INSERTION	UNP P60617
H	168	ALA	-	INSERTION	UNP P60617
H	169	GLY	-	INSERTION	UNP P60617
H	170	ASN	-	INSERTION	UNP P60617
H	171	ALA	-	INSERTION	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	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 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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	UNP P60618
M	194	ALA	-	INSERTION	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

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

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S			
			579	346	116	112	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	INSERTION	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

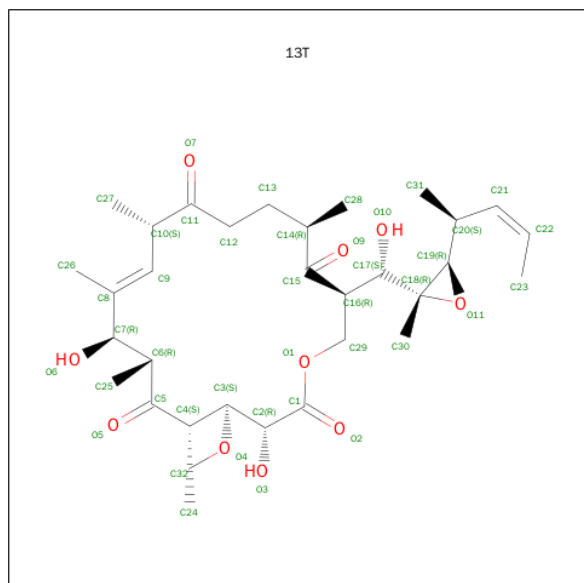
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is 13-DEOXYTEDANOLIDE (three-letter code: 13T) (formula: C₃₂H₅₀O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	0	1	Total	C	O	0	0
			42	32	10		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
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	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	2	Total	Mg	0	0
			2	2		

- 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	74	Total	Na	0	0
			74	74		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	H	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	9	2	Total 2	Na 2	0	0
35	L	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	9	Total 9	Cl 9	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	2	Total 2	Cl 2	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 CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5905	Total O 5905 5905	0	0
38	9	140	Total O 140 140	0	0
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	170	Total O 170 170	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	19	Total O 19 19	0	0
38	H	70	Total O 70 70	0	0
38	J	58	Total O 58 58	0	0
38	K	59	Total O 59 59	0	0
38	L	83	Total O 83 83	0	0
38	M	123	Total O 123 123	0	0
38	N	63	Total O 63 63	0	0

Continued on next page...

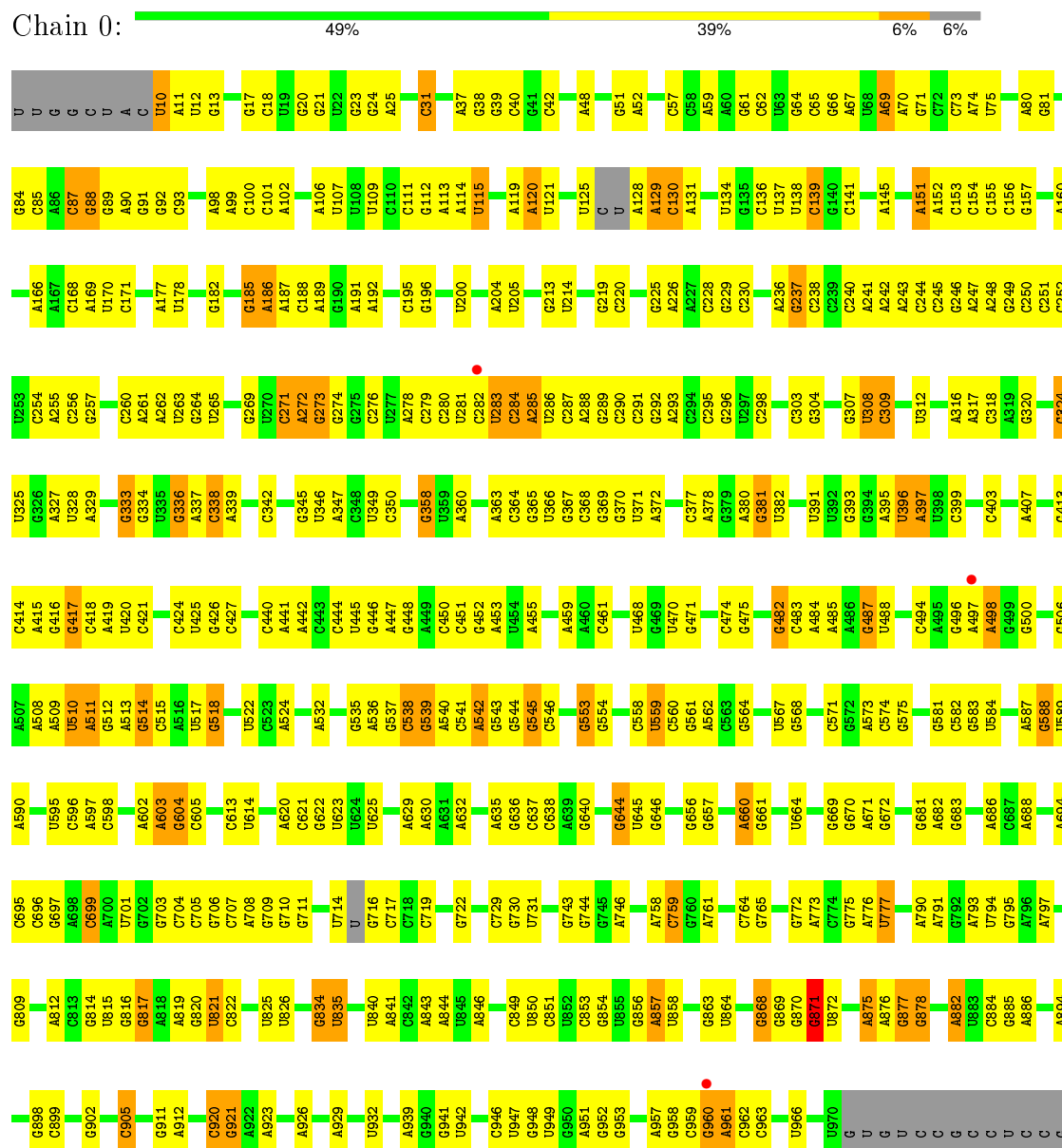
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	56	Total 56	O 56	0	0
38	Q	51	Total 51	O 51	0	0
38	R	80	Total 80	O 80	0	0
38	S	36	Total 36	O 36	0	0
38	T	33	Total 33	O 33	0	0
38	U	26	Total 26	O 26	0	0
38	V	11	Total 11	O 11	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	96	Total 96	O 96	0	0
38	Z	31	Total 31	O 31	0	0
38	1	56	Total 56	O 56	0	0
38	2	45	Total 45	O 45	0	0
38	3	66	Total 66	O 66	0	0
38	I	8	Total 8	O 8	0	0

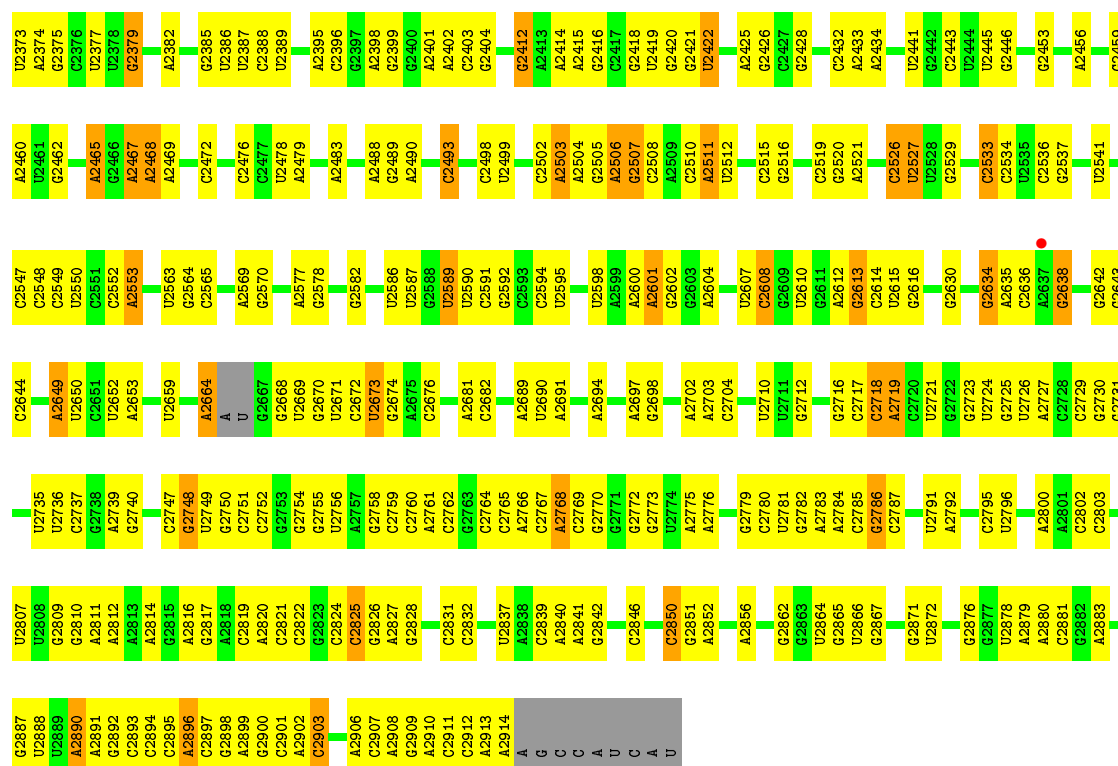
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

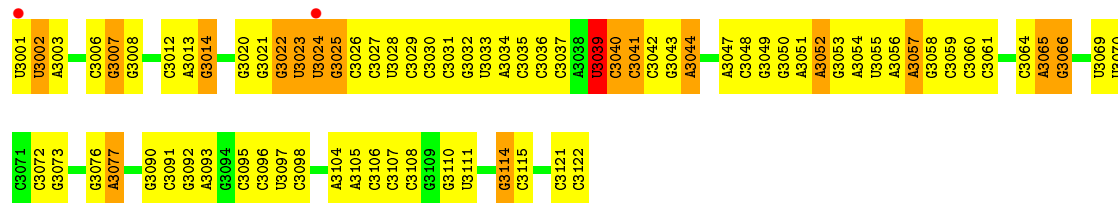
- Molecule 1: 23S ribosomal RNA







• Molecule 2: 5S ribosomal RNA

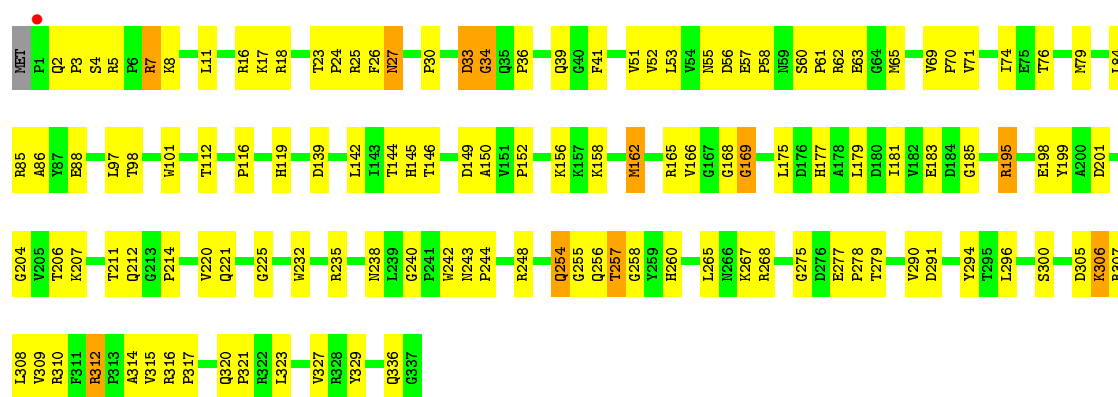


• Molecule 3: 50S ribosomal protein L2P

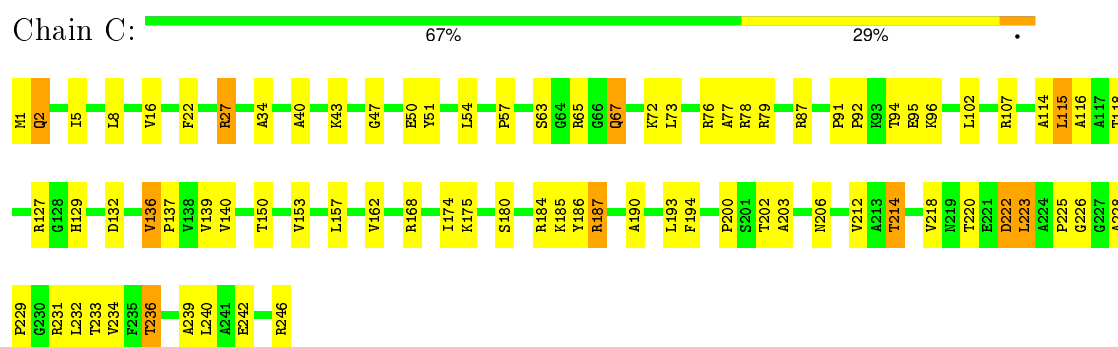


• Molecule 4: 50S ribosomal protein L3P

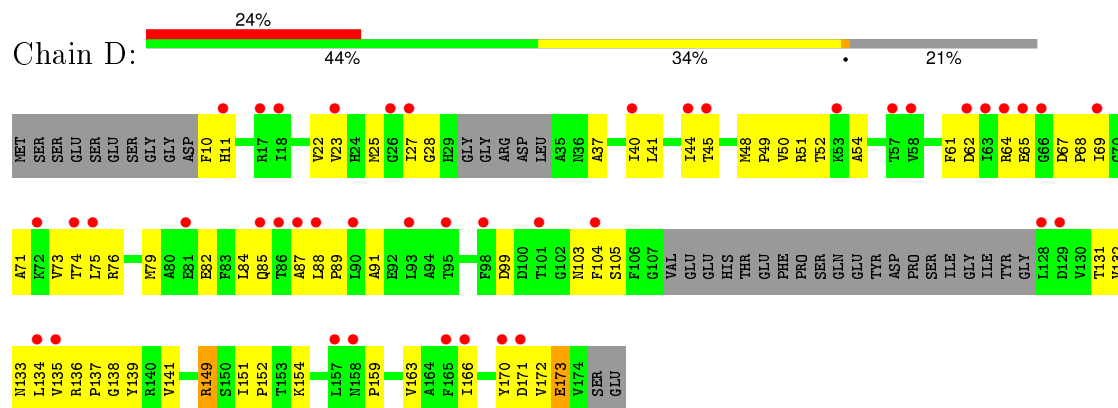




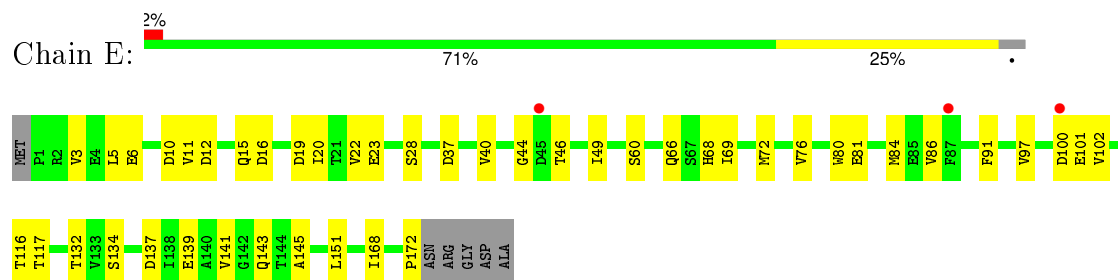
• Molecule 5: 50S ribosomal protein L4P



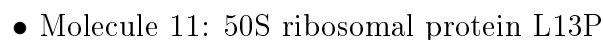
• Molecule 6: 50S ribosomal protein L5P



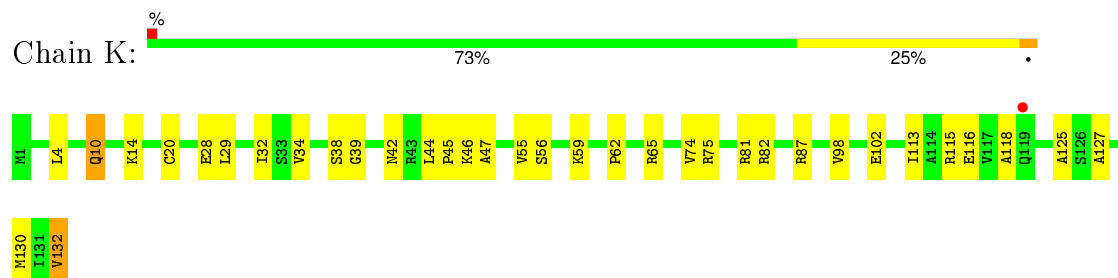
• Molecule 7: 50S ribosomal protein L6P



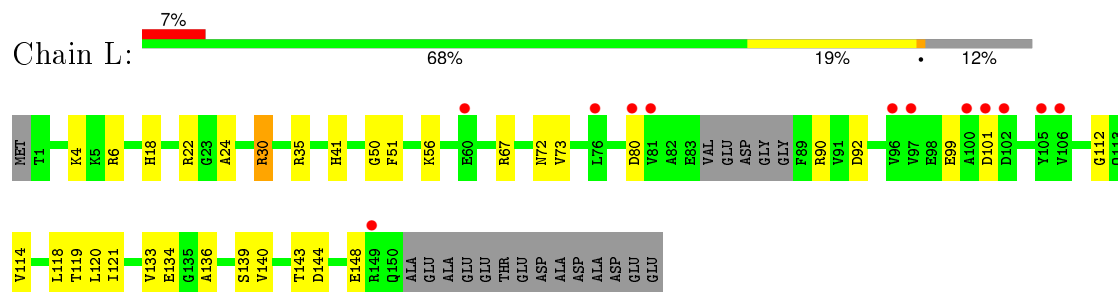
• Molecule 8: 50S ribosomal protein L7Ae



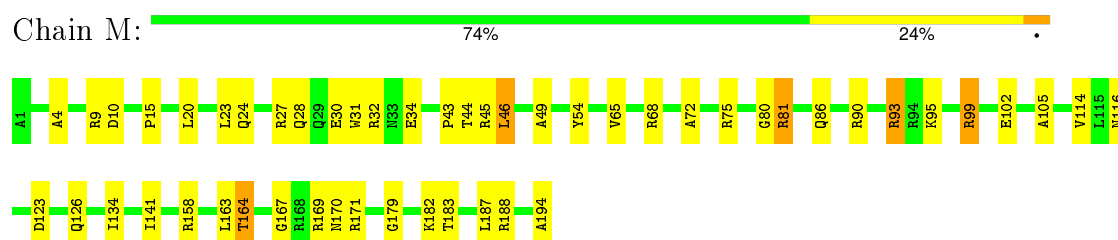
- Molecule 12: 50S ribosomal protein L14P



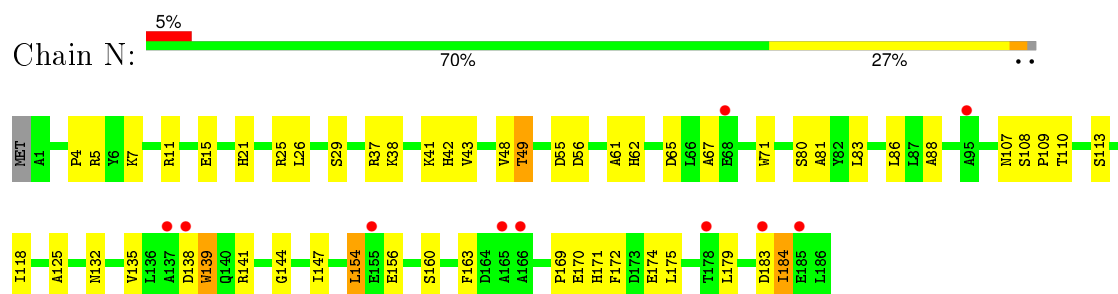
- Molecule 13: 50S ribosomal protein L15P



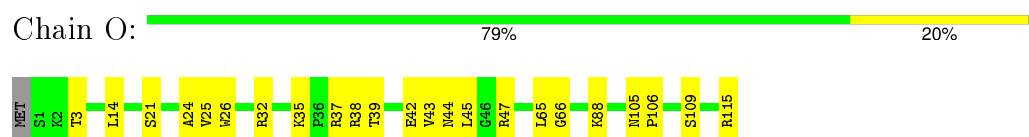
- Molecule 14: 50S ribosomal protein L15e



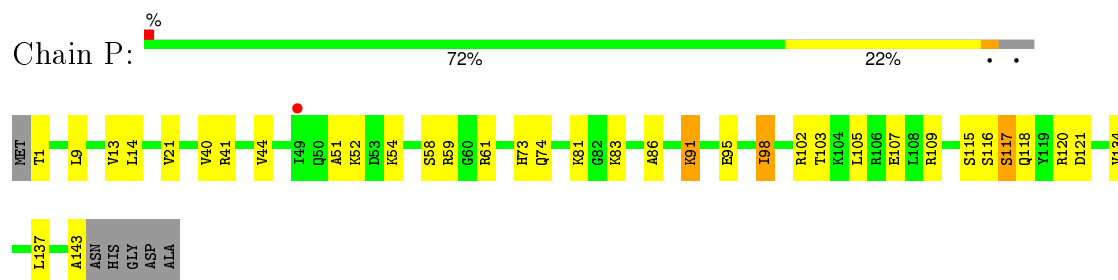
- Molecule 15: 50S ribosomal protein L18P



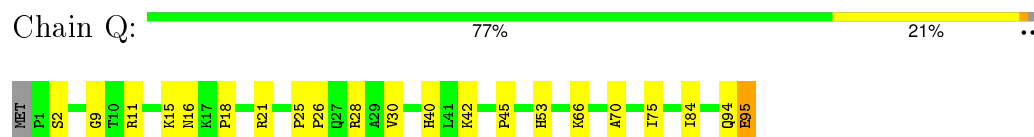
- Molecule 16: 50S ribosomal protein L18e



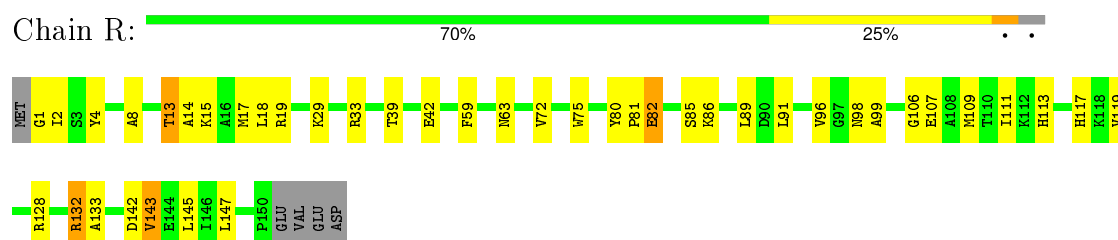
- Molecule 17: 50S ribosomal protein L19e



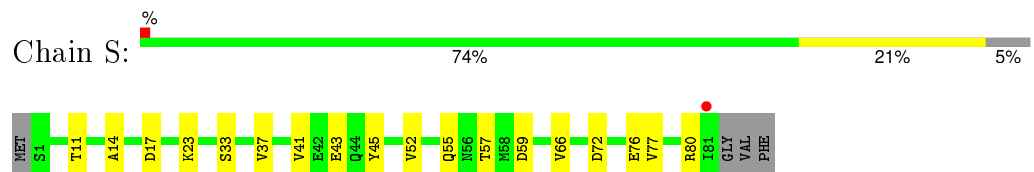
- Molecule 18: 50S ribosomal protein L21e



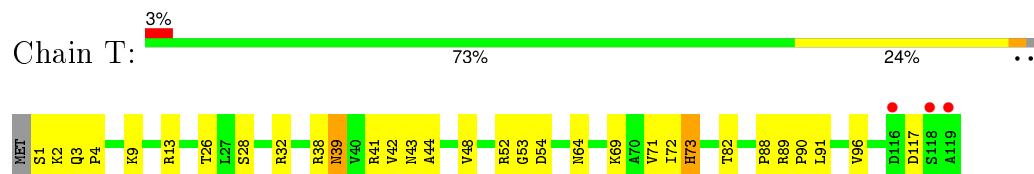
- Molecule 19: 50S ribosomal protein L22P



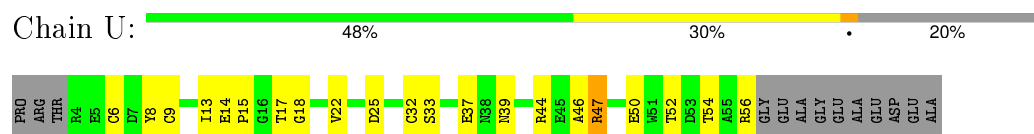
- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P

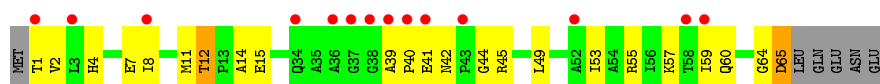


- Molecule 22: 50S ribosomal protein L24e



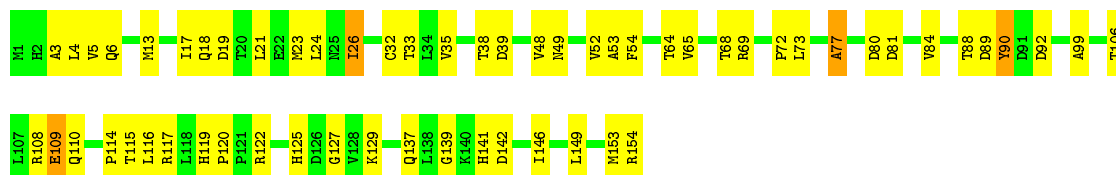
- Molecule 23: 50S ribosomal protein L29P





- Molecule 24: 50S ribosomal protein L30P

Chain W: 62% 36%



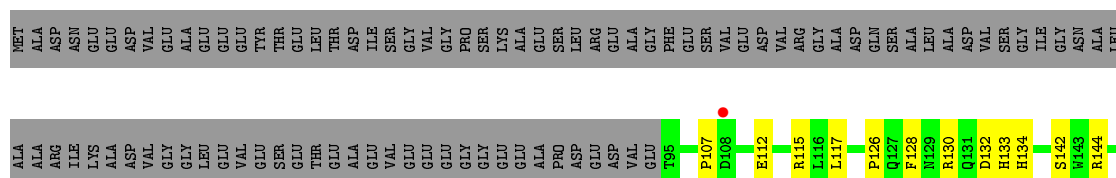
- Molecule 25: 50S ribosomal protein L31e

Chain X: 8% 60% 26% 11%



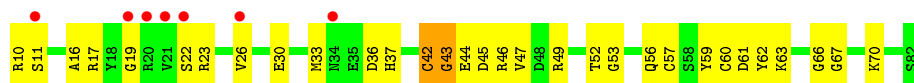
- Molecule 26: 50S ribosomal protein L32e

Chain Y: 42% 15% 41%



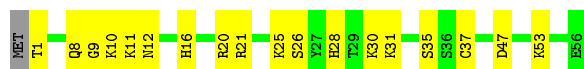
- Molecule 27: 50S ribosomal protein L37Ae

Chain Z: 10% 58% 40%



- Molecule 28: 50S ribosomal protein L37e

Chain 1: 67% 32%

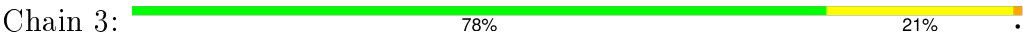


- Molecule 29: 50S ribosomal protein L39e

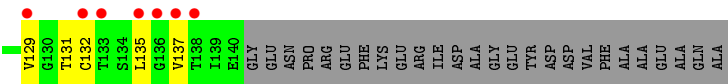
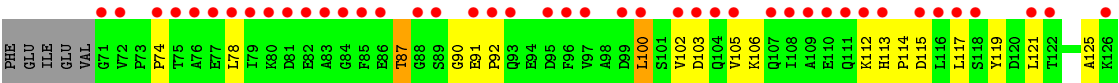
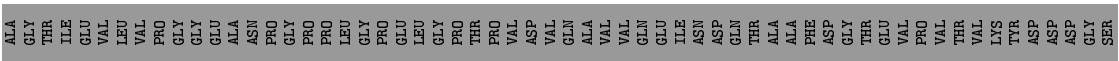
Chain 2: 6% 54% 38% 8%



• Molecule 30: 50S ribosomal protein L44E



• Molecule 31: 50S ribosomal protein L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.90 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.90) 91.7 (85.48-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.238 0.209 , 0.238	Depositor DCC
R_{free} test set	3898 reflections (1.06%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 422682 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99043	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, UR3, CD, OMU, 13T, 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	0.39	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.69	1/4528 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.34	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.58	0/1498
7	E	0.34	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.33	0/241	0.49	0/324
10	H	0.38	0/1287	0.65	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.35	0/1130	0.64	0/1509
14	M	0.37	0/1584	0.63	0/2119
15	N	0.31	0/1474	0.65	1/1999 (0.1%)
16	O	0.36	0/874	0.61	1/1181 (0.1%)
17	P	0.35	0/1147	0.55	0/1528
18	Q	0.37	0/749	0.68	0/1005
19	R	0.36	0/1172	0.64	0/1578
20	S	0.35	0/648	0.59	0/875
21	T	0.34	0/958	0.63	0/1289
22	U	0.36	0/417	0.56	0/562
23	V	0.35	0/502	0.56	0/675
24	W	0.34	0/1219	0.63	0/1655
25	X	0.35	0/664	0.59	0/895
26	Y	0.36	0/1146	0.63	0/1536
27	Z	0.39	0/590	0.64	0/787
28	1	0.40	0/438	0.63	0/578
29	2	0.37	0/401	0.56	0/529
30	3	0.37	0/771	0.57	0/1024
31	I	0.35	0/526	0.57	0/716
All	All	0.38	0/98693	0.67	17/147577 (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	42
2	9	0	2
24	W	0	1
All	All	1	45

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.37	130.11	109.50
2	9	3039	U	N1-C1'-C2'	6.50	122.45	114.00
1	0	2316	G	C5'-C4'-C3'	-6.49	105.61	116.00
1	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
1	0	1942	A	C5'-C4'-C3'	6.20	125.92	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	131	A	Sidechain
1	0	220	C	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	48	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	59021	0	29812	1337	0
2	9	2600	0	1326	95	0
3	A	1753	0	1766	78	0
4	B	2625	0	2533	112	0
5	C	1859	0	1816	74	0
6	D	1094	0	1085	56	0
7	E	1357	0	1266	38	0
8	F	890	0	843	32	0
9	G	240	0	231	9	0
10	H	1266	0	1268	39	0
11	J	1120	0	1098	49	0
12	K	992	0	1031	40	0
13	L	1118	0	1076	28	0
14	M	1560	0	1568	45	0
15	N	1445	0	1401	45	0
16	O	865	0	873	21	0
17	P	1136	0	1123	33	0
18	Q	735	0	728	22	0
19	R	1149	0	1122	41	0
20	S	641	0	605	14	0
21	T	950	0	923	25	0
22	U	410	0	364	21	0
23	V	499	0	511	19	0
24	W	1196	0	1137	57	0
25	X	654	0	653	25	0
26	Y	1130	0	1133	46	0
27	Z	579	0	539	25	0
28	1	431	0	426	21	0
29	2	396	0	413	18	0
30	3	755	0	728	18	0
31	I	519	0	500	23	0
32	0	42	0	50	24	0
33	0	108	0	0	0	0
33	3	2	0	0	0	0
33	9	1	0	0	0	0
33	A	2	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
35	0	74	0	0	2	0
35	9	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	2	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	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	2	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5905	0	0	199	0
38	1	56	0	0	1	0
38	2	45	0	0	4	0
38	3	66	0	0	2	0
38	9	140	0	0	10	0
38	A	112	0	0	8	0
38	B	142	0	0	21	0
38	C	170	0	0	16	0
38	D	45	0	0	8	0
38	E	42	0	0	5	0
38	F	26	0	0	2	0
38	G	19	0	0	0	0
38	H	70	0	0	6	0
38	I	8	0	0	1	0
38	J	58	0	0	3	0
38	K	59	0	0	1	0
38	L	83	0	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	123	0	0	4	0
38	N	63	0	0	6	0
38	O	44	0	0	3	0
38	P	56	0	0	2	0
38	Q	51	0	0	5	0
38	R	80	0	0	2	0
38	S	36	0	0	2	0
38	T	33	0	0	1	0
38	U	26	0	0	2	0
38	V	11	0	0	1	0
38	W	67	0	0	6	0
38	X	21	0	0	2	0
38	Y	96	0	0	6	0
38	Z	31	0	0	2	0
All	All	99043	0	59948	2276	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 15.

The worst 5 of 2276 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)
1:0:871:G:C8	1:0:871:G:H5'	1.77	1.19
1:0:1160:G:C5'	1:0:1161:A:H5'	1.73	1.18
1:0:1160:G:H5'	1:0:1161:A:C5'	1.79	1.12
1:0:871:G:H8	1:0:871:G:H5'	1.01	1.09
1:0:1002:G:H2'	1:0:1003:U:H5''	1.37	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
3	A	235/240 (98%)	212 (90%)	21 (9%)	2 (1%)	21	57
4	B	335/338 (99%)	310 (92%)	21 (6%)	4 (1%)	16	48
5	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	24	60
6	D	134/177 (76%)	113 (84%)	18 (13%)	3 (2%)	8	31
7	E	170/178 (96%)	163 (96%)	6 (4%)	1 (1%)	30	67
8	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	7	26
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	10	35
11	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	14	44
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	121 (86%)	20 (14%)	0	100	100
14	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
15	N	184/187 (98%)	167 (91%)	13 (7%)	4 (2%)	8	31
16	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
17	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	26	63
18	Q	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	17	51
19	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
20	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	57
22	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
24	W	152/154 (99%)	150 (99%)	0	2 (1%)	15	46
25	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	15	46
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	60 (84%)	9 (13%)	2 (3%)	6	24
28	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
31	I	68/161 (42%)	62 (91%)	6 (9%)	0	100	100
All	All	3705/4419 (84%)	3436 (93%)	237 (6%)	32 (1%)	21	57

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	101	ALA
10	H	166	SER
11	J	5	GLU
15	N	154	LEU
15	N	183	ASP

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	
3	A	179/182 (98%)	170 (95%)	9 (5%)	30	65
4	B	282/283 (100%)	268 (95%)	14 (5%)	30	65
5	C	193/193 (100%)	178 (92%)	15 (8%)	16	41
6	D	117/148 (79%)	115 (98%)	2 (2%)	68	91
7	E	152/156 (97%)	149 (98%)	3 (2%)	63	88
8	F	93/94 (99%)	89 (96%)	4 (4%)	35	71
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	126 (96%)	6 (4%)	34	70
11	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
12	K	106/106 (100%)	104 (98%)	2 (2%)	65	89
13	L	113/127 (89%)	107 (95%)	6 (5%)	28	63
14	M	158/158 (100%)	149 (94%)	9 (6%)	25	59
15	N	149/150 (99%)	146 (98%)	3 (2%)	63	88
16	O	93/94 (99%)	92 (99%)	1 (1%)	80	95
17	P	113/117 (97%)	109 (96%)	4 (4%)	43	78
18	Q	79/80 (99%)	78 (99%)	1 (1%)	76	94
19	R	117/122 (96%)	113 (97%)	4 (3%)	44	79
20	S	71/74 (96%)	70 (99%)	1 (1%)	74	93
21	T	105/106 (99%)	99 (94%)	6 (6%)	25	59
22	U	44/52 (85%)	43 (98%)	1 (2%)	58	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	51/57 (90%)	49 (96%)	2 (4%)	39	75
24	W	130/130 (100%)	124 (95%)	6 (5%)	33	69
25	X	66/74 (89%)	61 (92%)	5 (8%)	16	43
26	Y	120/196 (61%)	114 (95%)	6 (5%)	30	65
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/47 (98%)	45 (98%)	1 (2%)	60	88
29	2	42/46 (91%)	40 (95%)	2 (5%)	31	67
30	3	79/79 (100%)	78 (99%)	1 (1%)	76	94
31	I	58/129 (45%)	56 (97%)	2 (3%)	44	79
All	All	3093/3602 (86%)	2969 (96%)	124 (4%)	38	74

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	79	PHE
14	M	10	ASP
26	Y	200	THR
11	J	93	ARG
12	K	132	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	137	ASN
18	Q	40	HIS
29	2	45	ASN
14	M	170	ASN
17	P	50	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	241 (8%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	259 (9%)	34 (1%)

5 of 259 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1246	A
1	0	1474	C
1	0	2718	C
1	0	1377	C
1	0	699	C

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

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	12,22,23	0.96	1 (8%)	19,31,34	3.15	2 (10%)
1	OMG	0	2588	1	17,26,27	1.00	1 (5%)	21,38,41	2.54	3 (14%)
1	UR3	0	2619	1	12,22,23	0.77	0	16,32,35	0.78	0
1	PSU	0	2621	1	13,21,22	1.65	2 (15%)	18,30,33	6.12	3 (16%)
1	1MA	0	628	1	14,25,26	0.94	1 (7%)	15,37,40	1.20	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.05	1.47	1.52
1	0	2587	OMU	C4-N3	2.31	1.37	1.33
1	0	2621	PSU	C4-N3	2.38	1.37	1.33
1	0	628	1MA	C6-N6	2.49	1.33	1.29
1	0	2588	OMG	C6-N1	3.08	1.38	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.44	114.65	128.33
1	0	2588	OMG	C5-C6-N1	-8.74	111.64	123.59
1	0	628	1MA	C2-N3-C4	-3.75	110.59	116.40
1	0	2587	OMU	C5-C4-N3	-3.32	114.61	123.12
1	0	2588	OMG	N3-C2-N1	-2.34	123.89	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	13T	0	9000	-	40,43,43	2.02	11 (27%)	43,63,63	1.90	5 (11%)

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
32	13T	0	9000	-	-	0/73/81/81	0/0/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	13T	O1-C1	2.06	1.37	1.33
32	0	9000	13T	C26-C8	2.21	1.54	1.50
32	0	9000	13T	C27-C10	2.33	1.57	1.53
32	0	9000	13T	C10-C11	2.35	1.54	1.52
32	0	9000	13T	C29-C16	2.42	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	13T	O11-C18-C19	-4.16	56.62	59.46
32	0	9000	13T	O11-C19-C18	-2.35	58.01	59.87
32	0	9000	13T	C27-C10-C9	2.61	113.14	110.72
32	0	9000	13T	O4-C3-C4	3.86	115.61	106.02
32	0	9000	13T	C18-O11-C19	8.40	65.36	60.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	13T	24	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.44	9 (0%) 94 94	23, 50, 93, 150	0
2	9	122/122 (100%)	-0.64	2 (1%) 74 72	43, 69, 91, 151	0
3	A	237/240 (98%)	-0.20	7 (2%) 54 47	32, 55, 86, 105	0
4	B	337/338 (99%)	-0.27	1 (0%) 94 94	33, 60, 82, 90	0
5	C	246/246 (100%)	-0.43	0 100 100	30, 50, 73, 82	0
6	D	140/177 (79%)	1.29	42 (30%) 1 0	63, 103, 124, 130	0
7	E	172/178 (96%)	-0.12	3 (1%) 73 70	55, 73, 90, 96	0
8	F	119/120 (99%)	0.40	6 (5%) 32 26	57, 74, 96, 106	0
9	G	29/348 (8%)	0.81	4 (13%) 4 2	81, 94, 103, 103	0
10	H	160/171 (93%)	0.45	15 (9%) 11 6	52, 67, 93, 100	0
11	J	142/145 (97%)	-0.36	2 (1%) 78 76	45, 56, 74, 94	0
12	K	132/132 (100%)	-0.43	1 (0%) 87 86	41, 54, 75, 81	0
13	L	145/165 (87%)	0.29	12 (8%) 14 9	32, 71, 107, 118	0
14	M	194/194 (100%)	-0.51	0 100 100	36, 47, 60, 64	0
15	N	186/187 (99%)	0.11	10 (5%) 29 23	50, 67, 110, 119	0
16	O	115/116 (99%)	-0.33	0 100 100	44, 59, 71, 76	0
17	P	143/149 (95%)	-0.29	1 (0%) 89 88	46, 60, 70, 75	0
18	Q	95/96 (98%)	-0.43	0 100 100	43, 52, 64, 72	0
19	R	150/155 (96%)	-0.42	0 100 100	38, 50, 68, 73	0
20	S	81/85 (95%)	-0.04	1 (1%) 81 78	52, 65, 81, 85	0
21	T	119/120 (99%)	-0.06	3 (2%) 61 55	47, 62, 83, 96	0
22	U	53/66 (80%)	-0.19	0 100 100	51, 61, 75, 81	0
23	V	65/71 (91%)	1.30	14 (21%) 1 0	59, 79, 109, 114	0
24	W	154/154 (100%)	-0.38	0 100 100	42, 56, 70, 77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.18	7 (8%) 13 8	52, 64, 87, 97	0
26	Y	142/241 (58%)	-0.56	2 (1%) 78 76	30, 51, 70, 86	0
27	Z	73/73 (100%)	0.31	7 (9%) 10 6	58, 69, 80, 94	0
28	1	56/57 (98%)	-0.42	0 100 100	31, 37, 43, 51	0
29	2	46/50 (92%)	0.17	3 (6%) 22 16	41, 69, 90, 99	0
30	3	92/92 (100%)	-0.34	0 100 100	42, 60, 71, 82	0
31	I	70/161 (43%)	3.26	50 (71%) 0 0	109, 119, 135, 135	0
All	All	6646/7463 (89%)	-0.21	202 (3%) 54 47	23, 57, 100, 151	0

The worst 5 of 202 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	I	75	THR	9.3
31	I	79	ILE	8.8
23	V	1	THR	8.5
31	I	109	ALA	8.2
6	D	63	ILE	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PSU	0	2621	20/21	0.97	0.12	-	30,32,39,40	0
1	OMG	0	2588	24/25	0.97	0.13	-	37,38,39,40	0
1	UR3	0	2619	21/22	0.96	0.15	-	36,38,39,40	0
1	OMU	0	2587	21/22	0.95	0.12	-	38,39,40,41	0
1	1MA	0	628	23/24	0.96	0.17	-	33,35,36,37	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8577	1/1	0.63	0.73	58.21	81,81,81,81	0
34	K	0	8401	1/1	0.87	0.73	46.07	84,84,84,84	0
35	NA	0	8574	1/1	0.92	0.62	40.12	67,67,67,67	0
35	NA	0	8550	1/1	0.66	0.61	29.90	65,65,65,65	0
35	NA	0	8525	1/1	0.98	0.39	20.43	59,59,59,59	0
35	NA	0	8531	1/1	0.54	0.38	19.66	57,57,57,57	0
35	NA	0	8559	1/1	0.47	0.38	19.17	53,53,53,53	0
35	NA	0	8562	1/1	0.82	0.48	16.17	70,70,70,70	0
35	NA	0	8556	1/1	0.87	0.46	15.97	61,61,61,61	0
35	NA	0	8571	1/1	0.61	0.30	15.84	59,59,59,59	0
33	MG	0	8114	1/1	0.91	0.34	14.37	54,54,54,54	0
35	NA	0	8565	1/1	0.82	0.59	13.87	47,47,47,47	0
35	NA	0	8526	1/1	0.94	0.30	12.44	70,70,70,70	0
35	NA	0	8521	1/1	0.83	0.41	12.28	77,77,77,77	0
35	NA	0	8555	1/1	0.88	1.00	12.03	85,85,85,85	0
35	NA	0	8572	1/1	0.88	0.39	11.50	73,73,73,73	0
35	NA	0	8564	1/1	0.78	0.37	10.28	49,49,49,49	0
35	NA	0	8503	1/1	0.99	0.30	10.12	1,1,1,1	0
35	NA	0	8568	1/1	0.84	0.20	9.83	87,87,87,87	0
35	NA	0	8540	1/1	0.93	0.26	9.76	50,50,50,50	0
35	NA	0	8532	1/1	0.90	0.23	9.20	44,44,44,44	0
35	NA	0	8561	1/1	0.87	0.33	9.02	50,50,50,50	0
35	NA	0	8539	1/1	0.93	0.30	8.52	40,40,40,40	0
33	MG	0	8102	1/1	0.72	0.28	8.08	50,50,50,50	0
35	NA	0	8573	1/1	0.97	0.20	7.40	56,56,56,56	0
35	NA	0	8535	1/1	0.74	0.34	7.34	54,54,54,54	0
33	MG	0	8062	1/1	0.90	0.22	7.18	13,13,13,13	0
35	NA	0	8566	1/1	0.83	0.17	5.90	48,48,48,48	0
35	NA	0	8520	1/1	0.96	0.23	5.50	36,36,36,36	0
35	NA	0	8527	1/1	0.79	0.24	5.24	61,61,61,61	0
35	NA	0	8515	1/1	0.87	0.22	4.77	49,49,49,49	0
35	NA	0	8579	1/1	0.86	0.23	4.76	65,65,65,65	0
35	NA	0	8523	1/1	0.99	0.23	4.29	38,38,38,38	0
35	NA	0	8582	1/1	0.73	0.21	4.22	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	R	8586	1/1	0.95	0.35	3.70	23,23,23,23	0
33	MG	0	8013	1/1	0.88	0.20	3.66	38,38,38,38	0
35	NA	0	8543	1/1	0.98	0.20	3.63	35,35,35,35	0
35	NA	L	8580	1/1	0.98	0.24	3.60	1,1,1,1	0
32	13T	0	9000	42/42	0.86	0.25	3.41	58,67,73,74	0
35	NA	0	8569	1/1	0.69	0.25	2.85	64,64,64,64	0
35	NA	0	8505	1/1	0.91	0.23	2.73	37,37,37,37	0
35	NA	9	8583	1/1	0.74	0.15	1.91	73,73,73,73	0
36	CL	0	8805	1/1	0.99	0.13	1.56	71,71,71,71	0
33	MG	B	8055	1/1	0.95	0.15	1.56	64,64,64,64	0
33	MG	0	8012	1/1	0.99	0.14	1.30	39,39,39,39	0
33	MG	0	8018	1/1	0.90	0.15	1.13	39,39,39,39	0
33	MG	0	8060	1/1	0.98	0.17	0.92	45,45,45,45	0
35	NA	0	8510	1/1	0.73	0.14	0.83	45,45,45,45	0
33	MG	0	8084	1/1	0.82	0.14	0.78	58,58,58,58	0
33	MG	0	8054	1/1	0.97	0.16	0.70	30,30,30,30	0
35	NA	J	8546	1/1	0.76	0.25	0.70	39,39,39,39	0
35	NA	0	8533	1/1	0.92	0.12	0.60	39,39,39,39	0
33	MG	0	8004	1/1	0.96	0.18	0.55	37,37,37,37	0
35	NA	A	8545	1/1	0.94	0.16	0.29	61,61,61,61	0
36	CL	J	8821	1/1	0.87	0.21	0.14	77,77,77,77	0
33	MG	Y	8109	1/1	0.88	0.16	-0.01	44,44,44,44	0
33	MG	0	8007	1/1	0.97	0.17	-0.14	26,26,26,26	0
33	MG	0	8096	1/1	0.48	0.11	-0.39	48,48,48,48	0
33	MG	0	8107	1/1	0.98	0.12	-0.40	38,38,38,38	0
33	MG	0	8038	1/1	0.95	0.12	-0.51	31,31,31,31	0
35	NA	0	8576	1/1	0.98	0.16	-0.61	33,33,33,33	0
36	CL	0	8816	1/1	0.80	0.13	-0.63	69,69,69,69	0
37	CD	U	8701	1/1	0.99	0.10	-0.83	67,67,67,67	0
33	MG	0	8015	1/1	0.85	0.17	-0.83	35,35,35,35	0
35	NA	0	8524	1/1	0.80	0.11	-1.00	48,48,48,48	0
33	MG	0	8017	1/1	0.97	0.16	-1.09	31,31,31,31	0
33	MG	A	8065	1/1	0.96	0.14	-1.14	45,45,45,45	0
33	MG	0	8086	1/1	0.96	0.07	-1.14	42,42,42,42	0
35	NA	0	8509	1/1	0.72	0.11	-1.16	48,48,48,48	0
35	NA	Q	8548	1/1	0.94	0.11	-1.17	46,46,46,46	0
33	MG	0	8080	1/1	0.63	0.15	-1.18	39,39,39,39	0
34	K	0	8402	1/1	0.95	0.13	-1.20	61,61,61,61	0
35	NA	0	8517	1/1	0.77	0.12	-1.30	37,37,37,37	0
36	CL	0	8812	1/1	0.86	0.09	-1.33	49,49,49,49	0
33	MG	0	8077	1/1	0.96	0.16	-1.37	36,36,36,36	0
33	MG	0	8001	1/1	0.93	0.12	-1.39	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	CD	Z	8703	1/1	0.96	0.09	-1.42	71,71,71,71	0
33	MG	0	8020	1/1	0.90	0.12	-1.47	39,39,39,39	0
36	CL	3	8804	1/1	0.96	0.09	-1.51	56,56,56,56	0
37	CD	3	8704	1/1	0.98	0.08	-1.54	65,65,65,65	0
37	CD	O	8705	1/1	0.88	0.10	-1.63	186,186,186,186	0
33	MG	3	8078	1/1	0.94	0.10	-1.68	16,16,16,16	0
37	CD	1	8702	1/1	0.99	0.08	-1.76	65,65,65,65	0
33	MG	0	8053	1/1	0.96	0.13	-1.87	43,43,43,43	0
33	MG	0	8010	1/1	0.91	0.16	-1.95	11,11,11,11	0
33	MG	0	8074	1/1	0.95	0.04	-1.97	30,30,30,30	0
36	CL	M	8818	1/1	0.96	0.09	-2.00	44,44,44,44	0
36	CL	O	8808	1/1	0.88	0.09	-2.06	67,67,67,67	0
33	MG	0	8064	1/1	0.99	0.10	-2.10	41,41,41,41	0
33	MG	0	8035	1/1	0.84	0.11	-2.11	46,46,46,46	0
33	MG	T	8073	1/1	0.96	0.10	-2.15	57,57,57,57	0
33	MG	0	8091	1/1	0.91	0.10	-2.34	65,65,65,65	0
33	MG	0	8056	1/1	0.97	0.10	-2.47	56,56,56,56	0
33	MG	0	8032	1/1	0.97	0.07	-2.47	35,35,35,35	0
35	NA	0	8538	1/1	0.46	0.09	-2.60	55,55,55,55	0
36	CL	B	8819	1/1	0.91	0.10	-2.77	53,53,53,53	0
33	MG	0	8006	1/1	0.95	0.09	-2.80	36,36,36,36	0
33	MG	0	8028	1/1	0.90	0.06	-2.97	33,33,33,33	0
33	MG	0	8067	1/1	0.93	0.09	-3.03	37,37,37,37	0
35	NA	0	8578	1/1	0.97	0.10	-3.04	57,57,57,57	0
33	MG	0	8003	1/1	0.98	0.10	-3.06	36,36,36,36	0
33	MG	0	8014	1/1	1.00	0.10	-3.12	41,41,41,41	0
33	MG	0	8101	1/1	0.96	0.08	-3.28	45,45,45,45	0
33	MG	0	8008	1/1	0.89	0.08	-3.34	29,29,29,29	0
35	NA	0	8514	1/1	0.96	0.10	-3.35	38,38,38,38	0
33	MG	0	8058	1/1	0.86	0.11	-3.69	42,42,42,42	0
33	MG	0	8039	1/1	0.99	0.07	-3.79	64,64,64,64	0
35	NA	0	8553	1/1	0.98	0.11	-4.08	44,44,44,44	0
35	NA	M	8547	1/1	0.90	0.07	-4.37	41,41,41,41	0
33	MG	0	8021	1/1	0.94	0.09	-4.46	37,37,37,37	0
33	MG	0	8112	1/1	0.84	0.06	-5.25	39,39,39,39	0
33	MG	0	8088	1/1	0.92	0.10	-5.30	33,33,33,33	0
33	MG	0	8057	1/1	0.85	0.05	-5.46	41,41,41,41	0
33	MG	K	8069	1/1	0.82	0.06	-5.62	51,51,51,51	0
33	MG	0	8048	1/1	0.95	0.09	-5.78	49,49,49,49	0
33	MG	0	8002	1/1	0.97	0.03	-6.34	40,40,40,40	0
33	MG	0	8044	1/1	0.93	0.08	-7.01	55,55,55,55	0
35	NA	0	8544	1/1	0.86	0.07	-7.38	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8033	1/1	0.94	0.04	-8.56	38,38,38,38	0
33	MG	0	8108	1/1	0.95	0.03	-8.68	77,77,77,77	0
33	MG	0	8019	1/1	0.94	0.04	-10.99	34,34,34,34	0
35	NA	0	8541	1/1	0.94	0.10	-	46,46,46,46	0
35	NA	S	8512	1/1	0.87	0.43	-	57,57,57,57	0
33	MG	0	8041	1/1	0.96	0.22	-	68,68,68,68	0
33	MG	0	8090	1/1	0.90	0.23	-	73,73,73,73	0
35	NA	0	8516	1/1	0.78	0.43	-	49,49,49,49	0
35	NA	H	8522	1/1	0.79	0.35	-	77,77,77,77	0
33	MG	0	8024	1/1	0.84	0.99	-	65,65,65,65	0
33	MG	0	8100	1/1	0.71	0.10	-	42,42,42,42	0
33	MG	0	8117	1/1	0.69	0.09	-	34,34,34,34	0
36	CL	0	8815	1/1	0.64	0.14	-	89,89,89,89	0
35	NA	0	8585	1/1	0.61	0.38	-	65,65,65,65	0
33	MG	0	8046	1/1	0.72	0.07	-	56,56,56,56	0
33	MG	0	8113	1/1	0.23	0.16	-	44,44,44,44	0
35	NA	0	8560	1/1	0.74	0.24	-	60,60,60,60	0
35	NA	0	8507	1/1	0.54	0.24	-	69,69,69,69	0
35	NA	0	8529	1/1	0.83	0.10	-	68,68,68,68	0
33	MG	9	8095	1/1	0.77	0.15	-	77,77,77,77	0
33	MG	0	8116	1/1	0.86	0.10	-	56,56,56,56	0
33	MG	0	8106	1/1	0.99	0.07	-	71,71,71,71	0
33	MG	0	8045	1/1	0.76	0.12	-	67,67,67,67	0
33	MG	0	8076	1/1	0.87	0.06	-	49,49,49,49	0
35	NA	0	8534	1/1	0.94	0.07	-	40,40,40,40	0
33	MG	0	8023	1/1	0.92	0.24	-	61,61,61,61	0
33	MG	0	8093	1/1	0.92	0.10	-	61,61,61,61	0
33	MG	0	8068	1/1	0.98	0.09	-	56,56,56,56	0
35	NA	0	8542	1/1	0.91	0.29	-	15,15,15,15	0
33	MG	0	8071	1/1	0.82	0.07	-	50,50,50,50	0
33	MG	0	8011	1/1	0.89	0.18	-	39,39,39,39	0
33	MG	0	8043	1/1	0.95	0.13	-	47,47,47,47	0
36	CL	0	8813	1/1	0.95	0.06	-	54,54,54,54	0
35	NA	0	8519	1/1	0.99	0.16	-	17,17,17,17	0
33	MG	0	8083	1/1	0.93	0.07	-	41,41,41,41	0
33	MG	0	8059	1/1	0.97	0.05	-	39,39,39,39	0
33	MG	0	8087	1/1	0.96	0.09	-	63,63,63,63	0
33	MG	0	8027	1/1	0.99	0.03	-	40,40,40,40	0
33	MG	0	8098	1/1	0.95	0.11	-	42,42,42,42	0
33	MG	0	8111	1/1	0.68	0.08	-	46,46,46,46	0
33	MG	0	8115	1/1	0.90	0.07	-	45,45,45,45	0
35	NA	0	8528	1/1	0.68	0.51	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	0	8822	1/1	0.86	0.48	-	90,90,90,90	0
35	NA	0	8552	1/1	0.92	0.13	-	68,68,68,68	0
36	CL	J	8801	1/1	0.95	0.06	-	58,58,58,58	0
33	MG	0	8104	1/1	0.54	0.37	-	78,78,78,78	0
35	NA	0	8549	1/1	0.93	0.26	-	53,53,53,53	0
33	MG	0	8029	1/1	0.89	0.12	-	42,42,42,42	0
33	MG	0	8082	1/1	0.97	0.34	-	84,84,84,84	0
33	MG	0	8009	1/1	0.97	0.15	-	36,36,36,36	0
33	MG	0	8042	1/1	0.95	0.05	-	33,33,33,33	0
36	CL	N	8807	1/1	0.88	0.14	-	71,71,71,71	0
33	MG	0	8050	1/1	0.93	0.19	-	74,74,74,74	0
33	MG	0	8061	1/1	0.84	0.15	-	44,44,44,44	0
33	MG	3	8118	1/1	0.98	0.21	-	50,50,50,50	0
33	MG	0	8092	1/1	0.95	0.12	-	72,72,72,72	0
33	MG	0	8103	1/1	0.92	0.19	-	78,78,78,78	0
36	CL	L	8810	1/1	0.84	0.10	-	59,59,59,59	0
35	NA	0	8536	1/1	0.95	0.07	-	54,54,54,54	0
33	MG	0	8049	1/1	0.93	0.17	-	36,36,36,36	0
33	MG	0	8094	1/1	0.79	0.15	-	59,59,59,59	0
33	MG	A	8066	1/1	0.96	0.05	-	73,73,73,73	0
35	NA	0	8563	1/1	0.90	0.42	-	68,68,68,68	0
36	CL	Y	8817	1/1	0.95	0.15	-	70,70,70,70	0
35	NA	R	8537	1/1	0.94	0.14	-	45,45,45,45	0
33	MG	0	8016	1/1	0.97	0.07	-	18,18,18,18	0
36	CL	0	8814	1/1	0.96	0.11	-	57,57,57,57	0
35	NA	0	8584	1/1	0.77	0.69	-	90,90,90,90	0
35	NA	0	8567	1/1	0.91	0.46	-	61,61,61,61	0
33	MG	0	8040	1/1	0.92	0.34	-	53,53,53,53	0
35	NA	0	8518	1/1	0.89	0.35	-	58,58,58,58	0
33	MG	0	8110	1/1	0.99	0.10	-	53,53,53,53	0
35	NA	0	8554	1/1	0.90	0.15	-	42,42,42,42	0
35	NA	0	8506	1/1	0.77	0.74	-	49,49,49,49	0
33	MG	0	8079	1/1	0.93	0.15	-	27,27,27,27	0
35	NA	9	8551	1/1	0.39	0.39	-	92,92,92,92	0
33	MG	0	8047	1/1	0.83	0.12	-	57,57,57,57	0
36	CL	A	8809	1/1	0.95	0.19	-	82,82,82,82	0
35	NA	0	8530	1/1	0.95	0.09	-	45,45,45,45	0
33	MG	0	8022	1/1	0.90	0.08	-	37,37,37,37	0
36	CL	0	8803	1/1	0.92	0.16	-	56,56,56,56	0
33	MG	0	8075	1/1	0.77	0.06	-	56,56,56,56	0
33	MG	0	8031	1/1	0.91	0.10	-	30,30,30,30	0
33	MG	0	8081	1/1	0.90	0.13	-	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8558	1/1	0.89	0.55	-	75,75,75,75	0
36	CL	0	8811	1/1	0.99	0.11	-	58,58,58,58	0
35	NA	0	8557	1/1	0.87	0.13	-	45,45,45,45	0
33	MG	0	8063	1/1	0.82	0.09	-	63,63,63,63	0
35	NA	C	8504	1/1	0.85	0.08	-	35,35,35,35	0
33	MG	0	8025	1/1	0.93	0.10	-	43,43,43,43	0
33	MG	0	8070	1/1	0.93	0.15	-	43,43,43,43	0
33	MG	0	8034	1/1	0.96	0.10	-	25,25,25,25	0
36	CL	R	8806	1/1	0.99	0.03	-	49,49,49,49	0
35	NA	0	8501	1/1	0.99	0.06	-	50,50,50,50	0
33	MG	0	8099	1/1	0.95	0.33	-	70,70,70,70	0
35	NA	0	8502	1/1	0.67	0.20	-	57,57,57,57	0
33	MG	0	8005	1/1	0.96	0.10	-	32,32,32,32	0
35	NA	0	8570	1/1	0.94	0.39	-	65,65,65,65	0
33	MG	0	8072	1/1	0.85	0.09	-	57,57,57,57	0
35	NA	0	8511	1/1	0.98	0.12	-	56,56,56,56	0
33	MG	0	8030	1/1	0.99	0.07	-	35,35,35,35	0
35	NA	0	8513	1/1	0.55	0.07	-	72,72,72,72	0
36	CL	J	8802	1/1	0.91	0.15	-	76,76,76,76	0
33	MG	0	8036	1/1	0.92	0.06	-	41,41,41,41	0
33	MG	0	8085	1/1	0.95	0.12	-	48,48,48,48	0
35	NA	0	8581	1/1	0.81	0.08	-	42,42,42,42	0
35	NA	0	8508	1/1	0.96	0.26	-	58,58,58,58	0
33	MG	0	8089	1/1	0.92	0.13	-	62,62,62,62	0
33	MG	0	8097	1/1	0.85	0.07	-	45,45,45,45	0
33	MG	0	8051	1/1	0.95	0.12	-	56,56,56,56	0
33	MG	0	8052	1/1	0.81	0.13	-	68,68,68,68	0
35	NA	0	8575	1/1	0.75	0.32	-	72,72,72,72	0
36	CL	Y	8820	1/1	0.98	0.05	-	44,44,44,44	0
33	MG	0	8026	1/1	0.98	0.09	-	33,33,33,33	0
33	MG	0	8037	1/1	0.93	0.07	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.