



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:12 PM UTC

PDB ID : 1VQ7 / pdb_00001vq7
Title : The structure of the transition state analogue "DCA" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

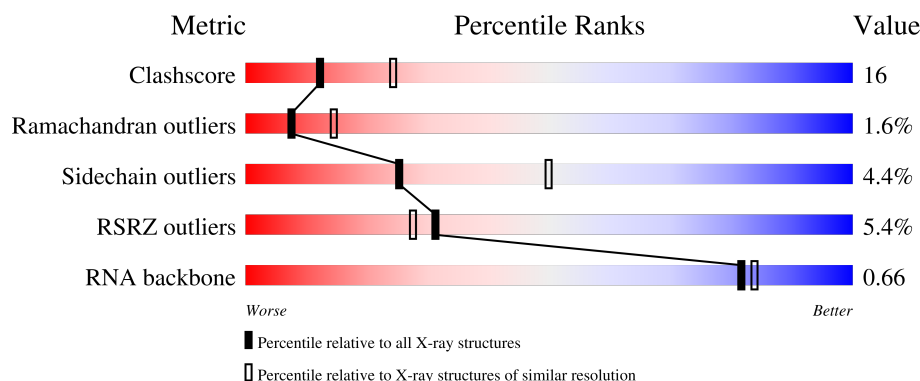
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

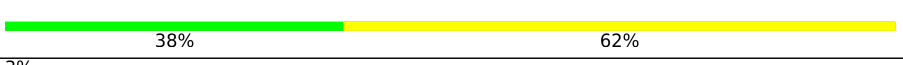
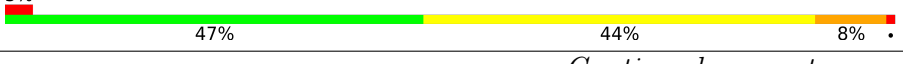
The reported resolution of this entry is 2.50 Å.

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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	
2	9	122	
3	4	8	
4	A	240	
5	B	338	

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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Mol	Chain	Length	Quality of chain
31	3	92	2% 64% 33%
32	I	162	31% 17% 24% 57%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99063 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 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			130	63	23	39	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total	C	N	O	S	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	S	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	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	53	Total	C	N	O	S	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	V	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	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	3	Total	K	0	0
			3	3		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	72	Total 72	Na 72	0	0
35	9	2	Total 2	Na 2	0	0
35	A	1	Total 1	Na 1	0	0
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	H	2	Total 2	Na 2	0	0
35	J	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	11	Total 11	Cl 11	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	3	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5809	Total 5809	O 5809	0	0
38	9	137	Total 137	O 137	0	0
38	4	8	Total 8	O 8	0	0
38	A	119	Total 119	O 119	0	0
38	B	153	Total 153	O 153	0	0
38	C	168	Total 168	O 168	0	0
38	D	47	Total 47	O 47	0	0
38	E	43	Total 43	O 43	0	0

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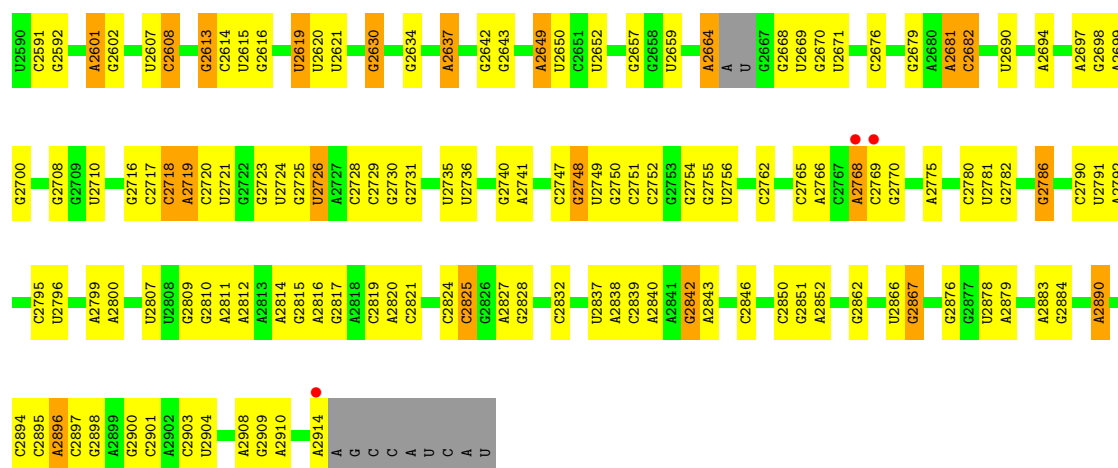
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38	F	23	Total 23	O 23	0	0
38	G	18	Total 18	O 18	0	0
38	H	65	Total 65	O 65	0	0
38	J	51	Total 51	O 51	0	0
38	K	58	Total 58	O 58	0	0
38	L	82	Total 82	O 82	0	0
38	M	116	Total 116	O 116	0	0
38	N	63	Total 63	O 63	0	0
38	O	42	Total 42	O 42	0	0
38	P	64	Total 64	O 64	0	0
38	Q	51	Total 51	O 51	0	0
38	R	84	Total 84	O 84	0	0
38	S	30	Total 30	O 30	0	0
38	T	42	Total 42	O 42	0	0
38	U	29	Total 29	O 29	0	0
38	V	14	Total 14	O 14	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	96	Total 96	O 96	0	0
38	Z	32	Total 32	O 32	0	0
38	1	53	Total 53	O 53	0	0

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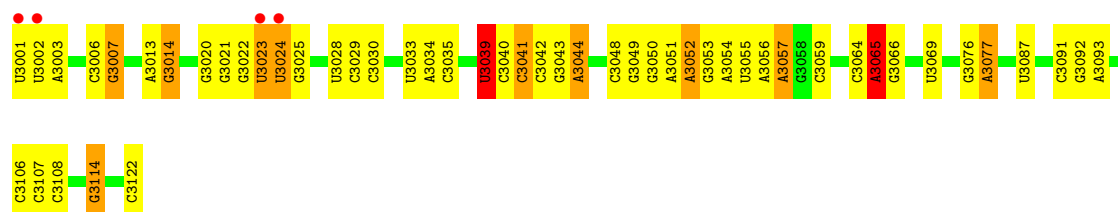
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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38	3	74	Total 74	O 74	0	0
38	I	9	Total 9	O 9	0	0





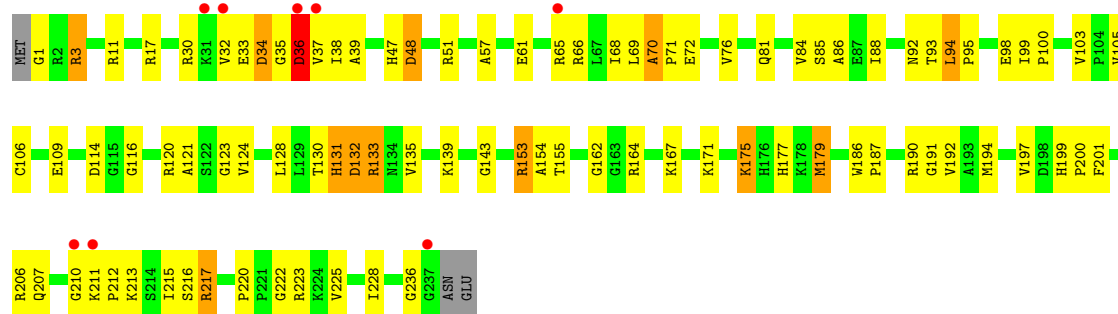
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3'

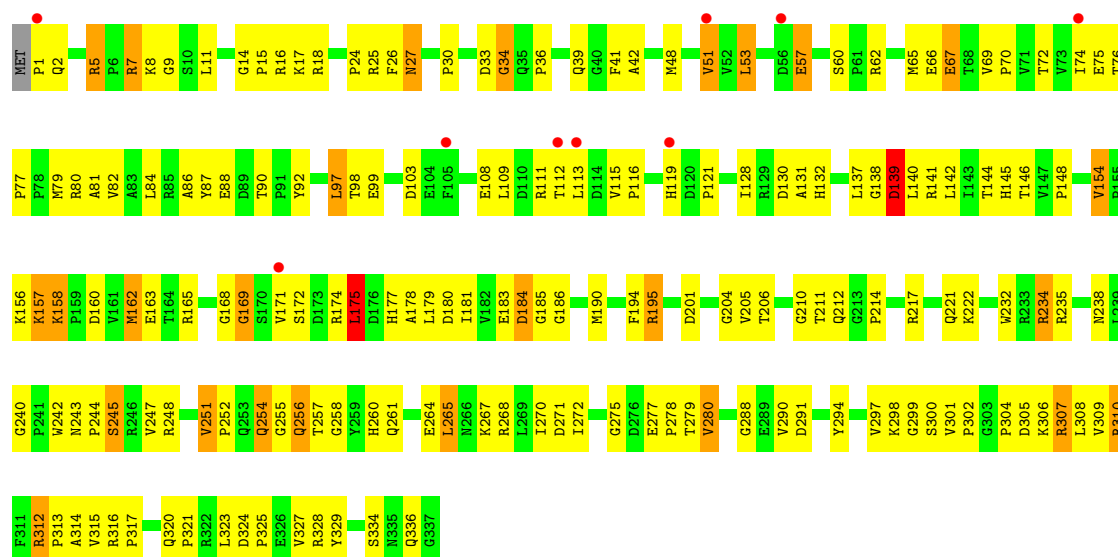


• Molecule 4: 50S ribosomal protein L2P

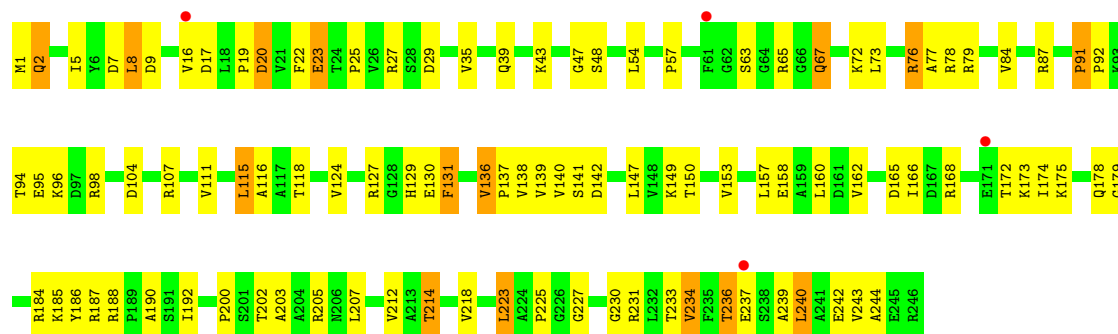


• Molecule 5: 50S ribosomal protein L3P

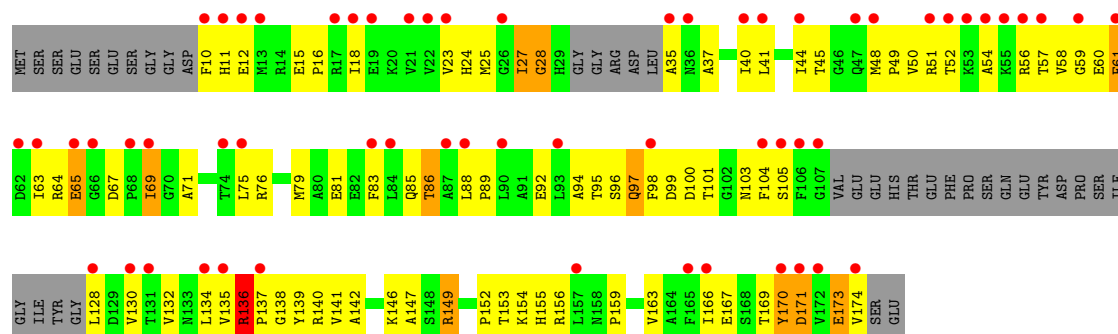




- Molecule 6: 50S ribosomal protein L4E

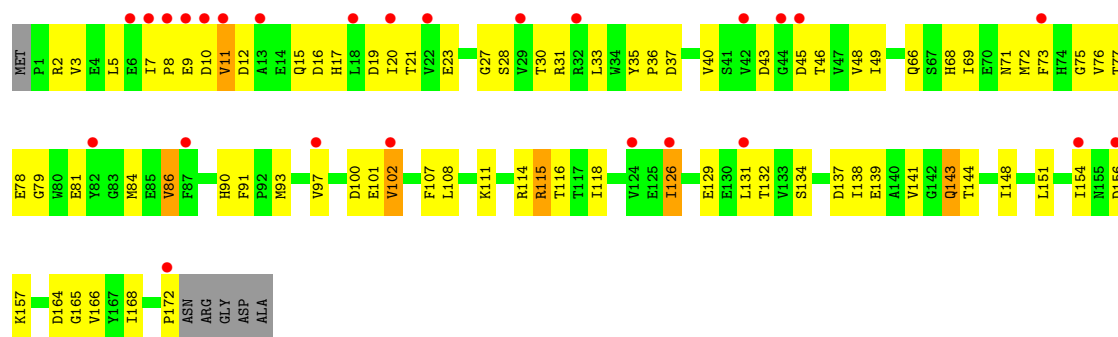


- Molecule 7: 50S ribosomal protein L5P

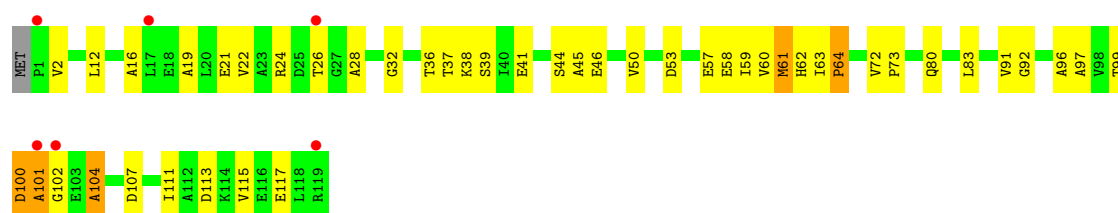


- Molecule 8: 50S ribosomal protein L6P





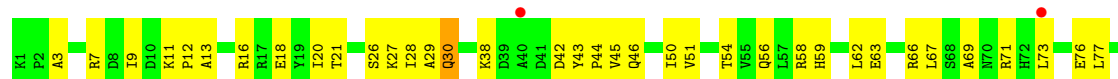
• Molecule 9: 50S ribosomal protein L7AE

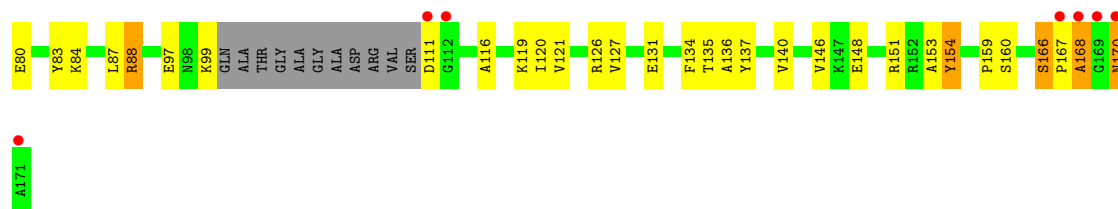


• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

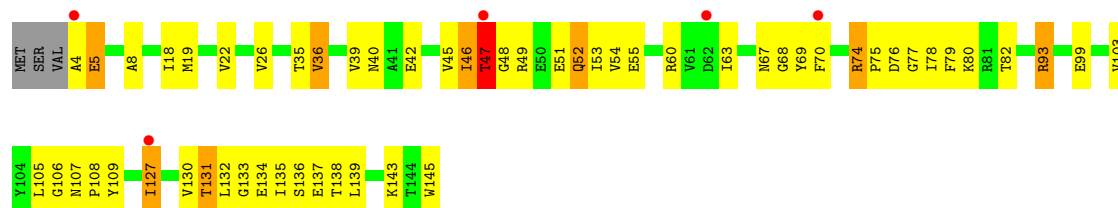


• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

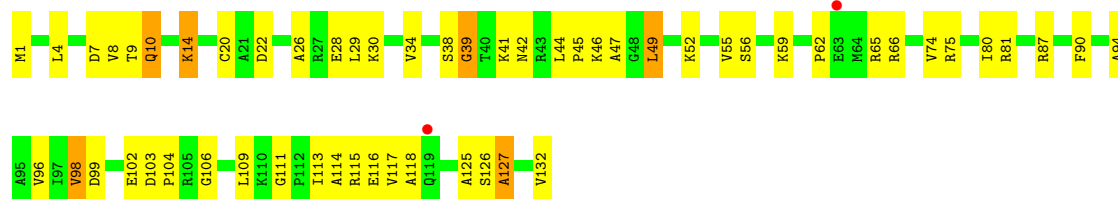




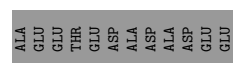
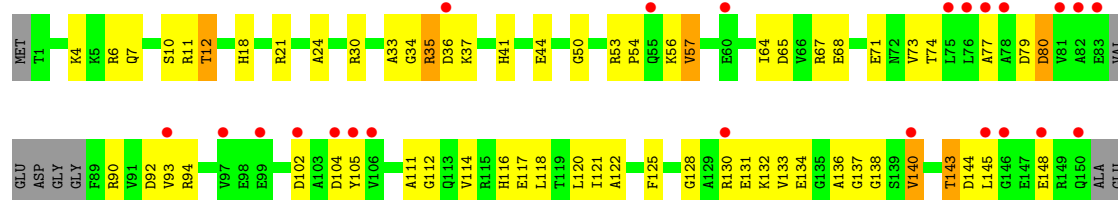
• Molecule 12: 50S ribosomal protein L13P



• Molecule 13: 50S ribosomal protein L14P



• Molecule 14: 50S ribosomal protein L15P

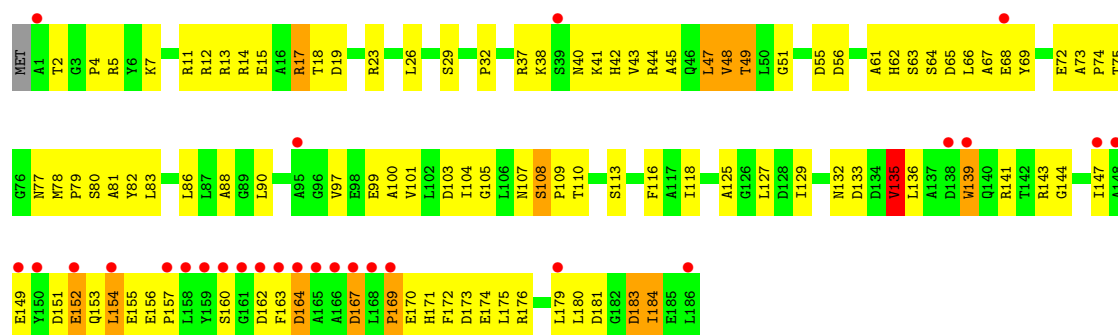
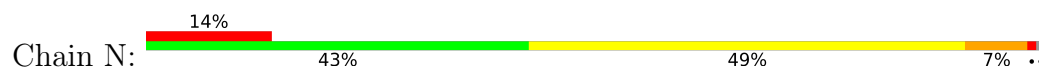


• Molecule 15: 50S Ribosomal Protein L15E

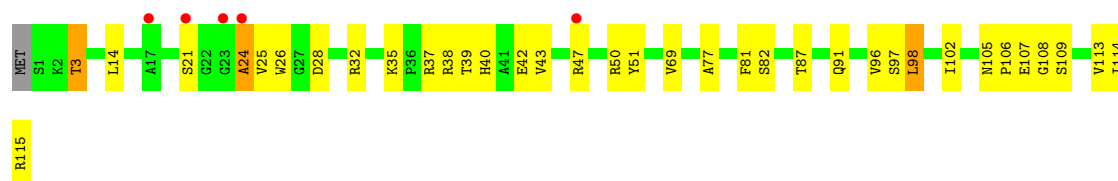




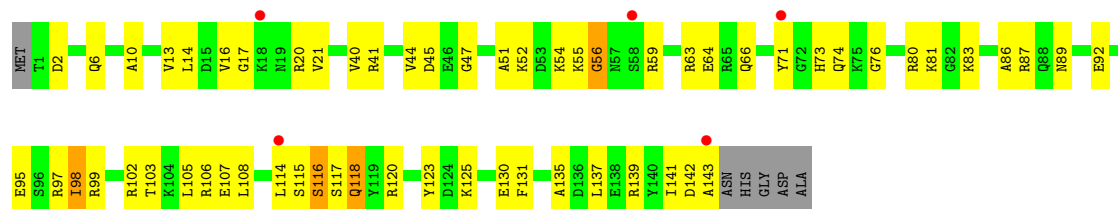
• Molecule 16: 50S ribosomal protein L18P



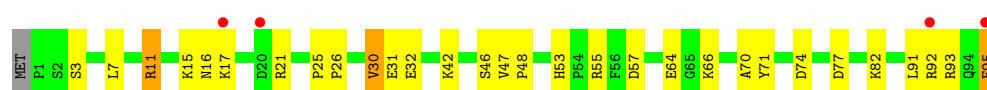
• Molecule 17: 50S ribosomal protein L18e



• Molecule 18: 50S ribosomal protein L19E

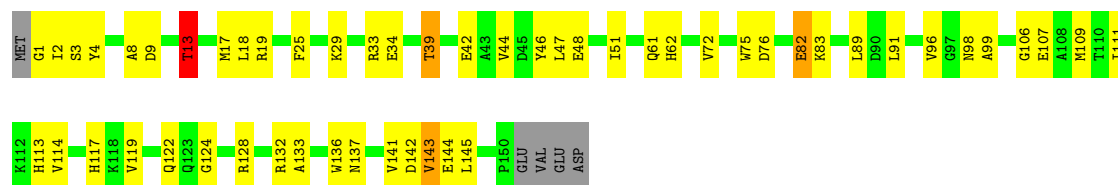


• Molecule 19: 50S ribosomal protein L21e



• Molecule 20: 50S ribosomal protein L22P





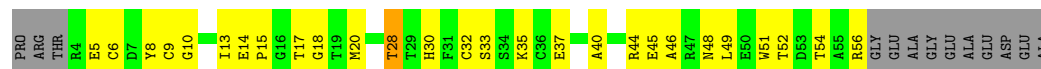
• Molecule 21: 50S ribosomal protein L23P



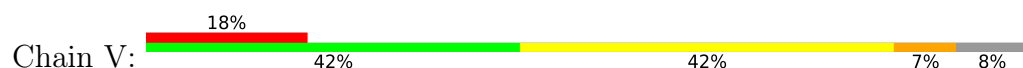
• Molecule 22: 50S ribosomal protein L24P



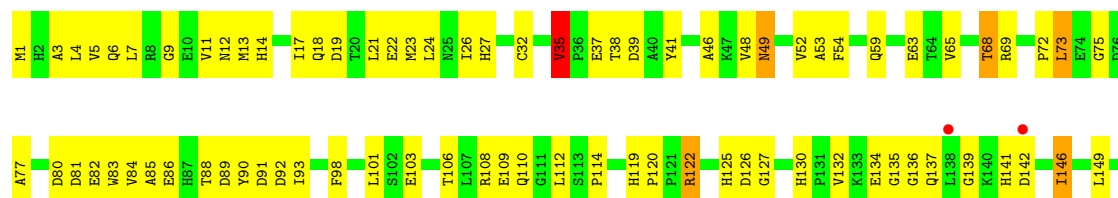
• Molecule 23: 50S ribosomal protein L24E



• Molecule 24: 50S ribosomal protein L29P



• Molecule 25: 50S ribosomal protein L30P



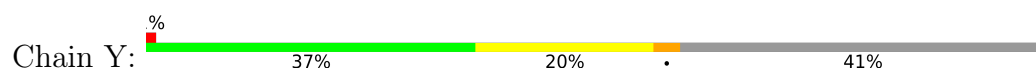
A152
M153
R154

• Molecule 26: 50S ribosomal protein L31e



MET SER ALA ASP PHE GLU E7 R8 V9 I12 R15 H23 K24 R25 A26 K30 I31 R34 E35 H36 L37 R40 F41 S42 V43 D44 A47 V48 R55 A58 W59 A64 R65 T66 R71 V72 R73 A74 A75 R76 F77 E78 E79 E80 A83 I84 V85
 E86 A87 E88 THR ALA GLU
 E86 A87 E88

• Molecule 27: 50S ribosomal protein L32E



MET ALA ASP ASN GLU ASP VAL GLU ALA LEU GLU TYR THR LEU THR ASP ILE SER VAL GLY VAL PRO SER LYS ALA GLU PRO LEU ARG GLU ALA PHE GLU SER VAL GLU ASP T103 R100 T104 E104 T106 P107 S110 D111 E112 R115 L116 L117 D132 H133 H134 K135 LEU
 ALA ALA ARG ILE LYS ALA ASP VAL GLY LEU VAL GLU SER THR LEU GLU VAL VAL GLU VAL GLU GLY GLY GLU GLU GLU VAL ASP T95 A99 R100 T103 E104 T106 P107 S110 D111 E112 R115 L116 L117 D132 H133 H134 K135
 V139 S140 T141 S142 W143 R144 G148 S151 R154 R155 K158 T163 V164 E165 R169 T172 A173 V174 K177 H178 P179 F182 E183 E184 V186 V187 H188 N189 V190 D191 D192 D197 T200 E201 A202 V203 R204 I205 K213 R214 E215 R216 I217 N230 Y233
 V234 E235 V236 VAL SER GLU
 V234 E235 V236

• Molecule 28: 50S ribosomal protein L37Ae



R10 S11 G12 R13 Y18 G19 R20 V21 R22 R23 R24 R25 V26 I29 E30 E31 E32 E35 D36 C39 C42 E43 E44 D45 R46 V47 G53 Q56 C57 S58 Y59 Y62 K63 G66 G67 K70 V79 R80 R81 S82 ILE ARG ALA ALA LEU SER GLU ASP GLU
 R10 S11 G12 R13 Y18 G19 R20 V21 R22 R23 R24 R25 V26 I29 E30 E31 E32 E35 D36 C39 C42 E43 E44 D45 R46 V47 G53 Q56 C57 S58 Y59 Y62 K63 G66 G67 K70 V79 R80 R81 S82 ILE ARG ALA ALA LEU SER GLU ASP GLU

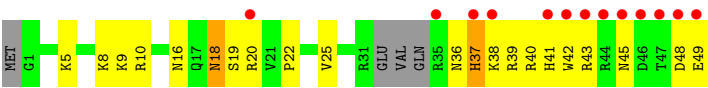
• Molecule 29: 50S ribosomal protein L37e



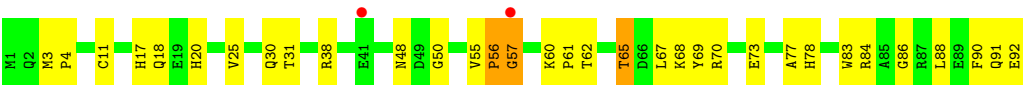
MET T1 Q8 G9 K10 K11 N12 H16 R20 R21 K25 H28 T29 K30 K31 K32 C37 A43 K44 R45 A54 G55 E56
 MET T1 Q8 G9 K10 K11 N12 H16 R20 R21 K25 H28 T29 K30 K31 K32 C37 A43 K44 R45 A54 G55 E56

• Molecule 30: 50S ribosomal protein L39e

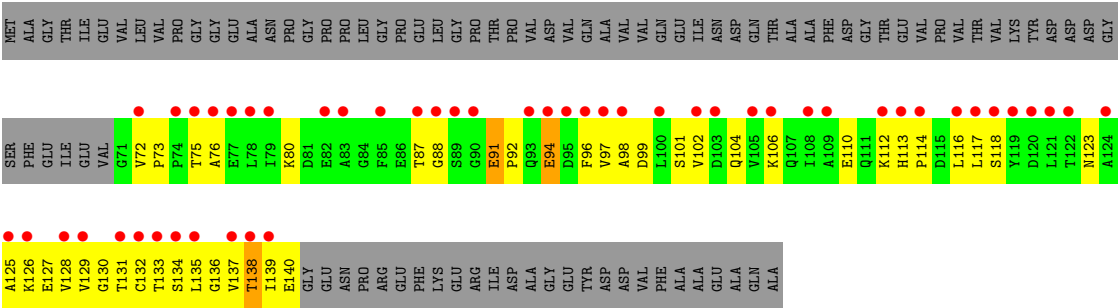




● Molecule 31: 50S ribosomal protein L44E



● Molecule 32: 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	211.15Å 300.13Å 573.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 89.0 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.244 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99063	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: MG, 1MA, 2OP, OMG, K, UR3, 5AA, PAE, NA, PSU, CD, OMU, 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	0.38	0/65959	0.61	27/102870 (0.0%)
2	9	0.37	0/2905	0.60	3/4528 (0.1%)
3	4	0.37	0/102	0.77	0/149
4	A	0.43	0/1786	1.01	8/2408 (0.3%)
5	B	0.41	0/2690	0.98	10/3652 (0.3%)
6	C	0.48	0/1884	1.00	8/2551 (0.3%)
7	D	0.34	0/1111	0.87	4/1498 (0.3%)
8	E	0.37	0/1382	0.87	4/1880 (0.2%)
9	F	0.38	0/901	0.86	1/1224 (0.1%)
10	G	0.34	0/241	0.71	0/324
11	H	0.37	0/1287	0.98	5/1725 (0.3%)
12	J	0.42	0/1136	0.96	5/1530 (0.3%)
13	K	0.43	0/1001	1.01	5/1347 (0.4%)
14	L	0.38	0/1130	0.97	4/1509 (0.3%)
15	M	0.42	0/1584	0.91	8/2119 (0.4%)
16	N	0.37	0/1474	1.05	12/1999 (0.6%)
17	O	0.43	0/874	0.97	4/1181 (0.3%)
18	P	0.40	0/1147	0.88	4/1528 (0.3%)
19	Q	0.43	0/749	1.05	3/1005 (0.3%)
20	R	0.43	0/1172	0.93	6/1578 (0.4%)
21	S	0.36	0/648	0.91	4/875 (0.5%)
22	T	0.39	0/958	0.97	2/1289 (0.2%)
23	U	0.38	0/417	0.85	0/562
24	V	0.37	0/502	0.94	3/675 (0.4%)
25	W	0.46	0/1219	1.03	8/1655 (0.5%)
26	X	0.42	0/664	0.96	2/895 (0.2%)
27	Y	0.44	0/1146	0.97	5/1536 (0.3%)
28	Z	0.39	0/589	0.94	1/787 (0.1%)
29	1	0.44	0/438	0.94	3/578 (0.5%)
30	2	0.40	0/401	0.71	0/529
31	3	0.42	0/771	0.96	2/1024 (0.2%)
32	I	0.37	0/526	0.94	3/716 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98794	0.72	154/147726 (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	1	54
2	9	0	3
All	All	1	57

There are no bond length outliers.

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	14.19	130.79	109.50
1	0	1979	G	C2'-C3'-O3'	11.32	126.49	109.50
19	Q	17	LYS	N-CA-C	-9.65	97.57	109.83
1	0	1942	A	C5'-C4'-C3'	8.95	129.43	116.00
1	0	1563	G	C4'-C3'-O3'	8.93	122.80	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	191	A	Sidechain
1	0	221	G	Sidechain
1	0	246	G	Sidechain
1	0	26	U	Sidechain

5.2 Too-close contacts [i](#)

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	29813	823	0
2	9	2600	0	1326	58	0
3	4	130	0	77	5	0
4	A	1753	0	1766	108	0
5	B	2625	0	2533	179	0
6	C	1859	0	1816	103	0
7	D	1094	0	1085	93	0
8	E	1357	0	1266	85	0
9	F	890	0	843	43	0
10	G	240	0	231	13	0
11	H	1266	0	1268	66	0
12	J	1120	0	1098	76	0
13	K	992	0	1031	59	0
14	L	1118	0	1076	57	0
15	M	1560	0	1568	60	0
16	N	1445	0	1401	108	0
17	O	865	0	873	32	0
18	P	1136	0	1123	53	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	59	0
21	S	641	0	605	22	0
22	T	950	0	923	56	0
23	U	410	0	364	30	0
24	V	499	0	511	37	0
25	W	1196	0	1137	99	0
26	X	654	0	653	38	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	25	0
29	1	431	0	426	22	0
30	2	396	0	413	30	0
31	3	755	0	728	27	0
32	I	519	0	500	50	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	B	2	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	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	11	0	0	1	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	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	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	5809	0	0	103	0
38	1	53	0	0	2	0
38	2	40	0	0	3	0
38	3	74	0	0	4	0
38	4	8	0	0	1	0
38	9	137	0	0	5	0
38	A	119	0	0	13	0
38	B	153	0	0	15	0
38	C	168	0	0	12	0
38	D	47	0	0	10	0
38	E	43	0	0	7	0
38	F	23	0	0	3	0
38	G	18	0	0	2	0
38	H	65	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	I	9	0	0	2	0
38	J	51	0	0	3	0
38	K	58	0	0	6	0
38	L	82	0	0	12	0
38	M	116	0	0	5	0
38	N	63	0	0	10	0
38	O	42	0	0	3	0
38	P	64	0	0	3	0
38	Q	51	0	0	3	0
38	R	84	0	0	2	0
38	S	30	0	0	1	0
38	T	42	0	0	2	0
38	U	29	0	0	2	0
38	V	14	0	0	1	0
38	W	68	0	0	2	0
38	X	27	0	0	2	0
38	Y	96	0	0	5	0
38	Z	32	0	0	2	0
All	All	99063	0	59977	2340	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 16.

The worst 5 of 2340 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:46:GLN:HB3	11:H:167:PRO:HD2	1.28	1.16
1:O:156:C:H5''	15:M:171:ARG:HD3	1.29	1.14
1:O:1160:G:H5'	1:O:1161:A:H5'	1.20	1.11
1:O:1242:A:H5'	12:J:82:THR:HG23	1.34	1.09
6:C:236:THR:HG22	6:C:239:ALA:H	1.16	1.08

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	7	13
5	B	335/338 (99%)	298 (89%)	31 (9%)	6 (2%)	6	12
6	C	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	30	49
7	D	134/177 (76%)	101 (75%)	23 (17%)	10 (8%)	1	0
8	E	170/178 (96%)	158 (93%)	12 (7%)	0	100	100
9	F	117/120 (98%)	108 (92%)	3 (3%)	6 (5%)	1	2
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	145 (93%)	8 (5%)	3 (2%)	6	11
12	J	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	9	17
13	K	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	5	8
14	L	141/165 (86%)	121 (86%)	16 (11%)	4 (3%)	4	6
15	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	2	3
17	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	14	27
18	P	141/149 (95%)	138 (98%)	2 (1%)	1 (1%)	18	34
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
21	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	27
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	3	4
25	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	18	34
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	9	18
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	9 (13%)	2 (3%)	4	6
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	4	8
31	3	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	5	9
32	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	8	16
All	All	3705/4430 (84%)	3373 (91%)	273 (7%)	59 (2%)	7	14

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	34	GLY
5	B	139	ASP
5	B	184	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	
4	A	179/182 (98%)	168 (94%)	11 (6%)	17	35
5	B	282/283 (100%)	261 (93%)	21 (7%)	13	27
6	C	193/193 (100%)	178 (92%)	15 (8%)	11	24
7	D	117/148 (79%)	112 (96%)	5 (4%)	26	51
8	E	152/156 (97%)	148 (97%)	4 (3%)	40	68
9	F	93/94 (99%)	92 (99%)	1 (1%)	65	84
10	G	27/283 (10%)	26 (96%)	1 (4%)	30	57
11	H	132/138 (96%)	124 (94%)	8 (6%)	17	35
12	J	118/121 (98%)	111 (94%)	7 (6%)	18	37
13	K	106/106 (100%)	102 (96%)	4 (4%)	29	56
14	L	113/127 (89%)	111 (98%)	2 (2%)	51	77
15	M	158/158 (100%)	153 (97%)	5 (3%)	34	62
16	N	149/150 (99%)	142 (95%)	7 (5%)	23	47
17	O	93/94 (99%)	90 (97%)	3 (3%)	34	62
18	P	113/117 (97%)	110 (97%)	3 (3%)	39	67
19	Q	79/80 (99%)	75 (95%)	4 (5%)	21	43
20	R	117/122 (96%)	113 (97%)	4 (3%)	32	60
21	S	71/74 (96%)	69 (97%)	2 (3%)	38	66
22	T	105/106 (99%)	101 (96%)	4 (4%)	29	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	44/52 (85%)	43 (98%)	1 (2%)	44	72
24	V	51/57 (90%)	49 (96%)	2 (4%)	28	55
25	W	130/130 (100%)	125 (96%)	5 (4%)	29	56
26	X	66/74 (89%)	62 (94%)	4 (6%)	17	35
27	Y	120/196 (61%)	110 (92%)	10 (8%)	10	22
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	45	73
30	2	42/46 (91%)	41 (98%)	1 (2%)	43	70
31	3	79/79 (100%)	77 (98%)	2 (2%)	42	69
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2956 (96%)	137 (4%)	25	50

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	W	73	LEU
26	X	15	ARG
27	Y	191	ASP
7	D	61	PHE
7	D	24	HIS

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

Mol	Chain	Res	Type
18	P	101	GLN
21	S	55	GLN
31	3	2	GLN
19	Q	40	HIS
20	R	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	32 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
3	4	1/8 (12%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2867/3052 (93%)	261 (9%)	33 (1%)

5 of 261 RNA backbone outliers are listed below:

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

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2649	A
1	0	2718	C
2	9	3065	A
1	0	1237	U
1	0	1232	A

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

6 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	OMG	0	2588	3,1	23,26,27	0.31	0	32,38,41	0.35	0
1	PSU	0	2621	1	18,21,22	1.56	2 (11%)	21,30,33	1.43	3 (14%)
3	5AA	4	76	3,1	23,26,27	0.76	1 (4%)	29,38,41	0.80	1 (3%)
1	OMU	0	2587	1	19,22,23	0.22	0	25,31,34	0.35	0
1	UR3	0	2619	1	19,22,23	0.38	0	26,32,35	0.73	1 (3%)
1	1MA	0	628	1	21,25,26	0.73	1 (4%)	30,37,40	0.81	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	3,1	-	0/9/27/28	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	5AA	4	76	3,1	-	0/11/29/30	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	1/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.20	1.43	1.36
3	4	76	5AA	C3'-N3'	-3.39	1.42	1.47
1	0	2621	PSU	C6-C5	2.75	1.38	1.35
1	0	628	1MA	C6-N6	2.61	1.34	1.28

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.82	120.75	118.17
1	0	2621	PSU	C6-N1-C2	-3.33	119.60	122.69
3	4	76	5AA	C2-N1-C6	2.86	118.82	111.83
1	0	2619	UR3	C4-N3-C2	2.85	126.88	124.58
1	0	628	1MA	N1-C2-N3	2.80	129.32	126.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2619	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 234 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 [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%)	-0.34	54 (1%) 65 61	24, 49, 93, 155	0
2	9	122/122 (100%)	0.12	4 (3%) 49 45	45, 66, 91, 152	0
3	4	5/8 (62%)	-0.44	0 100 100	41, 45, 47, 49	0
4	A	237/240 (98%)	0.26	8 (3%) 48 43	30, 51, 89, 114	0
5	B	337/338 (99%)	0.56	9 (2%) 56 51	31, 61, 90, 100	0
6	C	246/246 (100%)	0.24	4 (1%) 70 67	28, 48, 71, 82	0
7	D	140/177 (79%)	2.02	59 (42%) 0 0	59, 106, 130, 136	0
8	E	172/178 (96%)	1.16	26 (15%) 5 4	52, 76, 101, 111	0
9	F	119/120 (99%)	0.83	6 (5%) 34 30	52, 74, 100, 116	0
10	G	29/348 (8%)	1.57	8 (27%) 1 1	74, 92, 104, 108	0
11	H	160/171 (93%)	0.52	9 (5%) 30 26	42, 60, 91, 100	0
12	J	142/145 (97%)	0.47	5 (3%) 47 42	40, 56, 76, 99	0
13	K	132/132 (100%)	0.66	2 (1%) 72 68	35, 58, 80, 85	0
14	L	145/165 (87%)	0.88	23 (15%) 5 4	28, 69, 114, 127	0
15	M	194/194 (100%)	-0.08	1 (0%) 87 85	32, 43, 59, 66	0
16	N	186/187 (99%)	0.90	27 (14%) 6 5	40, 64, 113, 119	0
17	O	115/116 (99%)	0.70	5 (4%) 40 35	39, 58, 75, 90	0
18	P	143/149 (95%)	0.59	5 (3%) 47 42	43, 58, 70, 78	0
19	Q	95/96 (98%)	0.25	4 (4%) 40 36	38, 47, 60, 72	0
20	R	150/155 (96%)	-0.06	0 100 100	33, 48, 65, 76	0
21	S	81/85 (95%)	0.33	1 (1%) 76 73	45, 59, 78, 88	0
22	T	119/120 (99%)	0.46	1 (0%) 82 80	40, 58, 85, 96	0
23	U	53/66 (80%)	0.59	0 100 100	46, 62, 76, 86	0
24	V	65/71 (91%)	1.40	13 (20%) 3 2	56, 76, 112, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.43	2 (1%) 75 71	39, 55, 74, 86	0
26	X	82/92 (89%)	0.71	6 (7%) 21 19	46, 63, 85, 101	0
27	Y	142/241 (58%)	0.25	2 (1%) 73 70	30, 49, 70, 92	0
28	Z	73/83 (87%)	0.76	8 (10%) 10 8	46, 60, 76, 94	0
29	1	56/57 (98%)	-0.38	0 100 100	27, 34, 39, 52	0
30	2	46/50 (92%)	1.38	13 (28%) 1 1	36, 65, 120, 122	0
31	3	92/92 (100%)	0.26	2 (2%) 62 58	35, 55, 71, 87	0
32	I	70/162 (43%)	3.06	50 (71%) 0 0	108, 126, 148, 149	0
All	All	6651/7482 (88%)	0.21	357 (5%) 31 27	24, 55, 103, 155	0

The worst 5 of 357 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	10.2
32	I	133	THR	9.9
7	D	10	PHE	7.2
32	I	102	VAL	6.5
16	N	168	LEU	6.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	OMU	0	2587	21/22	0.97	0.07	31,34,37,38	0
1	OMG	0	2588	24/25	0.97	0.06	30,34,37,38	0
1	1MA	0	628	23/24	0.98	0.06	31,35,37,38	0
1	UR3	0	2619	21/22	0.98	0.07	33,38,40,43	0
1	PSU	0	2621	20/21	0.98	0.05	28,31,39,40	0
3	5AA	4	76	24/25	0.98	0.07	39,44,45,46	0

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
35	NA	9	9151	1/1	0.72	0.28	76,76,76,76	0
33	MG	0	8047	1/1	0.74	0.21	102,102,102,102	0
35	NA	S	9112	1/1	0.77	0.20	76,76,76,76	0
33	MG	0	8082	1/1	0.78	0.18	66,66,66,66	0
33	MG	9	8095	1/1	0.80	0.20	72,72,72,72	0
35	NA	0	9186	1/1	0.81	0.31	75,75,75,75	0
33	MG	0	8092	1/1	0.81	0.31	95,95,95,95	0
35	NA	0	9182	1/1	0.81	0.23	74,74,74,74	0
35	NA	0	9174	1/1	0.82	0.21	59,59,59,59	0
35	NA	0	9185	1/1	0.83	0.28	60,60,60,60	0
35	NA	0	9124	1/1	0.83	0.21	59,59,59,59	0
35	NA	H	9122	1/1	0.84	0.29	77,77,77,77	0
35	NA	0	9166	1/1	0.85	0.20	77,77,77,77	0
33	MG	0	8087	1/1	0.86	0.16	57,57,57,57	0
35	NA	0	9113	1/1	0.87	0.11	59,59,59,59	0
35	NA	0	9163	1/1	0.87	0.26	71,71,71,71	0
35	NA	0	9117	1/1	0.88	0.10	72,72,72,72	0
35	NA	0	9176	1/1	0.88	0.11	43,43,43,43	0
35	NA	0	9164	1/1	0.88	0.12	52,52,52,52	0
33	MG	0	8050	1/1	0.88	0.09	63,63,63,63	0
34	K	0	9003	1/1	0.89	0.28	82,82,82,82	0
35	NA	0	9171	1/1	0.89	0.20	60,60,60,60	0
35	NA	0	9150	1/1	0.89	0.09	44,44,44,44	0
33	MG	0	8114	1/1	0.89	0.09	64,64,64,64	0
33	MG	0	8066	1/1	0.89	0.11	114,114,114,114	0
35	NA	0	9165	1/1	0.90	0.14	39,39,39,39	0
35	NA	0	9111	1/1	0.90	0.25	65,65,65,65	0
35	NA	0	9170	1/1	0.90	0.29	61,61,61,61	0
35	NA	0	9157	1/1	0.90	0.19	60,60,60,60	0
35	NA	0	9129	1/1	0.90	0.11	53,53,53,53	0
35	NA	0	9141	1/1	0.90	0.14	46,46,46,46	0
36	CL	0	9315	1/1	0.90	0.20	69,69,69,69	0
35	NA	0	9107	1/1	0.91	0.07	43,43,43,43	0
33	MG	0	8090	1/1	0.91	0.16	80,80,80,80	0
35	NA	0	9172	1/1	0.91	0.19	59,59,59,59	0
33	MG	0	8101	1/1	0.91	0.13	69,69,69,69	0
35	NA	R	9137	1/1	0.91	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9142	1/1	0.91	0.11	52,52,52,52	0
33	MG	0	8103	1/1	0.91	0.11	66,66,66,66	0
36	CL	J	9302	1/1	0.91	0.12	70,70,70,70	0
33	MG	0	8049	1/1	0.92	0.17	90,90,90,90	0
35	NA	B	9158	1/1	0.92	0.43	69,69,69,69	0
33	MG	0	8024	1/1	0.92	0.08	49,49,49,49	0
33	MG	0	8113	1/1	0.92	0.07	45,45,45,45	0
35	NA	0	9184	1/1	0.92	0.21	75,75,75,75	0
35	NA	0	9110	1/1	0.92	0.09	37,37,37,37	0
33	MG	0	8085	1/1	0.92	0.09	93,93,93,93	0
37	CD	O	9205	1/1	0.92	0.15	137,137,137,137	0
35	NA	0	9162	1/1	0.93	0.24	58,58,58,58	0
35	NA	0	9140	1/1	0.93	0.12	49,49,49,49	0
35	NA	0	9102	1/1	0.93	0.09	42,42,42,42	0
35	NA	0	9179	1/1	0.93	0.12	57,57,57,57	0
33	MG	0	8102	1/1	0.93	0.06	51,51,51,51	0
33	MG	0	8041	1/1	0.93	0.09	59,59,59,59	0
33	MG	0	8045	1/1	0.93	0.18	65,65,65,65	0
35	NA	0	9161	1/1	0.93	0.09	49,49,49,49	0
33	MG	0	8118	1/1	0.94	0.08	63,63,63,63	0
33	MG	0	8057	1/1	0.94	0.09	39,39,39,39	0
35	NA	0	9175	1/1	0.94	0.27	42,42,42,42	0
35	NA	0	9155	1/1	0.94	0.13	60,60,60,60	0
35	NA	0	9114	1/1	0.94	0.16	66,66,66,66	0
35	NA	0	9181	1/1	0.94	0.07	51,51,51,51	0
35	NA	0	9160	1/1	0.94	0.19	41,41,41,41	0
35	NA	0	9115	1/1	0.94	0.08	37,37,37,37	0
33	MG	0	8091	1/1	0.94	0.06	74,74,74,74	0
35	NA	0	9121	1/1	0.94	0.19	50,50,50,50	0
33	MG	0	8106	1/1	0.94	0.06	51,51,51,51	0
35	NA	0	9126	1/1	0.94	0.10	40,40,40,40	0
35	NA	0	9105	1/1	0.94	0.05	35,35,35,35	0
35	NA	0	9167	1/1	0.94	0.09	40,40,40,40	0
35	NA	0	9168	1/1	0.94	0.17	52,52,52,52	0
35	NA	0	9169	1/1	0.94	0.09	46,46,46,46	0
33	MG	0	8053	1/1	0.94	0.07	51,51,51,51	0
33	MG	0	8072	1/1	0.94	0.08	51,51,51,51	0
33	MG	0	8046	1/1	0.95	0.05	52,52,52,52	0
33	MG	0	8063	1/1	0.95	0.06	53,53,53,53	0
35	NA	0	9173	1/1	0.95	0.06	42,42,42,42	0
35	NA	9	9183	1/1	0.95	0.06	55,55,55,55	0
33	MG	0	8098	1/1	0.95	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	C	9104	1/1	0.95	0.05	32,32,32,32	0
35	NA	O	9152	1/1	0.95	0.27	60,60,60,60	0
35	NA	O	9116	1/1	0.95	0.09	36,36,36,36	0
35	NA	O	9156	1/1	0.95	0.12	50,50,50,50	0
36	CL	O	9313	1/1	0.95	0.09	62,62,62,62	0
35	NA	O	9133	1/1	0.95	0.08	27,27,27,27	0
36	CL	O	9322	1/1	0.95	0.39	76,76,76,76	0
36	CL	J	9301	1/1	0.95	0.11	72,72,72,72	0
35	NA	O	9135	1/1	0.95	0.08	43,43,43,43	0
36	CL	O	9308	1/1	0.95	0.11	68,68,68,68	0
33	MG	O	8116	1/1	0.95	0.08	50,50,50,50	0
37	CD	3	9204	1/1	0.95	0.06	62,62,62,62	0
35	NA	A	9145	1/1	0.96	0.07	39,39,39,39	0
35	NA	O	9101	1/1	0.96	0.09	46,46,46,46	0
33	MG	O	8043	1/1	0.96	0.06	42,42,42,42	0
33	MG	O	8115	1/1	0.96	0.05	52,52,52,52	0
35	NA	L	9180	1/1	0.96	0.20	50,50,50,50	0
35	NA	O	9177	1/1	0.96	0.12	55,55,55,55	0
35	NA	O	9178	1/1	0.96	0.19	53,53,53,53	0
35	NA	O	9119	1/1	0.96	0.07	42,42,42,42	0
33	MG	O	8059	1/1	0.96	0.08	51,51,51,51	0
36	CL	O	9316	1/1	0.96	0.11	56,56,56,56	0
36	CL	O	9320	1/1	0.96	0.07	48,48,48,48	0
35	NA	O	9108	1/1	0.96	0.07	48,48,48,48	0
36	CL	A	9309	1/1	0.96	0.08	58,58,58,58	0
33	MG	O	8117	1/1	0.96	0.04	32,32,32,32	0
33	MG	O	8070	1/1	0.96	0.07	53,53,53,53	0
36	CL	J	9321	1/1	0.96	0.07	54,54,54,54	0
35	NA	O	9130	1/1	0.96	0.06	36,36,36,36	0
36	CL	3	9304	1/1	0.96	0.08	47,47,47,47	0
33	MG	O	8112	1/1	0.96	0.05	37,37,37,37	0
33	MG	O	8062	1/1	0.96	0.06	53,53,53,53	0
33	MG	O	8051	1/1	0.97	0.06	56,56,56,56	0
35	NA	O	9103	1/1	0.97	0.07	44,44,44,44	0
35	NA	O	9131	1/1	0.97	0.04	35,35,35,35	0
35	NA	O	9132	1/1	0.97	0.04	29,29,29,29	0
35	NA	H	9109	1/1	0.97	0.05	31,31,31,31	0
33	MG	O	8108	1/1	0.97	0.10	56,56,56,56	0
35	NA	J	9146	1/1	0.97	0.04	37,37,37,37	0
33	MG	O	8039	1/1	0.97	0.05	49,49,49,49	0
35	NA	Q	9148	1/1	0.97	0.08	36,36,36,36	0
35	NA	O	9139	1/1	0.97	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8093	1/1	0.97	0.06	56,56,56,56	0
36	CL	0	9303	1/1	0.97	0.08	54,54,54,54	0
36	CL	0	9305	1/1	0.97	0.08	52,52,52,52	0
33	MG	0	8094	1/1	0.97	0.10	62,62,62,62	0
36	CL	0	9314	1/1	0.97	0.07	50,50,50,50	0
33	MG	0	8071	1/1	0.97	0.05	53,53,53,53	0
33	MG	0	8099	1/1	0.97	0.07	59,59,59,59	0
36	CL	0	9317	1/1	0.97	0.07	61,61,61,61	0
33	MG	0	8100	1/1	0.97	0.07	68,68,68,68	0
33	MG	0	8088	1/1	0.97	0.04	39,39,39,39	0
33	MG	9	8052	1/1	0.97	0.05	50,50,50,50	0
36	CL	B	9319	1/1	0.97	0.10	47,47,47,47	0
33	MG	0	8089	1/1	0.97	0.06	60,60,60,60	0
35	NA	0	9159	1/1	0.97	0.13	50,50,50,50	0
34	K	0	9001	1/1	0.97	0.15	66,66,66,66	0
36	CL	N	9307	1/1	0.97	0.07	61,61,61,61	0
34	K	0	9002	1/1	0.97	0.13	43,43,43,43	0
36	CL	R	9306	1/1	0.97	0.07	53,53,53,53	0
33	MG	0	8042	1/1	0.97	0.06	45,45,45,45	0
33	MG	0	8104	1/1	0.97	0.07	53,53,53,53	0
35	NA	0	9127	1/1	0.97	0.12	39,39,39,39	0
33	MG	0	8060	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8007	1/1	0.98	0.03	23,23,23,23	0
33	MG	0	8018	1/1	0.98	0.04	40,40,40,40	0
35	NA	0	9118	1/1	0.98	0.08	54,54,54,54	0
33	MG	A	8065	1/1	0.98	0.04	42,42,42,42	0
33	MG	B	8055	1/1	0.98	0.09	60,60,60,60	0
35	NA	M	9147	1/1	0.98	0.03	18,18,18,18	0
33	MG	K	8069	1/1	0.98	0.04	41,41,41,41	0
35	NA	0	9125	1/1	0.98	0.08	64,64,64,64	0
33	MG	T	8073	1/1	0.98	0.05	49,49,49,49	0
33	MG	Y	8109	1/1	0.98	0.06	40,40,40,40	0
35	NA	0	9128	1/1	0.98	0.05	40,40,40,40	0
36	CL	0	9311	1/1	0.98	0.08	51,51,51,51	0
36	CL	0	9312	1/1	0.98	0.06	52,52,52,52	0
33	MG	3	8078	1/1	0.98	0.03	46,46,46,46	0
33	MG	0	8064	1/1	0.98	0.03	25,25,25,25	0
33	MG	0	8040	1/1	0.98	0.04	45,45,45,45	0
33	MG	0	8067	1/1	0.98	0.07	52,52,52,52	0
33	MG	0	8107	1/1	0.98	0.04	45,45,45,45	0
33	MG	0	8068	1/1	0.98	0.03	58,58,58,58	0
35	NA	0	9136	1/1	0.98	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8110	1/1	0.98	0.05	34,34,34,34	0
33	MG	0	8111	1/1	0.98	0.04	57,57,57,57	0
35	NA	0	9106	1/1	0.98	0.13	34,34,34,34	0
33	MG	0	8048	1/1	0.98	0.06	60,60,60,60	0
35	NA	0	9144	1/1	0.98	0.03	35,35,35,35	0
36	CL	L	9310	1/1	0.98	0.09	58,58,58,58	0
33	MG	0	8058	1/1	0.98	0.03	45,45,45,45	0
33	MG	0	8044	1/1	0.98	0.04	47,47,47,47	0
35	NA	0	9154	1/1	0.98	0.10	26,26,26,26	0
33	MG	0	8097	1/1	0.98	0.06	45,45,45,45	0
33	MG	0	8076	1/1	0.98	0.04	57,57,57,57	0
33	MG	0	8080	1/1	0.98	0.04	37,37,37,37	0
33	MG	0	8083	1/1	0.99	0.03	35,35,35,35	0
33	MG	0	8084	1/1	0.99	0.04	40,40,40,40	0
33	MG	0	8013	1/1	0.99	0.03	33,33,33,33	0
35	NA	0	9134	1/1	0.99	0.15	34,34,34,34	0
33	MG	B	8056	1/1	0.99	0.02	49,49,49,49	0
33	MG	0	8086	1/1	0.99	0.04	50,50,50,50	0
35	NA	0	9138	1/1	0.99	0.07	51,51,51,51	0
33	MG	0	8014	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	8015	1/1	0.99	0.03	30,30,30,30	0
33	MG	0	8002	1/1	0.99	0.07	28,28,28,28	0
33	MG	0	8019	1/1	0.99	0.03	33,33,33,33	0
33	MG	0	8020	1/1	0.99	0.02	32,32,32,32	0
35	NA	0	9149	1/1	0.99	0.03	36,36,36,36	0
33	MG	0	8021	1/1	0.99	0.02	25,25,25,25	0
33	MG	0	8022	1/1	0.99	0.04	35,35,35,35	0
35	NA	0	9153	1/1	0.99	0.09	17,17,17,17	0
33	MG	0	8023	1/1	0.99	0.08	53,53,53,53	0
33	MG	0	8096	1/1	0.99	0.04	38,38,38,38	0
35	NA	T	9143	1/1	0.99	0.04	31,31,31,31	0
33	MG	0	8054	1/1	0.99	0.03	24,24,24,24	0
33	MG	0	8003	1/1	0.99	0.03	26,26,26,26	0
33	MG	0	8026	1/1	0.99	0.04	24,24,24,24	0
33	MG	0	8027	1/1	0.99	0.05	44,44,44,44	0
33	MG	0	8029	1/1	0.99	0.05	32,32,32,32	0
33	MG	0	8030	1/1	0.99	0.03	35,35,35,35	0
33	MG	0	8032	1/1	0.99	0.03	39,39,39,39	0
33	MG	0	8034	1/1	0.99	0.02	39,39,39,39	0
33	MG	0	8035	1/1	0.99	0.03	50,50,50,50	0
33	MG	0	8036	1/1	0.99	0.03	39,39,39,39	0
33	MG	0	8037	1/1	0.99	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8038	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	8006	1/1	0.99	0.03	32,32,32,32	0
35	NA	0	9120	1/1	0.99	0.07	56,56,56,56	0
33	MG	0	8001	1/1	0.99	0.03	36,36,36,36	0
35	NA	0	9123	1/1	0.99	0.09	52,52,52,52	0
33	MG	0	8074	1/1	0.99	0.03	34,34,34,34	0
36	CL	M	9318	1/1	0.99	0.06	36,36,36,36	0
33	MG	0	8075	1/1	0.99	0.05	39,39,39,39	0
33	MG	0	8008	1/1	0.99	0.03	35,35,35,35	0
33	MG	0	8079	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	8011	1/1	0.99	0.04	23,23,23,23	0
33	MG	0	8081	1/1	0.99	0.04	43,43,43,43	0
37	CD	U	9201	1/1	0.99	0.03	73,73,73,73	0
37	CD	Z	9203	1/1	0.99	0.03	61,61,61,61	0
37	CD	1	9202	1/1	0.99	0.10	54,54,54,54	0
33	MG	0	8012	1/1	0.99	0.05	35,35,35,35	0
33	MG	0	8061	1/1	1.00	0.02	34,34,34,34	0
33	MG	0	8028	1/1	1.00	0.04	43,43,43,43	0
33	MG	0	8077	1/1	1.00	0.02	29,29,29,29	0
33	MG	0	8005	1/1	1.00	0.03	24,24,24,24	0
33	MG	0	8016	1/1	1.00	0.06	35,35,35,35	0
33	MG	0	8031	1/1	1.00	0.02	30,30,30,30	0
33	MG	4	8119	1/1	1.00	0.02	41,41,41,41	0
33	MG	0	8017	1/1	1.00	0.02	31,31,31,31	0
33	MG	0	8033	1/1	1.00	0.01	39,39,39,39	0
33	MG	0	8004	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8025	1/1	1.00	0.04	48,48,48,48	0
33	MG	0	8009	1/1	1.00	0.01	31,31,31,31	0
33	MG	0	8010	1/1	1.00	0.03	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.