



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 07:08 AM EDT

PDB ID : 3CPW  
Title : The structure of the antibiotic LINEZOLID bound to the large ribosomal subunit of HALOARCULA MARISMORTUI  
Authors : Ippolito, J.A.; Kanyo, Z.K.; Wang, D.; Franceschi, F.J.; Moore, P.B.; Steitz, T.A.; Duffy, E.M.  
Deposited on : 2008-04-01  
Resolution : 2.70 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

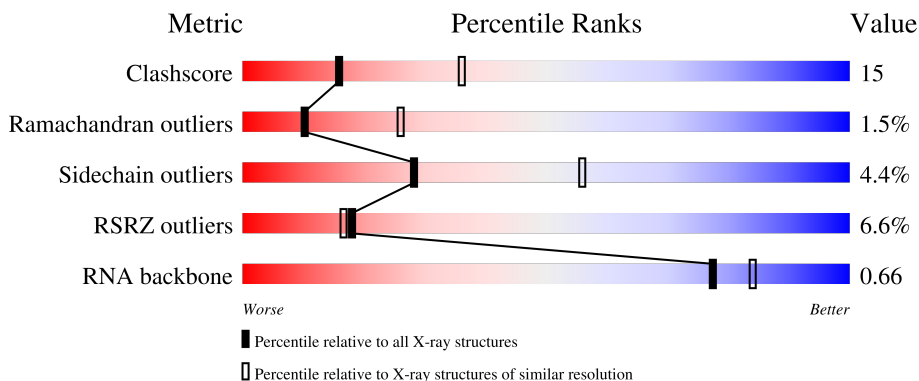
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



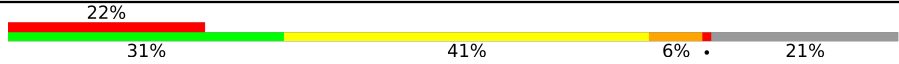
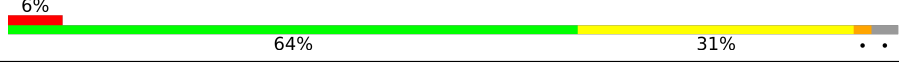
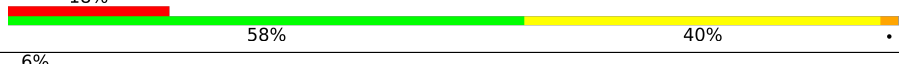
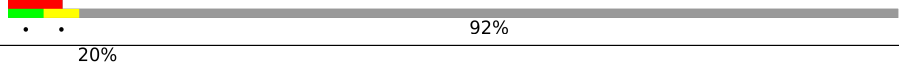

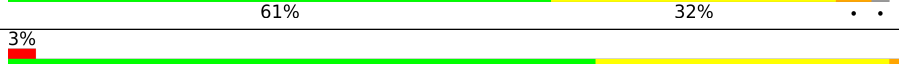
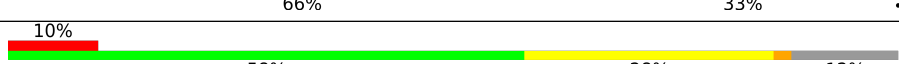
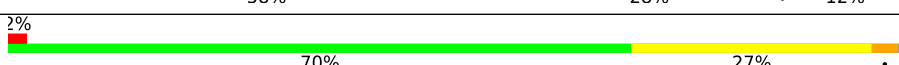
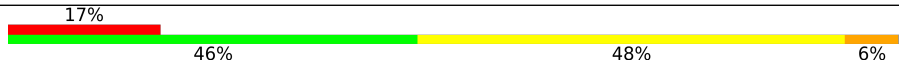


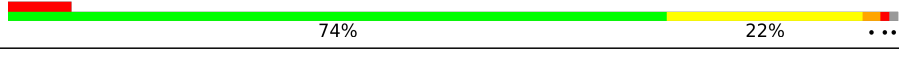
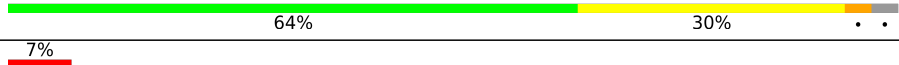


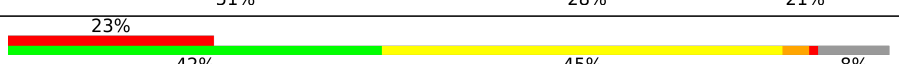


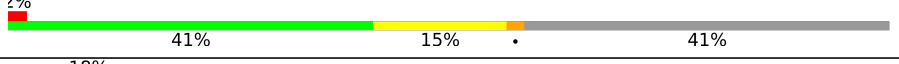
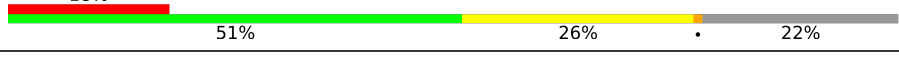





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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  $\geq 3$ , 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	 4% 55% 34% 5% 6%
2	9	122	 11% 48% 39% 11%
3	A	240	 4% 60% 32% 6%
4	B	338	 % 61% 36%
5	C	246	 2% 66% 30%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	145	
12	J	132	
13	K	165	
14	L	196	
15	M	187	
16	N	116	
17	O	149	
18	P	96	
19	Q	155	
20	R	85	
21	S	120	
22	T	67	
23	U	71	
24	V	154	
25	W	92	
26	X	241	
27	Y	92	
28	Z	57	
29	1	50	
30	2	92	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
31	4	4	<p>100% 25% 25% 50%</p>

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
33	MG	0	8017	-	-	-	X
33	MG	0	8030	-	-	-	X
33	MG	0	8037	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8071	-	-	-	X
33	MG	0	8073	-	-	-	X
33	MG	0	8082	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8518	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8544	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8543	-	-	-	X
35	NA	9	8572	-	-	-	X
37	SR	0	9006	-	-	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98629 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
			Total	C	N	O	P			
1	0	2754	59016	26346	10879	19046	2745	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	559	C	U	conflict	GB 3377779
0	560	C	U	conflict	GB 3377779
0	2099	A	G	engineered mutation	GB 3377779

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	246	1860	1130	345	384	1	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	H	160	1282	798	240	238	6	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	J	132	994	609	189	192	4	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	L	194	1558	943	333	281	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	T	53	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
			Total	C	N	O	S			
23	U	65	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
			Total	C	N	O	S			
24	V	154	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
			Total	C	N	O	S			
25	W	82	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
			Total	C	N	O			
26	X	142	1130	686	228	216	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	Y	72	567	340	112	110	5	0	0	0

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

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

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

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

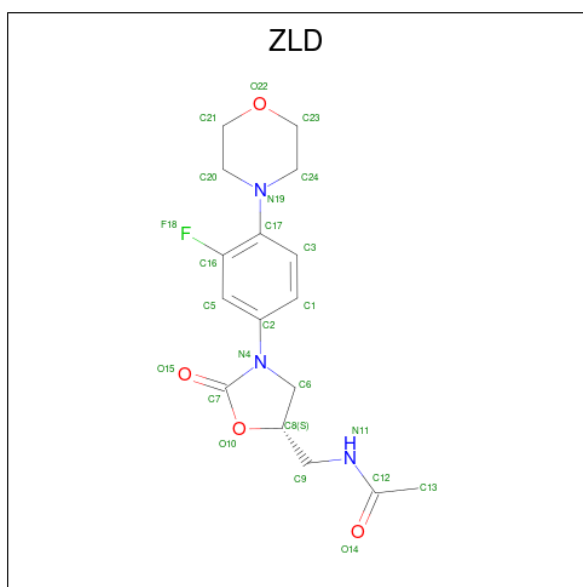
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	2	92	755	458	153	137	7	0	0	0

- Molecule 31 is a RNA chain called 5'-R(\*CP\*CP\*AP\*(PHE)\*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
31	4	4	70	37	12	19	2	0	0	0

- Molecule 32 is N-[[[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl]acetamide (three-letter code: ZLD) (formula: C<sub>16</sub>H<sub>20</sub>FN<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
32	0	1	24	16	1	3	4	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
33	0	84	84	84	0	0
33	9	1	1	1	0	0
33	A	2	2	2	0	0
33	B	1	1	1	0	0
33	J	1	1	1	0	0
33	S	1	1	1	0	0
33	X	1	1	1	0	0
33	1	1	1	1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	64	Total Na 64 64	0	0
35	9	2	Total Na 2 2	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	I	1	Total Na 1 1	0	0
35	K	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	P	1	Total Na 1 1	0	0
35	Q	2	Total Na 2 2	0	0
35	R	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	J	1	Total Cl 1 1	0	0
36	K	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	Q	1	Total Cl 1 1	0	0
36	X	1	Total Cl 1 1	0	0
36	2	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	92	Total Sr 92 92	0	0
37	9	3	Total Sr 3 3	0	0
37	A	3	Total Sr 3 3	0	0
37	B	2	Total Sr 2 2	0	0
37	F	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	Q	1	Total Sr 1 1	0	0
37	R	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	Z	2	Total Sr 2 2	0	0
37	2	1	Total Sr 1 1	0	0

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

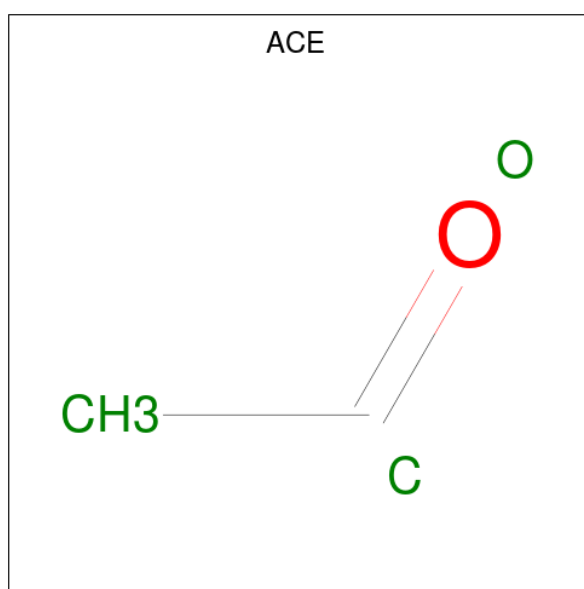
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	N	1	Total Cd 1 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	1	Total 1	Cd 1	0	0
38	Y	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	2	1	Total 1	Cd 1	0	0

- Molecule 39 is ACETYL GROUP (three-letter code: ACE) (formula: C<sub>2</sub>H<sub>4</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	4	1	Total 3	C 2	O 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5757	Total 5757	O 5757	0	0
40	9	144	Total 144	O 144	0	0
40	A	129	Total 129	O 129	0	0
40	B	158	Total 158	O 158	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	183	Total 183	O 183	0	0
40	D	53	Total 53	O 53	0	0
40	E	50	Total 50	O 50	0	0
40	F	25	Total 25	O 25	0	0
40	G	22	Total 22	O 22	0	0
40	H	66	Total 66	O 66	0	0
40	I	57	Total 57	O 57	0	0
40	J	59	Total 59	O 59	0	0
40	K	84	Total 84	O 84	0	0
40	L	136	Total 136	O 136	0	0
40	M	66	Total 66	O 66	0	0
40	N	45	Total 45	O 45	0	0
40	O	70	Total 70	O 70	0	0
40	P	51	Total 51	O 51	0	0
40	Q	84	Total 84	O 84	0	0
40	R	38	Total 38	O 38	0	0
40	S	43	Total 43	O 43	0	0
40	T	28	Total 28	O 28	0	0
40	U	15	Total 15	O 15	0	0
40	V	75	Total 75	O 75	0	0
40	W	28	Total 28	O 28	0	0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
40	X	99	Total O 99 99	0	0
40	Y	23	Total O 23 23	0	0
40	Z	58	Total O 58 58	0	0
40	1	40	Total O 40 40	0	0
40	2	73	Total O 73 73	0	0
40	4	3	Total O 3 3	0	0











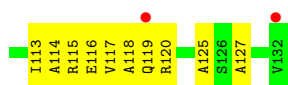
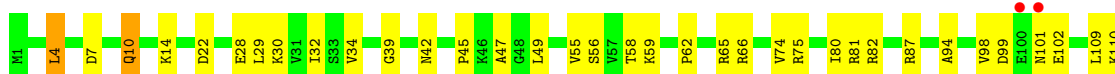




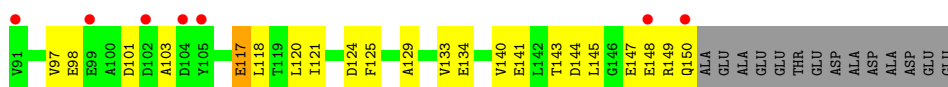
- Molecule 11: 50S ribosomal protein L13P



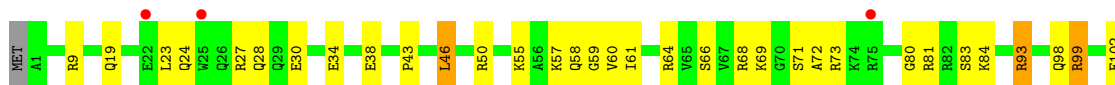
- Molecule 12: 50S ribosomal protein L14P



- Molecule 13: 50S ribosomal protein L15P

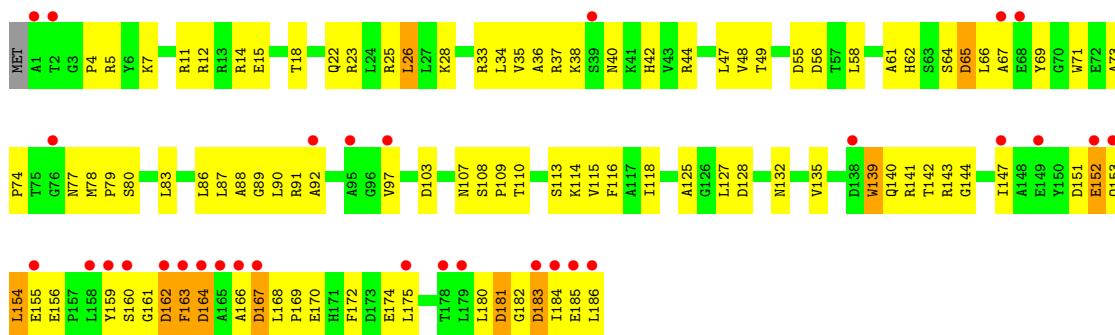


- Molecule 14: 50S ribosomal protein L15e

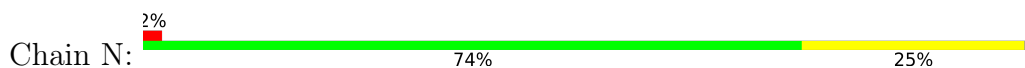


- Molecule 15: 50S ribosomal protein L18P

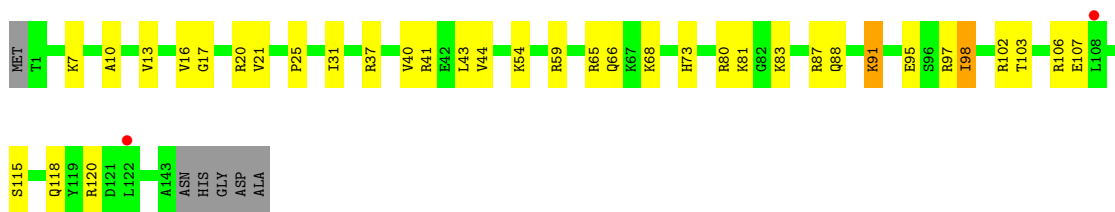




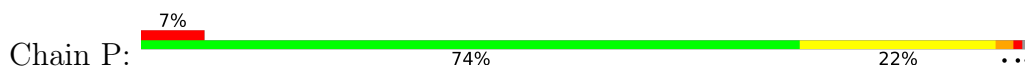
• Molecule 16: 50S ribosomal protein L18e



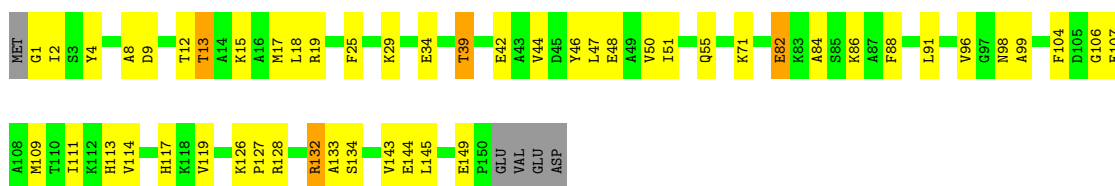
• Molecule 17: 50S ribosomal protein L19e



• Molecule 18: 50S ribosomal protein L21e



• Molecule 19: 50S ribosomal protein L22P

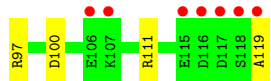
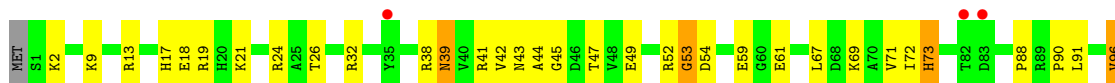


• Molecule 20: 50S ribosomal protein L23P

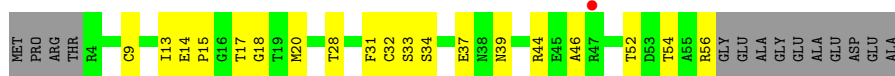




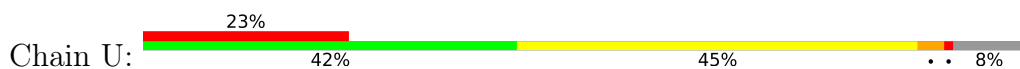
• Molecule 21: 50S ribosomal protein L24P



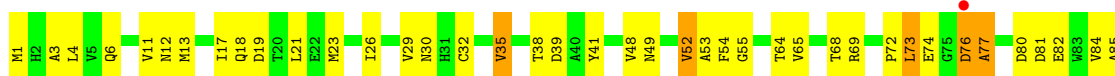
• Molecule 22: 50S ribosomal protein L24e



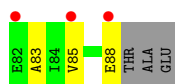
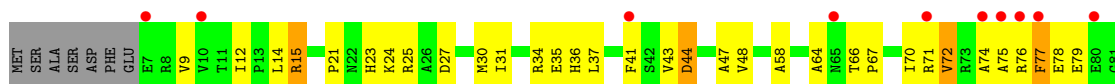
• Molecule 23: 50S ribosomal protein L29P



• Molecule 24: 50S ribosomal protein L30P



• Molecule 25: 50S ribosomal protein L31e









## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.73Å 298.58Å 575.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 91.4 (39.62-2.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.69Å)	Xtrriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.191 , 0.230 0.193 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtrriage
Anisotropy	0.107	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 74.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	98629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.37	2/66075 (0.0%)	0.69	25/103050 (0.0%)
2	9	0.34	0/2905	0.75	2/4528 (0.0%)
3	A	0.35	0/1786	0.65	0/2408
4	B	0.33	0/2690	0.64	0/3652
5	C	0.37	0/1885	0.63	0/2552
6	D	0.31	0/1111	0.57	0/1498
7	E	0.32	0/1382	0.57	0/1880
8	F	0.38	0/901	0.57	0/1224
9	G	0.28	0/241	0.48	0/324
10	H	0.51	0/1302	0.70	1/1743 (0.1%)
11	I	0.35	0/1136	0.59	0/1530
12	J	0.32	0/1004	0.65	0/1351
13	K	0.33	0/1130	0.65	0/1509
14	L	0.48	0/1582	0.67	0/2116
15	M	0.29	0/1474	0.62	0/1999
16	N	0.32	0/874	0.59	0/1181
17	O	0.35	0/1147	0.56	0/1528
18	P	0.33	0/749	0.65	0/1005
19	Q	0.34	0/1172	0.64	0/1578
20	R	0.31	0/648	0.57	0/875
21	S	0.31	0/958	0.62	0/1289
22	T	0.34	0/417	0.54	0/562
23	U	0.28	0/502	0.53	0/675
24	V	0.34	0/1219	0.62	0/1655
25	W	0.33	0/664	0.58	0/895
26	X	0.34	0/1146	0.64	0/1536
27	Y	0.46	0/578	0.69	0/773
28	Z	0.40	0/438	0.66	0/578
29	1	0.35	0/401	0.59	0/529
30	2	0.37	0/771	0.58	0/1024
31	4	1.99	3/76 (3.9%)	1.29	1/112 (0.9%)
All	All	0.37	5/98364 (0.0%)	0.68	29/147159 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	54
2	9	0	2
24	V	0	1
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	559	C	C4-N4	-11.17	1.23	1.33
1	0	559	C	N3-C4	6.65	1.38	1.33
31	4	74	C	N1-C6	6.21	1.40	1.37
31	4	75	C	N1-C6	5.85	1.40	1.37
31	4	76	A	N3-C4	5.43	1.38	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	559	C	N3-C4-C5	-18.22	114.61	121.90
1	0	559	C	C2-N3-C4	14.39	127.10	119.90
2	9	3024	U	C2'-C3'-O3'	8.50	128.19	109.50
1	0	559	C	C5-C4-N4	7.84	125.69	120.20
1	0	871	G	C5'-C4'-O4'	-7.72	99.84	109.10

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	270	U	Sidechain
1	0	324	G	Sidechain
1	0	332	G	Sidechain
1	0	50	G	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	59016	0	29807	894	0
2	9	2600	0	1326	75	0
3	A	1753	0	1766	102	0
4	B	2625	0	2532	132	0
5	C	1860	0	1813	85	0
6	D	1094	0	1085	92	0
7	E	1357	0	1266	62	0
8	F	890	0	843	46	0
9	G	240	0	231	15	0
10	H	1282	0	1295	61	0
11	I	1120	0	1098	56	0
12	J	994	0	1027	48	0
13	K	1118	0	1076	47	0
14	L	1558	0	1573	57	0
15	M	1445	0	1401	113	0
16	N	865	0	873	28	0
17	O	1136	0	1123	38	0
18	P	735	0	728	19	0
19	Q	1149	0	1122	49	0
20	R	641	0	605	21	0
21	S	950	0	923	37	0
22	T	410	0	364	21	0
23	U	499	0	511	36	0
24	V	1196	0	1137	87	0
25	W	654	0	653	35	0
26	X	1130	0	1133	43	0
27	Y	567	0	526	18	0
28	Z	431	0	426	26	0
29	1	396	0	413	25	0
30	2	755	0	728	29	0
31	4	70	0	42	4	0
32	0	24	0	20	0	0
33	0	84	0	0	0	0
33	1	1	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	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
34	0	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	0	64	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	9	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	0	92	0	0	0	0
37	2	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	Q	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
37	Z	2	0	0	0	0
38	2	1	0	0	0	0
38	N	1	0	0	0	0
38	T	1	0	0	0	0
38	Y	1	0	0	0	0
38	Z	1	0	0	0	0
39	4	3	0	3	0	0
40	0	5757	0	0	72	0
40	1	40	0	0	1	0
40	2	73	0	0	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	4	3	0	0	0	0
40	9	144	0	0	5	0
40	A	129	0	0	10	0
40	B	158	0	0	12	0
40	C	183	0	0	12	0
40	D	53	0	0	4	0
40	E	50	0	0	4	0
40	F	25	0	0	2	0
40	G	22	0	0	2	0
40	H	66	0	0	6	0
40	I	57	0	0	3	0
40	J	59	0	0	4	0
40	K	84	0	0	9	0
40	L	136	0	0	5	0
40	M	66	0	0	10	0
40	N	45	0	0	3	0
40	O	70	0	0	1	0
40	P	51	0	0	2	0
40	Q	84	0	0	1	0
40	R	38	0	0	0	0
40	S	43	0	0	4	0
40	T	28	0	0	1	0
40	U	15	0	0	1	0
40	V	75	0	0	4	0
40	W	28	0	0	1	0
40	X	99	0	0	4	0
40	Y	23	0	0	2	0
40	Z	58	0	0	1	0
All	All	98629	0	59469	2191	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 2191 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.21	1.14
5:C:236:THR:HG22	5:C:239:ALA:H	1.07	1.11
2:9:3023:U:H3'	2:9:3024:U:H5''	1.29	1.09
1:0:156:C:H5''	14:L:171:ARG:HD3	1.37	1.04
1:0:2637:A:H2'	31:4:74:C:H5''	1.35	1.04

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%)	210 (89%)	19 (8%)	6 (3%)	5	13
4	B	335/338 (99%)	311 (93%)	18 (5%)	6 (2%)	8	21
5	C	244/246 (99%)	227 (93%)	17 (7%)	0	100	100
6	D	134/177 (76%)	99 (74%)	25 (19%)	10 (8%)	1	1
7	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	5	13
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	140 (90%)	15 (10%)	1 (1%)	25	50
11	I	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	4	10
12	J	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	19	43
13	K	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	22	46
14	L	192/196 (98%)	179 (93%)	12 (6%)	1 (0%)	29	54
15	M	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	3	7
16	N	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
17	O	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
18	P	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	6	17
19	Q	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	R	79/85 (93%)	77 (98%)	1 (1%)	1 (1%)	12	30
21	S	117/120 (98%)	108 (92%)	7 (6%)	2 (2%)	9	23
22	T	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
23	U	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	4	9
24	V	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	12	30

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	W	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	12	30
26	X	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
27	Y	70/92 (76%)	61 (87%)	6 (9%)	3 (4%)	2	5
28	Z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	1	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	6	17
All	All	3636/4286 (85%)	3345 (92%)	236 (6%)	55 (2%)	10	26

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO

### 5.3.2 Protein sidechains [i](#)

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%)	167 (93%)	12 (7%)	16	37
4	B	282/283 (100%)	268 (95%)	14 (5%)	24	51
5	C	193/193 (100%)	178 (92%)	15 (8%)	12	29
6	D	117/148 (79%)	107 (92%)	10 (8%)	10	24
7	E	152/156 (97%)	149 (98%)	3 (2%)	55	81
8	F	93/94 (99%)	91 (98%)	2 (2%)	52	79
9	G	27/282 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	127 (95%)	7 (5%)	23	49
11	I	118/121 (98%)	108 (92%)	10 (8%)	10	24
12	J	106/106 (100%)	102 (96%)	4 (4%)	33	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	113/127 (89%)	108 (96%)	5 (4%)	28	56
14	L	158/160 (99%)	152 (96%)	6 (4%)	33	62
15	M	149/150 (99%)	144 (97%)	5 (3%)	37	66
16	N	93/94 (99%)	92 (99%)	1 (1%)	73	90
17	O	113/117 (97%)	111 (98%)	2 (2%)	59	83
18	P	79/80 (99%)	75 (95%)	4 (5%)	24	50
19	Q	117/122 (96%)	113 (97%)	4 (3%)	37	66
20	R	71/74 (96%)	71 (100%)	0	100	100
21	S	105/106 (99%)	102 (97%)	3 (3%)	42	71
22	T	44/53 (83%)	44 (100%)	0	100	100
23	U	51/57 (90%)	49 (96%)	2 (4%)	32	61
24	V	130/130 (100%)	122 (94%)	8 (6%)	18	40
25	W	66/74 (89%)	62 (94%)	4 (6%)	18	41
26	X	120/196 (61%)	111 (92%)	9 (8%)	13	31
27	Y	59/74 (80%)	58 (98%)	1 (2%)	60	84
28	Z	46/47 (98%)	46 (100%)	0	100	100
29	1	42/46 (91%)	41 (98%)	1 (2%)	49	77
30	2	79/79 (100%)	78 (99%)	1 (1%)	69	87
All	All	3036/3496 (87%)	2903 (96%)	133 (4%)	28	56

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

Mol	Chain	Res	Type
24	V	146	ILE
25	W	44	ASP
27	Y	44	GLU
6	D	137	PRO
6	D	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	60	GLN
29	1	18	ASN
24	V	110	GLN

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
26	X	149	GLN
30	2	30	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	239 (8%)	29 (1%)
2	9	121/122 (99%)	17 (14%)	2 (1%)
31	4	2/4 (50%)	1 (50%)	0
All	All	2869/3048 (94%)	257 (8%)	31 (1%)

5 of 257 RNA backbone outliers are listed below:

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

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1164	U
1	0	2726	U
1	0	1352	A
2	9	3024	U
1	0	2467	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 306 ligands modelled in this entry, 304 are monoatomic - leaving 2 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
39	ACE	4	78	31	1,2,2	1.04	0	1,1,1	0.52	0
32	ZLD	0	9500	-	26,26,26	3.08	14 (53%)	36,36,36	3.54	15 (41%)

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	ZLD	0	9500	-	-	0/13/33/33	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZLD	C3-C17	6.25	1.50	1.39
32	0	9500	ZLD	C3-C1	6.07	1.49	1.38
32	0	9500	ZLD	C17-C16	5.49	1.51	1.40
32	0	9500	ZLD	C1-C2	5.09	1.49	1.39
32	0	9500	ZLD	C20-N19	4.76	1.54	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZLD	C6-C8-C9	9.87	124.01	113.08
32	0	9500	ZLD	C6-N4-C7	-9.81	105.60	111.28
32	0	9500	ZLD	C2-N4-C7	7.48	133.92	125.91
32	0	9500	ZLD	O15-C7-N4	-6.35	123.88	128.91
32	0	9500	ZLD	O10-C7-N4	6.27	114.16	109.83

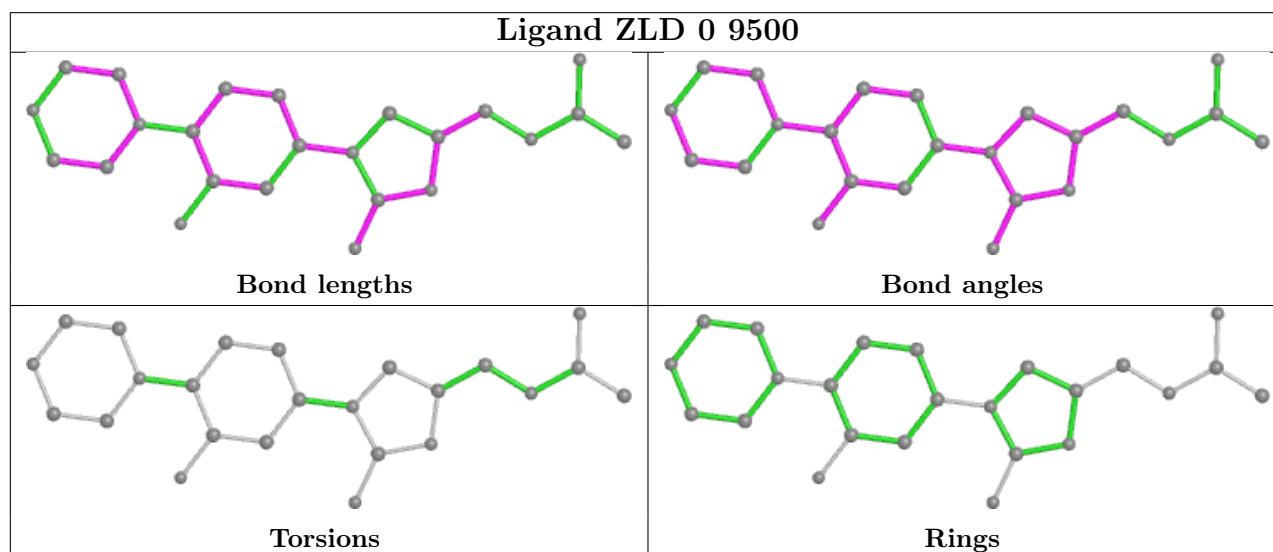
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2754/2922 (94%)	-0.24	118 (4%) 35 33	29, 53, 97, 144	0
2	9	122/122 (100%)	0.53	14 (11%) 4 4	45, 75, 98, 149	0
3	A	237/240 (98%)	0.13	10 (4%) 36 35	34, 58, 90, 107	0
4	B	337/338 (99%)	0.06	5 (1%) 73 76	35, 60, 86, 96	0
5	C	246/246 (100%)	-0.12	4 (1%) 72 74	28, 53, 75, 86	0
6	D	140/177 (79%)	1.50	39 (27%) 0 0	67, 101, 122, 127	0
7	E	172/178 (96%)	0.49	10 (5%) 23 22	48, 74, 93, 98	0
8	F	119/120 (99%)	0.69	21 (17%) 1 1	57, 78, 99, 108	0
9	G	29/348 (8%)	2.66	21 (72%) 0 0	79, 99, 105, 109	0
10	H	160/177 (90%)	0.82	36 (22%) 0 0	41, 55, 80, 88	0
11	I	142/145 (97%)	-0.01	2 (1%) 75 77	43, 56, 75, 94	0
12	J	132/132 (100%)	-0.08	4 (3%) 50 51	40, 54, 78, 90	0
13	K	145/165 (87%)	0.54	16 (11%) 5 4	34, 73, 107, 120	0
14	L	194/196 (98%)	-0.23	3 (1%) 73 76	33, 42, 65, 70	0
15	M	186/187 (99%)	0.87	31 (16%) 1 1	52, 72, 110, 120	0
16	N	115/116 (99%)	0.17	2 (1%) 70 72	45, 62, 77, 82	0
17	O	143/149 (95%)	0.36	2 (1%) 75 77	46, 59, 71, 82	0
18	P	95/96 (98%)	0.14	7 (7%) 14 12	46, 55, 72, 84	0
19	Q	150/155 (96%)	-0.14	0 100 100	37, 51, 70, 76	0
20	R	81/85 (95%)	0.25	6 (7%) 14 12	50, 65, 85, 90	0
21	S	119/120 (99%)	0.53	10 (8%) 11 9	47, 61, 87, 108	0
22	T	53/67 (79%)	0.33	1 (1%) 66 69	47, 59, 78, 86	0
23	U	65/71 (91%)	1.48	16 (24%) 0 0	59, 79, 115, 121	0
24	V	154/154 (100%)	0.17	3 (1%) 66 69	43, 58, 76, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	82/92 (89%)	0.73	13 (15%) 1 1	48, 64, 88, 106	0
26	X	142/241 (58%)	-0.02	4 (2%) 53 54	32, 49, 71, 91	0
27	Y	72/92 (78%)	0.75	17 (23%) 0 0	43, 59, 70, 76	0
28	Z	56/57 (98%)	-0.21	0 100 100	33, 40, 46, 57	0
29	1	46/50 (92%)	0.95	10 (21%) 0 0	41, 62, 87, 99	0
30	2	92/92 (100%)	0.35	6 (6%) 18 17	47, 64, 77, 86	0
31	4	4/4 (100%)	3.21	4 (100%) 0 0	78, 83, 85, 88	0
All	All	6584/7334 (89%)	0.10	435 (6%) 18 16	28, 57, 98, 149	0

The worst 5 of 435 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	13.4
21	S	119	ALA	10.2
15	M	186	LEU	10.1
23	U	1	THR	10.0
23	U	39	ALA	9.8

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
35	NA	9	8543	1/1	-0.00	0.93	116,116,116,116	0
35	NA	R	8510	1/1	0.33	0.39	127,127,127,127	0
35	NA	0	8571	1/1	0.40	0.79	103,103,103,103	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	MG	0	8066	1/1	0.42	0.33	103,103,103,103	0
33	MG	0	8038	1/1	0.50	0.85	88,88,88,88	0
33	MG	0	8081	1/1	0.54	0.34	82,82,82,82	0
33	MG	0	8017	1/1	0.55	0.51	121,121,121,121	0
35	NA	0	8544	1/1	0.56	0.52	86,86,86,86	0
35	NA	0	8518	1/1	0.58	0.65	107,107,107,107	0
35	NA	9	8572	1/1	0.59	0.56	99,99,99,99	0
33	MG	B	8042	1/1	0.59	0.19	85,85,85,85	0
33	MG	0	8037	1/1	0.60	0.48	102,102,102,102	0
35	NA	0	8573	1/1	0.63	1.09	92,92,92,92	0
34	K	0	8401	1/1	0.64	0.90	129,129,129,129	0
37	SR	0	8971	1/1	0.67	0.13	150,150,150,150	0
35	NA	0	8525	1/1	0.69	0.29	92,92,92,92	0
35	NA	0	8561	1/1	0.69	0.17	122,122,122,122	0
33	MG	0	8040	1/1	0.70	0.18	97,97,97,97	0
35	NA	0	8512	1/1	0.70	0.57	72,72,72,72	0
35	NA	0	8555	1/1	0.71	0.66	75,75,75,75	0
35	NA	0	8574	1/1	0.71	0.53	66,66,66,66	0
35	NA	0	8548	1/1	0.72	0.14	59,59,59,59	0
35	NA	0	8575	1/1	0.73	0.56	104,104,104,104	0
35	NA	0	8535	1/1	0.74	0.50	79,79,79,79	0
37	SR	0	9006	1/1	0.74	0.70	150,150,150,150	0
37	SR	9	8980	1/1	0.74	0.07	137,137,137,137	0
33	MG	0	8089	1/1	0.75	0.10	49,49,49,49	0
37	SR	0	8986	1/1	0.75	0.08	131,131,131,131	0
37	SR	0	8989	1/1	0.76	0.14	150,150,150,150	0
33	MG	0	8082	1/1	0.77	0.41	78,78,78,78	0
37	SR	0	8982	1/1	0.77	0.22	144,144,144,144	0
33	MG	0	8071	1/1	0.77	1.23	84,84,84,84	0
35	NA	0	8567	1/1	0.77	0.69	83,83,83,83	0
33	MG	0	8030	1/1	0.77	0.44	99,99,99,99	0
35	NA	0	8522	1/1	0.77	0.81	77,77,77,77	0
33	MG	0	8035	1/1	0.78	0.28	80,80,80,80	0
35	NA	0	8554	1/1	0.78	0.27	63,63,63,63	0
37	SR	0	8919	1/1	0.78	0.15	131,131,131,131	0
33	MG	0	8073	1/1	0.79	0.69	105,105,105,105	0
35	NA	0	8536	1/1	0.80	0.34	71,71,71,71	0
35	NA	0	8550	1/1	0.81	0.29	66,66,66,66	0
35	NA	0	8570	1/1	0.81	0.30	57,57,57,57	0
37	SR	0	8955	1/1	0.81	0.08	122,122,122,122	0
37	SR	B	8987	1/1	0.81	0.39	150,150,150,150	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8069	1/1	0.82	0.35	78,78,78,78	0
33	MG	0	8063	1/1	0.82	0.35	94,94,94,94	0
35	NA	0	8563	1/1	0.82	0.69	69,69,69,69	0
35	NA	0	8556	1/1	0.83	0.36	66,66,66,66	0
35	NA	0	8508	1/1	0.83	0.67	55,55,55,55	0
33	MG	0	8010	1/1	0.83	0.42	70,70,70,70	0
35	NA	0	8541	1/1	0.83	0.36	62,62,62,62	0
37	SR	0	8960	1/1	0.83	0.10	116,116,116,116	0
35	NA	0	8517	1/1	0.83	0.34	53,53,53,53	0
37	SR	0	9001	1/1	0.84	0.08	150,150,150,150	0
37	SR	0	9002	1/1	0.84	0.12	125,125,125,125	0
35	NA	0	8569	1/1	0.84	0.20	61,61,61,61	0
33	MG	0	8092	1/1	0.84	0.15	72,72,72,72	0
37	SR	0	8943	1/1	0.84	0.14	110,110,110,110	0
37	SR	0	8988	1/1	0.85	0.07	125,125,125,125	0
35	NA	0	8562	1/1	0.85	0.84	78,78,78,78	0
37	SR	0	8991	1/1	0.85	0.11	150,150,150,150	0
37	SR	0	8956	1/1	0.85	0.07	128,128,128,128	0
33	MG	0	8007	1/1	0.86	0.24	53,53,53,53	0
32	ZLD	0	9500	24/24	0.86	0.37	69,77,79,80	0
37	SR	0	8997	1/1	0.86	0.12	142,142,142,142	0
35	NA	0	8542	1/1	0.86	0.58	68,68,68,68	0
33	MG	0	8064	1/1	0.86	0.12	69,69,69,69	0
35	NA	0	8528	1/1	0.86	0.28	57,57,57,57	0
37	SR	0	9007	1/1	0.86	0.42	150,150,150,150	0
33	MG	0	8031	1/1	0.86	0.09	57,57,57,57	0
37	SR	0	8946	1/1	0.86	0.17	99,99,99,99	0
35	NA	0	8504	1/1	0.87	0.21	42,42,42,42	0
35	NA	0	8516	1/1	0.87	0.73	52,52,52,52	0
37	SR	0	8944	1/1	0.87	0.34	135,135,135,135	0
35	NA	0	8502	1/1	0.87	0.32	75,75,75,75	0
37	SR	0	8958	1/1	0.88	0.07	96,96,96,96	0
37	SR	0	8939	1/1	0.88	0.14	100,100,100,100	0
37	SR	0	8967	1/1	0.88	0.12	113,113,113,113	0
35	NA	0	8565	1/1	0.88	0.43	66,66,66,66	0
33	MG	0	8085	1/1	0.88	0.26	105,105,105,105	0
36	CL	B	8819	1/1	0.88	0.39	72,72,72,72	0
35	NA	0	8553	1/1	0.88	0.43	63,63,63,63	0
37	SR	0	8931	1/1	0.88	0.15	94,94,94,94	0
39	ACE	4	78	3/3	0.88	0.38	79,79,80,81	0
35	NA	0	8529	1/1	0.89	0.11	46,46,46,46	0
33	MG	0	8036	1/1	0.89	0.08	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8039	1/1	0.89	0.37	68,68,68,68	0
33	MG	A	8051	1/1	0.89	0.14	71,71,71,71	0
35	NA	0	8507	1/1	0.89	0.17	51,51,51,51	0
36	CL	I	8802	1/1	0.89	0.19	71,71,71,71	0
37	SR	0	8908	1/1	0.89	0.16	90,90,90,90	0
35	NA	0	8559	1/1	0.89	0.36	85,85,85,85	0
33	MG	0	8087	1/1	0.89	0.18	61,61,61,61	0
37	SR	0	8976	1/1	0.89	0.23	139,139,139,139	0
33	MG	1	8060	1/1	0.89	0.14	58,58,58,58	0
38	CD	N	8705	1/1	0.89	0.41	150,150,150,150	0
37	SR	0	8985	1/1	0.89	0.24	116,116,116,116	0
37	SR	0	8957	1/1	0.90	0.13	120,120,120,120	0
37	SR	0	8975	1/1	0.90	0.08	133,133,133,133	0
36	CL	0	8815	1/1	0.90	0.13	61,61,61,61	0
37	SR	0	8959	1/1	0.90	0.07	150,150,150,150	0
33	MG	0	8062	1/1	0.90	0.20	61,61,61,61	0
35	NA	0	8501	1/1	0.90	0.15	46,46,46,46	0
37	SR	0	8990	1/1	0.91	0.10	131,131,131,131	0
37	SR	0	8920	1/1	0.91	0.09	96,96,96,96	0
37	SR	0	8994	1/1	0.91	0.83	150,150,150,150	0
37	SR	0	8973	1/1	0.91	0.13	101,101,101,101	0
35	NA	0	8509	1/1	0.91	0.39	83,83,83,83	0
33	MG	0	8065	1/1	0.91	0.78	100,100,100,100	0
33	MG	0	8011	1/1	0.91	0.09	33,33,33,33	0
37	SR	0	8983	1/1	0.91	0.15	150,150,150,150	0
33	MG	0	8002	1/1	0.91	0.36	82,82,82,82	0
33	MG	0	8045	1/1	0.91	0.62	71,71,71,71	0
37	SR	H	8972	1/1	0.91	0.10	148,148,148,148	0
37	SR	R	8961	1/1	0.91	0.15	122,122,122,122	0
37	SR	0	8964	1/1	0.91	0.13	101,101,101,101	0
37	SR	0	8947	1/1	0.91	0.24	109,109,109,109	0
33	MG	0	8029	1/1	0.92	0.26	100,100,100,100	0
33	MG	0	8076	1/1	0.92	0.21	68,68,68,68	0
33	MG	0	8078	1/1	0.92	0.20	64,64,64,64	0
37	SR	0	8965	1/1	0.92	0.10	108,108,108,108	0
35	NA	0	8564	1/1	0.92	0.38	74,74,74,74	0
37	SR	0	9000	1/1	0.92	0.08	111,111,111,111	0
35	NA	0	8514	1/1	0.92	0.23	51,51,51,51	0
35	NA	I	8538	1/1	0.92	0.12	51,51,51,51	0
35	NA	P	8540	1/1	0.92	0.13	73,73,73,73	0
35	NA	Q	8533	1/1	0.92	0.09	68,68,68,68	0
37	SR	0	8981	1/1	0.92	0.11	150,150,150,150	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
37	SR	A	8977	1/1	0.92	0.19	99,99,99,99	0
37	SR	B	8950	1/1	0.92	0.17	106,106,106,106	0
33	MG	S	8057	1/1	0.92	0.19	55,55,55,55	0
35	NA	0	8506	1/1	0.92	0.38	66,66,66,66	0
33	MG	0	8068	1/1	0.92	0.61	86,86,86,86	0
35	NA	0	8521	1/1	0.92	0.44	110,110,110,110	0
36	CL	I	8821	1/1	0.92	0.15	67,67,67,67	0
35	NA	Q	8532	1/1	0.93	0.09	49,49,49,49	0
35	NA	0	8511	1/1	0.93	0.18	71,71,71,71	0
33	MG	0	8001	1/1	0.93	0.32	31,31,31,31	0
33	MG	0	8079	1/1	0.93	0.13	72,72,72,72	0
33	MG	0	8046	1/1	0.93	0.40	65,65,65,65	0
33	MG	0	8047	1/1	0.93	0.38	98,98,98,98	0
35	NA	0	8549	1/1	0.93	0.31	75,75,75,75	0
36	CL	2	8804	1/1	0.93	0.12	88,88,88,88	0
33	MG	0	8067	1/1	0.93	0.06	58,58,58,58	0
33	MG	0	8049	1/1	0.93	0.23	85,85,85,85	0
35	NA	0	8505	1/1	0.93	0.37	51,51,51,51	0
37	SR	0	9008	1/1	0.93	0.13	91,91,91,91	0
37	SR	0	8974	1/1	0.93	0.23	134,134,134,134	0
37	SR	9	9003	1/1	0.93	0.34	150,150,150,150	0
37	SR	0	8924	1/1	0.93	0.24	112,112,112,112	0
33	MG	0	8053	1/1	0.93	0.20	64,64,64,64	0
35	NA	0	8527	1/1	0.93	0.30	51,51,51,51	0
33	MG	0	8056	1/1	0.93	0.36	83,83,83,83	0
33	MG	0	8033	1/1	0.93	0.07	58,58,58,58	0
35	NA	L	8539	1/1	0.93	0.35	43,43,43,43	0
33	MG	0	8043	1/1	0.93	0.27	72,72,72,72	0
35	NA	0	8546	1/1	0.94	0.29	77,77,77,77	0
33	MG	0	8090	1/1	0.94	0.38	83,83,83,83	0
36	CL	K	8810	1/1	0.94	0.13	55,55,55,55	0
36	CL	M	8807	1/1	0.94	0.35	71,71,71,71	0
37	SR	0	8993	1/1	0.94	0.08	139,139,139,139	0
35	NA	0	8531	1/1	0.94	0.08	41,41,41,41	0
35	NA	C	8503	1/1	0.94	0.14	34,34,34,34	0
35	NA	0	8534	1/1	0.94	0.15	61,61,61,61	0
35	NA	0	8551	1/1	0.94	0.35	46,46,46,46	0
37	SR	0	8966	1/1	0.94	0.09	98,98,98,98	0
33	MG	0	8044	1/1	0.94	0.57	79,79,79,79	0
37	SR	0	8969	1/1	0.94	0.13	127,127,127,127	0
37	SR	0	8927	1/1	0.94	0.15	90,90,90,90	0
33	MG	9	8074	1/1	0.94	0.20	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	8933	1/1	0.94	0.08	103,103,103,103	0
35	NA	0	8526	1/1	0.94	0.15	50,50,50,50	0
35	NA	0	8513	1/1	0.94	0.21	50,50,50,50	0
36	CL	0	8813	1/1	0.94	0.10	59,59,59,59	0
37	SR	0	8945	1/1	0.94	0.11	92,92,92,92	0
35	NA	0	8557	1/1	0.94	0.19	67,67,67,67	0
35	NA	0	8519	1/1	0.94	0.33	49,49,49,49	0
37	SR	0	8948	1/1	0.94	0.16	102,102,102,102	0
37	SR	0	8915	1/1	0.95	0.08	93,93,93,93	0
33	MG	0	8019	1/1	0.95	0.23	37,37,37,37	0
33	MG	0	8091	1/1	0.95	0.05	54,54,54,54	0
36	CL	0	8805	1/1	0.95	0.10	65,65,65,65	0
36	CL	0	8811	1/1	0.95	0.14	83,83,83,83	0
37	SR	0	8995	1/1	0.95	0.21	107,107,107,107	0
35	NA	0	8545	1/1	0.95	0.44	57,57,57,57	0
33	MG	0	8052	1/1	0.95	0.19	49,49,49,49	0
37	SR	0	8938	1/1	0.95	0.26	105,105,105,105	0
36	CL	0	8822	1/1	0.95	0.26	69,69,69,69	0
37	SR	0	9004	1/1	0.95	0.15	150,150,150,150	0
36	CL	A	8809	1/1	0.95	0.20	65,65,65,65	0
33	MG	0	8022	1/1	0.95	0.27	46,46,46,46	0
33	MG	0	8084	1/1	0.95	0.10	66,66,66,66	0
33	MG	0	8025	1/1	0.95	0.08	43,43,43,43	0
37	SR	0	8979	1/1	0.95	0.28	150,150,150,150	0
33	MG	0	8058	1/1	0.95	0.22	28,28,28,28	0
33	MG	0	8088	1/1	0.95	0.08	57,57,57,57	0
37	SR	0	8951	1/1	0.95	0.13	113,113,113,113	0
37	SR	F	9005	1/1	0.95	0.20	116,116,116,116	0
37	SR	0	8984	1/1	0.95	0.10	109,109,109,109	0
36	CL	Q	8806	1/1	0.95	0.12	49,49,49,49	0
33	MG	0	8059	1/1	0.95	0.09	56,56,56,56	0
35	NA	0	8523	1/1	0.95	0.20	51,51,51,51	0
35	NA	0	8530	1/1	0.96	0.17	56,56,56,56	0
33	MG	0	8077	1/1	0.96	0.09	47,47,47,47	0
36	CL	0	8816	1/1	0.96	0.19	77,77,77,77	0
33	MG	0	8032	1/1	0.96	0.09	56,56,56,56	0
35	NA	0	8566	1/1	0.96	0.58	54,54,54,54	0
35	NA	0	8547	1/1	0.96	0.34	75,75,75,75	0
36	CL	I	8801	1/1	0.96	0.13	61,61,61,61	0
37	SR	9	8968	1/1	0.96	0.11	132,132,132,132	0
37	SR	0	8937	1/1	0.96	0.13	80,80,80,80	0
33	MG	0	8075	1/1	0.96	0.17	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
37	SR	A	8929	1/1	0.96	0.10	103,103,103,103	0
35	NA	0	8558	1/1	0.96	0.08	63,63,63,63	0
33	MG	X	8086	1/1	0.96	0.13	51,51,51,51	0
35	NA	0	8560	1/1	0.96	0.49	88,88,88,88	0
36	CL	0	8803	1/1	0.96	0.20	61,61,61,61	0
36	CL	X	8820	1/1	0.96	0.07	49,49,49,49	0
33	MG	0	8080	1/1	0.96	0.07	78,78,78,78	0
37	SR	0	8996	1/1	0.96	0.51	150,150,150,150	0
33	MG	0	8027	1/1	0.96	0.24	53,53,53,53	0
37	SR	0	8910	1/1	0.97	0.18	59,59,59,59	0
33	MG	0	8008	1/1	0.97	0.13	34,34,34,34	0
37	SR	0	8962	1/1	0.97	0.06	108,108,108,108	0
37	SR	0	8963	1/1	0.97	0.12	83,83,83,83	0
35	NA	B	8552	1/1	0.97	0.42	59,59,59,59	0
33	MG	0	8070	1/1	0.97	0.07	62,62,62,62	0
33	MG	0	8020	1/1	0.97	0.17	52,52,52,52	0
37	SR	0	8926	1/1	0.97	0.19	82,82,82,82	0
33	MG	0	8016	1/1	0.97	0.20	94,94,94,94	0
37	SR	0	8970	1/1	0.97	0.10	80,80,80,80	0
37	SR	0	8928	1/1	0.97	0.12	91,91,91,91	0
37	SR	0	8954	1/1	0.97	0.15	94,94,94,94	0
33	MG	0	8024	1/1	0.97	0.21	81,81,81,81	0
33	MG	0	8004	1/1	0.97	0.11	36,36,36,36	0
33	MG	0	8026	1/1	0.97	0.11	61,61,61,61	0
37	SR	S	8911	1/1	0.97	0.15	72,72,72,72	0
37	SR	Z	8952	1/1	0.97	0.11	71,71,71,71	0
37	SR	0	8978	1/1	0.97	0.06	85,85,85,85	0
35	NA	0	8537	1/1	0.97	0.09	43,43,43,43	0
33	MG	0	8023	1/1	0.98	0.16	39,39,39,39	0
36	CL	L	8818	1/1	0.98	0.21	48,48,48,48	0
35	NA	K	8568	1/1	0.98	0.23	57,57,57,57	0
36	CL	N	8808	1/1	0.98	0.27	76,76,76,76	0
34	K	0	8402	1/1	0.98	0.09	70,70,70,70	0
37	SR	0	8949	1/1	0.98	0.12	80,80,80,80	0
33	MG	0	8041	1/1	0.98	0.13	44,44,44,44	0
37	SR	0	8992	1/1	0.98	0.09	115,115,115,115	0
37	SR	0	8953	1/1	0.98	0.17	96,96,96,96	0
35	NA	0	8520	1/1	0.98	0.14	61,61,61,61	0
37	SR	0	8906	1/1	0.98	0.18	56,56,56,56	0
37	SR	0	8907	1/1	0.98	0.15	63,63,63,63	0
33	MG	0	8009	1/1	0.98	0.28	23,23,23,23	0
37	SR	0	8998	1/1	0.98	0.11	133,133,133,133	0

*Continued on next page...*

*Continued from previous page...*

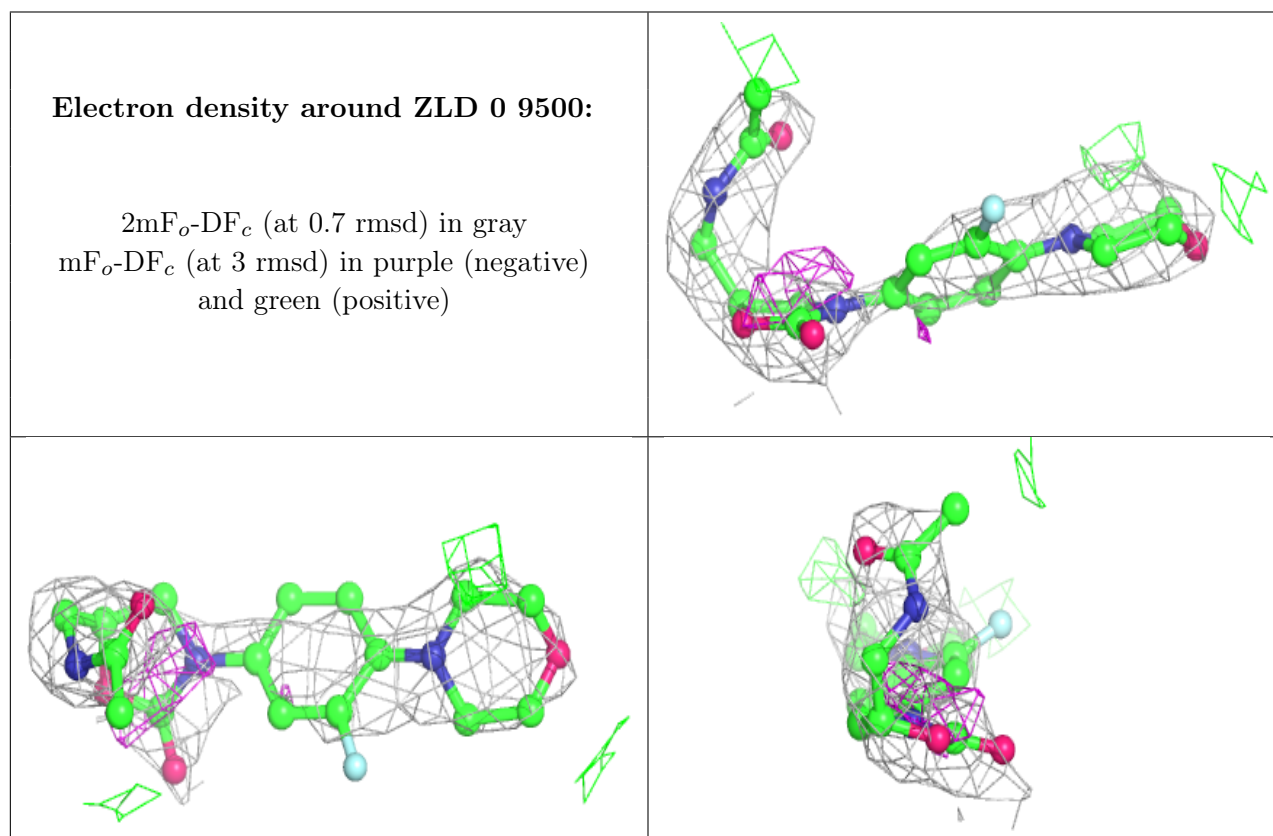
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	8909	1/1	0.98	0.18	74,74,74,74	0
33	MG	0	8018	1/1	0.98	0.29	44,44,44,44	0
33	MG	0	8034	1/1	0.98	0.07	44,44,44,44	0
37	SR	0	8916	1/1	0.98	0.17	85,85,85,85	0
37	SR	0	8917	1/1	0.98	0.16	81,81,81,81	0
35	NA	0	8524	1/1	0.98	0.38	56,56,56,56	0
33	MG	0	8012	1/1	0.98	0.10	30,30,30,30	0
37	SR	0	8923	1/1	0.98	0.13	83,83,83,83	0
33	MG	0	8093	1/1	0.98	0.07	41,41,41,41	0
37	SR	0	8925	1/1	0.98	0.21	79,79,79,79	0
33	MG	0	8015	1/1	0.98	0.13	62,62,62,62	0
37	SR	A	8930	1/1	0.98	0.18	81,81,81,81	0
33	MG	A	8050	1/1	0.98	0.47	93,93,93,93	0
36	CL	0	8817	1/1	0.98	0.13	56,56,56,56	0
33	MG	0	8048	1/1	0.98	0.07	64,64,64,64	0
33	MG	0	8028	1/1	0.98	0.23	29,29,29,29	0
37	SR	0	8934	1/1	0.98	0.17	90,90,90,90	0
33	MG	0	8021	1/1	0.98	0.15	38,38,38,38	0
33	MG	0	8003	1/1	0.98	0.17	35,35,35,35	0
35	NA	0	8515	1/1	0.98	0.15	34,34,34,34	0
37	SR	0	8941	1/1	0.98	0.15	81,81,81,81	0
33	MG	0	8055	1/1	0.98	0.16	40,40,40,40	0
37	SR	0	8999	1/1	0.99	0.09	88,88,88,88	0
37	SR	0	8922	1/1	0.99	0.12	77,77,77,77	0
37	SR	0	8902	1/1	0.99	0.21	49,49,49,49	0
37	SR	0	8903	1/1	0.99	0.14	59,59,59,59	0
37	SR	0	8904	1/1	0.99	0.18	52,52,52,52	0
37	SR	0	8905	1/1	0.99	0.21	59,59,59,59	0
33	MG	0	8005	1/1	0.99	0.07	39,39,39,39	0
36	CL	J	8812	1/1	0.99	0.13	54,54,54,54	0
33	MG	0	8061	1/1	0.99	0.17	36,36,36,36	0
33	MG	0	8006	1/1	0.99	0.25	27,27,27,27	0
33	MG	0	8014	1/1	0.99	0.21	37,37,37,37	0
37	SR	0	8935	1/1	0.99	0.18	80,80,80,80	0
37	SR	0	8936	1/1	0.99	0.15	70,70,70,70	0
37	SR	0	8914	1/1	0.99	0.25	84,84,84,84	0
33	MG	0	8083	1/1	0.99	0.16	55,55,55,55	0
33	MG	0	8072	1/1	0.99	0.13	47,47,47,47	0
37	SR	0	8940	1/1	0.99	0.10	77,77,77,77	0
33	MG	J	8054	1/1	0.99	0.20	37,37,37,37	0
37	SR	0	8942	1/1	0.99	0.12	89,89,89,89	0
37	SR	0	8918	1/1	0.99	0.21	59,59,59,59	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	Z	8913	1/1	0.99	0.14	52,52,52,52	0
36	CL	0	8814	1/1	0.99	0.18	57,57,57,57	0
37	SR	2	8932	1/1	0.99	0.12	76,76,76,76	0
37	SR	0	8901	1/1	0.99	0.14	75,75,75,75	0
38	CD	T	8701	1/1	0.99	0.10	64,64,64,64	0
38	CD	Z	8702	1/1	0.99	0.09	67,67,67,67	0
37	SR	0	8921	1/1	0.99	0.17	70,70,70,70	0
37	SR	Q	8912	1/1	1.00	0.17	75,75,75,75	0
38	CD	2	8704	1/1	1.00	0.07	65,65,65,65	0
38	CD	Y	8703	1/1	1.00	0.08	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.