



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:00 PM UTC

PDB ID : 3CPW / pdb_00003cpw
Title : The structure of the antibiotic LINEZOLID bound to the large ribosomal subunit of HALOARCUA 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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

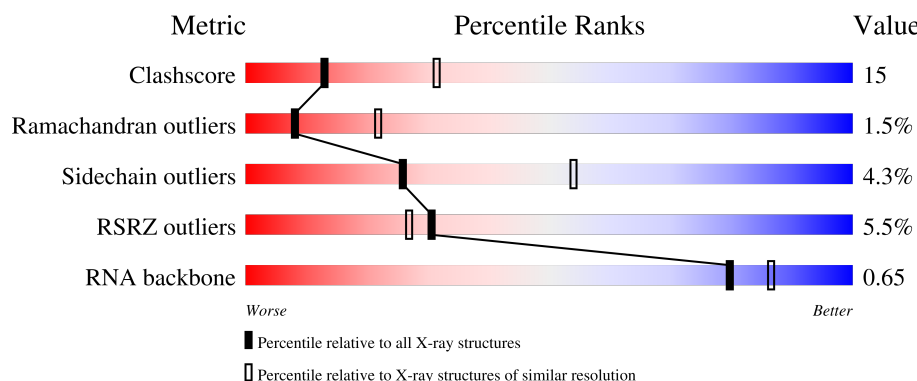
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	5% 54% 34% 5% • 6%
2	9	122	7% 47% 40% 11% •
3	A	240	4% 59% 32% 8% •
4	B	338	4% 59% 36% 5%

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Mol	Chain	Length	Quality of chain
5	C	246	
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	

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Mol	Chain	Length	Quality of chain
30	2	92	
31	4	4	

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	8071	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8544	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	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
1	0	2754	Total	C	N	O	P	0	0	0
			59016	26346	10879	19046	2745			

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
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	72	Total	C	N	O	S			
			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
28	Z	56	Total	C	N	O	S			
			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
29	1	46	Total	C	N	O	S			
			396	239	89	67	1	0	0	0

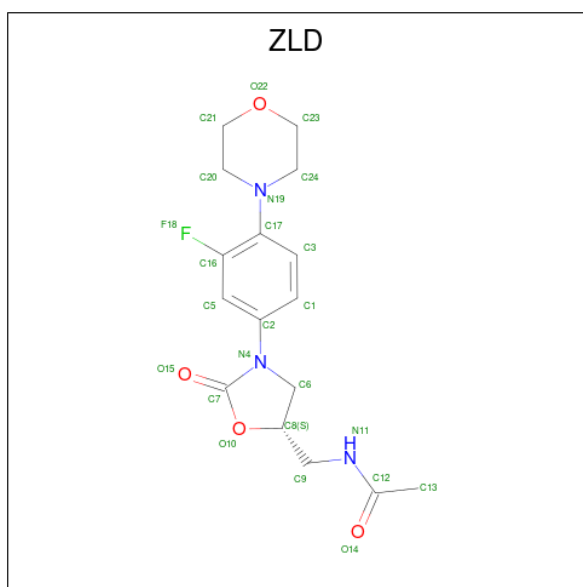
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S			
			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
31	4	4	Total	C	N	O	P			
			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 (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



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

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

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

- Molecule 35 is SODIUM ION (CCD ID: 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 (CCD ID: 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

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

- Molecule 37 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

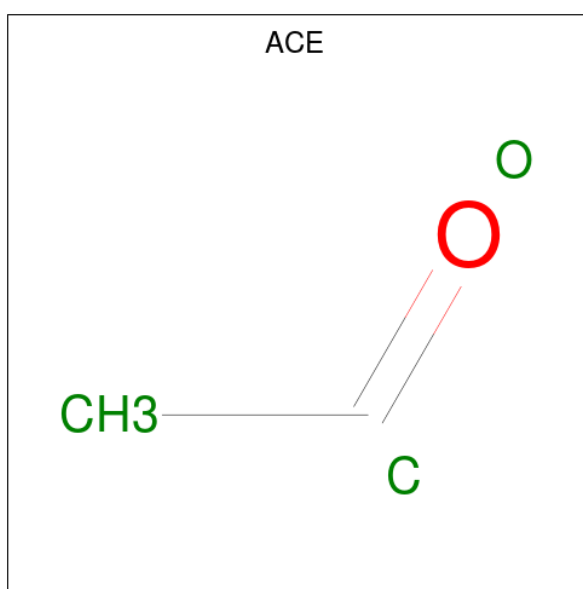
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	N	1	Total 1	Cd 1	0	0

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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 (CCD ID: ACE) (formula: C₂H₄O).



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

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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

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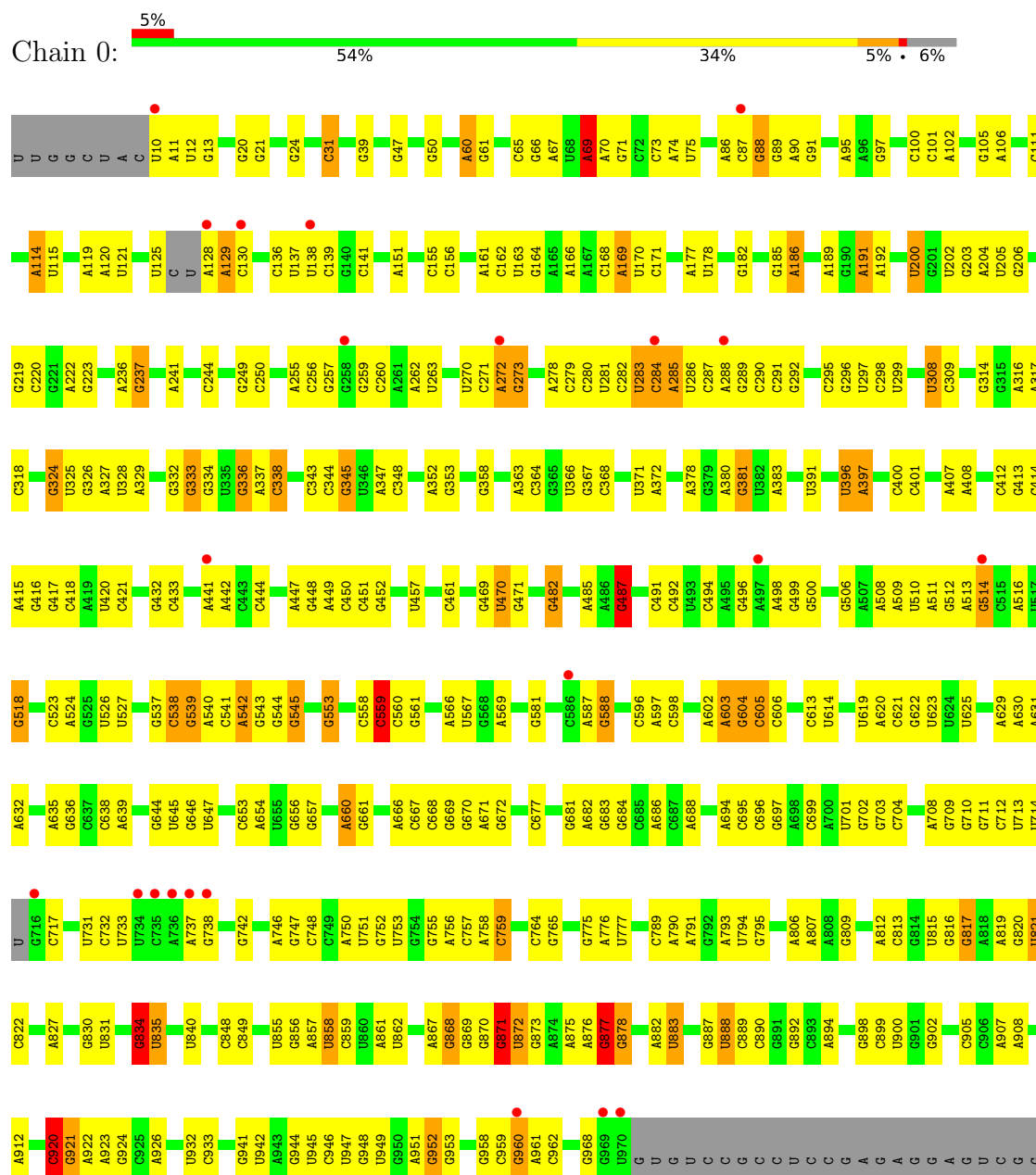
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	99	Total 99	O 99	0	0
40	Y	23	Total 23	O 23	0	0
40	Z	58	Total 58	O 58	0	0
40	1	40	Total 40	O 40	0	0
40	2	73	Total 73	O 73	0	0
40	4	3	Total 3	O 3	0	0

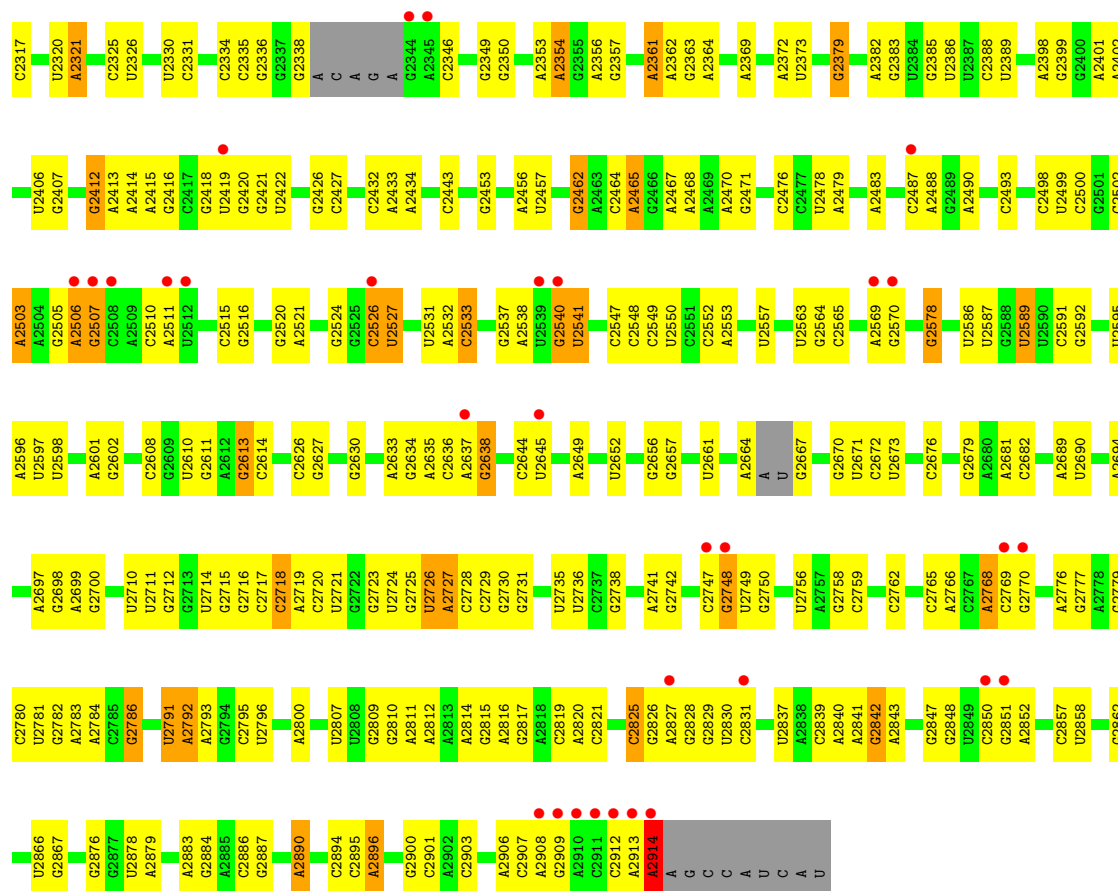
3 Residue-property plots

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

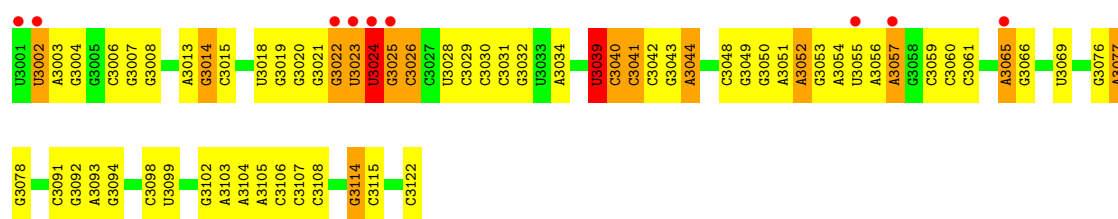
• Molecule 1: 23S RIBOSOMAL RNA



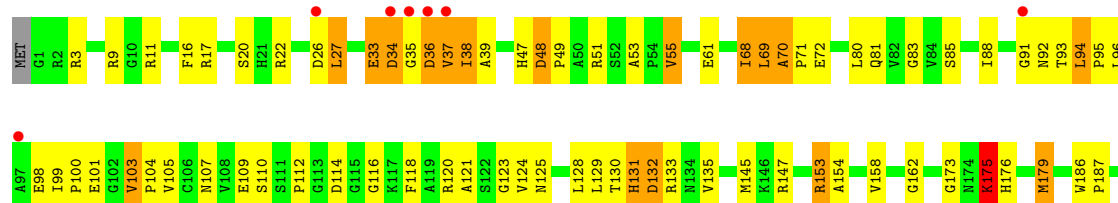




• Molecule 2: 5S RIBOSOMAL RNA

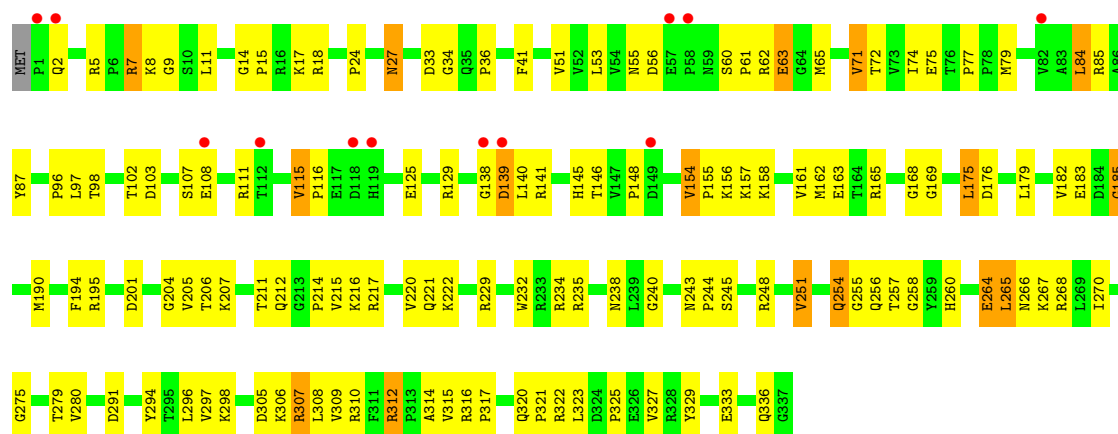


• Molecule 3: 50S ribosomal protein L2P

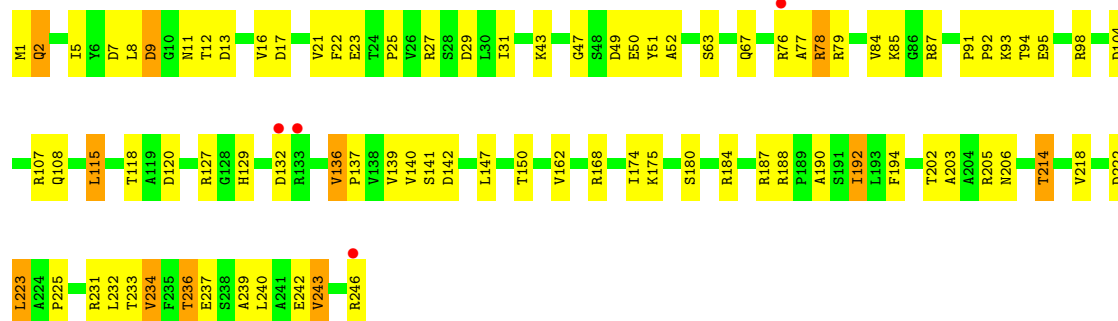




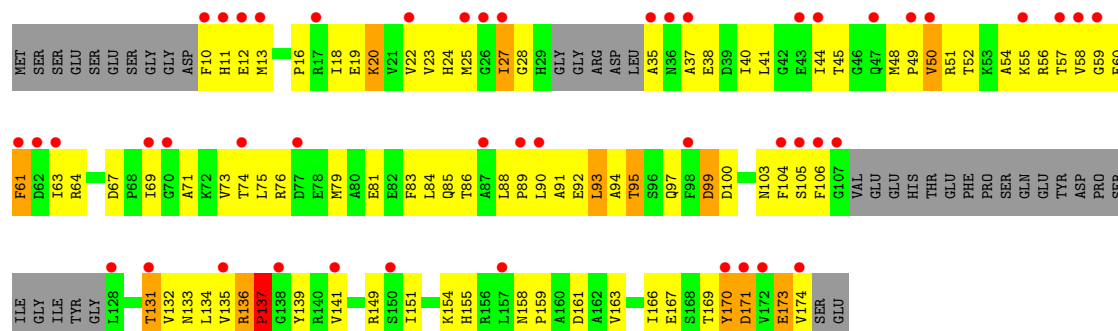
• Molecule 4: 50S ribosomal protein L3P



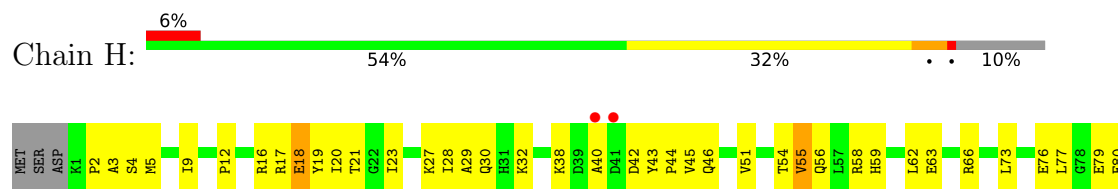
• Molecule 5: 50S ribosomal protein L4P



• Molecule 6: 50S ribosomal protein L5P



• Molecule 7: 50S ribosomal protein L6P

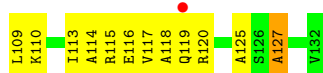
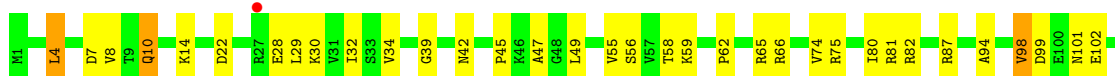




• Molecule 11: 50S ribosomal protein L13P



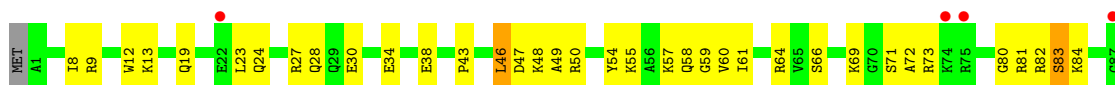
• Molecule 12: 50S ribosomal protein L14P



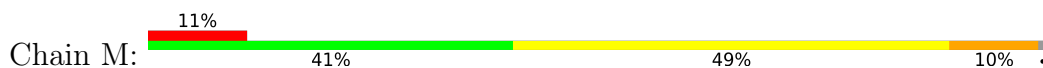
• Molecule 13: 50S ribosomal protein L15P

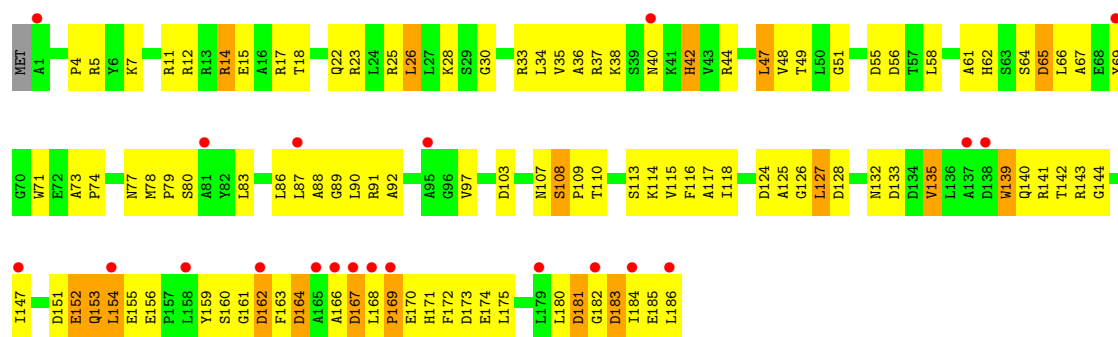


• Molecule 14: 50S ribosomal protein L15e

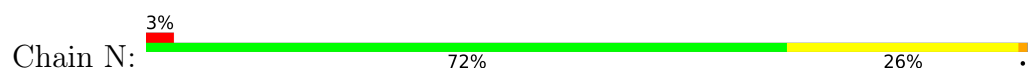


• Molecule 15: 50S ribosomal protein L18P

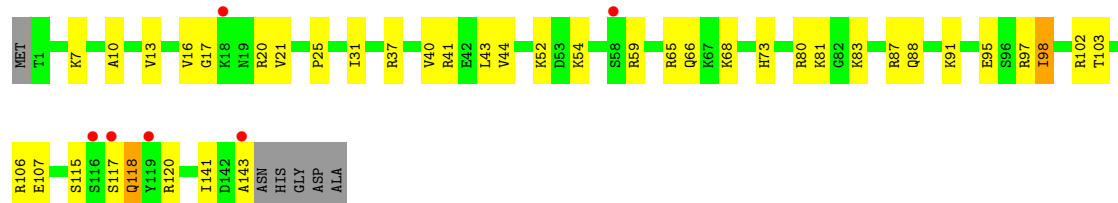




• Molecule 16: 50S ribosomal protein L18e



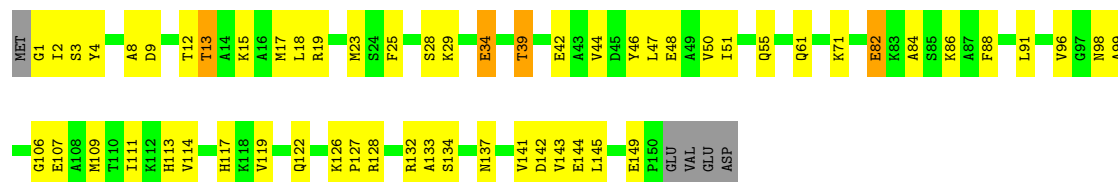
• Molecule 17: 50S ribosomal protein L19e



• Molecule 18: 50S ribosomal protein L21e



• Molecule 19: 50S ribosomal protein L22P



• Molecule 20: 50S ribosomal protein L23P





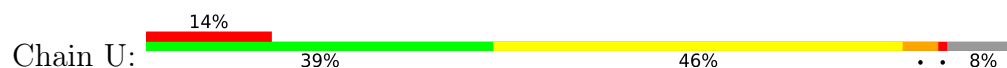
- Molecule 21: 50S ribosomal protein L24P



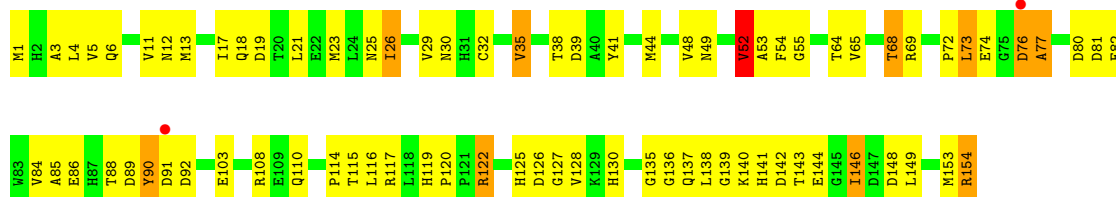
- Molecule 22: 50S ribosomal protein L24e



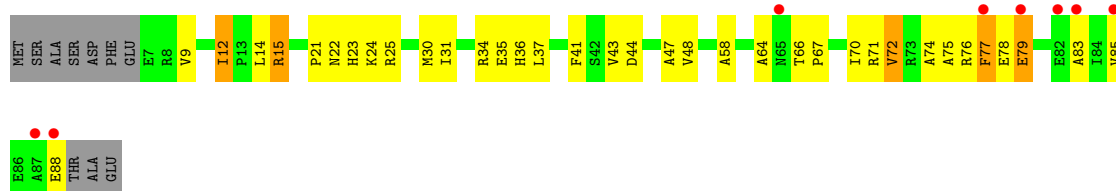
- Molecule 23: 50S ribosomal protein L29P



- Molecule 24: 50S ribosomal protein L30P



- Molecule 25: 50S ribosomal protein L31e



- Molecule 31: 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'

Chain 4: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.73Å 298.58Å 575.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 91.5 (40.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.69Å)	Xtriage
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 ²)	57.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.9	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	0.94	EDS
Total number of atoms	98629	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: ZLD, K, NA, MG, SR, ACE, CD, 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	0.36	1/66075 (0.0%)	0.59	24/103050 (0.0%)
2	9	0.37	0/2905	0.66	4/4528 (0.1%)
3	A	0.46	0/1786	1.00	9/2408 (0.4%)
4	B	0.41	0/2690	0.99	10/3652 (0.3%)
5	C	0.46	0/1885	0.98	6/2552 (0.2%)
6	D	0.36	0/1111	0.95	8/1498 (0.5%)
7	E	0.38	0/1382	0.87	1/1880 (0.1%)
8	F	0.47	0/901	0.87	1/1224 (0.1%)
9	G	0.38	0/241	0.81	0/324
10	H	0.54	0/1302	1.00	8/1743 (0.5%)
11	I	0.41	0/1136	0.91	0/1530
12	J	0.39	0/1004	0.96	2/1351 (0.1%)
13	K	0.37	0/1130	0.98	5/1509 (0.3%)
14	L	0.58	1/1582 (0.1%)	0.95	4/2116 (0.2%)
15	M	0.36	0/1474	1.03	13/1999 (0.7%)
16	N	0.41	0/874	0.93	2/1181 (0.2%)
17	O	0.42	0/1147	0.90	1/1528 (0.1%)
18	P	0.41	0/749	1.04	6/1005 (0.6%)
19	Q	0.43	0/1172	0.96	5/1578 (0.3%)
20	R	0.36	0/648	0.89	3/875 (0.3%)
21	S	0.37	0/958	0.91	4/1289 (0.3%)
22	T	0.39	0/417	0.83	1/562 (0.2%)
23	U	0.36	0/502	0.93	3/675 (0.4%)
24	V	0.46	0/1219	0.96	4/1655 (0.2%)
25	W	0.42	0/664	0.92	3/895 (0.3%)
26	X	0.43	0/1146	0.96	4/1536 (0.3%)
27	Y	0.56	1/578 (0.2%)	1.01	1/773 (0.1%)
28	Z	0.46	0/438	0.96	2/578 (0.3%)
29	1	0.45	0/401	0.82	0/529
30	2	0.39	0/771	0.86	5/1024 (0.5%)
31	4	1.07	0/76	1.15	1/112 (0.9%)
All	All	0.39	3/98364 (0.0%)	0.71	140/147159 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	12	TRP	C-O	-6.94	1.14	1.24
27	Y	33	MET	SD-CE	5.73	1.93	1.79
1	0	559	C	C4-N4	-5.03	1.23	1.33

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	12.46	128.19	109.50
1	0	1563	G	C2'-C3'-O3'	10.89	125.84	109.50
1	0	1979	G	C2'-C3'-O3'	10.51	125.27	109.50
6	D	136	ARG	CA-C-N	8.88	130.94	119.84
6	D	136	ARG	C-N-CA	8.88	130.94	119.84

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

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	897	0
2	9	2600	0	1326	76	0
3	A	1753	0	1766	107	0
4	B	2625	0	2532	134	0
5	C	1860	0	1813	87	0
6	D	1094	0	1085	96	0
7	E	1357	0	1266	70	0
8	F	890	0	843	46	0
9	G	240	0	231	15	0
10	H	1282	0	1295	62	0
11	I	1120	0	1098	59	0
12	J	994	0	1027	50	0
13	K	1118	0	1076	50	0
14	L	1558	0	1573	60	0
15	M	1445	0	1401	117	0
16	N	865	0	873	28	0
17	O	1136	0	1123	41	0
18	P	735	0	728	19	0
19	Q	1149	0	1122	50	0
20	R	641	0	605	22	0
21	S	950	0	923	38	0
22	T	410	0	364	22	0
23	U	499	0	511	40	0
24	V	1196	0	1137	93	0
25	W	654	0	653	34	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	31	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
35	0	64	0	0	0	0
35	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
40	4	3	0	0	0	0
40	9	144	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	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	2247	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 2247 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:O:1160:G:H5'	1:O:1161:A:H5'	1.21	1.14
5:C:236:THR:HG22	5:C:239:ALA:H	1.07	1.11
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.33	1.10
2:9:3023:U:H3'	2:9:3024:U:H5''	1.29	1.09
1:O:156:C:H5''	14:L:171:ARG:HD3	1.37	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	210 (89%)	19 (8%)	6 (3%)	4	11
4	B	335/338 (99%)	311 (93%)	18 (5%)	6 (2%)	6	18
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%)	4	11
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	140 (90%)	15 (10%)	1 (1%)	21	44
11	I	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	3	9
12	J	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	37
13	K	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	18	41
14	L	192/196 (98%)	179 (93%)	12 (6%)	1 (0%)	24	48
15	M	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	2	5
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%)	5	14
19	Q	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	R	79/85 (93%)	77 (98%)	1 (1%)	1 (1%)	9	25
21	S	117/120 (98%)	108 (92%)	7 (6%)	2 (2%)	7	19
22	T	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
23	U	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	3	7
24	V	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	9	25
25	W	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	9	25
26	X	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
27	Y	70/92 (76%)	61 (87%)	6 (9%)	3 (4%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	5	14
All	All	3636/4286 (85%)	3345 (92%)	236 (6%)	55 (2%)	8	22

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 ⓘ

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%)	15	36
4	B	282/283 (100%)	266 (94%)	16 (6%)	18	43
5	C	193/193 (100%)	179 (93%)	14 (7%)	13	32
6	D	117/148 (79%)	111 (95%)	6 (5%)	21	48
7	E	152/156 (97%)	149 (98%)	3 (2%)	48	76
8	F	93/94 (99%)	90 (97%)	3 (3%)	34	64
9	G	27/282 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	128 (96%)	6 (4%)	24	52
11	I	118/121 (98%)	110 (93%)	8 (7%)	14	35
12	J	106/106 (100%)	102 (96%)	4 (4%)	29	58
13	K	113/127 (89%)	109 (96%)	4 (4%)	32	61
14	L	158/160 (99%)	154 (98%)	4 (2%)	42	71
15	M	149/150 (99%)	142 (95%)	7 (5%)	23	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	93/94 (99%)	91 (98%)	2 (2%)	45	74
17	O	113/117 (97%)	111 (98%)	2 (2%)	51	78
18	P	79/80 (99%)	75 (95%)	4 (5%)	21	48
19	Q	117/122 (96%)	114 (97%)	3 (3%)	40	70
20	R	71/74 (96%)	70 (99%)	1 (1%)	59	82
21	S	105/106 (99%)	102 (97%)	3 (3%)	37	67
22	T	44/53 (83%)	44 (100%)	0	100	100
23	U	51/57 (90%)	50 (98%)	1 (2%)	48	76
24	V	130/130 (100%)	121 (93%)	9 (7%)	14	34
25	W	66/74 (89%)	64 (97%)	2 (3%)	36	66
26	X	120/196 (61%)	109 (91%)	11 (9%)	8	22
27	Y	59/74 (80%)	57 (97%)	2 (3%)	32	62
28	Z	46/47 (98%)	46 (100%)	0	100	100
29	1	42/46 (91%)	41 (98%)	1 (2%)	43	72
30	2	79/79 (100%)	77 (98%)	2 (2%)	42	71
All	All	3036/3496 (87%)	2906 (96%)	130 (4%)	26	54

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	X	115	ARG
26	X	172	THR
7	E	7	ILE
6	D	149	ARG
26	X	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
19	Q	113	HIS
24	V	59	GLN
19	Q	140	GLN
21	S	73	HIS
24	V	141	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	245 (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%)	263 (9%)	31 (1%)

5 of 263 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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
32	ZLD	0	9500	-	26,26,26	3.18	13 (50%)	36,36,36	3.24	15 (41%)
39	ACE	4	78	31	1,2,2	1.09	0	0,1,1	-	-

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 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZLD	C3-C1	6.80	1.49	1.38
32	0	9500	ZLD	C3-C17	6.72	1.50	1.39
32	0	9500	ZLD	C17-C16	5.60	1.51	1.40
32	0	9500	ZLD	C1-C2	5.32	1.49	1.39
32	0	9500	ZLD	C24-C23	4.80	1.68	1.50

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	9.38	124.01	113.38
32	0	9500	ZLD	C2-N4-C7	7.57	133.92	125.98
32	0	9500	ZLD	C6-N4-C7	-7.53	105.60	111.17
32	0	9500	ZLD	O15-C7-N4	-5.32	123.88	128.80
32	0	9500	ZLD	O10-C7-N4	5.03	114.16	109.92

There are no chirality outliers.

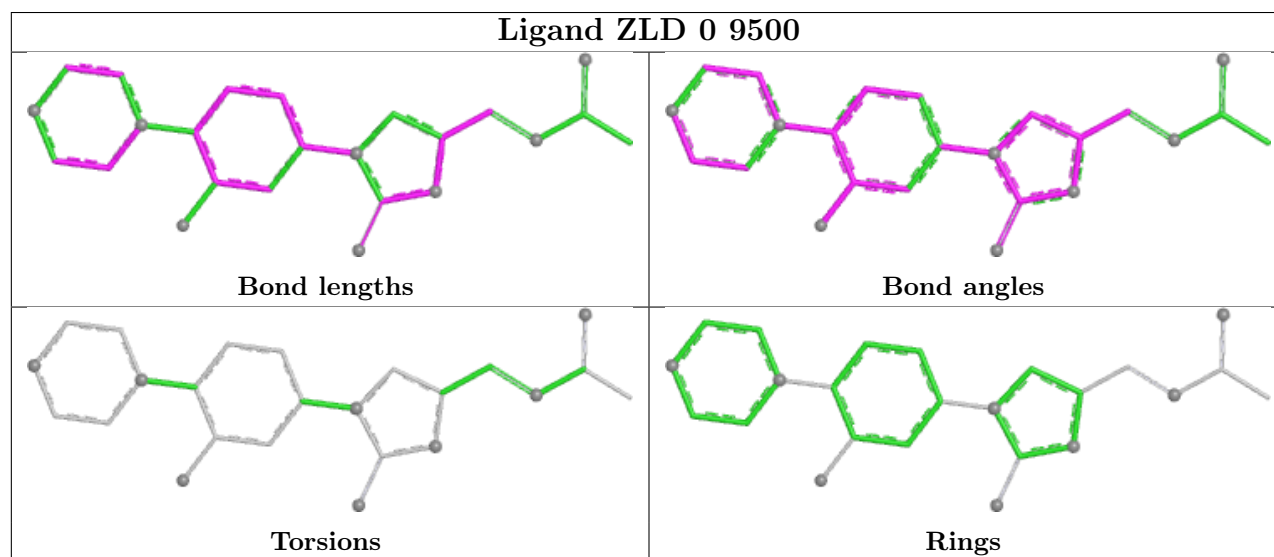
There are no torsion outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.09	138 (5%) 34 30	29, 53, 97, 144	0
2	9	122/122 (100%)	0.82	9 (7%) 20 18	45, 75, 98, 149	0
3	A	237/240 (98%)	0.25	10 (4%) 40 37	34, 58, 90, 107	0
4	B	337/338 (99%)	0.26	12 (3%) 46 42	35, 60, 86, 96	0
5	C	246/246 (100%)	0.10	4 (1%) 70 68	28, 53, 75, 86	0
6	D	140/177 (79%)	1.70	47 (33%) 1 1	67, 101, 122, 127	0
7	E	172/178 (96%)	0.59	8 (4%) 36 33	48, 74, 93, 98	0
8	F	119/120 (99%)	0.76	8 (6%) 24 21	57, 78, 99, 108	0
9	G	29/348 (8%)	1.48	7 (24%) 2 1	79, 99, 105, 109	0
10	H	160/177 (90%)	0.70	10 (6%) 26 23	41, 55, 80, 88	0
11	I	142/145 (97%)	0.23	3 (2%) 63 61	43, 56, 75, 94	0
12	J	132/132 (100%)	0.12	2 (1%) 72 70	40, 54, 78, 90	0
13	K	145/165 (87%)	0.71	18 (12%) 8 7	34, 73, 107, 120	0
14	L	194/196 (98%)	0.12	5 (2%) 57 54	33, 42, 65, 70	0
15	M	186/187 (99%)	0.91	21 (11%) 10 8	52, 72, 110, 120	0
16	N	115/116 (99%)	0.31	3 (2%) 57 54	45, 62, 77, 82	0
17	O	143/149 (95%)	0.38	6 (4%) 40 37	46, 59, 71, 82	0
18	P	95/96 (98%)	0.18	2 (2%) 63 61	46, 55, 72, 84	0
19	Q	150/155 (96%)	-0.22	0 100 100	37, 51, 70, 76	0
20	R	81/85 (95%)	0.29	2 (2%) 58 55	50, 65, 85, 90	0
21	S	119/120 (99%)	0.50	5 (4%) 40 37	47, 61, 87, 108	0
22	T	53/67 (79%)	0.41	0 100 100	47, 59, 78, 86	0
23	U	65/71 (91%)	0.99	10 (15%) 5 4	59, 79, 115, 121	0
24	V	154/154 (100%)	0.29	2 (1%) 75 73	43, 58, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	82/92 (89%)	0.60	8 (9%) 13 11	48, 64, 88, 106	0
26	X	142/241 (58%)	0.07	3 (2%) 63 61	32, 49, 71, 91	0
27	Y	72/92 (78%)	0.76	3 (4%) 40 37	43, 59, 70, 76	0
28	Z	56/57 (98%)	-0.27	0 100 100	33, 40, 46, 57	0
29	1	46/50 (92%)	0.81	7 (15%) 5 4	41, 62, 87, 99	0
30	2	92/92 (100%)	0.32	5 (5%) 31 27	47, 64, 77, 86	0
31	4	4/4 (100%)	2.52	2 (50%) 0 0	78, 83, 85, 88	0
All	All	6584/7334 (89%)	0.22	360 (5%) 30 27	28, 57, 98, 149	0

The worst 5 of 360 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	7.9
4	B	1	PRO	7.0
1	0	1161	A	7.0
1	0	737	A	6.7
6	D	107	GLY	6.5

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 oligosaccharides 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, 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	8543	1/1	0.44	0.21	116,116,116,116	0
35	NA	0	8525	1/1	0.51	0.31	92,92,92,92	0
35	NA	0	8571	1/1	0.54	0.41	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8035	1/1	0.57	0.26	80,80,80,80	0
33	MG	0	8071	1/1	0.59	0.48	84,84,84,84	0
33	MG	0	8038	1/1	0.59	0.17	88,88,88,88	0
35	NA	R	8510	1/1	0.60	0.26	127,127,127,127	0
34	K	0	8401	1/1	0.66	0.47	129,129,129,129	0
35	NA	9	8572	1/1	0.67	0.46	99,99,99,99	0
35	NA	0	8561	1/1	0.71	0.73	122,122,122,122	0
33	MG	0	8073	1/1	0.73	0.30	105,105,105,105	0
37	SR	0	9006	1/1	0.73	0.34	150,150,150,150	0
33	MG	0	8030	1/1	0.74	0.33	99,99,99,99	0
33	MG	0	8085	1/1	0.74	0.23	105,105,105,105	0
35	NA	0	8544	1/1	0.75	0.50	86,86,86,86	0
33	MG	0	8040	1/1	0.76	0.23	97,97,97,97	0
33	MG	0	8063	1/1	0.77	0.27	94,94,94,94	0
35	NA	0	8518	1/1	0.77	0.30	107,107,107,107	0
35	NA	0	8555	1/1	0.78	0.67	75,75,75,75	0
35	NA	0	8573	1/1	0.78	0.15	92,92,92,92	0
37	SR	0	8979	1/1	0.78	0.16	150,150,150,150	0
35	NA	0	8562	1/1	0.78	0.53	78,78,78,78	0
33	MG	0	8066	1/1	0.79	0.32	103,103,103,103	0
35	NA	0	8574	1/1	0.79	0.41	66,66,66,66	0
35	NA	0	8575	1/1	0.79	0.47	104,104,104,104	0
35	NA	0	8548	1/1	0.79	0.28	59,59,59,59	0
35	NA	0	8559	1/1	0.80	0.47	85,85,85,85	0
36	CL	B	8819	1/1	0.82	0.29	72,72,72,72	0
35	NA	0	8564	1/1	0.82	0.13	74,74,74,74	0
33	MG	9	8074	1/1	0.82	0.33	64,64,64,64	0
33	MG	0	8047	1/1	0.83	0.20	98,98,98,98	0
35	NA	0	8507	1/1	0.84	0.14	51,51,51,51	0
35	NA	0	8523	1/1	0.84	0.20	51,51,51,51	0
35	NA	0	8536	1/1	0.85	0.12	71,71,71,71	0
33	MG	0	8044	1/1	0.85	0.14	79,79,79,79	0
35	NA	0	8522	1/1	0.85	0.42	77,77,77,77	0
32	ZLD	0	9500	24/24	0.85	0.23	69,77,79,80	0
35	NA	0	8508	1/1	0.85	0.17	55,55,55,55	0
35	NA	0	8529	1/1	0.85	0.20	46,46,46,46	0
35	NA	0	8512	1/1	0.86	0.36	72,72,72,72	0
37	SR	0	8971	1/1	0.86	0.11	150,150,150,150	0
33	MG	0	8010	1/1	0.86	0.20	70,70,70,70	0
37	SR	0	8996	1/1	0.86	0.27	150,150,150,150	0
33	MG	0	8087	1/1	0.86	0.21	61,61,61,61	0
35	NA	0	8549	1/1	0.87	0.33	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8565	1/1	0.87	0.20	66,66,66,66	0
37	SR	9	9003	1/1	0.87	0.15	150,150,150,150	0
38	CD	N	8705	1/1	0.87	0.27	150,150,150,150	0
35	NA	0	8558	1/1	0.88	0.15	63,63,63,63	0
33	MG	0	8007	1/1	0.88	0.10	53,53,53,53	0
35	NA	0	8516	1/1	0.88	0.41	52,52,52,52	0
37	SR	0	8994	1/1	0.88	0.53	150,150,150,150	0
35	NA	0	8550	1/1	0.88	0.28	66,66,66,66	0
35	NA	0	8502	1/1	0.88	0.34	75,75,75,75	0
35	NA	0	8556	1/1	0.88	0.27	66,66,66,66	0
37	SR	B	8987	1/1	0.88	0.39	150,150,150,150	0
35	NA	0	8570	1/1	0.88	0.09	57,57,57,57	0
33	MG	0	8081	1/1	0.89	0.19	82,82,82,82	0
33	MG	0	8017	1/1	0.89	0.20	121,121,121,121	0
33	MG	0	8039	1/1	0.89	0.11	68,68,68,68	0
35	NA	0	8542	1/1	0.89	0.30	68,68,68,68	0
35	NA	0	8511	1/1	0.89	0.24	71,71,71,71	0
37	SR	0	8976	1/1	0.89	0.09	139,139,139,139	0
33	MG	0	8092	1/1	0.89	0.08	72,72,72,72	0
35	NA	0	8567	1/1	0.89	0.30	83,83,83,83	0
33	MG	0	8029	1/1	0.89	0.14	100,100,100,100	0
37	SR	0	9001	1/1	0.89	0.10	150,150,150,150	0
33	MG	B	8042	1/1	0.89	0.09	85,85,85,85	0
37	SR	0	9007	1/1	0.89	0.51	150,150,150,150	0
35	NA	0	8551	1/1	0.89	0.14	46,46,46,46	0
33	MG	S	8057	1/1	0.89	0.23	55,55,55,55	0
33	MG	0	8076	1/1	0.89	0.14	68,68,68,68	0
37	SR	0	8982	1/1	0.90	0.24	144,144,144,144	0
35	NA	0	8517	1/1	0.90	0.13	53,53,53,53	0
37	SR	0	8995	1/1	0.90	0.13	107,107,107,107	0
35	NA	0	8535	1/1	0.90	0.28	79,79,79,79	0
33	MG	0	8043	1/1	0.90	0.15	72,72,72,72	0
37	SR	0	8944	1/1	0.90	0.18	135,135,135,135	0
33	MG	0	8036	1/1	0.90	0.17	58,58,58,58	0
37	SR	0	8975	1/1	0.90	0.14	133,133,133,133	0
33	MG	0	8069	1/1	0.90	0.16	78,78,78,78	0
33	MG	0	8033	1/1	0.90	0.07	58,58,58,58	0
35	NA	0	8514	1/1	0.91	0.15	51,51,51,51	0
33	MG	0	8016	1/1	0.91	0.17	94,94,94,94	0
33	MG	0	8037	1/1	0.91	0.21	102,102,102,102	0
36	CL	0	8813	1/1	0.91	0.09	59,59,59,59	0
35	NA	0	8569	1/1	0.91	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8541	1/1	0.91	0.09	62,62,62,62	0
33	MG	A	8051	1/1	0.91	0.10	71,71,71,71	0
33	MG	0	8001	1/1	0.91	0.18	31,31,31,31	0
33	MG	0	8065	1/1	0.91	0.37	100,100,100,100	0
33	MG	1	8060	1/1	0.91	0.06	58,58,58,58	0
37	SR	0	8989	1/1	0.92	0.12	150,150,150,150	0
35	NA	0	8545	1/1	0.92	0.30	57,57,57,57	0
33	MG	0	8002	1/1	0.92	0.19	82,82,82,82	0
37	SR	0	8959	1/1	0.92	0.09	150,150,150,150	0
35	NA	I	8538	1/1	0.92	0.07	51,51,51,51	0
37	SR	0	9002	1/1	0.92	0.11	125,125,125,125	0
37	SR	0	9004	1/1	0.92	0.11	150,150,150,150	0
35	NA	L	8539	1/1	0.92	0.10	43,43,43,43	0
35	NA	Q	8533	1/1	0.92	0.17	68,68,68,68	0
33	MG	0	8090	1/1	0.92	0.08	83,83,83,83	0
37	SR	0	8981	1/1	0.92	0.11	150,150,150,150	0
35	NA	0	8509	1/1	0.92	0.23	83,83,83,83	0
39	ACE	4	78	3/3	0.92	0.26	79,79,80,81	0
37	SR	0	8960	1/1	0.93	0.10	116,116,116,116	0
33	MG	0	8048	1/1	0.93	0.06	64,64,64,64	0
33	MG	0	8049	1/1	0.93	0.08	85,85,85,85	0
35	NA	0	8553	1/1	0.93	0.18	63,63,63,63	0
35	NA	0	8554	1/1	0.93	0.10	63,63,63,63	0
35	NA	0	8530	1/1	0.93	0.12	56,56,56,56	0
35	NA	0	8534	1/1	0.93	0.07	61,61,61,61	0
37	SR	0	8983	1/1	0.93	0.10	150,150,150,150	0
37	SR	0	8986	1/1	0.93	0.09	131,131,131,131	0
35	NA	0	8557	1/1	0.93	0.22	67,67,67,67	0
37	SR	0	8990	1/1	0.93	0.10	131,131,131,131	0
35	NA	C	8503	1/1	0.93	0.07	34,34,34,34	0
33	MG	0	8053	1/1	0.93	0.23	64,64,64,64	0
33	MG	0	8078	1/1	0.93	0.14	64,64,64,64	0
35	NA	P	8540	1/1	0.93	0.10	73,73,73,73	0
35	NA	0	8501	1/1	0.93	0.10	46,46,46,46	0
33	MG	0	8056	1/1	0.93	0.14	83,83,83,83	0
35	NA	0	8505	1/1	0.93	0.13	51,51,51,51	0
35	NA	0	8520	1/1	0.93	0.24	61,61,61,61	0
36	CL	I	8802	1/1	0.93	0.10	71,71,71,71	0
33	MG	A	8050	1/1	0.93	0.12	93,93,93,93	0
37	SR	0	8951	1/1	0.93	0.14	113,113,113,113	0
33	MG	0	8082	1/1	0.93	0.12	78,78,78,78	0
37	SR	0	8985	1/1	0.94	0.25	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8506	1/1	0.94	0.14	66,66,66,66	0
33	MG	0	8024	1/1	0.94	0.14	81,81,81,81	0
37	SR	0	8943	1/1	0.94	0.11	110,110,110,110	0
37	SR	0	8991	1/1	0.94	0.11	150,150,150,150	0
33	MG	0	8089	1/1	0.94	0.08	49,49,49,49	0
33	MG	0	8077	1/1	0.94	0.08	47,47,47,47	0
33	MG	0	8068	1/1	0.94	0.15	86,86,86,86	0
37	SR	0	8997	1/1	0.94	0.09	142,142,142,142	0
35	NA	0	8546	1/1	0.94	0.20	77,77,77,77	0
37	SR	0	8966	1/1	0.94	0.08	98,98,98,98	0
35	NA	0	8526	1/1	0.94	0.11	50,50,50,50	0
35	NA	0	8563	1/1	0.94	0.30	69,69,69,69	0
35	NA	0	8528	1/1	0.94	0.10	57,57,57,57	0
33	MG	0	8019	1/1	0.94	0.12	37,37,37,37	0
37	SR	A	8977	1/1	0.94	0.12	99,99,99,99	0
33	MG	0	8046	1/1	0.94	0.09	65,65,65,65	0
35	NA	0	8504	1/1	0.94	0.10	42,42,42,42	0
33	MG	0	8052	1/1	0.94	0.14	49,49,49,49	0
36	CL	I	8821	1/1	0.95	0.10	67,67,67,67	0
36	CL	M	8807	1/1	0.95	0.07	71,71,71,71	0
36	CL	2	8804	1/1	0.95	0.16	88,88,88,88	0
37	SR	0	8908	1/1	0.95	0.09	90,90,90,90	0
37	SR	0	8939	1/1	0.95	0.08	100,100,100,100	0
33	MG	0	8059	1/1	0.95	0.05	56,56,56,56	0
33	MG	0	8020	1/1	0.95	0.15	52,52,52,52	0
35	NA	Q	8532	1/1	0.95	0.12	49,49,49,49	0
37	SR	0	8993	1/1	0.95	0.10	139,139,139,139	0
37	SR	0	8955	1/1	0.95	0.09	122,122,122,122	0
37	SR	0	8956	1/1	0.95	0.07	128,128,128,128	0
37	SR	0	8957	1/1	0.95	0.08	120,120,120,120	0
37	SR	0	8958	1/1	0.95	0.06	96,96,96,96	0
37	SR	0	8998	1/1	0.95	0.13	133,133,133,133	0
35	NA	0	8566	1/1	0.95	0.26	54,54,54,54	0
33	MG	0	8064	1/1	0.95	0.06	69,69,69,69	0
37	SR	0	8964	1/1	0.95	0.10	101,101,101,101	0
36	CL	0	8805	1/1	0.95	0.10	65,65,65,65	0
36	CL	0	8811	1/1	0.95	0.12	83,83,83,83	0
37	SR	9	8980	1/1	0.95	0.07	137,137,137,137	0
37	SR	0	8973	1/1	0.95	0.08	101,101,101,101	0
37	SR	0	8974	1/1	0.95	0.12	134,134,134,134	0
33	MG	0	8045	1/1	0.95	0.15	71,71,71,71	0
33	MG	0	8031	1/1	0.95	0.06	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8519	1/1	0.95	0.10	49,49,49,49	0
35	NA	0	8547	1/1	0.96	0.16	75,75,75,75	0
33	MG	0	8067	1/1	0.96	0.06	58,58,58,58	0
37	SR	0	8984	1/1	0.96	0.06	109,109,109,109	0
37	SR	0	8946	1/1	0.96	0.07	99,99,99,99	0
37	SR	0	8947	1/1	0.96	0.13	109,109,109,109	0
37	SR	0	8988	1/1	0.96	0.09	125,125,125,125	0
37	SR	0	8948	1/1	0.96	0.08	102,102,102,102	0
35	NA	B	8552	1/1	0.96	0.19	59,59,59,59	0
36	CL	0	8815	1/1	0.96	0.15	61,61,61,61	0
36	CL	0	8816	1/1	0.96	0.12	77,77,77,77	0
36	CL	A	8809	1/1	0.96	0.08	65,65,65,65	0
35	NA	0	8537	1/1	0.96	0.05	43,43,43,43	0
34	K	0	8402	1/1	0.96	0.07	70,70,70,70	0
35	NA	0	8560	1/1	0.96	0.23	88,88,88,88	0
35	NA	0	8513	1/1	0.96	0.09	50,50,50,50	0
37	SR	0	8965	1/1	0.96	0.09	108,108,108,108	0
33	MG	0	8032	1/1	0.96	0.07	56,56,56,56	0
37	SR	0	8967	1/1	0.96	0.11	113,113,113,113	0
37	SR	0	8969	1/1	0.96	0.24	127,127,127,127	0
33	MG	0	8080	1/1	0.96	0.09	78,78,78,78	0
37	SR	0	8915	1/1	0.96	0.07	93,93,93,93	0
37	SR	0	8919	1/1	0.96	0.08	131,131,131,131	0
37	SR	0	8924	1/1	0.96	0.15	112,112,112,112	0
37	SR	B	8950	1/1	0.96	0.06	106,106,106,106	0
37	SR	0	8931	1/1	0.96	0.11	94,94,94,94	0
37	SR	F	9005	1/1	0.96	0.12	116,116,116,116	0
37	SR	R	8961	1/1	0.96	0.08	122,122,122,122	0
37	SR	0	8938	1/1	0.96	0.15	105,105,105,105	0
33	MG	0	8062	1/1	0.96	0.14	61,61,61,61	0
33	MG	0	8070	1/1	0.97	0.04	62,62,62,62	0
36	CL	0	8803	1/1	0.97	0.12	61,61,61,61	0
33	MG	0	8091	1/1	0.97	0.06	54,54,54,54	0
37	SR	0	8918	1/1	0.97	0.09	59,59,59,59	0
37	SR	0	8992	1/1	0.97	0.12	115,115,115,115	0
37	SR	0	8962	1/1	0.97	0.06	108,108,108,108	0
37	SR	0	8963	1/1	0.97	0.08	83,83,83,83	0
35	NA	0	8521	1/1	0.97	0.15	110,110,110,110	0
37	SR	0	8920	1/1	0.97	0.06	96,96,96,96	0
33	MG	0	8008	1/1	0.97	0.06	34,34,34,34	0
33	MG	0	8006	1/1	0.97	0.18	27,27,27,27	0
37	SR	0	8999	1/1	0.97	0.06	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8933	1/1	0.97	0.08	103,103,103,103	0
37	SR	0	8970	1/1	0.97	0.08	80,80,80,80	0
37	SR	0	8937	1/1	0.97	0.09	80,80,80,80	0
35	NA	0	8524	1/1	0.97	0.09	56,56,56,56	0
36	CL	0	8817	1/1	0.97	0.05	56,56,56,56	0
37	SR	9	8968	1/1	0.97	0.08	132,132,132,132	0
33	MG	0	8083	1/1	0.97	0.05	55,55,55,55	0
33	MG	0	8022	1/1	0.97	0.13	46,46,46,46	0
37	SR	A	8929	1/1	0.97	0.10	103,103,103,103	0
36	CL	I	8801	1/1	0.97	0.12	61,61,61,61	0
33	MG	0	8018	1/1	0.97	0.21	44,44,44,44	0
33	MG	0	8027	1/1	0.97	0.07	53,53,53,53	0
37	SR	0	8949	1/1	0.97	0.06	80,80,80,80	0
36	CL	K	8810	1/1	0.97	0.09	55,55,55,55	0
33	MG	X	8086	1/1	0.97	0.09	51,51,51,51	0
36	CL	X	8820	1/1	0.97	0.04	49,49,49,49	0
37	SR	0	8945	1/1	0.98	0.07	92,92,92,92	0
33	MG	0	8072	1/1	0.98	0.04	47,47,47,47	0
36	CL	L	8818	1/1	0.98	0.04	48,48,48,48	0
33	MG	0	8093	1/1	0.98	0.03	41,41,41,41	0
36	CL	N	8808	1/1	0.98	0.06	76,76,76,76	0
36	CL	Q	8806	1/1	0.98	0.05	49,49,49,49	0
37	SR	0	8953	1/1	0.98	0.07	96,96,96,96	0
37	SR	0	8954	1/1	0.98	0.07	94,94,94,94	0
33	MG	0	8011	1/1	0.98	0.04	33,33,33,33	0
35	NA	0	8515	1/1	0.98	0.05	34,34,34,34	0
37	SR	0	8901	1/1	0.98	0.09	75,75,75,75	0
37	SR	0	8907	1/1	0.98	0.05	63,63,63,63	0
35	NA	0	8527	1/1	0.98	0.06	51,51,51,51	0
37	SR	0	8910	1/1	0.98	0.06	59,59,59,59	0
33	MG	0	8075	1/1	0.98	0.04	50,50,50,50	0
37	SR	0	9000	1/1	0.98	0.05	111,111,111,111	0
36	CL	0	8814	1/1	0.98	0.11	57,57,57,57	0
33	MG	0	8084	1/1	0.98	0.12	66,66,66,66	0
33	MG	0	8026	1/1	0.98	0.03	61,61,61,61	0
37	SR	0	8921	1/1	0.98	0.10	70,70,70,70	0
37	SR	0	8923	1/1	0.98	0.05	83,83,83,83	0
37	SR	0	9008	1/1	0.98	0.07	91,91,91,91	0
35	NA	0	8531	1/1	0.98	0.03	41,41,41,41	0
37	SR	0	8926	1/1	0.98	0.09	82,82,82,82	0
37	SR	0	8927	1/1	0.98	0.09	90,90,90,90	0
37	SR	0	8928	1/1	0.98	0.08	91,91,91,91	0

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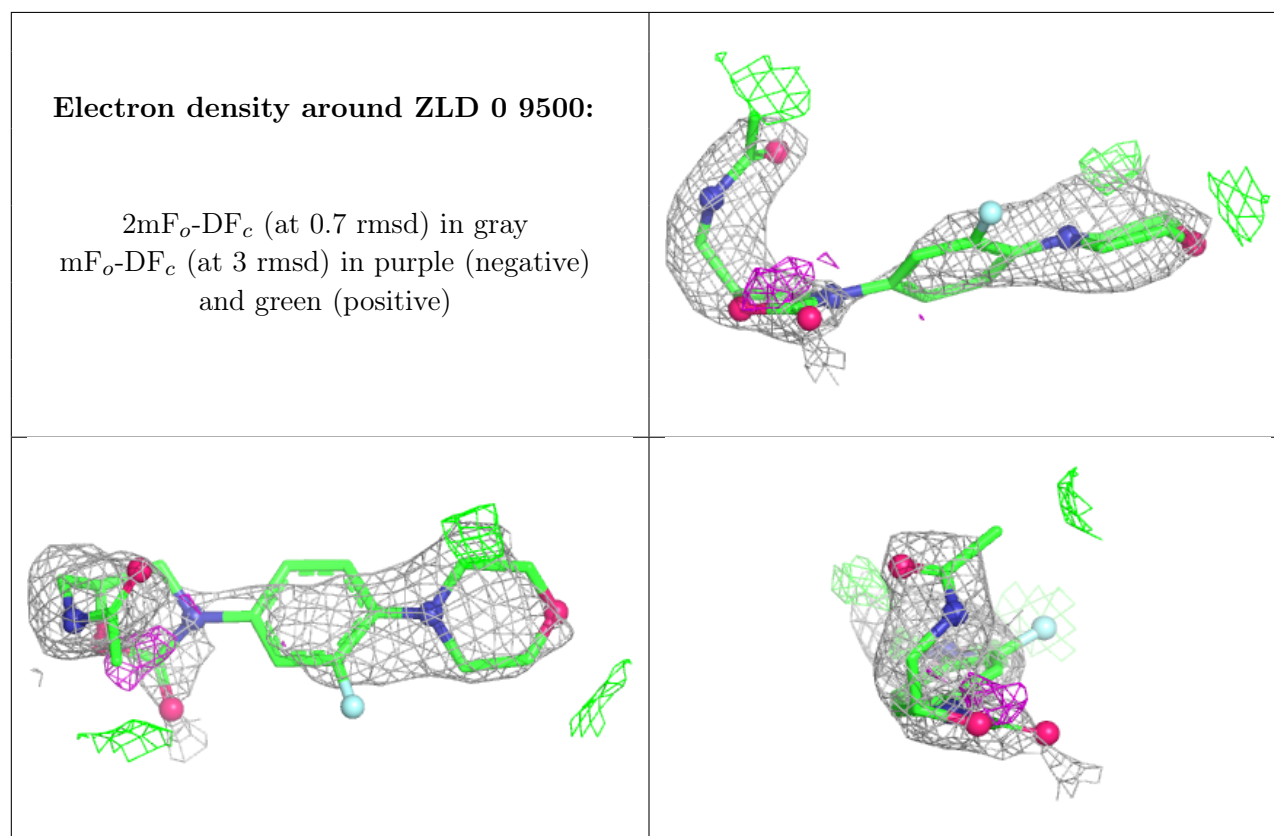
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	A	8930	1/1	0.98	0.10	81,81,81,81	0
36	CL	0	8822	1/1	0.98	0.23	69,69,69,69	0
33	MG	0	8055	1/1	0.98	0.11	40,40,40,40	0
35	NA	K	8568	1/1	0.98	0.09	57,57,57,57	0
33	MG	0	8034	1/1	0.98	0.04	44,44,44,44	0
37	SR	H	8972	1/1	0.98	0.16	148,148,148,148	0
33	MG	0	8079	1/1	0.98	0.06	72,72,72,72	0
37	SR	S	8911	1/1	0.98	0.06	72,72,72,72	0
37	SR	Z	8952	1/1	0.98	0.04	71,71,71,71	0
33	MG	0	8015	1/1	0.98	0.05	62,62,62,62	0
36	CL	J	8812	1/1	0.98	0.10	54,54,54,54	0
37	SR	0	8914	1/1	0.99	0.11	84,84,84,84	0
37	SR	0	8940	1/1	0.99	0.04	77,77,77,77	0
37	SR	0	8942	1/1	0.99	0.05	89,89,89,89	0
33	MG	0	8003	1/1	0.99	0.03	35,35,35,35	0
37	SR	0	8916	1/1	0.99	0.06	85,85,85,85	0
37	SR	0	8917	1/1	0.99	0.09	81,81,81,81	0
33	MG	0	8088	1/1	0.99	0.07	57,57,57,57	0
33	MG	0	8023	1/1	0.99	0.02	39,39,39,39	0
37	SR	0	8978	1/1	0.99	0.03	85,85,85,85	0
33	MG	0	8012	1/1	0.99	0.03	30,30,30,30	0
33	MG	0	8025	1/1	0.99	0.06	43,43,43,43	0
37	SR	0	8922	1/1	0.99	0.04	77,77,77,77	0
33	MG	0	8041	1/1	0.99	0.04	44,44,44,44	0
37	SR	0	8902	1/1	0.99	0.10	49,49,49,49	0
37	SR	0	8925	1/1	0.99	0.13	79,79,79,79	0
37	SR	0	8904	1/1	0.99	0.06	52,52,52,52	0
37	SR	0	8905	1/1	0.99	0.13	59,59,59,59	0
37	SR	0	8906	1/1	0.99	0.08	56,56,56,56	0
33	MG	0	8009	1/1	0.99	0.16	23,23,23,23	0
33	MG	0	8004	1/1	0.99	0.05	36,36,36,36	0
37	SR	Q	8912	1/1	0.99	0.07	75,75,75,75	0
37	SR	0	8934	1/1	0.99	0.07	90,90,90,90	0
37	SR	0	8935	1/1	0.99	0.07	80,80,80,80	0
37	SR	Z	8913	1/1	0.99	0.04	52,52,52,52	0
37	SR	0	8936	1/1	0.99	0.05	70,70,70,70	0
37	SR	2	8932	1/1	0.99	0.03	76,76,76,76	0
37	SR	0	8909	1/1	0.99	0.07	74,74,74,74	0
38	CD	Z	8702	1/1	0.99	0.03	67,67,67,67	0
38	CD	2	8704	1/1	0.99	0.02	65,65,65,65	0
33	MG	0	8021	1/1	0.99	0.03	38,38,38,38	0
33	MG	0	8058	1/1	1.00	0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8014	1/1	1.00	0.03	37,37,37,37	0
37	SR	0	8941	1/1	1.00	0.07	81,81,81,81	0
33	MG	J	8054	1/1	1.00	0.04	37,37,37,37	0
33	MG	0	8061	1/1	1.00	0.06	36,36,36,36	0
38	CD	T	8701	1/1	1.00	0.01	64,64,64,64	0
38	CD	Y	8703	1/1	1.00	0.02	59,59,59,59	0
33	MG	0	8005	1/1	1.00	0.02	39,39,39,39	0
37	SR	0	8903	1/1	1.00	0.07	59,59,59,59	0
33	MG	0	8028	1/1	1.00	0.09	29,29,29,29	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 ⓘ

There are no such residues in this entry.