



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 08:57 PM BST

PDB ID : 3I56
Title : Co-crystal structure of Triacetyloleandomycin Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13
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) : 2.13

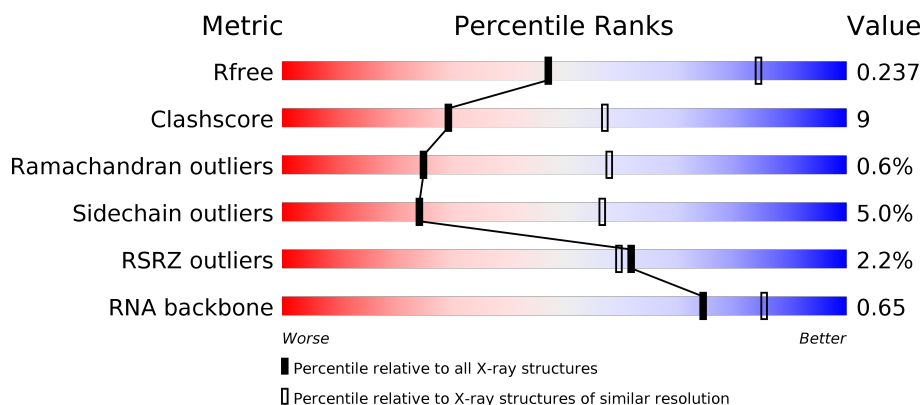
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



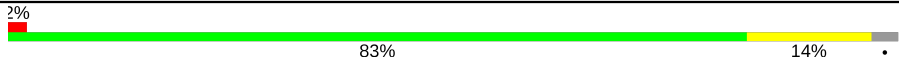
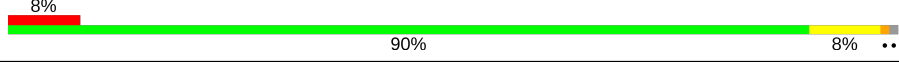
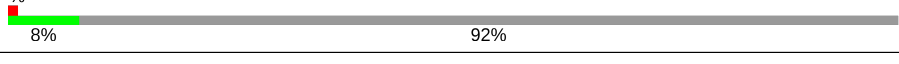


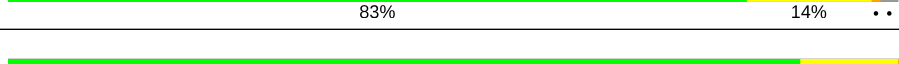
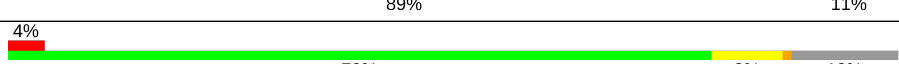
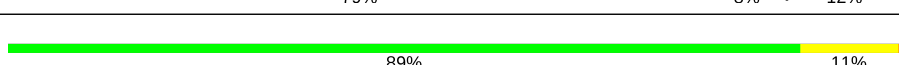
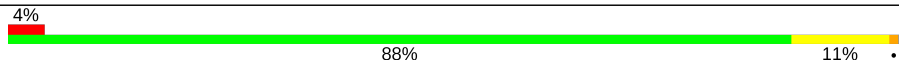
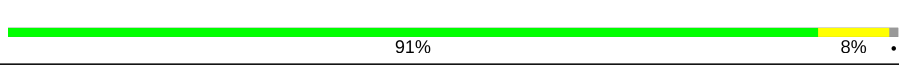

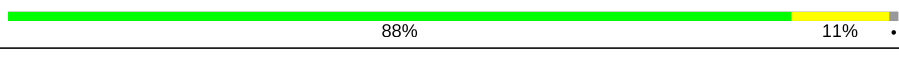

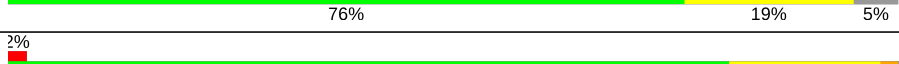
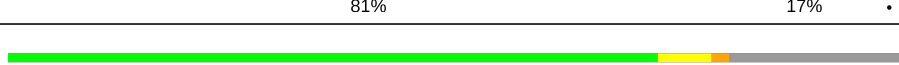










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A	240	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
2	B	338	<div> <div></div> <div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
3	C	246	<div> <div></div> <div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>18%</div> <div> <div>64%</div> <div>14%</div> <div>..</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	174	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	194	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	66	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8034	-	-	-	X
32	MG	0	8037	-	-	-	X
33	CL	K	8812	-	-	X	-
34	SR	0	8920	-	-	-	X
34	SR	0	8922	-	-	-	X
34	SR	0	8923	-	-	-	X
34	SR	0	8928	-	-	-	X
34	SR	0	8934	-	-	-	X
34	SR	0	8938	-	-	-	X
34	SR	0	8946	-	-	-	X
34	SR	0	8954	-	-	-	X
34	SR	0	8959	-	-	-	X
34	SR	0	8964	-	-	-	X
34	SR	0	8970	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8997	-	-	-	X
34	SR	0	9000	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	1	8952	-	-	-	X
34	SR	A	8929	-	-	-	X
34	SR	A	8930	-	-	-	X
34	SR	B	8950	-	-	-	X
34	SR	T	8939	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8549	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	0	8568	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8570	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	C	8558	-	-	-	X
38	TAO	0	2924	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99181 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

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

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1283	798	240	239	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

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

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	EXPRESSION TAG	UNP P60619
Z	2	SER	-	EXPRESSION TAG	UNP P60619
Z	3	PRO	-	EXPRESSION TAG	UNP P60619
Z	4	ARG	-	EXPRESSION TAG	UNP P60619
Z	5	ALA	-	EXPRESSION TAG	UNP P60619
Z	6	ARG	-	EXPRESSION TAG	UNP P60619

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	7	ARG	-	EXPRESSION TAG	UNP P60619
Z	8	GLU	-	EXPRESSION TAG	UNP P60619
Z	9	PRO	-	EXPRESSION TAG	UNP P60619
Z	10	ASN	-	EXPRESSION TAG	UNP P60619
Z	11	LEU	-	EXPRESSION TAG	UNP P60619
Z	12	GLU	-	EXPRESSION TAG	UNP P60619
Z	13	GLY	-	EXPRESSION TAG	UNP P60619
Z	14	LEU	-	EXPRESSION TAG	UNP P60619
Z	15	MET	-	EXPRESSION TAG	UNP P60619
Z	16	TRP	-	EXPRESSION TAG	UNP P60619
Z	17	PRO	-	EXPRESSION TAG	UNP P60619
Z	18	LEU	-	EXPRESSION TAG	UNP P60619
Z	19	GLY	-	EXPRESSION TAG	UNP P60619
Z	20	GLY	-	EXPRESSION TAG	UNP P60619
Z	21	GLN	-	EXPRESSION TAG	UNP P60619
Z	22	GLN	-	EXPRESSION TAG	UNP P60619
Z	23	THR	-	EXPRESSION TAG	UNP P60619
Z	24	THR	-	EXPRESSION TAG	UNP P60619

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	82	Total	Mg	0	0
			82	82		
32	9	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	C	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	7	Total	Cl	0	0
			7	7		
33	J	3	Total	Cl	0	0
			3	3		
33	Q	1	Total	Cl	0	0
			1	1		
33	K	1	Total	Cl	0	0
			1	1		
33	B	1	Total	Cl	0	0
			1	1		
33	A	1	Total	Cl	0	0
			1	1		
33	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	2	Total 2	Cl 2	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	91	Total 91	Sr 91	0	0
34	9	2	Total 2	Sr 2	0	0
34	1	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	3	Total 3	Sr 3	0	0
34	A	3	Total 3	Sr 3	0	0
34	T	1	Total 1	Sr 1	0	0
34	R	1	Total 1	Sr 1	0	0
34	Y	1	Total 1	Sr 1	0	0
34	S	1	Total 1	Sr 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	60	Total Na 60 60	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	3	Total Na 3 3	0	0
35	2	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

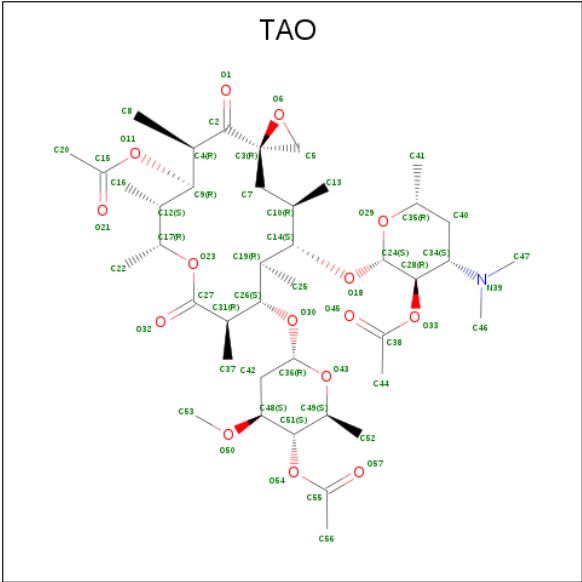
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is TROLEANDOMYCIN (three-letter code: TAO) (formula: C₄₁H₆₇NO₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	0	1	Total	C	N	O	0	0
			57	41	1	15		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	106	Total	O	0	0
			106	106		
39	B	135	Total	O	0	0
			135	135		
39	C	168	Total	O	0	0
			168	168		
39	D	45	Total	O	0	0
			45	45		
39	E	40	Total	O	0	0
			40	40		
39	F	23	Total	O	0	0
			23	23		
39	G	18	Total	O	0	0
			18	18		
39	H	71	Total	O	0	0
			71	71		
39	I	7	Total	O	0	0
			7	7		
39	J	46	Total	O	0	0
			46	46		
39	K	52	Total	O	0	0
			52	52		

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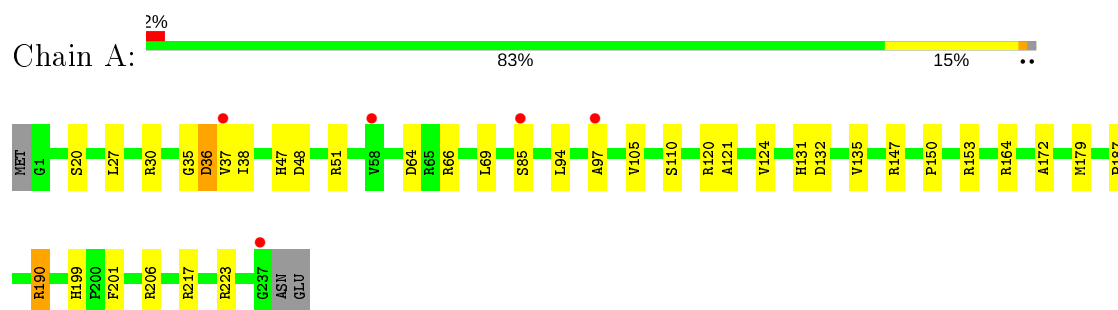
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	L	87	Total 87	O 87	0	0
39	M	123	Total 123	O 123	0	0
39	N	66	Total 66	O 66	0	0
39	O	44	Total 44	O 44	0	0
39	P	55	Total 55	O 55	0	0
39	Q	42	Total 42	O 42	0	0
39	R	78	Total 78	O 78	0	0
39	S	28	Total 28	O 28	0	0
39	T	35	Total 35	O 35	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	66	Total 66	O 66	0	0
39	X	22	Total 22	O 22	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	27	Total 27	O 27	0	0
39	1	49	Total 49	O 49	0	0
39	2	34	Total 34	O 34	0	0
39	3	62	Total 62	O 62	0	0
39	0	6021	Total 6021	O 6021	0	0
39	9	142	Total 142	O 142	0	0

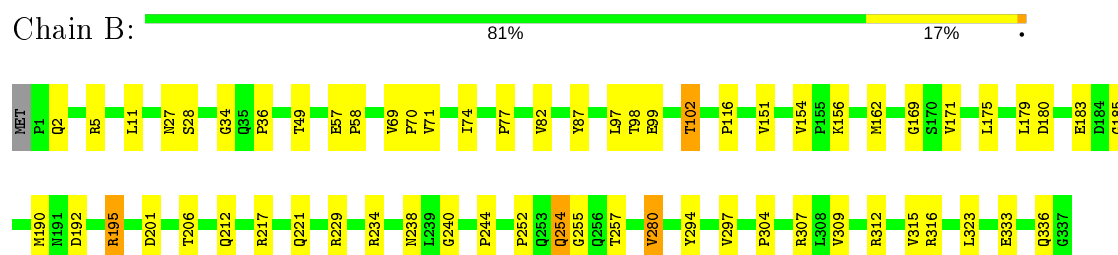
3 Residue-property plots [i](#)

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.

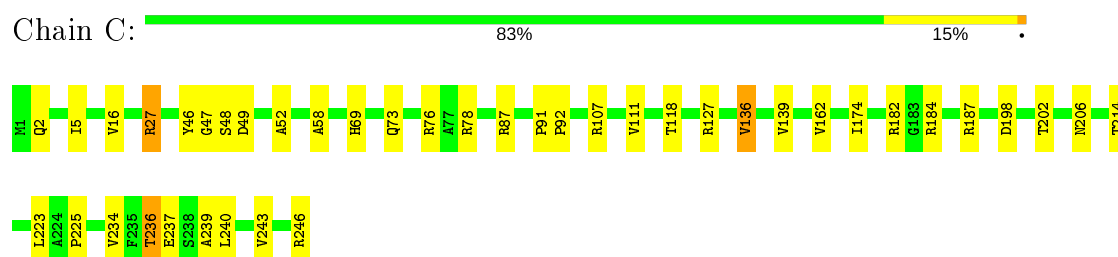
- Molecule 1: 50S ribosomal protein L2P



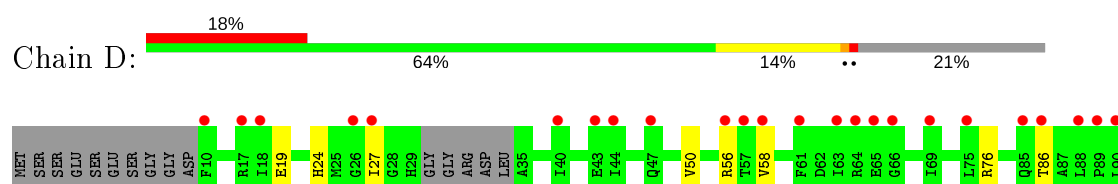
- Molecule 2: 50S ribosomal protein L3P

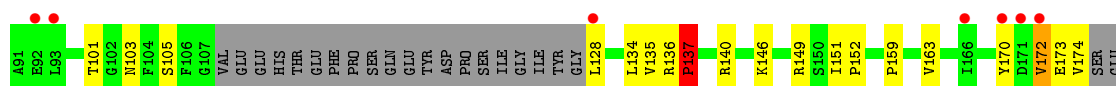


- Molecule 3: 50S ribosomal protein L4P

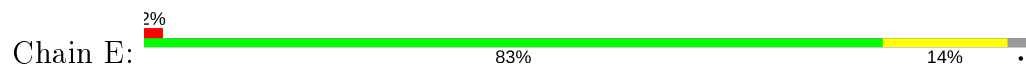


- Molecule 4: 50S ribosomal protein L5P

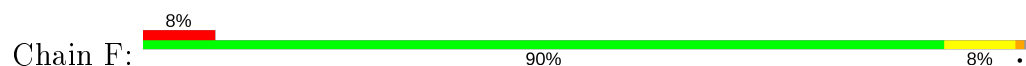




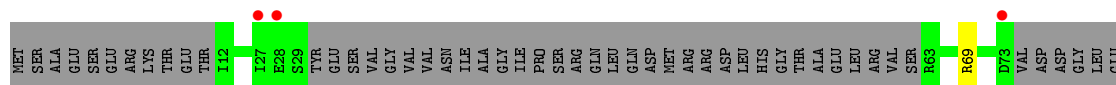
- Molecule 5: 50S ribosomal protein L6P



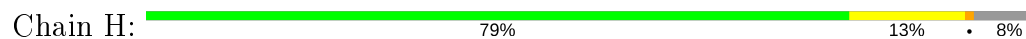
- Molecule 6: 50S ribosomal protein L7Ae



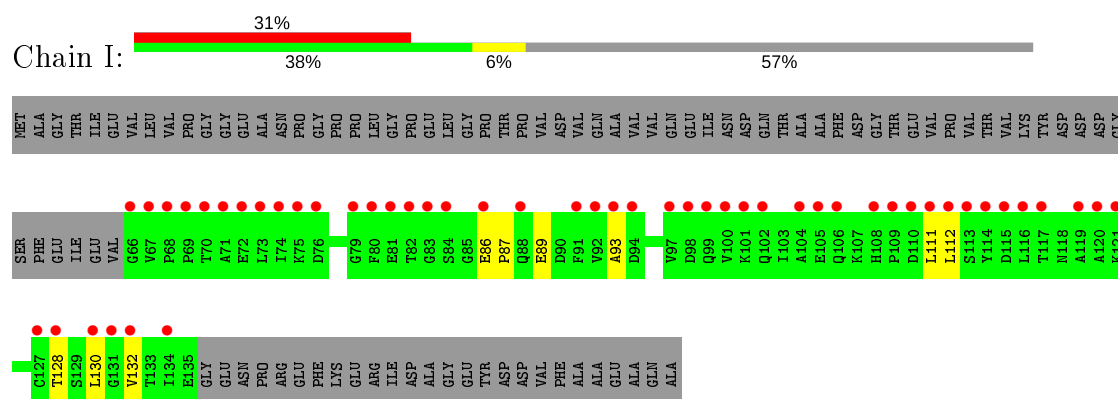
- Molecule 7: 50S ribosomal protein L10E



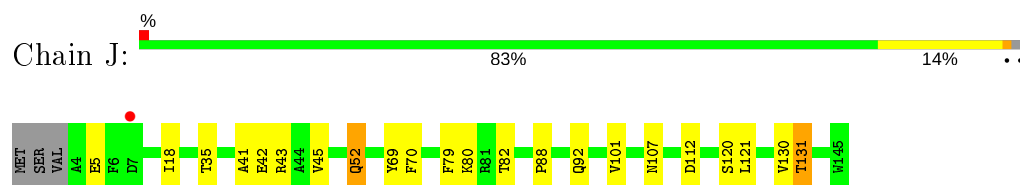
- Molecule 8: 50S ribosomal protein L10e



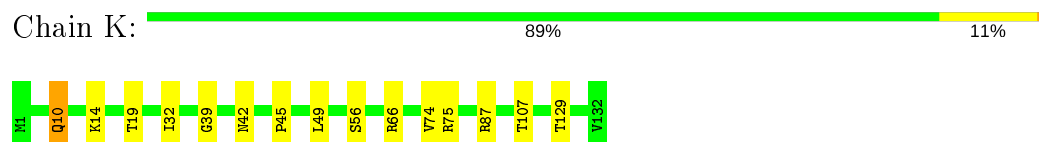
- Molecule 9: 50S ribosomal protein L11P



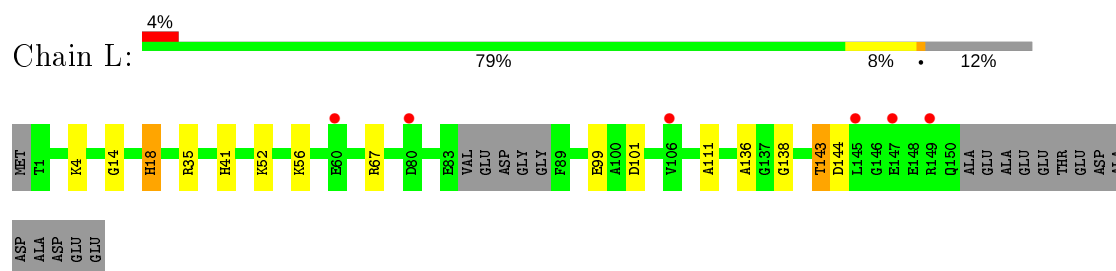
- Molecule 10: 50S ribosomal protein L13P



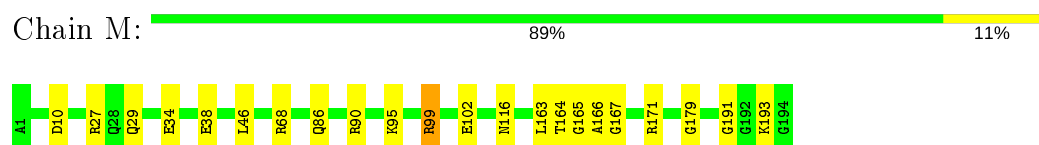
- Molecule 11: 50S ribosomal protein L14P



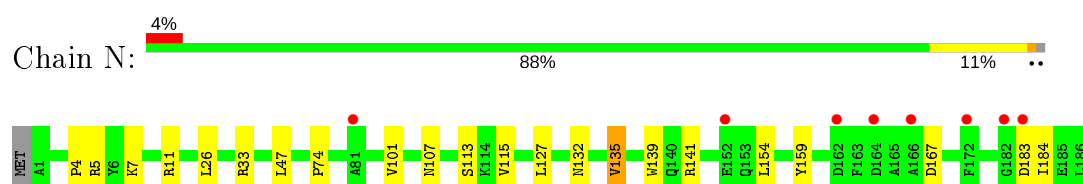
- Molecule 12: 50S ribosomal protein L15P



- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P




- Molecule 15: 50S ribosomal protein L18e

Chain O:  91% 8%




- Molecule 16: 50S ribosomal protein L19e

Chain P:  83% 13%




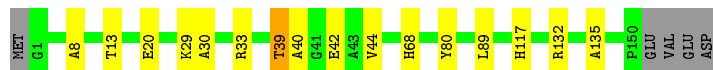
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  88% 11%




- Molecule 18: 50S ribosomal protein L22P

Chain R:  86% 10%




- Molecule 19: 50S ribosomal protein L23P

Chain S:  76% 19% 5%



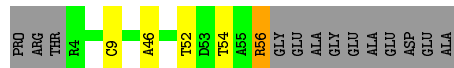
- Molecule 20: 50S ribosomal protein L24P

Chain T:  81% 17% 2%

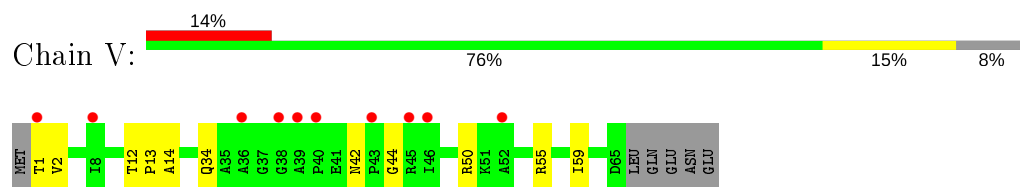


- Molecule 21: 50S ribosomal protein L24e

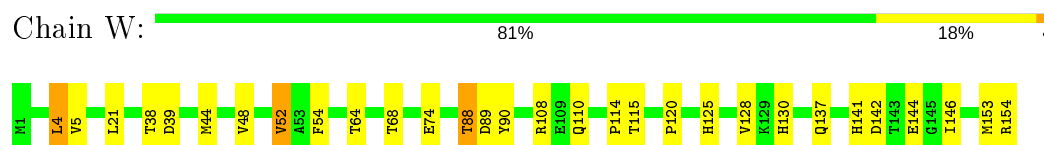
Chain U:  73% 6% 20%



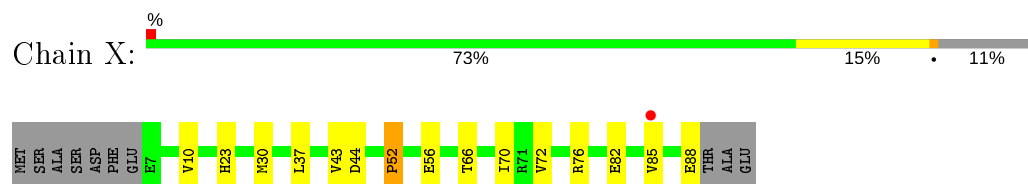
- Molecule 22: 50S ribosomal protein L29P



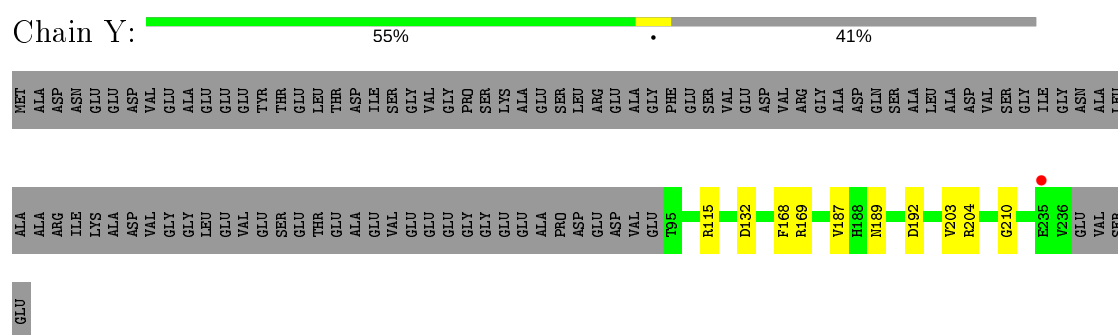
- Molecule 23: 50S ribosomal protein L30P



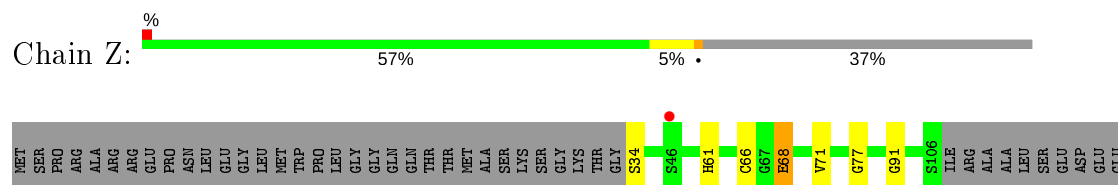
- Molecule 24: 50S ribosomal protein L31e



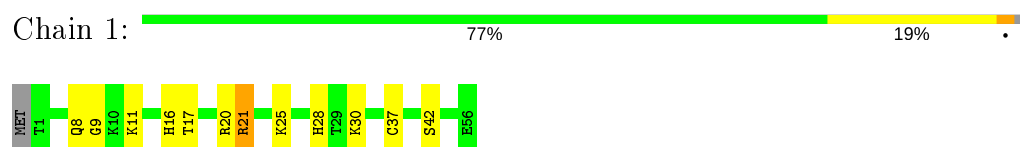
- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae



- Molecule 27: 50S ribosomal protein L37e




- Molecule 28: 50S ribosomal protein L39e

Chain 2:  66% 26% 8%



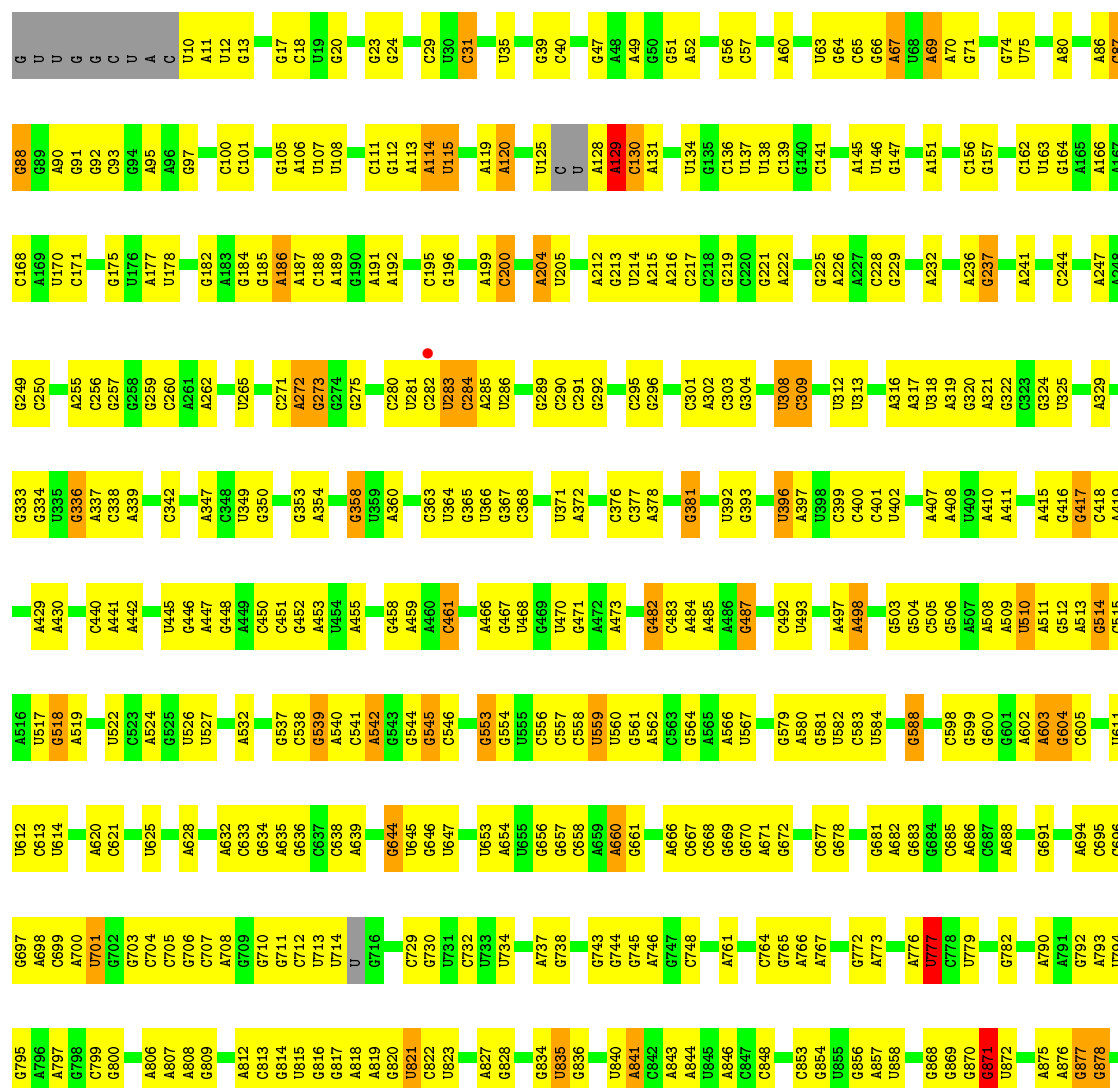
• Molecule 29: 50S ribosomal protein L44E

Chain 3:  84% 14% 2%

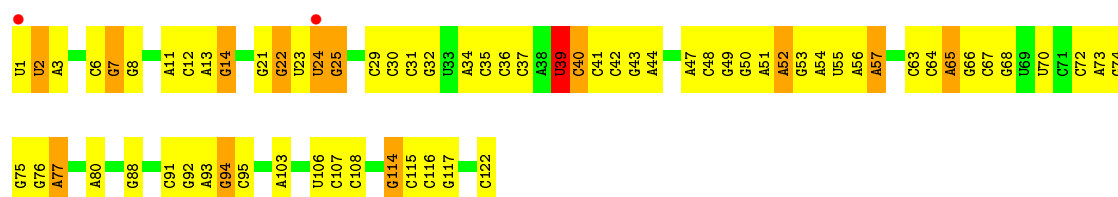


• Molecule 30: 23S ribosomal RNA

Chain 0:  49% 40% 5% 6%



G2110	C2020	G1756	C1666	G1592	U1500	G1409	G1224	C1156	G1063	C	C881
G2111	C2021	U1757	A1667	C1593	U1503	G1410	C1225	C1157	U1066	C	A882
A2112	G1939	U1758	A1668	G1594	U1504	A1413	C1228	G1158	C	G885	
C2113	C1940	U1759	U1596	G1595	A1504	A1414	C1229	G1159	A1067	U	A886
C2114	U1835	U1760	G1669	U1597	U1505	G1415	C1230	G1160	C	G887	
U2115	U1836	G1761	A1670	A1597	U1506	A1416	U1230	A1161	G	U888	
U2116	C1943	C1762	U1598	U1598	U1511	G1417	U1234	G1162	A	C889	
U2120	G1947	C1763	U1599	U1599	G1512	U1418	G1235	G1163	G	G890	
G2121	G1948	U1766	U1602	U1602	G1513	U1419	G1236	A1164	A	C896	
A2135	G1949	A1767	A1603	A1603	C1514	U1420	A1237	G1165	G	A897	
A2136	G1950	C1768	G1604	G1604	A1515	U1421	C1238	G1166	G	G898	
A	G1951	C1769	G1605	G1605	U1516	A1422	G1239	G1167	A	G902	
C	U	U1770	A1606	A1606	C1521	A1424	G1240	C1168	U	U903	
C	A	C1772	A1607	A1607	A1522	G1425	G1241	A1171	C	U904	
C	A	G1773	G1608	G1608	U1523	A1427	A1242	G1172	C	G905	
C	C	G1774	A1609	A1609	U1524	U1428	C1243	A1173	G	A906	
C	U	U1775	G1610	G1610	G1525	G1433	C1244	A1174	C	A907	
C	A	A1776	G1611	G1611	A1526	A1434	A1246	G1175	A	C920	
C	U	A1779	U1612	U1612	A1527	U1435	C1250	C1176	A	G921	
C	G	U1780	U1613	U1613	U1528	C1439	C1251	A1177	C	A922	
C	A	U1781	A1614	A1614	A1529	U1440	C1252	U1180	A	A923	
C	C	U1782	G1615	G1615	G1535	G1441	C1253	A1181	C	G924	
C	C	U1783	A1616	A1616	C1536	A1442	C1254	C1182	C	G925	
C	C	U1784	G1617	G1617	U1537	G1443	G1260	C1183	U	G940	
C	C	U1785	U1618	U1618	C1538	G1444	U1266	U1185	U	G941	
C	C	U1786	U1619	U1619	U1539	U1445	C1267	C1186	U	U942	
C	C	U1787	G1620	G1620	U1544	U1447	C1268	U1187	U	A943	
C	C	U1788	U1621	U1621	C1545	U1448	G1269	A1188	U	U944	
C	C	U1789	U1622	U1622	G1546	U1449	U1270	U1189	U	U945	
C	C	U1790	U1623	U1623	A1550	C1450	A1271	G1190	C	U946	
C	C	U1791	U1624	U1624	C1551	U1451	U1272	A1191	C	U947	
C	C	U1792	U1625	U1625	G1552	U1452	A1273	A1192	C	G948	
C	C	U1793	U1626	U1626	U1553	U1453	G1283	U1193	U	A951	
C	C	U1794	U1627	U1627	C1554	C1454	G1284	C1127	U	G952	
C	C	U1795	U1628	U1628	G1555	U1455	U1285	U1128	U	G953	
C	C	U1796	U1629	U1629	U1556	U1456	A1286	C1129	U	U954	
C	C	U1797	U1630	U1630	U1557	U1457	A1287	U1130	U	A955	
C	C	U1798	U1631	U1631	A1558	U1458	U1288	G1131	U	G958	
C	C	U1799	U1632	U1632	U1559	U1459	U1289	A1132	U	C959	
C	C	U1800	U1633	U1633	U1560	U1460	G1290	A1133	U	G960	
C	C	U1801	U1634	U1634	U1561	U1461	G1291	G1134	U	A961	
C	C	U1802	U1635	U1635	U1562	U1462	G1292	U1135	U	C962	
C	C	U1803	U1636	U1636	U1563	U1463	U1293	U1136	U	C963	
C	C	U1804	U1637	U1637	U1564	U1464	G1294	G1137	U	G968	
C	C	U1805	U1638	U1638	U1565	U1465	U1295	U1138	U	G969	
C	C	U1806	U1639	U1639	U1566	U1466	G1296	U1139	U	G	
C	C	U1807	U1640	U1640	U1567	U1467	G1297	G1052	U	U	
C	C	U1808	U1641	U1641	U1568	U1468	G1298	G1053	U	U	
C	C	U1809	U1642	U1642	U1569	U1469	U1299	G1054	U	U	
C	C	U1810	U1643	U1643	U1570	U1470	G1300	G1055	U	U	
C	C	U1811	U1644	U1644	U1571	U1471	U1301	U1056	U	U	
C	C	U1812	U1645	U1645	U1572	U1472	U1302	A1057	U	U	
C	C	U1813	U1646	U1646	U1573	U1473	U1303	A1058	U	U	
C	C	U1814	U1647	U1647	U1574	U1474	U1304	A1152	U	U	
C	C	U1815	U1648	U1648	U1575	U1475	U1305	C1153	U	U	
C	C	U1816	U1649	U1649	U1576	U1476	U1306	A1154	U	U	
C	C	U1817	U1650	U1650	U1577	U1477	U1307	C1155	U	U	
C	C	U1818	U1651	U1651	U1578	U1478	U1308	A1156	U	U	
C	C	U1819	U1652	U1652	U1579	U1479	U1309	C1157	U	U	
C	C	U1820	U1653	U1653	U1580	U1480	U1310	A1158	U	U	
C	C	U1821	U1654	U1654	U1581	U1481	U1311	C1159	U	U	
C	C	U1822	U1655	U1655	U1582	U1482	U1312	A1159	U	U	
C	C	U1823	U1656	U1656	U1583	U1483	U1313	C1160	U	U	
C	C	U1824	U1657	U1657	U1584	U1484	U1314	C1161	U	U	
C	C	U1825	U1658	U1658	U1585	U1485	U1315	C1162	U	U	
C	C	U1826	U1659	U1659	U1586	U1486	U1316	C1163	U	U	
C	C	U1827	U1660	U1660	U1587	U1487	U1317	C1164	U	U	
C	C	U1828	U1661	U1661	U1588	U1488	U1318	C1165	U	U	
C	C	U1829	U1662	U1662	U1589	U1489	U1319	C1166	U	U	
C	C	U1830	U1663	U1663	U1590	U1490	U1320	C1167	U	U	
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C	C	U1832	U1665	U1665	U1592	U1492	U1322	C1169	U	U	
C	C	U1833	U1666	U1666	U1593	U1493	U1323	C1170	U	U	
C	C	U1834	U1667	U1667	U1594	U1494	U1324	C1171	U	U	
C	C	U1835	U1668	U1668	U1595	U1495	U1325	C1172	U	U	
C	C	U1836	U1669	U1669	U1596	U1496	U1326	C1173	U	U	
C	C	U1837	U1670	U1670	U1597	U1497	U1327	C1174	U	U	
C	C	U1838	U1671	U1671	U1598	U1498	U1328	C1175	U	U	
C	C	U1839	U1672	U1672	U1599	U1499	U1329	C1176	U	U	
C	C	U1840	U1673	U1673	U1600	U1500	U1330	C1177	U	U	
C	C	U1841	U1674	U1674	U1601	U1501	U1331	C1178	U	U	
C	C	U1842	U1675	U1675	U1602	U1502	U1332	C1179	U	U	
C	C	U1843	U1676	U1676	U1603	U1503	U1333	C1180	U	U	
C	C	U1844	U1677	U1677	U1604	U1504	U1334	C1181	U	U	
C	C	U1845	U1678	U1678	U1605	U1505	U1335	C1182	U	U	
C	C	U1846	U1679	U1679	U1606	U1506	U1336	C1183	U	U	
C	C	U1847	U1680	U1680	U1607	U1507	U1337	C1184	U	U	
C	C	U1848	U1681	U1681	U1608	U1508	U1338	C1185	U	U	
C	C	U1849	U1682	U1682	U1609	U1509	U1339	C1186	U	U	
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C	C	U1853	U1686	U1686	U1613	U1513	U1343	C1190	U	U	
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C	C	U1856	U1689	U1689	U1616	U1516	U1346	C1193	U	U	
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C	C	U1861	U1694	U1694	U1621	U1521	U1351	C1198	U	U	
C	C	U1862	U1695	U1695	U1622	U1522	U1352	C1199	U	U	
C	C	U1863	U1696	U1696	U1623	U1523	U1353	C1200	U	U	
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C	C	U1866	U1699	U1699	U1626	U1526	U1356	C1203	U	U	
C	C	U1867	U1700	U1700	U1627	U1527	U1357	C1204	U	U	
C	C	U1868	U1701	U1701	U1628	U1528	U1358	C1205	U	U	
C	C	U1869	U1702	U1702	U1629	U1529	U1359	C1206	U	U	
C	C	U1870	U1703	U1703	U1630	U1530	U1360	C1207	U	U	
C	C	U1871	U1704	U1704	U1631	U1531	U1361	C1208	U	U	
C	C	U1872	U1705	U1705	U1632	U1532	U1362	C1209	U	U	
C	C	U1873	U1706	U1706	U1633	U1533	U1363	C1210	U	U	
C	C	U1874	U1707	U1707	U1634	U1534	U1364	C1211	U	U	
C	C	U1875	U1708	U1708	U1635	U1535	U1365	C1212	U	U	
C	C	U1876	U1709	U1709	U1636	U1536	U1366	C1213	U	U	
C	C	U1877	U1710	U1710	U1637	U1537	U1367	C1214	U	U	
C	C	U1878	U1711	U1711	U1638	U1538	U1368	C1215	U	U	
C	C	U1879	U1712	U1712	U1639	U1539	U1369	C1216	U	U	
C	C	U1880	U1713	U1713	U1640	U1540	U1370	C1217	U	U	
C	C	U1881	U1714	U1714	U1641	U1541	U1371	C1218	U	U	
C	C	U1882	U1715	U1715	U1642	U1542	U1372	C1219	U	U	
C	C	U1883	U1716	U1716	U1643	U1543	U1373	C1220	U	U	
C	C	U1884	U1717	U1717	U1644	U1544	U1374	C1221	U	U	
C	C	U1885	U1718	U1718	U1645	U1545	U1375	C1222	U	U	
C	C	U1886	U1719	U1719							



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.43 Å 300.77 Å 575.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 85.79 – 2.41	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.00-2.90) 90.7 (85.79-2.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.243 0.189 , 0.237	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99181	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, TAO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/1786	0.76	0/2408
2	B	0.53	0/2690	0.76	0/3652
3	C	0.54	0/1885	0.76	0/2552
4	D	0.63	0/1111	0.74	2/1498 (0.1%)
5	E	0.59	0/1382	0.70	0/1880
6	F	0.53	0/901	0.72	0/1224
7	G	0.51	0/241	0.63	0/324
8	H	0.59	0/1303	0.77	0/1743
9	I	0.59	0/526	0.68	0/716
10	J	0.61	0/1136	0.74	0/1530
11	K	0.50	0/1004	0.78	0/1351
12	L	0.50	0/1130	0.76	0/1509
13	M	0.50	0/1583	0.74	0/2116
14	N	0.54	0/1474	0.79	0/1999
15	O	0.49	0/874	0.72	1/1181 (0.1%)
16	P	0.54	0/1147	0.65	0/1528
17	Q	0.51	0/749	0.77	0/1005
18	R	0.57	0/1172	0.73	0/1578
19	S	0.52	0/648	0.66	0/875
20	T	0.49	0/958	0.75	1/1289 (0.1%)
21	U	0.56	0/417	0.69	0/562
22	V	0.44	0/502	0.71	0/675
23	W	0.52	0/1219	0.76	1/1655 (0.1%)
24	X	0.53	0/664	0.76	0/895
25	Y	0.49	0/1146	0.74	0/1536
26	Z	0.62	0/584	0.77	0/781
27	1	0.55	0/438	0.74	0/578
28	2	0.45	0/401	0.69	0/529
29	3	0.55	0/771	0.68	0/1024
30	0	0.41	0/65957	0.69	12/102867 (0.0%)
31	9	0.36	0/2904	0.69	1/4526 (0.0%)
All	All	0.45	0/98703	0.70	18/147586 (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
23	W	0	1
30	0	0	35
31	9	0	2
All	All	0	38

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
30	0	2291	A	N9-C1'-C2'	6.13	121.97	114.00
30	0	871	G	C5'-C4'-O4'	-6.06	101.83	109.10
30	0	1942	A	C5'-C4'-C3'	5.87	125.38	116.00
31	9	39	U	N1-C1'-C2'	5.60	121.29	114.00

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	482	G	Sidechain
30	0	49	A	Sidechain
23	W	90	TYR	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	A	1753	0	1766	22	0
2	B	2625	0	2533	35	0
3	C	1860	0	1813	28	0
4	D	1094	0	1085	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	14	0
6	F	890	0	843	5	0
7	G	240	0	231	0	0
8	H	1283	0	1292	17	0
9	I	519	0	500	6	0
10	J	1120	0	1098	15	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	11	0
13	M	1559	0	1573	18	0
14	N	1445	0	1401	13	0
15	O	865	0	873	7	0
16	P	1136	0	1123	12	0
17	Q	735	0	729	9	0
18	R	1149	0	1122	11	0
19	S	641	0	605	8	0
20	T	950	0	924	10	0
21	U	410	0	364	4	0
22	V	499	0	511	7	0
23	W	1196	0	1137	20	0
24	X	654	0	653	7	0
25	Y	1130	0	1133	10	0
26	Z	573	0	531	5	0
27	1	431	0	426	14	0
28	2	396	0	413	10	0
29	3	755	0	728	9	0
30	0	59020	0	29812	1178	0
31	9	2599	0	1325	71	0
32	0	82	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	C	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	7	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	0	0
33	K	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	2	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	91	0	0	0	0
34	1	2	0	0	0	0
34	3	3	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	60	0	0	0	0
35	2	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	3	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	57	0	67	14	0
39	0	6021	0	0	144	0
39	1	49	0	0	0	0
39	2	34	0	0	0	0
39	3	62	0	0	0	0
39	9	142	0	0	3	0
39	A	106	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	135	0	0	4	0
39	C	168	0	0	2	0
39	D	45	0	0	0	0
39	E	40	0	0	1	0
39	F	23	0	0	0	0
39	G	18	0	0	0	0
39	H	71	0	0	1	0
39	I	7	0	0	0	0
39	J	46	0	0	1	0
39	K	52	0	0	0	0
39	L	87	0	0	2	0
39	M	123	0	0	0	0
39	N	66	0	0	2	0
39	O	44	0	0	1	0
39	P	55	0	0	0	0
39	Q	42	0	0	0	0
39	R	78	0	0	2	0
39	S	28	0	0	0	0
39	T	35	0	0	1	0
39	U	26	0	0	0	0
39	V	11	0	0	0	0
39	W	66	0	0	1	0
39	X	22	0	0	0	0
39	Y	94	0	0	3	0
39	Z	27	0	0	0	0
All	All	99181	0	59980	1428	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 9.

The worst 5 of 1428 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)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.25	1.16
30:0:871:G:H8	30:0:871:G:H5'	1.06	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.90	1.06
30:0:2717:C:H2'	30:0:2718:C:H5''	1.42	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.42	1.01

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	
1	A	235/240 (98%)	219 (93%)	14 (6%)	2 (1%)	17	48
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	17	48
3	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
4	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	6	24
5	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
6	F	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	5	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/174 (90%)	146 (94%)	9 (6%)	1 (1%)	25	58
9	I	68/162 (42%)	62 (91%)	6 (9%)	0	100	100
10	J	140/145 (97%)	133 (95%)	6 (4%)	1 (1%)	22	54
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	131 (93%)	10 (7%)	0	100	100
13	M	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	5	19
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	42
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	22	54
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	111 (95%)	4 (3%)	2 (2%)	9	31
21	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	5	21
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	3705/4466 (83%)	3492 (94%)	189 (5%)	24 (1%)	25	58

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
10	J	5	GLU
14	N	154	LEU

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	
1	A	179/182 (98%)	165 (92%)	14 (8%)	12	34
2	B	282/283 (100%)	265 (94%)	17 (6%)	19	49
3	C	193/193 (100%)	175 (91%)	18 (9%)	9	27
4	D	117/148 (79%)	107 (92%)	10 (8%)	10	31
5	E	152/156 (97%)	147 (97%)	5 (3%)	38	72
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	134/143 (94%)	128 (96%)	6 (4%)	27	61
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	86
10	J	118/121 (98%)	109 (92%)	9 (8%)	13	36
11	K	106/106 (100%)	101 (95%)	5 (5%)	26	59
12	L	113/127 (89%)	107 (95%)	6 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/158 (100%)	153 (97%)	5 (3%)	39	73
14	N	149/150 (99%)	143 (96%)	6 (4%)	31	65
15	O	93/94 (99%)	91 (98%)	2 (2%)	52	81
16	P	113/117 (97%)	108 (96%)	5 (4%)	28	61
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	56
18	R	117/122 (96%)	115 (98%)	2 (2%)	60	86
19	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
20	T	105/106 (99%)	96 (91%)	9 (9%)	10	30
21	U	44/52 (85%)	43 (98%)	1 (2%)	50	80
22	V	51/57 (90%)	49 (96%)	2 (4%)	32	66
23	W	130/130 (100%)	124 (95%)	6 (5%)	27	60
24	X	66/74 (89%)	60 (91%)	6 (9%)	9	28
25	Y	120/196 (61%)	118 (98%)	2 (2%)	60	86
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60	86
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	81
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	74 (94%)	5 (6%)	18	46
All	All	3095/3641 (85%)	2940 (95%)	155 (5%)	24	57

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	87	LYS
11	K	107	THR
24	X	82	GLU
8	H	169	GLU
10	J	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	50	GLN
18	R	98	ASN
28	2	18	ASN
16	P	57	ASN

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Mol	Chain	Res	Type
17	Q	16	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	235 (8%)	22 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	251 (8%)	23 (0%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1237	U
30	0	1352	A
30	0	2791	U
30	0	1246	A
30	0	1377	C

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	1MA	0	628	30	15,25,26	0.70	0	15,37,40	1.37	1 (6%)
30	OMU	0	2587	30,35	14,22,23	1.03	1 (7%)	14,31,34	1.12	1 (7%)
30	PSU	0	2621	30	17,21,22	1.59	3 (17%)	20,30,33	5.40	4 (20%)
30	UR3	0	2619	30	14,22,23	0.73	0	15,32,35	0.59	0
30	OMG	0	2588	30	18,26,27	1.10	2 (11%)	20,38,41	2.61	5 (25%)

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
30	1MA	0	628	30	-	0/3/25/26	0/3/3/3
30	OMU	0	2587	30,35	-	0/7/27/28	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.90	1.48	1.52
30	0	2588	OMG	C6-N1	3.52	1.39	1.33
30	0	2587	OMU	C4-N3	2.67	1.37	1.33
30	0	2621	PSU	C2-N1	2.61	1.43	1.38
30	0	2621	PSU	C4-N3	2.57	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.10	114.84	128.43
30	0	2621	PSU	C4-N3-C2	14.28	127.20	115.14
30	0	2588	OMG	C5-C6-N1	-8.74	111.48	123.43
30	0	2621	PSU	C5-C4-N3	-8.04	115.00	125.36
30	0	2588	OMG	C6-N1-C2	5.84	125.21	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
38	TAO	0	2924	-	59,60,60	0.68	1 (1%)	77,89,89	1.85	16 (20%)

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
38	TAO	0	2924	-	2/2/24/24	14/77/113/113	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	TAO	C5-C3	2.28	1.52	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	O33-C38-C44	5.91	121.97	111.09
38	0	2924	TAO	C17-O23-C27	-4.89	110.42	117.51
38	0	2924	TAO	O54-C55-C56	4.65	119.65	111.09
38	0	2924	TAO	O11-C15-C20	4.37	119.13	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	C51-O54-C55	-4.27	111.12	117.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
38	0	2924	TAO	C10
38	0	2924	TAO	C9

5 of 14 torsion outliers are listed below:

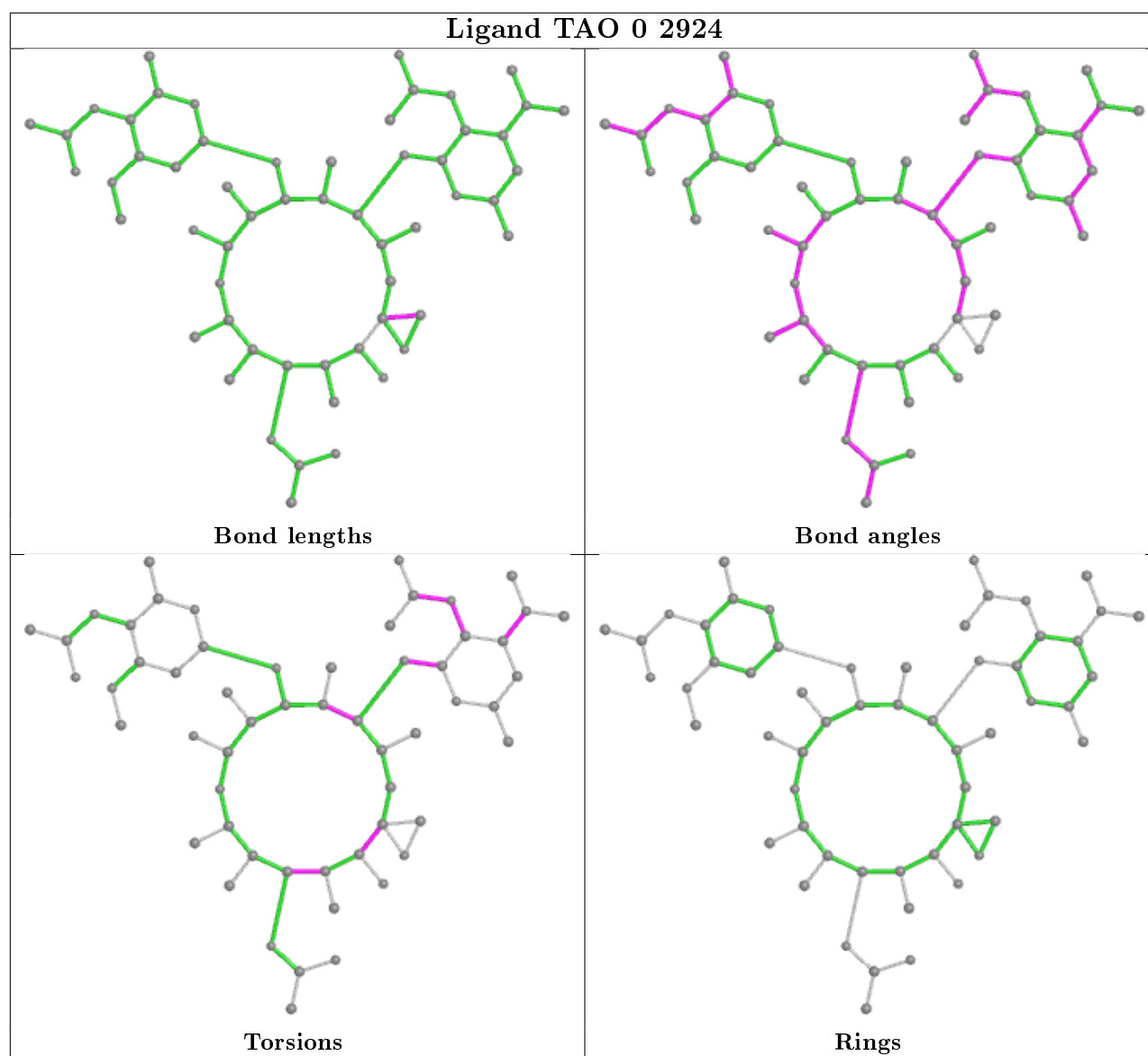
Mol	Chain	Res	Type	Atoms
38	0	2924	TAO	C44-C38-O33-C28
38	0	2924	TAO	O45-C38-O33-C28
38	0	2924	TAO	C10-C14-C19-C25
38	0	2924	TAO	C34-C28-O33-C38
38	0	2924	TAO	C40-C34-N39-C47

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	TAO	14	0

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	A	237/240 (98%)	-0.33	5 (2%) 63 61	19, 43, 83, 105	0
2	B	337/338 (99%)	-0.47	0 100 100	17, 47, 75, 90	0
3	C	246/246 (100%)	-0.39	0 100 100	12, 41, 66, 78	0
4	D	140/177 (79%)	0.97	31 (22%) 0 0	51, 92, 120, 131	0
5	E	172/178 (96%)	-0.19	4 (2%) 60 58	39, 62, 89, 96	0
6	F	119/120 (99%)	0.40	10 (8%) 11 8	43, 70, 104, 120	0
7	G	29/348 (8%)	0.80	3 (10%) 6 5	62, 88, 97, 98	0
8	H	160/174 (91%)	-0.35	0 100 100	24, 48, 85, 99	0
9	I	70/162 (43%)	3.17	51 (72%) 0 0	124, 138, 160, 161	0
10	J	142/145 (97%)	-0.51	1 (0%) 87 87	25, 43, 65, 80	0
11	K	132/132 (100%)	-0.54	0 100 100	25, 43, 68, 75	0
12	L	145/165 (87%)	0.06	6 (4%) 37 32	13, 60, 107, 118	0
13	M	194/194 (100%)	-0.61	0 100 100	22, 36, 55, 62	0
14	N	186/187 (99%)	0.08	8 (4%) 35 31	32, 58, 111, 119	0
15	O	115/116 (99%)	-0.38	0 100 100	30, 49, 66, 74	0
16	P	143/149 (95%)	-0.42	0 100 100	30, 49, 64, 67	0
17	Q	95/96 (98%)	-0.60	0 100 100	25, 36, 51, 71	0
18	R	150/155 (96%)	-0.64	0 100 100	21, 37, 61, 73	0
19	S	81/85 (95%)	-0.08	1 (1%) 79 79	35, 57, 74, 82	0
20	T	119/120 (99%)	-0.17	2 (1%) 70 69	32, 53, 80, 100	0
21	U	53/66 (80%)	-0.51	0 100 100	30, 49, 70, 74	0
22	V	65/71 (91%)	0.90	10 (15%) 2 1	49, 72, 108, 116	0
23	W	154/154 (100%)	-0.66	0 100 100	26, 40, 59, 70	0
24	X	82/92 (89%)	-0.22	1 (1%) 79 79	36, 49, 73, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.52	1 (0%) 87 87	18, 39, 64, 81	0
26	Z	73/116 (62%)	-0.32	1 (1%) 75 75	34, 54, 77, 93	0
27	1	56/57 (98%)	-0.63	0 100 100	16, 26, 35, 43	0
28	2	46/50 (92%)	-0.16	0 100 100	29, 56, 81, 98	0
29	3	92/92 (100%)	-0.41	0 100 100	27, 47, 62, 73	0
30	0	2749/2923 (94%)	-0.67	8 (0%) 94 94	11, 36, 81, 154	0
31	9	122/122 (100%)	-0.76	2 (1%) 72 71	22, 51, 78, 129	0
All	All	6646/7511 (88%)	-0.41	145 (2%) 62 59	11, 44, 93, 161	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	112	LEU	9.2
9	I	97	VAL	8.9
9	I	72	GLU	8.0
22	V	40	PRO	7.4
9	I	109	PRO	7.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.98	0.14	13,18,20,21	0
30	OMU	0	2587	21/22	0.98	0.11	22,25,29,32	0
30	PSU	0	2621	20/21	0.98	0.13	18,19,25,25	0
30	OMG	0	2588	24/25	0.98	0.13	20,23,24,28	0
30	UR3	0	2619	21/22	0.98	0.12	21,24,26,29	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	8938	1/1	-0.47	0.70	200,200,200,200	0
34	SR	0	8928	1/1	-0.11	1.41	200,200,200,200	0
34	SR	0	8959	1/1	-0.06	0.67	195,195,195,195	0
34	SR	A	8993	1/1	0.03	0.21	200,200,200,200	0
32	MG	0	8091	1/1	0.09	0.28	79,79,79,79	0
34	SR	A	8930	1/1	0.10	2.72	200,200,200,200	0
34	SR	9	8980	1/1	0.10	0.39	200,200,200,200	0
35	NA	0	8525	1/1	0.13	1.03	107,107,107,107	0
34	SR	0	9000	1/1	0.15	1.26	200,200,200,200	0
34	SR	0	9006	1/1	0.18	0.41	192,192,192,192	0
35	NA	0	8548	1/1	0.19	0.23	59,59,59,59	0
35	NA	0	8509	1/1	0.22	0.33	53,53,53,53	0
34	SR	0	8908	1/1	0.23	0.27	200,200,200,200	0
34	SR	0	8903	1/1	0.23	0.12	168,168,168,168	0
34	SR	0	8966	1/1	0.27	0.27	178,178,178,178	0
34	SR	0	8907	1/1	0.27	0.22	180,180,180,180	0
34	SR	0	8965	1/1	0.28	0.09	143,143,143,143	0
34	SR	0	8920	1/1	0.28	0.56	200,200,200,200	0
34	SR	0	8935	1/1	0.33	0.11	159,159,159,159	0
34	SR	0	8911	1/1	0.35	0.38	200,200,200,200	0
34	SR	0	8984	1/1	0.37	0.08	170,170,170,170	0
34	SR	0	8991	1/1	0.38	0.11	162,162,162,162	0
34	SR	0	8926	1/1	0.39	0.39	199,199,199,199	0
34	SR	0	8997	1/1	0.40	1.21	200,200,200,200	0
34	SR	B	8987	1/1	0.42	0.29	199,199,199,199	0
34	SR	A	8929	1/1	0.44	0.46	174,174,174,174	0
35	NA	0	8511	1/1	0.44	0.20	56,56,56,56	0
35	NA	0	8535	1/1	0.45	0.39	68,68,68,68	0
34	SR	0	8922	1/1	0.45	0.55	155,155,155,155	0
35	NA	0	8557	1/1	0.45	0.24	89,89,89,89	0
34	SR	3	8999	1/1	0.45	0.23	200,200,200,200	0
35	NA	J	8538	1/1	0.46	0.22	49,49,49,49	0
34	SR	0	8933	1/1	0.47	0.14	137,137,137,137	0
34	SR	1	8952	1/1	0.48	0.68	200,200,200,200	0
34	SR	0	8970	1/1	0.51	0.46	200,200,200,200	0
34	SR	0	9004	1/1	0.51	0.53	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8901	1/1	0.53	0.12	73,73,73,73	0
34	SR	B	8950	1/1	0.53	0.62	196,196,196,196	0
34	SR	0	8968	1/1	0.55	0.14	170,170,170,170	0
34	SR	0	8995	1/1	0.56	0.38	164,164,164,164	0
34	SR	0	8982	1/1	0.57	1.21	200,200,200,200	0
34	SR	0	8934	1/1	0.57	0.76	168,168,168,168	0
34	SR	0	8925	1/1	0.57	0.18	178,178,178,178	0
34	SR	T	8939	1/1	0.58	0.64	200,200,200,200	0
34	SR	Y	9002	1/1	0.58	0.39	200,200,200,200	0
32	MG	0	8037	1/1	0.58	0.94	88,88,88,88	0
34	SR	0	8949	1/1	0.58	0.20	132,132,132,132	0
34	SR	0	8919	1/1	0.59	0.40	188,188,188,188	0
35	NA	C	8558	1/1	0.61	0.45	33,33,33,33	0
35	NA	0	8519	1/1	0.62	0.37	76,76,76,76	0
34	SR	0	8964	1/1	0.62	0.42	188,188,188,188	0
34	SR	0	8956	1/1	0.64	0.10	147,147,147,147	0
32	MG	0	8034	1/1	0.65	0.50	60,60,60,60	0
35	NA	0	8570	1/1	0.65	0.55	81,81,81,81	0
35	NA	0	8560	1/1	0.65	0.45	104,104,104,104	0
35	NA	0	8565	1/1	0.66	1.06	79,79,79,79	0
34	SR	0	8988	1/1	0.66	0.20	177,177,177,177	0
34	SR	0	8931	1/1	0.66	0.16	193,193,193,193	0
34	SR	0	8927	1/1	0.67	0.23	184,184,184,184	0
34	SR	0	8958	1/1	0.67	0.10	147,147,147,147	0
34	SR	0	8973	1/1	0.68	0.14	178,178,178,178	0
34	SR	0	8960	1/1	0.68	0.35	200,200,200,200	0
34	SR	0	8909	1/1	0.69	0.25	189,189,189,189	0
32	MG	2	8060	1/1	0.70	0.28	67,67,67,67	0
34	SR	0	8946	1/1	0.70	0.40	190,190,190,190	0
34	SR	0	8954	1/1	0.70	0.87	198,198,198,198	0
34	SR	0	8945	1/1	0.70	0.09	131,131,131,131	0
34	SR	0	8998	1/1	0.71	0.37	196,196,196,196	0
34	SR	3	8932	1/1	0.71	0.11	133,133,133,133	0
34	SR	0	8979	1/1	0.71	0.09	180,180,180,180	0
32	MG	0	8053	1/1	0.72	0.11	78,78,78,78	0
34	SR	0	8910	1/1	0.72	0.10	92,92,92,92	0
34	SR	0	8977	1/1	0.72	0.12	194,194,194,194	0
35	NA	0	8502	1/1	0.72	0.29	54,54,54,54	0
34	SR	0	8962	1/1	0.73	0.26	197,197,197,197	0
34	SR	0	8923	1/1	0.73	0.59	165,165,165,165	0
35	NA	0	8568	1/1	0.73	0.44	46,46,46,46	0
35	NA	0	8505	1/1	0.74	0.52	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8924	1/1	0.74	0.12	184,184,184,184	0
34	SR	0	8942	1/1	0.74	0.34	162,162,162,162	0
35	NA	0	8529	1/1	0.74	0.08	33,33,33,33	0
34	SR	0	8916	1/1	0.75	0.34	178,178,178,178	0
35	NA	0	8567	1/1	0.76	0.46	63,63,63,63	0
35	NA	0	8571	1/1	0.76	0.21	73,73,73,73	0
35	NA	9	8572	1/1	0.76	0.68	103,103,103,103	0
32	MG	0	8036	1/1	0.77	0.08	46,46,46,46	0
34	SR	0	8943	1/1	0.77	0.38	179,179,179,179	0
32	MG	0	8039	1/1	0.77	0.31	56,56,56,56	0
35	NA	0	8549	1/1	0.77	0.43	60,60,60,60	0
35	NA	S	8510	1/1	0.77	0.18	35,35,35,35	0
32	MG	0	8083	1/1	0.78	0.09	41,41,41,41	0
35	NA	R	8532	1/1	0.78	0.12	39,39,39,39	0
34	SR	0	8947	1/1	0.78	0.32	200,200,200,200	0
32	MG	0	8052	1/1	0.79	0.23	59,59,59,59	0
32	MG	0	8027	1/1	0.80	0.16	37,37,37,37	0
34	SR	0	8986	1/1	0.80	1.32	200,200,200,200	0
35	NA	0	8507	1/1	0.80	0.58	68,68,68,68	0
34	SR	0	9001	1/1	0.80	0.71	187,187,187,187	0
38	TAO	0	2924	57/57	0.80	0.35	83,95,107,109	0
34	SR	9	9003	1/1	0.80	0.23	195,195,195,195	0
34	SR	0	8978	1/1	0.81	0.79	200,200,200,200	0
35	NA	Q	8540	1/1	0.81	0.11	34,34,34,34	0
35	NA	0	8561	1/1	0.81	0.46	52,52,52,52	0
35	NA	0	8555	1/1	0.82	0.37	38,38,38,38	0
34	SR	0	8989	1/1	0.82	0.70	200,200,200,200	0
32	MG	0	8020	1/1	0.82	0.11	36,36,36,36	0
32	MG	0	8059	1/1	0.82	0.11	33,33,33,33	0
35	NA	0	8559	1/1	0.82	0.34	94,94,94,94	0
34	SR	0	8917	1/1	0.82	0.62	199,199,199,199	0
37	K	0	8401	1/1	0.82	0.40	150,150,150,150	0
34	SR	0	8971	1/1	0.82	0.09	195,195,195,195	0
34	SR	0	8955	1/1	0.83	0.13	184,184,184,184	0
34	SR	0	9005	1/1	0.83	0.24	190,190,190,190	0
35	NA	0	8546	1/1	0.83	0.68	106,106,106,106	0
34	SR	0	8906	1/1	0.83	0.40	191,191,191,191	0
34	SR	0	8992	1/1	0.83	0.13	151,151,151,151	0
34	SR	0	9007	1/1	0.84	0.40	200,200,200,200	0
34	SR	0	8969	1/1	0.84	0.25	181,181,181,181	0
33	CL	J	8802	1/1	0.84	0.07	66,66,66,66	0
32	MG	0	8081	1/1	0.84	0.49	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8981	1/1	0.84	0.51	200,200,200,200	0
34	SR	0	8957	1/1	0.84	0.76	200,200,200,200	0
35	NA	0	8528	1/1	0.84	0.09	49,49,49,49	0
34	SR	0	8983	1/1	0.84	0.35	170,170,170,170	0
34	SR	0	8990	1/1	0.84	0.08	91,91,91,91	0
32	MG	0	8082	1/1	0.85	0.33	39,39,39,39	0
35	NA	0	8520	1/1	0.85	0.11	44,44,44,44	0
34	SR	H	8972	1/1	0.85	0.14	131,131,131,131	0
34	SR	0	8940	1/1	0.85	0.28	159,159,159,159	0
34	SR	0	8994	1/1	0.85	0.23	192,192,192,192	0
35	NA	0	8531	1/1	0.85	0.22	47,47,47,47	0
34	SR	0	8921	1/1	0.85	0.14	155,155,155,155	0
32	MG	B	8043	1/1	0.85	0.13	37,37,37,37	0
35	NA	0	8526	1/1	0.85	0.09	51,51,51,51	0
35	NA	0	8564	1/1	0.86	0.95	91,91,91,91	0
34	SR	0	8904	1/1	0.86	0.35	200,200,200,200	0
34	SR	0	8996	1/1	0.86	0.62	200,200,200,200	0
34	SR	0	8948	1/1	0.86	0.11	94,94,94,94	0
32	MG	0	8092	1/1	0.86	0.06	61,61,61,61	0
32	MG	0	8049	1/1	0.86	0.32	43,43,43,43	0
34	SR	0	8944	1/1	0.86	0.21	200,200,200,200	0
34	SR	0	8915	1/1	0.86	0.14	200,200,200,200	0
35	NA	M	8539	1/1	0.86	0.10	19,19,19,19	0
35	NA	0	8501	1/1	0.87	0.25	29,29,29,29	0
33	CL	L	8810	1/1	0.87	0.07	69,69,69,69	0
34	SR	0	9008	1/1	0.87	0.08	135,135,135,135	0
35	NA	0	8521	1/1	0.87	0.08	28,28,28,28	0
35	NA	0	8522	1/1	0.87	0.85	73,73,73,73	0
32	MG	0	8005	1/1	0.87	0.21	26,26,26,26	0
35	NA	0	8524	1/1	0.87	0.19	43,43,43,43	0
32	MG	A	8050	1/1	0.88	0.16	18,18,18,18	0
34	SR	R	8912	1/1	0.88	0.12	157,157,157,157	0
32	MG	0	8035	1/1	0.88	0.21	65,65,65,65	0
35	NA	0	8553	1/1	0.88	0.41	59,59,59,59	0
32	MG	0	8071	1/1	0.88	0.45	136,136,136,136	0
35	NA	0	8574	1/1	0.88	0.28	52,52,52,52	0
34	SR	3	8953	1/1	0.88	0.20	200,200,200,200	0
32	MG	0	8055	1/1	0.88	0.15	49,49,49,49	0
32	MG	0	8002	1/1	0.88	0.16	14,14,14,14	0
35	NA	0	8530	1/1	0.89	0.36	46,46,46,46	0
32	MG	0	8069	1/1	0.89	0.34	38,38,38,38	0
32	MG	0	8029	1/1	0.89	0.23	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	CL	0	8822	1/1	0.89	0.10	59,59,59,59	0
32	MG	0	8063	1/1	0.89	0.12	47,47,47,47	0
32	MG	0	8056	1/1	0.89	0.19	37,37,37,37	0
35	NA	0	8547	1/1	0.89	0.22	49,49,49,49	0
35	NA	0	8508	1/1	0.90	0.76	41,41,41,41	0
32	MG	0	8033	1/1	0.90	0.12	78,78,78,78	0
34	SR	0	8905	1/1	0.90	0.21	161,161,161,161	0
32	MG	9	8074	1/1	0.90	0.08	45,45,45,45	0
35	NA	0	8506	1/1	0.90	0.31	50,50,50,50	0
32	MG	0	8068	1/1	0.90	0.13	54,54,54,54	0
32	MG	0	8032	1/1	0.90	0.09	47,47,47,47	0
35	NA	0	8556	1/1	0.90	0.32	41,41,41,41	0
32	MG	0	8079	1/1	0.90	0.15	51,51,51,51	0
35	NA	0	8573	1/1	0.91	0.26	65,65,65,65	0
32	MG	K	8054	1/1	0.91	0.27	62,62,62,62	0
35	NA	0	8550	1/1	0.91	0.12	25,25,25,25	0
32	MG	0	8004	1/1	0.91	0.18	23,23,23,23	0
32	MG	0	8075	1/1	0.91	0.06	32,32,32,32	0
34	SR	0	8936	1/1	0.91	0.11	100,100,100,100	0
32	MG	0	8093	1/1	0.92	0.05	13,13,13,13	0
34	SR	0	8967	1/1	0.92	0.24	191,191,191,191	0
34	SR	0	8914	1/1	0.92	0.49	198,198,198,198	0
32	MG	T	8057	1/1	0.92	0.05	60,60,60,60	0
34	SR	0	8902	1/1	0.92	0.18	107,107,107,107	0
33	CL	L	8814	1/1	0.92	0.19	51,51,51,51	0
32	MG	0	8019	1/1	0.92	0.25	1,1,1,1	0
32	MG	9	8040	1/1	0.92	0.64	71,71,71,71	0
35	NA	0	8541	1/1	0.93	0.73	86,86,86,86	0
32	MG	0	8072	1/1	0.93	0.21	44,44,44,44	0
35	NA	0	8551	1/1	0.93	0.12	36,36,36,36	0
32	MG	0	8026	1/1	0.93	0.11	22,22,22,22	0
34	SR	0	8937	1/1	0.93	0.28	155,155,155,155	0
33	CL	J	8801	1/1	0.93	0.09	58,58,58,58	0
34	SR	0	8974	1/1	0.93	0.21	165,165,165,165	0
33	CL	J	8821	1/1	0.93	0.10	61,61,61,61	0
35	NA	C	8503	1/1	0.93	0.17	31,31,31,31	0
33	CL	Y	8820	1/1	0.93	0.09	33,33,33,33	0
35	NA	0	8516	1/1	0.94	0.12	18,18,18,18	0
34	SR	0	8918	1/1	0.94	0.12	122,122,122,122	0
32	MG	0	8031	1/1	0.94	0.10	69,69,69,69	0
35	NA	0	8562	1/1	0.94	0.28	45,45,45,45	0
33	CL	0	8805	1/1	0.94	0.18	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8941	1/1	0.94	0.20	180,180,180,180	0
32	MG	0	8078	1/1	0.94	0.17	28,28,28,28	0
32	MG	0	8021	1/1	0.94	0.07	16,16,16,16	0
32	MG	0	8023	1/1	0.94	0.13	14,14,14,14	0
35	NA	0	8536	1/1	0.94	0.16	46,46,46,46	0
34	SR	0	8963	1/1	0.94	0.20	182,182,182,182	0
32	MG	B	8042	1/1	0.94	0.14	41,41,41,41	0
32	MG	0	8067	1/1	0.94	0.37	51,51,51,51	0
32	MG	0	8028	1/1	0.94	0.18	16,16,16,16	0
33	CL	0	8803	1/1	0.94	0.14	50,50,50,50	0
32	MG	0	8089	1/1	0.94	0.27	56,56,56,56	0
34	SR	S	8961	1/1	0.94	0.21	165,165,165,165	0
32	MG	0	8030	1/1	0.94	0.30	45,45,45,45	0
35	NA	0	8566	1/1	0.94	0.15	69,69,69,69	0
35	NA	0	8545	1/1	0.95	0.18	41,41,41,41	0
34	SR	1	8913	1/1	0.95	0.35	179,179,179,179	0
32	MG	0	8046	1/1	0.95	0.12	25,25,25,25	0
32	MG	A	8051	1/1	0.95	0.47	117,117,117,117	0
33	CL	O	8808	1/1	0.95	0.13	68,68,68,68	0
32	MG	0	8018	1/1	0.95	0.26	53,53,53,53	0
32	MG	0	8047	1/1	0.95	0.25	34,34,34,34	0
37	K	0	8402	1/1	0.95	0.17	78,78,78,78	0
32	MG	0	8006	1/1	0.95	0.06	7,7,7,7	0
35	NA	0	8537	1/1	0.95	0.14	22,22,22,22	0
35	NA	0	8534	1/1	0.95	0.14	15,15,15,15	0
32	MG	0	8073	1/1	0.95	0.09	47,47,47,47	0
35	NA	9	8543	1/1	0.95	0.09	22,22,22,22	0
35	NA	0	8512	1/1	0.95	0.30	32,32,32,32	0
32	MG	0	8066	1/1	0.96	0.40	87,87,87,87	0
33	CL	0	8815	1/1	0.96	0.22	72,72,72,72	0
32	MG	0	8088	1/1	0.96	0.12	33,33,33,33	0
32	MG	0	8064	1/1	0.96	0.15	29,29,29,29	0
35	NA	0	8544	1/1	0.96	0.19	49,49,49,49	0
33	CL	0	8816	1/1	0.96	0.19	60,60,60,60	0
34	SR	0	8951	1/1	0.96	0.15	164,164,164,164	0
32	MG	0	8008	1/1	0.96	0.09	8,8,8,8	0
33	CL	K	8812	1/1	0.96	0.07	39,39,39,39	0
32	MG	0	8085	1/1	0.96	0.14	51,51,51,51	0
35	NA	0	8569	1/1	0.96	0.12	40,40,40,40	0
32	MG	0	8062	1/1	0.96	0.32	64,64,64,64	0
32	MG	0	8045	1/1	0.96	0.11	13,13,13,13	0
33	CL	3	8804	1/1	0.96	0.11	59,59,59,59	0

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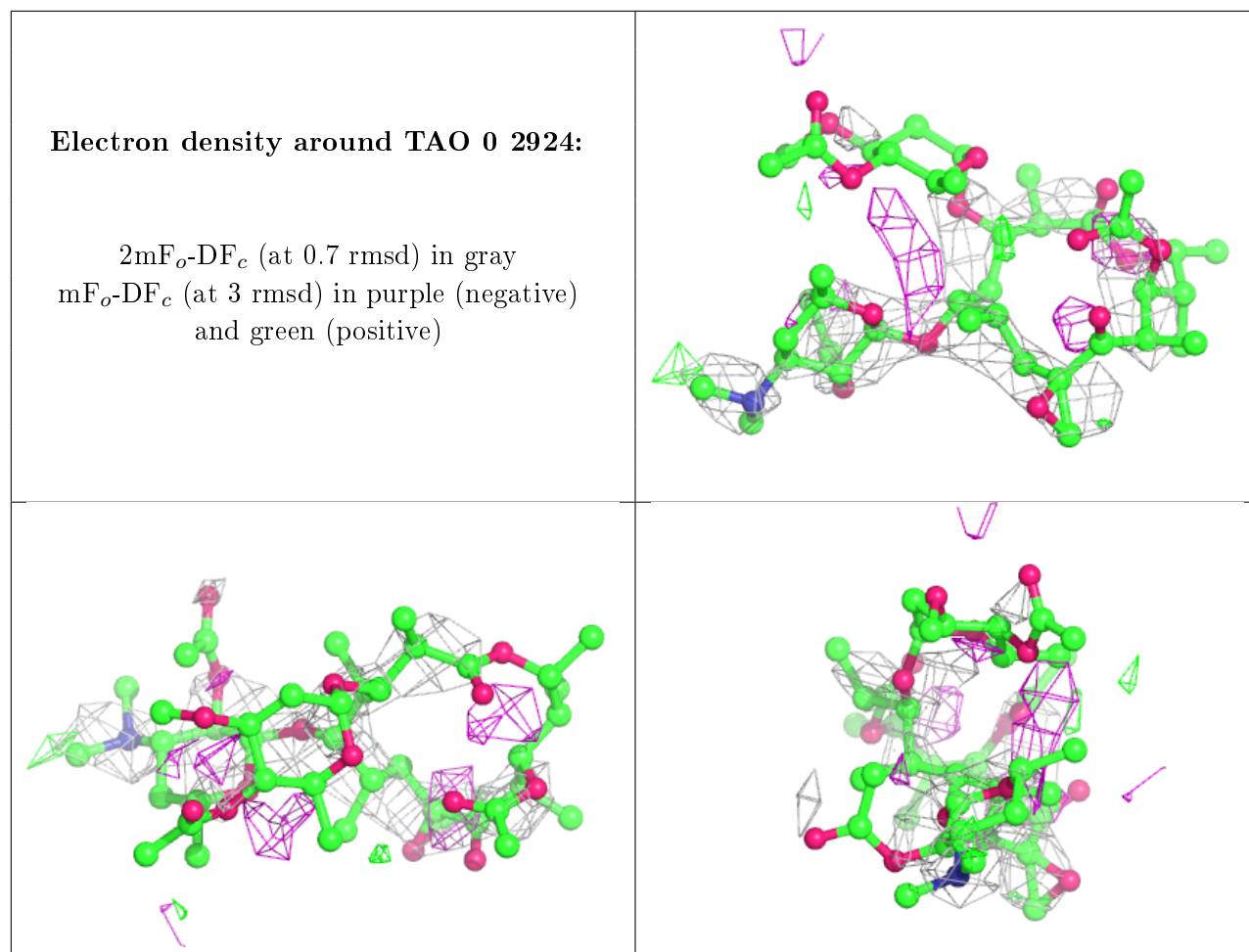
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8007	1/1	0.96	0.17	3,3,3,3	0
35	NA	R	8533	1/1	0.96	0.20	51,51,51,51	0
32	MG	0	8077	1/1	0.96	0.09	36,36,36,36	0
32	MG	0	8041	1/1	0.96	0.24	28,28,28,28	0
32	MG	0	8038	1/1	0.96	0.07	52,52,52,52	0
32	MG	0	8022	1/1	0.96	0.13	20,20,20,20	0
34	SR	0	8985	1/1	0.96	0.14	128,128,128,128	0
32	MG	0	8080	1/1	0.97	0.16	39,39,39,39	0
32	MG	0	8084	1/1	0.97	0.16	37,37,37,37	0
35	NA	0	8527	1/1	0.97	0.21	44,44,44,44	0
35	NA	B	8552	1/1	0.97	0.23	56,56,56,56	0
32	MG	0	8087	1/1	0.97	0.09	14,14,14,14	0
32	MG	0	8024	1/1	0.97	0.27	43,43,43,43	0
34	SR	0	8976	1/1	0.97	0.20	195,195,195,195	0
32	MG	0	8003	1/1	0.97	0.12	16,16,16,16	0
32	MG	0	8025	1/1	0.97	0.10	10,10,10,10	0
32	MG	0	8065	1/1	0.97	0.09	16,16,16,16	0
35	NA	0	8563	1/1	0.97	0.21	61,61,61,61	0
34	SR	0	8975	1/1	0.97	0.06	131,131,131,131	0
33	CL	N	8807	1/1	0.97	0.14	45,45,45,45	0
35	NA	0	8542	1/1	0.97	0.30	36,36,36,36	0
35	NA	0	8504	1/1	0.97	0.13	18,18,18,18	0
35	NA	R	8575	1/1	0.97	0.39	65,65,65,65	0
35	NA	0	8513	1/1	0.97	0.14	34,34,34,34	0
33	CL	R	8806	1/1	0.97	0.07	32,32,32,32	0
32	MG	0	8090	1/1	0.97	0.16	50,50,50,50	0
33	CL	0	8813	1/1	0.98	0.06	43,43,43,43	0
32	MG	0	8014	1/1	0.98	0.12	15,15,15,15	0
32	MG	0	8044	1/1	0.98	0.27	38,38,38,38	0
32	MG	0	8009	1/1	0.98	0.22	15,15,15,15	0
32	MG	0	8070	1/1	0.98	0.18	31,31,31,31	0
33	CL	0	8817	1/1	0.98	0.07	57,57,57,57	0
33	CL	A	8809	1/1	0.98	0.11	86,86,86,86	0
35	NA	0	8514	1/1	0.98	0.40	40,40,40,40	0
33	CL	M	8818	1/1	0.98	0.06	36,36,36,36	0
32	MG	0	8013	1/1	0.98	0.09	11,11,11,11	0
32	MG	0	8017	1/1	0.98	0.07	31,31,31,31	0
33	CL	B	8819	1/1	0.98	0.10	42,42,42,42	0
32	MG	Y	8086	1/1	0.98	0.20	69,69,69,69	0
32	MG	0	8061	1/1	0.98	0.17	23,23,23,23	0
35	NA	0	8523	1/1	0.98	0.29	46,46,46,46	0
36	CD	1	8702	1/1	0.98	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	CL	Q	8811	1/1	0.98	0.04	51,51,51,51	0
36	CD	O	8705	1/1	0.98	0.09	91,91,91,91	0
32	MG	C	8012	1/1	0.98	0.15	10,10,10,10	0
36	CD	U	8701	1/1	0.99	0.11	58,58,58,58	0
35	NA	H	8518	1/1	0.99	0.13	48,48,48,48	0
32	MG	0	8016	1/1	0.99	0.22	2,2,2,2	0
32	MG	0	8076	1/1	0.99	0.05	9,9,9,9	0
32	MG	0	8001	1/1	0.99	0.16	2,2,2,2	0
32	MG	0	8011	1/1	0.99	0.23	1,1,1,1	0
35	NA	2	8515	1/1	0.99	0.09	19,19,19,19	0
32	MG	0	8058	1/1	0.99	0.08	1,1,1,1	0
32	MG	0	8015	1/1	0.99	0.15	5,5,5,5	0
35	NA	C	8554	1/1	0.99	0.51	52,52,52,52	0
32	MG	0	8048	1/1	0.99	0.27	44,44,44,44	0
32	MG	0	8010	1/1	0.99	0.29	3,3,3,3	0
35	NA	0	8517	1/1	0.99	0.15	14,14,14,14	0
36	CD	3	8704	1/1	0.99	0.10	56,56,56,56	0
36	CD	Z	8703	1/1	1.00	0.12	55,55,55,55	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.