



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:00 am BST

PDB ID : 6CAR  
Title : Serial Femtosecond X-ray Crystal Structure of 30S ribosomal subunit from  
Thermus thermophilus in complex with Sisomicin  
Authors : DeMirci, H.  
Deposited on : 2018-01-31  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.11  
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) : 2.11

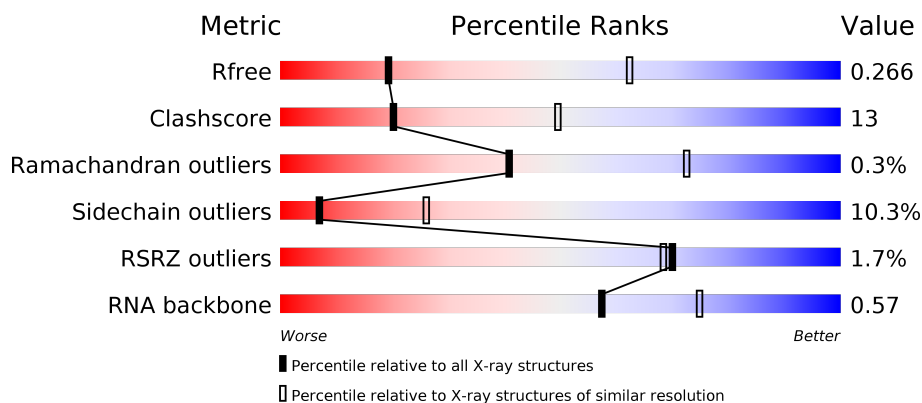
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1517	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>44%</div> <div>11%</div> <div>.</div> </div> </div>
2	B	255	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>6%</div> <div>8%</div> </div> </div>
3	C	238	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>.</div> <div>13%</div> </div> </div>
4	D	208	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	104	
11	K	128	
12	L	131	
13	M	125	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	87	
19	S	92	
20	T	105	
21	U	26	
22	Y	6	
23	W	15	

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
24	MG	A	1602	-	-	-	X
24	MG	A	1626	-	-	-	X
24	MG	A	1656	-	-	-	X
24	MG	A	1658	-	-	-	X
24	MG	A	1677	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1678	-	-	-	X
24	MG	A	1685	-	-	-	X
24	MG	A	1693	-	-	-	X
24	MG	A	1694	-	-	-	X
24	MG	A	1700	-	-	-	X
24	MG	A	1701	-	-	-	X
24	MG	A	1710	-	-	-	X
24	MG	A	1756	-	-	-	X
24	MG	A	1775	-	-	-	X
24	MG	A	1780	-	-	-	X
24	MG	A	1789	-	-	-	X
24	MG	A	1790	-	-	-	X
24	MG	A	1840	-	-	-	X
24	MG	A	1848	-	-	-	X
24	MG	A	1858	-	-	-	X
24	MG	C	302	-	-	-	X

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52778 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 16S Ribosomal RNA rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1511	Total	C	N	O	P	0	6	0
			32624	14531	6037	10539	1517			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	conflict	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP P0DOY7

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called RNA (5'-R(\*UP\*UP\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 23 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*AP\*UP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	3	Total	Mg	0	0
			3	3		
24	J	1	Total	Mg	0	0
			1	1		
24	Q	1	Total	Mg	0	0
			1	1		
24	D	3	Total	Mg	0	0
			3	3		
24	K	2	Total	Mg	0	0
			2	2		
24	E	1	Total	Mg	0	0
			1	1		

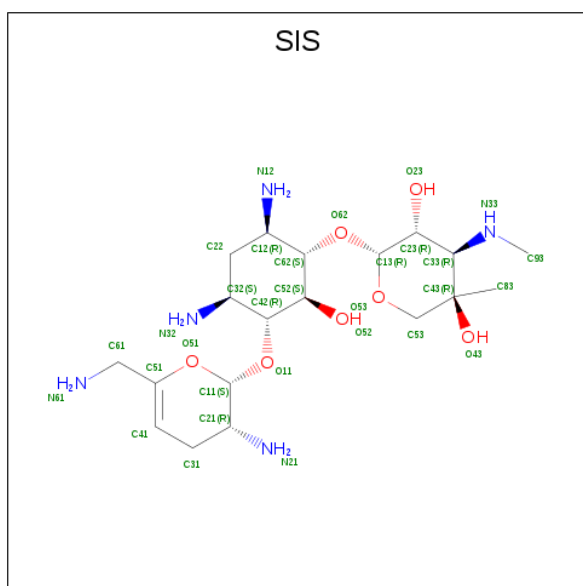
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	2	Total	Mg	0	0
			2	2		
24	I	1	Total	Mg	0	0
			1	1		
24	C	6	Total	Mg	0	0
			6	6		
24	A	258	Total	Mg	0	0
			258	258		
24	L	3	Total	Mg	0	0
			3	3		
24	S	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		

- Molecule 25 is (1S,2S,3R,4S,6R)-4,6-diamino-3-{[(2S,3R)-3-amino-6-(aminomethyl)-3,4-dihydro-2H-pyran-2-yl]oxy}-2-hydroxycyclohexyl 3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranoside (three-letter code: SIS) (formula: C<sub>19</sub>H<sub>37</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total Zn 1 1	0	0
26	N	1	Total Zn 1 1	0	0

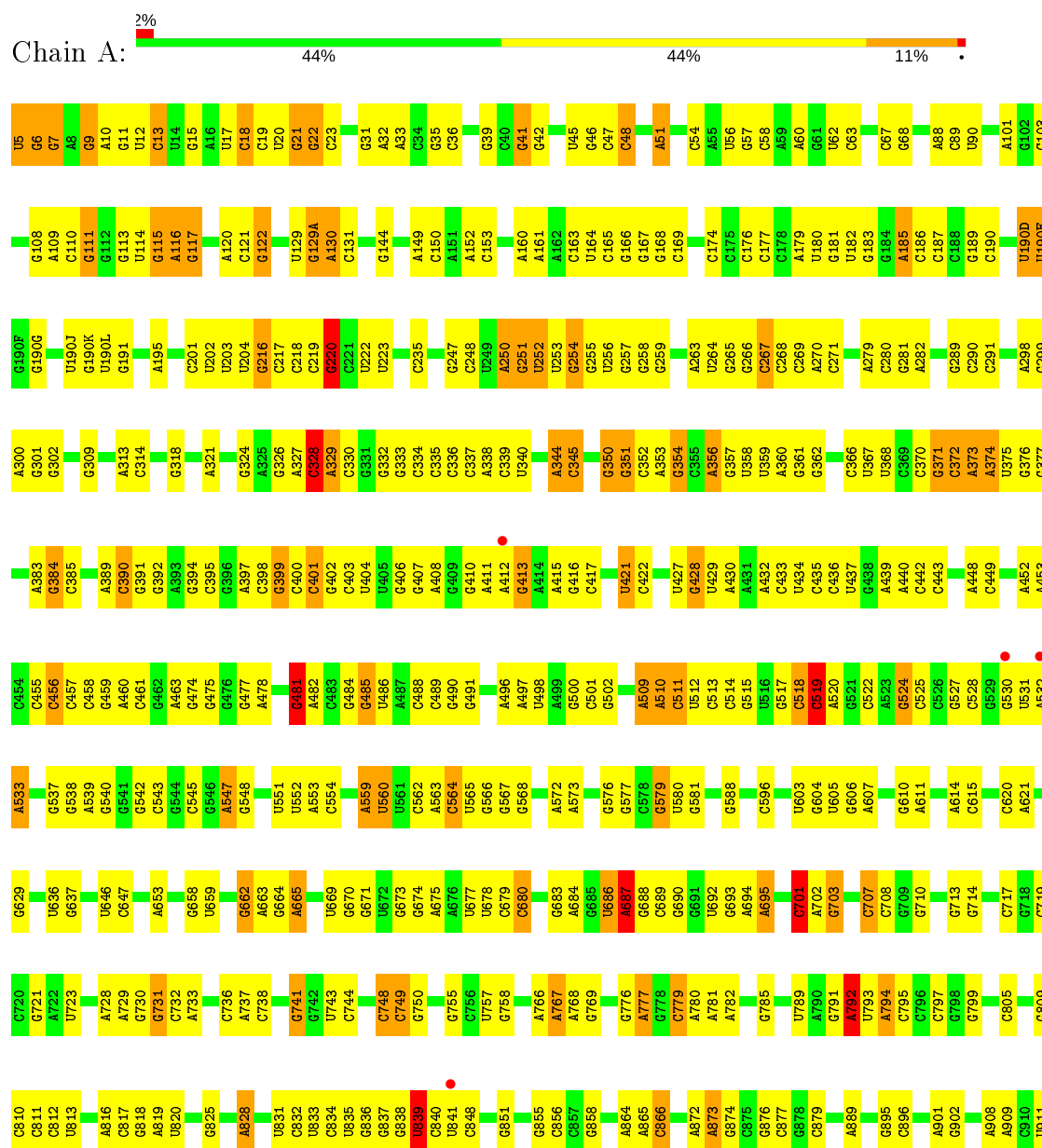
- Molecule 27 is water.

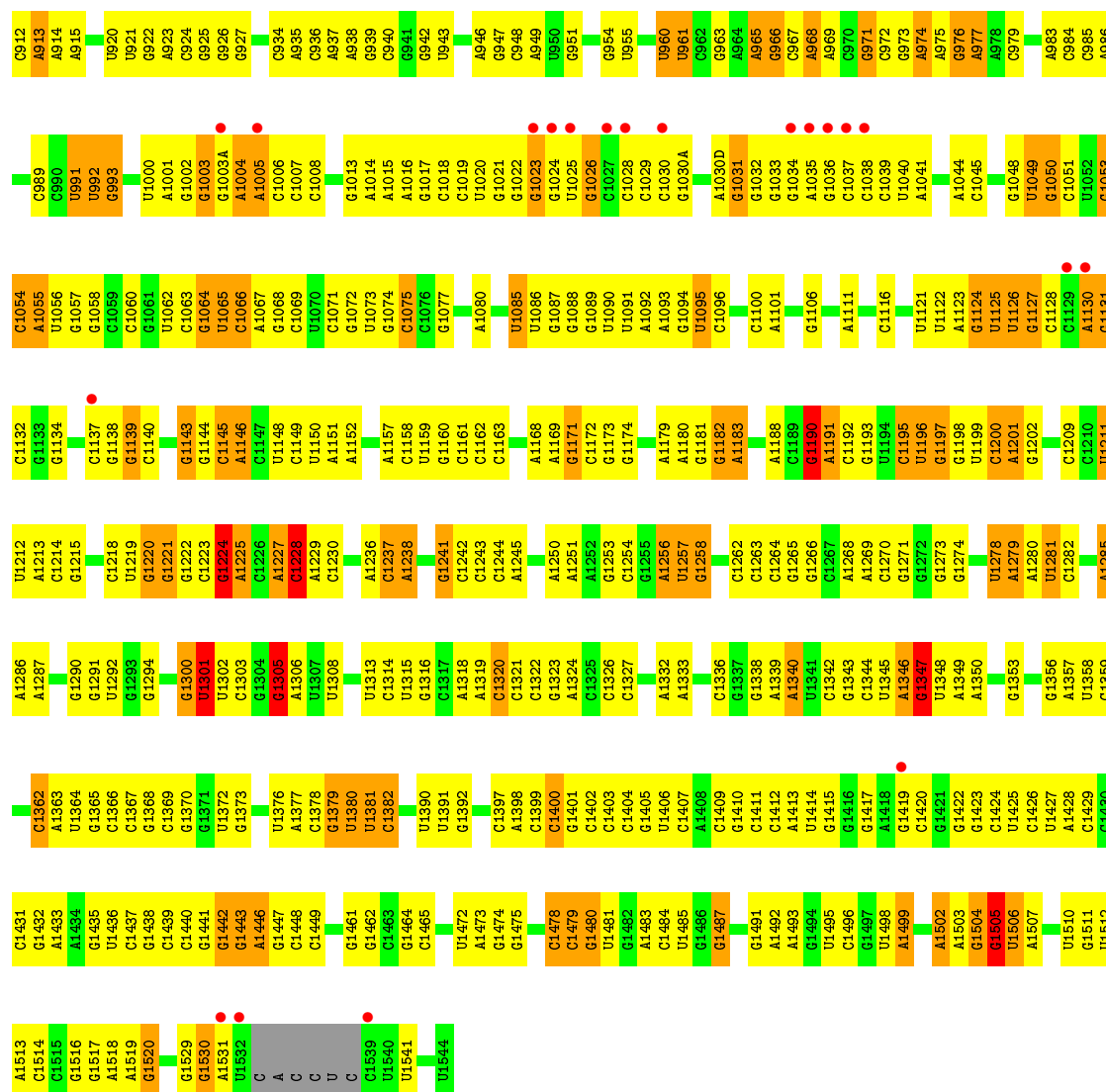
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	299	Total O 299 299	0	0
27	C	1	Total O 1 1	0	0
27	D	3	Total O 3 3	0	0
27	E	3	Total O 3 3	0	0
27	L	4	Total O 4 4	0	0
27	N	1	Total O 1 1	0	0
27	Q	1	Total O 1 1	0	0
27	T	2	Total O 2 2	0	0

### 3 Residue-property plots

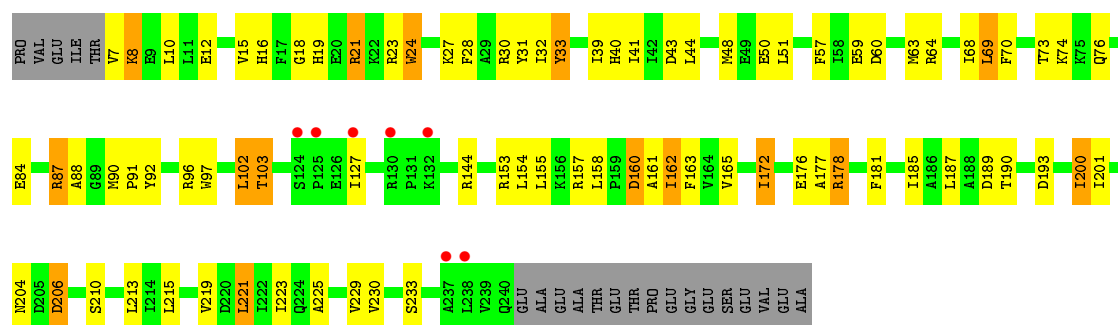
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S Ribosomal RNA rRNA



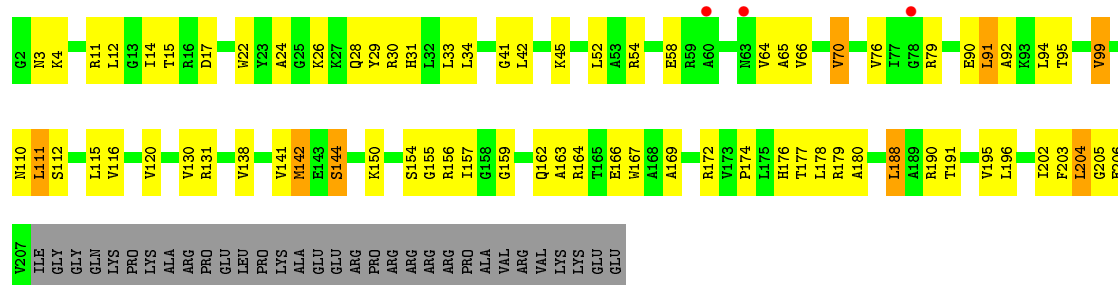


• Molecule 2: 30S ribosomal protein S2

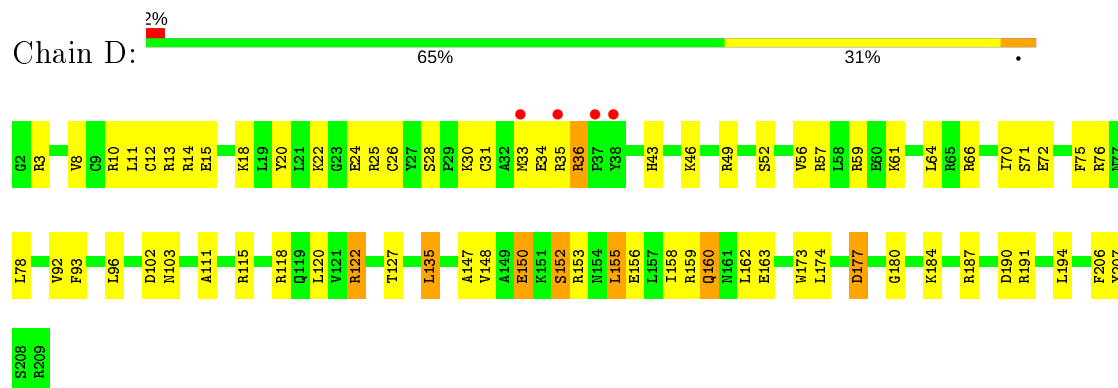


• Molecule 3: 30S ribosomal protein S3

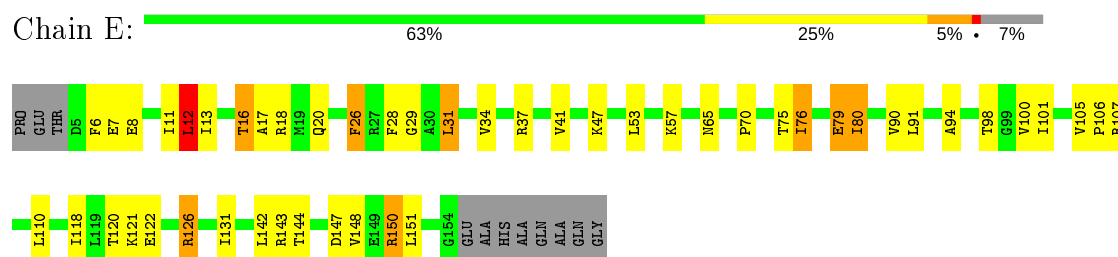




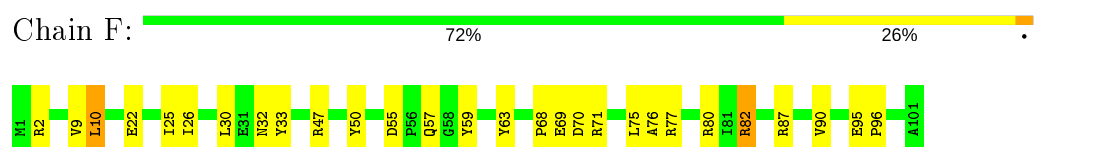
• Molecule 4: 30S ribosomal protein S4



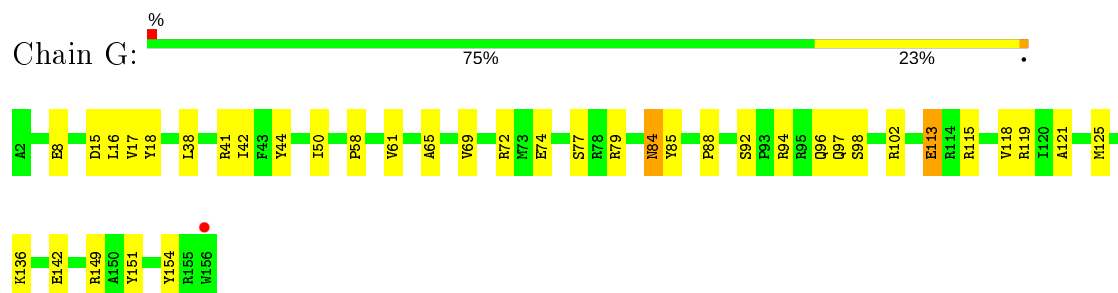
• Molecule 5: 30S ribosomal protein S5



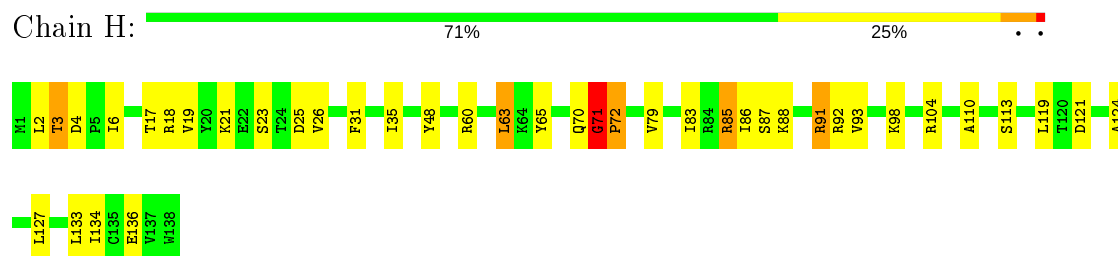
• Molecule 6: 30S ribosomal protein S6



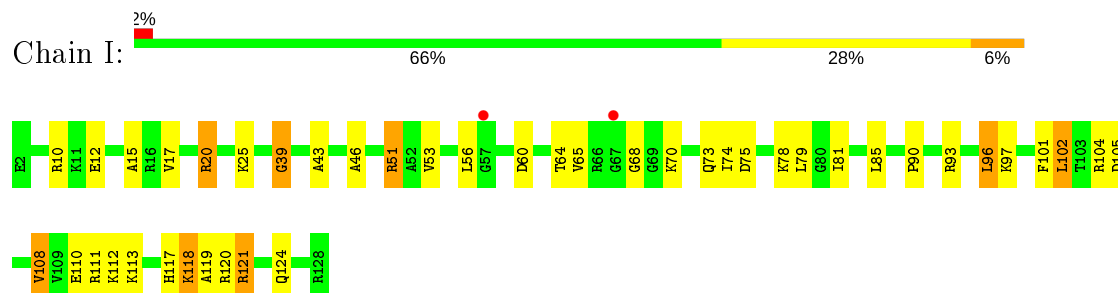
• Molecule 7: 30S ribosomal protein S7



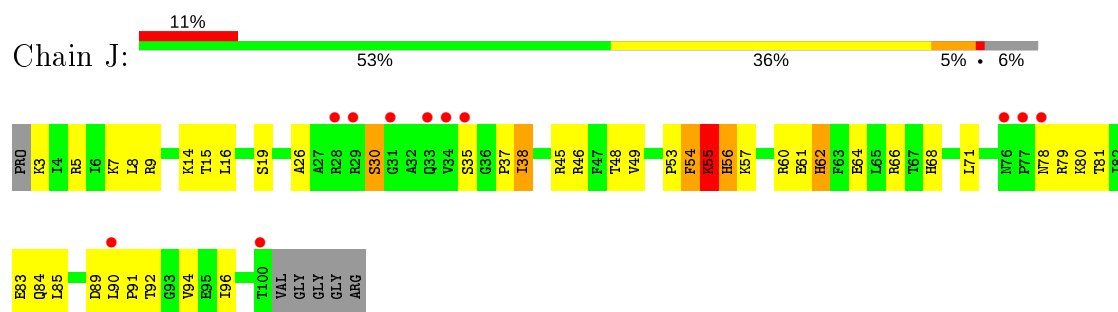
- Molecule 8: 30S ribosomal protein S8



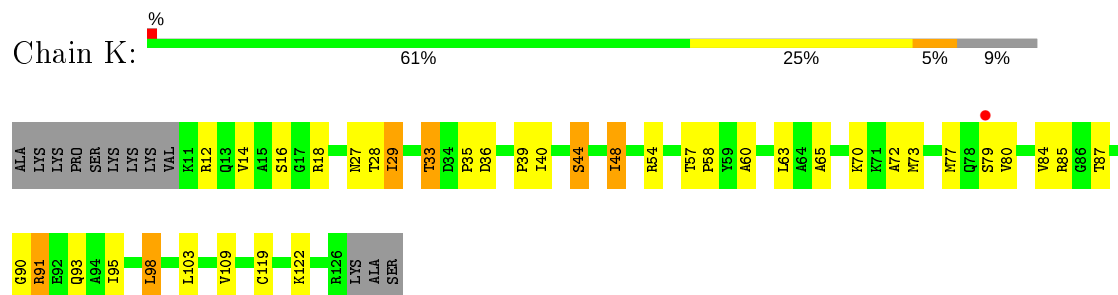
- Molecule 9: 30S ribosomal protein S9



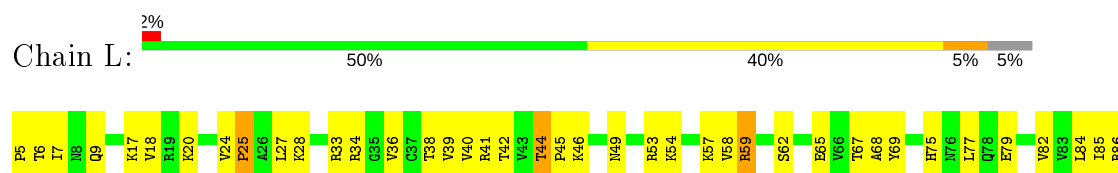
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12





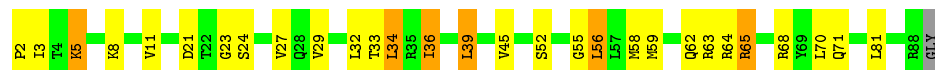
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



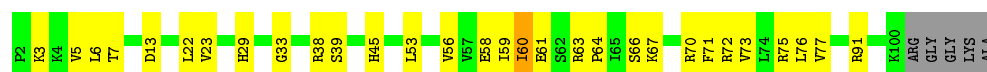
- Molecule 15: 30S ribosomal protein S15



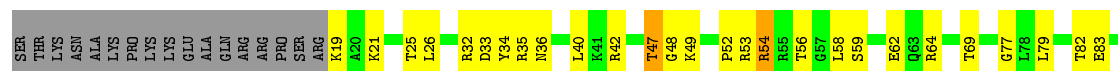
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

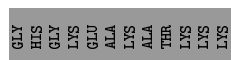
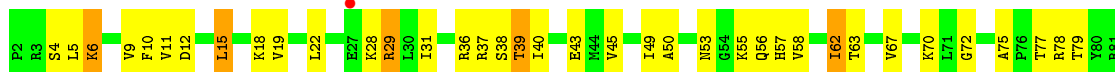


- Molecule 18: 30S ribosomal protein S18

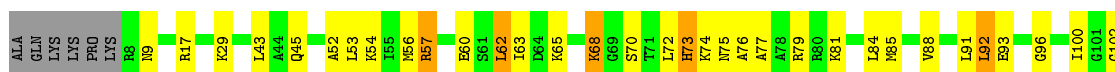




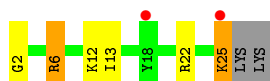
- Molecule 19: 30S ribosomal protein S19



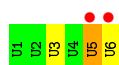
- Molecule 20: 30S ribosomal protein S20



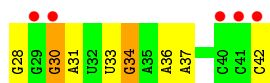
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-R(\*UP\*UP\*UP\*UP\*UP\*U)-3')



- Molecule 23: RNA (5'-R(\*GP\*GP\*GP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*AP\*UP\*CP\*CP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.60 Å   402.60 Å   175.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.26 – 3.40 39.26 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.26-3.40) 99.9 (39.26-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.222   ,   0.266 0.222   ,   0.266	Depositor DCC
$R_{free}$ test set	999 reflections (0.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 95.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	52778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIS, ZN, MA6, G7M, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 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	0.55	0/36117	1.13	125/56362 (0.2%)
2	B	0.33	0/1935	0.50	0/2609
3	C	0.32	0/1636	0.51	0/2205
4	D	0.33	0/1733	0.50	0/2318
5	E	0.37	0/1162	0.58	1/1564 (0.1%)
6	F	0.32	0/856	0.51	0/1154
7	G	0.34	0/1276	0.49	0/1709
8	H	0.39	0/1136	0.59	0/1527
9	I	0.32	0/1029	0.53	1/1379 (0.1%)
10	J	0.31	0/805	0.57	0/1082
11	K	0.33	0/879	0.55	0/1187
12	L	0.35	0/977	0.56	0/1306
13	M	0.32	0/947	0.51	0/1270
14	N	0.39	0/501	0.51	0/664
15	O	0.36	0/740	0.54	0/987
16	P	0.36	0/716	0.56	0/963
17	Q	0.38	0/836	0.58	0/1117
18	R	0.33	0/579	0.54	0/768
19	S	0.29	0/661	0.53	0/890
20	T	0.35	0/765	0.52	0/1007
21	U	0.30	0/212	0.46	0/277
22	Y	0.41	0/128	1.23	0/196
23	W	0.49	0/357	1.12	0/555
All	All	0.49	0/55983	0.99	127/83096 (0.2%)

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
3	C	0	1
8	H	0	1
10	J	0	2
12	L	0	1
13	M	0	2
All	All	0	7

There are no bond length outliers.

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	G	O5'-P-OP1	-9.09	97.52	105.70
1	A	1422	G	N3-C2-N2	-8.14	114.20	119.90
1	A	1143	G	N3-C2-N2	-8.08	114.24	119.90
1	A	792	A	P-O3'-C3'	7.91	129.19	119.70
1	A	1502	A	N1-C6-N6	7.84	123.31	118.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	71	GLY	Peptide
10	J	54	PHE	Peptide
10	J	55	LYS	Peptide
12	L	25	PRO	Peptide

## 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	32624	0	16496	664	0
2	B	1900	0	1951	49	0
3	C	1612	0	1677	46	0
4	D	1703	0	1763	48	0
5	E	1146	0	1207	36	0
6	F	843	0	857	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1257	0	1296	23	0
8	H	1116	0	1177	23	0
9	I	1010	0	1037	35	0
10	J	792	0	835	37	0
11	K	864	0	881	22	0
12	L	972	0	1058	39	0
13	M	937	0	995	27	0
14	N	492	0	529	24	0
15	O	729	0	768	15	0
16	P	700	0	720	16	0
17	Q	823	0	893	20	0
18	R	574	0	644	20	0
19	S	647	0	673	32	0
20	T	763	0	861	20	0
21	U	208	0	221	7	0
22	Y	117	0	62	3	0
23	W	319	0	164	6	0
24	A	258	0	0	0	0
24	B	2	0	0	0	0
24	C	6	0	0	0	0
24	D	3	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	I	1	0	0	0	0
24	J	1	0	0	0	0
24	K	2	0	0	0	0
24	L	3	0	0	0	0
24	P	3	0	0	0	0
24	Q	1	0	0	0	0
24	S	1	0	0	0	0
25	A	31	0	37	5	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	299	0	0	6	0
27	C	1	0	0	0	0
27	D	3	0	0	0	0
27	E	3	0	0	0	0
27	L	4	0	0	1	0
27	N	1	0	0	0	0
27	Q	1	0	0	0	0
27	T	2	0	0	0	0
All	All	52778	0	36802	1102	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 13.

The worst 5 of 1102 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:A:955:U:H1'	1:A:1227:A:H61	1.31	0.94
1:A:481:G:HO2'	1:A:482:A:H8	1.00	0.94
1:A:664:G:H22	1:A:741:G:H1	1.13	0.91
1:A:407:G:OP1	4:D:115:ARG:NH1	2.06	0.89
20:T:100:ILE:HG22	20:T:102:GLY:H	1.39	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/255 (91%)	214 (92%)	17 (7%)	1 (0%)	34	67
3	C	204/238 (86%)	180 (88%)	24 (12%)	0	100	100
4	D	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	148/161 (92%)	142 (96%)	6 (4%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/155 (99%)	147 (96%)	6 (4%)	0	100	100
8	H	136/138 (99%)	128 (94%)	6 (4%)	2 (2%)	10	36
9	I	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
10	J	96/104 (92%)	81 (84%)	13 (14%)	2 (2%)	7	30
11	K	114/128 (89%)	106 (93%)	8 (7%)	0	100	100
12	L	121/131 (92%)	111 (92%)	10 (8%)	0	100	100
13	M	116/125 (93%)	103 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	O	85/88 (97%)	82 (96%)	3 (4%)	0	100	100
16	P	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/104 (93%)	91 (94%)	6 (6%)	0	100	100
18	R	68/87 (78%)	65 (96%)	3 (4%)	0	100	100
19	S	78/92 (85%)	72 (92%)	6 (8%)	0	100	100
20	T	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	15	46
21	U	22/26 (85%)	22 (100%)	0	0	100	100
All	All	2336/2521 (93%)	2153 (92%)	177 (8%)	6 (0%)	41	72

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
10	J	56	HIS
8	H	71	GLY
8	H	72	PRO
20	T	73	HIS

### 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	
2	B	202/219 (92%)	172 (85%)	30 (15%)	3	12
3	C	160/187 (86%)	136 (85%)	24 (15%)	3	12
4	D	180/180 (100%)	168 (93%)	12 (7%)	16	46
5	E	115/122 (94%)	102 (89%)	13 (11%)	6	21
6	F	90/90 (100%)	86 (96%)	4 (4%)	28	58
7	G	126/126 (100%)	120 (95%)	6 (5%)	25	56
8	H	119/119 (100%)	106 (89%)	13 (11%)	6	23
9	I	98/98 (100%)	88 (90%)	10 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	87/91 (96%)	80 (92%)	7 (8%)	12	38
11	K	88/98 (90%)	77 (88%)	11 (12%)	4	17
12	L	103/107 (96%)	89 (86%)	14 (14%)	3	14
13	M	94/100 (94%)	83 (88%)	11 (12%)	5	20
14	N	49/49 (100%)	47 (96%)	2 (4%)	30	59
15	O	79/79 (100%)	66 (84%)	13 (16%)	2	9
16	P	72/74 (97%)	66 (92%)	6 (8%)	11	36
17	Q	94/96 (98%)	89 (95%)	5 (5%)	22	52
18	R	61/76 (80%)	57 (93%)	4 (7%)	16	46
19	S	71/79 (90%)	64 (90%)	7 (10%)	8	27
20	T	76/81 (94%)	66 (87%)	10 (13%)	4	15
21	U	19/21 (90%)	17 (90%)	2 (10%)	7	25
All	All	1983/2092 (95%)	1779 (90%)	204 (10%)	7	26

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	26	VAL
10	J	38	ILE
19	S	39	THR
8	H	83	ILE
9	I	51	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
9	I	3	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1517 (99%)	247 (16%)	45 (2%)
22	Y	5/6 (83%)	2 (40%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1522/1538 (98%)	253 (16%)	45 (2%)

5 of 253 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	13	C
1	A	39	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	748	C
1	A	965	A
1	A	1346	A
1	A	812	C
1	A	992	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MA6	A	1518[A]	1	19,26,27	0.79	0	18,38,41	0.76	0
1	5MC	A	967	1	15,22,23	0.97	0	19,32,35	1.09	2 (10%)
1	MA6	A	1518[B]	1	19,26,27	1.30	2 (10%)	18,38,41	0.69	0
1	PSU	A	516	1,24	17,21,22	1.03	1 (5%)	20,30,33	3.13	6 (30%)
1	4OC	A	1402	1	16,23,24	1.01	2 (12%)	17,32,35	0.65	0
1	2MG	A	1207	1	19,26,27	2.22	4 (21%)	21,38,41	2.02	3 (14%)
1	G7M	A	527	1	20,26,27	1.75	3 (15%)	20,39,42	1.93	5 (25%)
1	5MC	A	1400	1	15,22,23	0.94	0	19,32,35	1.00	1 (5%)
1	5MC	A	1404	1	15,22,23	0.89	0	19,32,35	1.00	1 (5%)
1	PSU	A	1541	1	17,21,22	1.11	1 (5%)	20,30,33	3.49	6 (30%)
1	MA6	A	1519[B]	1	19,26,27	1.29	3 (15%)	18,38,41	0.59	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1407	1	15,22,23	0.96	0	19,32,35	1.07	1 (5%)
12	0TD	L	92	12	4,9,10	1.43	1 (25%)	3,11,13	1.85	1 (33%)
1	MA6	A	1519[A]	1	19,26,27	1.18	2 (10%)	18,38,41	0.64	0
1	UR3	A	1498	1	14,22,23	0.82	1 (7%)	15,32,35	1.11	1 (6%)
1	M2G	A	966	1	20,27,28	2.17	5 (25%)	22,40,43	2.42	3 (13%)
1	PSU	A	1540	1	17,21,22	1.06	1 (5%)	20,30,33	3.11	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518[A]	1	-	3/7/29/30	0/3/3/3
1	5MC	A	967	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	1/7/29/30	0/3/3/3
1	PSU	A	516	1,24	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	G7M	A	527	1	-	2/3/25/26	0/3/3/3
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-
1	MA6	A	1519[A]	1	-	3/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	6.58	1.39	1.34
1	A	966	M2G	C6-N1	6.48	1.44	1.33
1	A	1207	2MG	C6-N1	5.94	1.43	1.33
1	A	527	G7M	C2-N2	5.83	1.45	1.33
1	A	966	M2G	C2-N1	4.30	1.42	1.34

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N1-C2-N3	-12.44	118.54	128.43
1	A	1540	PSU	N1-C2-N3	-10.73	119.90	128.43
1	A	516	PSU	N1-C2-N3	-10.57	120.03	128.43
1	A	966	M2G	C5-C6-N1	-8.46	111.86	123.43
1	A	1207	2MG	C5-C6-N1	-7.37	113.36	123.43

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
12	L	92	0TD	CG-CB-SB-CSB
1	A	966	M2G	C4'-C5'-O5'-P
1	A	967	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1518[A]	MA6	1	0
1	A	967	5MC	2	0
1	A	1518[B]	MA6	3	0
1	A	1402	4OC	2	0
1	A	527	G7M	1	0
1	A	1400	5MC	2	0
1	A	1404	5MC	1	0
1	A	1541	PSU	1	0
1	A	1519[B]	MA6	3	0
1	A	1407	5MC	2	0
12	L	92	0TD	3	0
1	A	1519[A]	MA6	2	0
1	A	1498	UR3	1	0
1	A	966	M2G	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 286 ligands modelled in this entry, 285 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$
25	SIS	A	1809	-	28,33,33	1.34	2 (7%)	28,49,49	1.30	2 (7%)

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
25	SIS	A	1809	-	-	2/9/65/65	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1809	SIS	C31-C41	-4.72	1.40	1.50
25	A	1809	SIS	C61-C51	-3.70	1.40	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1809	SIS	C93-N33-C33	-4.70	107.54	114.38
25	A	1809	SIS	C13-O62-C62	-2.09	112.80	117.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

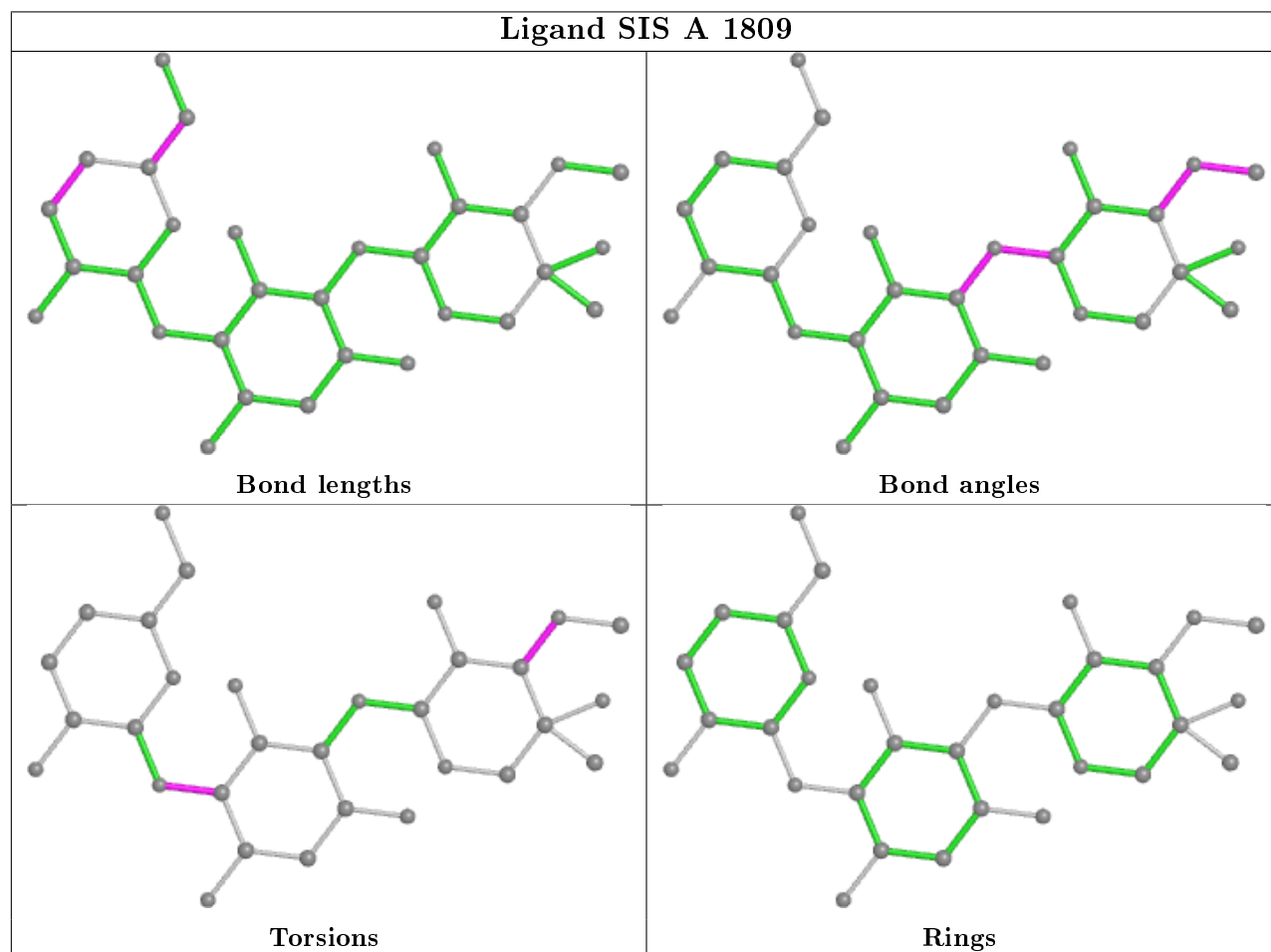
Mol	Chain	Res	Type	Atoms
25	A	1809	SIS	C23-C33-N33-C93
25	A	1809	SIS	C52-C42-O11-C11

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1809	SIS	5	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1497/1517 (98%)	0.18	24 (1%) 72 70	46, 82, 168, 310	0
2	B	234/255 (91%)	0.01	7 (2%) 50 49	68, 109, 179, 214	0
3	C	206/238 (86%)	0.09	3 (1%) 73 72	83, 128, 176, 190	0
4	D	208/208 (100%)	-0.19	4 (1%) 66 65	55, 98, 149, 205	0
5	E	150/161 (93%)	-0.30	0 100 100	40, 67, 101, 166	0
6	F	101/101 (100%)	-0.18	0 100 100	61, 94, 140, 175	0
7	G	155/155 (100%)	-0.15	1 (0%) 89 89	67, 97, 166, 204	0
8	H	138/138 (100%)	-0.47	0 100 100	37, 56, 85, 132	0
9	I	127/127 (100%)	0.07	2 (1%) 72 70	79, 121, 162, 195	0
10	J	98/104 (94%)	0.72	11 (11%) 5 6	88, 158, 233, 294	0
11	K	116/128 (90%)	-0.17	1 (0%) 84 83	56, 76, 110, 157	0
12	L	123/131 (93%)	-0.20	2 (1%) 72 70	46, 84, 135, 190	0
13	M	118/125 (94%)	-0.15	1 (0%) 86 85	74, 101, 147, 226	0
14	N	60/60 (100%)	-0.19	0 100 100	86, 111, 151, 202	0
15	O	87/88 (98%)	-0.27	0 100 100	44, 76, 119, 160	0
16	P	83/88 (94%)	-0.25	1 (1%) 79 77	56, 77, 111, 190	0
17	Q	99/104 (95%)	-0.28	0 100 100	43, 62, 98, 140	0
18	R	70/87 (80%)	-0.19	0 100 100	50, 81, 135, 168	0
19	S	80/92 (86%)	0.29	1 (1%) 77 76	94, 128, 185, 245	0
20	T	99/105 (94%)	-0.30	1 (1%) 82 81	56, 79, 134, 181	0
21	U	24/26 (92%)	0.41	2 (8%) 11 13	91, 123, 151, 154	0
22	Y	6/6 (100%)	1.62	2 (33%) 0 0	103, 112, 178, 209	0
23	W	15/15 (100%)	1.63	5 (33%) 0 0	89, 126, 196, 199	0
All	All	3894/4059 (95%)	0.01	68 (1%) 70 68	37, 89, 169, 310	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	10.6
10	J	33	GLN	7.4
12	L	128	ALA	5.8
10	J	100	THR	5.4
10	J	90	LEU	4.6

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1540	20/21	0.81	0.51	217,234,249,254	0
1	MA6	A	1518[B]	24/25	0.93	0.26	59,61,62,62	24
1	PSU	A	516	20/21	0.93	0.18	101,114,117,118	0
1	PSU	A	1541	20/21	0.93	0.33	218,237,269,281	0
1	MA6	A	1518[A]	24/25	0.93	0.26	60,62,62,62	24
1	2MG	A	1207	24/25	0.94	0.15	103,112,118,122	0
1	5MC	A	1407	21/22	0.95	0.23	64,67,69,73	0
1	MA6	A	1519[A]	24/25	0.95	0.25	58,59,60,60	24
1	M2G	A	966	25/26	0.95	0.19	72,88,97,99	0
1	MA6	A	1519[B]	24/25	0.95	0.25	57,59,60,60	24
12	0TD	L	92	10/11	0.96	0.19	74,79,85,86	0
1	4OC	A	1402	22/23	0.96	0.21	63,67,78,82	0
1	G7M	A	527	24/25	0.96	0.20	60,73,83,89	0
1	5MC	A	1404	21/22	0.96	0.20	59,60,63,73	0
1	UR3	A	1498	21/22	0.97	0.21	59,62,65,78	0
1	5MC	A	967	21/22	0.97	0.15	74,79,84,87	0
1	5MC	A	1400	21/22	0.97	0.17	58,66,88,93	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1710	1/1	0.33	0.85	255,255,255,255	0
24	MG	A	1700	1/1	0.36	1.29	261,261,261,261	0
24	MG	A	1602	1/1	0.43	1.26	201,201,201,201	0
24	MG	A	1790	1/1	0.48	0.43	189,189,189,189	0
24	MG	A	1619	1/1	0.55	0.30	71,71,71,71	0
24	MG	A	1789	1/1	0.57	0.78	247,247,247,247	0
24	MG	A	1685	1/1	0.61	0.62	82,82,82,82	0
24	MG	A	1678	1/1	0.61	0.81	78,78,78,78	0
24	MG	A	1693	1/1	0.62	0.60	91,91,91,91	0
24	MG	C	303	1/1	0.63	0.25	137,137,137,137	0
24	MG	A	1758	1/1	0.63	0.28	115,115,115,115	0
24	MG	A	1846	1/1	0.64	0.22	76,76,76,76	0
24	MG	A	1677	1/1	0.64	0.77	76,76,76,76	0
24	MG	A	1734	1/1	0.67	0.27	66,66,66,66	0
24	MG	A	1701	1/1	0.68	0.42	145,145,145,145	0
24	MG	A	1810	1/1	0.69	0.22	122,122,122,122	0
24	MG	A	1694	1/1	0.69	0.41	71,71,71,71	0
24	MG	A	1756	1/1	0.71	0.97	74,74,74,74	0
24	MG	A	1848	1/1	0.72	0.41	79,79,79,79	0
24	MG	A	1656	1/1	0.72	0.63	37,37,37,37	0
24	MG	A	1834	1/1	0.73	0.18	96,96,96,96	0
24	MG	A	1717	1/1	0.74	0.15	161,161,161,161	0
24	MG	A	1856	1/1	0.74	0.27	58,58,58,58	0
24	MG	L	201	1/1	0.74	0.32	83,83,83,83	0
24	MG	A	1858	1/1	0.74	0.85	66,66,66,66	0
24	MG	A	1775	1/1	0.74	0.57	81,81,81,81	0
24	MG	A	1841	1/1	0.74	0.37	58,58,58,58	0
24	MG	C	302	1/1	0.75	0.46	69,69,69,69	0
24	MG	A	1818	1/1	0.75	0.20	101,101,101,101	0
24	MG	E	201	1/1	0.75	0.36	70,70,70,70	0
24	MG	A	1692	1/1	0.76	0.32	184,184,184,184	0
24	MG	A	1624	1/1	0.76	0.39	56,56,56,56	0
24	MG	A	1658	1/1	0.77	0.52	94,94,94,94	0
24	MG	A	1712	1/1	0.77	0.39	67,67,67,67	0
24	MG	A	1722	1/1	0.78	0.35	59,59,59,59	0
24	MG	A	1703	1/1	0.78	0.38	214,214,214,214	0
24	MG	A	1612	1/1	0.78	0.28	182,182,182,182	0
24	MG	A	1626	1/1	0.78	0.49	48,48,48,48	0
24	MG	A	1780	1/1	0.78	0.56	67,67,67,67	0
24	MG	A	1755	1/1	0.78	0.39	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1800	1/1	0.79	0.38	99,99,99,99	0
24	MG	P	102	1/1	0.79	0.21	93,93,93,93	0
24	MG	A	1840	1/1	0.79	0.43	52,52,52,52	0
24	MG	A	1652	1/1	0.79	0.38	52,52,52,52	0
24	MG	A	1672	1/1	0.80	0.24	65,65,65,65	0
24	MG	A	1715	1/1	0.80	0.29	75,75,75,75	0
24	MG	Q	201	1/1	0.81	0.15	50,50,50,50	0
24	MG	A	1696	1/1	0.81	0.37	112,112,112,112	0
24	MG	I	301	1/1	0.81	0.17	89,89,89,89	0
24	MG	A	1617	1/1	0.81	0.43	179,179,179,179	0
24	MG	A	1857	1/1	0.81	0.32	103,103,103,103	0
24	MG	A	1659	1/1	0.81	0.42	135,135,135,135	0
24	MG	A	1682	1/1	0.81	0.12	53,53,53,53	0
24	MG	A	1728	1/1	0.81	0.52	78,78,78,78	0
24	MG	A	1799	1/1	0.81	0.43	51,51,51,51	0
24	MG	A	1632	1/1	0.82	0.72	180,180,180,180	0
24	MG	C	301	1/1	0.82	0.20	44,44,44,44	0
24	MG	A	1779	1/1	0.82	0.35	54,54,54,54	0
24	MG	A	1774	1/1	0.82	0.14	51,51,51,51	0
24	MG	A	1808	1/1	0.82	0.37	76,76,76,76	0
24	MG	A	1845	1/1	0.82	0.62	110,110,110,110	0
24	MG	A	1680	1/1	0.82	0.25	92,92,92,92	0
24	MG	A	1671	1/1	0.82	0.19	76,76,76,76	0
24	MG	A	1731	1/1	0.83	0.37	112,112,112,112	0
24	MG	A	1765	1/1	0.83	0.32	89,89,89,89	0
24	MG	A	1805	1/1	0.83	0.27	73,73,73,73	0
24	MG	A	1665	1/1	0.83	0.31	68,68,68,68	0
24	MG	A	1816	1/1	0.84	0.14	77,77,77,77	0
24	MG	A	1767	1/1	0.84	0.46	63,63,63,63	0
24	MG	A	1660	1/1	0.84	0.18	124,124,124,124	0
24	MG	A	1705	1/1	0.84	0.42	62,62,62,62	0
24	MG	A	1827	1/1	0.85	0.28	140,140,140,140	0
24	MG	A	1666	1/1	0.85	0.17	41,41,41,41	0
24	MG	A	1613	1/1	0.85	0.23	118,118,118,118	0
24	MG	A	1642	1/1	0.85	0.42	51,51,51,51	0
24	MG	A	1753	1/1	0.85	0.45	73,73,73,73	0
24	MG	A	1720	1/1	0.85	0.28	43,43,43,43	0
24	MG	A	1601	1/1	0.85	0.34	70,70,70,70	0
24	MG	A	1854	1/1	0.85	0.40	65,65,65,65	0
24	MG	A	1823	1/1	0.86	0.12	101,101,101,101	0
24	MG	A	1807	1/1	0.86	0.23	47,47,47,47	0
24	MG	A	1675	1/1	0.86	0.09	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1768	1/1	0.86	0.19	43,43,43,43	0
24	MG	A	1781	1/1	0.86	0.19	74,74,74,74	0
24	MG	A	1684	1/1	0.86	0.11	66,66,66,66	0
24	MG	A	1689	1/1	0.86	0.18	105,105,105,105	0
24	MG	A	1802	1/1	0.86	0.24	67,67,67,67	0
24	MG	A	1627	1/1	0.86	0.24	111,111,111,111	0
24	MG	L	202	1/1	0.86	0.14	67,67,67,67	0
24	MG	A	1773	1/1	0.86	0.38	64,64,64,64	0
24	MG	A	1713	1/1	0.86	0.25	53,53,53,53	0
24	MG	A	1674	1/1	0.86	0.24	45,45,45,45	0
24	MG	A	1826	1/1	0.87	0.32	110,110,110,110	0
24	MG	A	1721	1/1	0.87	0.26	59,59,59,59	0
24	MG	K	201	1/1	0.87	0.19	36,36,36,36	0
24	MG	A	1702	1/1	0.87	0.29	252,252,252,252	0
24	MG	A	1716	1/1	0.87	0.48	61,61,61,61	0
24	MG	A	1736	1/1	0.87	0.06	81,81,81,81	0
24	MG	A	1838	1/1	0.87	0.21	39,39,39,39	0
24	MG	K	202	1/1	0.87	0.10	72,72,72,72	0
24	MG	A	1825	1/1	0.88	0.12	86,86,86,86	0
24	MG	S	101	1/1	0.88	0.25	79,79,79,79	0
24	MG	L	203	1/1	0.88	0.15	45,45,45,45	0
24	MG	A	1806	1/1	0.88	0.62	201,201,201,201	0
24	MG	A	1616	1/1	0.88	0.24	62,62,62,62	0
24	MG	A	1832	1/1	0.88	0.28	38,38,38,38	0
24	MG	A	1745	1/1	0.88	0.20	64,64,64,64	0
24	MG	A	1770	1/1	0.88	0.18	61,61,61,61	0
24	MG	A	1766	1/1	0.88	0.26	23,23,23,23	0
24	MG	A	1673	1/1	0.88	0.22	51,51,51,51	0
24	MG	A	1795	1/1	0.88	0.30	60,60,60,60	0
24	MG	A	1653	1/1	0.88	0.39	64,64,64,64	0
24	MG	A	1730	1/1	0.89	0.23	67,67,67,67	0
24	MG	A	1631	1/1	0.89	0.23	54,54,54,54	0
24	MG	A	1695	1/1	0.89	0.42	211,211,211,211	0
24	MG	A	1706	1/1	0.89	0.30	91,91,91,91	0
24	MG	A	1740	1/1	0.89	0.19	55,55,55,55	0
24	MG	A	1637	1/1	0.89	0.21	63,63,63,63	0
24	MG	A	1847	1/1	0.89	0.15	47,47,47,47	0
24	MG	A	1639	1/1	0.89	0.66	115,115,115,115	0
24	MG	A	1844	1/1	0.89	0.25	75,75,75,75	0
24	MG	A	1811	1/1	0.89	0.10	76,76,76,76	0
24	MG	P	103	1/1	0.89	0.21	60,60,60,60	0
24	MG	A	1669	1/1	0.89	0.20	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1749	1/1	0.89	0.29	45,45,45,45	0
24	MG	D	304	1/1	0.89	0.28	61,61,61,61	0
24	MG	A	1817	1/1	0.89	0.13	73,73,73,73	0
24	MG	A	1742	1/1	0.89	0.16	40,40,40,40	0
24	MG	A	1615	1/1	0.90	0.49	44,44,44,44	0
24	MG	A	1836	1/1	0.90	0.39	36,36,36,36	0
24	MG	A	1759	1/1	0.90	0.36	66,66,66,66	0
24	MG	A	1726	1/1	0.90	0.17	40,40,40,40	0
24	MG	A	1718	1/1	0.90	0.22	54,54,54,54	0
24	MG	A	1843	1/1	0.90	0.33	48,48,48,48	0
24	MG	A	1792	1/1	0.90	0.21	73,73,73,73	0
24	MG	A	1837	1/1	0.90	0.44	66,66,66,66	0
24	MG	A	1839	1/1	0.90	0.52	57,57,57,57	0
24	MG	A	1668	1/1	0.90	0.29	53,53,53,53	0
24	MG	A	1764	1/1	0.90	0.44	93,93,93,93	0
24	MG	B	302	1/1	0.90	0.13	56,56,56,56	0
24	MG	A	1842	1/1	0.91	0.28	59,59,59,59	0
24	MG	A	1804	1/1	0.91	0.24	60,60,60,60	0
24	MG	A	1803	1/1	0.91	0.30	29,29,29,29	0
24	MG	A	1760	1/1	0.91	0.38	35,35,35,35	0
24	MG	A	1752	1/1	0.91	0.11	60,60,60,60	0
24	MG	A	1822	1/1	0.91	0.10	64,64,64,64	0
24	MG	A	1778	1/1	0.91	0.14	67,67,67,67	0
24	MG	A	1690	1/1	0.91	0.29	143,143,143,143	0
24	MG	A	1853	1/1	0.91	0.51	59,59,59,59	0
24	MG	A	1633	1/1	0.91	0.61	207,207,207,207	0
24	MG	A	1735	1/1	0.91	0.13	28,28,28,28	0
24	MG	A	1793	1/1	0.91	0.24	81,81,81,81	0
24	MG	A	1646	1/1	0.91	0.34	91,91,91,91	0
24	MG	A	1645	1/1	0.91	0.20	67,67,67,67	0
24	MG	A	1769	1/1	0.92	0.28	63,63,63,63	0
24	MG	A	1813	1/1	0.92	0.09	100,100,100,100	0
24	MG	A	1831	1/1	0.92	0.20	48,48,48,48	0
24	MG	A	1849	1/1	0.92	0.24	77,77,77,77	0
24	MG	A	1783	1/1	0.92	0.28	58,58,58,58	0
24	MG	D	303	1/1	0.92	0.10	78,78,78,78	0
24	MG	A	1748	1/1	0.92	0.38	63,63,63,63	0
24	MG	A	1691	1/1	0.92	0.21	59,59,59,59	0
24	MG	A	1657	1/1	0.92	0.24	80,80,80,80	0
24	MG	A	1851	1/1	0.92	0.51	56,56,56,56	0
24	MG	A	1787	1/1	0.92	0.28	169,169,169,169	0
24	MG	F	201	1/1	0.92	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1606	1/1	0.92	0.19	54,54,54,54	0
24	MG	A	1697	1/1	0.92	0.20	176,176,176,176	0
24	MG	A	1610	1/1	0.92	0.31	139,139,139,139	0
24	MG	A	1620	1/1	0.92	0.36	16,16,16,16	0
24	MG	A	1814	1/1	0.92	0.08	100,100,100,100	0
24	MG	A	1604	1/1	0.92	0.56	48,48,48,48	0
24	MG	A	1655	1/1	0.92	0.15	55,55,55,55	0
24	MG	A	1835	1/1	0.93	0.20	36,36,36,36	0
24	MG	A	1663	1/1	0.93	0.20	80,80,80,80	0
24	MG	A	1651	1/1	0.93	0.07	48,48,48,48	0
24	MG	A	1724	1/1	0.93	0.19	29,29,29,29	0
24	MG	A	1738	1/1	0.93	0.69	60,60,60,60	0
24	MG	A	1725	1/1	0.93	0.22	67,67,67,67	0
24	MG	A	1719	1/1	0.93	0.30	55,55,55,55	0
24	MG	A	1801	1/1	0.93	0.23	74,74,74,74	0
24	MG	C	306	1/1	0.93	0.15	41,41,41,41	0
24	MG	A	1641	1/1	0.93	0.42	112,112,112,112	0
24	MG	A	1737	1/1	0.93	0.21	52,52,52,52	0
24	MG	A	1628	1/1	0.93	0.44	72,72,72,72	0
24	MG	A	1634	1/1	0.93	0.15	42,42,42,42	0
24	MG	A	1733	1/1	0.93	0.17	34,34,34,34	0
24	MG	A	1704	1/1	0.93	0.17	61,61,61,61	0
24	MG	A	1852	1/1	0.94	0.42	58,58,58,58	0
24	MG	A	1732	1/1	0.94	0.11	28,28,28,28	0
24	MG	A	1640	1/1	0.94	0.11	59,59,59,59	0
24	MG	A	1776	1/1	0.94	0.34	63,63,63,63	0
24	MG	A	1667	1/1	0.94	0.40	197,197,197,197	0
24	MG	A	1707	1/1	0.94	0.12	50,50,50,50	0
24	MG	A	1681	1/1	0.94	0.23	104,104,104,104	0
24	MG	A	1855	1/1	0.94	0.28	26,26,26,26	0
24	MG	A	1622	1/1	0.94	0.28	103,103,103,103	0
24	MG	A	1729	1/1	0.94	0.13	29,29,29,29	0
24	MG	A	1603	1/1	0.94	0.11	84,84,84,84	0
24	MG	A	1625	1/1	0.94	0.21	117,117,117,117	0
24	MG	A	1796	1/1	0.94	0.12	87,87,87,87	0
24	MG	A	1611	1/1	0.94	0.29	132,132,132,132	0
24	MG	A	1761	1/1	0.94	0.23	34,34,34,34	0
24	MG	A	1727	1/1	0.94	0.13	53,53,53,53	0
24	MG	A	1833	1/1	0.94	0.20	97,97,97,97	0
24	MG	A	1782	1/1	0.94	0.19	34,34,34,34	0
24	MG	P	101	1/1	0.95	0.21	9,9,9,9	0
24	MG	A	1785	1/1	0.95	0.21	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1688	1/1	0.95	0.29	29,29,29,29	0
24	MG	A	1821	1/1	0.95	0.09	86,86,86,86	0
24	MG	A	1714	1/1	0.95	0.15	68,68,68,68	0
24	MG	A	1859	1/1	0.95	0.13	45,45,45,45	0
24	MG	A	1744	1/1	0.95	0.12	46,46,46,46	0
24	MG	A	1676	1/1	0.95	0.08	49,49,49,49	0
24	MG	A	1763	1/1	0.95	0.17	40,40,40,40	0
24	MG	A	1699	1/1	0.95	0.41	79,79,79,79	0
24	MG	A	1829	1/1	0.95	0.09	69,69,69,69	0
24	MG	A	1661	1/1	0.95	0.17	153,153,153,153	0
24	MG	A	1723	1/1	0.95	0.65	74,74,74,74	0
24	MG	A	1635	1/1	0.95	0.40	46,46,46,46	0
24	MG	A	1609	1/1	0.95	0.15	52,52,52,52	0
25	SIS	A	1809	31/31	0.95	0.23	32,57,79,80	0
24	MG	A	1824	1/1	0.95	0.14	83,83,83,83	0
24	MG	A	1623	1/1	0.95	0.22	72,72,72,72	0
24	MG	A	1786	1/1	0.95	0.07	80,80,80,80	0
24	MG	C	305	1/1	0.95	0.15	36,36,36,36	0
24	MG	A	1636	1/1	0.95	0.09	68,68,68,68	0
24	MG	A	1621	1/1	0.96	0.21	48,48,48,48	0
24	MG	A	1750	1/1	0.96	0.15	34,34,34,34	0
24	MG	A	1649	1/1	0.96	0.22	75,75,75,75	0
24	MG	A	1747	1/1	0.96	0.08	26,26,26,26	0
24	MG	C	304	1/1	0.96	0.09	77,77,77,77	0
24	MG	A	1711	1/1	0.96	0.15	37,37,37,37	0
24	MG	A	1638	1/1	0.96	0.83	159,159,159,159	0
24	MG	A	1687	1/1	0.96	0.17	132,132,132,132	0
24	MG	A	1708	1/1	0.96	0.16	58,58,58,58	0
24	MG	A	1751	1/1	0.96	0.11	25,25,25,25	0
24	MG	A	1815	1/1	0.96	0.09	88,88,88,88	0
24	MG	A	1605	1/1	0.96	0.29	115,115,115,115	0
24	MG	A	1772	1/1	0.96	0.19	40,40,40,40	0
24	MG	A	1650	1/1	0.96	0.15	80,80,80,80	0
24	MG	A	1664	1/1	0.96	0.16	64,64,64,64	0
24	MG	A	1741	1/1	0.96	0.18	32,32,32,32	0
24	MG	A	1754	1/1	0.96	0.15	39,39,39,39	0
24	MG	A	1771	1/1	0.96	0.21	39,39,39,39	0
24	MG	A	1643	1/1	0.97	0.20	96,96,96,96	0
24	MG	A	1797	1/1	0.97	0.12	48,48,48,48	0
24	MG	D	302	1/1	0.97	0.15	52,52,52,52	0
24	MG	A	1788	1/1	0.97	0.14	80,80,80,80	0
24	MG	A	1644	1/1	0.97	0.19	38,38,38,38	0

*Continued on next page...*

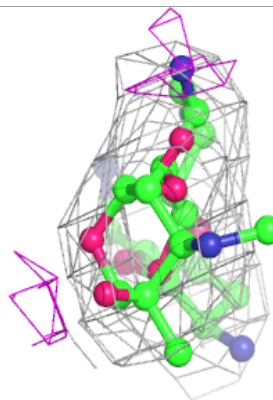
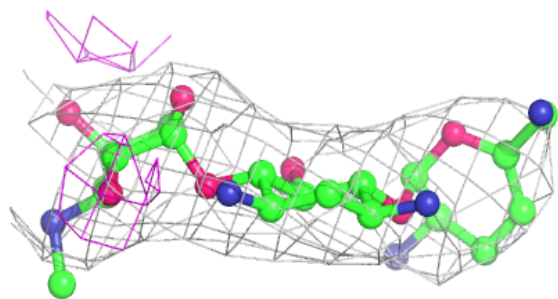
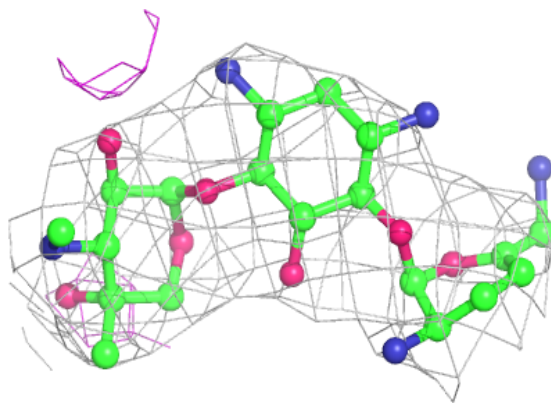
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1812	1/1	0.97	0.06	98,98,98,98	0
24	MG	A	1683	1/1	0.97	0.21	37,37,37,37	0
24	MG	J	201	1/1	0.97	0.09	36,36,36,36	0
24	MG	A	1618	1/1	0.97	0.25	64,64,64,64	0
24	MG	A	1777	1/1	0.97	0.21	46,46,46,46	0
24	MG	A	1630	1/1	0.97	0.17	61,61,61,61	0
24	MG	A	1654	1/1	0.97	0.12	57,57,57,57	0
24	MG	A	1820	1/1	0.97	0.09	107,107,107,107	0
24	MG	A	1647	1/1	0.97	0.20	36,36,36,36	0
24	MG	A	1828	1/1	0.97	0.07	43,43,43,43	0
24	MG	A	1709	1/1	0.97	0.29	57,57,57,57	0
24	MG	A	1762	1/1	0.97	0.19	22,22,22,22	0
24	MG	A	1608	1/1	0.97	0.10	38,38,38,38	0
24	MG	A	1679	1/1	0.97	0.18	54,54,54,54	0
24	MG	A	1830	1/1	0.97	0.10	36,36,36,36	0
24	MG	A	1607	1/1	0.97	0.10	108,108,108,108	0
24	MG	A	1686	1/1	0.97	0.18	67,67,67,67	0
24	MG	A	1746	1/1	0.97	0.10	35,35,35,35	0
24	MG	A	1794	1/1	0.97	0.22	64,64,64,64	0
24	MG	B	301	1/1	0.97	0.10	74,74,74,74	0
24	MG	A	1819	1/1	0.98	0.11	62,62,62,62	0
24	MG	A	1629	1/1	0.98	0.15	66,66,66,66	0
24	MG	A	1798	1/1	0.98	0.13	70,70,70,70	0
24	MG	A	1743	1/1	0.98	0.12	65,65,65,65	0
24	MG	A	1614	1/1	0.98	0.30	78,78,78,78	0
26	ZN	D	301	1/1	0.98	0.20	83,83,83,83	0
24	MG	A	1757	1/1	0.98	0.30	45,45,45,45	0
24	MG	A	1739	1/1	0.98	0.07	48,48,48,48	0
26	ZN	N	101	1/1	0.98	0.13	112,112,112,112	0
24	MG	A	1850	1/1	0.98	0.05	30,30,30,30	0
24	MG	A	1791	1/1	0.98	0.09	93,93,93,93	0
24	MG	A	1698	1/1	0.98	0.23	56,56,56,56	0
24	MG	A	1648	1/1	0.98	0.09	64,64,64,64	0
24	MG	A	1784	1/1	0.98	0.10	63,63,63,63	0
24	MG	A	1662	1/1	0.99	0.07	61,61,61,61	0
24	MG	A	1670	1/1	0.99	0.12	60,60,60,60	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.

**Electron density around SIS A 1809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.