



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 03:27 PM BST

PDB ID : 4DR5  
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered cognate transfer RNA anticodon stem-loop and streptomycin bound  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-16  
Resolution : 3.45 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 : 2.13  
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

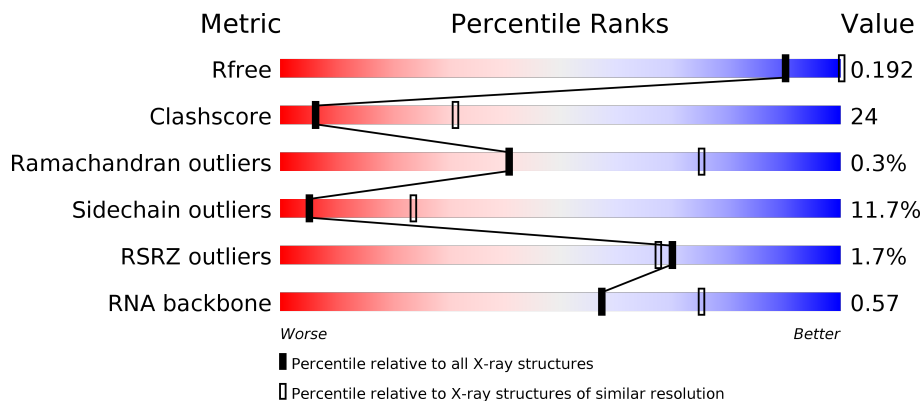
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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.






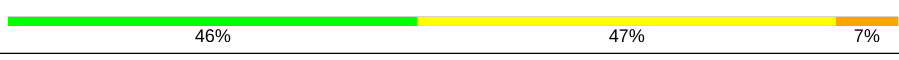
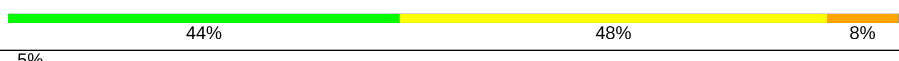
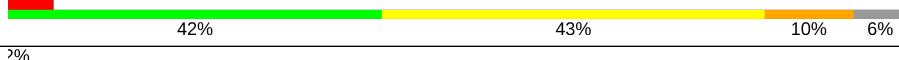
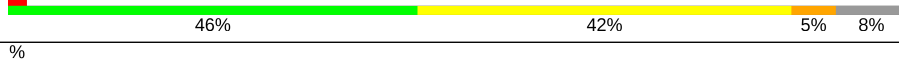

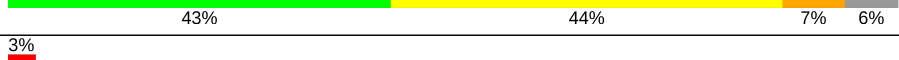

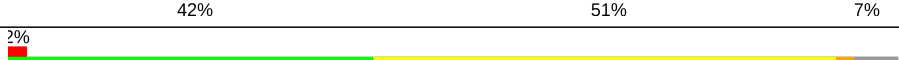
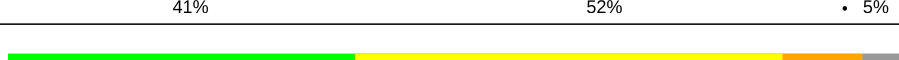
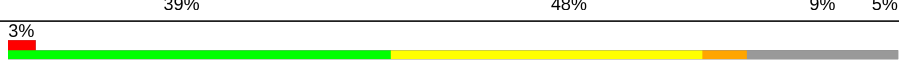
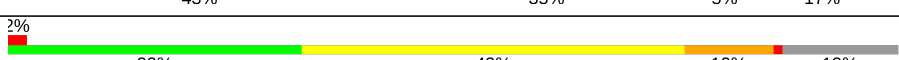
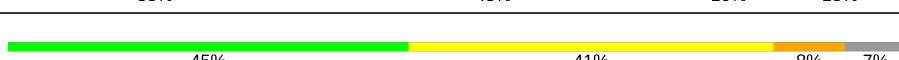




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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	1522	
2	B	256	
3	C	239	
4	D	209	

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	3	
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
1	UR3	A	1498	-	-	X	-
1	MA6	A	1518[B]	-	-	X	-
1	PSU	A	1540	-	-	-	X
1	PSU	A	1541	-	-	-	X
24	MG	A	1615	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
24	MG	A	1659	-	-	-	X
24	MG	A	1697	-	-	-	X
24	MG	A	1711	-	-	-	X
24	MG	A	1722	-	-	-	X
24	MG	A	1730	-	-	-	X
24	MG	A	1731	-	-	-	X
24	MG	A	1732	-	-	-	X
24	MG	A	1746	-	-	-	X
24	MG	A	1747	-	-	-	X
24	MG	A	1749	-	-	-	X
24	MG	A	1768	-	-	-	X
24	MG	A	1779	-	-	-	X
24	MG	A	1790	-	-	-	X
24	MG	A	1794	-	-	-	X
24	MG	A	1795	-	-	-	X
24	MG	A	1808	-	-	-	X
24	MG	A	1825	-	-	-	X
24	MG	A	1851	-	-	-	X
24	MG	F	201	-	-	-	X
24	MG	N	102	-	-	-	X

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 53065 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32641	14540	6039	10545	1517	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1896	1211	337	343	5	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	99	793	498	157	137	1	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	885	549	168	165	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	125	973	612	196	163	2	0	0	1

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	88	734	459	147	126	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	84	701	443	140	117	1	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	100	834	534	156	142	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	598	381	118	99	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	81	648	414	120	112	2	0	0	1

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	U	25	209	128	51	30	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	V	3	57	27	6	22	2	0	0	0

- Molecule 23 is a RNA chain called 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
			Total	C	N	O	P			
23	W	15	319	144	60	101	14	0	0	0

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

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

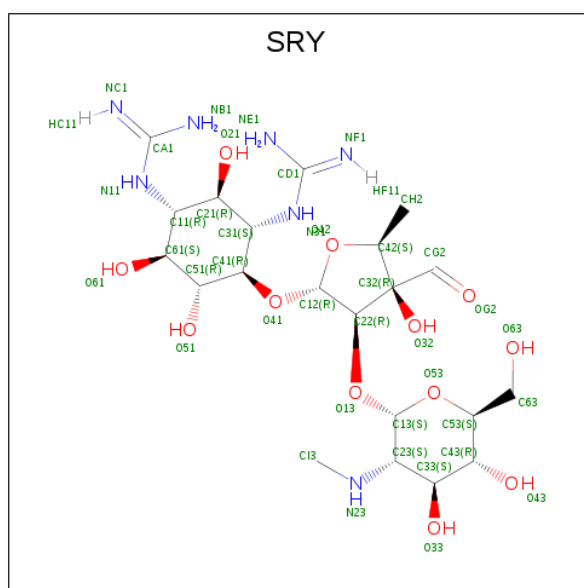
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	259	Total	Mg	0	0
			259	259		
24	N	1	Total	Mg	0	0
			1	1		
24	L	1	Total	Mg	0	0
			1	1		
24	S	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		

- Molecule 25 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
25	A	1	Total	C	N	O	0	0
			40	21	7	12		

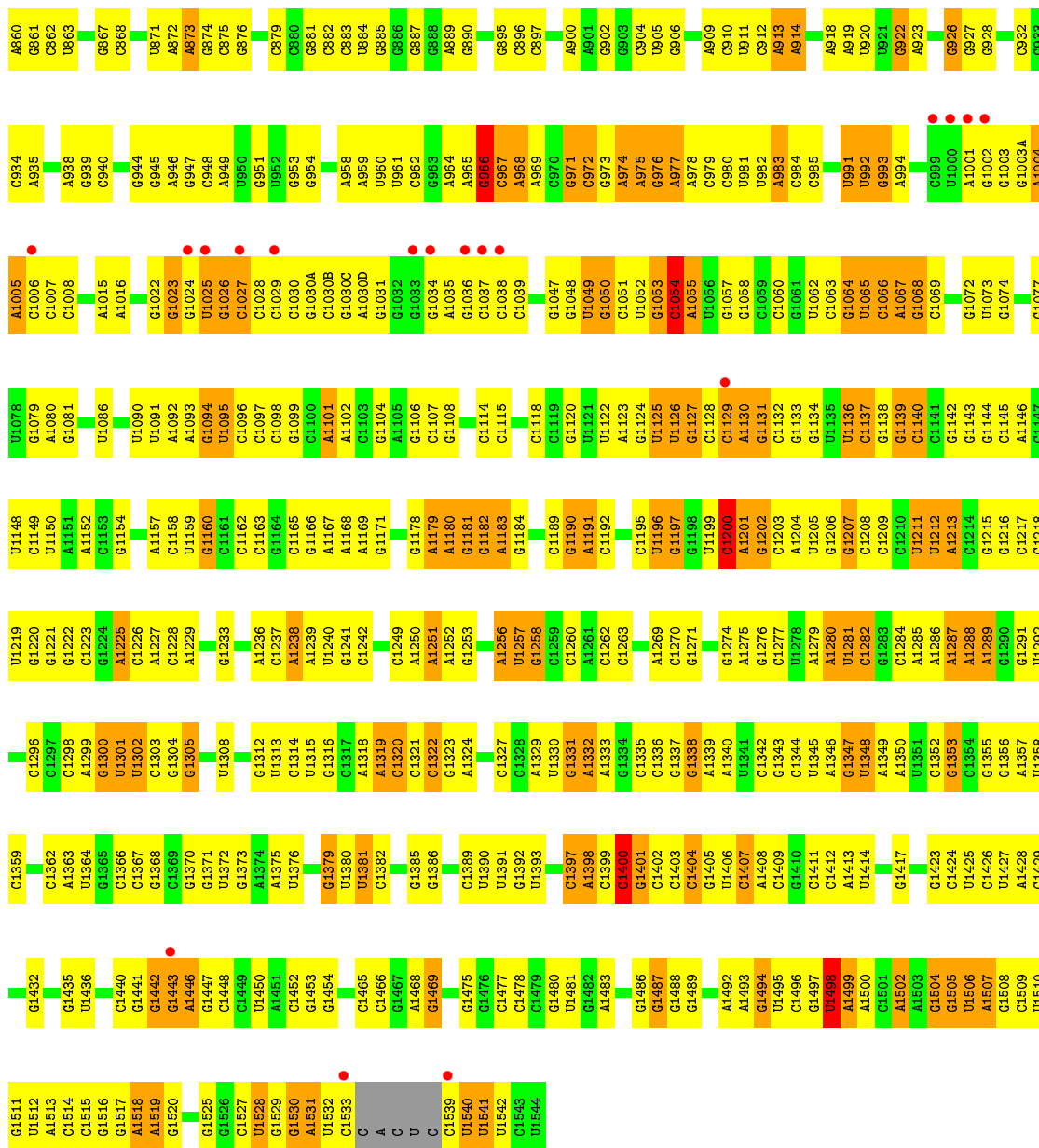
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

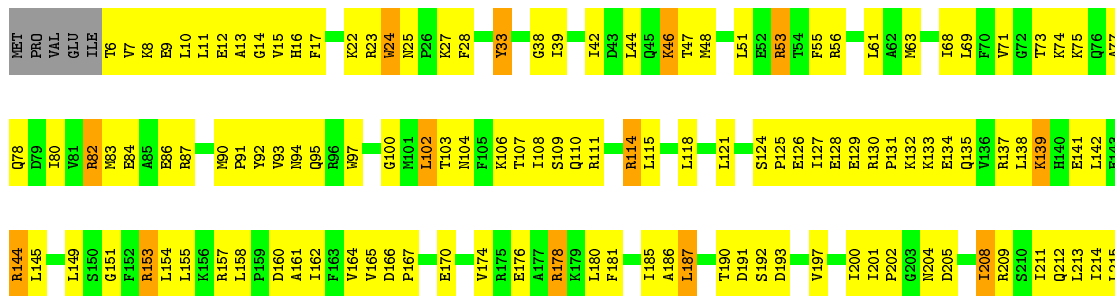
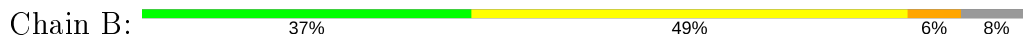
- Molecule 27 is water.

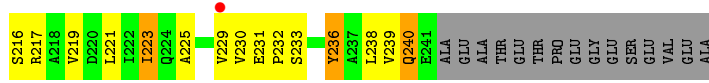
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	572	Total O 572 572	0	0
27	D	2	Total O 2 2	0	0
27	E	3	Total O 3 3	0	0
27	L	1	Total O 1 1	0	0
27	O	1	Total O 1 1	0	0
27	P	1	Total O 1 1	0	0
27	Q	1	Total O 1 1	0	0
27	T	1	Total O 1 1	0	0



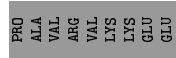
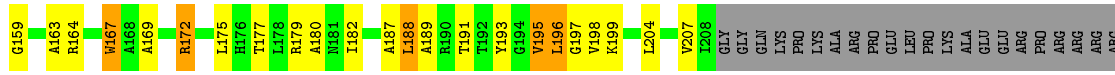
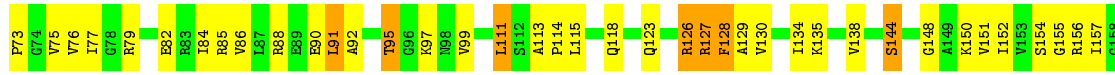
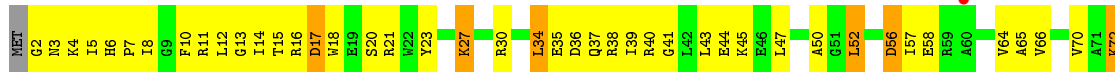


• Molecule 2: 30S ribosomal protein S2

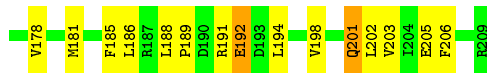
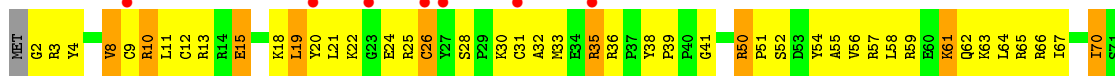




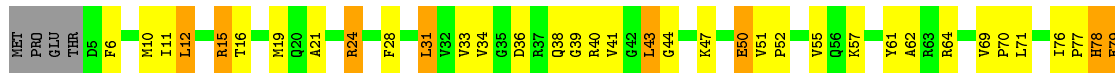
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

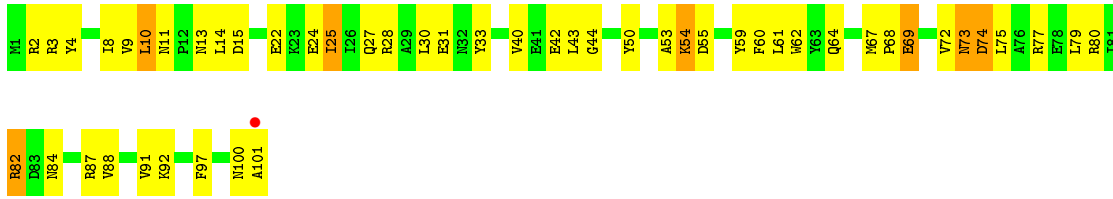


• Molecule 5: 30S ribosomal protein S5

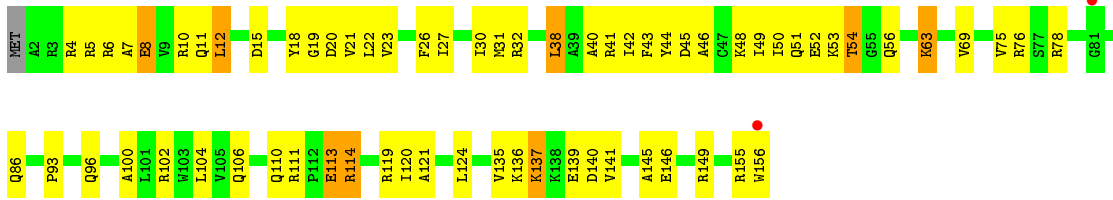


• Molecule 6: 30S ribosomal protein S6

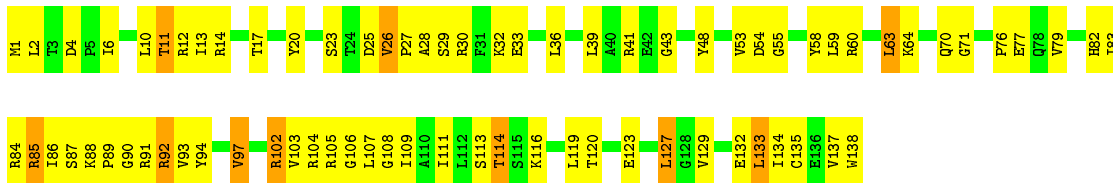




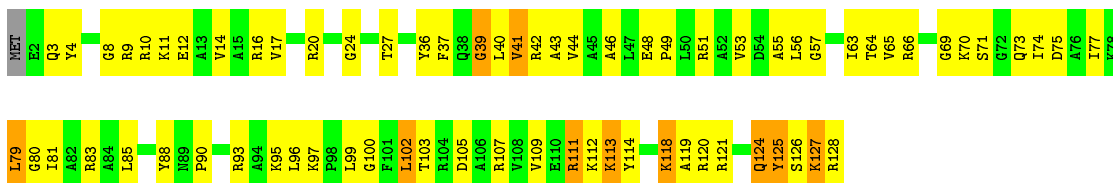
• Molecule 7: 30S ribosomal protein S7



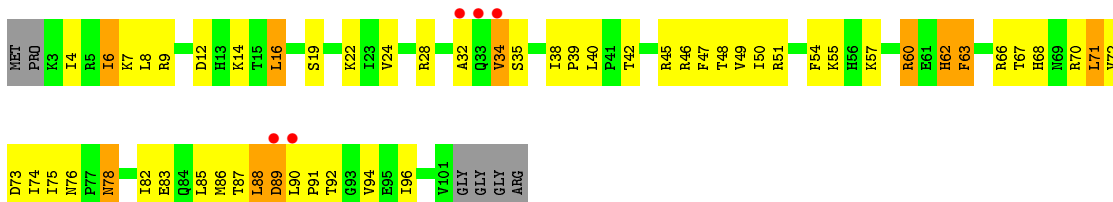
• Molecule 8: 30S ribosomal protein S8



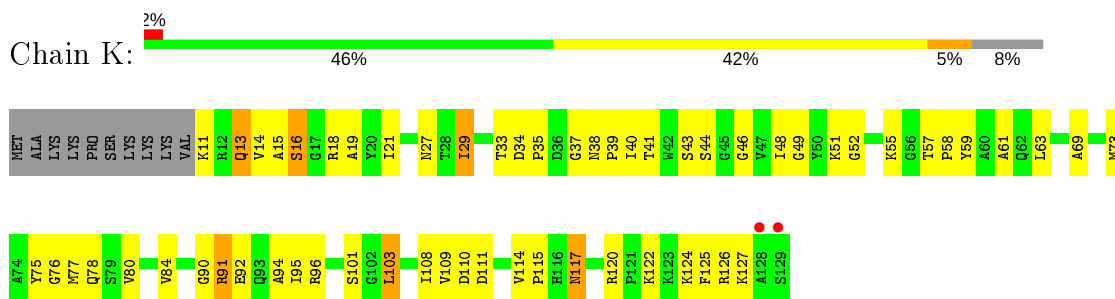
• Molecule 9: 30S ribosomal protein S9



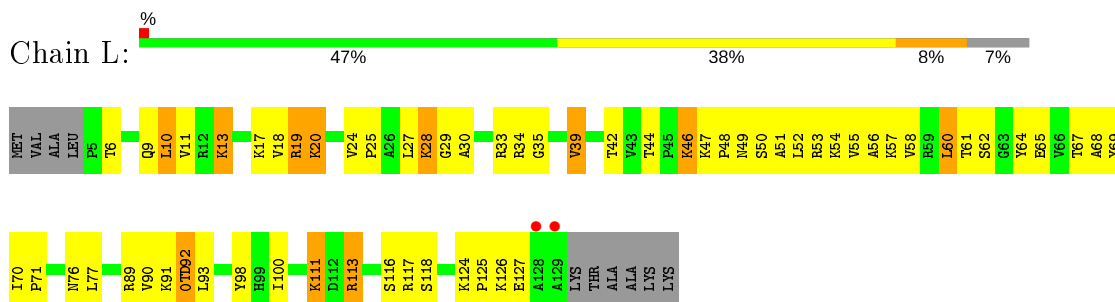
• Molecule 10: 30S ribosomal protein S10



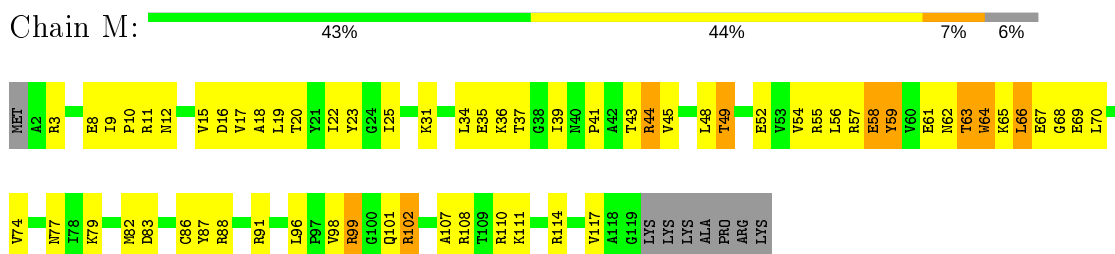
• Molecule 11: 30S ribosomal protein S11



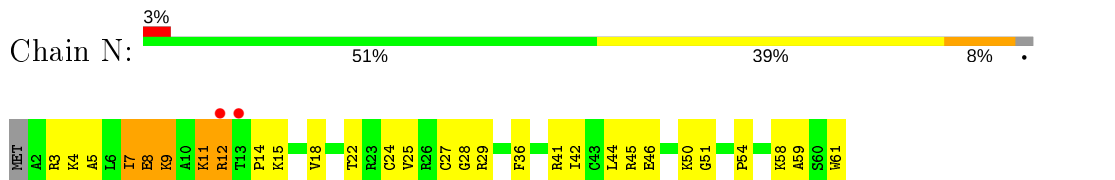
- Molecule 12: 30S ribosomal protein S12



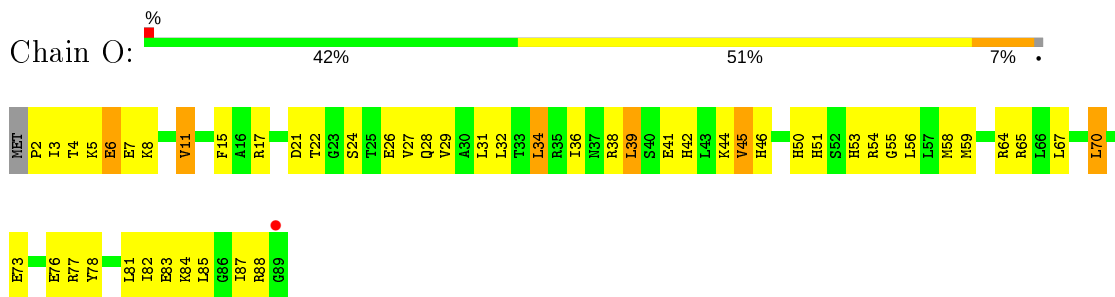
- Molecule 13: 30S ribosomal protein S13



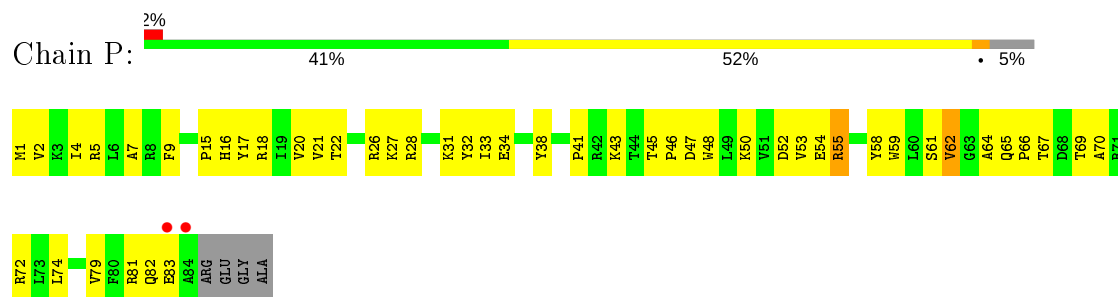
- Molecule 14: 30S ribosomal protein S14



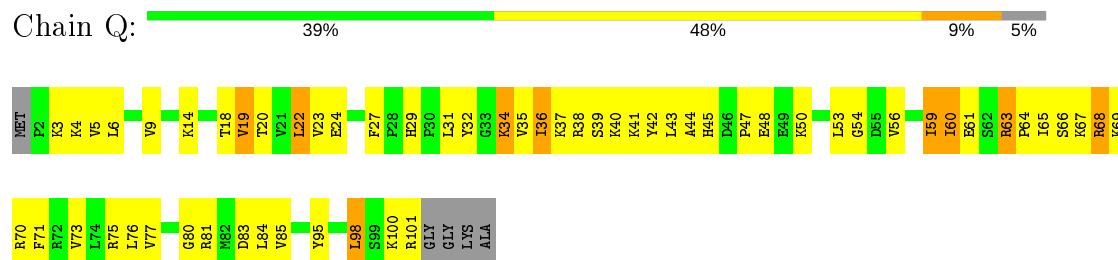
- Molecule 15: 30S ribosomal protein S15



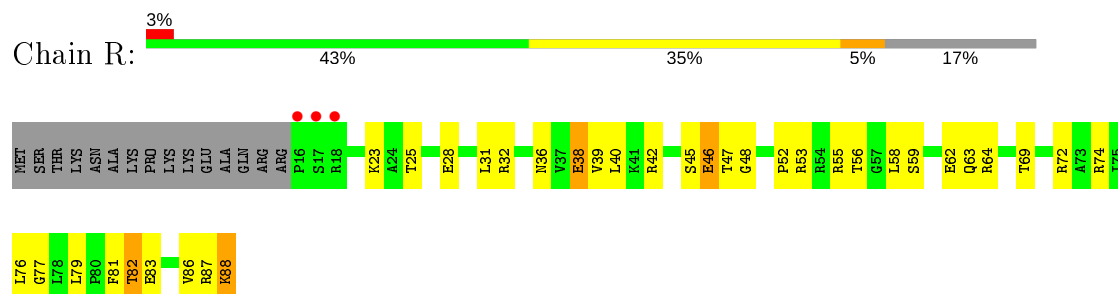
- Molecule 16: 30S ribosomal protein S16



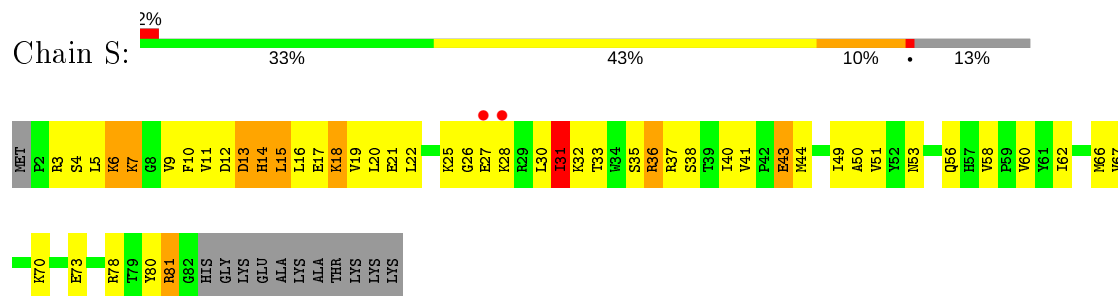
- Molecule 17: 30S ribosomal protein S17



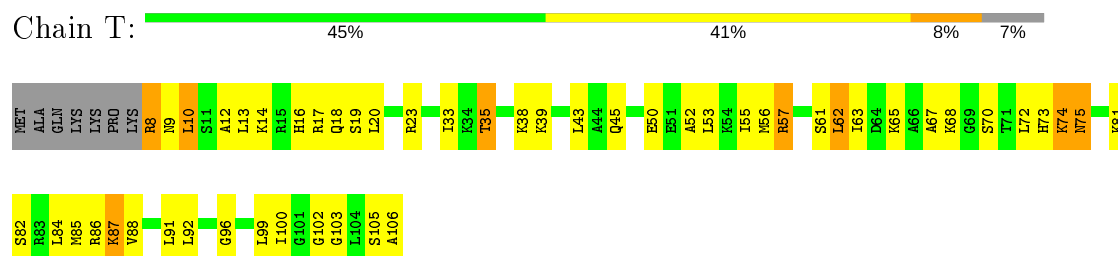
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20





- Molecule 21: 30S ribosomal protein THX

Chain U:  70% 15% 7% 7%




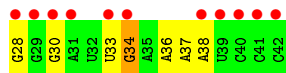
- Molecule 22: 5'-R(\*UP\*UP\*U)-3'

Chain V:  67% 100%



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

Chain W:  73% 53% 40% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.51Å 400.51Å 175.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 3.45 19.90 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.90-3.45) 100.0 (19.90-3.45)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.44Å)	Xtrriage
Refinement program	PHENIX dev_978	Depositor
R, $R_{free}$	0.152 , 0.192 0.152 , 0.192	Depositor DCC
$R_{free}$ test set	9323 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.7	Xtrriage
Anisotropy	0.223	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 83.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, 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	0/36136	0.87	37/56392 (0.1%)
2	B	0.31	0/1931	0.53	0/2607
3	C	0.31	0/1637	0.50	0/2207
4	D	0.34	0/1733	0.53	0/2318
5	E	0.43	0/1163	0.64	0/1566
6	F	0.31	0/856	0.51	0/1154
7	G	0.33	0/1276	0.52	0/1709
8	H	0.41	0/1136	0.62	0/1527
9	I	0.30	0/1029	0.56	1/1379 (0.1%)
10	J	0.32	0/806	0.57	0/1084
11	K	0.38	0/900	0.65	0/1213
12	L	0.38	0/978	0.67	0/1308
13	M	0.31	0/947	0.52	0/1270
14	N	0.36	0/501	0.54	0/664
15	O	0.36	0/745	0.54	0/992
16	P	0.42	0/717	0.62	0/965
17	Q	0.45	0/847	0.66	0/1131
18	R	0.33	0/604	0.54	0/801
19	S	0.27	0/662	0.54	0/892
20	T	0.39	0/765	0.67	0/1007
21	U	0.34	0/213	0.57	0/279
22	V	0.23	0/62	0.67	0/94
23	W	0.18	0/357	0.47	0/555
All	All	0.45	0/56001	0.78	38/83114 (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
2	B	0	1
8	H	0	1
12	L	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	108	G	C4-C5-N7	7.91	113.97	110.80
1	A	108	G	N7-C8-N9	7.26	116.73	113.10
1	A	108	G	C5-N7-C8	-7.26	100.67	104.30
1	A	108	G	C6-C5-N7	-7.07	126.16	130.40
1	A	108	G	C4-N9-C1'	7.03	135.64	126.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
8	H	90	GLY	Peptide
12	L	46	LYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32641	0	16508	1073	1
2	B	1896	0	1936	125	0
3	C	1613	0	1677	108	0
4	D	1703	0	1763	85	0
5	E	1147	0	1207	73	0
6	F	843	0	857	45	0
7	G	1257	0	1296	64	0
8	H	1116	0	1177	69	0
9	I	1010	0	1037	77	0
10	J	793	0	835	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	885	0	904	48	0
12	L	973	0	1058	67	0
13	M	937	0	995	71	0
14	N	492	0	529	34	0
15	O	734	0	771	50	0
16	P	701	0	720	44	0
17	Q	834	0	906	69	0
18	R	598	0	670	38	0
19	S	648	0	673	59	0
20	T	763	0	861	64	0
21	U	209	0	221	10	0
22	V	57	0	32	0	0
23	W	319	0	164	8	0
24	A	259	0	0	0	0
24	D	2	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	G	1	0	0	0	0
24	H	1	0	0	0	0
24	L	1	0	0	0	0
24	N	1	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	40	0	37	9	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	572	0	0	21	0
27	D	2	0	0	0	0
27	E	3	0	0	0	0
27	L	1	0	0	0	0
27	O	1	0	0	0	0
27	P	1	0	0	0	0
27	Q	1	0	0	0	0
27	T	1	0	0	0	0
All	All	53065	0	36834	2136	1

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 24.

The worst 5 of 2136 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:ALA:HA	11:K:77:MET:HA	1.32	1.12
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.29	1.06
15:O:87:ILE:HG22	15:O:88:ARG:H	1.18	1.06
1:A:1498:UR3:O2'	1:A:1499:A:OP2	1.75	1.04
3:C:27:LYS:H	3:C:27:LYS:HD3	1.19	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:A:N6	1:A:1447:G:OP1[4_554]	2.18	0.02

## 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	234/256 (91%)	209 (89%)	24 (10%)	1 (0%)	34	70
3	C	205/239 (86%)	183 (89%)	22 (11%)	0	100	100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	19	57
10	J	97/105 (92%)	80 (82%)	16 (16%)	1 (1%)	15	52
11	K	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	17	54
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	19	57
13	M	116/126 (92%)	105 (90%)	11 (10%)	0	100	100
14	N	58/61 (95%)	54 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	P	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
19	S	79/93 (85%)	69 (87%)	8 (10%)	2 (2%)	5	32
20	T	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2353/2541 (93%)	2152 (92%)	194 (8%)	7 (0%)	41	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
19	S	6	LYS
11	K	117	ASN
9	I	119	ALA

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	201/220 (91%)	181 (90%)	20 (10%)	7	31
3	C	160/188 (85%)	136 (85%)	24 (15%)	3	15
4	D	180/181 (99%)	161 (89%)	19 (11%)	6	28
5	E	115/123 (94%)	101 (88%)	14 (12%)	5	22
6	F	90/90 (100%)	78 (87%)	12 (13%)	4	19
7	G	126/127 (99%)	114 (90%)	12 (10%)	8	33
8	H	119/119 (100%)	105 (88%)	14 (12%)	5	23
9	I	98/99 (99%)	83 (85%)	15 (15%)	2	15
10	J	87/92 (95%)	76 (87%)	11 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	90/99 (91%)	81 (90%)	9 (10%)	7	31
12	L	103/110 (94%)	90 (87%)	13 (13%)	4	21
13	M	94/101 (93%)	83 (88%)	11 (12%)	5	24
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	17
15	O	79/80 (99%)	72 (91%)	7 (9%)	9	36
16	P	72/74 (97%)	67 (93%)	5 (7%)	15	47
17	Q	95/97 (98%)	84 (88%)	11 (12%)	5	24
18	R	64/77 (83%)	58 (91%)	6 (9%)	8	33
19	S	71/80 (89%)	61 (86%)	10 (14%)	3	17
20	T	76/82 (93%)	65 (86%)	11 (14%)	3	16
21	U	19/22 (86%)	17 (90%)	2 (10%)	7	29
All	All	1988/2111 (94%)	1755 (88%)	233 (12%)	5	24

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	85	ARG
10	J	6	ILE
19	S	30	LEU
8	H	97	VAL
9	I	66	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	135	GLN
9	I	73	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	248 (16%)	43 (2%)
22	V	2/3 (66%)	0	0
23	W	14/15 (93%)	3 (21%)	0
All	All	1519/1540 (98%)	251 (16%)	43 (2%)



5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	1026	G
1	A	1397	C
1	A	812	C
1	A	913	A

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

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	M2G	A	966	1	20,27,28	1.57	4 (20%)	22,40,43	2.42	4 (18%)
1	PSU	A	1540	1	17,21,22	1.17	1 (5%)	20,30,33	3.58	6 (30%)
1	UR3	A	1498	1	14,22,23	0.65	0	15,32,35	1.00	1 (6%)
1	4OC	A	1402	1	16,23,24	0.82	0	17,32,35	0.76	0
1	7MG	A	527	1	22,26,27	2.09	5 (22%)	28,39,42	1.66	7 (25%)
1	5MC	A	1407	1	15,22,23	1.20	1 (6%)	19,32,35	0.99	1 (5%)
1	5MC	A	967	1	15,22,23	1.04	1 (6%)	19,32,35	0.96	1 (5%)
1	PSU	A	1541	1	17,21,22	0.95	1 (5%)	20,30,33	3.62	7 (35%)
12	0TD	L	92	12	4,9,10	1.17	0	3,11,13	2.77	1 (33%)
1	2MG	A	1207	1	19,26,27	2.22	3 (15%)	21,38,41	2.06	4 (19%)
1	5MC	A	1404	1	15,22,23	1.48	1 (6%)	19,32,35	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1400	1	15,22,23	0.88	0	19,32,35	1.07	2 (10%)
1	MA6	A	1519[A]	1	19,26,27	0.70	0	18,38,41	0.75	0
1	MA6	A	1518[B]	1	19,26,27	1.20	3 (15%)	18,38,41	0.75	0
1	MA6	A	1518[A]	1	19,26,27	1.07	2 (10%)	18,38,41	0.60	0
1	MA6	A	1519[B]	1	19,26,27	1.28	3 (15%)	18,38,41	0.57	0
1	PSU	A	516	1,24	17,21,22	0.98	1 (5%)	20,30,33	3.23	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	M2G	A	966	1	-	5/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1404	1	-	2/5/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	3/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	5/7/29/30	0/3/3/3
1	PSU	A	516	1,24	-	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	6.98	1.40	1.34
1	A	1207	2MG	C6-N1	5.46	1.42	1.33
1	A	527	7MG	C2-N2	5.16	1.44	1.33
1	A	527	7MG	C8-N9	-5.09	1.33	1.45
1	A	966	M2G	C6-N1	4.84	1.41	1.33

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-11.30	119.45	128.43
1	A	516	PSU	N1-C2-N3	-11.04	119.65	128.43
1	A	1541	PSU	N1-C2-N3	-10.83	119.82	128.43
1	A	966	M2G	C5-C6-N1	-8.15	112.29	123.43
1	A	1207	2MG	C5-C6-N1	-7.42	113.28	123.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1400	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	966	M2G	3	0
1	A	1540	PSU	6	0
1	A	1498	UR3	9	0
1	A	1402	4OC	4	0
1	A	527	7MG	2	0
1	A	1407	5MC	3	0
1	A	967	5MC	3	0
1	A	1541	PSU	3	0
12	L	92	0TD	3	0
1	A	1207	2MG	3	0
1	A	1404	5MC	1	0
1	A	1400	5MC	3	0
1	A	1519[A]	MA6	3	0
1	A	1518[B]	MA6	9	0
1	A	1518[A]	MA6	3	0
1	A	1519[B]	MA6	7	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 275 ligands modelled in this entry, 274 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	SRY	A	1860	-	40,42,42	2.36	10 (25%)	49,63,63	2.01	11 (22%)

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	SRY	A	1860	-	-	3/20/87/87	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1860	SRY	CD1-N31	9.04	1.49	1.33
25	A	1860	SRY	CA1-N11	7.10	1.45	1.33
25	A	1860	SRY	O53-C53	-3.48	1.35	1.44
25	A	1860	SRY	C23-N23	-2.97	1.42	1.47
25	A	1860	SRY	C32-CG2	-2.79	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1860	SRY	C13-O13-C22	-7.51	103.22	116.25
25	A	1860	SRY	CI3-N23-C23	-4.77	107.43	114.38
25	A	1860	SRY	C12-O42-C42	-4.68	101.02	108.38
25	A	1860	SRY	C61-C11-N11	-3.98	103.10	110.62
25	A	1860	SRY	C43-C33-C23	-3.50	105.21	110.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

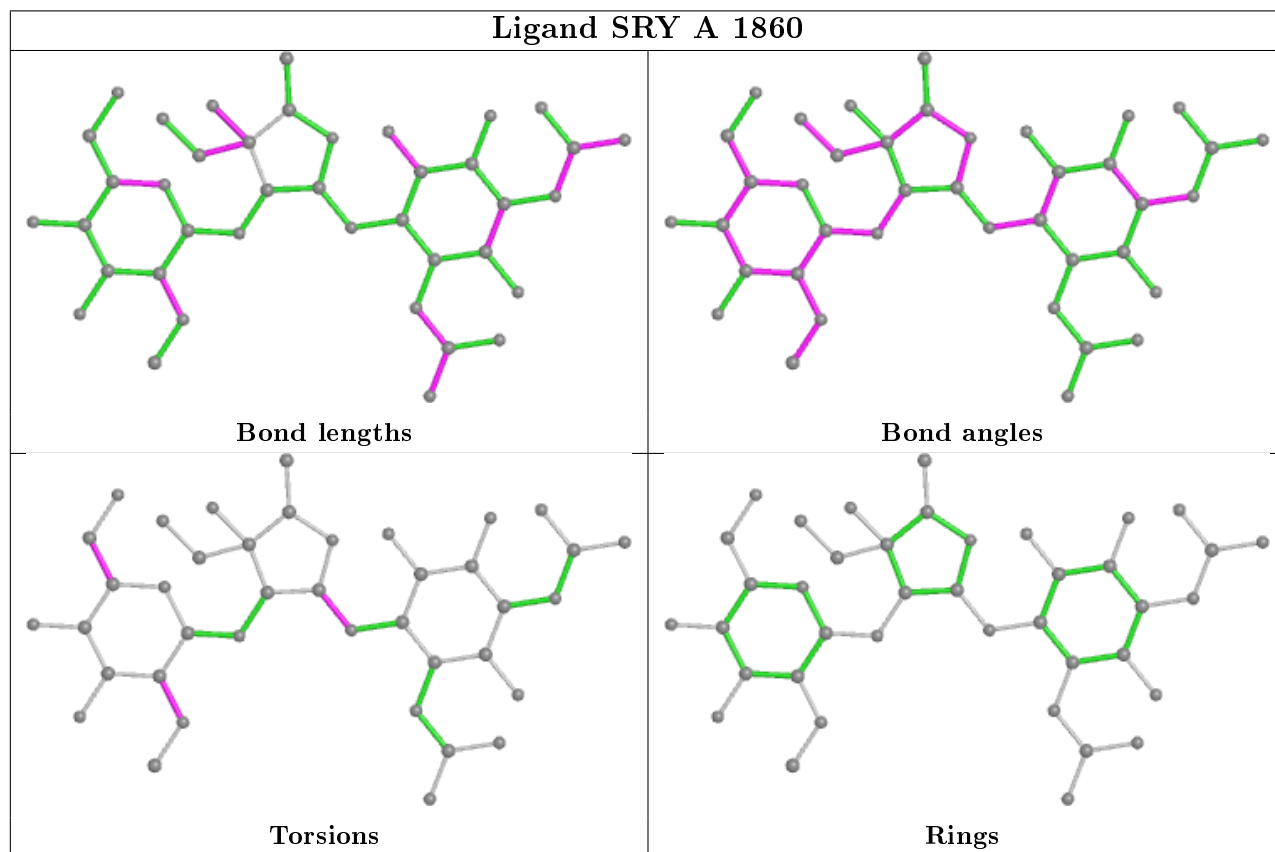
Mol	Chain	Res	Type	Atoms
25	A	1860	SRY	C13-C23-N23-CI3
25	A	1860	SRY	C43-C53-C63-O63
25	A	1860	SRY	O42-C12-O41-C41

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1860	SRY	9	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	1498/1522 (98%)	-0.24	20 (1%) 77 73	63, 101, 189, 333	0
2	B	236/256 (92%)	-0.33	1 (0%) 92 90	93, 136, 194, 231	0
3	C	207/239 (86%)	-0.35	1 (0%) 91 89	106, 142, 183, 216	0
4	D	208/209 (99%)	-0.29	7 (3%) 45 43	77, 113, 175, 202	0
5	E	151/162 (93%)	-0.44	1 (0%) 87 85	68, 95, 131, 177	0
6	F	101/101 (100%)	-0.44	1 (0%) 82 79	93, 133, 164, 185	0
7	G	155/156 (99%)	-0.34	2 (1%) 77 73	90, 120, 183, 219	0
8	H	138/138 (100%)	-0.55	0 100 100	62, 85, 115, 146	0
9	I	127/128 (99%)	-0.29	0 100 100	95, 144, 180, 216	0
10	J	99/105 (94%)	-0.01	5 (5%) 28 27	105, 165, 237, 271	0
11	K	119/129 (92%)	-0.26	2 (1%) 70 67	72, 101, 148, 212	0
12	L	124/135 (91%)	-0.33	2 (1%) 72 69	64, 110, 146, 220	0
13	M	118/126 (93%)	-0.59	0 100 100	92, 124, 162, 204	0
14	N	60/61 (98%)	-0.28	2 (3%) 46 44	107, 133, 172, 248	0
15	O	88/89 (98%)	-0.45	1 (1%) 80 77	68, 102, 144, 210	0
16	P	84/88 (95%)	-0.45	2 (2%) 59 56	75, 96, 122, 171	0
17	Q	100/105 (95%)	-0.34	0 100 100	63, 89, 126, 182	0
18	R	73/88 (82%)	-0.27	3 (4%) 37 36	86, 109, 197, 245	0
19	S	81/93 (87%)	-0.27	2 (2%) 57 54	120, 154, 199, 254	0
20	T	99/106 (93%)	-0.61	0 100 100	73, 96, 140, 176	0
21	U	25/27 (92%)	-0.37	0 100 100	101, 121, 153, 171	0
22	V	3/3 (100%)	2.48	2 (66%) 0 0	191, 191, 198, 226	3 (100%)
23	W	15/15 (100%)	3.28	11 (73%) 0 0	194, 222, 273, 301	8 (53%)
All	All	3909/4081 (95%)	-0.30	65 (1%) 70 67	62, 112, 188, 333	11 (0%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	129	ALA	7.4
11	K	129	SER	6.8
23	W	28	G	6.6
18	R	17	SER	6.1
23	W	42	C	5.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1541	20/21	0.71	0.47	188,196,202,203	0
1	PSU	A	1540	20/21	0.72	0.47	193,205,213,214	0
1	5MC	A	1400	21/22	0.92	0.23	71,102,119,121	0
1	M2G	A	966	25/26	0.95	0.15	88,105,117,123	0
1	MA6	A	1518[B]	24/25	0.95	0.19	79,88,110,112	24
1	MA6	A	1518[A]	24/25	0.95	0.19	81,85,92,101	24
1	UR3	A	1498	21/22	0.96	0.21	87,96,109,112	0
1	5MC	A	1407	21/22	0.96	0.23	107,119,130,134	0
1	4OC	A	1402	22/23	0.97	0.18	89,101,107,111	0
1	MA6	A	1519[A]	24/25	0.97	0.17	77,81,91,95	24
12	0TD	L	92	10/11	0.97	0.15	83,93,97,207	0
1	2MG	A	1207	24/25	0.97	0.15	120,123,131,135	0
1	MA6	A	1519[B]	24/25	0.97	0.17	76,83,90,91	24
1	5MC	A	1404	21/22	0.98	0.15	84,88,103,117	0
1	5MC	A	967	21/22	0.98	0.13	90,98,107,115	0
1	7MG	A	527	24/25	0.98	0.13	66,86,94,104	0
1	PSU	A	516	20/21	0.98	0.15	120,125,133,136	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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



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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1853	1/1	0.32	0.23	96,96,96,96	0
24	MG	A	1746	1/1	0.42	0.48	99,99,99,99	0
24	MG	A	1779	1/1	0.56	1.20	94,94,94,94	0
24	MG	A	1825	1/1	0.62	0.41	401,401,401,401	0
24	MG	A	1659	1/1	0.65	0.51	121,121,121,121	0
24	MG	A	1794	1/1	0.66	0.47	120,120,120,120	0
24	MG	A	1790	1/1	0.67	0.61	88,88,88,88	0
24	MG	A	1731	1/1	0.69	0.67	114,114,114,114	0
24	MG	A	1722	1/1	0.70	0.43	118,118,118,118	0
24	MG	A	1711	1/1	0.70	0.52	109,109,109,109	0
24	MG	A	1808	1/1	0.70	0.44	377,377,377,377	0
24	MG	A	1749	1/1	0.71	0.63	98,98,98,98	0
24	MG	A	1851	1/1	0.72	0.68	92,92,92,92	0
24	MG	A	1762	1/1	0.73	0.27	83,83,83,83	0
24	MG	A	1812	1/1	0.73	0.23	290,290,290,290	0
24	MG	A	1768	1/1	0.73	0.51	99,99,99,99	0
24	MG	A	1697	1/1	0.74	1.14	102,102,102,102	0
24	MG	F	201	1/1	0.74	0.45	79,79,79,79	0
24	MG	A	1732	1/1	0.75	0.71	97,97,97,97	0
24	MG	A	1633	1/1	0.75	0.15	85,85,85,85	0
24	MG	A	1795	1/1	0.76	0.41	85,85,85,85	0
24	MG	A	1646	1/1	0.76	0.37	79,79,79,79	0
24	MG	A	1765	1/1	0.77	0.11	93,93,93,93	0
24	MG	A	1777	1/1	0.78	0.39	100,100,100,100	0
24	MG	N	102	1/1	0.78	0.63	99,99,99,99	0
24	MG	A	1856	1/1	0.78	0.15	104,104,104,104	0
24	MG	A	1747	1/1	0.79	0.46	111,111,111,111	0
24	MG	A	1615	1/1	0.79	0.44	72,72,72,72	0
24	MG	A	1730	1/1	0.80	0.42	90,90,90,90	0
24	MG	A	1673	1/1	0.80	0.36	102,102,102,102	0
24	MG	A	1781	1/1	0.80	0.42	75,75,75,75	0
24	MG	A	1815	1/1	0.81	0.29	309,309,309,309	0
24	MG	A	1727	1/1	0.81	0.29	79,79,79,79	0
24	MG	A	1683	1/1	0.81	0.60	110,110,110,110	0
24	MG	L	201	1/1	0.81	0.14	81,81,81,81	0
24	MG	A	1848	1/1	0.81	0.37	87,87,87,87	0
24	MG	A	1724	1/1	0.82	0.23	99,99,99,99	0
24	MG	A	1773	1/1	0.82	0.78	88,88,88,88	0
24	MG	A	1740	1/1	0.82	0.32	89,89,89,89	0
24	MG	G	201	1/1	0.82	0.64	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1827	1/1	0.82	0.27	244,244,244,244	0
24	MG	A	1687	1/1	0.82	0.28	116,116,116,116	0
24	MG	A	1761	1/1	0.82	0.24	107,107,107,107	0
24	MG	A	1852	1/1	0.82	0.39	84,84,84,84	0
24	MG	A	1789	1/1	0.83	0.50	92,92,92,92	0
24	MG	A	1855	1/1	0.83	0.37	115,115,115,115	0
24	MG	A	1767	1/1	0.83	0.57	64,64,64,64	0
24	MG	A	1857	1/1	0.83	0.29	89,89,89,89	0
24	MG	A	1655	1/1	0.83	0.35	210,210,210,210	0
24	MG	A	1858	1/1	0.83	0.32	98,98,98,98	0
24	MG	A	1672	1/1	0.84	0.89	92,92,92,92	0
24	MG	A	1771	1/1	0.84	0.41	82,82,82,82	0
24	MG	A	1709	1/1	0.84	0.35	250,250,250,250	0
24	MG	A	1816	1/1	0.84	0.28	318,318,318,318	0
24	MG	A	1609	1/1	0.84	0.16	74,74,74,74	0
24	MG	A	1757	1/1	0.84	0.37	83,83,83,83	0
24	MG	A	1784	1/1	0.84	0.78	92,92,92,92	0
24	MG	A	1809	1/1	0.84	0.21	355,355,355,355	0
24	MG	D	303	1/1	0.85	0.94	97,97,97,97	0
24	MG	A	1634	1/1	0.85	0.27	243,243,243,243	0
24	MG	P	103	1/1	0.85	0.16	93,93,93,93	0
24	MG	A	1801	1/1	0.85	0.25	248,248,248,248	0
24	MG	A	1819	1/1	0.85	0.78	371,371,371,371	0
24	MG	A	1725	1/1	0.85	0.59	109,109,109,109	0
24	MG	A	1755	1/1	0.86	0.13	131,131,131,131	0
24	MG	A	1850	1/1	0.86	0.59	117,117,117,117	0
24	MG	A	1753	1/1	0.86	0.81	110,110,110,110	0
24	MG	A	1772	1/1	0.86	0.37	78,78,78,78	0
24	MG	A	1744	1/1	0.86	0.29	109,109,109,109	0
24	MG	A	1726	1/1	0.87	0.28	86,86,86,86	0
24	MG	A	1807	1/1	0.87	0.31	397,397,397,397	0
24	MG	A	1800	1/1	0.87	0.32	203,203,203,203	0
24	MG	A	1656	1/1	0.87	0.28	177,177,177,177	0
24	MG	A	1770	1/1	0.87	0.78	98,98,98,98	0
24	MG	H	201	1/1	0.87	0.26	63,63,63,63	0
24	MG	A	1682	1/1	0.87	0.28	228,228,228,228	0
24	MG	A	1791	1/1	0.87	0.20	109,109,109,109	0
24	MG	A	1766	1/1	0.87	0.27	95,95,95,95	0
24	MG	A	1622	1/1	0.88	0.78	75,75,75,75	0
24	MG	A	1657	1/1	0.88	0.31	189,189,189,189	0
24	MG	A	1641	1/1	0.88	0.42	92,92,92,92	0
24	MG	A	1718	1/1	0.89	0.24	220,220,220,220	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1818	1/1	0.89	0.25	249,249,249,249	0
24	MG	P	102	1/1	0.89	0.73	96,96,96,96	0
24	MG	A	1836	1/1	0.89	0.32	300,300,300,300	0
24	MG	A	1666	1/1	0.89	0.19	103,103,103,103	0
24	MG	A	1792	1/1	0.89	0.23	91,91,91,91	0
24	MG	A	1798	1/1	0.89	0.20	115,115,115,115	0
24	MG	A	1739	1/1	0.89	0.65	103,103,103,103	0
24	MG	A	1769	1/1	0.89	0.27	92,92,92,92	0
24	MG	A	1625	1/1	0.89	0.25	194,194,194,194	0
24	MG	A	1676	1/1	0.89	0.21	138,138,138,138	0
24	MG	A	1859	1/1	0.89	0.54	94,94,94,94	0
24	MG	A	1774	1/1	0.90	0.66	61,61,61,61	0
24	MG	A	1750	1/1	0.90	0.59	92,92,92,92	0
24	MG	A	1667	1/1	0.90	0.64	168,168,168,168	0
24	MG	A	1719	1/1	0.90	0.32	88,88,88,88	0
24	MG	A	1720	1/1	0.90	0.20	64,64,64,64	0
24	MG	A	1679	1/1	0.90	0.24	168,168,168,168	0
24	MG	A	1847	1/1	0.90	0.35	334,334,334,334	0
24	MG	A	1652	1/1	0.90	0.32	96,96,96,96	0
24	MG	A	1644	1/1	0.90	0.51	95,95,95,95	0
24	MG	A	1695	1/1	0.91	0.44	88,88,88,88	0
24	MG	A	1603	1/1	0.91	0.23	97,97,97,97	0
24	MG	A	1658	1/1	0.91	0.18	102,102,102,102	0
24	MG	A	1689	1/1	0.91	0.16	132,132,132,132	0
24	MG	A	1803	1/1	0.91	0.54	324,324,324,324	0
24	MG	A	1752	1/1	0.91	0.24	90,90,90,90	0
24	MG	A	1745	1/1	0.91	0.69	82,82,82,82	0
24	MG	A	1653	1/1	0.91	0.65	89,89,89,89	0
24	MG	A	1764	1/1	0.91	0.27	104,104,104,104	0
24	MG	A	1751	1/1	0.91	0.25	83,83,83,83	0
24	MG	A	1717	1/1	0.91	0.53	125,125,125,125	0
24	MG	A	1661	1/1	0.91	0.22	121,121,121,121	0
24	MG	A	1688	1/1	0.92	0.15	120,120,120,120	0
24	MG	A	1817	1/1	0.92	0.28	180,180,180,180	0
24	MG	A	1756	1/1	0.92	0.18	101,101,101,101	0
24	MG	A	1780	1/1	0.92	0.70	80,80,80,80	0
24	MG	A	1685	1/1	0.92	0.26	134,134,134,134	0
24	MG	A	1849	1/1	0.92	0.25	74,74,74,74	0
24	MG	A	1742	1/1	0.92	0.35	89,89,89,89	0
24	MG	A	1824	1/1	0.92	0.17	202,202,202,202	0
24	MG	Q	201	1/1	0.92	0.26	84,84,84,84	0
24	MG	A	1680	1/1	0.92	0.22	250,250,250,250	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1737	1/1	0.92	0.35	81,81,81,81	0
24	MG	A	1793	1/1	0.92	0.46	80,80,80,80	0
24	MG	A	1670	1/1	0.92	0.21	109,109,109,109	0
24	MG	A	1681	1/1	0.92	0.10	160,160,160,160	0
24	MG	A	1785	1/1	0.92	0.41	92,92,92,92	0
24	MG	A	1854	1/1	0.92	0.64	89,89,89,89	0
24	MG	A	1845	1/1	0.92	0.20	293,293,293,293	0
24	MG	A	1802	1/1	0.93	0.42	206,206,206,206	0
24	MG	E	201	1/1	0.93	0.57	87,87,87,87	0
24	MG	A	1705	1/1	0.93	0.43	69,69,69,69	0
24	MG	A	1728	1/1	0.93	0.17	95,95,95,95	0
24	MG	A	1844	1/1	0.93	0.44	310,310,310,310	0
24	MG	A	1714	1/1	0.93	0.53	99,99,99,99	0
24	MG	A	1830	1/1	0.93	0.25	273,273,273,273	0
24	MG	A	1786	1/1	0.93	0.31	96,96,96,96	0
24	MG	A	1796	1/1	0.93	0.28	98,98,98,98	0
24	MG	A	1639	1/1	0.93	0.32	73,73,73,73	0
24	MG	A	1684	1/1	0.93	0.28	90,90,90,90	0
24	MG	A	1846	1/1	0.93	0.13	225,225,225,225	0
24	MG	A	1826	1/1	0.93	0.28	354,354,354,354	0
24	MG	A	1782	1/1	0.93	0.17	65,65,65,65	0
24	MG	A	1813	1/1	0.94	0.27	181,181,181,181	0
24	MG	A	1797	1/1	0.94	0.19	94,94,94,94	0
24	MG	A	1810	1/1	0.94	0.34	295,295,295,295	0
24	MG	A	1805	1/1	0.94	0.39	280,280,280,280	0
24	MG	A	1837	1/1	0.94	0.14	244,244,244,244	0
24	MG	A	1748	1/1	0.94	0.26	77,77,77,77	0
24	MG	A	1637	1/1	0.94	0.20	86,86,86,86	0
24	MG	A	1638	1/1	0.94	0.32	87,87,87,87	0
24	MG	A	1832	1/1	0.94	0.18	112,112,112,112	0
24	MG	A	1618	1/1	0.94	0.60	85,85,85,85	0
24	MG	A	1833	1/1	0.94	0.15	335,335,335,335	0
24	MG	A	1806	1/1	0.94	0.51	211,211,211,211	0
24	MG	A	1723	1/1	0.94	0.22	117,117,117,117	0
24	MG	A	1702	1/1	0.94	0.11	163,163,163,163	0
24	MG	A	1620	1/1	0.94	0.19	141,141,141,141	0
24	MG	A	1834	1/1	0.94	0.41	231,231,231,231	0
24	MG	A	1776	1/1	0.94	0.23	96,96,96,96	0
24	MG	A	1692	1/1	0.94	0.17	119,119,119,119	0
24	MG	A	1678	1/1	0.94	0.19	133,133,133,133	0
24	MG	A	1700	1/1	0.94	0.19	272,272,272,272	0
24	MG	A	1698	1/1	0.94	0.16	218,218,218,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1754	1/1	0.95	0.24	105,105,105,105	0
24	MG	A	1699	1/1	0.95	0.49	100,100,100,100	0
24	MG	A	1701	1/1	0.95	0.54	73,73,73,73	0
24	MG	A	1613	1/1	0.95	0.14	88,88,88,88	0
24	MG	A	1647	1/1	0.95	0.17	127,127,127,127	0
24	MG	A	1843	1/1	0.95	0.12	115,115,115,115	0
24	MG	A	1822	1/1	0.95	0.25	209,209,209,209	0
24	MG	A	1829	1/1	0.95	0.19	267,267,267,267	0
24	MG	A	1821	1/1	0.95	0.18	178,178,178,178	0
24	MG	A	1706	1/1	0.95	0.28	174,174,174,174	0
24	MG	A	1788	1/1	0.95	0.19	84,84,84,84	0
24	MG	A	1842	1/1	0.95	0.65	334,334,334,334	0
24	MG	A	1663	1/1	0.95	0.33	94,94,94,94	0
24	MG	A	1840	1/1	0.95	0.21	289,289,289,289	0
24	MG	A	1804	1/1	0.95	0.26	304,304,304,304	0
24	MG	A	1733	1/1	0.95	0.34	68,68,68,68	0
24	MG	A	1734	1/1	0.95	0.19	99,99,99,99	0
24	MG	A	1799	1/1	0.95	0.29	277,277,277,277	0
24	MG	A	1696	1/1	0.95	0.39	99,99,99,99	0
24	MG	A	1839	1/1	0.96	0.23	205,205,205,205	1
24	MG	A	1759	1/1	0.96	0.30	75,75,75,75	0
24	MG	A	1831	1/1	0.96	0.33	160,160,160,160	0
24	MG	A	1629	1/1	0.96	0.06	151,151,151,151	0
24	MG	A	1708	1/1	0.96	0.12	211,211,211,211	0
24	MG	A	1654	1/1	0.96	0.15	97,97,97,97	0
24	MG	A	1729	1/1	0.96	0.72	111,111,111,111	0
24	MG	A	1607	1/1	0.96	0.10	102,102,102,102	0
24	MG	P	101	1/1	0.96	0.41	67,67,67,67	0
24	MG	A	1710	1/1	0.96	0.30	177,177,177,177	0
24	MG	A	1838	1/1	0.96	0.25	181,181,181,181	0
24	MG	A	1627	1/1	0.96	0.23	102,102,102,102	0
24	MG	A	1617	1/1	0.96	0.14	81,81,81,81	0
24	MG	A	1674	1/1	0.96	0.10	125,125,125,125	0
24	MG	A	1716	1/1	0.96	0.09	70,70,70,70	0
25	SRY	A	1860	40/40	0.96	0.17	60,79,97,101	0
24	MG	A	1811	1/1	0.96	0.06	121,121,121,121	0
24	MG	A	1783	1/1	0.96	0.29	89,89,89,89	0
24	MG	A	1635	1/1	0.97	0.15	75,75,75,75	0
24	MG	A	1636	1/1	0.97	0.19	94,94,94,94	0
26	ZN	D	301	1/1	0.97	0.34	114,114,114,114	0
24	MG	A	1713	1/1	0.97	0.08	112,112,112,112	0
24	MG	A	1841	1/1	0.97	0.14	266,266,266,266	0

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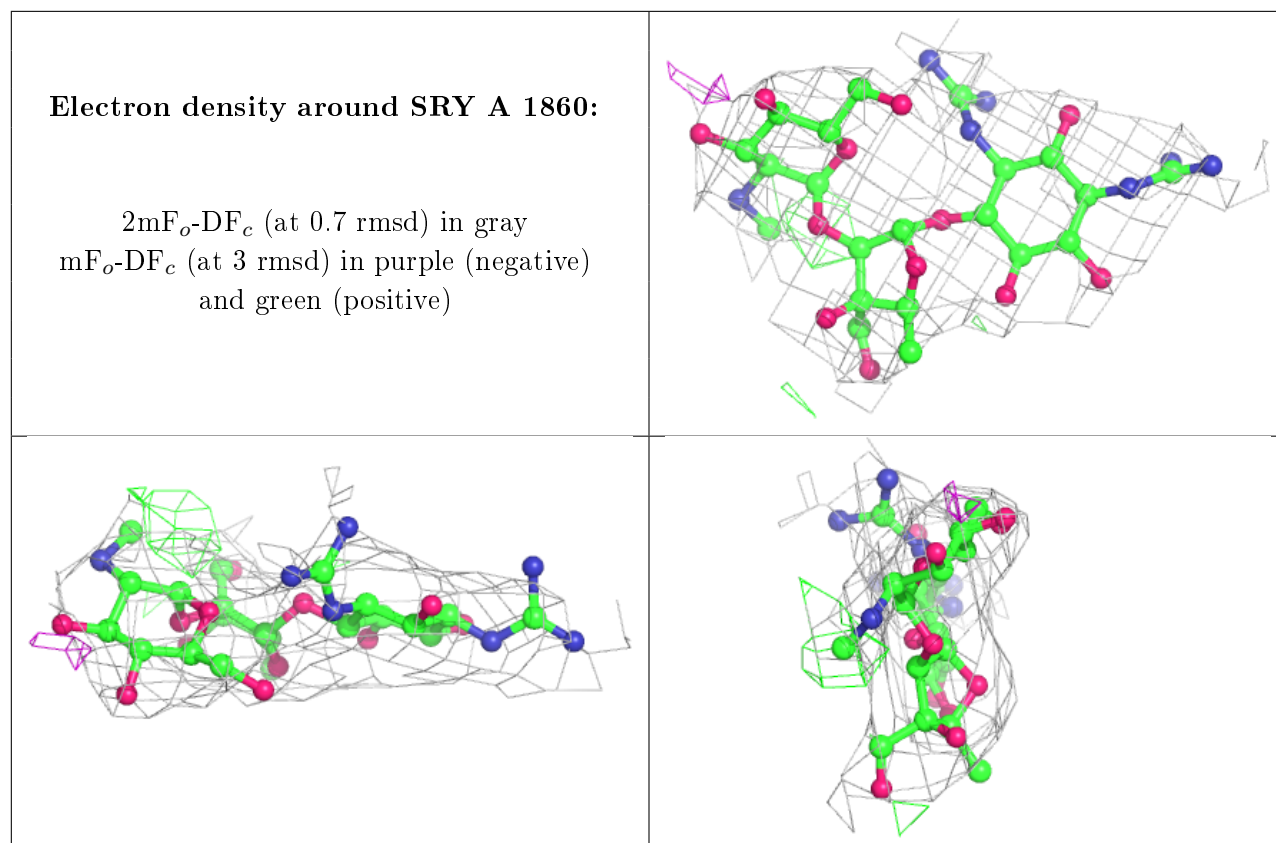
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1675	1/1	0.97	0.12	223,223,223,223	0
24	MG	A	1601	1/1	0.97	0.12	86,86,86,86	0
24	MG	A	1621	1/1	0.97	0.46	131,131,131,131	0
24	MG	D	302	1/1	0.97	0.13	86,86,86,86	0
24	MG	S	101	1/1	0.97	0.22	80,80,80,80	0
24	MG	A	1645	1/1	0.97	0.09	108,108,108,108	0
24	MG	A	1758	1/1	0.97	0.15	70,70,70,70	0
24	MG	A	1778	1/1	0.97	0.33	78,78,78,78	0
24	MG	A	1721	1/1	0.97	0.21	95,95,95,95	0
24	MG	A	1665	1/1	0.97	0.15	99,99,99,99	0
24	MG	A	1823	1/1	0.97	0.22	281,281,281,281	0
24	MG	A	1691	1/1	0.97	0.19	139,139,139,139	0
24	MG	A	1835	1/1	0.97	0.16	299,299,299,299	0
24	MG	A	1763	1/1	0.97	0.16	72,72,72,72	0
24	MG	A	1820	1/1	0.97	0.30	152,152,152,152	0
24	MG	A	1690	1/1	0.97	0.35	193,193,193,193	0
24	MG	A	1604	1/1	0.97	0.10	153,153,153,153	0
24	MG	A	1671	1/1	0.98	0.33	99,99,99,99	0
24	MG	A	1787	1/1	0.98	0.15	78,78,78,78	0
24	MG	A	1602	1/1	0.98	0.11	108,108,108,108	0
24	MG	A	1611	1/1	0.98	0.14	120,120,120,120	0
24	MG	A	1606	1/1	0.98	0.29	87,87,87,87	0
24	MG	A	1648	1/1	0.98	0.10	96,96,96,96	0
24	MG	A	1738	1/1	0.98	0.24	58,58,58,58	0
24	MG	A	1712	1/1	0.98	0.16	107,107,107,107	0
24	MG	A	1741	1/1	0.98	0.20	101,101,101,101	0
24	MG	A	1736	1/1	0.98	0.14	119,119,119,119	0
24	MG	A	1669	1/1	0.98	0.43	134,134,134,134	0
24	MG	A	1608	1/1	0.98	0.48	84,84,84,84	0
24	MG	A	1628	1/1	0.98	0.43	104,104,104,104	0
24	MG	A	1760	1/1	0.98	0.15	101,101,101,101	0
24	MG	A	1612	1/1	0.98	0.19	97,97,97,97	0
24	MG	A	1614	1/1	0.98	0.19	79,79,79,79	0
24	MG	A	1814	1/1	0.98	0.07	113,113,113,113	0
24	MG	A	1610	1/1	0.98	0.14	71,71,71,71	0
24	MG	A	1650	1/1	0.98	0.08	107,107,107,107	0
24	MG	A	1686	1/1	0.98	0.14	194,194,194,194	0
24	MG	A	1735	1/1	0.98	0.38	96,96,96,96	0
24	MG	A	1630	1/1	0.98	0.06	82,82,82,82	0
24	MG	A	1662	1/1	0.98	0.17	145,145,145,145	0
24	MG	A	1668	1/1	0.98	0.19	138,138,138,138	0
24	MG	A	1743	1/1	0.98	0.07	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1640	1/1	0.98	0.07	98,98,98,98	0
24	MG	A	1642	1/1	0.98	0.04	112,112,112,112	0
24	MG	A	1664	1/1	0.98	0.35	131,131,131,131	0
24	MG	A	1619	1/1	0.98	0.14	72,72,72,72	0
24	MG	A	1660	1/1	0.98	0.06	104,104,104,104	0
24	MG	A	1707	1/1	0.99	0.27	163,163,163,163	0
24	MG	A	1704	1/1	0.99	0.26	116,116,116,116	0
24	MG	A	1616	1/1	0.99	0.04	93,93,93,93	0
24	MG	A	1677	1/1	0.99	0.11	113,113,113,113	0
24	MG	A	1693	1/1	0.99	0.11	192,192,192,192	0
24	MG	A	1703	1/1	0.99	0.26	106,106,106,106	0
24	MG	A	1828	1/1	0.99	0.15	284,284,284,284	0
24	MG	A	1624	1/1	0.99	0.26	97,97,97,97	0
26	ZN	N	101	1/1	0.99	0.11	129,129,129,129	0
24	MG	A	1651	1/1	0.99	0.14	143,143,143,143	0
24	MG	A	1631	1/1	0.99	0.13	101,101,101,101	0
24	MG	A	1632	1/1	0.99	0.12	76,76,76,76	0
24	MG	A	1605	1/1	0.99	0.08	72,72,72,72	0
24	MG	A	1643	1/1	0.99	0.26	99,99,99,99	0
24	MG	A	1715	1/1	0.99	0.13	89,89,89,89	0
24	MG	A	1649	1/1	0.99	0.30	51,51,51,51	0
24	MG	A	1623	1/1	0.99	0.12	84,84,84,84	0
24	MG	A	1694	1/1	0.99	0.14	116,116,116,116	0
24	MG	A	1626	1/1	0.99	0.20	103,103,103,103	0
24	MG	A	1775	1/1	0.99	0.10	114,114,114,114	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.