



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:45 PM UTC

PDB ID : 4LF5 / pdb\_00004lf5  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Belardinelli, R.; Carr, J.; Murphy IV, F.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-06-26  
Resolution : 3.75 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

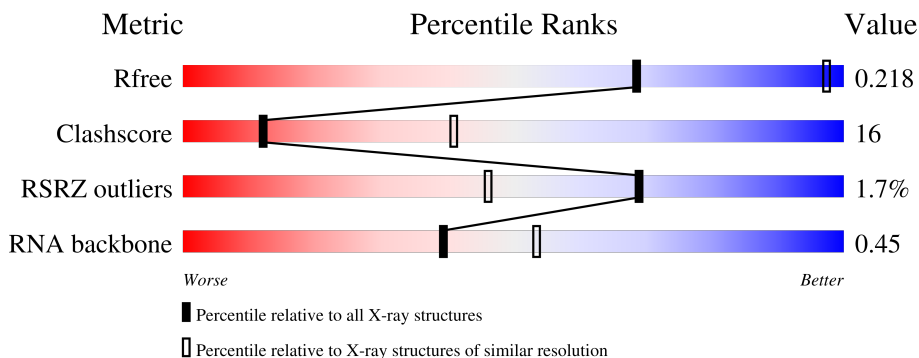
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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))
$R_{free}$	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)
RNA backbone	3983	1001 (4.40-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	 % 45% 44% 10% ..
2	B	256	 % 54% 37% 8%
3	C	239	 2% 45% 41% 13%
4	D	209	 5% 52% 45%
5	E	162	 51% 41% 7%
6	F	101	 62% 36%

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Mol	Chain	Length	Quality of chain
7	G	156	<p>2% 63% 34% ..</p>
8	H	138	<p>48% 50% .</p>
9	I	128	<p>3% 59% 40% .</p>
10	J	105	<p>50% 39% 5% . 6%</p>
11	K	129	<p>2% 51% 40% . 8%</p>
12	L	135	<p>2% 62% 29% . 7%</p>
13	M	126	<p>3% 56% 36% . 6%</p>
14	N	61	<p>8% 39% 59% .</p>
15	O	89	<p>60% 39% .</p>
16	P	88	<p>68% 26% . 5%</p>
17	Q	105	<p>58% 34% . 6%</p>
18	R	88	<p>39% 44% 17%</p>
19	S	93	<p>5% 53% 33% . 13%</p>
20	T	106	<p>3% 54% 37% . 7%</p>
21	U	27	<p>11% 41% 52% 7%</p>

## 2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 51823 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	1513	32522	14483	6016	10511	1512	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1533	C	A	conflict	GB M26923.1
A	1534	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1874	1195	336	338	5	0	0	1

- Molecule 3 is a protein called 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 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 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 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 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 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 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 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 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 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 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 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 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 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 ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called 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 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 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 ribosomal protein THX.

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

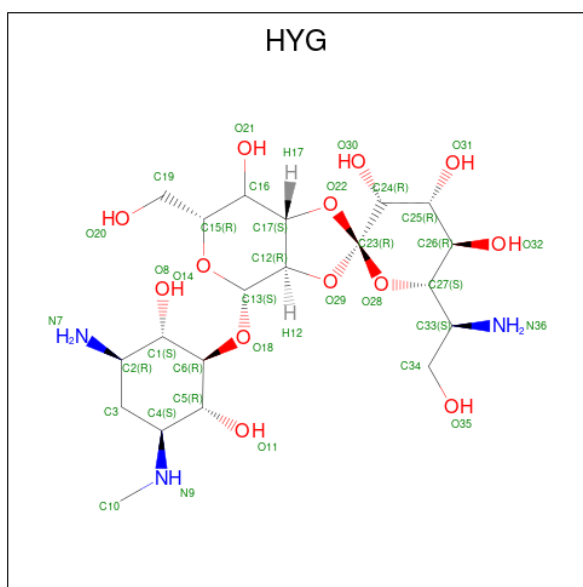
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	108	Total	Mg	0	0
			108	108		
22	B	1	Total	Mg	0	0
			1	1		
22	D	2	Total	Mg	0	0
			2	2		
22	E	1	Total	Mg	0	0
			1	1		
22	H	2	Total	Mg	0	0
			2	2		
22	K	1	Total	Mg	0	0
			1	1		
22	L	1	Total	Mg	0	0
			1	1		
22	M	1	Total	Mg	0	0
			1	1		
22	S	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total	K	0	0
			8	8		

- Molecule 24 is HYGROMYCIN B (CCD ID: HYG) (formula: C<sub>20</sub>H<sub>37</sub>N<sub>3</sub>O<sub>13</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	36	20	3	13	0	0

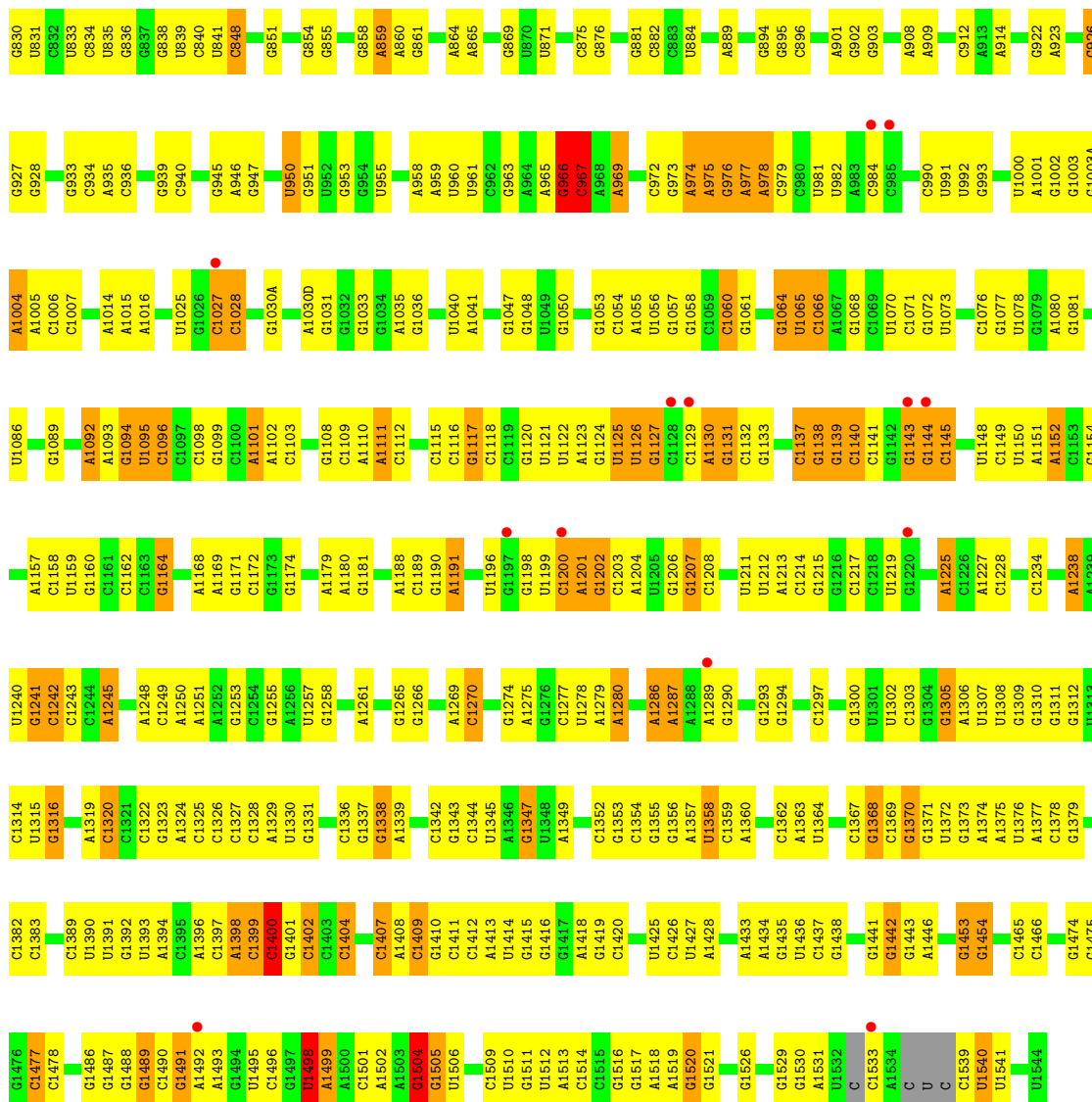
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

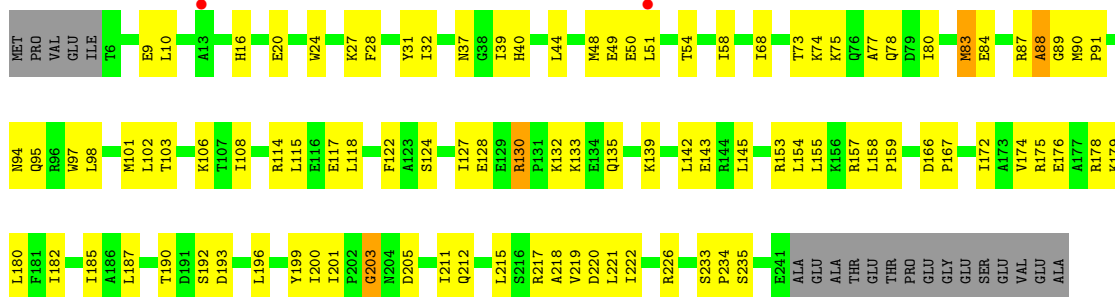
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
26	A	11	11	11	0	0
26	E	6	6	6	0	0
26	Q	1	1	1	0	0

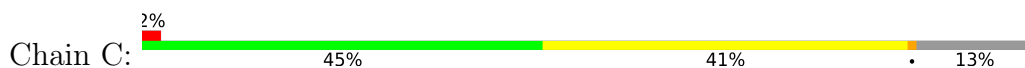




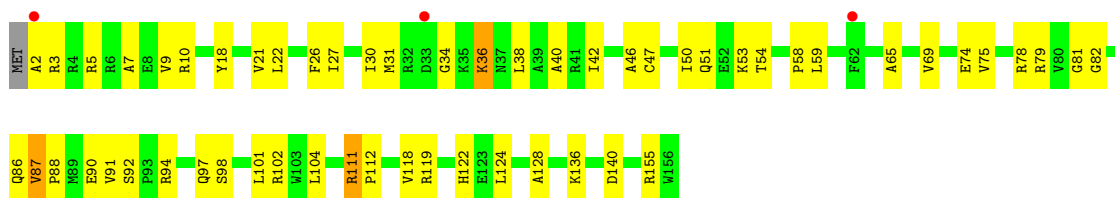
• Molecule 2: ribosomal protein S2



• Molecule 3: ribosomal protein S3

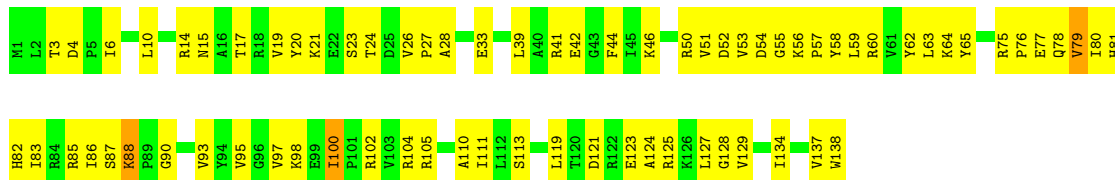






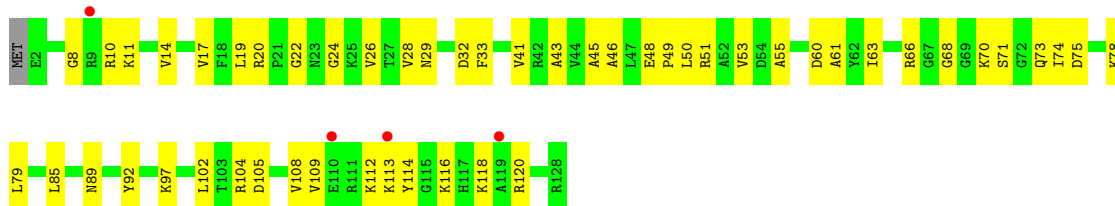
- Molecule 8: ribosomal protein S8

Chain H: 48% 50%



- Molecule 9: ribosomal protein S9

Chain I: 3% 59% 40%



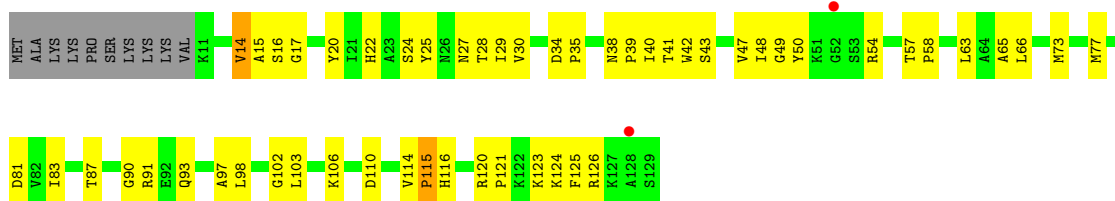
- Molecule 10: ribosomal protein S10

Chain J: 50% 39% 5% 6%

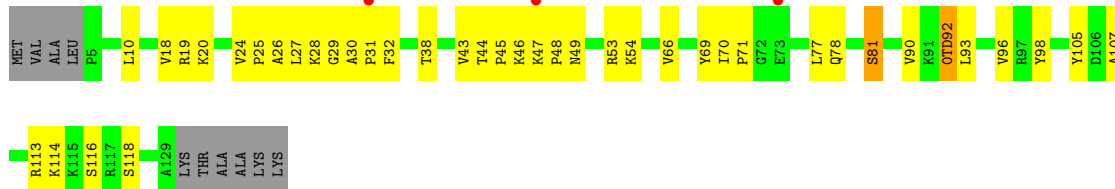


- Molecule 11: ribosomal protein S11

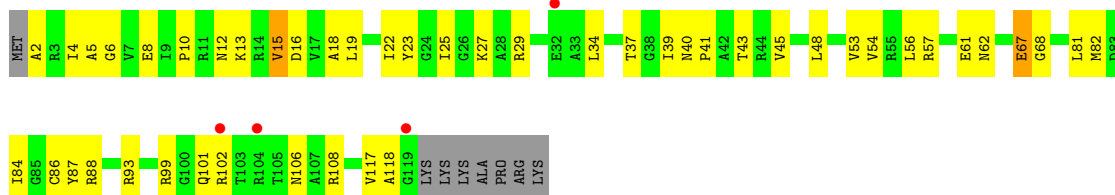
Chain K: 2% 51% 40% 8%



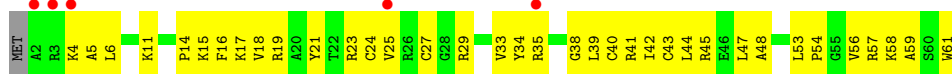
- Molecule 12: ribosomal protein S12



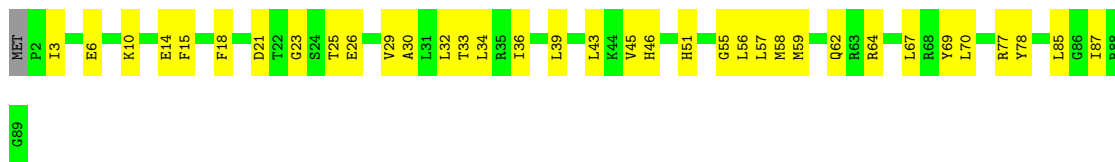
- Molecule 13: ribosomal protein S13



- Molecule 14: ribosomal protein S14



- Molecule 15: ribosomal protein S15



- Molecule 16: ribosomal protein S16



- Molecule 17: ribosomal protein S17





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.83Å 401.83Å 174.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.59 – 3.75 34.59 – 3.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.59-3.75) 97.4 (34.59-3.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.76Å)	Xtrriage
Refinement program	PHENIX dev_1119	Depositor
R, $R_{free}$	0.163 , 0.218 (Not available) , 0.218	Depositor DCC
$R_{free}$ test set	7022 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	137.9	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 115.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	51823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: M2G, 7MG, 0TD, K, PSU, 4OC, HYG, ZN, MG, 5MC, 2MG, UR3

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	0.45	0/36113	0.63	7/56360 (0.0%)
2	B	0.75	0/1909	1.08	5/2579 (0.2%)
3	C	0.54	0/1637	0.98	5/2207 (0.2%)
4	D	0.67	0/1733	1.14	16/2318 (0.7%)
5	E	0.96	1/1163 (0.1%)	1.32	11/1566 (0.7%)
6	F	0.60	0/856	1.04	5/1154 (0.4%)
7	G	0.62	0/1276	1.03	6/1709 (0.4%)
8	H	1.03	1/1136 (0.1%)	1.31	10/1527 (0.7%)
9	I	0.61	0/1029	1.01	1/1379 (0.1%)
10	J	0.58	0/806	1.19	9/1084 (0.8%)
11	K	0.74	0/900	1.19	7/1213 (0.6%)
12	L	0.77	0/978	1.24	9/1308 (0.7%)
13	M	0.68	1/947 (0.1%)	1.09	4/1270 (0.3%)
14	N	0.59	0/501	0.96	0/664
15	O	0.84	0/745	1.01	0/992
16	P	0.79	0/717	1.16	4/965 (0.4%)
17	Q	0.91	1/836 (0.1%)	1.24	3/1117 (0.3%)
18	R	0.68	0/604	1.13	5/801 (0.6%)
19	S	0.58	0/662	1.03	3/892 (0.3%)
20	T	0.74	0/765	1.14	6/1007 (0.6%)
21	U	0.51	0/213	0.90	0/279
All	All	0.56	4/55526 (0.0%)	0.82	116/82391 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
10	J	0	2
18	R	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	11	ILE	CA-CB	-6.07	1.47	1.54
17	Q	9	VAL	CA-CB	-5.27	1.48	1.54
8	H	79	VAL	CA-CB	-5.24	1.47	1.54
13	M	106	ASN	CA-C	-5.09	1.48	1.53

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	13	HIS	CB-CA-C	-10.11	104.91	116.54
4	D	26	CYS	N-CA-C	-9.18	102.08	113.28
12	L	26	ALA	N-CA-C	-8.99	102.45	113.15
10	J	13	HIS	N-CA-C	8.35	121.00	108.31
7	G	111	ARG	CA-C-N	8.13	127.71	118.85

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	ARG	Peptide
2	B	88	ALA	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
10	J	12	ASP	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32522	0	16437	647	0
2	B	1874	0	1887	78	0
3	C	1613	0	1677	79	0
4	D	1703	0	1763	84	0
5	E	1147	0	1207	53	0
6	F	843	0	857	34	0
7	G	1257	0	1296	48	0
8	H	1116	0	1177	52	0
9	I	1010	0	1037	42	0
10	J	793	0	835	43	0
11	K	885	0	904	37	0
12	L	973	0	1058	35	0
13	M	937	0	995	42	0
14	N	492	0	529	44	0
15	O	734	0	771	32	0
16	P	701	0	720	16	0
17	Q	823	0	891	36	0
18	R	598	0	670	30	0
19	S	648	0	673	24	0
20	T	763	0	861	34	0
21	U	209	0	221	20	0
22	A	108	0	0	0	0
22	B	1	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	H	2	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
22	S	1	0	0	0	0
23	A	8	0	0	0	0
24	A	36	0	37	4	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	11	0	0	0	0
26	E	6	0	0	0	0
26	Q	1	0	0	0	0
All	All	51823	0	36503	1355	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 16.

The worst 5 of 1355 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:538:G:H5''	12:L:114:LYS:HB2	1.55	0.88
16:P:57:ARG:NH1	16:P:79:VAL:O	2.07	0.86
1:A:279:A:OP2	17:Q:95:TYR:OH	1.93	0.85
1:A:959:A:HO2'	1:A:984:C:HO2'	1.18	0.85
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.57	0.85

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	288 (19%)	0

5 of 288 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	38	G
1	A	39	G

There are no RNA pucker outliers to report.

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

13 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	PSU	A	516	22,1	18,21,22	1.11	1 (5%)	21,30,33	1.62	3 (14%)
1	7MG	A	527	1	23,26,27	4.08	4 (17%)	27,39,42	2.26	9 (33%)
1	5MC	A	1404	1	19,22,23	0.93	2 (10%)	26,32,35	1.04	4 (15%)
1	UR3	A	1498	1	19,22,23	0.91	1 (5%)	26,32,35	1.14	0
1	5MC	A	1407	1	19,22,23	1.66	3 (15%)	26,32,35	1.28	4 (15%)
1	PSU	A	1541	1	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
1	PSU	A	1540	1	18,21,22	1.17	2 (11%)	21,30,33	1.94	6 (28%)
1	M2G	A	966	1	24,27,28	1.32	2 (8%)	33,40,43	0.90	2 (6%)
12	0TD	L	92	12	8,9,10	1.70	1 (12%)	6,11,13	2.64	4 (66%)
1	4OC	A	1402	1	20,23,24	1.13	1 (5%)	25,32,35	0.68	0
1	2MG	A	1207	1	23,26,27	1.51	5 (21%)	33,38,41	1.10	3 (9%)
1	5MC	A	1400	1	19,22,23	1.34	2 (10%)	26,32,35	0.99	1 (3%)
1	5MC	A	967	1	19,22,23	0.95	0	26,32,35	1.02	1 (3%)

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	PSU	A	516	22,1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	4/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	0TD	L	92	12	-	2/7/12/14	-
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	1/9/27/28	0/3/3/3
1	5MC	A	1400	1	-	6/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-17.79	1.34	1.45
1	A	527	7MG	C5-N7	4.99	1.42	1.35
1	A	1407	5MC	C5-C4	4.88	1.47	1.44
1	A	527	7MG	C2-N2	4.57	1.44	1.34
1	A	966	M2G	C2-N2	4.05	1.42	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.37	120.40	110.94
1	A	1540	PSU	C4-N3-C2	-4.82	119.73	126.37
1	A	1541	PSU	N1-C2-N3	4.78	120.21	115.17
1	A	1541	PSU	C4-N3-C2	-4.73	119.86	126.37
1	A	527	7MG	C2-N3-C4	4.73	120.44	112.30

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	527	7MG	1	0
1	A	1404	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	1	0
1	A	1407	5MC	1	0
1	A	1540	PSU	1	0
1	A	966	M2G	1	0
12	L	92	0TD	5	0
1	A	1207	2MG	3	0
1	A	1400	5MC	2	0
1	A	967	5MC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 128 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
24	HYG	A	1717	-	36,39,39	1.94	8 (22%)	44,60,60	2.69	14 (31%)

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
24	HYG	A	1717	-	-	6/12/87/87	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1717	HYG	C27-C33	6.55	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1717	HYG	C34-C33	3.73	1.58	1.52
24	A	1717	HYG	C5-C4	3.51	1.59	1.52
24	A	1717	HYG	C4-N9	3.23	1.50	1.47
24	A	1717	HYG	C16-C15	3.22	1.59	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1717	HYG	O29-C12-C13	7.25	129.40	110.89
24	A	1717	HYG	O18-C13-C12	7.20	123.08	109.09
24	A	1717	HYG	O28-C27-C26	6.21	117.19	108.50
24	A	1717	HYG	C13-O14-C15	4.73	122.96	113.72
24	A	1717	HYG	O14-C15-C16	4.61	118.00	109.70

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

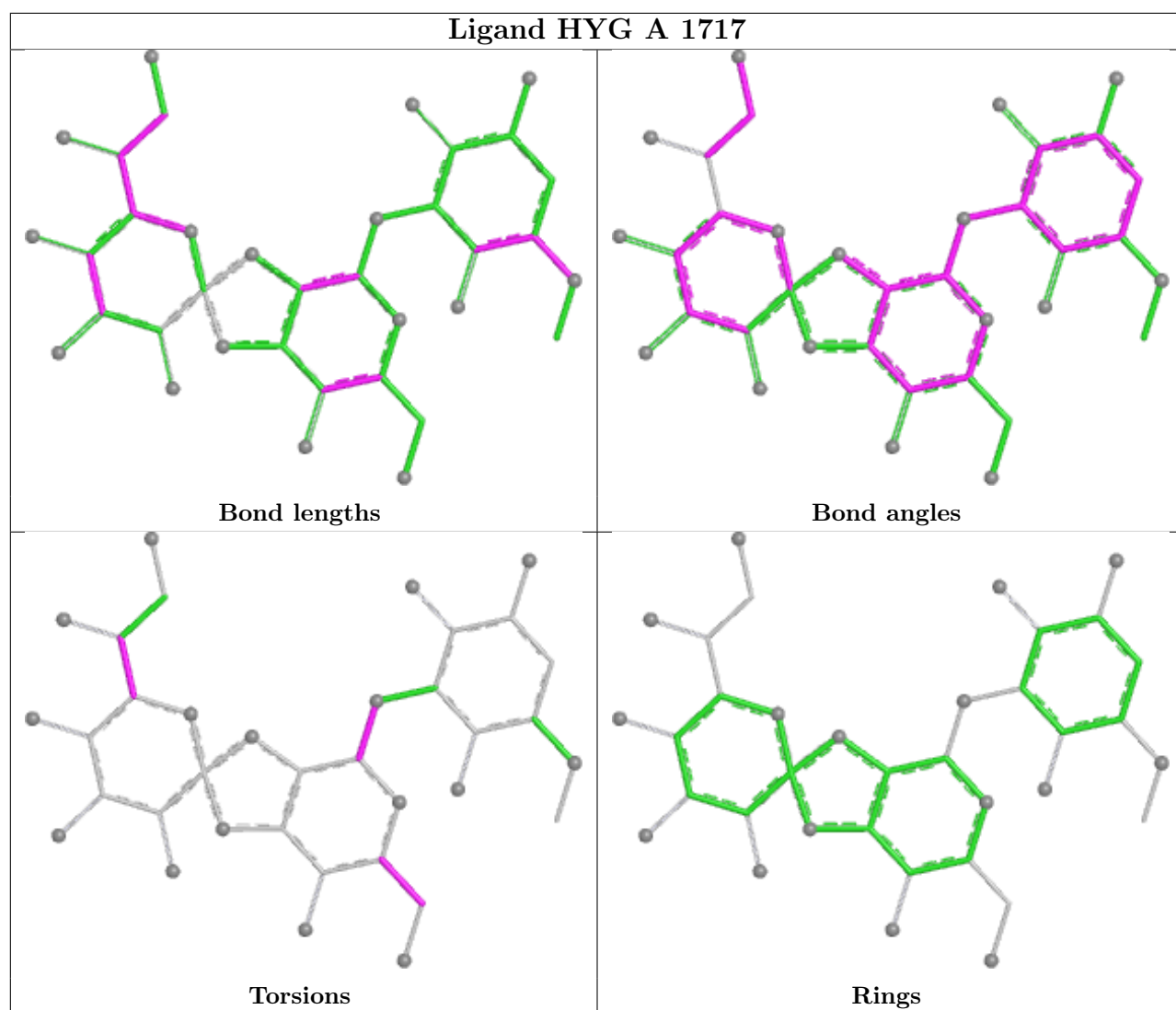
Mol	Chain	Res	Type	Atoms
24	A	1717	HYG	C26-C27-C33-C34
24	A	1717	HYG	O28-C27-C33-C34
24	A	1717	HYG	O14-C13-O18-C6
24	A	1717	HYG	O14-C15-C19-O20
24	A	1717	HYG	C16-C15-C19-O20

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1717	HYG	4	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	1501/1522 (98%)	-0.38	20 (1%) 75 52	69, 132, 256, 360	0
2	B	236/256 (92%)	-0.46	2 (0%) 82 62	77, 136, 231, 275	0
3	C	207/239 (86%)	-0.17	4 (1%) 66 44	94, 196, 235, 248	0
4	D	208/209 (99%)	-0.16	10 (4%) 35 26	87, 136, 186, 207	0
5	E	151/162 (93%)	-0.55	0 100 100	62, 100, 148, 192	0
6	F	101/101 (100%)	-0.52	0 100 100	114, 152, 178, 202	0
7	G	155/156 (99%)	-0.25	3 (1%) 66 44	125, 174, 240, 276	0
8	H	138/138 (100%)	-0.67	0 100 100	65, 91, 134, 149	0
9	I	127/128 (99%)	0.01	4 (3%) 51 34	145, 190, 236, 264	0
10	J	99/105 (94%)	-0.02	0 100 100	81, 213, 309, 332	0
11	K	119/129 (92%)	-0.38	2 (1%) 69 46	88, 126, 169, 206	0
12	L	124/135 (91%)	-0.23	3 (2%) 59 40	64, 126, 162, 245	0
13	M	118/126 (93%)	-0.17	4 (3%) 48 32	133, 163, 190, 230	0
14	N	60/61 (98%)	0.41	5 (8%) 17 16	152, 187, 233, 271	0
15	O	88/89 (98%)	-0.48	0 100 100	85, 119, 169, 220	0
16	P	84/88 (95%)	-0.31	0 100 100	89, 128, 167, 247	0
17	Q	99/105 (94%)	-0.45	0 100 100	73, 110, 148, 169	0
18	R	73/88 (82%)	-0.48	0 100 100	82, 126, 207, 231	0
19	S	81/93 (87%)	0.08	5 (6%) 26 21	96, 206, 253, 294	0
20	T	99/106 (93%)	-0.23	3 (3%) 52 35	98, 133, 180, 200	0
21	U	25/27 (92%)	0.58	3 (12%) 9 11	80, 173, 190, 263	0
All	All	3893/4063 (95%)	-0.32	68 (1%) 69 46	62, 141, 236, 360	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	3	ARG	5.5
1	A	202	U	5.2
20	T	106	ALA	4.9
12	L	73	GLU	4.0
1	A	985	C	3.9

## 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	1540	20/21	0.85	0.12	325,348,352,353	0
1	PSU	A	1541	20/21	0.91	0.10	333,344,359,360	0
1	PSU	A	516	20/21	0.94	0.10	137,146,155,158	0
1	2MG	A	1207	24/25	0.95	0.09	200,220,224,230	0
1	7MG	A	527	24/25	0.96	0.07	97,110,123,130	0
1	5MC	A	1407	21/22	0.96	0.10	142,156,190,190	0
1	UR3	A	1498	21/22	0.96	0.11	115,129,138,150	0
1	M2G	A	966	25/26	0.96	0.09	130,149,169,172	0
1	5MC	A	967	21/22	0.96	0.07	128,135,143,146	0
1	5MC	A	1400	21/22	0.97	0.06	100,115,125,129	0
1	5MC	A	1404	21/22	0.97	0.06	97,110,130,136	0
12	0TD	L	92	10/11	0.97	0.09	130,150,216,313	0
1	4OC	A	1402	22/23	0.98	0.09	102,122,130,137	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
22	MG	A	1711	1/1	0.33	0.27	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1609	1/1	0.69	0.22	119,119,119,119	0
23	K	A	1704	1/1	0.70	0.22	148,148,148,148	0
22	MG	D	302	1/1	0.73	0.23	112,112,112,112	0
22	MG	A	1709	1/1	0.74	0.20	130,130,130,130	0
22	MG	A	1643	1/1	0.74	0.27	131,131,131,131	0
22	MG	H	202	1/1	0.75	0.14	100,100,100,100	0
22	MG	A	1641	1/1	0.77	0.21	80,80,80,80	0
22	MG	A	1663	1/1	0.79	0.11	107,107,107,107	0
22	MG	A	1715	1/1	0.80	0.06	434,434,434,434	0
22	MG	A	1710	1/1	0.80	0.13	71,71,71,71	0
22	MG	A	1633	1/1	0.81	0.12	92,92,92,92	0
22	MG	A	1666	1/1	0.81	0.20	130,130,130,130	0
22	MG	A	1690	1/1	0.81	0.27	84,84,84,84	0
22	MG	A	1608	1/1	0.81	0.36	70,70,70,70	0
22	MG	A	1629	1/1	0.81	0.21	46,46,46,46	0
23	K	A	1706	1/1	0.81	0.15	146,146,146,146	0
22	MG	A	1610	1/1	0.82	0.30	62,62,62,62	0
22	MG	A	1664	1/1	0.82	0.22	75,75,75,75	0
22	MG	A	1635	1/1	0.82	0.36	74,74,74,74	0
22	MG	A	1713	1/1	0.83	0.15	136,136,136,136	0
22	MG	A	1646	1/1	0.84	0.08	127,127,127,127	0
23	K	A	1699	1/1	0.85	0.24	142,142,142,142	0
22	MG	D	303	1/1	0.85	0.18	88,88,88,88	0
22	MG	A	1712	1/1	0.85	0.21	88,88,88,88	0
22	MG	A	1619	1/1	0.86	0.21	79,79,79,79	0
23	K	A	1702	1/1	0.86	0.18	161,161,161,161	0
22	MG	H	201	1/1	0.86	0.18	72,72,72,72	0
23	K	A	1705	1/1	0.86	0.17	157,157,157,157	0
22	MG	A	1606	1/1	0.86	0.48	99,99,99,99	0
22	MG	A	1655	1/1	0.87	0.20	102,102,102,102	0
22	MG	A	1658	1/1	0.87	0.34	70,70,70,70	0
22	MG	A	1644	1/1	0.87	0.21	109,109,109,109	0
22	MG	A	1648	1/1	0.88	0.20	81,81,81,81	0
22	MG	A	1603	1/1	0.88	0.15	64,64,64,64	0
22	MG	S	101	1/1	0.88	0.19	114,114,114,114	0
22	MG	A	1637	1/1	0.88	0.27	63,63,63,63	0
24	HYG	A	1717	36/36	0.88	0.15	144,215,236,246	0
22	MG	A	1657	1/1	0.89	0.08	127,127,127,127	0
22	MG	A	1670	1/1	0.89	0.11	91,91,91,91	0
22	MG	A	1651	1/1	0.89	0.21	73,73,73,73	0
22	MG	A	1654	1/1	0.89	0.42	84,84,84,84	0
22	MG	A	1614	1/1	0.89	0.33	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1630	1/1	0.90	0.18	56,56,56,56	0
22	MG	A	1650	1/1	0.90	0.28	59,59,59,59	0
22	MG	A	1616	1/1	0.90	0.16	101,101,101,101	0
22	MG	B	301	1/1	0.90	0.16	101,101,101,101	0
22	MG	A	1652	1/1	0.90	0.36	71,71,71,71	0
22	MG	A	1665	1/1	0.91	0.34	86,86,86,86	0
22	MG	A	1645	1/1	0.91	0.08	135,135,135,135	0
22	MG	A	1634	1/1	0.91	0.30	83,83,83,83	0
22	MG	A	1671	1/1	0.91	0.23	94,94,94,94	0
22	MG	A	1675	1/1	0.91	0.16	91,91,91,91	0
22	MG	A	1611	1/1	0.91	0.23	106,106,106,106	0
22	MG	A	1612	1/1	0.92	0.21	66,66,66,66	0
22	MG	A	1632	1/1	0.92	0.29	86,86,86,86	0
22	MG	A	1667	1/1	0.92	0.14	73,73,73,73	0
22	MG	A	1618	1/1	0.92	0.25	40,40,40,40	0
23	K	A	1701	1/1	0.92	0.13	100,100,100,100	0
22	MG	A	1692	1/1	0.93	0.22	167,167,167,167	0
22	MG	A	1696	1/1	0.93	0.29	73,73,73,73	0
22	MG	A	1628	1/1	0.93	0.16	55,55,55,55	0
22	MG	M	201	1/1	0.93	0.08	113,113,113,113	0
22	MG	A	1685	1/1	0.93	0.19	91,91,91,91	0
22	MG	A	1668	1/1	0.93	0.31	77,77,77,77	0
22	MG	A	1615	1/1	0.94	0.23	40,40,40,40	0
22	MG	A	1631	1/1	0.94	0.18	57,57,57,57	0
22	MG	A	1687	1/1	0.94	0.20	89,89,89,89	0
22	MG	A	1642	1/1	0.94	0.15	103,103,103,103	0
22	MG	A	1607	1/1	0.94	0.26	90,90,90,90	0
22	MG	A	1649	1/1	0.94	0.29	80,80,80,80	0
22	MG	A	1707	1/1	0.94	0.08	76,76,76,76	0
22	MG	A	1673	1/1	0.94	0.17	48,48,48,48	0
22	MG	A	1674	1/1	0.94	0.25	49,49,49,49	0
22	MG	A	1677	1/1	0.95	0.12	40,40,40,40	0
22	MG	K	201	1/1	0.95	0.14	59,59,59,59	0
22	MG	A	1684	1/1	0.95	0.05	141,141,141,141	0
22	MG	A	1669	1/1	0.95	0.30	59,59,59,59	0
22	MG	A	1636	1/1	0.95	0.26	54,54,54,54	0
23	K	A	1700	1/1	0.95	0.16	130,130,130,130	0
22	MG	A	1604	1/1	0.95	0.14	98,98,98,98	0
22	MG	A	1617	1/1	0.95	0.17	29,29,29,29	0
23	K	A	1703	1/1	0.95	0.20	166,166,166,166	0
22	MG	A	1602	1/1	0.95	0.33	54,54,54,54	0
22	MG	A	1647	1/1	0.95	0.10	50,50,50,50	0

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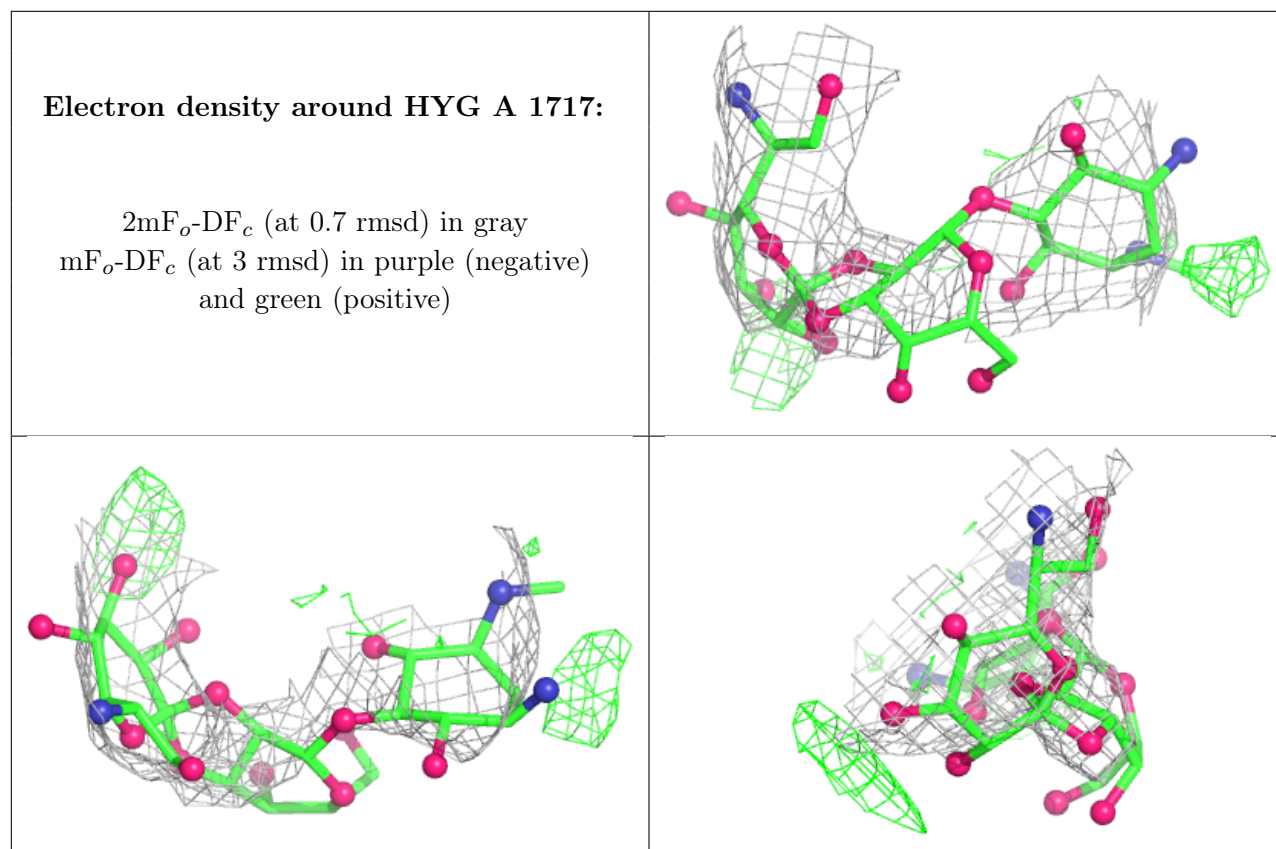
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	E	201	1/1	0.95	0.05	301,301,301,301	0
22	MG	A	1676	1/1	0.95	0.13	89,89,89,89	0
22	MG	A	1682	1/1	0.96	0.30	61,61,61,61	0
22	MG	A	1672	1/1	0.96	0.24	37,37,37,37	0
22	MG	A	1662	1/1	0.96	0.55	64,64,64,64	0
22	MG	A	1639	1/1	0.96	0.23	72,72,72,72	0
22	MG	A	1656	1/1	0.96	0.50	66,66,66,66	0
22	MG	A	1716	1/1	0.96	0.05	320,320,320,320	0
22	MG	A	1653	1/1	0.96	0.09	74,74,74,74	0
22	MG	A	1694	1/1	0.96	0.11	82,82,82,82	0
22	MG	A	1627	1/1	0.96	0.19	47,47,47,47	0
22	MG	A	1679	1/1	0.96	0.26	78,78,78,78	0
22	MG	A	1708	1/1	0.96	0.07	65,65,65,65	0
22	MG	A	1681	1/1	0.96	0.10	76,76,76,76	0
22	MG	A	1625	1/1	0.97	0.10	65,65,65,65	0
22	MG	A	1686	1/1	0.97	0.32	102,102,102,102	0
22	MG	A	1601	1/1	0.97	0.40	52,52,52,52	0
22	MG	A	1688	1/1	0.97	0.09	62,62,62,62	0
22	MG	A	1678	1/1	0.97	0.11	72,72,72,72	0
22	MG	A	1714	1/1	0.97	0.08	118,118,118,118	0
22	MG	A	1638	1/1	0.97	0.13	55,55,55,55	0
22	MG	A	1613	1/1	0.97	0.21	65,65,65,65	0
22	MG	A	1695	1/1	0.97	0.04	103,103,103,103	0
22	MG	A	1620	1/1	0.97	0.15	89,89,89,89	0
22	MG	A	1697	1/1	0.97	0.11	117,117,117,117	0
22	MG	A	1683	1/1	0.97	0.11	76,76,76,76	0
22	MG	A	1623	1/1	0.97	0.22	55,55,55,55	0
22	MG	A	1622	1/1	0.98	0.24	55,55,55,55	0
22	MG	A	1640	1/1	0.98	0.07	88,88,88,88	0
22	MG	A	1698	1/1	0.98	0.07	70,70,70,70	0
22	MG	A	1689	1/1	0.98	0.05	86,86,86,86	0
22	MG	A	1605	1/1	0.98	0.14	67,67,67,67	0
22	MG	A	1691	1/1	0.98	0.07	81,81,81,81	0
22	MG	A	1621	1/1	0.98	0.10	61,61,61,61	0
22	MG	A	1693	1/1	0.98	0.04	60,60,60,60	0
22	MG	A	1626	1/1	0.98	0.03	88,88,88,88	0
22	MG	A	1660	1/1	0.98	0.04	64,64,64,64	0
22	MG	L	201	1/1	0.98	0.03	107,107,107,107	0
25	ZN	D	301	1/1	0.98	0.21	119,119,119,119	0
22	MG	A	1659	1/1	0.99	0.10	84,84,84,84	0
22	MG	A	1624	1/1	0.99	0.04	71,71,71,71	0
22	MG	A	1661	1/1	0.99	0.04	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1680	1/1	0.99	0.11	88,88,88,88	0
25	ZN	N	101	1/1	0.99	0.06	199,199,199,199	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.