



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 09:31 AM EDT

PDB ID : 4LF6  
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 : 3.31 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

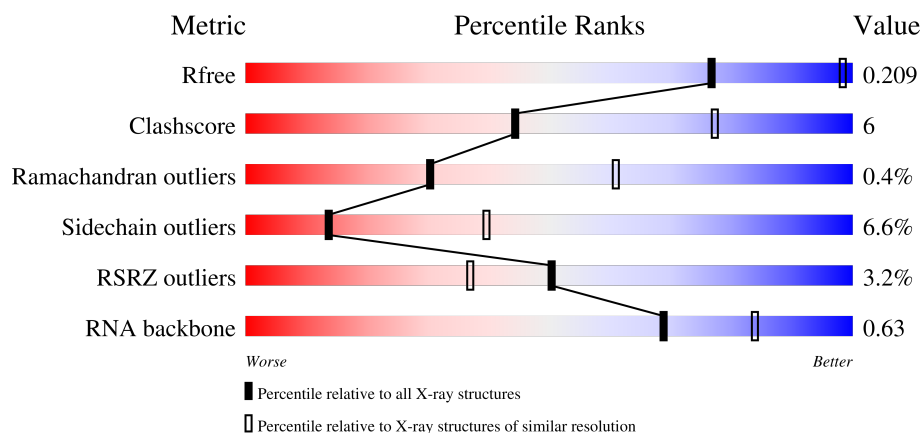
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 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))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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 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	<div> <div>4%</div> <div>69% 25% 5% ..</div> </div>
2	B	256	<div> <div>4%</div> <div>72% 20% 8%</div> </div>
3	C	239	<div> <div>4%</div> <div>64% 21% 13%</div> </div>
4	D	209	<div> <div>4%</div> <div>78% 18% .</div> </div>

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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	

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
22	MG	A	1602	-	-	-	X
22	MG	A	1615	-	-	-	X
22	MG	A	1655	-	-	-	X
22	MG	A	1658	-	-	-	X
22	MG	A	1667	-	-	-	X
22	MG	A	1762	-	-	-	X
22	MG	A	1772	-	-	-	X
22	MG	A	1781	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1787	-	-	-	X
22	MG	A	1788	-	-	-	X
22	MG	A	1795	-	-	-	X
22	MG	A	1800	-	-	-	X
22	MG	A	1802	-	-	-	X
22	MG	N	102	-	-	-	X
23	K	A	1735	-	-	-	X
23	K	A	1741	-	-	-	X
23	K	A	1750	-	-	-	X
23	K	A	1755	-	-	-	X

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52131 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
1	A	1510	Total	C	N	O	P	0	0	0
			32462	14456	6009	10488	1509			

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
2	B	236	Total	C	N	O	S	0	0	1
			1874	1195	336	338	5			

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

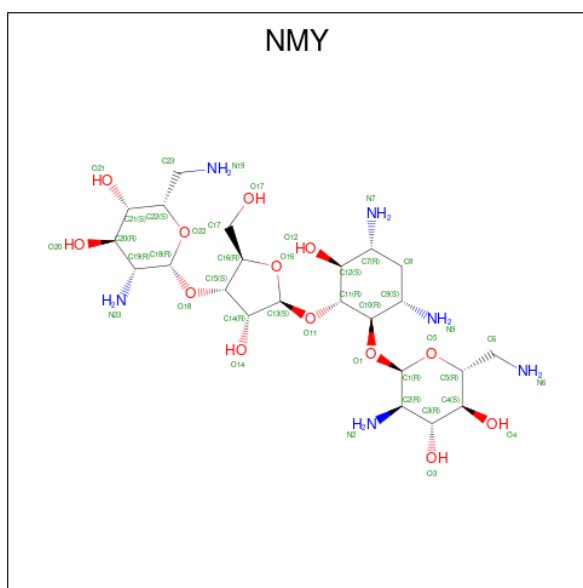
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	201	Total	Mg	0	0
			201	201		
22	B	3	Total	Mg	0	0
			3	3		
22	C	2	Total	Mg	0	0
			2	2		
22	D	2	Total	Mg	0	0
			2	2		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	H	2	Total	Mg	0	0
			2	2		
22	L	1	Total	Mg	0	0
			1	1		
22	M	2	Total	Mg	0	0
			2	2		
22	N	2	Total	Mg	0	0
			2	2		
22	P	2	Total	Mg	0	0
			2	2		
22	Q	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	30	Total	K	0	0
			30	30		



- Molecule 24 is NEOMYCIN (three-letter code: NMY) (formula:  $C_{23}H_{46}N_6O_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	6	13		
24	A	1	Total	C	N	O	0	0
			42	23	6	13		
24	A	1	Total	C	N	O	0	0
			42	23	6	13		
24	A	1	Total	C	N	O	0	0
			42	23	6	13		
24	A	1	Total	C	N	O	0	0
			42	23	6	13		
24	A	1	Total	C	N	O	0	0
			42	23	6	13		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

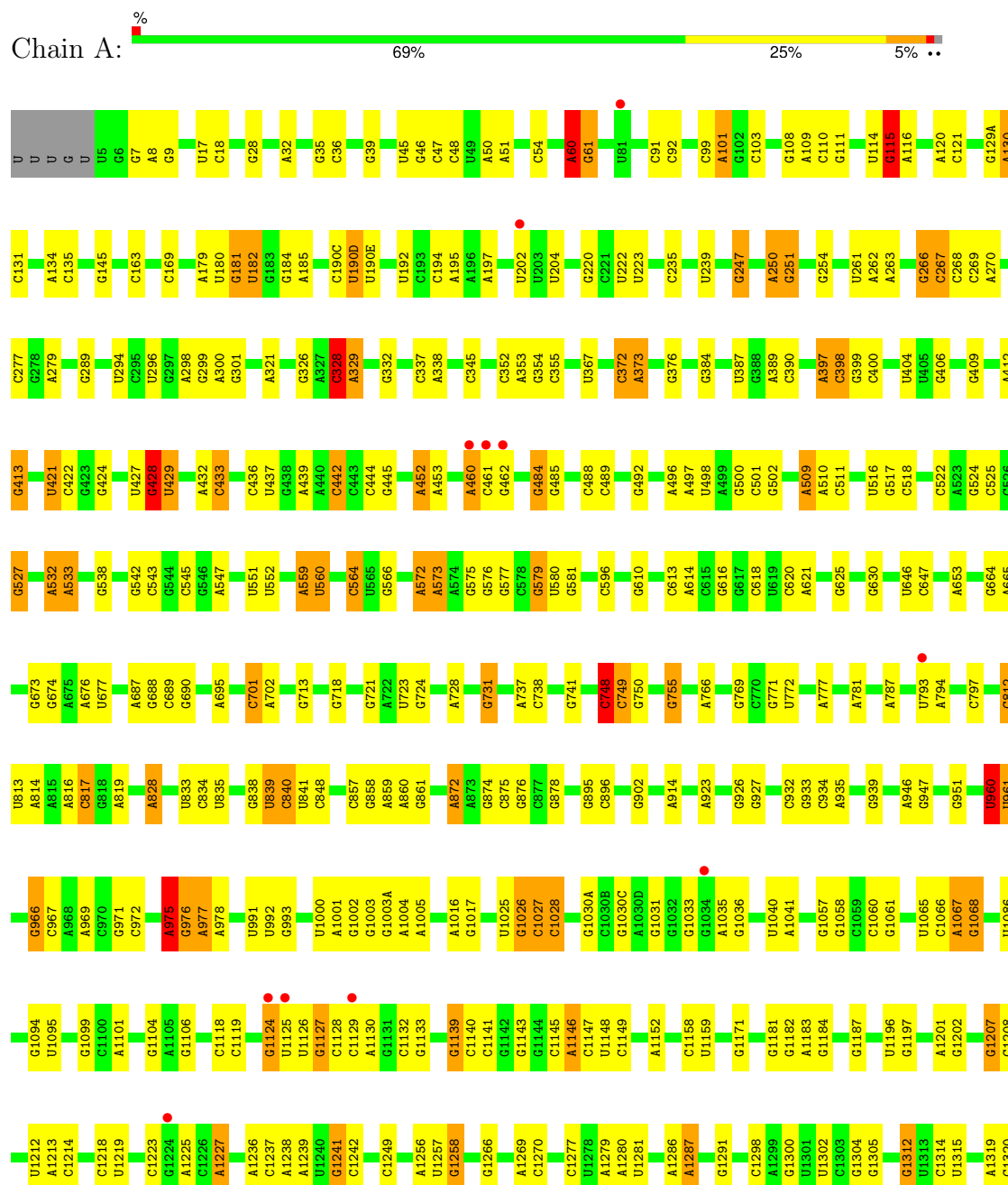
- Molecule 26 is water.

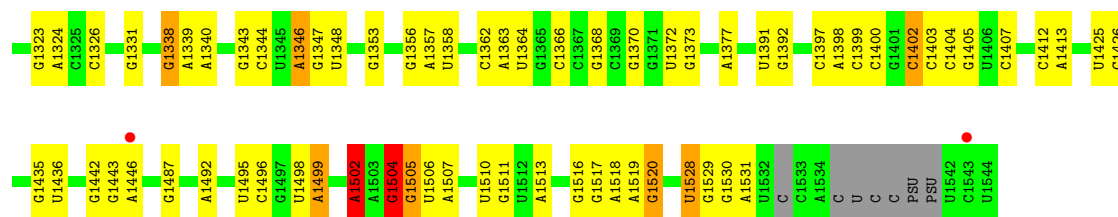
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	12	Total	O	0	0
			12	12		

### 3 Residue-property plots

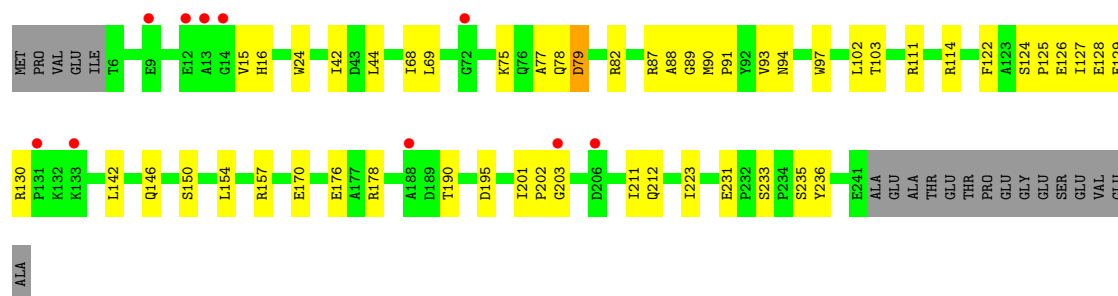
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 16S rRNA

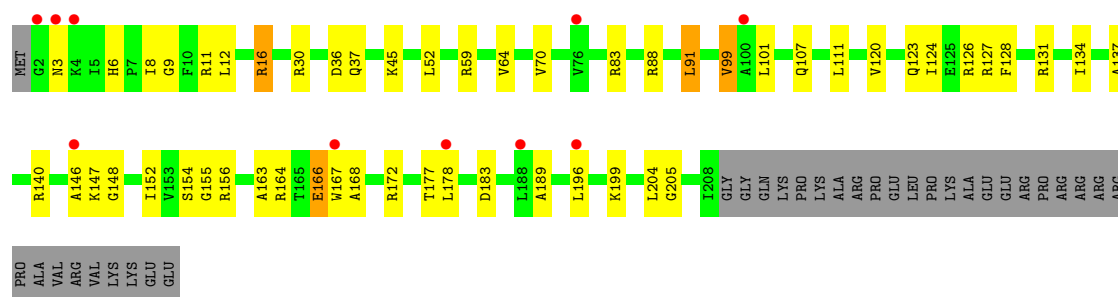




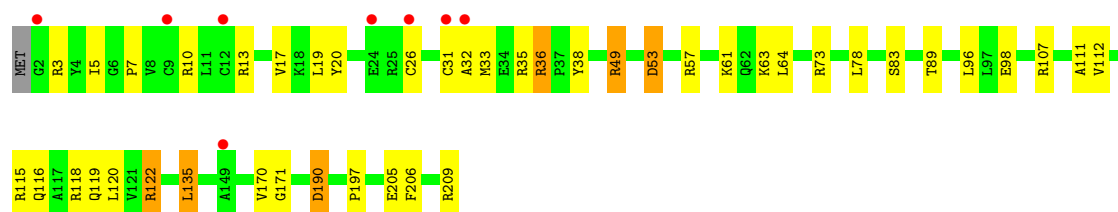
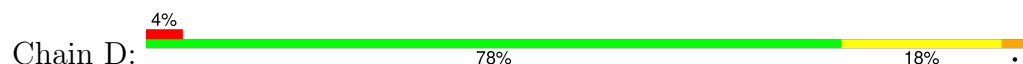
• Molecule 2: ribosomal protein S2



• Molecule 3: ribosomal protein S3

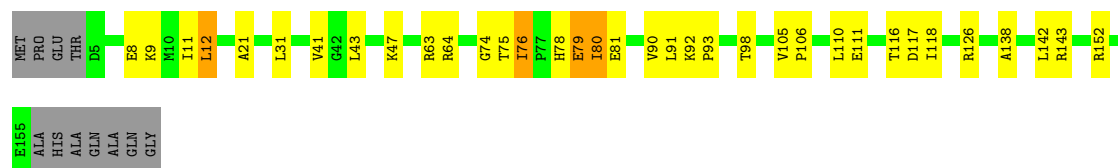


• Molecule 4: ribosomal protein S4

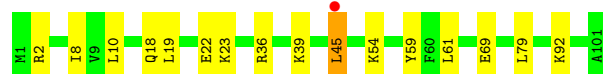
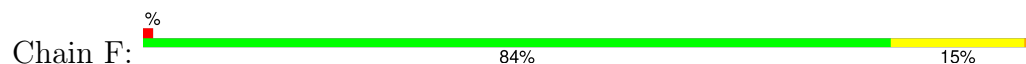


• Molecule 5: ribosomal protein S5

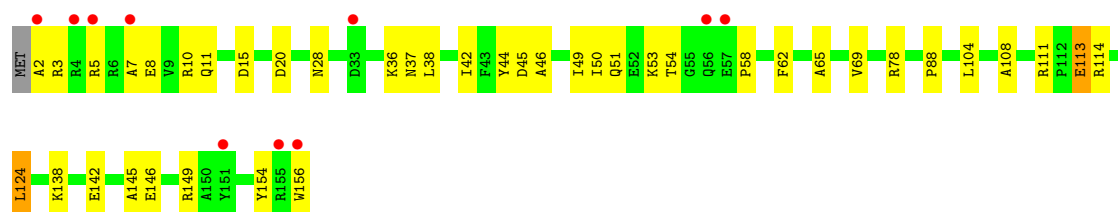




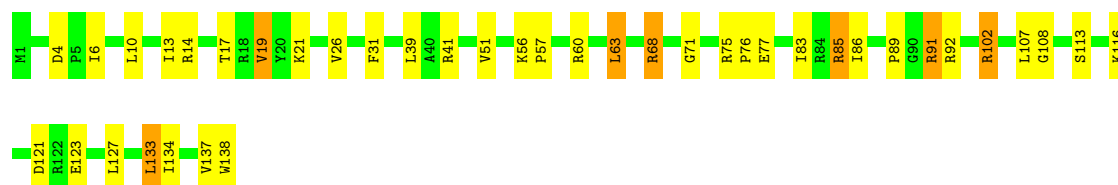
- Molecule 6: ribosomal protein S6



- Molecule 7: ribosomal protein S7



- Molecule 8: ribosomal protein S8

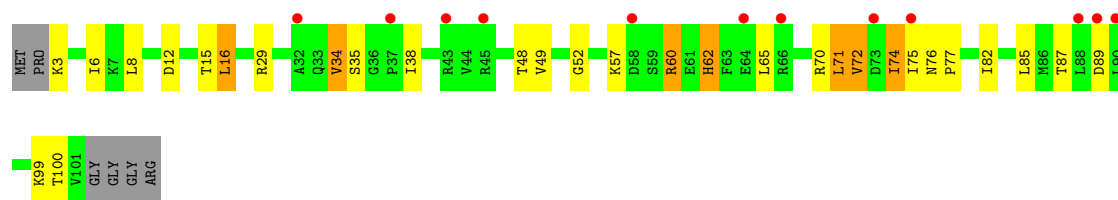


- Molecule 9: ribosomal protein S9

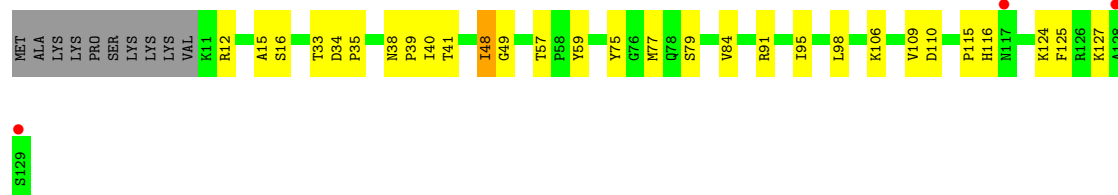


- Molecule 10: ribosomal protein S10

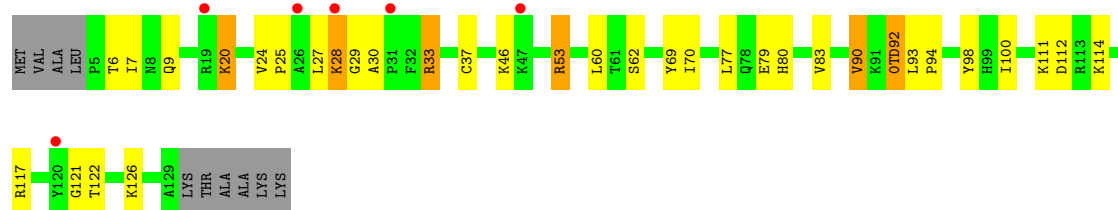




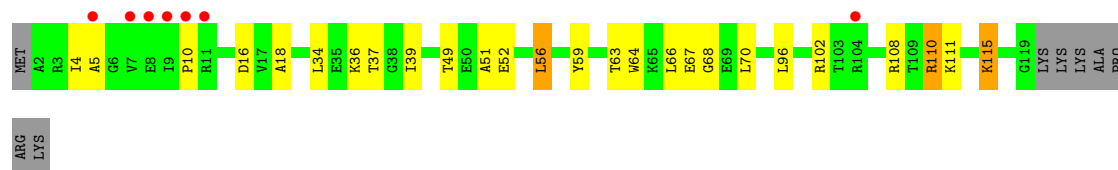
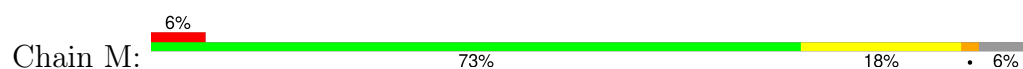
- Molecule 11: ribosomal protein S11



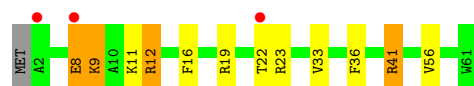
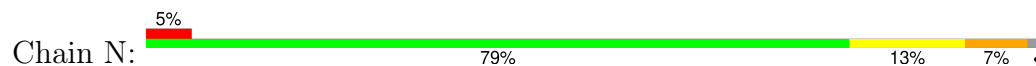
- Molecule 12: ribosomal protein S12



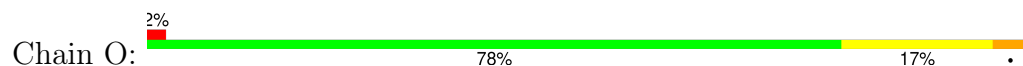
- Molecule 13: ribosomal protein S13

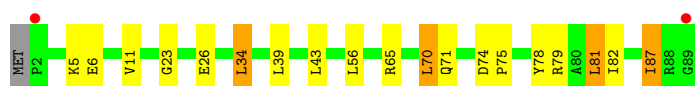


- Molecule 14: ribosomal protein S14



- Molecule 15: ribosomal protein S15

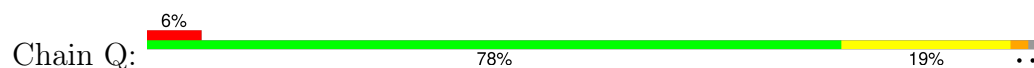




- Molecule 16: ribosomal protein S16



- Molecule 17: ribosomal protein S17



- Molecule 18: ribosomal protein S18



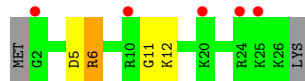
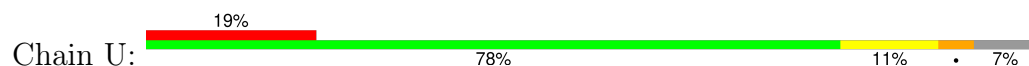
- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	403.18Å 403.18Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 3.31 34.90 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.90-3.31) 98.4 (34.90-3.31)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, $R_{free}$	0.175 , 0.210 0.176 , 0.209	Depositor DCC
$R_{free}$ test set	10690 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	52131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, MG, UR3, PSU, K, NMY, 0TD, M2G, 7MG, ZN, 2MG, 5MC

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	0.35	0/36091	0.80	30/56326 (0.1%)
2	B	0.28	0/1909	0.49	0/2579
3	C	0.27	0/1637	0.47	0/2207
4	D	0.31	0/1733	0.48	0/2318
5	E	0.34	0/1163	0.56	0/1566
6	F	0.25	0/856	0.45	0/1154
7	G	0.26	0/1276	0.43	0/1709
8	H	0.34	0/1136	0.52	0/1527
9	I	0.26	0/1029	0.50	0/1379
10	J	0.28	0/806	0.54	0/1084
11	K	0.28	0/900	0.51	0/1213
12	L	0.31	0/978	0.59	0/1308
13	M	0.26	0/947	0.45	0/1270
14	N	0.29	0/501	0.48	0/664
15	O	0.28	0/745	0.46	0/992
16	P	0.29	0/717	0.52	0/965
17	Q	0.34	0/870	0.57	0/1159
18	R	0.27	0/604	0.49	0/801
19	S	0.24	0/662	0.46	0/892
20	T	0.32	0/765	0.53	0/1007
21	U	0.26	0/213	0.44	0/279
All	All	0.33	0/55538	0.72	30/82399 (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
18	R	0	1
20	T	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	C	C2-N1-C1'	8.28	127.91	118.80
1	A	328	C	N1-C2-O2	8.10	123.76	118.90
1	A	328	C	N3-C2-O2	-7.05	116.96	121.90
1	A	254	G	O5'-P-OP1	-6.99	99.41	105.70
1	A	1528	U	C2-N1-C1'	6.52	125.52	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	20	ALA	Peptide
20	T	73	HIS	Peptide
20	T	93	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32462	0	16406	218	0
2	B	1874	0	1887	25	0
3	C	1613	0	1677	28	0
4	D	1703	0	1763	26	0
5	E	1147	0	1207	24	0
6	F	843	0	857	10	0
7	G	1257	0	1296	25	0
8	H	1116	0	1177	27	0
9	I	1010	0	1037	24	0
10	J	793	0	835	23	0
11	K	885	0	904	19	0
12	L	973	0	1058	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	937	0	995	15	0
14	N	492	0	529	9	0
15	O	734	0	771	11	0
16	P	701	0	720	14	0
17	Q	857	0	928	13	0
18	R	598	0	670	11	0
19	S	648	0	673	11	0
20	T	763	0	861	19	0
21	U	209	0	221	3	0
22	A	201	0	0	0	0
22	B	3	0	0	0	0
22	C	2	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	2	0	0	0	0
22	L	1	0	0	0	0
22	M	2	0	0	0	0
22	N	2	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	A	30	0	0	0	0
24	A	252	0	276	13	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	12	0	0	0	0
All	All	52131	0	36748	518	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 6.

The worst 5 of 518 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:1086:U:H3	1:A:1099:G:H22	1.23	0.86
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.60	0.83
1:A:664:G:H22	1:A:741:G:H1	1.27	0.81
1:A:279:A:OP2	17:Q:95:TYR:OH	1.98	0.81
19:S:33:THR:HG22	19:S:35:SER:H	1.47	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	208 (89%)	24 (10%)	2 (1%)	14	44
3	C	205/239 (86%)	190 (93%)	15 (7%)	0	100	100
4	D	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	25	56
5	E	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	46
10	J	97/105 (92%)	78 (80%)	17 (18%)	2 (2%)	5	27
11	K	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
12	L	122/135 (90%)	110 (90%)	10 (8%)	2 (2%)	8	32
13	M	116/126 (92%)	109 (94%)	7 (6%)	0	100	100
14	N	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	Q	102/105 (97%)	95 (93%)	7 (7%)	0	100	100
18	R	71/88 (81%)	66 (93%)	4 (6%)	1 (1%)	9	34
19	S	79/93 (85%)	72 (91%)	7 (9%)	0	100	100
20	T	97/106 (92%)	88 (91%)	8 (8%)	1 (1%)	13	42
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2357/2541 (93%)	2189 (93%)	158 (7%)	10 (0%)	30	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS

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Mol	Chain	Res	Type
10	J	34	VAL
18	R	19	LYS
10	J	72	VAL
20	T	74	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/220 (88%)	185 (95%)	9 (5%)	23	52
3	C	160/188 (85%)	145 (91%)	15 (9%)	7	25
4	D	180/181 (99%)	166 (92%)	14 (8%)	10	33
5	E	115/123 (94%)	107 (93%)	8 (7%)	12	37
6	F	90/90 (100%)	87 (97%)	3 (3%)	33	60
7	G	126/127 (99%)	119 (94%)	7 (6%)	17	45
8	H	119/119 (100%)	109 (92%)	10 (8%)	9	30
9	I	98/99 (99%)	90 (92%)	8 (8%)	9	31
10	J	87/92 (95%)	81 (93%)	6 (7%)	13	38
11	K	90/99 (91%)	88 (98%)	2 (2%)	47	69
12	L	103/110 (94%)	97 (94%)	6 (6%)	17	44
13	M	94/101 (93%)	88 (94%)	6 (6%)	14	40
14	N	49/50 (98%)	43 (88%)	6 (12%)	4	16
15	O	79/80 (99%)	71 (90%)	8 (10%)	6	23
16	P	72/74 (97%)	71 (99%)	1 (1%)	62	78
17	Q	96/97 (99%)	90 (94%)	6 (6%)	15	41
18	R	64/77 (83%)	63 (98%)	1 (2%)	58	76
19	S	71/80 (89%)	65 (92%)	6 (8%)	8	30
20	T	76/82 (93%)	69 (91%)	7 (9%)	7	26
21	U	19/22 (86%)	18 (95%)	1 (5%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1982/2111 (94%)	1852 (93%)	130 (7%)	14	40

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

Mol	Chain	Res	Type
18	R	18	ARG
19	S	61	TYR
6	F	54	LYS
6	F	45	LEU
19	S	81	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	GLN
3	C	6	HIS
7	G	51	GLN
9	I	73	GLN
13	M	106	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	201 (13%)	28 (1%)

5 of 201 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	575	G
1	A	1528	U
1	A	723	U

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Mol	Chain	Res	Type
1	A	1201	A
1	A	701	C

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

11 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	1.45	4 (20%)	19,40,43	1.13	2 (10%)
1	4OC	A	1402	1	20,23,24	0.97	2 (10%)	25,32,35	0.79	0
1	7MG	A	527	1	23,26,27	3.69	4 (17%)	27,39,42	2.35	9 (33%)
1	5MC	A	1407	1	19,22,23	1.15	2 (10%)	26,32,35	1.11	2 (7%)
1	5MC	A	1404	1	19,22,23	0.93	1 (5%)	26,32,35	0.91	2 (7%)
1	PSU	A	516	22,1	18,21,22	1.14	1 (5%)	21,30,33	1.76	4 (19%)
1	UR3	A	1498	1	19,22,23	0.51	0	26,32,35	0.96	0
12	0TD	L	92	12	8,9,10	1.92	1 (12%)	6,11,13	2.06	3 (50%)
1	5MC	A	967	1	19,22,23	0.96	1 (5%)	26,32,35	0.85	1 (3%)
1	2MG	A	1207	1	18,26,27	1.45	4 (22%)	16,38,41	1.44	2 (12%)
1	5MC	A	1400	1	19,22,23	1.05	2 (10%)	26,32,35	0.95	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	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	516	22,1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.27	1.35	1.45
12	L	92	0TD	CB-CA	-4.78	1.53	1.54
1	A	527	7MG	C2-N2	4.17	1.43	1.34
1	A	516	PSU	C6-C5	3.85	1.39	1.35
1	A	966	M2G	C6-N1	3.44	1.43	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	N9-C4-N3	5.14	133.00	125.46
1	A	527	7MG	C5-C6-N1	5.12	119.95	110.94
1	A	527	7MG	C2-N3-C4	4.88	120.71	112.30
1	A	527	7MG	C5-C4-N3	-4.58	119.53	128.13
1	A	516	PSU	N1-C2-N3	4.35	119.76	115.17

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	1	0
12	L	92	0TD	2	0
1	A	1207	2MG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 258 ligands modelled in this entry, 252 are monoatomic - leaving 6 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	NMY	A	1835	-	43,45,45	1.33	5 (11%)	62,67,67	1.46	12 (19%)
24	NMY	A	1836	-	43,45,45	1.39	6 (13%)	62,67,67	2.16	15 (24%)
24	NMY	A	1833	-	43,45,45	1.33	4 (9%)	62,67,67	1.83	12 (19%)
24	NMY	A	1834	-	43,45,45	1.49	7 (16%)	62,67,67	1.85	15 (24%)
24	NMY	A	1837	-	43,45,45	1.47	8 (18%)	62,67,67	1.89	16 (25%)
24	NMY	A	1832	-	43,45,45	1.33	6 (13%)	62,67,67	1.44	8 (12%)

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	NMY	A	1835	-	-	3/18/94/94	0/4/4/4
24	NMY	A	1836	-	-	11/18/94/94	0/4/4/4
24	NMY	A	1833	-	-	6/18/94/94	0/4/4/4
24	NMY	A	1834	-	-	7/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	NMY	A	1837	-	-	8/18/94/94	0/4/4/4
24	NMY	A	1832	-	-	5/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1834	NMY	C13-C14	4.69	1.58	1.52
24	A	1837	NMY	C1-C2	3.91	1.60	1.52
24	A	1833	NMY	C3-C2	3.47	1.57	1.53
24	A	1837	NMY	C3-C2	3.35	1.57	1.53
24	A	1836	NMY	C1-C2	3.34	1.58	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1836	NMY	C13-C14-C15	-10.11	89.95	102.10
24	A	1836	NMY	C14-C15-C16	-6.61	91.66	103.24
24	A	1837	NMY	O1-C10-C11	5.71	121.92	107.42
24	A	1833	NMY	O11-C13-O16	-5.69	105.56	111.37
24	A	1834	NMY	O18-C18-C19	5.47	117.03	108.08

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

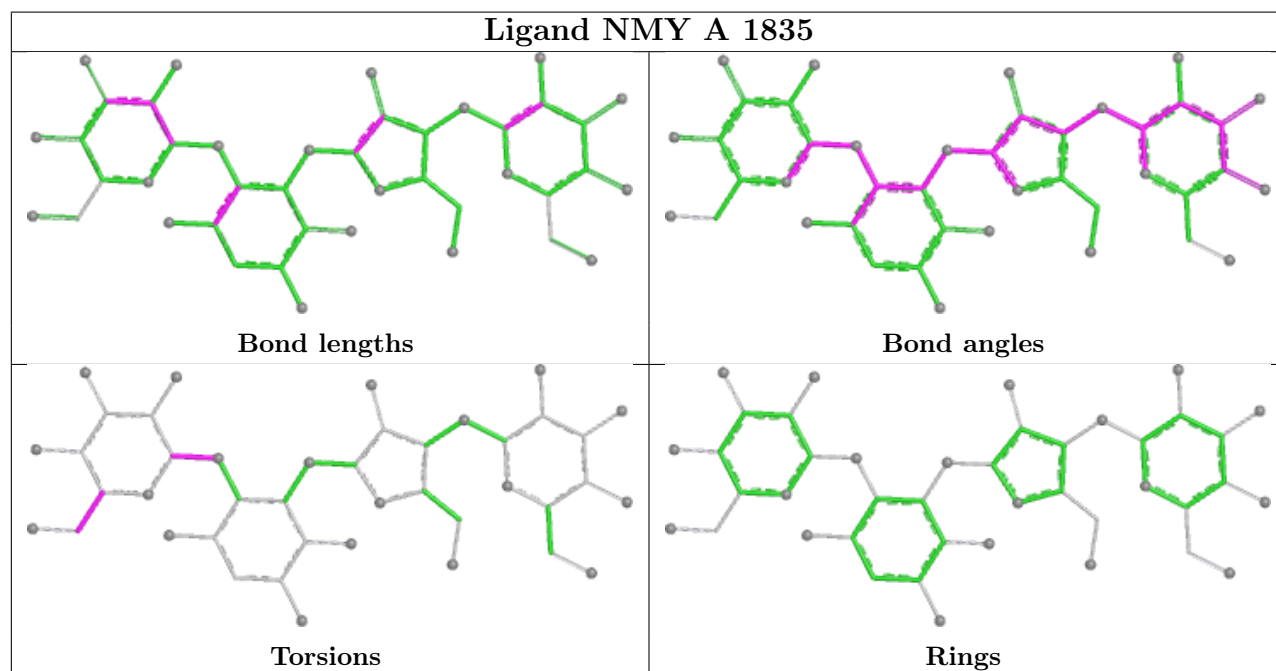
Mol	Chain	Res	Type	Atoms
24	A	1833	NMY	C16-C15-O18-C18
24	A	1833	NMY	C19-C18-O18-C15
24	A	1833	NMY	O22-C22-C23-N19
24	A	1834	NMY	C4-C5-C6-N6
24	A	1834	NMY	O5-C5-C6-N6

There are no ring outliers.

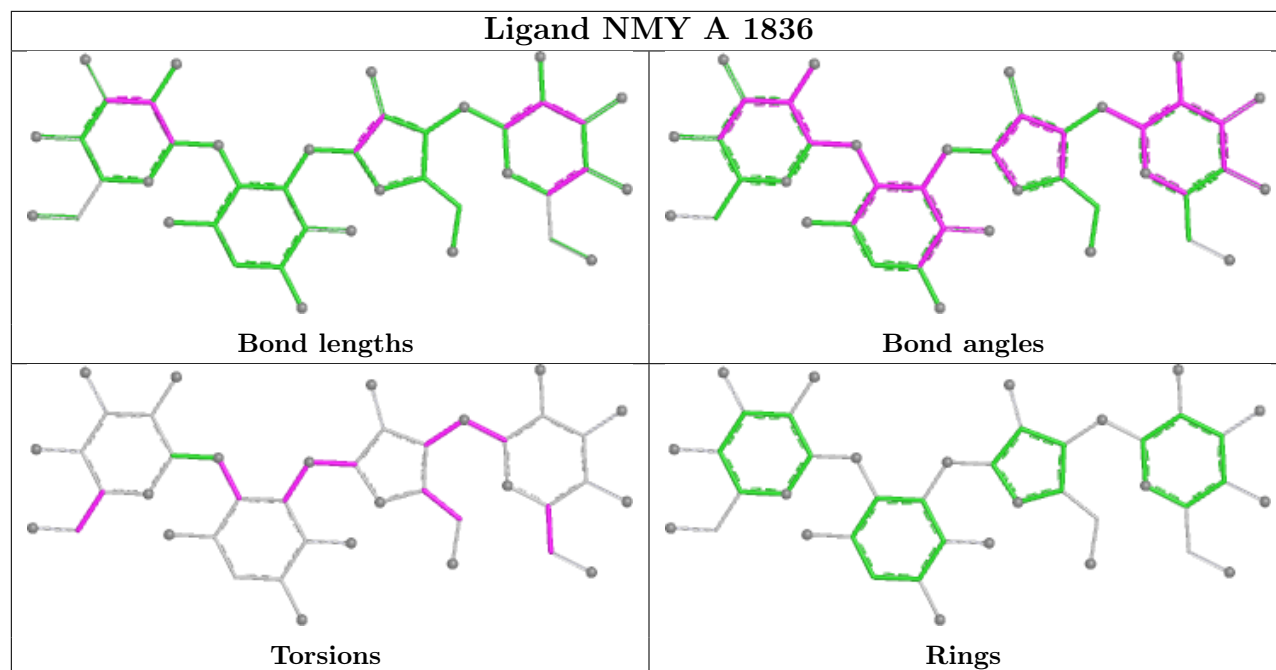
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1835	NMY	4	0
24	A	1836	NMY	2	0
24	A	1833	NMY	1	0
24	A	1834	NMY	3	0
24	A	1837	NMY	2	0
24	A	1832	NMY	1	0

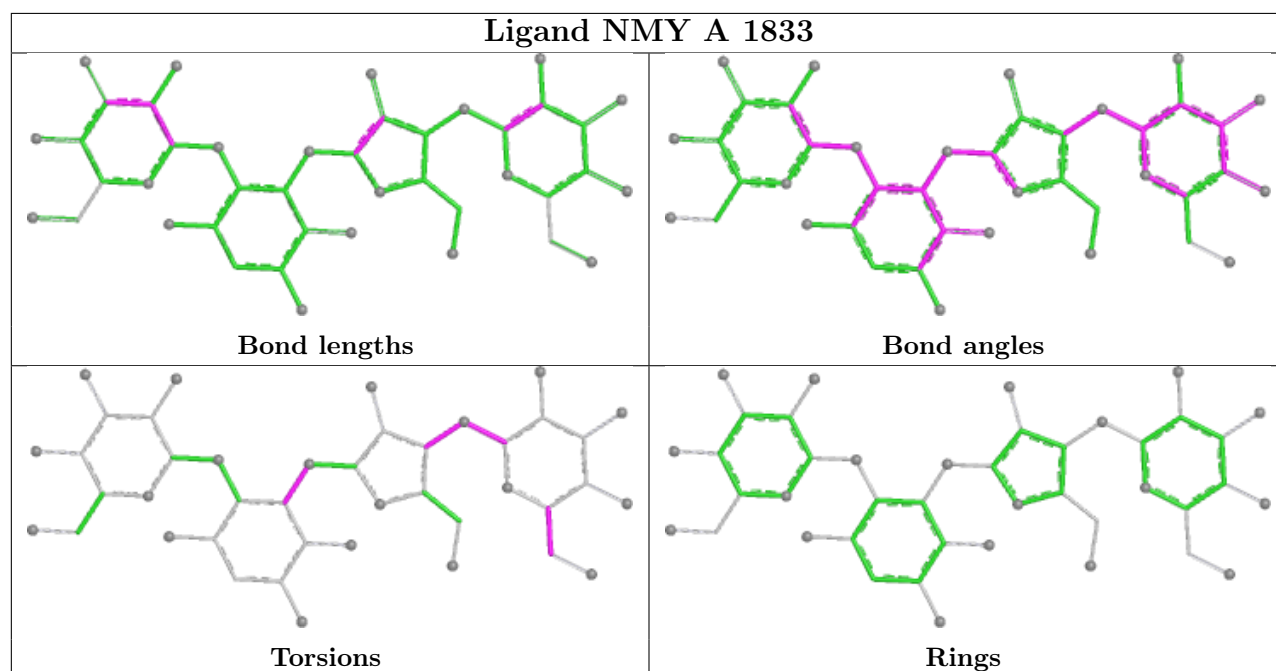
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

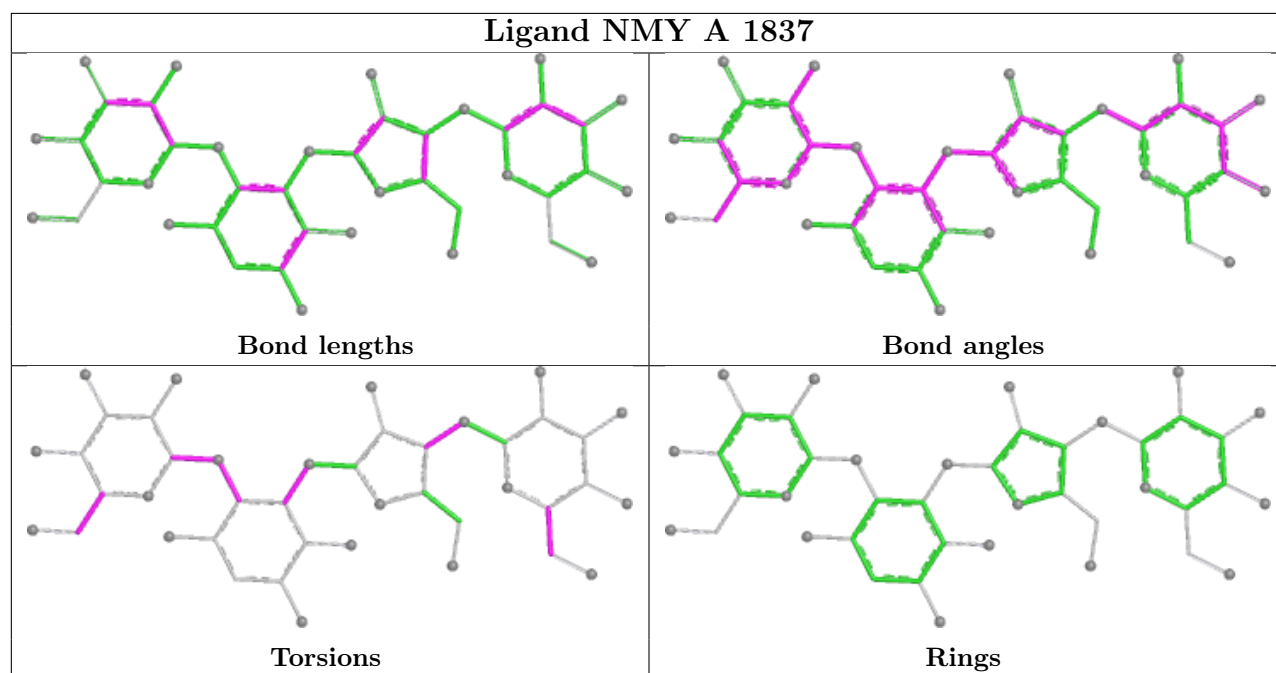
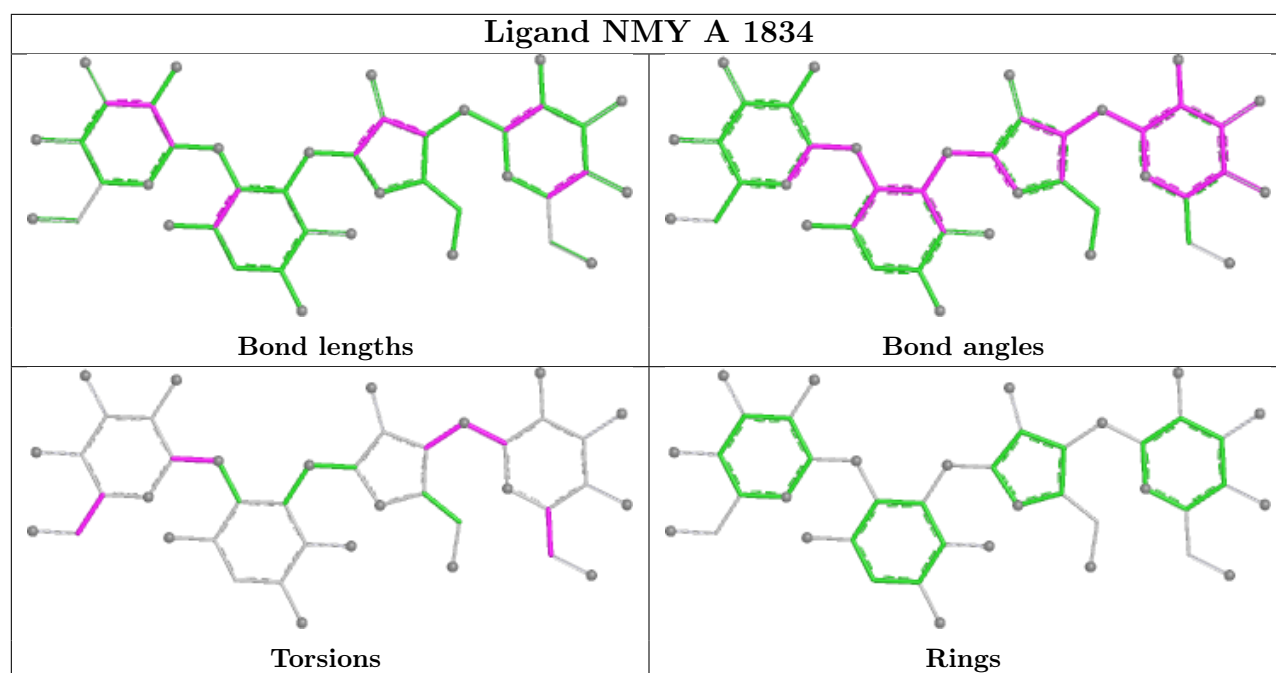


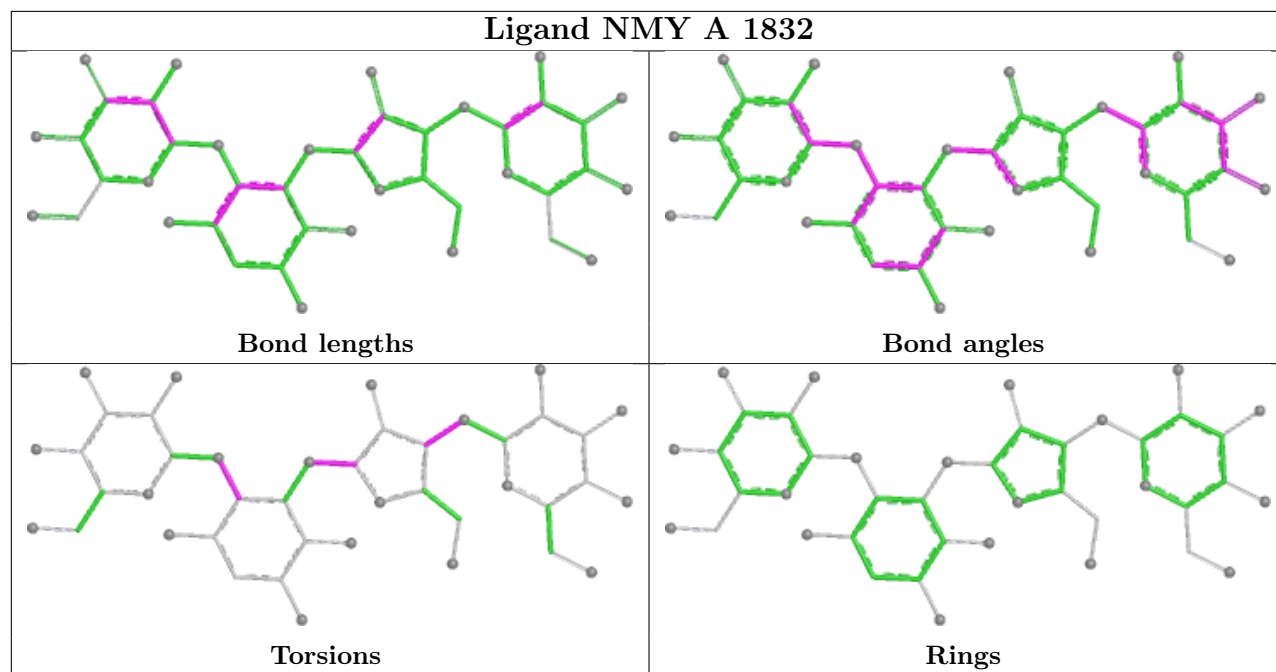
## Ligand NMY A 1836



## Ligand NMY A 1833







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1500/1522 (98%)	-0.53	13 (0%) 81 70	51, 84, 177, 283	0
2	B	236/256 (92%)	0.03	10 (4%) 41 31	60, 109, 189, 249	0
3	C	207/239 (86%)	0.03	10 (4%) 36 28	50, 115, 158, 195	0
4	D	208/209 (99%)	-0.02	8 (3%) 44 33	63, 94, 134, 166	0
5	E	151/162 (93%)	-0.31	0 100 100	56, 75, 113, 167	0
6	F	101/101 (100%)	-0.17	1 (0%) 79 68	78, 118, 149, 179	0
7	G	155/156 (99%)	0.17	10 (6%) 26 21	82, 115, 183, 212	0
8	H	138/138 (100%)	-0.56	0 100 100	46, 72, 102, 140	0
9	I	127/128 (99%)	0.35	8 (6%) 27 22	79, 121, 162, 198	0
10	J	99/105 (94%)	0.85	12 (12%) 10 10	73, 140, 218, 252	0
11	K	119/129 (92%)	-0.00	3 (2%) 58 43	68, 93, 129, 150	0
12	L	124/135 (91%)	0.12	6 (4%) 36 28	58, 87, 126, 215	0
13	M	118/126 (93%)	0.10	7 (5%) 29 24	84, 114, 146, 183	0
14	N	60/61 (98%)	0.51	3 (5%) 35 28	81, 108, 151, 202	0
15	O	88/89 (98%)	-0.10	2 (2%) 61 46	57, 89, 135, 169	0
16	P	84/88 (95%)	-0.16	1 (1%) 76 64	62, 80, 107, 189	0
17	Q	104/105 (99%)	-0.04	6 (5%) 30 24	59, 78, 125, 196	0
18	R	73/88 (82%)	0.00	3 (4%) 42 31	65, 97, 177, 232	0
19	S	81/93 (87%)	0.46	9 (11%) 12 11	47, 137, 180, 209	0
20	T	99/106 (93%)	0.26	8 (8%) 19 17	64, 86, 136, 182	0
21	U	25/27 (92%)	0.90	5 (20%) 3 3	73, 106, 130, 206	0
All	All	3897/4063 (95%)	-0.17	125 (3%) 50 37	46, 94, 169, 283	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	12.5
1	A	1129	C	10.5
11	K	129	SER	7.4
19	S	2	PRO	7.1
17	Q	105	ALA	6.9

## 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	5MC	A	1407	21/22	0.94	0.12	83,120,143,145	0
1	PSU	A	516	20/21	0.95	0.09	87,90,100,100	0
1	UR3	A	1498	21/22	0.95	0.10	71,77,98,103	0
12	0TD	L	92	10/11	0.95	0.16	96,102,168,273	0
1	5MC	A	1404	21/22	0.96	0.09	72,81,90,95	0
1	7MG	A	527	24/25	0.97	0.08	66,72,94,98	0
1	M2G	A	966	25/26	0.97	0.06	70,81,95,98	0
1	2MG	A	1207	24/25	0.97	0.07	101,107,113,115	0
1	5MC	A	1400	21/22	0.97	0.09	67,83,106,112	0
1	5MC	A	967	21/22	0.98	0.06	59,76,83,84	0
1	4OC	A	1402	22/23	0.98	0.08	70,75,83,91	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
22	MG	A	1802	1/1	0.31	0.42	108,108,108,108	0
22	MG	C	302	1/1	0.34	0.21	106,106,106,106	0
23	K	A	1742	1/1	0.47	0.34	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1667	1/1	0.52	0.62	98,98,98,98	0
22	MG	A	1829	1/1	0.52	0.26	104,104,104,104	0
22	MG	A	1655	1/1	0.53	0.42	93,93,93,93	0
22	MG	A	1602	1/1	0.54	0.47	114,114,114,114	0
22	MG	A	1830	1/1	0.54	0.18	293,293,293,293	0
22	MG	N	102	1/1	0.56	0.55	92,92,92,92	0
22	MG	A	1776	1/1	0.57	0.33	85,85,85,85	0
22	MG	A	1762	1/1	0.58	0.41	89,89,89,89	0
22	MG	A	1772	1/1	0.61	0.47	66,66,66,66	0
23	K	A	1753	1/1	0.61	0.37	127,127,127,127	0
22	MG	A	1788	1/1	0.62	0.42	88,88,88,88	0
22	MG	A	1823	1/1	0.62	0.25	107,107,107,107	0
22	MG	A	1814	1/1	0.63	0.38	87,87,87,87	0
23	K	A	1760	1/1	0.63	0.36	145,145,145,145	0
23	K	A	1755	1/1	0.64	0.42	147,147,147,147	0
23	K	A	1751	1/1	0.65	0.19	160,160,160,160	0
22	MG	A	1633	1/1	0.65	0.34	93,93,93,93	0
23	K	A	1748	1/1	0.66	0.33	136,136,136,136	0
22	MG	A	1787	1/1	0.67	0.44	117,117,117,117	0
22	MG	A	1615	1/1	0.67	0.48	95,95,95,95	0
22	MG	A	1782	1/1	0.67	0.36	82,82,82,82	0
22	MG	A	1795	1/1	0.68	0.47	96,96,96,96	0
22	MG	A	1774	1/1	0.68	0.35	98,98,98,98	0
22	MG	A	1660	1/1	0.70	0.35	75,75,75,75	0
22	MG	A	1789	1/1	0.70	0.33	97,97,97,97	0
23	K	A	1747	1/1	0.71	0.25	112,112,112,112	0
22	MG	F	201	1/1	0.71	0.20	95,95,95,95	0
22	MG	A	1642	1/1	0.72	0.39	68,68,68,68	0
23	K	A	1741	1/1	0.73	0.63	154,154,154,154	0
22	MG	A	1822	1/1	0.74	0.16	101,101,101,101	0
23	K	A	1735	1/1	0.74	0.46	152,152,152,152	0
22	MG	A	1781	1/1	0.74	0.44	87,87,87,87	0
22	MG	A	1800	1/1	0.74	0.42	98,98,98,98	0
22	MG	L	201	1/1	0.74	0.34	99,99,99,99	0
22	MG	A	1658	1/1	0.75	0.45	76,76,76,76	0
23	K	A	1739	1/1	0.75	0.33	140,140,140,140	0
22	MG	A	1791	1/1	0.76	0.39	78,78,78,78	0
23	K	A	1731	1/1	0.76	0.21	121,121,121,121	0
22	MG	A	1778	1/1	0.76	0.30	88,88,88,88	0
22	MG	A	1725	1/1	0.76	0.26	76,76,76,76	0
23	K	A	1750	1/1	0.77	0.42	143,143,143,143	0
23	K	A	1733	1/1	0.77	0.19	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1824	1/1	0.77	0.21	103,103,103,103	0
22	MG	A	1796	1/1	0.77	0.12	89,89,89,89	0
23	K	A	1740	1/1	0.77	0.24	135,135,135,135	0
22	MG	A	1775	1/1	0.78	0.35	84,84,84,84	0
22	MG	A	1809	1/1	0.78	0.23	74,74,74,74	0
22	MG	A	1827	1/1	0.79	0.23	102,102,102,102	0
22	MG	A	1784	1/1	0.79	0.34	90,90,90,90	0
22	MG	A	1773	1/1	0.79	0.21	69,69,69,69	0
22	MG	A	1777	1/1	0.80	0.47	96,96,96,96	0
22	MG	A	1763	1/1	0.80	0.28	68,68,68,68	0
22	MG	A	1688	1/1	0.80	0.37	41,41,41,41	0
23	K	A	1757	1/1	0.80	0.28	143,143,143,143	0
23	K	A	1759	1/1	0.80	0.18	145,145,145,145	0
22	MG	A	1818	1/1	0.80	0.34	90,90,90,90	0
22	MG	A	1622	1/1	0.81	0.27	65,65,65,65	0
22	MG	A	1799	1/1	0.81	0.37	98,98,98,98	0
22	MG	A	1710	1/1	0.81	0.34	90,90,90,90	0
22	MG	A	1819	1/1	0.81	0.25	85,85,85,85	0
22	MG	A	1720	1/1	0.81	0.50	75,75,75,75	0
22	MG	A	1826	1/1	0.82	0.25	81,81,81,81	0
22	MG	A	1621	1/1	0.82	0.47	82,82,82,82	0
22	MG	A	1647	1/1	0.82	0.41	83,83,83,83	0
24	NMY	A	1837	42/42	0.82	0.16	57,138,186,186	0
22	MG	A	1766	1/1	0.83	0.27	61,61,61,61	0
22	MG	A	1798	1/1	0.83	0.58	85,85,85,85	0
23	K	A	1737	1/1	0.83	0.19	134,134,134,134	0
22	MG	A	1728	1/1	0.83	0.31	55,55,55,55	0
22	MG	M	202	1/1	0.83	0.18	85,85,85,85	0
22	MG	A	1783	1/1	0.83	0.17	73,73,73,73	0
22	MG	N	103	1/1	0.83	0.18	57,57,57,57	0
23	K	A	1744	1/1	0.83	0.35	121,121,121,121	0
22	MG	C	301	1/1	0.83	0.21	66,66,66,66	0
22	MG	A	1805	1/1	0.84	0.52	79,79,79,79	0
22	MG	B	301	1/1	0.84	0.17	96,96,96,96	0
22	MG	A	1659	1/1	0.84	0.19	94,94,94,94	0
22	MG	A	1686	1/1	0.84	0.30	54,54,54,54	0
22	MG	D	303	1/1	0.84	0.29	89,89,89,89	0
22	MG	A	1815	1/1	0.84	0.49	81,81,81,81	0
22	MG	H	201	1/1	0.84	0.21	74,74,74,74	0
22	MG	A	1726	1/1	0.84	0.24	70,70,70,70	0
22	MG	A	1828	1/1	0.84	0.14	95,95,95,95	0
24	NMY	A	1834	42/42	0.84	0.23	62,120,200,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1797	1/1	0.84	0.18	68,68,68,68	0
22	MG	A	1682	1/1	0.85	0.46	84,84,84,84	0
22	MG	A	1785	1/1	0.85	0.27	67,67,67,67	0
23	K	A	1756	1/1	0.85	0.15	151,151,151,151	0
23	K	A	1746	1/1	0.85	0.19	149,149,149,149	0
22	MG	A	1801	1/1	0.85	0.36	80,80,80,80	0
22	MG	A	1790	1/1	0.85	0.36	72,72,72,72	0
22	MG	A	1803	1/1	0.85	0.16	66,66,66,66	0
22	MG	A	1771	1/1	0.85	0.48	58,58,58,58	0
22	MG	A	1604	1/1	0.86	0.23	79,79,79,79	0
23	K	A	1754	1/1	0.86	0.27	135,135,135,135	0
23	K	A	1743	1/1	0.86	0.11	137,137,137,137	0
22	MG	A	1724	1/1	0.86	0.12	51,51,51,51	0
22	MG	A	1804	1/1	0.86	0.16	56,56,56,56	0
22	MG	A	1601	1/1	0.86	0.21	76,76,76,76	0
22	MG	A	1808	1/1	0.86	0.61	79,79,79,79	0
22	MG	A	1627	1/1	0.86	0.27	90,90,90,90	0
22	MG	A	1770	1/1	0.86	0.51	102,102,102,102	0
22	MG	A	1706	1/1	0.87	0.38	73,73,73,73	0
22	MG	A	1611	1/1	0.87	0.30	49,49,49,49	0
22	MG	A	1631	1/1	0.87	0.28	63,63,63,63	0
22	MG	A	1723	1/1	0.87	0.27	55,55,55,55	0
23	K	A	1749	1/1	0.87	0.30	115,115,115,115	0
22	MG	D	302	1/1	0.87	0.16	63,63,63,63	0
22	MG	A	1657	1/1	0.87	0.28	70,70,70,70	0
24	NMY	A	1835	42/42	0.87	0.16	105,127,145,147	0
22	MG	A	1661	1/1	0.87	0.26	69,69,69,69	0
22	MG	A	1817	1/1	0.88	0.28	103,103,103,103	0
22	MG	A	1646	1/1	0.88	0.43	58,58,58,58	0
22	MG	A	1640	1/1	0.88	0.21	47,47,47,47	0
22	MG	A	1813	1/1	0.88	0.18	88,88,88,88	0
22	MG	A	1761	1/1	0.88	0.36	51,51,51,51	0
22	MG	A	1689	1/1	0.88	0.29	67,67,67,67	0
22	MG	A	1764	1/1	0.89	0.21	65,65,65,65	0
23	K	A	1752	1/1	0.89	0.35	115,115,115,115	0
22	MG	A	1668	1/1	0.89	0.33	66,66,66,66	0
22	MG	A	1672	1/1	0.89	0.39	83,83,83,83	0
22	MG	A	1663	1/1	0.89	0.49	67,67,67,67	0
22	MG	A	1709	1/1	0.89	0.34	66,66,66,66	0
22	MG	A	1792	1/1	0.89	0.32	68,68,68,68	0
22	MG	A	1683	1/1	0.89	0.39	77,77,77,77	0
22	MG	A	1685	1/1	0.89	0.41	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1807	1/1	0.89	0.49	78,78,78,78	0
22	MG	A	1619	1/1	0.89	0.25	77,77,77,77	0
23	K	A	1738	1/1	0.89	0.29	133,133,133,133	0
22	MG	A	1821	1/1	0.90	0.18	73,73,73,73	0
22	MG	A	1705	1/1	0.90	0.39	61,61,61,61	0
22	MG	A	1616	1/1	0.90	0.35	84,84,84,84	0
22	MG	A	1644	1/1	0.90	0.33	62,62,62,62	0
22	MG	A	1645	1/1	0.90	0.54	79,79,79,79	0
22	MG	A	1767	1/1	0.90	0.33	62,62,62,62	0
22	MG	A	1617	1/1	0.90	0.64	112,112,112,112	0
22	MG	A	1721	1/1	0.90	0.26	77,77,77,77	0
22	MG	A	1630	1/1	0.90	0.48	60,60,60,60	0
22	MG	A	1651	1/1	0.90	0.34	77,77,77,77	0
22	MG	A	1652	1/1	0.90	0.32	64,64,64,64	0
22	MG	A	1664	1/1	0.90	0.35	94,94,94,94	0
22	MG	A	1665	1/1	0.90	0.33	84,84,84,84	0
22	MG	A	1729	1/1	0.90	0.18	64,64,64,64	0
22	MG	A	1730	1/1	0.90	0.38	74,74,74,74	0
22	MG	A	1699	1/1	0.90	0.09	64,64,64,64	0
23	K	A	1734	1/1	0.91	0.25	119,119,119,119	0
22	MG	A	1624	1/1	0.91	0.31	39,39,39,39	0
22	MG	A	1656	1/1	0.91	0.19	57,57,57,57	0
22	MG	A	1711	1/1	0.91	0.38	90,90,90,90	0
22	MG	A	1713	1/1	0.91	0.43	61,61,61,61	0
22	MG	A	1603	1/1	0.91	0.36	69,69,69,69	0
22	MG	A	1673	1/1	0.91	0.15	57,57,57,57	0
22	MG	A	1693	1/1	0.91	0.32	72,72,72,72	0
22	MG	A	1632	1/1	0.91	0.30	64,64,64,64	0
23	K	A	1758	1/1	0.91	0.52	130,130,130,130	0
22	MG	A	1831	1/1	0.91	0.08	285,285,285,285	0
23	K	A	1745	1/1	0.91	0.30	142,142,142,142	0
22	MG	A	1653	1/1	0.91	0.51	63,63,63,63	0
23	K	A	1732	1/1	0.91	0.18	104,104,104,104	0
24	NMY	A	1836	42/42	0.91	0.23	75,119,177,188	0
22	MG	A	1684	1/1	0.91	0.41	68,68,68,68	0
22	MG	A	1768	1/1	0.92	0.28	50,50,50,50	0
22	MG	A	1769	1/1	0.92	0.47	73,73,73,73	0
22	MG	A	1609	1/1	0.92	0.28	86,86,86,86	0
22	MG	P	102	1/1	0.92	0.28	84,84,84,84	0
22	MG	Q	201	1/1	0.92	0.12	71,71,71,71	0
22	MG	A	1666	1/1	0.92	0.43	72,72,72,72	0
22	MG	A	1806	1/1	0.92	0.26	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1727	1/1	0.92	0.15	54,54,54,54	0
22	MG	A	1637	1/1	0.92	0.19	67,67,67,67	0
22	MG	A	1613	1/1	0.92	0.49	86,86,86,86	0
22	MG	A	1662	1/1	0.92	0.20	51,51,51,51	0
22	MG	B	302	1/1	0.92	0.37	84,84,84,84	0
22	MG	A	1712	1/1	0.92	0.24	75,75,75,75	0
22	MG	A	1623	1/1	0.92	0.67	86,86,86,86	0
22	MG	A	1679	1/1	0.92	0.34	62,62,62,62	0
22	MG	A	1779	1/1	0.92	0.22	82,82,82,82	0
22	MG	A	1697	1/1	0.92	0.25	36,36,36,36	0
22	MG	A	1610	1/1	0.92	0.20	89,89,89,89	0
22	MG	A	1701	1/1	0.92	0.29	44,44,44,44	0
22	MG	A	1825	1/1	0.93	0.27	63,63,63,63	0
22	MG	A	1812	1/1	0.93	0.28	103,103,103,103	0
22	MG	H	202	1/1	0.93	0.07	49,49,49,49	0
22	MG	A	1675	1/1	0.93	0.60	75,75,75,75	0
22	MG	A	1715	1/1	0.93	0.11	68,68,68,68	0
22	MG	A	1676	1/1	0.93	0.08	60,60,60,60	0
22	MG	A	1816	1/1	0.93	0.35	67,67,67,67	0
22	MG	A	1643	1/1	0.93	0.26	54,54,54,54	0
22	MG	A	1608	1/1	0.93	0.14	73,73,73,73	0
22	MG	A	1690	1/1	0.93	0.40	70,70,70,70	0
22	MG	A	1614	1/1	0.93	0.24	72,72,72,72	0
22	MG	A	1694	1/1	0.93	0.39	83,83,83,83	0
22	MG	A	1786	1/1	0.93	0.34	71,71,71,71	0
22	MG	A	1606	1/1	0.93	0.85	72,72,72,72	0
22	MG	A	1810	1/1	0.94	0.30	65,65,65,65	0
23	K	A	1736	1/1	0.94	0.22	108,108,108,108	0
22	MG	A	1714	1/1	0.94	0.51	94,94,94,94	0
22	MG	A	1704	1/1	0.94	0.24	60,60,60,60	0
22	MG	A	1691	1/1	0.94	0.23	82,82,82,82	0
22	MG	A	1780	1/1	0.94	0.34	75,75,75,75	0
22	MG	A	1639	1/1	0.94	0.26	28,28,28,28	0
22	MG	A	1670	1/1	0.94	0.21	57,57,57,57	0
22	MG	A	1794	1/1	0.94	0.32	73,73,73,73	0
22	MG	A	1696	1/1	0.94	0.34	45,45,45,45	0
22	MG	A	1820	1/1	0.94	0.26	65,65,65,65	0
24	NMY	A	1832	42/42	0.94	0.13	54,85,153,163	0
22	MG	B	303	1/1	0.94	0.23	83,83,83,83	0
22	MG	A	1629	1/1	0.94	0.41	43,43,43,43	0
22	MG	A	1654	1/1	0.94	0.20	50,50,50,50	0
22	MG	A	1618	1/1	0.94	0.36	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1636	1/1	0.95	0.37	64,64,64,64	0
22	MG	A	1612	1/1	0.95	0.67	93,93,93,93	0
22	MG	E	201	1/1	0.95	0.30	64,64,64,64	0
22	MG	A	1717	1/1	0.95	0.14	66,66,66,66	0
22	MG	A	1638	1/1	0.95	0.11	64,64,64,64	0
22	MG	A	1811	1/1	0.95	0.18	79,79,79,79	0
22	MG	A	1793	1/1	0.95	0.31	69,69,69,69	0
22	MG	A	1698	1/1	0.95	0.35	47,47,47,47	0
22	MG	A	1626	1/1	0.95	0.46	79,79,79,79	0
22	MG	A	1692	1/1	0.95	0.48	72,72,72,72	0
22	MG	P	101	1/1	0.95	0.27	68,68,68,68	0
22	MG	A	1635	1/1	0.95	0.35	41,41,41,41	0
22	MG	A	1718	1/1	0.96	0.55	84,84,84,84	0
22	MG	A	1719	1/1	0.96	0.10	62,62,62,62	0
22	MG	A	1678	1/1	0.96	0.12	35,35,35,35	0
22	MG	A	1649	1/1	0.96	0.31	40,40,40,40	0
22	MG	A	1628	1/1	0.96	0.37	57,57,57,57	0
24	NMY	A	1833	42/42	0.96	0.10	55,78,103,105	0
22	MG	A	1620	1/1	0.96	0.50	53,53,53,53	0
22	MG	A	1648	1/1	0.96	0.27	56,56,56,56	0
22	MG	A	1716	1/1	0.96	0.10	49,49,49,49	0
22	MG	A	1677	1/1	0.96	0.46	63,63,63,63	0
22	MG	A	1680	1/1	0.97	0.41	46,46,46,46	0
22	MG	A	1681	1/1	0.97	0.49	75,75,75,75	0
22	MG	A	1765	1/1	0.97	0.42	55,55,55,55	0
22	MG	A	1669	1/1	0.97	0.05	51,51,51,51	0
22	MG	A	1700	1/1	0.97	0.17	38,38,38,38	0
22	MG	A	1641	1/1	0.97	0.35	37,37,37,37	0
22	MG	A	1702	1/1	0.97	0.23	40,40,40,40	0
22	MG	A	1703	1/1	0.97	0.21	51,51,51,51	0
22	MG	A	1671	1/1	0.97	0.42	50,50,50,50	0
22	MG	M	201	1/1	0.97	0.12	72,72,72,72	0
22	MG	A	1625	1/1	0.97	0.62	57,57,57,57	0
22	MG	A	1634	1/1	0.97	0.20	40,40,40,40	0
22	MG	A	1687	1/1	0.97	0.46	60,60,60,60	0
25	ZN	D	301	1/1	0.97	0.22	92,92,92,92	0
22	MG	A	1722	1/1	0.98	0.03	35,35,35,35	0
22	MG	A	1708	1/1	0.98	0.15	63,63,63,63	0
22	MG	A	1605	1/1	0.98	0.42	44,44,44,44	0
22	MG	A	1607	1/1	0.98	0.46	59,59,59,59	0
22	MG	A	1674	1/1	0.98	0.06	38,38,38,38	0
22	MG	A	1695	1/1	0.98	0.11	53,53,53,53	0

*Continued on next page...*

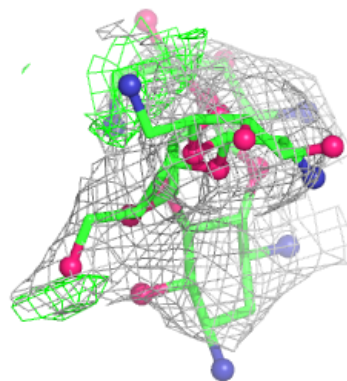
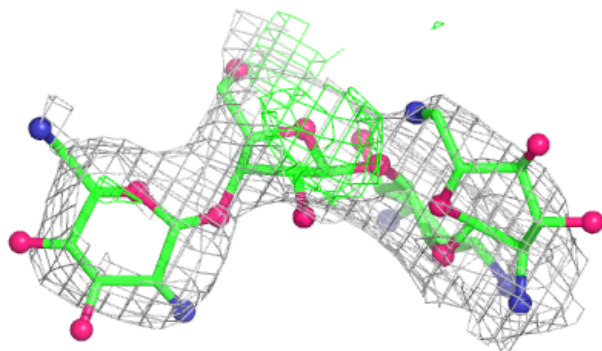
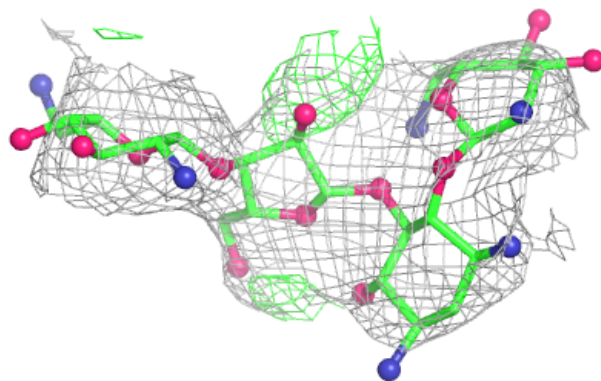
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1650	1/1	0.98	0.11	41,41,41,41	0
22	MG	A	1707	1/1	0.98	0.15	85,85,85,85	0
25	ZN	N	101	1/1	1.00	0.06	106,106,106,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NMY A 1837:**

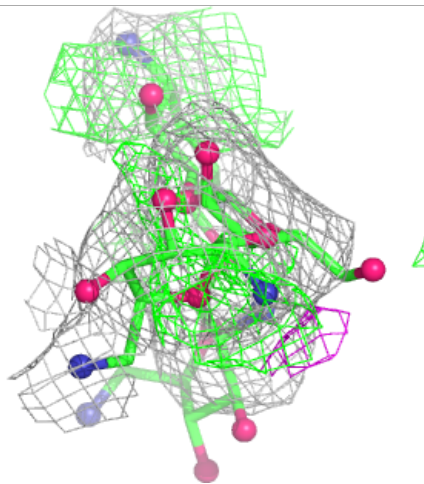
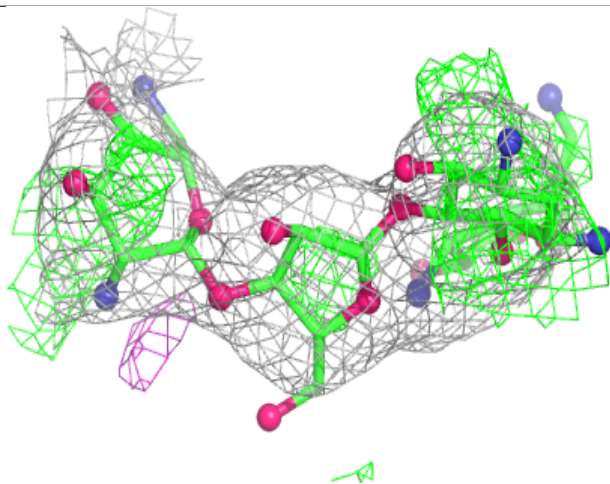
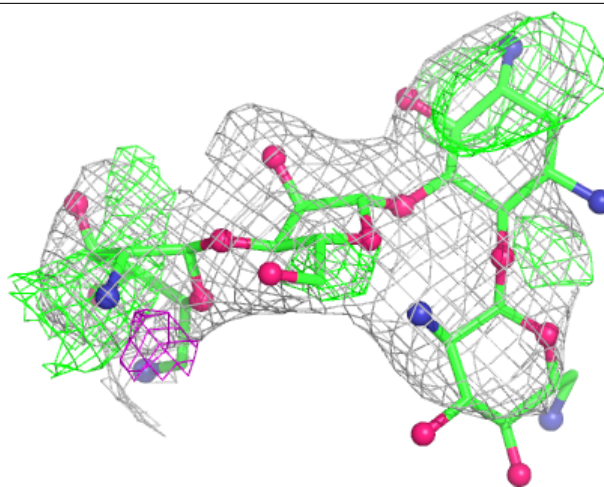
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





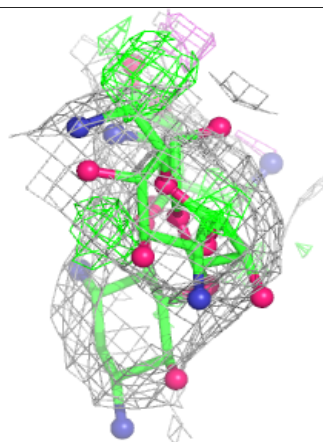
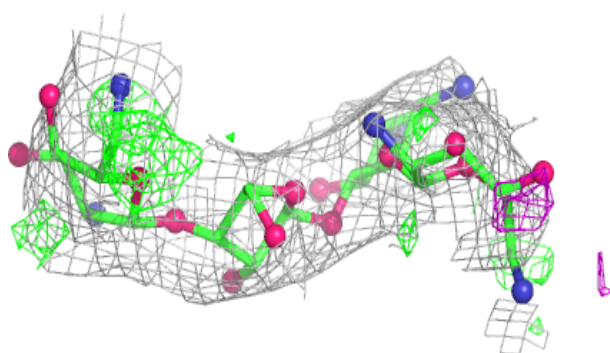
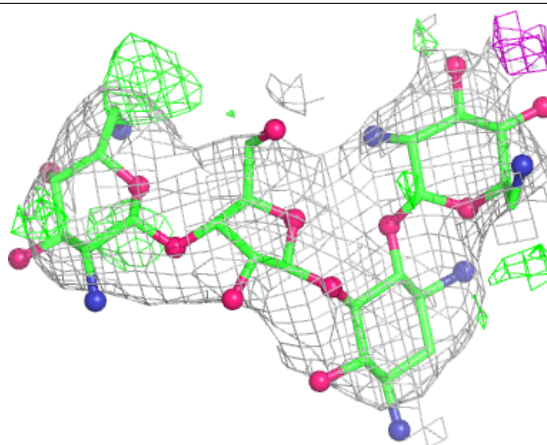
**Electron density around NMY A 1834:**

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



**Electron density around NMY A 1835:**

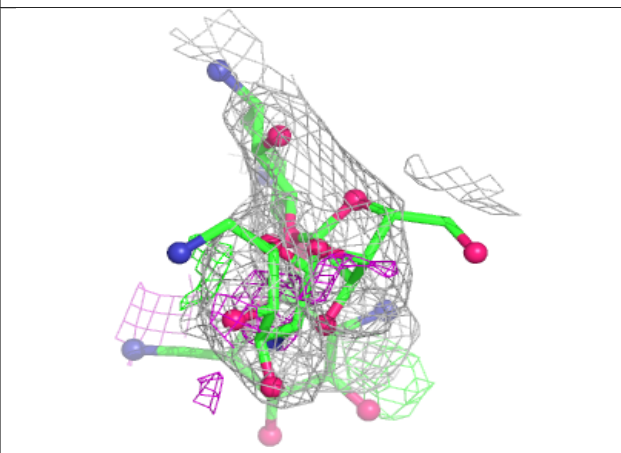
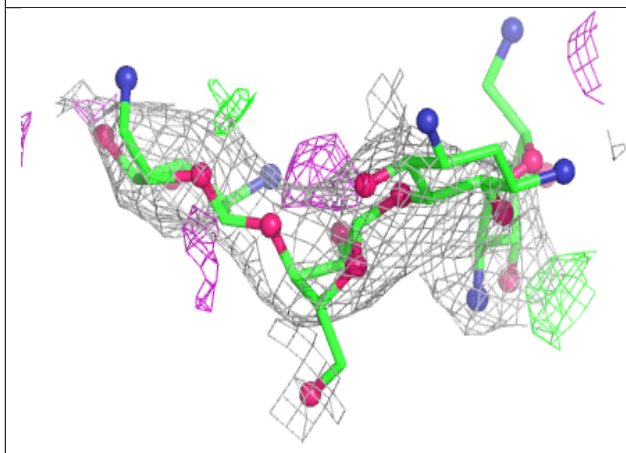
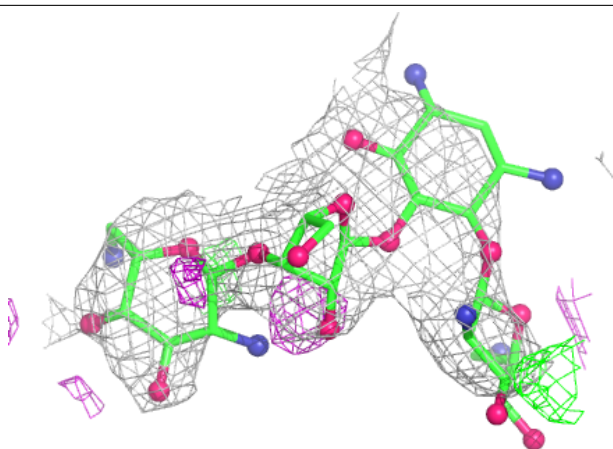
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



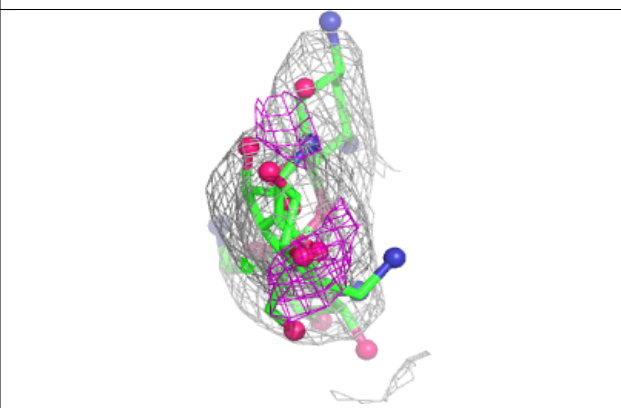
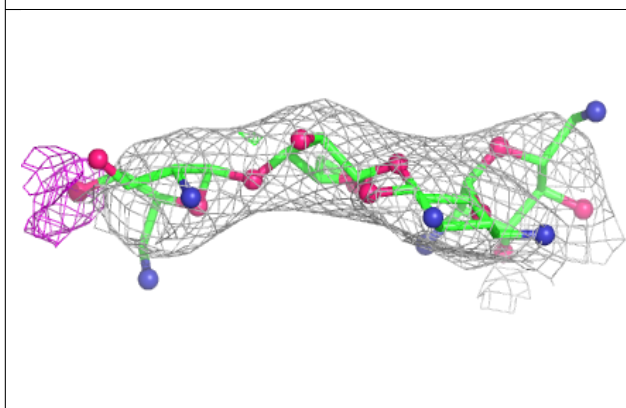
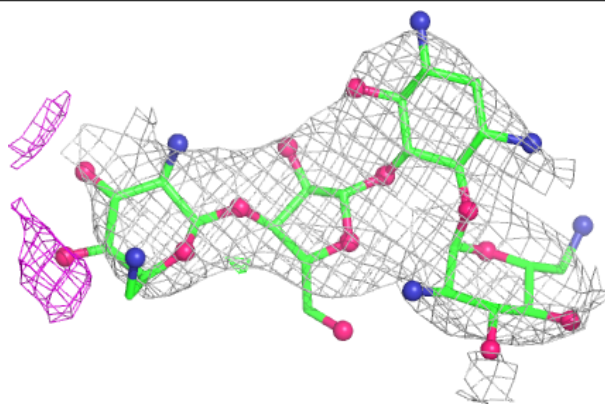


**Electron density around NMY A 1836:**

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

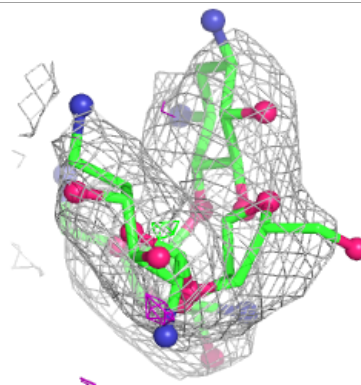
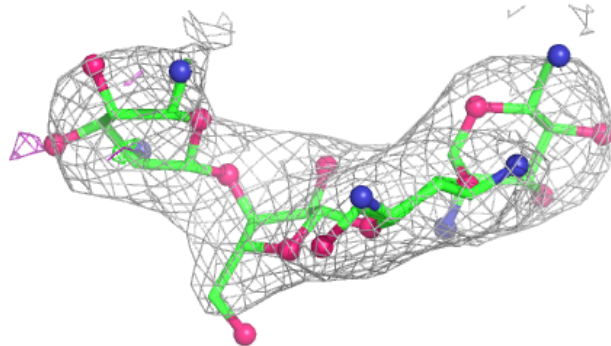
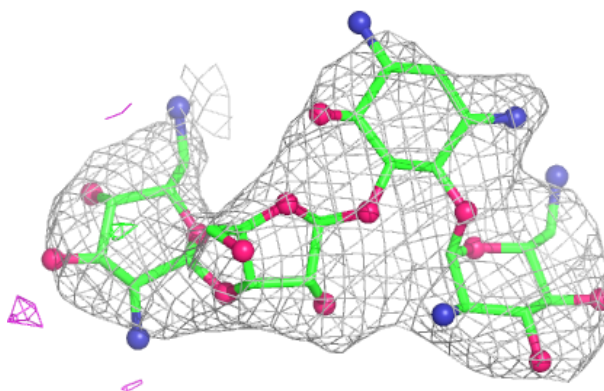
**Electron density around NMY A 1832:**

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



**Electron density around NMY A 1833:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.