



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:37 AM UTC

PDB ID : 4LFB / pdb_00004lfb
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 : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

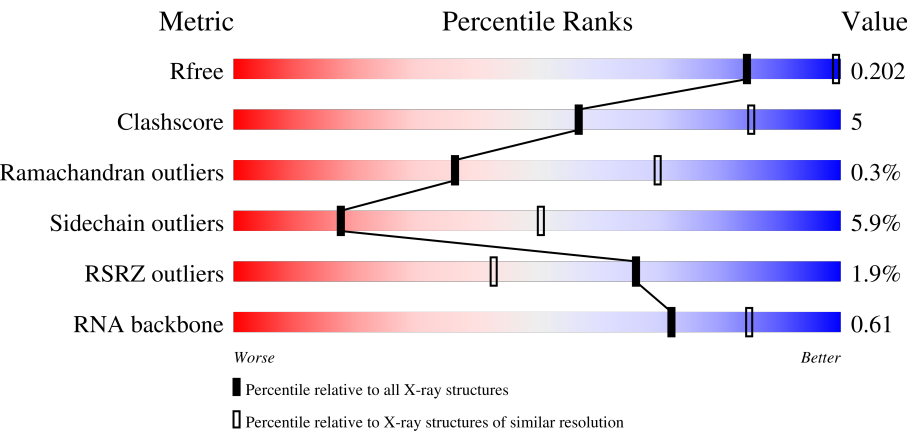
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.



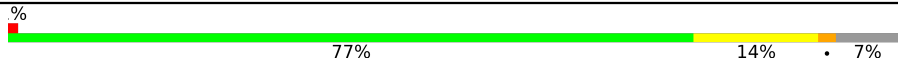
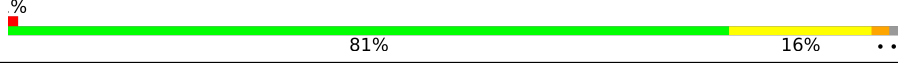
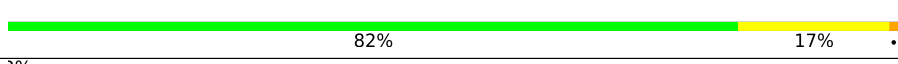
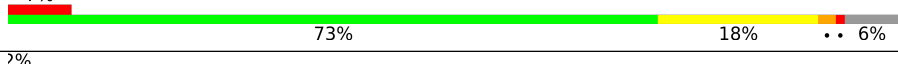
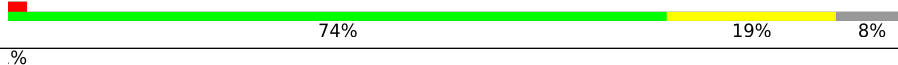
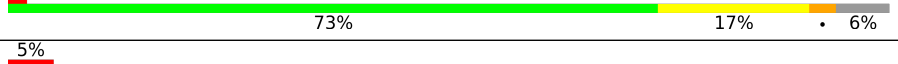
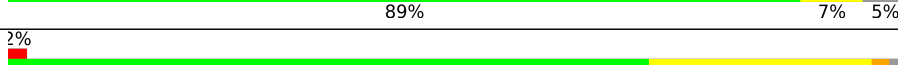
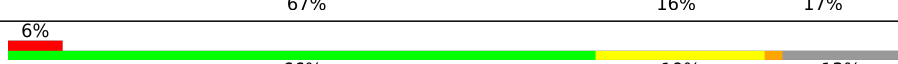
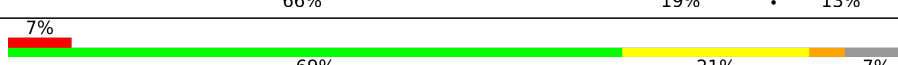
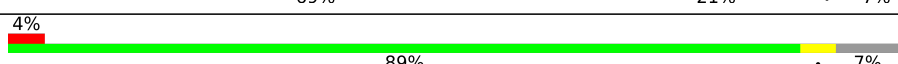
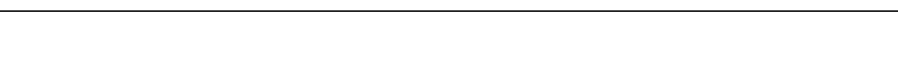
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 ≥ 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	73%22%.
2	B	256	3% 74%17%.8%
3	C	239	2% 64%20%.13%
4	D	209	6% 75%22%.

Continued on next page...

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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	1608	-	-	-	X
22	MG	A	1731	-	-	-	X
22	MG	A	1762	-	-	-	X
22	MG	A	1783	-	-	-	X
23	K	A	1750	-	-	-	X
23	K	A	1752	-	-	-	X
23	K	A	1757	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52046 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	1512	Total	C	N	O	P	0	0	0
			32504	14477	6011	10505	1511			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 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			

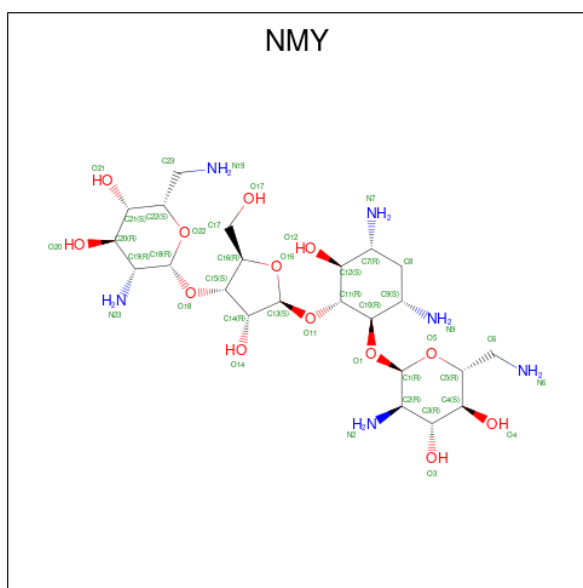
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	197	Total	Mg	0	0
			197	197		
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	N	1	Total	Mg	0	0
			1	1		
22	P	3	Total	Mg	0	0
			3	3		
22	Q	1	Total	Mg	0	0
			1	1		
22	S	2	Total	Mg	0	0
			2	2		
22	U	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	24	Total	K	0	0
			24	24		

- Molecule 24 is NEOMYCIN (CCD ID: 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		

- Molecule 25 is ZINC ION (CCD ID: 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		

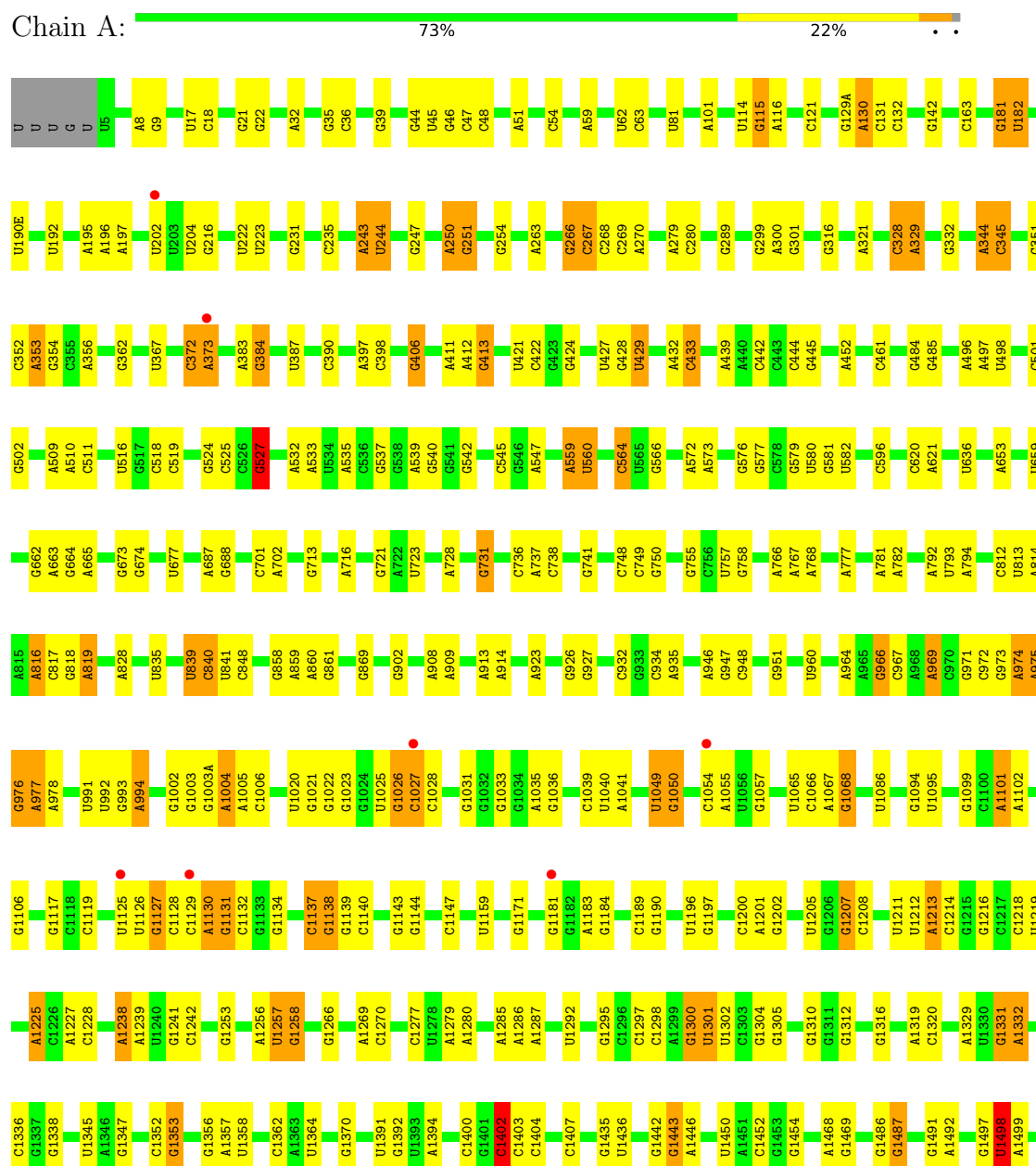
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	20	Total	O	0	0
			20	20		
26	H	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

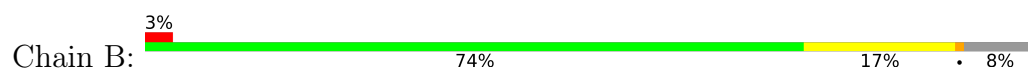
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

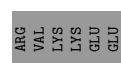
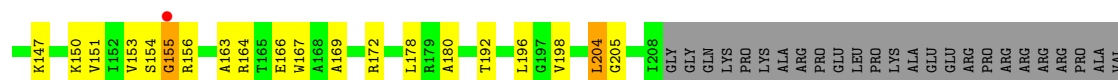
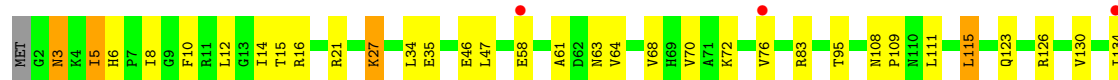




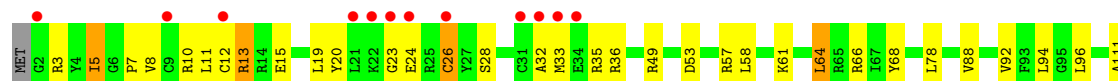
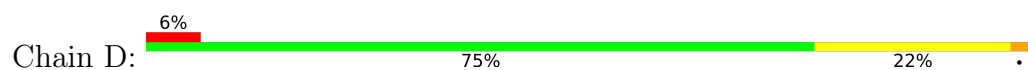
• Molecule 2: ribosomal protein S2



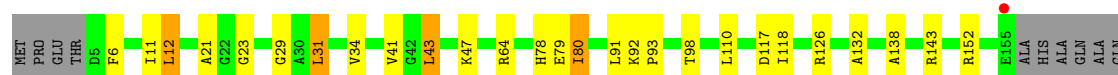
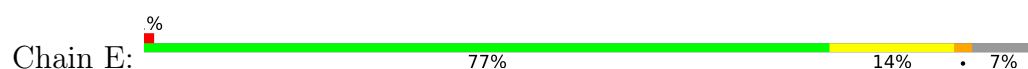
• Molecule 3: ribosomal protein S3



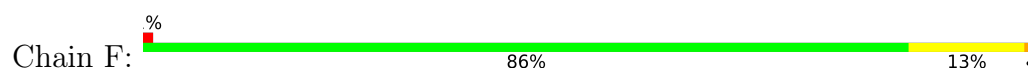
• Molecule 4: ribosomal protein S4



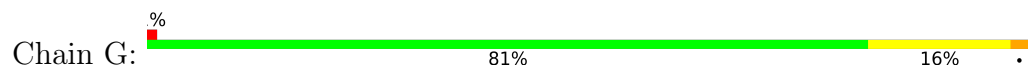
• Molecule 5: ribosomal protein S5



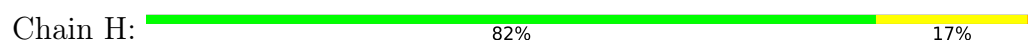
• Molecule 6: ribosomal protein S6



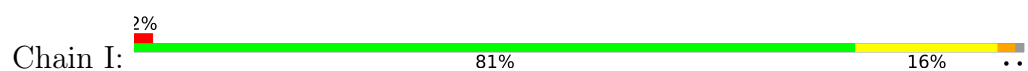
- Molecule 7: ribosomal protein S7



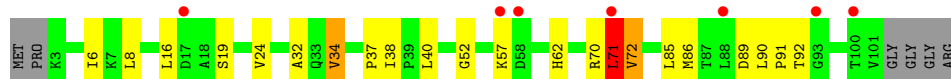
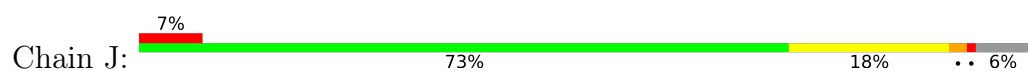
- Molecule 8: ribosomal protein S8



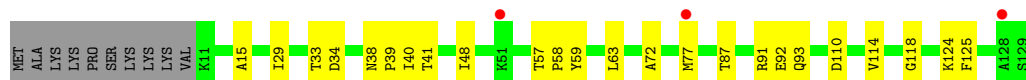
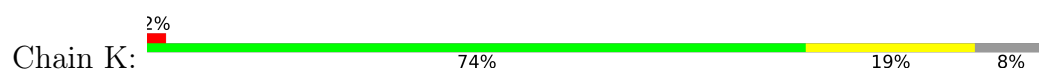
- Molecule 9: ribosomal protein S9



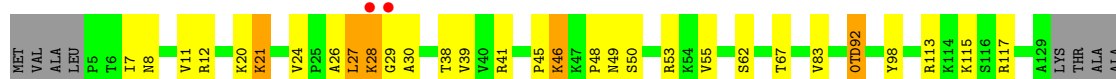
- Molecule 10: ribosomal protein S10



- Molecule 11: ribosomal protein S11



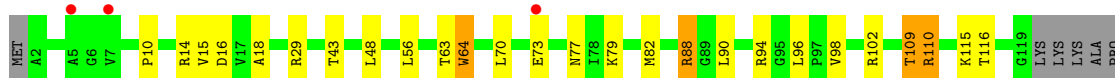
- Molecule 12: ribosomal protein S12



LYS
LYS

• Molecule 13: ribosomal protein S13

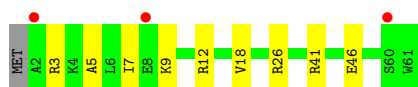
Chain M: 2% 73% 17% 6%



ARG
LYS

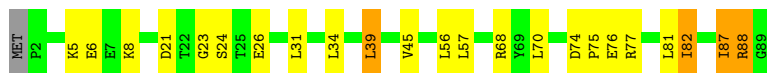
• Molecule 14: ribosomal protein S14

Chain N: 5% 84% 15%



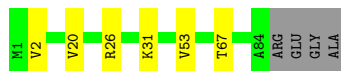
• Molecule 15: ribosomal protein S15

Chain O: 73% 21% 6%



• Molecule 16: ribosomal protein S16

Chain P: 89% 7% 5%



• Molecule 17: ribosomal protein S17

Chain Q: 2% 72% 25% 1%



• Molecule 18: ribosomal protein S18

Chain R: 3% 67% 16% 17%



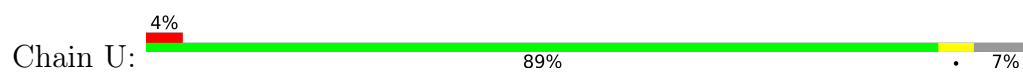
• Molecule 19: ribosomal protein S19



- 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, α , β , γ	402.76Å 402.76Å 177.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 3.01 34.54 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (34.54-3.01) 96.2 (34.54-3.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.00Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.169 , 0.203 0.170 , 0.202	Depositor DCC
R_{free} test set	13980 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52046	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMY, 2MG, ZN, MG, 4OC, 5MC, UR3, 0TD, PSU, MA6, 7MG, K, M2G

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	0.19	0/36037	0.37	1/56239 (0.0%)
2	B	0.35	0/1909	0.80	0/2579
3	C	0.36	0/1637	0.76	4/2207 (0.2%)
4	D	0.38	0/1733	0.83	6/2318 (0.3%)
5	E	0.46	0/1163	0.86	1/1566 (0.1%)
6	F	0.29	0/856	0.77	0/1154
7	G	0.34	0/1276	0.78	1/1709 (0.1%)
8	H	0.42	0/1136	0.88	0/1527
9	I	0.37	0/1029	0.83	1/1379 (0.1%)
10	J	0.38	0/806	0.89	1/1084 (0.1%)
11	K	0.41	0/900	0.87	0/1213
12	L	0.38	0/978	0.97	6/1308 (0.5%)
13	M	0.34	0/947	0.79	0/1270
14	N	0.36	0/501	0.74	0/664
15	O	0.35	0/745	0.72	0/992
16	P	0.39	0/717	0.78	0/965
17	Q	0.38	0/870	0.81	0/1159
18	R	0.34	0/604	0.75	0/801
19	S	0.30	0/662	0.81	0/892
20	T	0.42	0/765	0.87	2/1007 (0.2%)
21	U	0.30	0/213	0.77	0/279
All	All	0.27	0/55484	0.56	23/82312 (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
8	H	0	1
12	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-9.97	101.39	114.85
4	D	26	CYS	N-CA-C	-8.31	103.14	113.28
20	T	73	HIS	CB-CA-C	-6.96	107.51	115.79
12	L	26	ALA	N-CA-C	-6.89	104.75	113.02
20	T	74	LYS	CB-CA-C	-6.55	108.00	115.79
5	E	23	GLY	N-CA-C	6.53	119.77	111.09
4	D	33	MET	N-CA-C	-5.84	105.65	112.89
12	L	30	ALA	CA-C-N	5.72	125.09	118.85
12	L	30	ALA	C-N-CA	5.72	125.09	118.85
4	D	28	SER	CA-C-N	-5.67	112.76	119.84
4	D	28	SER	C-N-CA	-5.67	112.76	119.84
12	L	27	LEU	CB-CA-C	-5.61	109.11	115.79
4	D	12	CYS	N-CA-C	-5.54	104.47	111.11
3	C	155	GLY	N-CA-C	5.46	121.47	112.30
1	A	1498	UR3	P-O3'-C3'	5.27	126.02	119.70
10	J	71	LEU	N-CA-C	5.12	117.99	111.69
12	L	115	LYS	CA-C-N	-5.11	115.20	122.77
12	L	115	LYS	C-N-CA	-5.11	115.20	122.77
7	G	87	VAL	N-CA-C	5.10	113.48	107.77
4	D	13	ARG	N-CA-C	5.08	116.62	111.14
3	C	108	ASN	CA-C-N	5.03	124.69	119.56
3	C	108	ASN	C-N-CA	5.03	124.69	119.56
3	C	180	ALA	N-CA-C	5.01	118.16	111.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	90	GLY	Peptide
12	L	46	LYS	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	32504	0	16434	169	0
2	B	1874	0	1887	22	0
3	C	1613	0	1677	34	0
4	D	1703	0	1763	28	0
5	E	1147	0	1207	15	0
6	F	843	0	857	8	0
7	G	1257	0	1296	15	0
8	H	1116	0	1177	14	0
9	I	1010	0	1037	12	0
10	J	793	0	835	15	0
11	K	885	0	904	14	0
12	L	973	0	1058	16	0
13	M	937	0	995	17	0
14	N	492	0	529	6	0
15	O	734	0	771	9	0
16	P	701	0	720	1	0
17	Q	857	0	928	15	0
18	R	598	0	670	11	0
19	S	648	0	673	10	0
20	T	763	0	861	18	0
21	U	209	0	221	1	0
22	A	197	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	N	1	0	0	0	0
22	P	3	0	0	0	0
22	Q	1	0	0	0	0
22	S	2	0	0	0	0
22	U	1	0	0	0	0
23	A	24	0	0	0	0
24	A	126	0	138	4	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	20	0	0	0	0
26	H	4	0	0	0	0
All	All	52046	0	36638	394	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 5.

All (394) 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:975:A:H4'	1:A:976:G:H5''	1.58	0.85
1:A:664:G:H22	1:A:741:G:H1	1.28	0.82
1:A:279:A:OP2	17:Q:95:TYR:OH	1.98	0.81
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.63	0.80
1:A:1502:A:H2	1:A:1505:G:H1	1.28	0.80
1:A:1086:U:H3	1:A:1099:G:H22	1.28	0.78
1:A:406:G:H21	4:D:119:GLN:HE22	1.32	0.78
1:A:387:U:OP1	24:A:1824:NMY:N9	2.18	0.77
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.17	0.76
13:M:88:ARG:HD3	19:S:3:ARG:HH21	1.50	0.74
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.69	0.74
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.70	0.73
19:S:33:THR:HG22	19:S:35:SER:H	1.54	0.73
12:L:48:PRO:HD2	12:L:92:0TD:H3	1.69	0.73
1:A:542:G:OP1	4:D:10:ARG:NH2	2.22	0.72
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.73	0.71
1:A:427:U:OP1	4:D:13:ARG:NH2	2.23	0.71
1:A:951:G:OP2	13:M:102:ARG:NH2	2.24	0.71
1:A:413:G:N2	1:A:429:U:OP2	2.16	0.70
10:J:19:SER:HB3	10:J:91:PRO:HG3	1.74	0.70
20:T:50:GLU:HG3	20:T:100:ILE:HD12	1.73	0.69
11:K:15:ALA:HA	11:K:77:MET:HA	1.74	0.69
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.25	0.69
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.73	0.69
1:A:1128:C:O2'	1:A:1130:A:N7	2.25	0.69
1:A:560:U:H5'	1:A:566:G:N2	2.07	0.69
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.75	0.68
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.26	0.67
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.26	0.67
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.75	0.67
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:26:ARG:HD2	16:P:31:LYS:O	1.95	0.66
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.76	0.65
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.78	0.65
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.29	0.65
1:A:266:G:H5''	1:A:267:C:H5	1.61	0.65
1:A:501:C:OP1	12:L:117:ARG:NH2	2.29	0.64
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.78	0.64
1:A:1147:C:O2	9:I:16:ARG:NH1	2.31	0.64
20:T:10:LEU:HG	20:T:12:ALA:H	1.63	0.64
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.79	0.64
1:A:266:G:H5''	1:A:267:C:C5	2.33	0.64
1:A:537:G:OP1	12:L:113:ARG:NH2	2.28	0.63
1:A:975:A:H5'	1:A:975:A:H8	1.64	0.63
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.78	0.63
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.64	0.63
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.81	0.63
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.81	0.63
3:C:156:ARG:H	3:C:163:ALA:HA	1.64	0.63
7:G:140:ASP:OD1	7:G:143:ARG:NH2	2.33	0.62
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.81	0.62
6:F:11:ASN:HD22	6:F:14:LEU:HG	1.66	0.61
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.81	0.61
7:G:78:ARG:NH1	7:G:154:TYR:O	2.33	0.61
1:A:427:U:OP2	4:D:36:ARG:NH2	2.34	0.60
20:T:89:ARG:NH2	20:T:105:SER:O	2.33	0.60
3:C:46:GLU:HG3	3:C:83:ARG:HH21	1.67	0.60
11:K:57:THR:HG22	11:K:59:TYR:H	1.67	0.59
1:A:1392:G:H21	1:A:1502:A:H8	1.50	0.59
5:E:80:ILE:HD12	5:E:91:LEU:HD12	1.83	0.59
1:A:948:C:OP1	13:M:109:THR:HG22	2.03	0.59
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.20	0.58
1:A:266:G:H5'	1:A:268:C:H41	1.67	0.58
1:A:559:A:OP1	5:E:126:ARG:NH2	2.29	0.58
1:A:1266:G:N2	1:A:1269:A:OP2	2.34	0.58
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.85	0.58
12:L:8:ASN:O	12:L:12:ARG:HG3	2.04	0.58
1:A:362:G:O2'	12:L:28:LYS:NZ	2.37	0.57
3:C:6:HIS:HD2	3:C:8:ILE:H	1.50	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.39	0.57
2:B:223:ILE:HD13	2:B:230:VAL:H	1.69	0.57
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:O	12:L:29:GLY:N	2.37	0.57
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.39	0.57
3:C:21:ARG:HG3	3:C:58:GLU:HG2	1.87	0.56
18:R:47:THR:HA	18:R:83:GLU:HB2	1.85	0.56
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.87	0.56
1:A:972:C:H4'	10:J:57:LYS:HG2	1.88	0.56
4:D:49:ARG:H	4:D:49:ARG:HD2	1.69	0.56
1:A:1305:G:N2	1:A:1331:G:H1'	2.21	0.56
20:T:67:ALA:HA	20:T:73:HIS:H	1.69	0.56
1:A:976:G:H5'	1:A:1358:U:O2'	2.06	0.56
18:R:32:ARG:HA	18:R:69:THR:HG21	1.88	0.56
1:A:1295:G:O2'	13:M:14:ARG:NH1	2.39	0.55
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	1.88	0.55
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.87	0.55
5:E:152:ARG:NH2	8:H:107:LEU:O	2.39	0.55
1:A:818:G:H3'	1:A:819:A:H5''	1.89	0.55
1:A:1026:G:H3'	1:A:1027:C:H5''	1.88	0.55
1:A:580:U:H2'	1:A:581:G:O4'	2.06	0.55
1:A:1049:U:H4'	1:A:1050:G:O5'	2.07	0.55
1:A:1305:G:H22	1:A:1331:G:H1'	1.71	0.55
1:A:1435:G:H2'	1:A:1436:U:C6	2.42	0.55
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.89	0.54
1:A:353:A:H5'	1:A:353:A:H8	1.72	0.54
2:B:87:ARG:NH2	2:B:220:ASP:OD1	2.33	0.54
11:K:110:ASP:OD1	18:R:88:LYS:NZ	2.39	0.54
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.89	0.54
1:A:582:U:OP1	15:O:68:ARG:NH2	2.40	0.54
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.40	0.54
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.90	0.54
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.90	0.54
1:A:328:C:H4'	1:A:329:A:H5'	1.89	0.53
13:M:63:THR:HG23	13:M:64:TRP:H	1.72	0.53
1:A:1225:A:H2'	1:A:1225:A:N3	2.24	0.53
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.38	0.53
1:A:1510:U:H2'	1:A:1511:G:C8	2.43	0.53
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.73	0.53
20:T:41:ILE:HD13	20:T:87:LYS:HD2	1.91	0.53
1:A:132:C:O3'	20:T:74:LYS:NZ	2.38	0.53
1:A:1003:G:N2	1:A:1039:C:O2	2.41	0.53
1:A:1319:A:H5'	19:S:5:LEU:HD22	1.91	0.53
4:D:24:GLU:C	4:D:26:CYS:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:16:ASP:OD1	13:M:16:ASP:N	2.41	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.53
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.89	0.53
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.90	0.53
15:O:87:ILE:HG22	15:O:88:ARG:H	1.74	0.52
20:T:75:ASN:OD1	20:T:75:ASN:N	2.42	0.52
1:A:243:A:H4'	1:A:244:U:O5'	2.08	0.52
5:E:98:THR:HB	5:E:117:ASP:HB3	1.91	0.52
1:A:372:C:H4'	1:A:373:A:O5'	2.09	0.52
3:C:153:VAL:HG22	3:C:198:VAL:HG22	1.91	0.52
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.90	0.52
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.92	0.52
1:A:344:A:H5''	1:A:345:C:H5	1.75	0.52
1:A:250:A:H4'	1:A:251:G:O5'	2.09	0.52
1:A:1502:A:H2	1:A:1505:G:N1	2.01	0.52
1:A:1391:U:H2'	1:A:1392:G:C8	2.44	0.52
1:A:1238:A:H5'	1:A:1336:C:H41	1.74	0.52
1:A:673:G:H2'	1:A:674:G:C8	2.45	0.51
1:A:1127:G:H5'	9:I:66:ARG:HH12	1.74	0.51
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.51
1:A:1392:G:N2	1:A:1502:A:H8	2.07	0.51
13:M:73:GLU:O	13:M:77:ASN:ND2	2.42	0.51
1:A:1218:C:H2'	1:A:1219:U:C6	2.46	0.51
3:C:68:VAL:HG12	3:C:70:VAL:HG23	1.93	0.51
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.93	0.51
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.44	0.51
10:J:52:GLY:O	14:N:41:ARG:NH2	2.43	0.51
8:H:121:ASP:OD1	8:H:121:ASP:N	2.42	0.50
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.93	0.50
1:A:579:G:H5'	1:A:728:A:H1'	1.92	0.50
1:A:1292:U:OP1	7:G:41:ARG:NH2	2.44	0.50
18:R:47:THR:HG22	18:R:48:GLY:H	1.76	0.50
1:A:818:G:C3'	1:A:819:A:H5''	2.41	0.50
24:A:1822:NMY:O11	24:A:1822:NMY:H1	2.12	0.50
2:B:122:PHE:HA	2:B:127:ILE:HD13	1.94	0.50
7:G:46:ALA:O	7:G:50:ILE:HG12	2.11	0.50
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.94	0.50
1:A:35:G:H2'	1:A:36:C:C6	2.47	0.50
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.94	0.49
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.93	0.49
7:G:54:THR:HG22	7:G:56:GLN:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:90:LEU:N	10:J:91:PRO:HD2	2.27	0.49
1:A:1504:G:OP1	1:A:1507:A:H4'	2.12	0.49
5:E:6:PHE:HB3	5:E:34:VAL:HG22	1.95	0.49
1:A:181:G:H4'	1:A:182:U:H5'	1.93	0.49
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.93	0.49
9:I:37:PHE:HD2	9:I:40:LEU:HD12	1.77	0.49
9:I:55:ALA:O	9:I:58:HIS:ND1	2.36	0.49
1:A:130:A:OP2	1:A:190(E):U:O2'	2.21	0.49
1:A:1068:G:H8	1:A:1068:G:OP2	1.96	0.49
3:C:47:LEU:HG	3:C:76:VAL:HG12	1.95	0.49
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.93	0.49
1:A:1228:C:H4'	13:M:116:THR:HA	1.94	0.49
5:E:29:GLY:HA2	5:E:47:LYS:HG3	1.94	0.49
1:A:527:7MG:O2'	1:A:535:A:N1	2.40	0.48
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.95	0.48
3:C:123:GLN:O	3:C:126:ARG:HG2	2.13	0.48
1:A:1331:G:H4'	1:A:1332:A:O5'	2.14	0.48
1:A:1128:C:O2	1:A:1144:G:N2	2.47	0.48
2:B:47:THR:HA	2:B:202:PRO:HG2	1.95	0.48
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.48	0.48
12:L:45:PRO:HB2	12:L:92:0TD:SB	2.53	0.48
3:C:109:PRO:HB3	3:C:115:LEU:HD23	1.95	0.48
13:M:15:VAL:HG23	13:M:43:THR:O	2.14	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.48
1:A:1035:A:H2'	1:A:1036:G:H8	1.79	0.48
12:L:46:LYS:HG3	12:L:92:0TD:H8	1.95	0.48
13:M:88:ARG:HG3	13:M:98:VAL:HG13	1.96	0.48
11:K:57:THR:HG22	11:K:59:TYR:N	2.29	0.47
1:A:444:C:H2'	1:A:445:G:H8	1.79	0.47
1:A:59:A:OP1	24:A:1824:NMY:N2	2.47	0.47
1:A:564:C:O2'	8:H:91:ARG:NH2	2.48	0.47
1:A:923:A:OP1	5:E:21:ALA:HB2	2.14	0.47
1:A:1006:C:H42	1:A:1023:G:H1	1.61	0.47
1:A:1468:A:H2'	1:A:1469:G:O4'	2.14	0.47
1:A:263:A:OP2	20:T:79:ARG:NH1	2.48	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.47
2:B:44:LEU:HD12	2:B:44:LEU:H	1.80	0.47
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.96	0.47
1:A:1101:A:H4'	1:A:1102:A:O5'	2.15	0.47
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.49	0.47
8:H:19:VAL:HG23	8:H:21:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:73:HIS:HB3	20:T:74:LYS:H	1.55	0.47
1:A:1498:UR3:O4'	1:A:1519:MA6:H2	2.15	0.47
6:F:11:ASN:OD1	6:F:86:ARG:NH2	2.48	0.47
1:A:1352:C:H2'	1:A:1353:G:C8	2.50	0.46
20:T:92:LEU:O	20:T:96:GLY:N	2.44	0.46
1:A:501:C:H2'	1:A:502:G:C8	2.51	0.46
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.46
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.97	0.46
1:A:62:U:H2'	1:A:63:C:C6	2.51	0.46
1:A:750:G:N3	15:O:23:GLY:HA3	2.30	0.46
1:A:1131:G:H2'	1:A:1132:C:C6	2.50	0.46
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.97	0.46
1:A:192:U:H1'	20:T:103:GLY:HA2	1.98	0.46
1:A:1450:U:H2'	1:A:1452:C:C5	2.50	0.46
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.97	0.46
6:F:11:ASN:HD21	6:F:13:ASN:HB2	1.79	0.46
19:S:27:GLU:HG3	19:S:47:HIS:CE1	2.51	0.46
6:F:45:LEU:HD23	6:F:45:LEU:H	1.80	0.46
18:R:19:LYS:H	18:R:19:LYS:HD2	1.79	0.46
1:A:858:G:O6	1:A:869:G:H3'	2.16	0.46
1:A:1127:G:H21	1:A:1147:C:N4	2.14	0.46
3:C:6:HIS:CD2	3:C:8:ILE:H	2.33	0.46
1:A:1486:G:H2'	1:A:1487:G:O4'	2.15	0.46
1:A:383:A:C5	1:A:384:G:H1'	2.50	0.45
1:A:1300:G:HO2'	1:A:1301:U:P	2.38	0.45
1:A:973:G:H3'	1:A:974:A:H5''	1.98	0.45
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.99	0.45
1:A:1131:G:H1	1:A:1143:G:H21	1.64	0.45
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.98	0.45
1:A:1057:G:H5''	3:C:154:SER:HB2	1.98	0.45
1:A:1137:C:H4'	1:A:1138:G:C2	2.51	0.45
3:C:147:LYS:HG3	3:C:205:GLY:H	1.81	0.45
1:A:192:U:C1'	20:T:103:GLY:HA2	2.47	0.45
1:A:432:A:H3'	1:A:433:C:H5''	1.98	0.45
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.28	0.45
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.99	0.45
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.76	0.45
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.85	0.45
1:A:114:U:O2'	1:A:115:G:H5'	2.17	0.45
1:A:1040:U:H2'	1:A:1041:A:H8	1.81	0.45
7:G:145:ALA:C	7:G:147:ALA:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:ALA:O	10:J:34:VAL:HG23	2.16	0.45
1:A:964:A:N3	1:A:969:A:O2'	2.47	0.45
6:F:25:ILE:HG21	6:F:82:ARG:HD2	1.97	0.45
1:A:1200:C:O2'	1:A:1205:U:O4	2.22	0.45
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.99	0.45
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.18	0.44
4:D:53:ASP:O	4:D:57:ARG:HG2	2.17	0.44
11:K:87:THR:HA	11:K:91:ARG:HH21	1.83	0.44
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.50	0.44
1:A:994:A:OP1	1:A:994:A:C8	2.71	0.44
1:A:545:C:OP1	4:D:61:LYS:NZ	2.50	0.44
1:A:677:U:H3	1:A:713:G:H22	1.66	0.44
1:A:767:A:H2'	1:A:768:A:O4'	2.18	0.44
17:Q:94:ASN:O	17:Q:97:SER:HB3	2.18	0.44
19:S:44:MET:C	19:S:62:ILE:HD11	2.43	0.44
1:A:17:U:H2'	1:A:18:C:C6	2.52	0.44
1:A:519:C:OP2	12:L:50:SER:OG	2.34	0.44
4:D:5:ILE:H	4:D:115:ARG:HH22	1.65	0.44
1:A:21:G:H2'	1:A:22:G:C8	2.53	0.44
2:B:98:LEU:HG	2:B:101:MET:HE3	1.98	0.44
10:J:40:LEU:HD11	10:J:71:LEU:HD23	1.99	0.44
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.51	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.53	0.44
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.52	0.44
1:A:977:A:H2'	1:A:978:A:H5''	2.00	0.44
10:J:6:ILE:HB	10:J:72:VAL:HB	1.99	0.44
1:A:1002:G:H2'	1:A:1003:G:C8	2.54	0.43
3:C:61:ALA:O	3:C:63:ASN:ND2	2.47	0.43
1:A:908:A:H2'	1:A:909:A:C8	2.53	0.43
2:B:73:THR:HG23	2:B:95:GLN:O	2.17	0.43
3:C:14:ILE:HG22	3:C:15:THR:HG23	2.00	0.43
9:I:39:GLY:O	9:I:40:LEU:HD23	2.18	0.43
11:K:124:LYS:HE3	11:K:125:PHE:CZ	2.53	0.43
1:A:731:G:OP1	1:A:766:A:H1'	2.18	0.43
15:O:39:LEU:HD13	15:O:56:LEU:HB2	2.00	0.43
1:A:1277:C:O2'	1:A:1279:A:H1'	2.18	0.43
1:A:1443:G:H5''	1:A:1443:G:N3	2.34	0.43
10:J:85:LEU:HB3	10:J:86:MET:H	1.68	0.43
17:Q:53:LEU:HG	17:Q:82:MET:HE1	2.00	0.43
20:T:10:LEU:HD12	20:T:11:SER:H	1.83	0.43
8:H:6:ILE:HD11	8:H:31:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:G:C6	1:A:1305:G:N1	2.86	0.43
12:L:21:LYS:HE3	12:L:21:LYS:HB3	1.89	0.43
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.89	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.54	0.43
3:C:134:ILE:HG23	3:C:151:VAL:HB	2.00	0.43
15:O:21:ASP:OD1	15:O:24:SER:OG	2.31	0.43
1:A:839:U:H5'	1:A:840:C:H5	1.84	0.43
20:T:8:ARG:N	20:T:8:ARG:HH11	2.16	0.43
20:T:51:GLU:O	20:T:55:ILE:HG12	2.19	0.43
1:A:45:U:H2'	1:A:46:G:C8	2.54	0.43
1:A:716:A:N3	11:K:118:GLY:HA2	2.34	0.43
1:A:975:A:H5'	1:A:975:A:C8	2.48	0.43
1:A:1316:G:H4'	14:N:18:VAL:HG11	2.00	0.43
3:C:155:GLY:HA2	3:C:164:ARG:H	1.84	0.43
8:H:116:LYS:HD3	8:H:127:LEU:HD13	1.99	0.43
2:B:74:LYS:C	2:B:76:GLN:H	2.27	0.43
3:C:130:VAL:O	3:C:134:ILE:HG13	2.19	0.43
8:H:17:THR:HG22	8:H:63:LEU:HG	2.01	0.43
14:N:3:ARG:O	14:N:7:ILE:HG13	2.19	0.43
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.46	0.43
20:T:74:LYS:HB3	20:T:74:LYS:HE3	1.75	0.43
1:A:1035:A:H2'	1:A:1036:G:C8	2.54	0.42
17:Q:93:GLN:O	17:Q:96:GLU:HG2	2.18	0.42
1:A:8:A:N6	4:D:205:GLU:O	2.52	0.42
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.54	0.42
1:A:1239:A:C4	1:A:1298:C:N4	2.87	0.42
1:A:1356:G:H2'	1:A:1357:A:C8	2.54	0.42
3:C:70:VAL:HG12	3:C:72:LYS:H	1.84	0.42
1:A:1020:U:H2'	1:A:1021:G:C8	2.55	0.42
1:A:1257:U:O2'	1:A:1258:G:OP2	2.30	0.42
13:M:90:LEU:O	13:M:94:ARG:HG2	2.19	0.42
6:F:10:LEU:HD12	6:F:10:LEU:HA	1.89	0.42
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.94	0.42
1:A:280:C:O2	17:Q:38:ARG:HG3	2.19	0.42
1:A:328:C:H4'	1:A:329:A:C5'	2.49	0.42
3:C:6:HIS:HD2	3:C:8:ILE:N	2.16	0.42
3:C:35:GLU:HG3	3:C:95:THR:HG21	2.01	0.42
1:A:932:C:H4'	7:G:4:ARG:HH21	1.84	0.42
1:A:1022:G:H2'	1:A:1023:G:H8	1.85	0.42
1:A:1211:U:H1'	1:A:1213:A:C2	2.54	0.42
1:A:1329:A:H5'	13:M:29:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.35	0.42
1:A:316:G:OP2	1:A:351:G:O2'	2.36	0.42
1:A:1057:G:H5''	3:C:154:SER:CB	2.50	0.42
1:A:1329:A:N7	21:U:7:ARG:NH2	2.68	0.42
19:S:33:THR:HG22	19:S:35:SER:N	2.29	0.42
1:A:620:C:H2'	1:A:621:A:O4'	2.20	0.42
1:A:222:U:H2'	1:A:223:U:C6	2.55	0.41
1:A:659:U:OP2	15:O:8:LYS:NZ	2.53	0.41
10:J:89:ASP:OD2	10:J:91:PRO:HG2	2.20	0.41
13:M:96:LEU:C	13:M:110:ARG:HG2	2.45	0.41
1:A:835:U:OP1	18:R:64:ARG:NH2	2.45	0.41
1:A:1491:G:N7	24:A:1822:NMY:O17	2.46	0.41
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.88	0.41
1:A:539:A:H2'	1:A:540:G:C8	2.55	0.41
1:A:1040:U:H2'	1:A:1041:A:C8	2.56	0.41
1:A:1106:G:H5''	3:C:172:ARG:HG2	2.03	0.41
8:H:13:ILE:O	8:H:17:THR:HG23	2.21	0.41
1:A:662:G:H2'	1:A:663:A:C8	2.55	0.41
2:B:146:GLN:O	2:B:150:SER:HB3	2.20	0.41
4:D:68:TYR:OH	4:D:196:LEU:HD11	2.20	0.41
4:D:127:THR:HG23	4:D:147:ALA:HB3	2.02	0.41
4:D:140:VAL:HG11	4:D:146:ILE:HD11	2.02	0.41
19:S:41:VAL:HG23	19:S:43:GLU:HG2	2.01	0.41
1:A:1297:C:O2'	7:G:114:ARG:NH2	2.54	0.41
3:C:111:LEU:HD22	3:C:204:LEU:HD23	2.01	0.41
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.50	0.41
18:R:52:PRO:HB2	18:R:54:ARG:HG2	2.02	0.41
1:A:1028:C:H42	1:A:1033:G:H1	1.66	0.41
12:L:7:ILE:O	12:L:11:VAL:HG23	2.20	0.41
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.90	0.41
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.41
2:B:83:MET:HA	2:B:86:GLU:HB2	2.03	0.41
12:L:49:ASN:HB2	12:L:92:OTD:SB	2.61	0.41
17:Q:9:VAL:O	17:Q:21:VAL:HA	2.21	0.41
18:R:47:THR:HG22	18:R:48:GLY:N	2.36	0.41
1:A:737:A:H2'	1:A:738:C:C6	2.56	0.41
1:A:814:A:H2'	1:A:816:A:H5''	2.03	0.41
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.04	0.41
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.92	0.41
3:C:58:GLU:HB3	10:J:92:THR:HG21	2.03	0.41
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:89:ARG:HG3	20:T:104:LEU:HD13	2.03	0.41
1:A:142:G:O2'	1:A:196:A:N1	2.41	0.41
2:B:122:PHE:HA	2:B:127:ILE:HG21	2.02	0.41
4:D:32:ALA:O	4:D:36:ARG:N	2.42	0.41
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.92	0.41
11:K:33:THR:HG22	11:K:39:PRO:HA	2.03	0.41
2:B:25:ASN:HA	2:B:26:PRO:HD2	1.94	0.40
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.56	0.40
3:C:27:LYS:HD3	3:C:27:LYS:H	1.86	0.40
3:C:70:VAL:HG12	3:C:72:LYS:N	2.37	0.40
9:I:24:GLY:N	9:I:60:ASP:OD1	2.45	0.40
10:J:38:ILE:HB	10:J:71:LEU:HB2	2.02	0.40
1:A:254:G:OP1	17:Q:67:LYS:O	2.39	0.40
1:A:1134:G:N2	1:A:1140:C:O2	2.49	0.40
3:C:12:LEU:HA	3:C:12:LEU:HD23	1.88	0.40
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.40
11:K:34:ASP:OD1	11:K:38:ASN:N	2.54	0.40
3:C:3:ASN:OD1	3:C:3:ASN:N	2.54	0.40
4:D:11:LEU:HD13	4:D:66:ARG:HD3	2.03	0.40
4:D:57:ARG:HE	4:D:202:LEU:HD22	1.86	0.40
4:D:150:GLU:OE1	4:D:150:GLU:N	2.42	0.40
11:K:63:LEU:HD23	11:K:63:LEU:HA	1.90	0.40
1:A:736:C:H2'	1:A:737:A:C8	2.57	0.40
2:B:101:MET:HA	2:B:108:ILE:HG13	2.02	0.40
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.95	0.40
4:D:32:ALA:HA	4:D:35:ARG:HB2	2.04	0.40
4:D:88:VAL:O	4:D:92:VAL:HG23	2.22	0.40
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.80	0.40
5:E:80:ILE:HD12	5:E:138:ALA:HB1	2.03	0.40
7:G:63:LYS:HE3	7:G:63:LYS:HB2	1.90	0.40
7:G:69:VAL:HG21	7:G:104:LEU:HD21	2.03	0.40
14:N:12:ARG:HD2	14:N:12:ARG:H	1.87	0.40
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.21	0.40
13:M:79:LYS:HA	13:M:82:MET:HE2	2.03	0.40
15:O:82:ILE:HD13	15:O:88:ARG:HB2	2.03	0.40

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%)	216 (92%)	17 (7%)	1 (0%)	30	65
3	C	205/239 (86%)	189 (92%)	16 (8%)	0	100	100
4	D	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	60
5	E	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	99 (100%)	0	0	100	100
7	G	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
10	J	97/105 (92%)	82 (84%)	13 (13%)	2 (2%)	5	27
11	K	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
12	L	122/135 (90%)	114 (93%)	7 (6%)	1 (1%)	16	50
13	M	116/126 (92%)	113 (97%)	3 (3%)	0	100	100
14	N	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	Q	102/105 (97%)	96 (94%)	6 (6%)	0	100	100
18	R	71/88 (81%)	64 (90%)	7 (10%)	0	100	100
19	S	79/93 (85%)	71 (90%)	7 (9%)	1 (1%)	9	38
20	T	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2357/2541 (93%)	2218 (94%)	133 (6%)	6 (0%)	36	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS

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Mol	Chain	Res	Type
19	S	31	ILE
10	J	72	VAL
10	J	34	VAL
4	D	5	ILE
2	B	229	VAL

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%)	183 (94%)	11 (6%)	18	52
3	C	160/188 (85%)	148 (92%)	12 (8%)	12	41
4	D	180/181 (99%)	170 (94%)	10 (6%)	19	52
5	E	115/123 (94%)	108 (94%)	7 (6%)	17	49
6	F	90/90 (100%)	86 (96%)	4 (4%)	25	60
7	G	126/127 (99%)	120 (95%)	6 (5%)	23	57
8	H	119/119 (100%)	113 (95%)	6 (5%)	22	56
9	I	98/99 (99%)	93 (95%)	5 (5%)	21	55
10	J	87/92 (95%)	85 (98%)	2 (2%)	44	74
11	K	90/99 (91%)	86 (96%)	4 (4%)	25	60
12	L	103/110 (94%)	96 (93%)	7 (7%)	14	45
13	M	94/101 (93%)	87 (93%)	7 (7%)	13	42
14	N	49/50 (98%)	48 (98%)	1 (2%)	48	76
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	12
16	P	72/74 (97%)	68 (94%)	4 (6%)	19	52
17	Q	96/97 (99%)	90 (94%)	6 (6%)	16	48
18	R	64/77 (83%)	63 (98%)	1 (2%)	55	79
19	S	71/80 (89%)	66 (93%)	5 (7%)	14	44
20	T	76/82 (93%)	71 (93%)	5 (7%)	15	46
21	U	19/22 (86%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1982/2111 (94%)	1866 (94%)	116 (6%)	18 50

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	LYS
2	B	61	LEU
2	B	75	LYS
2	B	86	GLU
2	B	97	TRP
2	B	102	LEU
2	B	121	LEU
2	B	175	ARG
2	B	187	LEU
2	B	221	LEU
2	B	236	TYR
3	C	3	ASN
3	C	5	ILE
3	C	27	LYS
3	C	34	LEU
3	C	64	VAL
3	C	115	LEU
3	C	166	GLU
3	C	167	TRP
3	C	178	LEU
3	C	192	THR
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	15	GLU
4	D	19	LEU
4	D	58	LEU
4	D	64	LEU
4	D	96	LEU
4	D	122	ARG
4	D	135	LEU
4	D	170	VAL
5	E	12	LEU
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU

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Mol	Chain	Res	Type
5	E	64	ARG
5	E	79	GLU
5	E	80	ILE
6	F	10	LEU
6	F	39	LYS
6	F	69	GLU
6	F	75	LEU
7	G	75	VAL
7	G	113	GLU
7	G	114	ARG
7	G	124	LEU
7	G	126	ASP
7	G	156	TRP
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	91	ARG
8	H	102	ARG
8	H	133	LEU
9	I	25	LYS
9	I	79	LEU
9	I	112	LYS
9	I	118	LYS
9	I	128	ARG
10	J	62	HIS
10	J	71	LEU
11	K	29	ILE
11	K	48	ILE
11	K	92	GLU
11	K	114	VAL
12	L	20	LYS
12	L	21	LYS
12	L	41	ARG
12	L	55	VAL
12	L	62	SER
12	L	67	THR
12	L	83	VAL
13	M	56	LEU
13	M	64	TRP
13	M	70	LEU
13	M	88	ARG
13	M	109	THR

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Mol	Chain	Res	Type
13	M	110	ARG
13	M	115	LYS
14	N	9	LYS
15	O	5	LYS
15	O	6	GLU
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	45	VAL
15	O	57	LEU
15	O	70	LEU
15	O	76	GLU
15	O	81	LEU
15	O	82	ILE
15	O	87	ILE
15	O	88	ARG
16	P	2	VAL
16	P	20	VAL
16	P	53	VAL
16	P	67	THR
17	Q	9	VAL
17	Q	38	ARG
17	Q	59	ILE
17	Q	74	LEU
17	Q	98	LEU
17	Q	101	ARG
18	R	86	VAL
19	S	6	LYS
19	S	7	LYS
19	S	15	LEU
19	S	43	GLU
19	S	81	ARG
20	T	8	ARG
20	T	31	SER
20	T	56	MET
20	T	75	ASN
20	T	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	78	GLN

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Mol	Chain	Res	Type
2	B	212	GLN
3	C	6	HIS
3	C	31	HIS
3	C	69	HIS
3	C	108	ASN
4	D	74	GLN
4	D	119	GLN
6	F	11	ASN
9	I	3	GLN
11	K	116	HIS
13	M	62	ASN
13	M	106	ASN
15	O	71	GLN
20	T	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	204 (13%)	31 (2%)

All (204) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	54	C
1	A	81	U
1	A	101	A
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U

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Mol	Chain	Res	Type
1	A	195	A
1	A	197	A
1	A	202	U
1	A	204	U
1	A	216	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A

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Mol	Chain	Res	Type
1	A	461	C
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	596	C
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A
1	A	721	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U

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Mol	Chain	Res	Type
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1031	G
1	A	1050	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C

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Mol	Chain	Res	Type
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1312	G
1	A	1320	C
1	A	1332	A
1	A	1338	G
1	A	1347	G
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1394	A

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Mol	Chain	Res	Type
1	A	1402	4OC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1519	MA6
1	A	1520	G
1	A	1529	G
1	A	1530	G

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	1049	U

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Mol	Chain	Res	Type
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1201	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1443	G
1	A	1505	G

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

15 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	$\# Z > 2$
12	0TD	L	92	12	8,9,10	1.39	1 (12%)	6,11,13	1.86	2 (33%)
1	UR3	A	1498	1	19,22,23	0.73	1 (5%)	26,32,35	1.05	1 (3%)
1	PSU	A	1540	1	18,21,22	1.12	1 (5%)	21,30,33	1.75	4 (19%)
1	5MC	A	1400	1	19,22,23	1.11	3 (15%)	26,32,35	0.95	1 (3%)
1	2MG	A	1207	1	23,26,27	1.39	5 (21%)	33,38,41	1.17	4 (12%)
1	PSU	A	516	22,1	18,21,22	1.13	1 (5%)	21,30,33	1.86	5 (23%)
1	MA6	A	1518	1	23,26,27	1.04	2 (8%)	33,38,41	0.83	1 (3%)
1	5MC	A	967	1	19,22,23	1.09	2 (10%)	26,32,35	0.94	2 (7%)
1	M2G	A	966	1	24,27,28	1.23	3 (12%)	33,40,43	0.79	1 (3%)
1	PSU	A	1541	22,1	18,21,22	1.08	1 (5%)	21,30,33	1.88	6 (28%)
1	4OC	A	1402	1	20,23,24	0.99	2 (10%)	25,32,35	0.76	0
1	MA6	A	1519	1	23,26,27	1.15	2 (8%)	33,38,41	0.93	0
1	5MC	A	1407	1	19,22,23	1.01	2 (10%)	26,32,35	0.94	1 (3%)
1	7MG	A	527	1	23,26,27	3.93	4 (17%)	27,39,42	2.30	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1404	1	19,22,23	0.99	2 (10%)	26,32,35	1.01	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	0TD	L	92	12	-	2/7/12/14	-
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	PSU	A	516	22,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	2/11/29/30	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/11/29/30	0/3/3/3
1	PSU	A	1541	22,1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
1	5MC	A	1407	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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-17.54	1.34	1.45
1	A	527	7MG	C2-N2	4.16	1.43	1.34
1	A	516	PSU	C6-C5	3.82	1.39	1.35
1	A	1540	PSU	C6-C5	3.80	1.39	1.35
1	A	527	7MG	C5-N7	3.75	1.40	1.35
1	A	1541	PSU	C6-C5	3.46	1.39	1.35
1	A	527	7MG	C4-N3	3.26	1.41	1.34
1	A	1207	2MG	C2-N2	3.25	1.40	1.33
1	A	966	M2G	C2-N2	3.12	1.40	1.35
12	L	92	0TD	CB-CA	-2.93	1.53	1.54
1	A	966	M2G	C4-N3	2.90	1.40	1.34
1	A	1407	5MC	C2-N1	2.74	1.45	1.40
1	A	1207	2MG	C2-N1	2.66	1.40	1.36
1	A	1400	5MC	C2-N1	2.65	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C2-N3	2.56	1.41	1.36
1	A	1519	MA6	C2-N1	2.53	1.38	1.33
1	A	1207	2MG	C4-N3	2.52	1.40	1.34
1	A	1519	MA6	C5-C4	2.52	1.43	1.39
1	A	967	5MC	C2-N1	2.50	1.45	1.40
1	A	1207	2MG	C8-N9	2.36	1.42	1.37
1	A	1404	5MC	C2-N1	2.34	1.45	1.40
1	A	1400	5MC	C2-N3	2.34	1.41	1.36
1	A	966	M2G	C8-N9	2.27	1.42	1.37
1	A	1402	4OC	C2-N3	2.25	1.40	1.36
1	A	1207	2MG	C2-N3	2.22	1.36	1.32
1	A	1518	MA6	C8-N9	2.21	1.41	1.37
1	A	1404	5MC	C2-N3	2.20	1.40	1.36
1	A	1407	5MC	C2-N3	2.16	1.40	1.36
1	A	1518	MA6	C5-C4	2.14	1.42	1.39
1	A	1498	UR3	C2-N1	2.09	1.41	1.38
1	A	1402	4OC	O2-C2	-2.06	1.19	1.23
1	A	1400	5MC	C6-C5	2.03	1.37	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C2-N3-C4	4.97	120.85	112.30
1	A	527	7MG	C5-C6-N1	4.95	119.65	110.94
1	A	1541	PSU	C4-N3-C2	-4.77	119.80	126.37
1	A	527	7MG	N9-C4-N3	4.60	132.20	125.46
1	A	1540	PSU	C4-N3-C2	-4.57	120.07	126.37
1	A	516	PSU	N1-C2-N3	4.55	119.97	115.17
1	A	1541	PSU	N1-C2-N3	4.55	119.96	115.17
1	A	516	PSU	C4-N3-C2	-4.52	120.15	126.37
1	A	1540	PSU	N1-C2-N3	4.34	119.75	115.17
1	A	527	7MG	C5-C4-N3	-4.24	120.18	128.13
1	A	527	7MG	N9-C8-N7	3.73	108.66	103.37
1	A	516	PSU	O2-C2-N1	-3.13	119.56	122.79
1	A	1207	2MG	C5-C4-N3	-2.90	123.78	128.39
1	A	1541	PSU	O2-C2-N1	-2.87	119.83	122.79
1	A	527	7MG	O6-C6-C5	-2.83	120.68	127.62
1	A	527	7MG	C6-C5-C4	-2.77	117.54	122.40
1	A	527	7MG	C2-N1-C6	-2.75	120.12	125.11
1	A	1498	UR3	C6-N1-C2	-2.69	119.60	121.80
1	A	1207	2MG	O6-C6-N1	-2.62	115.18	120.11
1	A	1207	2MG	N9-C4-N3	2.60	131.15	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-2.56	97.76	102.36
1	A	516	PSU	C6-N1-C2	-2.54	120.33	122.69
1	A	527	7MG	C6-C5-N7	2.52	135.84	131.93
1	A	1404	5MC	C5-C4-N3	2.52	124.34	121.75
12	L	92	0TD	OD1-CG-CB	-2.41	117.40	122.44
1	A	1404	5MC	N4-C4-N3	-2.40	114.16	118.51
1	A	1400	5MC	N4-C4-N3	-2.35	114.25	118.51
1	A	1540	PSU	O2-C2-N1	-2.23	120.49	122.79
1	A	967	5MC	C5-C4-N3	2.22	124.03	121.75
1	A	516	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	A	1540	PSU	C6-N1-C2	-2.14	120.70	122.69
1	A	1518	MA6	C2-N1-C6	2.14	117.05	111.83
1	A	1541	PSU	O4'-C1'-C2'	2.12	108.09	105.15
1	A	1407	5MC	N4-C4-N3	-2.12	114.67	118.51
1	A	1541	PSU	C6-N1-C2	-2.07	120.77	122.69
1	A	967	5MC	N4-C4-N3	-2.07	114.77	118.51
1	A	1541	PSU	C6-C5-C4	2.04	119.55	118.17
1	A	966	M2G	C5-C4-N3	-2.03	125.16	128.39
1	A	1207	2MG	C2-N1-C6	-2.01	122.12	124.55

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C5-C6-N6-C9
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	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1518	MA6	C3'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1
1	A	1518	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	92	0TD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	1	0
1	A	1207	2MG	1	0
1	A	1402	4OC	1	0
1	A	1519	MA6	1	0
1	A	527	7MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 239 are monoatomic - leaving 3 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	1822	-	43,45,45	1.30	4 (9%)	62,67,67	1.49	12 (19%)
24	NMY	A	1823	22	43,45,45	1.37	7 (16%)	62,67,67	1.74	11 (17%)
24	NMY	A	1824	-	43,45,45	1.53	7 (16%)	62,67,67	1.71	13 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	NMY	A	1822	-	-	6/18/94/94	0/4/4/4
24	NMY	A	1823	22	-	9/18/94/94	0/4/4/4
24	NMY	A	1824	-	-	8/18/94/94	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1824	NMY	C1-C2	4.29	1.60	1.52
24	A	1824	NMY	C3-C2	3.91	1.58	1.53
24	A	1823	NMY	C1-C2	3.29	1.58	1.52
24	A	1823	NMY	C3-C2	3.19	1.57	1.53
24	A	1824	NMY	C13-C14	3.19	1.57	1.52
24	A	1822	NMY	C3-C2	3.12	1.57	1.53
24	A	1823	NMY	C18-C19	2.89	1.58	1.52
24	A	1824	NMY	C18-C19	2.81	1.57	1.52
24	A	1822	NMY	C1-C2	2.67	1.57	1.52
24	A	1823	NMY	C13-C14	2.52	1.56	1.52
24	A	1822	NMY	C10-C11	2.42	1.57	1.52
24	A	1822	NMY	C13-C14	2.40	1.56	1.52
24	A	1824	NMY	C10-C11	2.29	1.57	1.52
24	A	1824	NMY	C10-C9	2.23	1.57	1.53
24	A	1823	NMY	C10-C11	2.17	1.56	1.52
24	A	1823	NMY	C10-C9	2.15	1.57	1.53
24	A	1823	NMY	C20-C19	2.11	1.56	1.53
24	A	1824	NMY	C20-C19	2.11	1.56	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1823	NMY	C13-C14-C15	-7.19	93.45	102.10
24	A	1824	NMY	C11-C10-C9	-5.04	101.97	111.31
24	A	1824	NMY	O1-C10-C11	4.65	119.23	107.42
24	A	1824	NMY	O1-C1-C2	4.25	115.03	108.08
24	A	1822	NMY	O20-C20-C19	-4.20	102.67	110.22
24	A	1822	NMY	O1-C10-C11	4.19	118.07	107.42
24	A	1823	NMY	C14-C15-C16	-3.65	96.84	103.24
24	A	1823	NMY	O1-C1-C2	3.56	113.91	108.08
24	A	1823	NMY	O16-C13-C14	-3.55	100.47	104.98
24	A	1823	NMY	O18-C18-C19	3.44	113.70	108.08
24	A	1824	NMY	O11-C13-O16	-3.43	107.86	111.37
24	A	1822	NMY	O11-C13-O16	-3.36	107.94	111.37
24	A	1823	NMY	O1-C10-C11	3.16	115.43	107.42
24	A	1824	NMY	O16-C13-C14	-3.06	101.08	104.98
24	A	1823	NMY	O20-C20-C19	-3.01	104.81	110.22
24	A	1824	NMY	O11-C11-C12	2.93	114.67	107.23
24	A	1822	NMY	O21-C21-C20	-2.85	103.65	110.38
24	A	1823	NMY	O18-C18-O22	-2.77	103.42	110.69
24	A	1824	NMY	O20-C20-C19	-2.69	105.39	110.22
24	A	1822	NMY	C13-C14-C15	-2.62	98.95	102.10
24	A	1823	NMY	O21-C21-C20	-2.56	104.35	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1824	NMY	O18-C18-C19	2.51	112.19	108.08
24	A	1824	NMY	O21-C21-C20	-2.48	104.53	110.38
24	A	1822	NMY	O16-C13-C14	-2.42	101.90	104.98
24	A	1822	NMY	C11-C10-C9	-2.41	106.85	111.31
24	A	1822	NMY	C8-C7-C12	-2.40	106.48	110.08
24	A	1822	NMY	C9-C8-C7	-2.31	107.06	111.02
24	A	1823	NMY	C11-C10-C9	-2.17	107.28	111.31
24	A	1822	NMY	O18-C18-C19	2.17	111.62	108.08
24	A	1824	NMY	O12-C12-C7	-2.13	105.91	109.90
24	A	1824	NMY	C13-C14-C15	-2.11	99.57	102.10
24	A	1824	NMY	O5-C5-C6	2.09	110.08	106.07
24	A	1822	NMY	O12-C12-C7	-2.07	106.02	109.90
24	A	1824	NMY	O11-C11-C10	2.07	112.68	107.42
24	A	1822	NMY	C18-O18-C15	-2.04	113.14	117.98
24	A	1823	NMY	C1-C2-N2	2.01	113.82	110.20

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1822	NMY	C21-C22-C23-N19
24	A	1822	NMY	O22-C22-C23-N19
24	A	1823	NMY	C4-C5-C6-N6
24	A	1823	NMY	O5-C5-C6-N6
24	A	1823	NMY	C14-C13-O11-C11
24	A	1823	NMY	O16-C13-O11-C11
24	A	1823	NMY	C19-C18-O18-C15
24	A	1823	NMY	O22-C22-C23-N19
24	A	1824	NMY	C9-C10-O1-C1
24	A	1824	NMY	C4-C5-C6-N6
24	A	1824	NMY	O5-C5-C6-N6
24	A	1824	NMY	O22-C22-C23-N19
24	A	1824	NMY	C12-C11-O11-C13
24	A	1823	NMY	O22-C18-O18-C15
24	A	1822	NMY	C11-C10-O1-C1
24	A	1824	NMY	C11-C10-O1-C1
24	A	1822	NMY	O16-C16-C17-O17
24	A	1822	NMY	O16-C13-O11-C11
24	A	1822	NMY	C9-C10-O1-C1
24	A	1824	NMY	O16-C13-O11-C11
24	A	1823	NMY	C16-C15-O18-C18
24	A	1824	NMY	C21-C22-C23-N19

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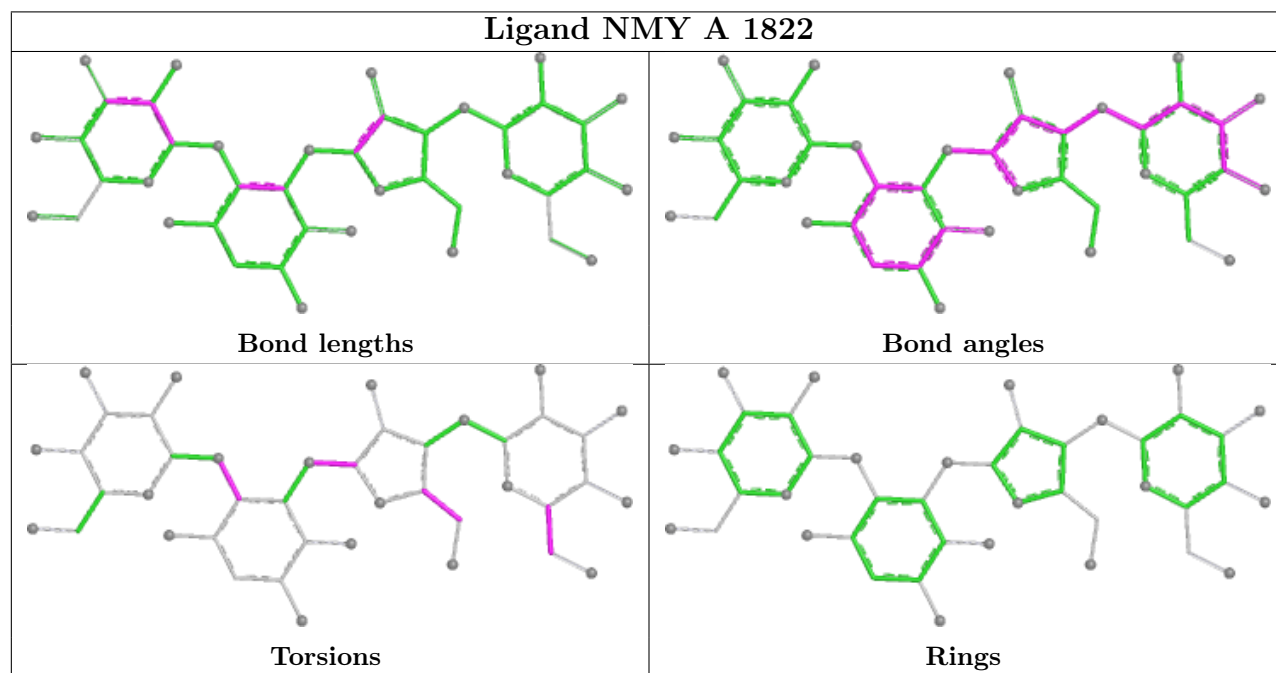
Mol	Chain	Res	Type	Atoms
24	A	1823	NMY	C14-C15-O18-C18

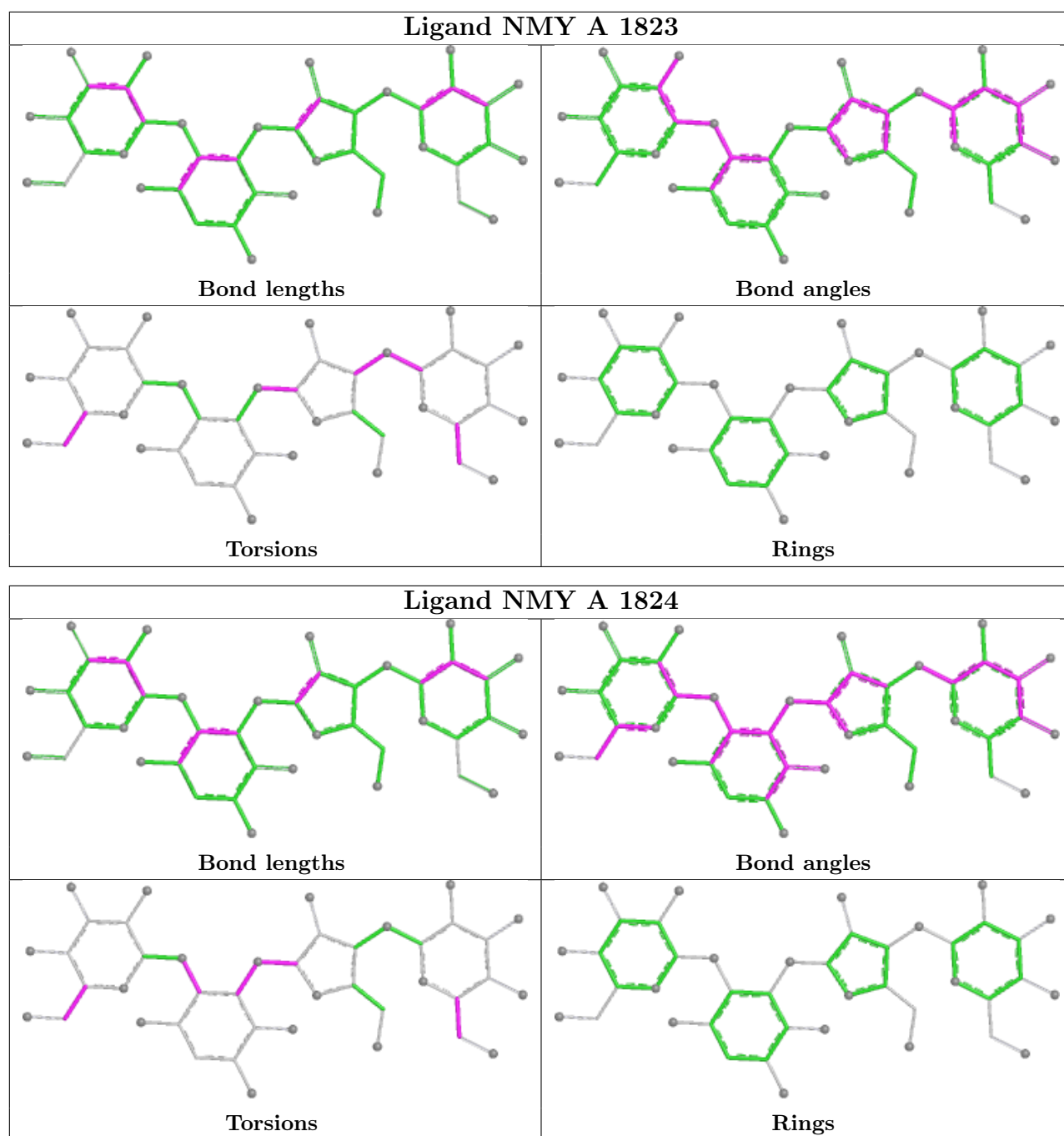
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1822	NMY	2	0
24	A	1824	NMY	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.59	7 (0%) 87 72	55, 85, 178, 278	0
2	B	236/256 (92%)	0.00	7 (2%) 52 30	75, 124, 211, 250	0
3	C	207/239 (86%)	0.05	4 (1%) 66 43	79, 122, 163, 202	0
4	D	208/209 (99%)	-0.01	12 (5%) 29 15	67, 97, 138, 164	0
5	E	151/162 (93%)	-0.30	1 (0%) 84 66	61, 84, 129, 175	0
6	F	101/101 (100%)	-0.09	1 (0%) 79 59	82, 126, 158, 192	0
7	G	155/156 (99%)	-0.09	2 (1%) 75 53	79, 106, 175, 211	0
8	H	138/138 (100%)	-0.42	0 100 100	55, 81, 111, 147	0
9	I	127/128 (99%)	0.15	3 (2%) 59 36	83, 125, 165, 203	0
10	J	99/105 (94%)	0.57	7 (7%) 22 11	77, 144, 225, 241	0
11	K	119/129 (92%)	0.02	3 (2%) 58 35	65, 95, 145, 203	0
12	L	124/135 (91%)	-0.12	2 (1%) 70 47	58, 91, 139, 235	0
13	M	118/126 (93%)	0.09	3 (2%) 58 35	79, 115, 155, 187	0
14	N	60/61 (98%)	0.18	3 (5%) 34 18	85, 107, 143, 191	0
15	O	88/89 (98%)	-0.04	0 100 100	68, 98, 147, 190	0
16	P	84/88 (95%)	-0.29	0 100 100	63, 84, 118, 197	0
17	Q	104/105 (99%)	-0.09	2 (1%) 66 43	60, 87, 143, 228	0
18	R	73/88 (82%)	0.06	3 (4%) 41 23	73, 105, 183, 211	0
19	S	81/93 (87%)	0.37	6 (7%) 20 10	70, 134, 199, 236	0
20	T	99/106 (93%)	0.19	7 (7%) 22 11	62, 92, 150, 207	0
21	U	25/27 (92%)	0.10	1 (4%) 42 23	81, 112, 129, 192	0
All	All	3895/4063 (95%)	-0.23	74 (1%) 66 43	55, 98, 173, 278	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	7.2
4	D	31	CYS	6.5
19	S	3	ARG	5.9
17	Q	103	GLY	5.4
19	S	4	SER	5.1
1	A	1129	C	5.0
19	S	2	PRO	4.9
4	D	26	CYS	4.9
4	D	33	MET	4.4
12	L	29	GLY	4.3
19	S	5	LEU	3.7
7	G	33	ASP	3.7
1	A	1027	C	3.7
4	D	21	LEU	3.5
4	D	2	GLY	3.5
4	D	9	CYS	3.5
1	A	1181	G	3.4
4	D	12	CYS	3.4
18	R	20	ALA	3.4
20	T	12	ALA	3.3
5	E	155	GLU	3.2
2	B	14	GLY	3.1
13	M	7	VAL	3.1
10	J	93	GLY	3.1
14	N	2	ALA	3.1
10	J	58	ASP	3.0
2	B	13	ALA	3.0
2	B	12	GLU	3.0
2	B	15	VAL	3.0
1	A	1125	U	3.0
20	T	100	ILE	2.9
10	J	88	LEU	2.9
13	M	5	ALA	2.9
7	G	5	ARG	2.9
4	D	32	ALA	2.8
10	J	100	THR	2.8
10	J	57	LYS	2.7
10	J	17	ASP	2.7
19	S	7	LYS	2.6
10	J	71	LEU	2.6
12	L	28	LYS	2.6
3	C	76	VAL	2.6
20	T	11	SER	2.5

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Mol	Chain	Res	Type	RSRZ
13	M	73	GLU	2.5
9	I	126	SER	2.5
20	T	106	ALA	2.5
4	D	23	GLY	2.5
1	A	373	A	2.5
14	N	60	SER	2.5
1	A	202	U	2.4
3	C	58	GLU	2.4
1	A	1054	C	2.4
21	U	6	ARG	2.4
18	R	83	GLU	2.4
3	C	155	GLY	2.3
11	K	51	LYS	2.3
3	C	134	ILE	2.3
2	B	88	ALA	2.2
9	I	8	GLY	2.2
4	D	34	GLU	2.2
18	R	16	PRO	2.2
9	I	128	ARG	2.2
6	F	14	LEU	2.2
14	N	8	GLU	2.1
20	T	64	ASP	2.1
2	B	31	TYR	2.1
2	B	44	LEU	2.1
20	T	103	GLY	2.1
11	K	128	ALA	2.1
4	D	24	GLU	2.1
20	T	73	HIS	2.1
19	S	10	PHE	2.0
11	K	77	MET	2.0
4	D	22	LYS	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.88	0.16	176,191,205,208	0
1	PSU	A	1541	20/21	0.91	0.14	178,188,205,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	A	516	20/21	0.94	0.09	83,98,104,105	0
12	0TD	L	92	10/11	0.95	0.17	81,88,186,306	0
1	5MC	A	1400	21/22	0.97	0.08	57,76,100,104	0
1	UR3	A	1498	21/22	0.97	0.10	52,64,74,99	0
1	7MG	A	527	24/25	0.97	0.08	66,74,91,95	0
1	M2G	A	966	25/26	0.97	0.06	74,84,102,116	0
1	2MG	A	1207	24/25	0.97	0.07	97,104,109,114	0
1	MA6	A	1519	24/25	0.98	0.08	54,71,82,89	0
1	5MC	A	1407	21/22	0.98	0.07	64,74,83,90	0
1	5MC	A	967	21/22	0.98	0.07	73,80,89,93	0
1	MA6	A	1518	24/25	0.98	0.07	57,65,79,84	0
1	5MC	A	1404	21/22	0.99	0.05	55,62,71,76	0
1	4OC	A	1402	22/23	0.99	0.07	59,69,78,79	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	K	A	1754	1/1	0.57	0.28	170,170,170,170	0
22	MG	A	1789	1/1	0.61	0.31	119,119,119,119	0
22	MG	A	1791	1/1	0.63	0.26	102,102,102,102	0
22	MG	A	1807	1/1	0.66	0.36	85,85,85,85	0
23	K	A	1741	1/1	0.67	0.21	150,150,150,150	0
23	K	A	1752	1/1	0.68	0.73	138,138,138,138	0
22	MG	A	1799	1/1	0.68	0.25	118,118,118,118	0
22	MG	A	1617	1/1	0.72	0.29	81,81,81,81	0
23	K	A	1757	1/1	0.72	0.70	145,145,145,145	0
22	MG	A	1765	1/1	0.73	0.29	94,94,94,94	0
22	MG	A	1723	1/1	0.73	0.36	77,77,77,77	0
22	MG	A	1731	1/1	0.73	0.64	95,95,95,95	0
23	K	A	1750	1/1	0.74	0.64	137,137,137,137	0
22	MG	A	1776	1/1	0.74	0.20	87,87,87,87	0
22	MG	A	1777	1/1	0.75	0.40	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1721	1/1	0.76	0.31	94,94,94,94	0
23	K	A	1746	1/1	0.77	0.08	186,186,186,186	0
23	K	A	1747	1/1	0.77	0.33	147,147,147,147	0
22	MG	A	1763	1/1	0.77	0.32	95,95,95,95	0
22	MG	A	1607	1/1	0.78	0.32	98,98,98,98	0
22	MG	A	1805	1/1	0.78	0.20	104,104,104,104	0
22	MG	A	1608	1/1	0.78	0.47	107,107,107,107	0
22	MG	N	102	1/1	0.78	0.24	71,71,71,71	0
22	MG	S	101	1/1	0.78	0.15	92,92,92,92	0
22	MG	A	1762	1/1	0.78	0.42	76,76,76,76	0
22	MG	A	1783	1/1	0.79	0.44	105,105,105,105	0
22	MG	Q	201	1/1	0.79	0.15	101,101,101,101	0
23	K	A	1755	1/1	0.80	0.13	165,165,165,165	0
22	MG	A	1682	1/1	0.80	0.23	108,108,108,108	0
22	MG	A	1724	1/1	0.81	0.18	74,74,74,74	0
22	MG	A	1808	1/1	0.81	0.51	91,91,91,91	0
23	K	A	1745	1/1	0.81	0.32	147,147,147,147	0
22	MG	A	1639	1/1	0.81	0.39	105,105,105,105	0
22	MG	A	1685	1/1	0.81	0.54	72,72,72,72	0
23	K	A	1759	1/1	0.81	0.19	167,167,167,167	0
22	MG	A	1780	1/1	0.82	0.53	95,95,95,95	0
22	MG	A	1711	1/1	0.82	0.39	79,79,79,79	0
22	MG	A	1818	1/1	0.82	0.32	113,113,113,113	0
22	MG	A	1656	1/1	0.82	0.10	113,113,113,113	0
22	MG	A	1814	1/1	0.83	0.26	109,109,109,109	0
22	MG	A	1683	1/1	0.83	0.69	100,100,100,100	0
23	K	A	1749	1/1	0.83	0.14	146,146,146,146	0
22	MG	A	1629	1/1	0.83	0.36	70,70,70,70	0
22	MG	A	1688	1/1	0.83	0.54	63,63,63,63	0
22	MG	A	1640	1/1	0.83	0.34	62,62,62,62	0
22	MG	A	1761	1/1	0.83	0.18	79,79,79,79	0
23	K	A	1744	1/1	0.83	0.14	195,195,195,195	0
22	MG	A	1716	1/1	0.83	0.32	61,61,61,61	0
24	NMY	A	1824	42/42	0.83	0.15	76,172,227,228	0
22	MG	A	1611	1/1	0.84	0.66	89,89,89,89	0
23	K	A	1737	1/1	0.84	0.21	135,135,135,135	0
22	MG	A	1719	1/1	0.84	0.26	60,60,60,60	0
22	MG	A	1624	1/1	0.84	0.38	113,113,113,113	0
22	MG	A	1613	1/1	0.84	0.29	87,87,87,87	0
23	K	A	1756	1/1	0.84	0.35	150,150,150,150	0
22	MG	A	1658	1/1	0.84	0.30	75,75,75,75	0
22	MG	A	1661	1/1	0.84	0.38	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	K	A	1748	1/1	0.84	0.26	119,119,119,119	0
22	MG	A	1619	1/1	0.85	0.65	99,99,99,99	0
23	K	A	1753	1/1	0.85	0.21	162,162,162,162	0
22	MG	A	1800	1/1	0.85	0.20	82,82,82,82	0
22	MG	A	1601	1/1	0.85	1.02	92,92,92,92	0
22	MG	A	1781	1/1	0.85	0.36	85,85,85,85	0
22	MG	A	1794	1/1	0.85	0.19	97,97,97,97	0
22	MG	A	1811	1/1	0.85	0.23	82,82,82,82	0
22	MG	A	1813	1/1	0.85	0.31	99,99,99,99	0
22	MG	A	1735	1/1	0.86	0.30	86,86,86,86	0
22	MG	L	201	1/1	0.86	0.26	109,109,109,109	0
22	MG	A	1778	1/1	0.86	0.19	91,91,91,91	0
22	MG	A	1804	1/1	0.86	0.20	98,98,98,98	0
22	MG	A	1760	1/1	0.86	0.29	73,73,73,73	0
22	MG	A	1659	1/1	0.86	0.25	61,61,61,61	0
23	K	A	1738	1/1	0.86	0.13	140,140,140,140	0
23	K	A	1739	1/1	0.86	0.35	137,137,137,137	0
22	MG	A	1710	1/1	0.86	0.22	86,86,86,86	0
22	MG	A	1615	1/1	0.86	0.09	107,107,107,107	0
22	MG	A	1670	1/1	0.86	0.53	92,92,92,92	0
22	MG	A	1717	1/1	0.86	0.38	108,108,108,108	0
23	K	A	1736	1/1	0.87	0.20	125,125,125,125	0
22	MG	A	1784	1/1	0.87	0.09	94,94,94,94	0
22	MG	A	1692	1/1	0.87	0.44	81,81,81,81	0
22	MG	A	1703	1/1	0.87	0.38	64,64,64,64	0
22	MG	A	1708	1/1	0.87	0.33	69,69,69,69	0
22	MG	A	1660	1/1	0.87	0.43	69,69,69,69	0
22	MG	A	1643	1/1	0.87	0.26	69,69,69,69	0
22	MG	A	1668	1/1	0.87	0.21	97,97,97,97	0
22	MG	A	1686	1/1	0.87	0.31	73,73,73,73	0
22	MG	A	1612	1/1	0.87	0.24	83,83,83,83	0
22	MG	A	1713	1/1	0.88	0.17	91,91,91,91	0
22	MG	A	1788	1/1	0.88	0.51	78,78,78,78	0
22	MG	A	1821	1/1	0.88	0.09	227,227,227,227	0
22	MG	A	1614	1/1	0.88	0.27	103,103,103,103	0
22	MG	A	1806	1/1	0.88	0.42	104,104,104,104	0
22	MG	A	1634	1/1	0.88	0.39	79,79,79,79	0
22	MG	A	1793	1/1	0.88	0.35	108,108,108,108	0
23	K	A	1758	1/1	0.88	0.22	168,168,168,168	0
22	MG	A	1628	1/1	0.88	0.58	64,64,64,64	0
22	MG	A	1702	1/1	0.88	0.23	64,64,64,64	0
22	MG	A	1646	1/1	0.89	0.62	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1817	1/1	0.89	0.16	101,101,101,101	0
22	MG	A	1635	1/1	0.89	0.12	81,81,81,81	0
22	MG	A	1790	1/1	0.89	0.12	69,69,69,69	0
22	MG	K	201	1/1	0.89	0.22	75,75,75,75	0
22	MG	A	1620	1/1	0.89	0.30	75,75,75,75	0
22	MG	A	1645	1/1	0.89	0.60	69,69,69,69	0
23	K	A	1743	1/1	0.89	0.20	136,136,136,136	0
22	MG	A	1667	1/1	0.90	0.41	69,69,69,69	0
22	MG	A	1733	1/1	0.90	0.25	89,89,89,89	0
22	MG	A	1785	1/1	0.90	0.22	95,95,95,95	0
22	MG	A	1630	1/1	0.90	0.34	77,77,77,77	0
22	MG	A	1712	1/1	0.90	0.10	78,78,78,78	0
22	MG	A	1633	1/1	0.90	0.48	55,55,55,55	0
22	MG	A	1693	1/1	0.90	0.16	104,104,104,104	0
22	MG	A	1698	1/1	0.90	0.44	69,69,69,69	0
22	MG	A	1699	1/1	0.90	0.26	51,51,51,51	0
22	MG	A	1774	1/1	0.90	0.32	76,76,76,76	0
22	MG	A	1622	1/1	0.90	0.34	56,56,56,56	0
22	MG	A	1722	1/1	0.90	0.17	83,83,83,83	0
22	MG	A	1625	1/1	0.90	0.53	97,97,97,97	0
22	MG	A	1779	1/1	0.90	0.52	88,88,88,88	0
22	MG	A	1636	1/1	0.90	0.34	21,21,21,21	0
22	MG	A	1730	1/1	0.90	0.29	83,83,83,83	0
23	K	A	1742	1/1	0.90	0.30	143,143,143,143	0
22	MG	A	1655	1/1	0.91	0.48	84,84,84,84	0
22	MG	A	1663	1/1	0.91	0.44	82,82,82,82	0
22	MG	A	1700	1/1	0.91	0.37	55,55,55,55	0
22	MG	A	1642	1/1	0.91	0.34	62,62,62,62	0
22	MG	A	1606	1/1	0.91	0.35	33,33,33,33	0
22	MG	A	1769	1/1	0.91	0.25	79,79,79,79	0
22	MG	A	1691	1/1	0.91	0.46	94,94,94,94	0
22	MG	A	1647	1/1	0.91	0.46	78,78,78,78	0
22	MG	A	1792	1/1	0.91	0.17	82,82,82,82	0
22	MG	A	1650	1/1	0.91	0.48	88,88,88,88	0
22	MG	A	1694	1/1	0.91	0.23	52,52,52,52	0
22	MG	A	1697	1/1	0.91	0.15	102,102,102,102	0
22	MG	A	1714	1/1	0.91	0.24	92,92,92,92	0
22	MG	A	1773	1/1	0.92	0.29	89,89,89,89	0
22	MG	A	1797	1/1	0.92	0.26	89,89,89,89	0
22	MG	A	1618	1/1	0.92	0.71	74,74,74,74	0
22	MG	A	1775	1/1	0.92	0.50	97,97,97,97	0
22	MG	A	1801	1/1	0.92	0.29	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1802	1/1	0.92	0.20	79,79,79,79	0
22	MG	A	1803	1/1	0.92	0.22	78,78,78,78	0
22	MG	A	1657	1/1	0.92	0.04	127,127,127,127	0
22	MG	A	1729	1/1	0.92	0.25	70,70,70,70	0
22	MG	A	1616	1/1	0.92	0.87	92,92,92,92	0
22	MG	A	1672	1/1	0.92	0.35	82,82,82,82	0
22	MG	A	1680	1/1	0.92	0.69	70,70,70,70	0
22	MG	A	1810	1/1	0.92	0.48	98,98,98,98	0
22	MG	A	1734	1/1	0.92	0.27	70,70,70,70	0
22	MG	A	1603	1/1	0.92	0.20	90,90,90,90	0
22	MG	A	1631	1/1	0.92	0.22	110,110,110,110	0
22	MG	A	1632	1/1	0.92	0.28	56,56,56,56	0
22	MG	A	1718	1/1	0.92	0.09	66,66,66,66	0
22	MG	A	1627	1/1	0.92	0.30	50,50,50,50	0
22	MG	H	201	1/1	0.92	0.19	90,90,90,90	0
22	MG	A	1764	1/1	0.92	0.59	81,81,81,81	0
22	MG	A	1665	1/1	0.92	0.34	103,103,103,103	0
22	MG	A	1707	1/1	0.92	0.39	63,63,63,63	0
24	NMY	A	1823	42/42	0.92	0.20	104,173,194,228	0
22	MG	A	1772	1/1	0.92	0.57	87,87,87,87	0
22	MG	P	102	1/1	0.93	0.19	88,88,88,88	0
22	MG	P	103	1/1	0.93	0.34	95,95,95,95	0
22	MG	A	1637	1/1	0.93	0.17	57,57,57,57	0
22	MG	A	1766	1/1	0.93	0.21	81,81,81,81	0
23	K	A	1751	1/1	0.93	0.15	153,153,153,153	0
22	MG	A	1767	1/1	0.93	0.14	116,116,116,116	0
22	MG	A	1768	1/1	0.93	0.19	113,113,113,113	0
22	MG	A	1662	1/1	0.93	0.26	83,83,83,83	0
22	MG	A	1819	1/1	0.93	0.07	257,257,257,257	0
22	MG	A	1638	1/1	0.93	0.34	80,80,80,80	0
22	MG	D	303	1/1	0.93	0.18	93,93,93,93	0
22	MG	A	1664	1/1	0.93	0.31	81,81,81,81	0
22	MG	A	1796	1/1	0.93	0.47	100,100,100,100	0
22	MG	A	1641	1/1	0.93	0.62	87,87,87,87	0
22	MG	A	1689	1/1	0.93	0.39	77,77,77,77	0
22	MG	A	1787	1/1	0.94	0.16	73,73,73,73	0
22	MG	A	1626	1/1	0.94	0.55	75,75,75,75	0
22	MG	A	1815	1/1	0.94	0.11	79,79,79,79	0
22	MG	A	1621	1/1	0.94	0.37	87,87,87,87	0
22	MG	A	1709	1/1	0.94	0.18	77,77,77,77	0
22	MG	A	1671	1/1	0.94	0.10	63,63,63,63	0
22	MG	A	1695	1/1	0.94	0.48	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1654	1/1	0.94	0.46	89,89,89,89	0
23	K	A	1740	1/1	0.94	0.20	122,122,122,122	0
22	MG	E	201	1/1	0.94	0.24	79,79,79,79	0
22	MG	A	1771	1/1	0.94	0.37	71,71,71,71	0
22	MG	H	202	1/1	0.94	0.07	204,204,204,204	0
22	MG	A	1705	1/1	0.94	0.29	68,68,68,68	0
22	MG	A	1706	1/1	0.94	0.21	71,71,71,71	0
22	MG	A	1715	1/1	0.94	0.30	102,102,102,102	0
22	MG	A	1602	1/1	0.95	0.59	84,84,84,84	0
22	MG	A	1812	1/1	0.95	0.46	102,102,102,102	0
22	MG	A	1644	1/1	0.95	0.42	80,80,80,80	0
22	MG	A	1798	1/1	0.95	0.22	81,81,81,81	0
22	MG	A	1673	1/1	0.95	0.17	53,53,53,53	0
22	MG	U	101	1/1	0.95	0.19	121,121,121,121	0
22	MG	A	1786	1/1	0.95	0.24	87,87,87,87	0
22	MG	A	1674	1/1	0.95	0.78	91,91,91,91	0
22	MG	A	1675	1/1	0.95	0.18	59,59,59,59	0
22	MG	A	1676	1/1	0.95	0.18	80,80,80,80	0
22	MG	A	1690	1/1	0.95	0.54	81,81,81,81	0
22	MG	A	1677	1/1	0.95	0.27	88,88,88,88	0
22	MG	A	1704	1/1	0.95	0.35	58,58,58,58	0
22	MG	A	1653	1/1	0.95	0.39	86,86,86,86	0
24	NMY	A	1822	42/42	0.95	0.10	42,78,109,159	0
22	MG	A	1681	1/1	0.95	0.48	89,89,89,89	0
22	MG	A	1795	1/1	0.95	0.23	71,71,71,71	0
25	ZN	D	301	1/1	0.95	0.28	95,95,95,95	0
22	MG	A	1679	1/1	0.96	0.39	79,79,79,79	0
22	MG	A	1727	1/1	0.96	0.08	92,92,92,92	0
22	MG	A	1605	1/1	0.96	0.63	72,72,72,72	0
22	MG	A	1701	1/1	0.96	0.16	76,76,76,76	0
22	MG	S	102	1/1	0.96	0.38	71,71,71,71	0
22	MG	A	1610	1/1	0.96	0.19	58,58,58,58	0
22	MG	A	1732	1/1	0.96	0.13	61,61,61,61	0
22	MG	D	302	1/1	0.96	0.10	73,73,73,73	0
22	MG	A	1623	1/1	0.96	0.45	62,62,62,62	0
22	MG	A	1720	1/1	0.96	0.08	103,103,103,103	0
22	MG	A	1782	1/1	0.96	0.19	82,82,82,82	0
22	MG	A	1770	1/1	0.96	0.41	86,86,86,86	0
22	MG	A	1696	1/1	0.96	0.22	70,70,70,70	0
22	MG	A	1678	1/1	0.96	0.24	46,46,46,46	0
22	MG	M	201	1/1	0.96	0.13	75,75,75,75	0
22	MG	A	1684	1/1	0.96	0.48	79,79,79,79	0

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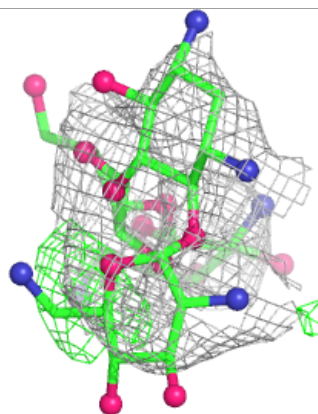
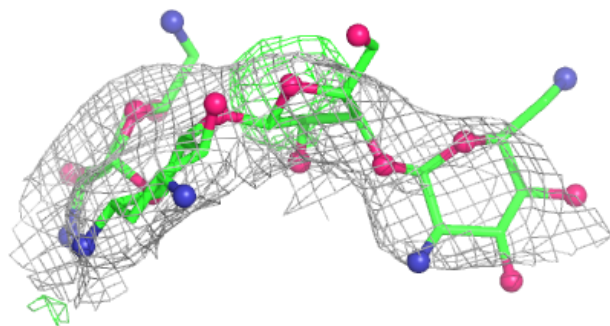
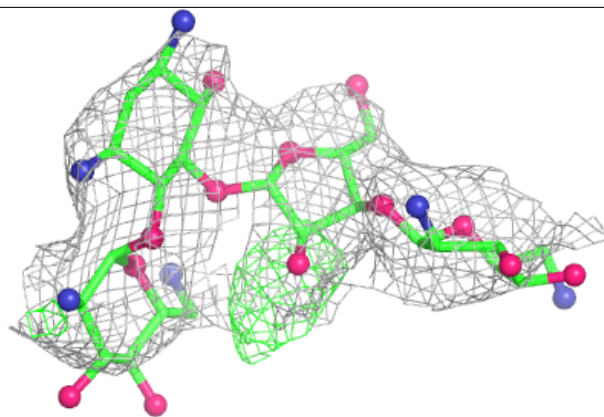
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	P	101	1/1	0.96	0.35	89,89,89,89	0
22	MG	A	1652	1/1	0.97	0.19	78,78,78,78	0
22	MG	A	1648	1/1	0.97	0.46	58,58,58,58	0
22	MG	A	1687	1/1	0.97	0.55	69,69,69,69	0
22	MG	A	1609	1/1	0.97	0.15	83,83,83,83	0
22	MG	A	1726	1/1	0.97	0.06	118,118,118,118	0
22	MG	A	1816	1/1	0.97	0.12	92,92,92,92	0
22	MG	A	1651	1/1	0.97	0.54	73,73,73,73	0
22	MG	A	1728	1/1	0.97	0.05	36,36,36,36	0
22	MG	A	1669	1/1	0.97	0.55	71,71,71,71	0
22	MG	A	1604	1/1	0.98	0.39	57,57,57,57	0
22	MG	A	1725	1/1	0.98	0.06	57,57,57,57	0
22	MG	A	1649	1/1	0.98	0.16	52,52,52,52	0
22	MG	A	1666	1/1	0.98	0.09	63,63,63,63	0
22	MG	A	1820	1/1	0.99	0.04	107,107,107,107	0
22	MG	A	1809	1/1	0.99	0.09	72,72,72,72	0
25	ZN	N	101	1/1	1.00	0.06	108,108,108,108	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.

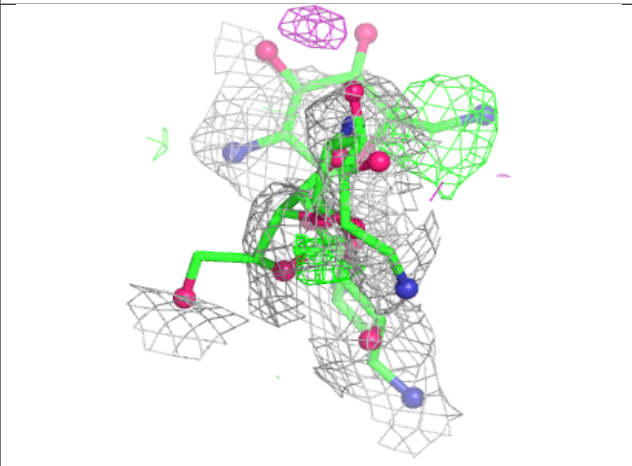
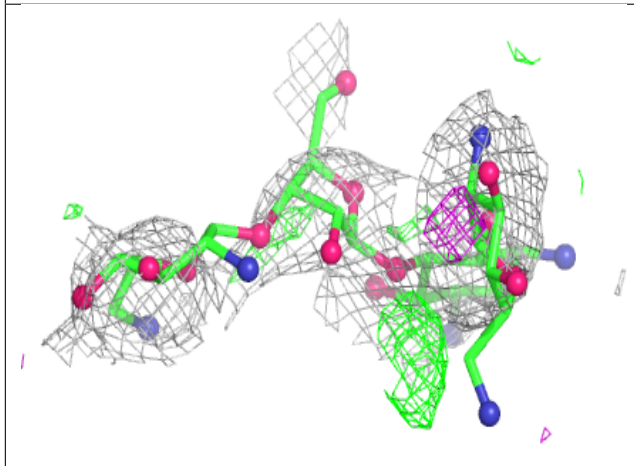
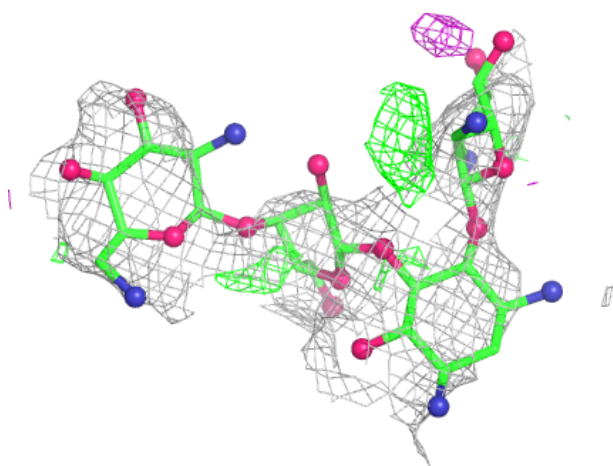
Electron density around NMY A 1824:

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



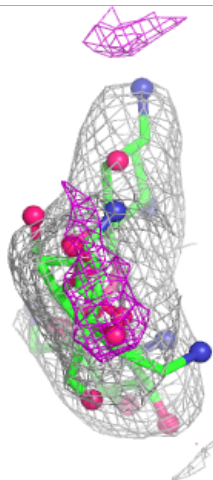
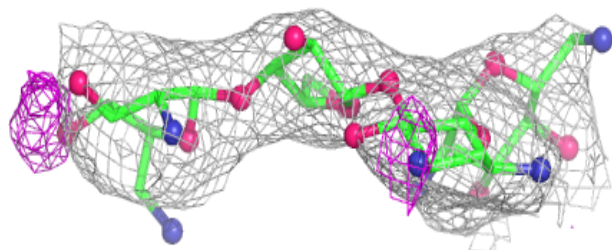
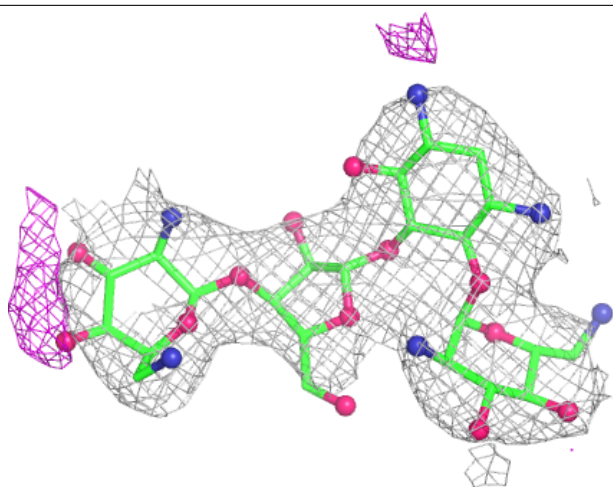
Electron density around NMY A 1823:

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



Electron density around NMY A 1822:

$2mF_o-DF_c$ (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.