



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:05 AM UTC

PDB ID : 5WNT / pdb_00005wnt
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : DeMirici, H.
Deposited on : 2017-08-01
Resolution : 3.30 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

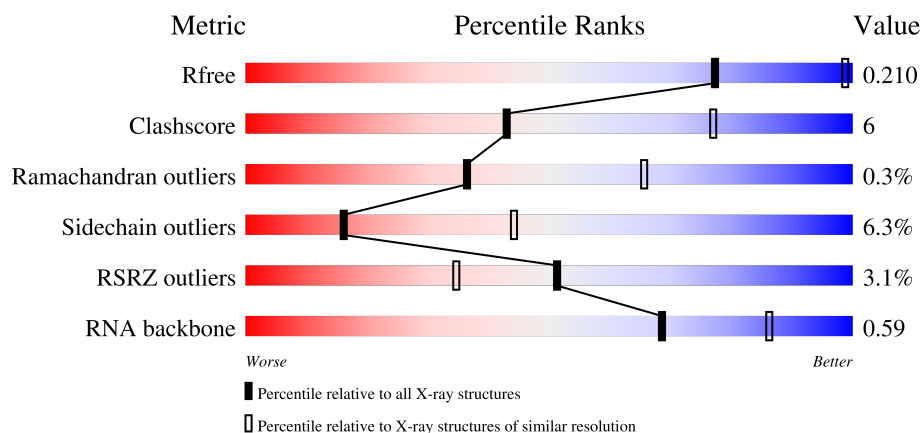
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



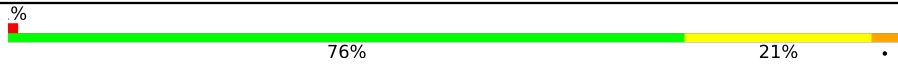
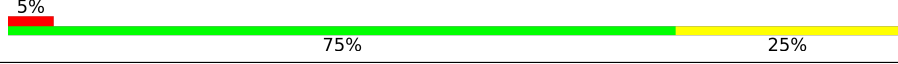
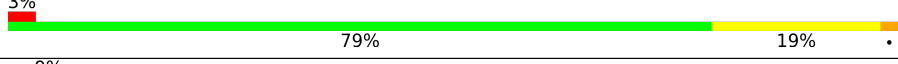
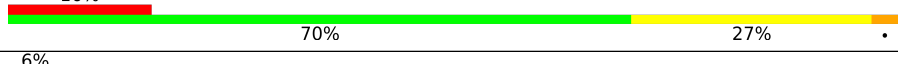
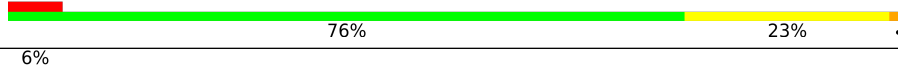
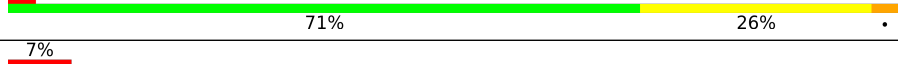
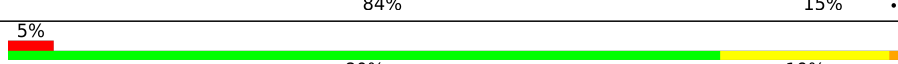
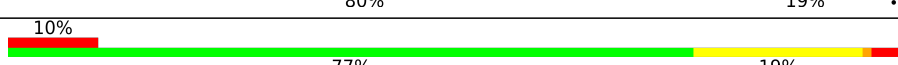
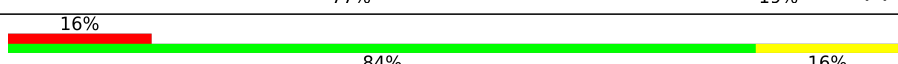
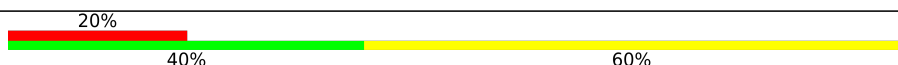
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	66% 27% 7%
2	B	236	3% 81% 18%
3	C	207	4% 81% 17%
4	D	208	6% 80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	99	
11	K	119	
12	L	125	
13	M	118	
14	N	60	
15	O	88	
16	P	84	
17	Q	99	
18	R	73	
19	S	81	
20	T	99	
21	U	25	
22	a	5	
23	b	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	12A	b	37	X	-	-	-
24	MG	A	1609	-	-	-	X
24	MG	A	1627	-	-	-	X
24	MG	A	1701	-	-	-	X
24	MG	A	1705	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1709	-	-	-	X
24	MG	A	1720	-	-	-	X
24	MG	A	1722	-	-	-	X
24	MG	A	1744	-	-	-	X
24	MG	A	1751	-	-	-	X
24	MG	A	1758	-	-	-	X
24	MG	A	1782	-	-	-	X
24	MG	A	1783	-	-	-	X
24	MG	A	1784	-	-	-	X
24	MG	A	1785	-	-	-	X
24	MG	A	1791	-	-	-	X
24	MG	A	1803	-	-	-	X
24	MG	A	1805	-	-	-	X
24	MG	A	1808	-	-	-	X
24	MG	A	1809	-	-	-	X
24	MG	A	1820	-	-	-	X
25	K	A	1837	-	-	-	X
25	K	A	1839	-	-	-	X
25	K	A	1846	-	-	-	X
25	K	A	1848	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 52602 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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 55771382
A	1535	A	C	conflict	GB 55771382

- 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	S	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	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 a RNA chain called RNA (5'-R(*(A2M)P*AP*AP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	a	5	Total	C	N	O	P	0	0	0
			104	49	19	32	4			

- Molecule 23 is a RNA chain called RNA (5'-R(P*UP*AP*GP*AP*CP*UP*(70U)P*UP*UP*(12A)P*AP*(PSU)P*CP*UP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	b	15	Total	C	N	O	P	S	0	0	0
			330	150	51	112	15	2			

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	236	Total	Mg	0	0
			236	236		
24	D	1	Total	Mg	0	0
			1	1		
24	E	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		
24	G	1	Total	Mg	0	0
			1	1		
24	H	2	Total	Mg	0	0
			2	2		
24	L	1	Total	Mg	0	0
			1	1		
24	P	3	Total	Mg	0	0
			3	3		
24	Q	2	Total	Mg	0	0
			2	2		

Continued on next page...

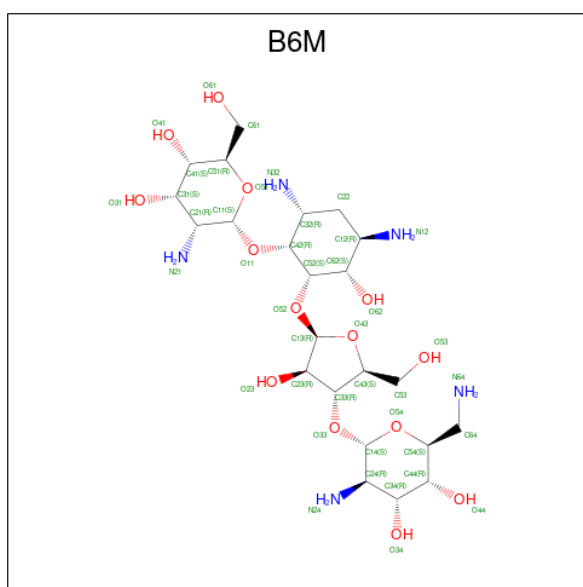
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	S	3	Total	Mg	0	0
			3	3		
24	T	1	Total	Mg	0	0
			1	1		

- Molecule 25 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	22	Total	K	0	0
			22	22		

- Molecule 26 is (1R,2S,3S,4R,6R)-4,6-diamino-2-{[3-O-(2,6-diamino-2,6-dideoxy-alpha-L-altr
opyranosyl)-beta-L-arabinofuranosyl]oxy}-3-hydroxycyclohexyl 2-amino-2-deoxy-alpha-D-al
lopyranoside (CCD ID: B6M) (formula: C₂₃H₄₅N₅O₁₄).

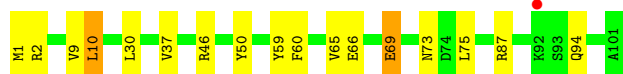
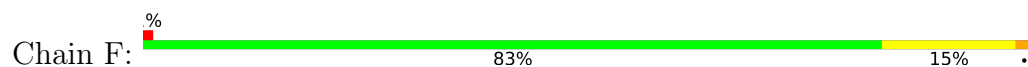


- Molecule 28 is water.

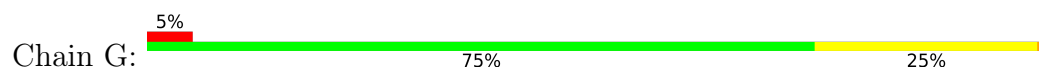
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	214	Total 214	O 214	0	0
28	D	3	Total 3	O 3	0	0
28	E	4	Total 4	O 4	0	0
28	K	1	Total 1	O 1	0	0
28	L	3	Total 3	O 3	0	0
28	N	1	Total 1	O 1	0	0
28	T	1	Total 1	O 1	0	0



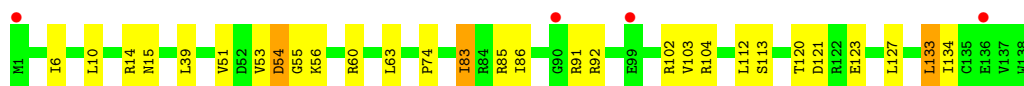
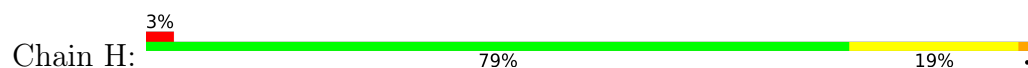
- Molecule 6: RIBOSOMAL PROTEIN S6



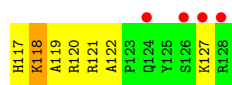
- Molecule 7: RIBOSOMAL PROTEIN S7



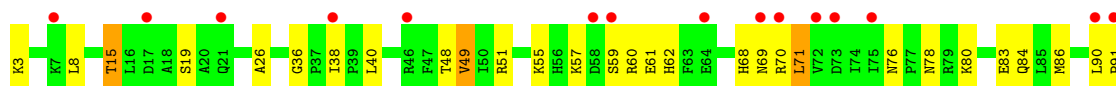
- Molecule 8: RIBOSOMAL PROTEIN S8



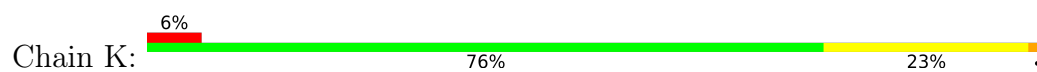
- Molecule 9: RIBOSOMAL PROTEIN S9



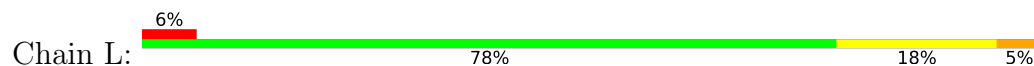
- Molecule 10: RIBOSOMAL PROTEIN S10



- Molecule 11: RIBOSOMAL PROTEIN S11



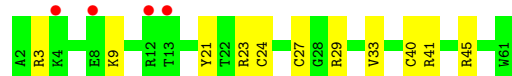
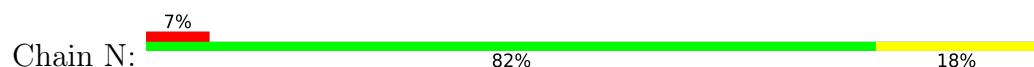
• Molecule 12: RIBOSOMAL PROTEIN S12



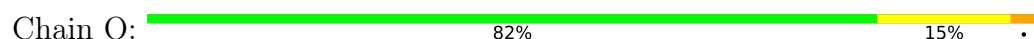
• Molecule 13: RIBOSOMAL PROTEIN S13



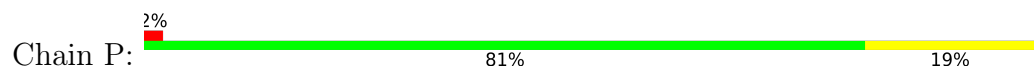
• Molecule 14: RIBOSOMAL PROTEIN S14



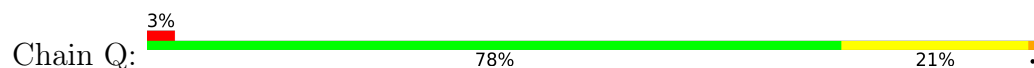
• Molecule 15: RIBOSOMAL PROTEIN S15



• Molecule 16: RIBOSOMAL PROTEIN S16

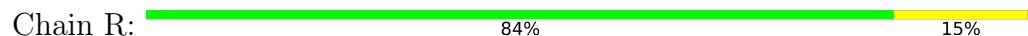


• Molecule 17: RIBOSOMAL PROTEIN S17

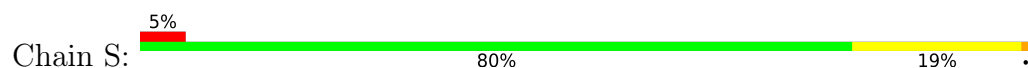




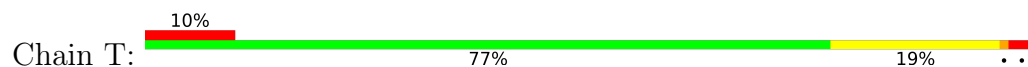
• Molecule 18: RIBOSOMAL PROTEIN S18



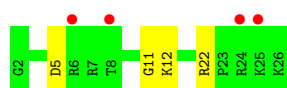
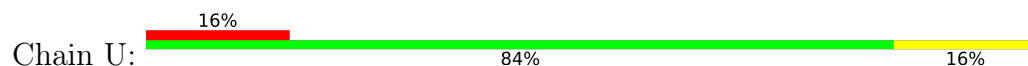
• Molecule 19: RIBOSOMAL PROTEIN S19



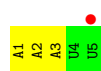
• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



• Molecule 22: RNA (5'-R*(A2M)P*AP*AP*UP*U)-3')



• Molecule 23: RNA (5'-R(P*UP*AP*GP*AP*CP*UP*(70U)P*UP*UP*(12A)P*AP*(PSU)P*C P*UP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.00Å 400.00Å 173.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 3.30 39.78 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.78-3.30) 91.8 (39.78-3.30)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.26 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.173 , 0.212 0.173 , 0.210	Depositor DCC
R_{free} test set	2000 reflections (0.68%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 84.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52602	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: 5MC, 0TD, B6M, A2M, UR3, 4OC, MG, MA6, M2G, 2MG, 70U, 7MG, PSU, K, 12A, ZN

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	0.10	1/36037 (0.0%)	0.28	0/56239
2	B	0.11	0/1909	0.34	0/2579
3	C	0.12	0/1637	0.32	0/2207
4	D	0.12	0/1733	0.35	0/2318
5	E	0.12	0/1163	0.33	0/1566
6	F	0.10	0/856	0.33	0/1154
7	G	0.13	0/1276	0.34	0/1709
8	H	0.13	0/1136	0.35	0/1527
9	I	0.12	0/1029	0.40	0/1379
10	J	0.15	0/806	0.49	0/1084
11	K	0.10	0/900	0.31	0/1213
12	L	0.12	0/978	0.42	0/1308
13	M	0.29	1/947 (0.1%)	0.53	1/1270 (0.1%)
14	N	0.12	0/501	0.35	0/664
15	O	0.12	0/745	0.31	0/992
16	P	0.12	0/717	0.35	0/965
17	Q	0.12	0/836	0.34	0/1117
18	R	0.11	0/604	0.31	0/801
19	S	0.11	0/662	0.34	0/892
20	T	0.34	0/765	0.50	1/1007 (0.1%)
21	U	0.12	0/213	0.36	0/279
22	a	0.49	0/94	0.22	0/146
23	b	0.08	0/277	0.24	0/423
All	All	0.12	2/55821 (0.0%)	0.31	2/82839 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
23	b	1	0
All	All	1	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.60	1.61	1.56
13	M	107	ALA	CA-C	-5.17	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	107	ALA	N-CA-C	-11.04	87.29	110.80
20	T	75	ASN	N-CA-C	-7.29	103.26	111.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	37	12A	C1'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	88	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16434	280	1
2	B	1874	0	1887	24	0
3	C	1613	0	1677	26	0
4	D	1703	0	1763	28	0
5	E	1147	0	1207	20	0
6	F	843	0	857	12	0
7	G	1257	0	1296	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1116	0	1177	17	0
9	I	1010	0	1037	30	0
10	J	793	0	835	19	0
11	K	885	0	904	15	0
12	L	973	0	1058	19	0
13	M	937	0	995	21	0
14	N	492	0	529	9	0
15	O	734	0	771	6	0
16	P	701	0	720	7	0
17	Q	823	0	891	15	0
18	R	598	0	670	9	0
19	S	648	0	673	7	0
20	T	763	0	861	23	0
21	U	209	0	221	3	0
22	a	104	0	56	1	0
23	b	330	0	171	4	0
24	A	236	0	0	0	0
24	D	1	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	G	1	0	0	0	0
24	H	2	0	0	0	0
24	L	1	0	0	0	0
24	P	3	0	0	0	0
24	Q	2	0	0	0	0
24	S	3	0	0	0	0
24	T	1	0	0	0	0
25	A	22	0	0	0	0
26	A	42	0	0	1	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	214	0	0	3	0
28	D	3	0	0	0	0
28	E	4	0	0	0	0
28	K	1	0	0	1	0
28	L	3	0	0	0	0
28	N	1	0	0	0	0
28	T	1	0	0	0	0
All	All	52602	0	36690	548	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (548) 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:948:C:C5	13:M:106:ASN:ND2	2.01	1.29
20:T:74:LYS:HA	20:T:74:LYS:HZ3	1.41	0.82
1:A:948:C:C4	13:M:106:ASN:ND2	2.48	0.81
1:A:948:C:H5	13:M:106:ASN:HD22	1.28	0.75
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.70	0.73
7:G:143:ARG:O	7:G:147:ALA:HB2	1.88	0.73
20:T:75:ASN:O	20:T:78:ALA:N	2.21	0.72
20:T:75:ASN:OD1	20:T:75:ASN:N	2.18	0.72
11:K:123:LYS:HA	11:K:126:ARG:HG3	1.72	0.72
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.73	0.71
1:A:975:A:H4'	1:A:976:G:H5''	1.74	0.70
11:K:15:ALA:HA	11:K:77:MET:HA	1.73	0.70
1:A:677:U:H3	1:A:713:G:H22	1.40	0.70
1:A:1422:G:H1	1:A:1478:C:H42	1.40	0.69
1:A:1518:MA6:H93	1:A:1519:MA6:H92	1.75	0.68
10:J:19:SER:HB3	10:J:91:PRO:HG3	1.75	0.68
1:A:948:C:C6	13:M:106:ASN:ND2	2.61	0.68
12:L:41:ARG:HE	12:L:57:LYS:HE2	1.59	0.68
1:A:235:C:N4	28:A:1902:HOH:O	2.27	0.67
1:A:1266:G:N2	1:A:1269:A:OP2	2.25	0.67
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.27	0.67
1:A:266:G:H5'	1:A:268:C:H41	1.59	0.67
1:A:537:G:OP1	12:L:113:ARG:NH2	2.27	0.67
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.59	0.67
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.76	0.67
1:A:1005:A:N6	1:A:1024:G:O2'	2.28	0.66
5:E:102:ALA:O	5:E:107:ARG:NH1	2.28	0.66
7:G:146:GLU:HG2	7:G:149:ARG:HD3	1.78	0.66
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.77	0.66
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.77	0.65
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.78	0.65
1:A:501:C:OP1	12:L:117:ARG:NH2	2.30	0.65
2:B:223:ILE:HD13	2:B:230:VAL:H	1.62	0.65
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.79	0.64
2:B:174:VAL:O	2:B:178:ARG:HG2	1.96	0.64
1:A:1124:G:N7	1:A:1145:C:O2'	2.29	0.64
1:A:1347:G:O6	9:I:10:ARG:NH2	2.29	0.64
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.78	0.64
3:C:27:LYS:HD3	3:C:27:LYS:H	1.63	0.64
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:140:ARG:O	5:E:143:ARG:NH2	2.31	0.63
1:A:509:A:N3	1:A:543:C:O2'	2.30	0.63
1:A:1319:A:H5'	19:S:5:LEU:HD22	1.80	0.63
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.79	0.63
3:C:131:ARG:HH11	3:C:166:GLU:HG3	1.64	0.63
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.81	0.63
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.80	0.63
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.80	0.63
20:T:74:LYS:HA	20:T:74:LYS:NZ	2.13	0.62
8:H:53:VAL:HG12	8:H:54:ASP:H	1.64	0.62
20:T:73:HIS:O	20:T:74:LYS:O	2.16	0.62
1:A:664:G:H22	1:A:741:G:H1	1.48	0.62
20:T:74:LYS:HB3	20:T:74:LYS:HZ2	1.65	0.62
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.33	0.61
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.83	0.61
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.34	0.61
11:K:18:ARG:NH1	11:K:35:PRO:O	2.34	0.61
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.81	0.61
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.82	0.61
7:G:54:THR:HG22	7:G:56:GLN:H	1.64	0.61
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.83	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.66	0.61
7:G:143:ARG:O	7:G:147:ALA:CB	2.47	0.61
1:A:8:A:N6	4:D:205:GLU:O	2.34	0.60
1:A:521:G:N7	12:L:53:ARG:NH2	2.48	0.60
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.83	0.60
3:C:70:VAL:HG12	3:C:72:LYS:H	1.65	0.60
12:L:59:ARG:NH1	12:L:65:GLU:OE2	2.34	0.60
1:A:372:C:H4'	1:A:373:A:O5'	2.02	0.60
1:A:1035:A:H2'	1:A:1036:G:H8	1.66	0.60
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.83	0.60
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.84	0.59
14:N:9:LYS:HE2	14:N:23:ARG:HB2	1.82	0.59
11:K:122:LYS:NZ	28:K:201:HOH:O	2.35	0.59
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.84	0.59
1:A:1073:U:O2	2:B:104:ASN:ND2	2.35	0.59
1:A:401:C:O2'	1:A:621:A:N3	2.33	0.59
12:L:36:VAL:HG22	12:L:82:VAL:HG22	1.85	0.59
1:A:542:G:OP1	4:D:10:ARG:NH2	2.35	0.58
13:M:23:TYR:HB3	13:M:67:GLU:HG2	1.85	0.58
1:A:298:A:N6	28:A:1904:HOH:O	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:C:H4'	1:A:1138:G:C2	2.39	0.58
1:A:1379:G:OP1	7:G:6:ARG:NH1	2.36	0.58
15:O:56:LEU:HA	15:O:59:MET:HE2	1.85	0.58
1:A:890:G:O2'	1:A:906:G:O6	2.21	0.58
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.84	0.58
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.58
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.86	0.58
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.85	0.58
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.85	0.58
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.86	0.57
1:A:1122:U:O4	1:A:1123:A:N6	2.38	0.57
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.86	0.57
1:A:1442:G:O6	1:A:1446:A:N6	2.37	0.57
1:A:1502:A:H2	1:A:1505:G:H1	1.50	0.57
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.87	0.57
1:A:1504:G:OP1	1:A:1507:A:H4'	2.05	0.57
1:A:1505:G:O2'	1:A:1506:U:OP2	2.16	0.57
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.87	0.57
1:A:1240:U:OP1	7:G:119:ARG:NH1	2.36	0.57
16:P:7:ALA:O	16:P:17:TYR:HA	2.05	0.56
18:R:48:GLY:O	18:R:74:ARG:NH2	2.36	0.56
1:A:250:A:H4'	1:A:251:G:O5'	2.04	0.56
1:A:1031:G:H2'	1:A:1032:G:H8	1.71	0.56
18:R:32:ARG:HA	18:R:69:THR:HG21	1.87	0.56
12:L:111:LYS:HE3	12:L:112:ASP:H	1.71	0.56
8:H:103:VAL:HG12	8:H:104:ARG:HG2	1.88	0.56
17:Q:53:LEU:HD23	17:Q:82:MET:HE1	1.87	0.56
1:A:316:G:OP2	1:A:351:G:O2'	2.24	0.56
1:A:300:A:O2'	1:A:564:C:N3	2.36	0.56
1:A:1425:U:H3	1:A:1475:G:H1	1.52	0.56
1:A:1031:G:H2'	1:A:1032:G:C8	2.41	0.56
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.88	0.56
11:K:57:THR:HG22	11:K:59:TYR:H	1.71	0.56
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.34	0.55
1:A:685:G:N2	1:A:704:A:OP2	2.37	0.55
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.88	0.55
9:I:32:ASP:OD1	9:I:33:PHE:N	2.40	0.55
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.55
1:A:45:U:H2'	1:A:46:G:C8	2.41	0.55
1:A:562:C:H1'	12:L:15:ARG:HG3	1.87	0.55
1:A:1035:A:H2'	1:A:1036:G:C8	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:U:H4'	1:A:1050:G:O5'	2.05	0.55
2:B:48:MET:HA	2:B:51:LEU:HB2	1.89	0.55
1:A:309:G:O2'	1:A:607:A:N1	2.40	0.54
1:A:1026:G:O6	1:A:1027:C:N4	2.41	0.54
1:A:1392:G:N2	1:A:1502:A:H8	2.06	0.54
5:E:80:ILE:HG13	5:E:91:LEU:HB2	1.88	0.54
1:A:765:G:N2	1:A:813:U:OP2	2.39	0.54
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.40	0.54
1:A:1412:C:H2'	1:A:1413:A:C8	2.41	0.54
1:A:1510:U:H2'	1:A:1511:G:C8	2.42	0.54
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.89	0.54
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.54
4:D:68:TYR:HB3	4:D:70:ILE:HD13	1.90	0.54
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.88	0.54
13:M:3:ARG:HE	13:M:7:VAL:HA	1.71	0.54
1:A:1034:G:H2'	1:A:1035:A:C8	2.43	0.54
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.72	0.54
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.73	0.54
1:A:413:G:N2	1:A:429:U:OP2	2.41	0.54
23:b:30:G:H22	23:b:40:C:H42	1.55	0.54
1:A:1250:A:H4'	9:I:68:GLY:N	2.22	0.54
2:B:101:MET:HA	2:B:108:ILE:HG13	1.89	0.54
3:C:6:HIS:HD2	3:C:8:ILE:H	1.54	0.54
3:C:59:ARG:HG2	3:C:64:VAL:HG22	1.89	0.54
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.90	0.54
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.90	0.53
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.91	0.53
1:A:1309:G:N7	13:M:99:ARG:NH2	2.56	0.53
5:E:33:VAL:HG22	5:E:43:LEU:HD23	1.90	0.53
13:M:16:ASP:OD1	13:M:16:ASP:N	2.40	0.53
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.40	0.53
1:A:1414:U:H2'	1:A:1415:G:H8	1.73	0.53
13:M:12:ASN:OD1	13:M:46:LYS:NZ	2.37	0.53
1:A:619:U:N3	4:D:134:ASP:OD1	2.39	0.53
10:J:3:LYS:O	10:J:101:VAL:N	2.41	0.53
12:L:48:PRO:HD2	12:L:92:OTD:H3	1.91	0.53
20:T:74:LYS:NZ	20:T:74:LYS:CB	2.72	0.53
3:C:11:ARG:NH1	3:C:177:THR:O	2.42	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.91	0.53
1:A:974:A:OP2	14:N:29:ARG:NH2	2.42	0.53
1:A:1251:A:N3	1:A:1369:C:O2'	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:U:O2'	1:A:1302:U:O5'	2.27	0.53
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.75	0.52
1:A:6:G:H4'	1:A:298:A:H4'	1.91	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.44	0.52
1:A:1435:G:H2'	1:A:1436:U:C6	2.45	0.52
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.41	0.52
7:G:152:ALA:O	7:G:155:ARG:NH1	2.43	0.52
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.91	0.52
10:J:38:ILE:HD12	10:J:71:LEU:HD12	1.92	0.52
1:A:7:G:H5'	1:A:298:A:O4'	2.09	0.52
1:A:28:G:O2'	1:A:296:U:OP1	2.24	0.52
1:A:811:C:O2'	1:A:901:A:N1	2.43	0.52
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.10	0.52
1:A:579:G:H5'	1:A:728:A:H1'	1.92	0.52
1:A:946:A:H2'	1:A:947:G:C8	2.45	0.52
1:A:21:G:H2'	1:A:22:G:C8	2.45	0.51
7:G:113:GLU:HB2	7:G:119:ARG:HG3	1.93	0.51
9:I:116:LYS:HD2	9:I:122:ALA:HA	1.92	0.51
1:A:673:G:H2'	1:A:674:G:C8	2.45	0.51
1:A:951:G:OP2	13:M:102:ARG:NH2	2.44	0.51
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.92	0.51
10:J:8:LEU:O	10:J:69:ASN:HA	2.10	0.51
1:A:1443:G:H4'	1:A:1446:A:O5'	2.09	0.51
12:L:27:LEU:O	12:L:33:ARG:NH1	2.43	0.51
13:M:86:CYS:SG	13:M:87:TYR:N	2.83	0.51
1:A:738:C:H5''	6:F:69:GLU:HB3	1.91	0.51
1:A:976:G:OP2	1:A:1358:U:O2'	2.22	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.46	0.51
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.92	0.51
20:T:74:LYS:N	20:T:74:LYS:HD2	2.26	0.51
1:A:580:U:H2'	1:A:581:G:O4'	2.10	0.50
2:B:55:PHE:HD2	2:B:221:LEU:HG	1.76	0.50
7:G:62:PHE:HA	7:G:124:LEU:HD12	1.93	0.50
18:R:25:THR:HB	18:R:42:ARG:HH22	1.76	0.50
1:A:1065:U:H4'	1:A:1066:C:O5'	2.11	0.50
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.93	0.50
2:B:44:LEU:HD12	2:B:44:LEU:H	1.76	0.50
23:b:37:12A:H2'	23:b:38:A:H8	1.75	0.50
1:A:60:A:H4'	1:A:61:G:O5'	2.10	0.50
1:A:1074:G:O2'	1:A:1101:A:N1	2.41	0.50
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:U:H2'	1:A:57:G:C8	2.47	0.50
1:A:181:G:H4'	1:A:182:U:H5'	1.93	0.50
1:A:243:A:H4'	1:A:244:U:H5'	1.94	0.50
1:A:362:G:N2	1:A:365:U:OP2	2.43	0.50
20:T:74:LYS:HZ2	20:T:74:LYS:CB	2.25	0.50
1:A:1080:A:H5''	5:E:16:THR:HG21	1.94	0.49
1:A:186:C:H5'	20:T:78:ALA:HB1	1.93	0.49
1:A:1498:UR3:H1'	1:A:1499:A:OP2	2.12	0.49
7:G:46:ALA:O	7:G:50:ILE:HG12	2.12	0.49
20:T:92:LEU:O	20:T:96:GLY:N	2.33	0.49
1:A:662:G:H2'	1:A:663:A:C8	2.46	0.49
1:A:1356:G:H2'	1:A:1357:A:C8	2.47	0.49
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.93	0.49
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.94	0.49
9:I:49:PRO:O	9:I:52:ALA:HB3	2.13	0.49
22:a:2:A:H2'	22:a:3:A:H8	1.78	0.49
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.93	0.49
1:A:560:U:H5'	1:A:566:G:N2	2.27	0.49
1:A:652:U:O4	1:A:752:G:O2'	2.23	0.49
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.45	0.49
1:A:1413:A:H2	1:A:1487:G:H22	1.59	0.49
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.94	0.49
1:A:390:C:H2'	1:A:391:G:C8	2.48	0.49
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.95	0.49
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.93	0.49
1:A:266:G:H5''	1:A:267:C:C5	2.48	0.49
1:A:1020:U:H2'	1:A:1021:G:H8	1.77	0.49
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.95	0.49
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.94	0.48
1:A:1124:G:O2'	1:A:1126:U:O4	2.31	0.48
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.45	0.48
20:T:30:LYS:HE3	20:T:72:LEU:HD23	1.95	0.48
2:B:112:VAL:O	2:B:116:GLU:HG2	2.13	0.48
9:I:44:VAL:O	9:I:51:ARG:NH2	2.46	0.48
20:T:73:HIS:O	20:T:74:LYS:C	2.56	0.48
1:A:967:5MC:H5''	1:A:968:A:OP2	2.13	0.48
1:A:1499:A:H1'	1:A:1520:G:H5'	1.95	0.48
4:D:24:GLU:HG2	4:D:25:ARG:H	1.78	0.48
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.95	0.48
1:A:1034:G:H2'	1:A:1035:A:H8	1.78	0.48
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:77:MET:HE3	11:K:80:VAL:HG12	1.94	0.48
13:M:33:ALA:O	13:M:37:THR:OG1	2.25	0.48
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.31	0.48
20:T:74:LYS:NZ	20:T:74:LYS:CA	2.76	0.48
2:B:68:ILE:O	2:B:90:MET:HB3	2.14	0.48
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.43	0.48
20:T:73:HIS:C	20:T:74:LYS:O	2.56	0.48
1:A:344:A:H5'	1:A:345:C:C5	2.49	0.48
1:A:1518:MA6:H93	1:A:1519:MA6:C9	2.42	0.48
2:B:239:VAL:O	2:B:241:GLU:N	2.47	0.47
1:A:1132:C:H2'	1:A:1133:G:H8	1.79	0.47
1:A:1301:U:HO2'	1:A:1302:U:P	2.36	0.47
7:G:51:GLN:C	7:G:53:LYS:H	2.23	0.47
1:A:335:C:O2'	1:A:1433:A:N3	2.36	0.47
1:A:973:G:H3'	1:A:974:A:H5''	1.95	0.47
6:F:46:ARG:HB2	6:F:60:PHE:CE2	2.49	0.47
1:A:663:A:H5''	18:R:61:LYS:HE3	1.96	0.47
11:K:69:ALA:O	11:K:73:MET:HG2	2.15	0.47
1:A:559:A:P	5:E:126:ARG:HH22	2.37	0.47
1:A:776:G:N2	1:A:802:A:OP2	2.46	0.47
1:A:673:G:O3'	6:F:87:ARG:NH2	2.47	0.47
1:A:826:C:O2	8:H:15:ASN:ND2	2.47	0.47
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.96	0.47
1:A:1305:G:N2	1:A:1331:G:H2'	2.29	0.47
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.50	0.47
7:G:152:ALA:HB1	7:G:155:ARG:HH12	1.80	0.47
9:I:16:ARG:O	9:I:63:ILE:HA	2.15	0.47
12:L:24:VAL:HG13	12:L:98:TYR:CE1	2.49	0.47
13:M:5:ALA:HB1	13:M:66:LEU:HD13	1.96	0.47
15:O:87:ILE:HG22	15:O:88:ARG:H	1.79	0.47
1:A:1054:C:H42	23:b:34:70U:H1'	1.79	0.47
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.50	0.47
1:A:1010:G:H2'	1:A:1011:G:H8	1.79	0.47
1:A:1532:U:H2'	1:A:1533:C:H3'	1.97	0.47
14:N:24:CYS:HB3	14:N:29:ARG:H	1.80	0.47
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.97	0.47
1:A:59:A:H5''	1:A:387:U:H5''	1.98	0.46
26:A:1858:B6M:O62	26:A:1858:B6M:O23	2.33	0.46
4:D:4:TYR:CG	4:D:4:TYR:O	2.68	0.46
11:K:80:VAL:HG11	11:K:103:LEU:HD13	1.98	0.46
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.49	0.46
1:A:191:G:O2'	20:T:102:GLY:O	2.29	0.46
1:A:1392:G:H21	1:A:1502:A:H8	1.61	0.46
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.80	0.46
1:A:1301:U:H1'	1:A:1302:U:OP1	2.15	0.46
1:A:976:G:H5'	1:A:1358:U:O2'	2.16	0.46
7:G:75:VAL:HG11	7:G:144:MET:HB3	1.97	0.46
1:A:558:G:OP2	1:A:559:A:O2'	2.30	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.16	0.46
8:H:121:ASP:N	8:H:121:ASP:OD1	2.47	0.46
5:E:98:THR:HB	5:E:117:ASP:HB3	1.98	0.46
20:T:74:LYS:HD2	20:T:74:LYS:H	1.79	0.46
1:A:737:A:H1'	6:F:73:ASN:HD21	1.81	0.46
4:D:151:LYS:H	4:D:151:LYS:HD2	1.79	0.46
8:H:53:VAL:O	8:H:55:GLY:N	2.49	0.46
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.14	0.46
1:A:727:G:N2	1:A:730:G:OP2	2.47	0.46
9:I:25:LYS:N	9:I:60:ASP:OD1	2.46	0.46
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.55	0.46
1:A:1366:C:H2'	1:A:1367:C:C6	2.51	0.46
5:E:6:PHE:HD1	5:E:6:PHE:HA	1.70	0.46
1:A:801:U:H2'	1:A:802:A:C8	2.51	0.46
1:A:947:G:H4'	1:A:1332:A:H2	1.81	0.46
6:F:94:GLN:HB3	18:R:32:ARG:HH11	1.80	0.46
9:I:65:VAL:HG21	9:I:77:ILE:HD11	1.98	0.46
1:A:1127:G:N2	1:A:1146:A:H62	2.14	0.45
1:A:1179:A:O2'	1:A:1180:A:OP1	2.31	0.45
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.98	0.45
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.45
1:A:836:G:C6	1:A:851:G:C6	3.04	0.45
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.15	0.45
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.98	0.45
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.98	0.45
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.98	0.45
1:A:277:C:H5''	17:Q:68:ARG:NH2	2.31	0.45
1:A:713:G:H2'	1:A:714:G:C8	2.51	0.45
1:A:1057:G:H5''	3:C:154:SER:HB2	1.97	0.45
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.98	0.45
13:M:96:LEU:O	13:M:110:ARG:NH1	2.50	0.45
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.98	0.45
1:A:103:C:OP1	20:T:17:ARG:NH1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:U:H2'	1:A:912:C:C6	2.51	0.45
14:N:9:LYS:HD3	14:N:21:TYR:O	2.16	0.45
1:A:1064:G:H21	1:A:1190:G:H2'	1.81	0.45
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.47	0.45
1:A:1182:G:H4'	1:A:1183:A:O5'	2.17	0.45
1:A:129:U:O3'	1:A:129(A):G:H3'	2.17	0.45
1:A:1431:C:H2'	1:A:1432:G:O4'	2.16	0.45
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.99	0.45
1:A:875:C:O2'	8:H:14:ARG:NH1	2.49	0.45
1:A:1128:C:H42	1:A:1143:G:H22	1.64	0.45
13:M:37:THR:HG22	13:M:55:ARG:HD2	1.98	0.45
1:A:184:G:H2'	1:A:185:A:H8	1.82	0.45
1:A:977:A:H2'	1:A:978:A:H5''	1.99	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.45
1:A:1177:G:O5'	9:I:97:LYS:NZ	2.48	0.45
1:A:1490:C:H2'	1:A:1491:G:H8	1.82	0.45
2:B:130:ARG:HA	2:B:130:ARG:HD3	1.71	0.45
2:B:223:ILE:HD13	2:B:230:VAL:HG23	1.98	0.45
1:A:1218:C:H2'	1:A:1219:U:C6	2.51	0.45
1:A:1305:G:H22	1:A:1331:G:H2'	1.81	0.45
2:B:88:ALA:O	2:B:90:MET:N	2.48	0.45
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.98	0.45
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.99	0.45
1:A:384:G:H2'	1:A:385:C:C6	2.52	0.44
1:A:1020:U:H2'	1:A:1021:G:C8	2.52	0.44
1:A:1026:G:H3'	1:A:1027:C:H5''	2.00	0.44
5:E:90:VAL:O	5:E:120:THR:HA	2.17	0.44
13:M:3:ARG:HA	13:M:9:ILE:HG13	1.99	0.44
1:A:994:A:N7	1:A:1216:G:H4'	2.33	0.44
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.00	0.44
5:E:145:LYS:O	5:E:149:GLU:HG2	2.18	0.44
3:C:3:ASN:OD1	3:C:3:ASN:N	2.49	0.44
10:J:51:ARG:HG2	10:J:61:GLU:HB2	1.98	0.44
21:U:5:ASP:O	21:U:11:GLY:HA3	2.17	0.44
7:G:45:ASP:O	7:G:48:LYS:HG2	2.16	0.44
1:A:452:A:HO2'	1:A:453:A:H8	1.61	0.44
1:A:501:C:H1'	1:A:549:C:H1'	1.98	0.44
1:A:1256:A:O2'	1:A:1257:U:O5'	2.33	0.44
1:A:1505:G:HO2'	1:A:1506:U:P	2.37	0.44
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.99	0.44
3:C:147:LYS:HE2	3:C:205:GLY:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:CYS:C	4:D:33:MET:H	2.26	0.44
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.99	0.44
10:J:26:ALA:O	10:J:84:GLN:NE2	2.49	0.44
1:A:1054:C:H2'	1:A:1055:A:H5''	2.00	0.44
1:A:1347:G:O2'	1:A:1348:U:P	2.76	0.44
5:E:79:GLU:HG3	5:E:93:PRO:HD2	2.00	0.44
5:E:142:LEU:O	5:E:143:ARG:NE	2.48	0.44
8:H:6:ILE:O	8:H:10:LEU:HG	2.18	0.44
1:A:62:U:O2'	1:A:379:C:O2	2.35	0.44
1:A:337:C:H2'	1:A:338:A:H8	1.82	0.44
1:A:501:C:H2'	1:A:502:G:C8	2.52	0.44
1:A:701:C:H4'	1:A:702:A:O5'	2.17	0.44
1:A:1298:C:H4'	1:A:1299:A:C4	2.52	0.44
7:G:44:TYR:HE2	9:I:41:VAL:HG11	1.82	0.44
7:G:65:ALA:O	7:G:69:VAL:HG23	2.18	0.44
1:A:1198:G:H2'	1:A:1199:U:C6	2.53	0.44
9:I:44:VAL:HG12	9:I:51:ARG:NH2	2.33	0.44
13:M:66:LEU:O	13:M:70:LEU:HB2	2.17	0.44
1:A:946:A:O2'	1:A:1333:A:N3	2.45	0.43
1:A:1029:C:H2'	1:A:1030:C:C6	2.53	0.43
1:A:1502:A:H2	1:A:1505:G:N1	2.16	0.43
1:A:1300:G:HO2'	1:A:1301:U:P	2.41	0.43
8:H:86:ILE:HD12	8:H:133:LEU:HD22	2.00	0.43
10:J:48:THR:HA	10:J:62:HIS:HB3	2.00	0.43
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.01	0.43
1:A:380:G:N2	1:A:383:A:OP2	2.39	0.43
1:A:739:C:O2'	15:O:42:HIS:ND1	2.42	0.43
1:A:757:U:H2'	1:A:758:G:O4'	2.18	0.43
1:A:1286:A:H2'	1:A:1287:A:H4'	1.99	0.43
4:D:24:GLU:C	4:D:26:CYS:H	2.26	0.43
4:D:110:PHE:HD1	4:D:162:LEU:HD21	1.83	0.43
1:A:1323:G:H2'	1:A:1324:A:C8	2.54	0.43
2:B:178:ARG:NH2	8:H:74:PRO:HB3	2.33	0.43
1:A:186:C:H2'	1:A:187:C:C6	2.53	0.43
1:A:555:C:H2'	1:A:556:C:C6	2.53	0.43
1:A:1497:G:H2'	1:A:1498:UR3:H5'	2.00	0.43
10:J:40:LEU:HB3	10:J:69:ASN:HB2	1.99	0.43
1:A:324:G:OP1	20:T:70:SER:OG	2.36	0.43
1:A:558:G:C8	1:A:559:A:H2'	2.54	0.43
1:A:1001:A:H2'	1:A:1002:G:C8	2.53	0.43
1:A:1256:A:H5'	1:A:1258:G:H1'	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:A:N6	1:A:1331:G:H1'	2.33	0.43
2:B:87:ARG:O	2:B:88:ALA:C	2.61	0.43
4:D:110:PHE:CD1	4:D:162:LEU:HD21	2.52	0.43
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.83	0.43
10:J:40:LEU:HD23	10:J:40:LEU:HA	1.90	0.43
15:O:6:GLU:CD	15:O:6:GLU:H	2.27	0.43
1:A:328:C:H4'	1:A:329:A:O5'	2.18	0.43
1:A:1021:G:H2'	1:A:1022:G:C8	2.53	0.43
1:A:1342:C:H2'	1:A:1343:G:C8	2.54	0.43
1:A:269:C:H2'	1:A:270:A:H8	1.82	0.43
14:N:24:CYS:SG	14:N:40:CYS:N	2.89	0.43
1:A:483:C:OP2	1:A:484:G:O2'	2.35	0.43
1:A:1065:U:H1'	1:A:1066:C:OP2	2.18	0.43
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.64	0.43
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.33	0.43
1:A:938:A:N6	28:A:1905:HOH:O	2.39	0.43
3:C:64:VAL:H	3:C:99:VAL:HB	1.84	0.43
7:G:74:GLU:HG2	7:G:91:VAL:HG22	2.01	0.43
8:H:120:THR:H	8:H:123:GLU:HB2	1.83	0.43
10:J:15:THR:HG22	10:J:91:PRO:HB3	2.00	0.43
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.54	0.42
1:A:564:C:O2'	8:H:91:ARG:NH2	2.53	0.42
1:A:958:A:N6	19:S:77:THR:O	2.50	0.42
1:A:1348:U:H4'	9:I:120:ARG:HD2	2.00	0.42
10:J:90:LEU:N	10:J:91:PRO:HD2	2.34	0.42
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.42
1:A:413:G:H1'	1:A:428:G:N2	2.33	0.42
1:A:714:G:H2'	1:A:715:A:C8	2.54	0.42
1:A:1346:A:N1	1:A:1374:A:H5''	2.35	0.42
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.19	0.42
4:D:64:LEU:HB2	4:D:198:VAL:HG11	2.01	0.42
13:M:90:LEU:O	13:M:94:ARG:HG2	2.19	0.42
15:O:62:GLN:OE1	15:O:65:ARG:NH2	2.52	0.42
1:A:363:A:H62	12:L:28:LYS:HE2	1.84	0.42
3:C:8:ILE:HG23	3:C:16:ARG:HG2	2.01	0.42
4:D:32:ALA:HA	4:D:35:ARG:HG2	2.01	0.42
4:D:57:ARG:HB3	4:D:206:PHE:HB2	2.01	0.42
19:S:33:THR:HG22	19:S:35:SER:H	1.84	0.42
1:A:514:C:H2'	1:A:515:G:C8	2.54	0.42
1:A:737:A:H2'	1:A:738:C:C6	2.54	0.42
1:A:1273:G:H2'	1:A:1274:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:GLU:HG2	5:E:88:LYS:HE2	2.00	0.42
1:A:991:U:O4	1:A:1212:U:O2'	2.25	0.42
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.49	0.42
18:R:47:THR:HA	18:R:83:GLU:HB2	2.01	0.42
1:A:106:C:H2'	1:A:107:G:H8	1.84	0.42
1:A:192:U:H1'	20:T:103:GLY:HA2	2.01	0.42
9:I:117:HIS:HB2	9:I:121:ARG:HB3	2.02	0.42
1:A:130:A:OP2	1:A:190(E):U:O2'	2.26	0.42
1:A:1236:A:H4'	1:A:1304:G:H4'	2.02	0.42
1:A:1376:U:H2'	1:A:1377:A:C8	2.55	0.42
3:C:148:GLY:HA3	3:C:172:ARG:O	2.19	0.42
7:G:45:ASP:O	7:G:49:ILE:HG13	2.19	0.42
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.84	0.42
13:M:115:LYS:HE2	13:M:115:LYS:HB2	1.89	0.42
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.55	0.42
1:A:184:G:H2'	1:A:185:A:C8	2.55	0.42
1:A:665:A:N3	1:A:732:C:H2'	2.34	0.42
1:A:578:C:O2'	1:A:728:A:N3	2.50	0.42
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.42
1:A:975:A:H62	10:J:60:ARG:HH12	1.68	0.42
1:A:1027:C:N4	1:A:1036:G:O6	2.53	0.42
1:A:1086:U:H3	1:A:1099:G:H22	1.66	0.42
1:A:1131:G:H2'	1:A:1132:C:C6	2.54	0.42
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.35	0.42
11:K:72:ALA:HB1	11:K:77:MET:HE2	2.02	0.42
1:A:339:C:H2'	1:A:340:U:C6	2.55	0.42
1:A:410:G:OP1	4:D:30:LYS:NZ	2.45	0.42
1:A:1118:C:H1'	1:A:1179:A:C5	2.55	0.41
6:F:30:LEU:HD23	6:F:75:LEU:HD11	2.02	0.41
1:A:1069:C:O2'	1:A:1192:C:H1'	2.20	0.41
9:I:127:LYS:HE3	9:I:127:LYS:HB3	1.84	0.41
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.56	0.41
20:T:74:LYS:HZ3	20:T:74:LYS:CA	2.20	0.41
1:A:51:A:N7	1:A:114:U:O2'	2.51	0.41
19:S:36:ARG:NH2	19:S:75:ALA:O	2.48	0.41
1:A:653:A:C8	8:H:56:LYS:HG2	2.56	0.41
1:A:1308:U:H2'	1:A:1309:G:H8	1.85	0.41
1:A:1311:G:N7	19:S:2:PRO:HA	2.36	0.41
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.41
2:B:108:ILE:O	2:B:112:VAL:HG23	2.21	0.41
11:K:34:ASP:OD1	11:K:38:ASN:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:C:H2'	1:A:502:G:H8	1.83	0.41
1:A:1112:C:O2	3:C:179:ARG:HG2	2.19	0.41
3:C:6:HIS:HD2	3:C:8:ILE:N	2.16	0.41
1:A:1054:C:N4	23:b:34:70U:H1'	2.34	0.41
6:F:2:ARG:NH1	6:F:69:GLU:HG2	2.36	0.41
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.49	0.41
19:S:23:ASN:OD1	19:S:47:HIS:NE2	2.45	0.41
1:A:748:C:H1'	1:A:749:C:OP2	2.21	0.41
1:A:789:U:O2'	1:A:791:G:N7	2.51	0.41
1:A:939:G:H2'	1:A:940:C:C6	2.56	0.41
1:A:1065:U:C5	1:A:1190:G:H1'	2.55	0.41
1:A:1338:G:H2'	1:A:1339:A:C8	2.55	0.41
1:A:1477:C:H2'	1:A:1478:C:C6	2.56	0.41
1:A:35:G:H2'	1:A:36:C:C6	2.55	0.41
1:A:603:U:H2'	1:A:604:G:C8	2.56	0.41
1:A:1306:A:H61	1:A:1331:G:H1'	1.86	0.41
1:A:1414:U:H2'	1:A:1415:G:C8	2.54	0.41
11:K:62:GLN:HG3	11:K:97:ALA:HB2	2.02	0.41
1:A:17:U:H2'	1:A:18:C:C6	2.55	0.41
1:A:110:C:O2'	16:P:25:ARG:O	2.36	0.41
1:A:299:G:H2'	1:A:300:A:C8	2.56	0.41
1:A:436:C:H2'	1:A:437:U:C6	2.56	0.41
1:A:514:C:H2'	1:A:515:G:H8	1.86	0.41
1:A:575:G:O2'	1:A:821:G:OP2	2.37	0.41
1:A:736:C:H2'	1:A:737:A:C8	2.56	0.41
1:A:986:A:H2'	1:A:987:G:O4'	2.20	0.41
1:A:1225:A:H5''	1:A:1226:C:OP2	2.21	0.41
1:A:1300:G:O2'	1:A:1301:U:P	2.78	0.41
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.21	0.41
6:F:1:MET:HE3	6:F:66:GLU:HG2	2.03	0.41
12:L:124:LYS:HG3	12:L:125:PRO:O	2.21	0.41
16:P:70:ALA:O	16:P:74:LEU:HG	2.20	0.41
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.20	0.41
1:A:691:G:H2'	1:A:692:U:C6	2.56	0.41
1:A:1148:U:H1'	9:I:16:ARG:HH21	1.85	0.41
9:I:118:LYS:C	9:I:120:ARG:H	2.27	0.41
1:A:401:C:H2'	1:A:402:G:H8	1.87	0.40
1:A:110:C:H2'	1:A:111:G:O4'	2.21	0.40
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.56	0.40
10:J:76:ASN:O	10:J:78:ASN:N	2.55	0.40
11:K:27:ASN:OD1	11:K:28:THR:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:59:TRP:HA	16:P:62:VAL:HG22	2.03	0.40
20:T:54:LYS:HE2	20:T:54:LYS:HB3	1.91	0.40
1:A:1010:G:H2'	1:A:1011:G:C8	2.56	0.40
1:A:1250:A:H2'	1:A:1251:A:C8	2.57	0.40
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.93	0.40
8:H:53:VAL:O	8:H:54:ASP:C	2.65	0.40
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.70	0.40
1:A:927:G:OP1	1:A:1505:G:N2	2.55	0.40
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.36	0.40
7:G:50:ILE:HB	7:G:58:PRO:HB3	2.04	0.40
18:R:47:THR:HG22	18:R:48:GLY:H	1.86	0.40
1:A:397:A:H5'	1:A:398:C:OP1	2.21	0.40
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.22	0.40
7:G:69:VAL:HG21	7:G:104:LEU:HD21	2.02	0.40
12:L:53:ARG:HD2	12:L:53:ARG:N	2.37	0.40
20:T:62:LEU:HD23	20:T:62:LEU:HA	1.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:U:OP2	1:A:1335:C:O2'[3_545]	2.17	0.03

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	234/236 (99%)	212 (91%)	20 (8%)	2 (1%)	14	43
3	C	205/207 (99%)	185 (90%)	20 (10%)	0	100	100
4	D	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
5	E	149/151 (99%)	144 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/101 (98%)	99 (100%)	0	0	100	100
7	G	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
8	H	136/138 (99%)	129 (95%)	6 (4%)	1 (1%)	18	49
9	I	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	J	97/99 (98%)	80 (82%)	16 (16%)	1 (1%)	12	40
11	K	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
12	L	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
13	M	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14	43
14	N	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
15	O	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
16	P	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
17	Q	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
18	R	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
19	S	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
20	T	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	3	20
21	U	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2393 (98%)	2194 (93%)	150 (6%)	8 (0%)	36	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	107	ALA
20	T	74	LYS
20	T	76	ALA
2	B	240	GLN
20	T	73	HIS
10	J	55	LYS
8	H	54	ASP
2	B	89	GLY

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	194/204 (95%)	186 (96%)	8 (4%)	27	55
3	C	160/161 (99%)	150 (94%)	10 (6%)	16	44
4	D	180/180 (100%)	173 (96%)	7 (4%)	28	56
5	E	115/116 (99%)	104 (90%)	11 (10%)	8	29
6	F	90/90 (100%)	88 (98%)	2 (2%)	45	66
7	G	126/126 (100%)	121 (96%)	5 (4%)	28	56
8	H	119/119 (100%)	111 (93%)	8 (7%)	15	42
9	I	98/98 (100%)	93 (95%)	5 (5%)	21	50
10	J	87/89 (98%)	80 (92%)	7 (8%)	11	36
11	K	90/90 (100%)	84 (93%)	6 (7%)	15	42
12	L	103/103 (100%)	95 (92%)	8 (8%)	11	36
13	M	94/94 (100%)	87 (93%)	7 (7%)	13	38
14	N	49/49 (100%)	48 (98%)	1 (2%)	48	68
15	O	79/79 (100%)	69 (87%)	10 (13%)	4	18
16	P	72/72 (100%)	68 (94%)	4 (6%)	19	47
17	Q	94/94 (100%)	89 (95%)	5 (5%)	20	49
18	R	64/64 (100%)	62 (97%)	2 (3%)	35	60
19	S	71/71 (100%)	65 (92%)	6 (8%)	10	33
20	T	76/76 (100%)	64 (84%)	12 (16%)	2	12
21	U	19/20 (95%)	19 (100%)	0	100	100
All	All	1980/1995 (99%)	1856 (94%)	124 (6%)	16	44

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	LYS
2	B	61	LEU
2	B	69	LEU
2	B	82	ARG
2	B	114	ARG
2	B	139	LYS
2	B	221	LEU
2	B	236	TYR
3	C	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	27	LYS
3	C	28	GLN
3	C	34	LEU
3	C	91	LEU
3	C	95	THR
3	C	126	ARG
3	C	166	GLU
3	C	204	LEU
3	C	206	GLU
4	D	15	GLU
4	D	64	LEU
4	D	96	LEU
4	D	122	ARG
4	D	127	THR
4	D	170	VAL
4	D	194	LEU
5	E	6	PHE
5	E	12	LEU
5	E	41	VAL
5	E	43	LEU
5	E	64	ARG
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	120	THR
5	E	150	ARG
6	F	10	LEU
6	F	69	GLU
7	G	8	GLU
7	G	11	GLN
7	G	52	GLU
7	G	75	VAL
7	G	156	TRP
8	H	39	LEU
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	92	ARG
8	H	102	ARG
8	H	127	LEU
8	H	133	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	2	GLU
9	I	79	LEU
9	I	102	LEU
9	I	103	THR
9	I	118	LYS
10	J	15	THR
10	J	49	VAL
10	J	59	SER
10	J	71	LEU
10	J	80	LYS
10	J	83	GLU
10	J	86	MET
11	K	11	LYS
11	K	29	ILE
11	K	48	ILE
11	K	80	VAL
11	K	92	GLU
11	K	114	VAL
12	L	20	LYS
12	L	27	LEU
12	L	28	LYS
12	L	39	VAL
12	L	47	LYS
12	L	53	ARG
12	L	100	ILE
12	L	111	LYS
13	M	37	THR
13	M	56	LEU
13	M	58	GLU
13	M	69	GLU
13	M	70	LEU
13	M	105	THR
13	M	109	THR
14	N	33	VAL
15	O	5	LYS
15	O	6	GLU
15	O	34	LEU
15	O	38	ARG
15	O	39	LEU
15	O	41	GLU
15	O	45	VAL
15	O	70	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	81	LEU
15	O	87	ILE
16	P	1	MET
16	P	20	VAL
16	P	53	VAL
16	P	67	THR
17	Q	38	ARG
17	Q	53	LEU
17	Q	74	LEU
17	Q	91	ARG
17	Q	98	LEU
18	R	25	THR
18	R	86	VAL
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	31	ILE
19	S	62	ILE
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU
20	T	48	LYS
20	T	56	MET
20	T	57	ARG
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
3	C	28	GLN
4	D	119	GLN
6	F	7	ASN
6	F	64	GLN
7	G	84	ASN
9	I	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	73	GLN
9	I	124	GLN
10	J	76	ASN
12	L	9	GLN
14	N	49	HIS
16	P	14	ASN
17	Q	26	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	205 (13%)	36 (2%)
22	a	4/5 (80%)	0	0
23	b	14/15 (93%)	5 (35%)	0
All	All	1528/1542 (99%)	210 (13%)	36 (2%)

All (210) 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
1	A	51	A
1	A	61	G
1	A	63	C
1	A	101	A
1	A	116	A
1	A	117	G
1	A	120	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
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	204	U
1	A	216	G
1	A	220	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	267	C
1	A	270	A
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	352	C
1	A	353	A
1	A	354	G
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	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	429	U
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	460	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	596	C
1	A	630	G
1	A	631	G
1	A	653	A
1	A	665	A
1	A	666	G
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	793	U
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	848	C
1	A	876	G
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	961	U
1	A	968	A
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	989	C
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	1050	G
1	A	1054	C
1	A	1064	G
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
1	A	1130	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1180	A
1	A	1181	G
1	A	1182	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	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1280	A
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1320	C
1	A	1332	A
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1397	C
1	A	1398	A
1	A	1421	G
1	A	1442	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1443	G
1	A	1446	A
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	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
23	b	32	C
23	b	33	U
23	b	34	70U
23	b	37	12A
23	b	38	A

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	960	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1179	A
1	A	1182	G
1	A	1201	A
1	A	1256	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1443	G
1	A	1505	G
1	A	1528	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518	1	23,26,27	0.81	1 (4%)	33,38,41	0.93	1 (3%)
23	12A	b	37	23	33,36,37	3.30	14 (42%)	46,52,55	3.13	19 (41%)
1	M2G	A	966	1	24,27,28	1.05	3 (12%)	33,40,43	0.81	1 (3%)
1	MA6	A	1519	1	23,26,27	0.78	1 (4%)	33,38,41	0.94	1 (3%)
1	PSU	A	1540	1	18,21,22	2.02	7 (38%)	21,30,33	1.51	4 (19%)
1	PSU	A	516	1	18,21,22	2.04	7 (38%)	21,30,33	1.51	4 (19%)
23	70U	b	34	22,23	22,26,27	3.54	10 (45%)	27,37,40	1.42	5 (18%)
22	A2M	a	1	22,23	22,22,26	1.35	3 (13%)	31,32,39	2.20	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1541	1,24	18,21,22	2.02	7 (38%)	21,30,33	1.53	4 (19%)
1	5MC	A	967	1	19,22,23	1.03	2 (10%)	26,32,35	0.95	2 (7%)
1	2MG	A	1207	1	23,26,27	1.14	3 (13%)	33,38,41	1.12	4 (12%)
1	UR3	A	1498	1	19,22,23	0.77	1 (5%)	26,32,35	1.13	2 (7%)
1	5MC	A	1400	1	19,22,23	1.02	2 (10%)	26,32,35	0.95	1 (3%)
1	5MC	A	1407	1	19,22,23	1.02	2 (10%)	26,32,35	1.00	2 (7%)
1	7MG	A	527	1	23,26,27	4.29	4 (17%)	27,39,42	2.22	9 (33%)
1	4OC	A	1402	1	20,23,24	0.95	2 (10%)	25,32,35	0.72	0
12	0TD	L	92	12	8,9,10	2.31	1 (12%)	6,11,13	2.06	2 (33%)
1	5MC	A	1404	1	19,22,23	1.02	2 (10%)	26,32,35	0.96	1 (3%)
23	PSU	b	39	23	18,21,22	2.03	7 (38%)	21,30,33	1.60	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
23	12A	b	37	23	1/1/9/11	8/25/43/44	0/3/3/3
1	M2G	A	966	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
23	70U	b	34	22,23	-	4/13/31/32	0/2/2/2
22	A2M	a	1	22,23	-	3/8/24/28	0/3/3/3
1	PSU	A	1541	1,24	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	1/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
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	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
23	PSU	b	39	23	-	0/7/25/26	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-19.57	1.33	1.45
23	b	34	70U	O4-C4	8.69	1.40	1.23
23	b	37	12A	O4'-C1'	8.38	1.61	1.42
23	b	34	70U	C2-S2	8.26	1.81	1.67
23	b	37	12A	C2-S2	7.33	1.81	1.75
23	b	37	12A	C2'-C1'	-7.17	1.30	1.53
23	b	37	12A	C6-N6	6.07	1.52	1.39
12	L	92	0TD	CB-CA	-5.92	1.52	1.54
23	b	34	70U	C6-N1	-5.88	1.28	1.38
23	b	37	12A	O4'-C4'	-5.58	1.32	1.45
23	b	34	70U	C4-N3	-5.06	1.29	1.38
22	a	1	A2M	C6-N6	4.37	1.45	1.34
23	b	37	12A	CC-N	4.11	1.46	1.35
23	b	34	70U	C5M-C5	4.10	1.57	1.51
23	b	37	12A	O2'-C2'	3.98	1.52	1.43
1	A	527	7MG	C2-N2	3.89	1.43	1.34
23	b	39	PSU	C2-N1	-3.75	1.31	1.36
23	b	34	70U	O9-C8	3.71	1.44	1.33
1	A	516	PSU	C2-N1	-3.70	1.31	1.36
1	A	1540	PSU	C6-C5	3.68	1.39	1.35
1	A	1540	PSU	C2-N1	-3.66	1.31	1.36
1	A	1541	PSU	C6-C5	3.66	1.39	1.35
1	A	1541	PSU	C2-N1	-3.65	1.31	1.36
1	A	516	PSU	C6-C5	3.59	1.39	1.35
23	b	39	PSU	C6-C5	3.58	1.39	1.35
23	b	37	12A	CC-N6	3.46	1.45	1.37
23	b	34	70U	O9-C9	-3.45	1.37	1.45
23	b	39	PSU	C4-N3	-3.42	1.32	1.38
1	A	516	PSU	C4-N3	-3.38	1.32	1.38
1	A	1541	PSU	C4-N3	-3.37	1.32	1.38
1	A	516	PSU	C2-N3	-3.35	1.32	1.37
1	A	1540	PSU	C4-N3	-3.34	1.32	1.38
23	b	34	70U	C4-C5	-3.34	1.37	1.45
1	A	1541	PSU	C2-N3	-3.31	1.32	1.37
23	b	39	PSU	C2-N3	-3.31	1.32	1.37
1	A	1540	PSU	C2-N3	-3.30	1.32	1.37
23	b	37	12A	OO-CC	-3.15	1.16	1.23
23	b	37	12A	O-C	3.09	1.31	1.22
23	b	37	12A	O3'-C3'	-3.01	1.35	1.43
23	b	34	70U	C6-C5	2.98	1.43	1.35
1	A	1207	2MG	C2-N2	2.86	1.39	1.33
1	A	966	M2G	C2-N2	2.83	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1	A2M	C2-N1	2.83	1.39	1.33
1	A	516	PSU	O4-C4	-2.75	1.18	1.23
1	A	1540	PSU	O4-C4	-2.72	1.18	1.23
23	b	39	PSU	O4-C4	-2.67	1.18	1.23
23	b	37	12A	CA-N	-2.67	1.40	1.45
1	A	527	7MG	C5-N7	2.64	1.39	1.35
1	A	1541	PSU	O4-C4	-2.63	1.18	1.23
23	b	34	70U	C2-N3	-2.56	1.31	1.38
1	A	966	M2G	C4-N3	2.53	1.40	1.34
1	A	1400	5MC	C2-N1	2.53	1.45	1.40
1	A	1498	UR3	C2-N1	2.52	1.42	1.38
1	A	967	5MC	C2-N1	2.49	1.45	1.40
1	A	1407	5MC	C2-N1	2.45	1.45	1.40
1	A	1404	5MC	C2-N1	2.42	1.45	1.40
1	A	1402	4OC	C2-N3	2.40	1.41	1.36
1	A	1407	5MC	C2-N3	2.38	1.41	1.36
1	A	1400	5MC	C2-N3	2.38	1.41	1.36
1	A	1207	2MG	C2-N1	2.36	1.40	1.36
1	A	967	5MC	C2-N3	2.36	1.41	1.36
1	A	1404	5MC	C2-N3	2.35	1.41	1.36
23	b	37	12A	O5'-C5'	-2.29	1.37	1.44
23	b	39	PSU	O2-C2	-2.24	1.18	1.23
1	A	516	PSU	O2-C2	-2.19	1.18	1.23
1	A	1402	4OC	O2-C2	-2.18	1.19	1.23
23	b	39	PSU	C6-N1	-2.18	1.32	1.36
1	A	527	7MG	C4-N3	2.18	1.39	1.34
1	A	1540	PSU	O2-C2	-2.18	1.18	1.23
1	A	1541	PSU	O2-C2	-2.15	1.18	1.23
1	A	966	M2G	C6-N1	2.08	1.42	1.38
22	a	1	A2M	C5-C6	2.07	1.46	1.41
1	A	1518	MA6	C5-C4	2.05	1.42	1.39
1	A	1207	2MG	C8-N9	2.05	1.42	1.37
1	A	1519	MA6	C5-C4	2.05	1.42	1.39
1	A	516	PSU	C6-N1	-2.04	1.33	1.36
23	b	37	12A	CA-C	2.04	1.55	1.52
1	A	1541	PSU	C6-N1	-2.04	1.33	1.36
1	A	1540	PSU	C6-N1	-2.03	1.33	1.36

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	37	12A	C2M-S2-C2	9.83	109.63	102.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	37	12A	O4'-C1'-N9	9.47	126.27	108.09
23	b	37	12A	C5-C4-N3	-8.34	118.39	127.18
23	b	37	12A	N3-C4-N9	6.01	134.62	126.99
22	a	1	A2M	C5-C4-N3	-5.75	118.80	126.72
22	a	1	A2M	N3-C2-N1	-5.35	120.48	128.58
1	A	527	7MG	C5-C6-N1	4.97	119.68	110.94
1	A	527	7MG	C2-N3-C4	4.79	120.55	112.30
23	b	37	12A	N6-CC-N	4.73	120.28	113.77
23	b	39	PSU	N1-C2-N3	4.34	119.75	115.17
22	a	1	A2M	N3-C4-N9	4.28	134.45	127.17
23	b	37	12A	C4'-O4'-C1'	-4.22	100.15	109.47
22	a	1	A2M	C2-N3-C4	4.19	122.06	111.83
23	b	34	70U	O9-C8-C5M	4.17	119.69	111.28
1	A	1498	UR3	C6-N1-C2	-4.00	118.53	121.80
1	A	1541	PSU	N1-C2-N3	3.93	119.31	115.17
1	A	1540	PSU	N1-C2-N3	3.92	119.30	115.17
1	A	527	7MG	C5-C4-N3	-3.87	120.86	128.13
1	A	516	PSU	N1-C2-N3	3.81	119.19	115.17
1	A	527	7MG	N9-C4-N3	3.71	130.90	125.46
1	A	527	7MG	N9-C8-N7	3.42	108.21	103.37
23	b	37	12A	C2-N3-C4	3.41	121.22	112.29
12	L	92	0TD	OD1-CG-CB	-3.20	115.74	122.44
12	L	92	0TD	CSB-SB-CB	-3.16	96.68	102.36
23	b	37	12A	C4-C5-N7	-3.13	107.00	110.58
23	b	37	12A	OO-CC-N6	-3.11	118.11	123.64
1	A	527	7MG	C6-C5-C4	-2.99	117.13	122.40
23	b	37	12A	C5-N7-C8	2.99	108.15	103.45
23	b	37	12A	C3'-C2'-C1'	-2.99	95.81	101.46
1	A	527	7MG	C6-C5-N7	2.98	136.55	131.93
23	b	39	PSU	C4-N3-C2	-2.90	122.38	126.37
22	a	1	A2M	C4-C5-N7	-2.87	107.30	110.58
1	A	516	PSU	C6-C5-C4	-2.83	116.26	118.17
23	b	34	70U	C5-C4-N3	2.82	119.51	115.21
22	a	1	A2M	C5-N7-C8	2.80	107.85	103.45
1	A	527	7MG	C2-N1-C6	-2.79	120.04	125.11
22	a	1	A2M	CM'-O2'-C2'	2.75	121.53	114.47
22	a	1	A2M	N9-C8-N7	-2.74	110.05	113.94
1	A	1541	PSU	C6-C5-C4	-2.74	116.33	118.17
23	b	39	PSU	O2-C2-N1	-2.73	119.97	122.79
1	A	1541	PSU	C4-N3-C2	-2.71	122.64	126.37
23	b	34	70U	C5-C6-N1	-2.70	119.30	122.94
1	A	527	7MG	O6-C6-C5	-2.70	121.00	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	C4-N3-C2	-2.69	122.67	126.37
23	b	37	12A	N3-C2-N1	-2.68	122.10	127.00
1	A	516	PSU	C4-N3-C2	-2.63	122.75	126.37
23	b	37	12A	N9-C8-N7	-2.61	110.23	113.94
1	A	1207	2MG	C5-C4-N3	-2.56	124.32	128.39
23	b	37	12A	O4'-C1'-C2'	-2.49	101.28	106.62
23	b	37	12A	CA-N-CC	2.48	126.12	121.99
1	A	1540	PSU	C6-C5-C4	-2.46	116.52	118.17
1	A	1404	5MC	N4-C4-N3	-2.39	114.17	118.51
1	A	967	5MC	N4-C4-N3	-2.39	114.18	118.51
1	A	1407	5MC	N4-C4-N3	-2.39	114.19	118.51
1	A	1400	5MC	N4-C4-N3	-2.35	114.26	118.51
1	A	1207	2MG	O6-C6-N1	-2.32	115.76	120.11
1	A	1541	PSU	O2-C2-N1	-2.30	120.41	122.79
23	b	37	12A	C5'-C4'-C3'	-2.25	107.10	115.21
1	A	1207	2MG	N9-C4-N3	2.23	130.41	125.95
22	a	1	A2M	C4-N9-C8	2.21	108.05	105.74
1	A	1407	5MC	C5-C4-N3	2.20	124.01	121.75
1	A	1540	PSU	O2-C2-N1	-2.16	120.56	122.79
23	b	34	70U	C5M-C5-C4	2.15	120.90	118.00
23	b	39	PSU	C6-C5-C4	-2.10	116.76	118.17
1	A	1518	MA6	C2-N1-C6	2.09	116.92	111.83
1	A	1207	2MG	C2-N1-C6	-2.07	122.05	124.55
23	b	37	12A	C6-C5-N7	2.05	134.67	132.43
1	A	1498	UR3	C1'-N1-C2	2.05	120.39	117.04
23	b	37	12A	OXT-C-O	-2.05	119.43	124.08
23	b	34	70U	O4-C4-C5	-2.05	121.27	124.71
1	A	967	5MC	C5-C4-N3	2.02	123.83	121.75
23	b	37	12A	OXT-C-CA	2.02	121.14	114.15
1	A	966	M2G	C5-C4-N3	-2.01	125.19	128.39
1	A	1519	MA6	C2-N1-C6	2.01	116.74	111.83
1	A	516	PSU	O2-C2-N1	-2.01	120.72	122.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	37	12A	C1'

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	92	0TD	CA-CB-SB-CSB
22	a	1	A2M	C1'-C2'-O2'-CM'
23	b	37	12A	N1-C2-S2-C2M
23	b	37	12A	N3-C2-S2-C2M
23	b	34	70U	C5M-C8-O9-C9
23	b	34	70U	O8-C8-O9-C9
22	a	1	A2M	O4'-C4'-C5'-O5'
22	a	1	A2M	C3'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
23	b	37	12A	O4'-C4'-C5'-O5'
23	b	37	12A	C2'-C1'-N9-C4
23	b	37	12A	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
23	b	37	12A	CB-CA-N-CC
23	b	34	70U	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
23	b	34	70U	O4'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
23	b	37	12A	C2'-C1'-N9-C8
1	A	1519	MA6	C4'-C5'-O5'-P
23	b	37	12A	C4'-C5'-O5'-P
1	A	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1518	MA6	3	0
23	b	37	12A	1	0
1	A	1519	MA6	2	0
23	b	34	70U	2	0
1	A	967	5MC	1	0
1	A	1207	2MG	1	0
1	A	1498	UR3	3	0
1	A	1400	5MC	1	0
1	A	1402	4OC	2	0
12	L	92	0TD	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 277 ligands modelled in this entry, 276 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	B6M	A	1858	-	44,45,45	3.31	13 (29%)	63,67,67	1.52	11 (17%)

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
26	B6M	A	1858	-	-	8/18/94/94	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1858	B6M	C23-C33	-13.77	1.22	1.53
26	A	1858	B6M	O43-C43	-7.65	1.28	1.45
26	A	1858	B6M	C34-C24	-5.28	1.46	1.53
26	A	1858	B6M	O43-C13	5.04	1.50	1.41
26	A	1858	B6M	C13-C23	5.01	1.59	1.52
26	A	1858	B6M	C33-C43	4.94	1.65	1.52
26	A	1858	B6M	O54-C54	4.77	1.56	1.44
26	A	1858	B6M	C31-C21	-4.04	1.48	1.53
26	A	1858	B6M	O51-C11	4.01	1.52	1.41
26	A	1858	B6M	O33-C33	3.94	1.53	1.43
26	A	1858	B6M	O23-C23	3.89	1.52	1.43
26	A	1858	B6M	O52-C13	-3.64	1.31	1.41
26	A	1858	B6M	C24-N24	2.42	1.50	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1858	B6M	C13-O52-C52	-4.22	107.97	117.98
26	A	1858	B6M	C14-O33-C33	-4.13	108.18	117.98
26	A	1858	B6M	C11-O11-C42	-3.16	110.49	117.98
26	A	1858	B6M	C41-C31-C21	2.76	115.58	110.99
26	A	1858	B6M	C22-C12-C62	2.74	114.18	110.08
26	A	1858	B6M	C31-C41-C51	2.42	114.62	110.23
26	A	1858	B6M	O51-C51-C41	2.32	113.88	109.70
26	A	1858	B6M	C13-C23-C33	2.26	104.82	102.10
26	A	1858	B6M	C61-C51-C41	-2.19	107.64	113.02
26	A	1858	B6M	O51-C11-C21	2.10	114.72	110.08
26	A	1858	B6M	O52-C52-C42	2.02	112.55	107.42

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	1858	B6M	C23-C13-O52-C52
26	A	1858	B6M	O43-C13-O52-C52
26	A	1858	B6M	C24-C14-O33-C33
26	A	1858	B6M	C44-C54-C64-N64
26	A	1858	B6M	C41-C51-C61-O61
26	A	1858	B6M	O51-C51-C61-O61
26	A	1858	B6M	O51-C11-O11-C42
26	A	1858	B6M	O54-C14-O33-C33

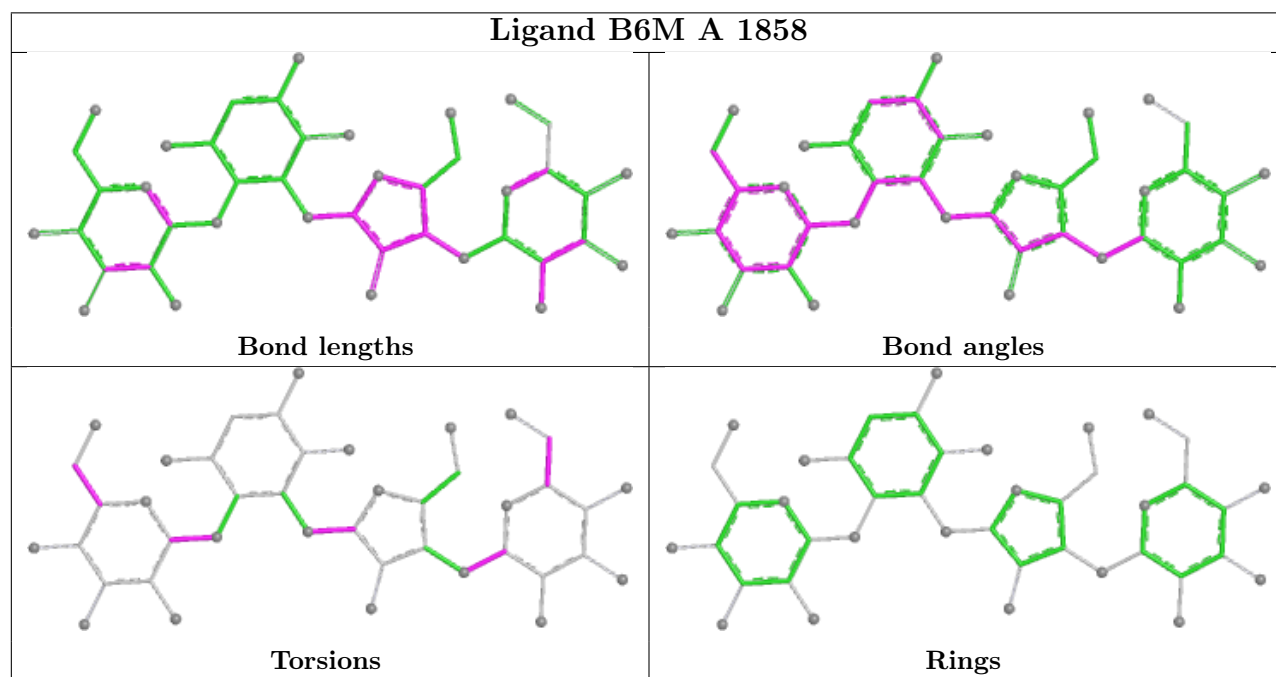
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	1858	B6M	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.



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%)	-0.65	5 (0%) 90 82	81, 114, 197, 306	0
2	B	236/236 (100%)	0.02	6 (2%) 58 39	106, 156, 232, 300	0
3	C	207/207 (100%)	-0.03	9 (4%) 40 25	82, 157, 207, 249	0
4	D	208/208 (100%)	0.26	13 (6%) 26 17	91, 132, 190, 261	0
5	E	151/151 (100%)	-0.10	2 (1%) 75 56	77, 114, 154, 219	0
6	F	101/101 (100%)	-0.22	1 (0%) 79 63	108, 148, 183, 215	0
7	G	155/155 (100%)	0.01	7 (4%) 38 25	104, 136, 198, 237	0
8	H	138/138 (100%)	-0.19	4 (2%) 53 35	79, 107, 151, 223	0
9	I	127/127 (100%)	0.53	11 (8%) 16 12	109, 159, 205, 292	0
10	J	99/99 (100%)	0.76	16 (16%) 4 4	110, 184, 266, 286	0
11	K	119/119 (100%)	0.28	7 (5%) 28 19	88, 117, 163, 245	0
12	L	124/125 (99%)	0.29	8 (6%) 25 17	85, 118, 181, 259	0
13	M	118/118 (100%)	0.15	3 (2%) 58 39	102, 137, 182, 283	0
14	N	60/60 (100%)	0.36	4 (6%) 24 16	114, 142, 181, 269	0
15	O	88/88 (100%)	-0.15	0 100 100	96, 126, 178, 229	0
16	P	84/84 (100%)	0.12	2 (2%) 59 40	77, 116, 153, 236	0
17	Q	99/99 (100%)	0.12	3 (3%) 52 35	83, 113, 165, 173	0
18	R	73/73 (100%)	-0.13	0 100 100	92, 129, 227, 288	0
19	S	81/81 (100%)	0.35	4 (4%) 35 23	104, 158, 223, 276	0
20	T	99/99 (100%)	0.37	10 (10%) 12 10	87, 117, 168, 208	0
21	U	25/25 (100%)	1.18	4 (16%) 5 4	101, 139, 192, 243	0
22	a	4/5 (80%)	1.49	1 (25%) 2 1	143, 144, 165, 211	0
23	b	12/15 (80%)	0.03	0 100 100	142, 232, 256, 264	0
All	All	3906/3935 (99%)	-0.16	120 (3%) 51 35	77, 127, 206, 306	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	128	ALA	8.3
4	D	2	GLY	8.1
11	K	129	SER	8.1
19	S	2	PRO	5.9
21	U	25	LYS	5.8
4	D	4	TYR	5.6
19	S	3	ARG	5.5
12	L	28	LYS	5.4
13	M	8	GLU	4.6
3	C	167	TRP	4.4
9	I	127	LYS	4.3
7	G	8	GLU	4.3
20	T	10	LEU	4.1
9	I	105	ASP	4.1
22	a	5	U	4.1
5	E	81	GLU	4.0
2	B	133	LYS	3.9
11	K	127	LYS	3.9
9	I	15	ALA	3.9
7	G	5	ARG	3.8
3	C	2	GLY	3.8
3	C	190	ARG	3.8
12	L	47	LYS	3.8
4	D	3	ARG	3.8
1	A	532	A	3.8
7	G	13	GLN	3.6
4	D	9	CYS	3.6
12	L	27	LEU	3.5
20	T	73	HIS	3.5
10	J	58	ASP	3.5
9	I	126	SER	3.5
12	L	26	ALA	3.5
2	B	134	GLU	3.4
10	J	64	GLU	3.4
14	N	8	GLU	3.4
11	K	126	ARG	3.4
13	M	10	PRO	3.4
10	J	73	ASP	3.3
14	N	13	THR	3.3
2	B	140	HIS	3.2
20	T	72	LEU	3.2
17	Q	100	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	5	ILE	3.1
7	G	6	ARG	3.0
12	L	62	SER	3.0
8	H	1	MET	3.0
3	C	206	GLU	3.0
10	J	7	LYS	2.9
10	J	59	SER	2.9
10	J	17	ASP	2.9
20	T	74	LYS	2.9
7	G	11	GLN	2.8
9	I	42	ARG	2.8
4	D	31	CYS	2.8
2	B	137	ARG	2.8
9	I	128	ARG	2.8
19	S	4	SER	2.7
3	C	207	VAL	2.7
9	I	66	ARG	2.7
20	T	8	ARG	2.7
9	I	67	GLY	2.6
7	G	4	ARG	2.6
8	H	99	GLU	2.6
10	J	70	ARG	2.6
16	P	29	ASP	2.6
12	L	19	ARG	2.6
10	J	96	ILE	2.6
20	T	12	ALA	2.6
19	S	5	LEU	2.5
4	D	6	GLY	2.5
17	Q	97	SER	2.5
11	K	111	ASP	2.5
4	D	23	GLY	2.5
17	Q	99	SER	2.5
7	G	2	ALA	2.5
21	U	24	ARG	2.5
4	D	26	CYS	2.5
10	J	46	ARG	2.5
14	N	12	ARG	2.4
20	T	23	ARG	2.4
3	C	192	THR	2.4
9	I	75	ASP	2.4
10	J	21	GLN	2.4
4	D	21	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	U	6	ARG	2.4
1	A	1251	A	2.4
3	C	201	TYR	2.3
10	J	75	ILE	2.3
4	D	118	ARG	2.3
14	N	4	LYS	2.3
1	A	82	U	2.3
4	D	72	GLU	2.3
1	A	1129	C	2.3
13	M	27	LYS	2.3
10	J	91	PRO	2.2
4	D	32	ALA	2.2
5	E	5	ASP	2.2
20	T	9	ASN	2.2
8	H	90	GLY	2.2
9	I	124	GLN	2.2
11	K	124	LYS	2.2
16	P	68	ASP	2.2
9	I	65	VAL	2.1
2	B	13	ALA	2.1
10	J	69	ASN	2.1
10	J	72	VAL	2.1
3	C	188	LEU	2.1
3	C	193	TYR	2.1
6	F	92	LYS	2.1
10	J	90	LEU	2.1
1	A	1286	A	2.1
8	H	136	GLU	2.1
10	J	38	ILE	2.1
21	U	8	THR	2.1
20	T	11	SER	2.1
12	L	88	GLY	2.1
11	K	125	PHE	2.1
20	T	75	ASN	2.0
12	L	29	GLY	2.0
2	B	7	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	PSU	b	39	20/21	0.86	0.09	172,224,242,250	0
1	PSU	A	1540	20/21	0.88	0.14	172,211,264,268	0
1	PSU	A	1541	20/21	0.90	0.14	153,186,208,212	0
22	A2M	a	1	20/24	0.90	0.14	165,193,216,224	0
1	PSU	A	516	20/21	0.90	0.09	98,122,152,152	0
23	70U	b	34	25/26	0.92	0.11	130,153,185,189	0
23	12A	b	37	34/35	0.93	0.13	134,187,202,205	0
1	UR3	A	1498	21/22	0.95	0.11	85,89,111,135	0
12	0TD	L	92	10/11	0.95	0.22	100,168,264,271	0
1	5MC	A	1400	21/22	0.96	0.10	76,100,129,136	0
1	2MG	A	1207	24/25	0.97	0.08	113,139,160,163	0
1	7MG	A	527	24/25	0.97	0.09	78,99,114,150	0
1	5MC	A	1407	21/22	0.97	0.06	89,98,111,133	0
1	M2G	A	966	25/26	0.97	0.09	83,122,147,168	0
1	MA6	A	1518	24/25	0.97	0.07	83,92,107,125	0
1	5MC	A	967	21/22	0.97	0.09	87,113,138,148	0
1	4OC	A	1402	22/23	0.98	0.07	91,98,124,134	0
1	MA6	A	1519	24/25	0.98	0.09	82,90,101,116	0
1	5MC	A	1404	21/22	0.98	0.07	83,87,106,112	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
24	MG	A	1815	1/1	0.13	0.28	141,141,141,141	0
24	MG	A	1805	1/1	0.14	0.48	141,141,141,141	0
25	K	A	1839	1/1	0.34	0.48	192,192,192,192	0
25	K	A	1845	1/1	0.36	0.17	195,195,195,195	0
24	MG	A	1670	1/1	0.43	0.29	141,141,141,141	0
24	MG	A	1803	1/1	0.45	0.52	129,129,129,129	0
25	K	A	1837	1/1	0.47	0.48	190,190,190,190	0
25	K	A	1834	1/1	0.51	0.23	190,190,190,190	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1793	1/1	0.54	0.40	115,115,115,115	0
24	MG	A	1709	1/1	0.54	0.62	134,134,134,134	0
24	MG	A	1785	1/1	0.55	0.43	129,129,129,129	0
24	MG	A	1671	1/1	0.55	0.38	121,121,121,121	0
24	MG	A	1627	1/1	0.55	0.85	158,158,158,158	0
25	K	A	1854	1/1	0.57	0.27	195,195,195,195	0
24	MG	A	1603	1/1	0.58	0.24	136,136,136,136	0
24	MG	A	1809	1/1	0.58	0.46	130,130,130,130	0
24	MG	A	1744	1/1	0.59	0.57	115,115,115,115	0
24	MG	A	1831	1/1	0.60	0.39	121,121,121,121	0
24	MG	A	1601	1/1	0.60	0.33	149,149,149,149	0
24	MG	A	1690	1/1	0.60	0.13	126,126,126,126	0
24	MG	A	1722	1/1	0.61	0.67	133,133,133,133	0
24	MG	A	1715	1/1	0.61	0.39	122,122,122,122	0
24	MG	A	1784	1/1	0.61	0.45	129,129,129,129	0
24	MG	A	1710	1/1	0.62	0.28	132,132,132,132	0
24	MG	A	1751	1/1	0.62	0.65	110,110,110,110	0
24	MG	A	1731	1/1	0.62	0.31	138,138,138,138	0
25	K	A	1850	1/1	0.64	0.23	174,174,174,174	0
24	MG	A	1711	1/1	0.64	0.40	124,124,124,124	0
24	MG	A	1808	1/1	0.66	0.50	123,123,123,123	0
24	MG	A	1712	1/1	0.66	0.28	131,131,131,131	0
25	K	A	1847	1/1	0.67	0.22	225,225,225,225	0
24	MG	A	1673	1/1	0.68	0.32	107,107,107,107	0
24	MG	A	1783	1/1	0.68	0.54	125,125,125,125	0
24	MG	A	1705	1/1	0.69	0.70	109,109,109,109	0
25	K	A	1842	1/1	0.69	0.18	169,169,169,169	0
24	MG	A	1716	1/1	0.69	0.36	134,134,134,134	0
24	MG	A	1758	1/1	0.70	0.43	139,139,139,139	0
25	K	A	1848	1/1	0.70	0.41	200,200,200,200	0
24	MG	A	1782	1/1	0.71	0.50	118,118,118,118	0
24	MG	A	1609	1/1	0.72	0.68	136,136,136,136	0
25	K	A	1853	1/1	0.72	0.13	180,180,180,180	0
25	K	A	1841	1/1	0.72	0.15	175,175,175,175	0
25	K	A	1846	1/1	0.73	0.45	192,192,192,192	0
24	MG	A	1774	1/1	0.73	0.29	108,108,108,108	0
25	K	A	1835	1/1	0.74	0.30	176,176,176,176	0
24	MG	A	1814	1/1	0.74	0.23	113,113,113,113	0
24	MG	A	1820	1/1	0.74	0.92	146,146,146,146	0
24	MG	A	1824	1/1	0.75	0.34	112,112,112,112	0
24	MG	A	1768	1/1	0.75	0.37	191,191,191,191	0
24	MG	A	1678	1/1	0.75	0.36	135,135,135,135	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	1828	1/1	0.76	0.18	129,129,129,129	0
24	MG	A	1779	1/1	0.76	0.15	175,175,175,175	0
24	MG	A	1634	1/1	0.76	0.40	106,106,106,106	0
24	MG	A	1791	1/1	0.76	0.79	148,148,148,148	0
24	MG	A	1702	1/1	0.76	0.30	118,118,118,118	0
24	MG	A	1826	1/1	0.77	0.16	142,142,142,142	0
24	MG	A	1827	1/1	0.77	0.19	108,108,108,108	0
25	K	A	1843	1/1	0.77	0.14	180,180,180,180	0
24	MG	A	1708	1/1	0.77	0.32	110,110,110,110	0
24	MG	A	1798	1/1	0.77	0.38	138,138,138,138	0
24	MG	A	1701	1/1	0.77	0.41	136,136,136,136	0
24	MG	A	1819	1/1	0.77	0.29	110,110,110,110	0
24	MG	A	1666	1/1	0.77	0.25	108,108,108,108	0
24	MG	A	1610	1/1	0.77	0.20	85,85,85,85	0
25	K	A	1840	1/1	0.77	0.34	175,175,175,175	0
24	MG	A	1664	1/1	0.78	0.19	115,115,115,115	0
24	MG	A	1625	1/1	0.78	0.18	132,132,132,132	0
25	K	A	1849	1/1	0.78	0.17	169,169,169,169	0
24	MG	A	1829	1/1	0.78	0.32	107,107,107,107	0
24	MG	A	1812	1/1	0.78	0.14	111,111,111,111	0
24	MG	D	302	1/1	0.78	0.17	119,119,119,119	0
24	MG	A	1786	1/1	0.79	0.38	101,101,101,101	0
24	MG	A	1787	1/1	0.79	0.16	90,90,90,90	0
24	MG	A	1631	1/1	0.79	0.28	111,111,111,111	0
24	MG	A	1620	1/1	0.79	0.18	114,114,114,114	0
25	K	A	1838	1/1	0.79	0.25	190,190,190,190	0
24	MG	A	1748	1/1	0.79	0.40	104,104,104,104	0
24	MG	A	1720	1/1	0.80	0.47	120,120,120,120	0
24	MG	A	1703	1/1	0.80	0.36	97,97,97,97	0
24	MG	A	1775	1/1	0.80	0.20	116,116,116,116	0
24	MG	L	201	1/1	0.80	0.15	123,123,123,123	0
24	MG	A	1723	1/1	0.80	0.35	98,98,98,98	0
24	MG	A	1718	1/1	0.80	0.31	103,103,103,103	0
24	MG	A	1818	1/1	0.80	0.19	121,121,121,121	0
24	MG	A	1734	1/1	0.81	0.67	112,112,112,112	0
24	MG	A	1763	1/1	0.81	0.49	113,113,113,113	0
24	MG	A	1822	1/1	0.81	0.37	98,98,98,98	0
24	MG	A	1754	1/1	0.81	0.15	118,118,118,118	0
24	MG	A	1800	1/1	0.81	0.31	114,114,114,114	0
24	MG	H	201	1/1	0.81	0.23	102,102,102,102	0
24	MG	A	1736	1/1	0.82	0.40	98,98,98,98	0
24	MG	A	1761	1/1	0.82	0.29	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1740	1/1	0.82	0.22	99,99,99,99	0
24	MG	A	1764	1/1	0.82	0.25	96,96,96,96	0
24	MG	A	1692	1/1	0.82	0.41	115,115,115,115	0
24	MG	P	102	1/1	0.83	0.09	101,101,101,101	0
24	MG	A	1769	1/1	0.83	0.11	138,138,138,138	0
24	MG	A	1770	1/1	0.83	0.22	112,112,112,112	0
24	MG	A	1665	1/1	0.83	0.26	100,100,100,100	0
24	MG	A	1647	1/1	0.83	0.16	89,89,89,89	0
24	MG	A	1629	1/1	0.83	0.52	91,91,91,91	0
24	MG	A	1681	1/1	0.83	0.36	94,94,94,94	0
24	MG	H	202	1/1	0.83	0.07	126,126,126,126	0
24	MG	A	1686	1/1	0.83	0.38	111,111,111,111	0
25	K	A	1855	1/1	0.83	0.24	159,159,159,159	0
24	MG	A	1616	1/1	0.84	0.51	109,109,109,109	0
24	MG	T	201	1/1	0.84	0.40	86,86,86,86	0
24	MG	A	1707	1/1	0.84	0.34	82,82,82,82	0
24	MG	A	1811	1/1	0.84	0.24	124,124,124,124	0
25	K	A	1836	1/1	0.84	0.29	145,145,145,145	0
24	MG	A	1675	1/1	0.84	0.16	149,149,149,149	0
24	MG	A	1794	1/1	0.84	0.29	97,97,97,97	0
24	MG	A	1743	1/1	0.85	0.17	111,111,111,111	0
24	MG	A	1663	1/1	0.85	0.38	113,113,113,113	0
24	MG	A	1688	1/1	0.85	0.11	149,149,149,149	0
24	MG	A	1801	1/1	0.85	0.38	96,96,96,96	0
24	MG	A	1802	1/1	0.85	0.19	88,88,88,88	0
24	MG	A	1749	1/1	0.85	0.16	120,120,120,120	0
24	MG	A	1737	1/1	0.85	0.17	79,79,79,79	0
24	MG	A	1617	1/1	0.85	0.21	92,92,92,92	0
24	MG	A	1726	1/1	0.86	0.32	117,117,117,117	0
24	MG	A	1766	1/1	0.86	0.07	157,157,157,157	0
24	MG	A	1767	1/1	0.86	0.11	139,139,139,139	0
24	MG	A	1721	1/1	0.86	0.23	113,113,113,113	0
24	MG	A	1796	1/1	0.86	0.35	110,110,110,110	0
24	MG	A	1604	1/1	0.86	0.16	126,126,126,126	0
25	K	A	1851	1/1	0.86	0.18	184,184,184,184	0
24	MG	A	1677	1/1	0.86	0.34	104,104,104,104	0
24	MG	A	1813	1/1	0.86	0.11	106,106,106,106	0
24	MG	A	1725	1/1	0.86	0.22	102,102,102,102	0
24	MG	A	1613	1/1	0.87	0.16	99,99,99,99	0
24	MG	A	1792	1/1	0.87	0.23	144,144,144,144	0
24	MG	A	1816	1/1	0.87	0.42	108,108,108,108	0
24	MG	A	1727	1/1	0.87	0.18	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1760	1/1	0.87	0.19	106,106,106,106	0
24	MG	A	1611	1/1	0.87	0.09	119,119,119,119	0
24	MG	A	1687	1/1	0.87	0.60	118,118,118,118	0
24	MG	A	1788	1/1	0.87	0.36	115,115,115,115	0
24	MG	A	1825	1/1	0.87	0.33	104,104,104,104	0
24	MG	A	1789	1/1	0.87	0.25	88,88,88,88	0
24	MG	A	1646	1/1	0.88	0.23	124,124,124,124	0
24	MG	A	1638	1/1	0.88	0.28	103,103,103,103	0
24	MG	A	1668	1/1	0.88	0.38	111,111,111,111	0
24	MG	A	1821	1/1	0.88	0.16	101,101,101,101	0
24	MG	A	1640	1/1	0.88	0.14	95,95,95,95	0
24	MG	A	1781	1/1	0.88	0.33	108,108,108,108	0
24	MG	A	1714	1/1	0.88	0.37	126,126,126,126	0
24	MG	A	1645	1/1	0.88	0.26	116,116,116,116	0
24	MG	Q	201	1/1	0.88	0.15	123,123,123,123	0
24	MG	A	1695	1/1	0.88	0.22	148,148,148,148	0
24	MG	A	1780	1/1	0.89	0.07	172,172,172,172	0
24	MG	A	1653	1/1	0.89	0.32	122,122,122,122	0
24	MG	A	1797	1/1	0.89	0.30	108,108,108,108	0
24	MG	A	1706	1/1	0.89	0.16	122,122,122,122	0
24	MG	A	1697	1/1	0.89	0.23	114,114,114,114	0
24	MG	A	1698	1/1	0.89	0.34	89,89,89,89	0
24	MG	A	1700	1/1	0.89	0.12	159,159,159,159	0
24	MG	A	1753	1/1	0.89	0.16	103,103,103,103	0
24	MG	A	1667	1/1	0.89	0.15	184,184,184,184	0
24	MG	A	1772	1/1	0.89	0.22	107,107,107,107	0
24	MG	A	1606	1/1	0.89	0.48	102,102,102,102	0
25	K	A	1852	1/1	0.89	0.10	149,149,149,149	0
24	MG	A	1738	1/1	0.89	0.28	108,108,108,108	0
24	MG	A	1776	1/1	0.89	0.40	88,88,88,88	0
24	MG	A	1694	1/1	0.89	0.23	106,106,106,106	0
24	MG	A	1661	1/1	0.90	0.10	110,110,110,110	0
24	MG	A	1773	1/1	0.90	0.55	138,138,138,138	0
24	MG	A	1696	1/1	0.90	0.12	103,103,103,103	0
24	MG	A	1810	1/1	0.90	0.13	91,91,91,91	0
24	MG	A	1739	1/1	0.90	0.31	93,93,93,93	0
24	MG	A	1730	1/1	0.90	0.10	111,111,111,111	0
24	MG	A	1624	1/1	0.90	0.41	101,101,101,101	0
24	MG	A	1615	1/1	0.90	0.21	113,113,113,113	0
24	MG	A	1614	1/1	0.90	0.14	86,86,86,86	0
24	MG	A	1771	1/1	0.90	0.44	98,98,98,98	0
24	MG	A	1691	1/1	0.91	0.19	123,123,123,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1635	1/1	0.91	0.09	138,138,138,138	0
24	MG	A	1857	1/1	0.91	0.09	129,129,129,129	0
24	MG	A	1656	1/1	0.91	0.18	130,130,130,130	0
24	MG	G	201	1/1	0.91	0.18	109,109,109,109	0
24	MG	A	1741	1/1	0.91	0.26	77,77,77,77	0
24	MG	A	1742	1/1	0.91	0.27	109,109,109,109	0
24	MG	A	1755	1/1	0.91	0.34	92,92,92,92	0
24	MG	A	1633	1/1	0.91	0.22	132,132,132,132	0
24	MG	A	1630	1/1	0.91	0.09	127,127,127,127	0
24	MG	Q	202	1/1	0.91	0.50	121,121,121,121	0
24	MG	A	1626	1/1	0.92	0.27	88,88,88,88	0
24	MG	S	101	1/1	0.92	0.20	87,87,87,87	0
25	K	A	1844	1/1	0.92	0.14	154,154,154,154	0
24	MG	S	102	1/1	0.92	0.19	95,95,95,95	0
24	MG	S	103	1/1	0.92	0.11	109,109,109,109	0
24	MG	A	1619	1/1	0.92	0.16	102,102,102,102	0
24	MG	A	1682	1/1	0.92	0.29	210,210,210,210	0
24	MG	A	1732	1/1	0.92	0.41	92,92,92,92	0
24	MG	A	1823	1/1	0.92	0.06	124,124,124,124	0
24	MG	A	1644	1/1	0.92	0.22	108,108,108,108	0
24	MG	A	1662	1/1	0.92	0.13	115,115,115,115	0
24	MG	A	1757	1/1	0.92	0.12	90,90,90,90	0
24	MG	A	1817	1/1	0.92	0.17	89,89,89,89	0
24	MG	A	1650	1/1	0.92	0.09	50,50,50,50	0
24	MG	A	1654	1/1	0.93	0.12	106,106,106,106	0
24	MG	A	1795	1/1	0.93	0.55	123,123,123,123	0
24	MG	A	1636	1/1	0.93	0.09	109,109,109,109	0
24	MG	A	1659	1/1	0.93	0.33	89,89,89,89	0
24	MG	A	1745	1/1	0.93	0.44	93,93,93,93	0
24	MG	A	1799	1/1	0.93	0.48	111,111,111,111	0
24	MG	A	1642	1/1	0.93	0.29	113,113,113,113	0
24	MG	A	1830	1/1	0.93	0.14	94,94,94,94	0
24	MG	A	1637	1/1	0.93	0.20	99,99,99,99	0
24	MG	A	1856	1/1	0.93	0.07	125,125,125,125	0
24	MG	A	1679	1/1	0.93	0.29	123,123,123,123	0
24	MG	A	1777	1/1	0.93	0.17	87,87,87,87	0
24	MG	A	1717	1/1	0.93	0.19	105,105,105,105	0
24	MG	A	1729	1/1	0.93	0.10	85,85,85,85	0
24	MG	A	1623	1/1	0.93	0.48	79,79,79,79	0
24	MG	A	1728	1/1	0.94	0.20	101,101,101,101	0
24	MG	A	1674	1/1	0.94	0.07	135,135,135,135	0
24	MG	A	1622	1/1	0.94	0.20	122,122,122,122	0

Continued on next page...

Continued from previous page...

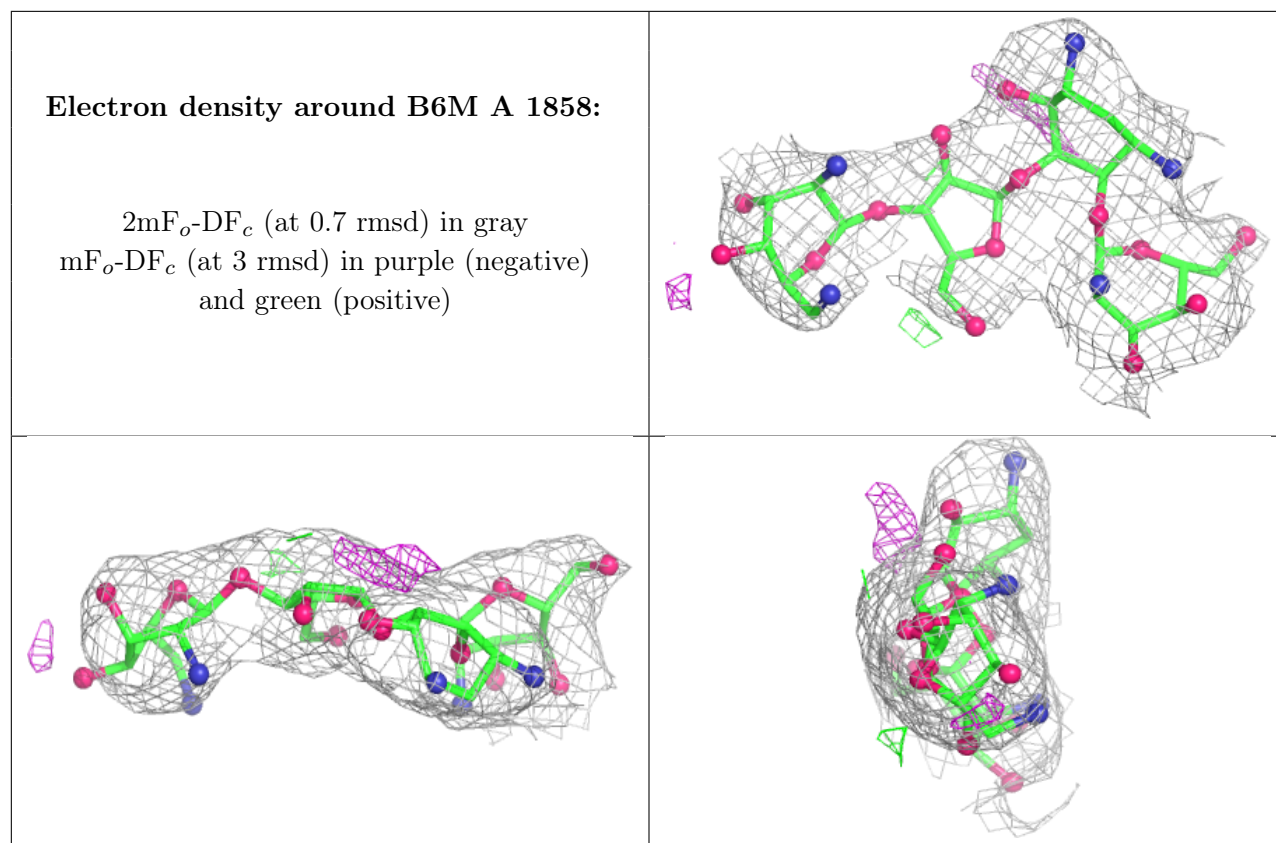
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1756	1/1	0.94	0.14	107,107,107,107	0
24	MG	A	1693	1/1	0.94	0.08	142,142,142,142	0
24	MG	A	1683	1/1	0.94	0.58	99,99,99,99	0
24	MG	A	1759	1/1	0.94	0.09	87,87,87,87	0
24	MG	P	101	1/1	0.94	0.42	90,90,90,90	0
24	MG	A	1807	1/1	0.94	0.18	91,91,91,91	0
24	MG	P	103	1/1	0.94	0.15	115,115,115,115	0
24	MG	A	1790	1/1	0.94	0.26	154,154,154,154	0
24	MG	A	1608	1/1	0.94	0.15	86,86,86,86	0
24	MG	A	1735	1/1	0.94	0.09	103,103,103,103	0
24	MG	A	1762	1/1	0.94	0.33	81,81,81,81	0
24	MG	A	1746	1/1	0.94	0.14	179,179,179,179	0
24	MG	A	1672	1/1	0.94	0.41	93,93,93,93	0
24	MG	A	1651	1/1	0.94	0.18	118,118,118,118	0
24	MG	A	1680	1/1	0.94	0.09	121,121,121,121	0
24	MG	A	1833	1/1	0.94	0.08	111,111,111,111	0
26	B6M	A	1858	42/42	0.94	0.10	70,99,121,163	0
24	MG	A	1859	1/1	0.95	0.10	101,101,101,101	0
24	MG	A	1699	1/1	0.95	0.07	143,143,143,143	0
24	MG	E	201	1/1	0.95	0.09	121,121,121,121	0
24	MG	A	1612	1/1	0.95	0.07	118,118,118,118	0
24	MG	A	1657	1/1	0.95	0.18	91,91,91,91	0
24	MG	A	1652	1/1	0.95	0.16	125,125,125,125	0
24	MG	A	1806	1/1	0.95	0.41	90,90,90,90	0
24	MG	A	1719	1/1	0.95	0.18	94,94,94,94	0
24	MG	A	1649	1/1	0.95	0.07	114,114,114,114	0
24	MG	A	1605	1/1	0.95	0.09	106,106,106,106	0
24	MG	A	1778	1/1	0.95	0.18	92,92,92,92	0
24	MG	A	1655	1/1	0.95	0.06	116,116,116,116	0
24	MG	A	1750	1/1	0.95	0.38	76,76,76,76	0
27	ZN	D	301	1/1	0.95	0.30	201,201,201,201	0
24	MG	A	1639	1/1	0.96	0.13	81,81,81,81	0
24	MG	A	1804	1/1	0.96	0.18	86,86,86,86	0
24	MG	A	1713	1/1	0.96	0.07	76,76,76,76	0
24	MG	A	1733	1/1	0.96	0.15	89,89,89,89	0
24	MG	A	1648	1/1	0.96	0.14	92,92,92,92	0
24	MG	A	1669	1/1	0.96	0.09	121,121,121,121	0
24	MG	A	1689	1/1	0.96	0.13	111,111,111,111	0
24	MG	A	1752	1/1	0.96	0.19	180,180,180,180	0
24	MG	A	1660	1/1	0.96	0.51	94,94,94,94	0
24	MG	A	1832	1/1	0.97	0.08	110,110,110,110	0
24	MG	A	1747	1/1	0.97	0.10	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1621	1/1	0.97	0.39	64,64,64,64	0
24	MG	A	1724	1/1	0.97	0.08	81,81,81,81	0
24	MG	A	1643	1/1	0.97	0.06	142,142,142,142	0
24	MG	A	1602	1/1	0.97	0.10	101,101,101,101	0
24	MG	A	1685	1/1	0.97	0.17	77,77,77,77	0
24	MG	F	201	1/1	0.97	0.08	100,100,100,100	0
24	MG	A	1676	1/1	0.97	0.17	97,97,97,97	0
24	MG	A	1765	1/1	0.98	0.14	131,131,131,131	0
24	MG	A	1684	1/1	0.98	0.22	126,126,126,126	0
24	MG	A	1607	1/1	0.98	0.05	123,123,123,123	0
24	MG	A	1618	1/1	0.98	0.14	87,87,87,87	0
24	MG	A	1641	1/1	0.98	0.04	69,69,69,69	0
24	MG	A	1632	1/1	0.98	0.11	82,82,82,82	0
24	MG	A	1704	1/1	0.98	0.09	88,88,88,88	0
24	MG	A	1628	1/1	0.99	0.05	109,109,109,109	0
24	MG	A	1658	1/1	0.99	0.08	82,82,82,82	0
27	ZN	N	101	1/1	0.99	0.06	142,142,142,142	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.