



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 6CAO / pdb_00006cao
Title : Structure of the ribosomal decoding complex at ambient temperature
Authors : DeMirici, H.
Deposited on : 2018-01-31
Resolution : 3.45 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

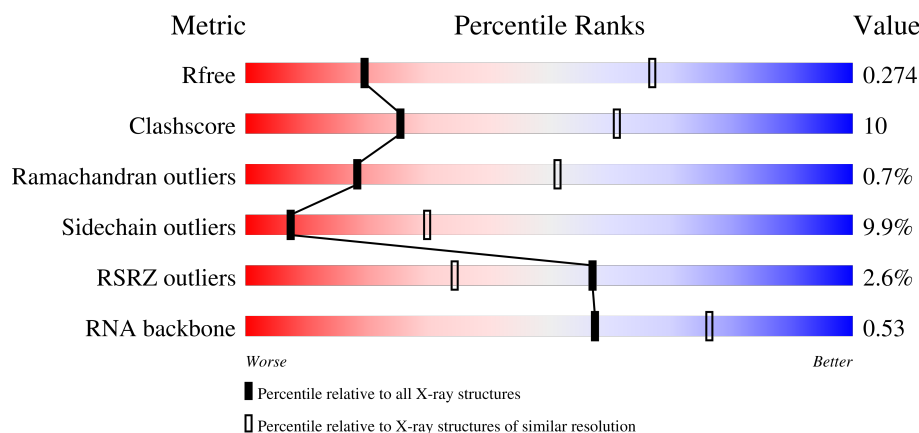
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



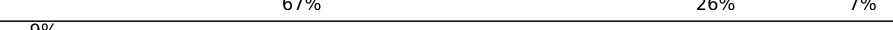
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

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	59% 32% 8% .
2	B	236	4% 65% 32% ..
3	C	207	68% 29% .
4	D	208	7% 67% 30% .

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	117	
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	W	15	
23	Y	6	

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
26	MG	A	1684	-	-	-	X
26	MG	A	1731	-	-	-	X
26	MG	A	1738	-	-	-	X
26	MG	A	1826	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 52855 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			

- Molecule 2 is a protein called 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S 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 30S 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 30S ribosomal protein S14 type Z.

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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein Thx.

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

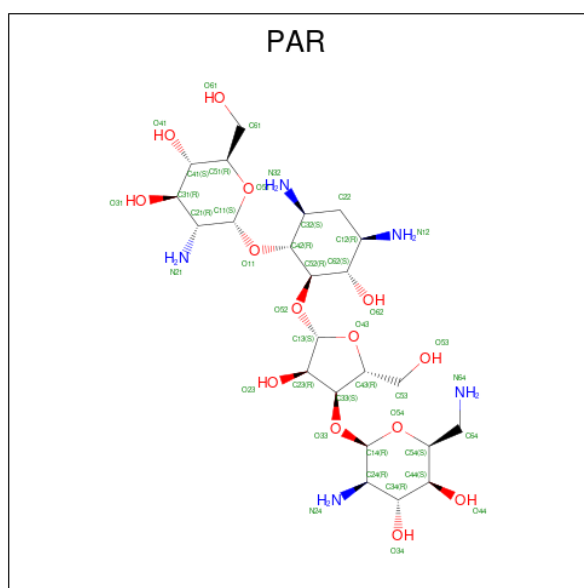
- Molecule 22 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 23 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	35	Total	K	0	0
			35	35		
25	E	2	Total	K	0	0
			2	2		

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	279	Total	Mg	0	0
			279	279		
26	C	1	Total	Mg	0	0
			1	1		
26	D	2	Total	Mg	0	0
			2	2		
26	E	2	Total	Mg	0	0
			2	2		
26	F	1	Total	Mg	0	0
			1	1		
26	G	1	Total	Mg	0	0
			1	1		
26	H	2	Total	Mg	0	0
			2	2		
26	L	2	Total	Mg	0	0
			2	2		
26	M	1	Total	Mg	0	0
			1	1		
26	P	3	Total	Mg	0	0
			3	3		
26	Q	4	Total	Mg	0	0
			4	4		
26	S	3	Total	Mg	0	0
			3	3		
26	T	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	Y	1	Total	Mg	0	0
			1	1		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

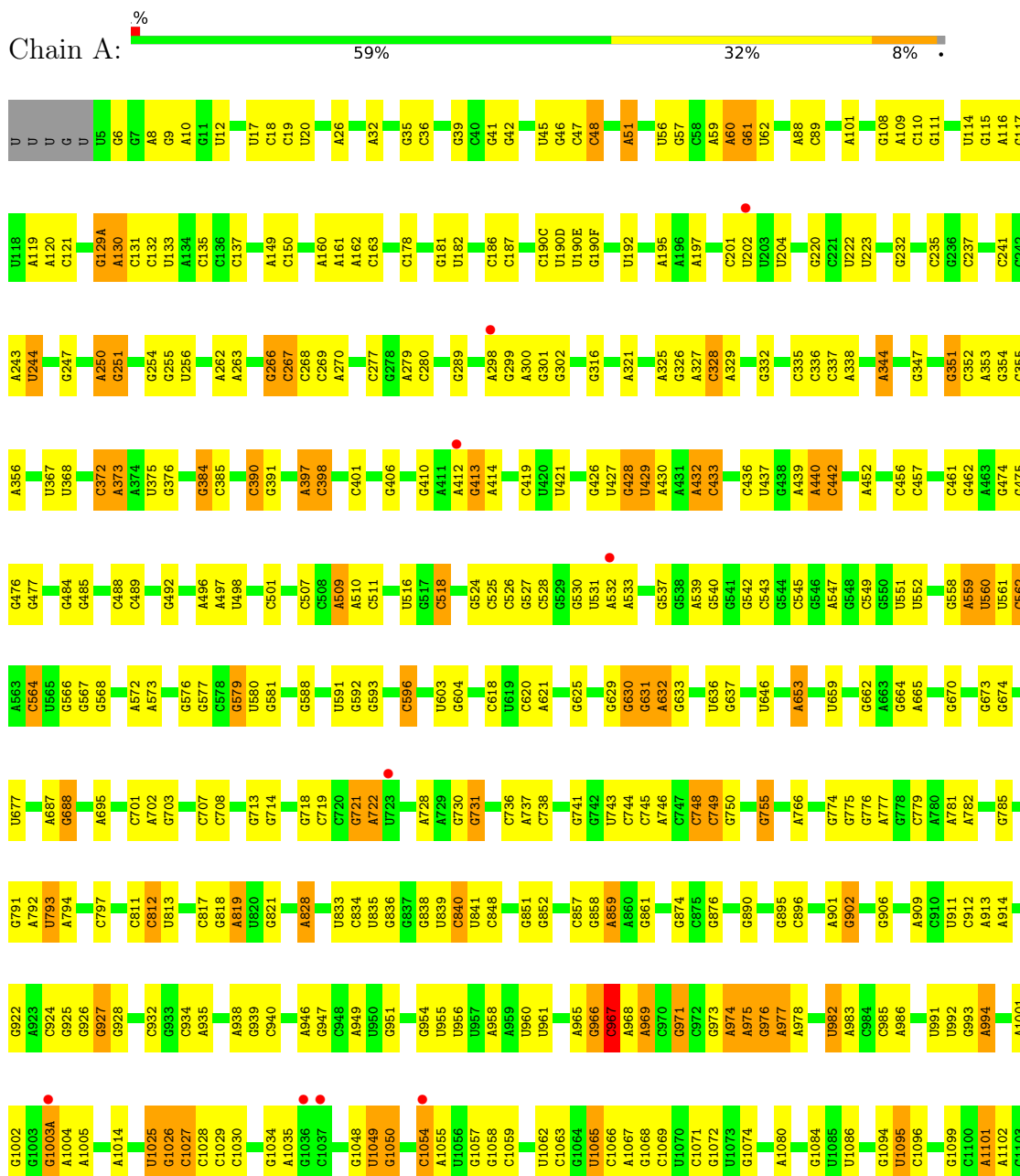
- Molecule 28 is water.

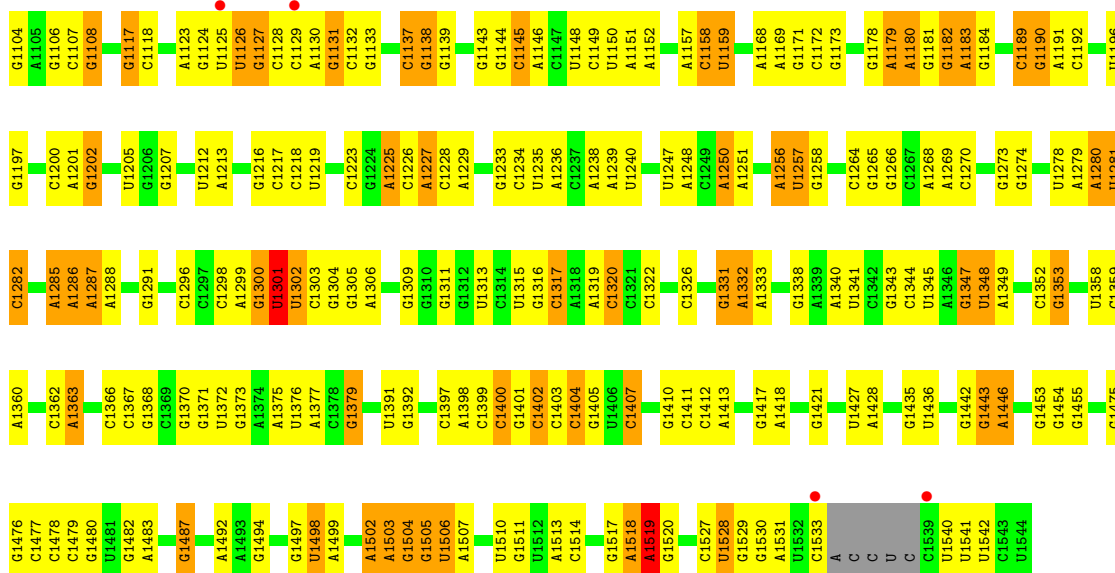
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	199	Total	O	0	0
			199	199		
28	D	2	Total	O	0	0
			2	2		
28	E	5	Total	O	0	0
			5	5		
28	I	1	Total	O	0	0
			1	1		
28	K	1	Total	O	0	0
			1	1		
28	L	2	Total	O	0	0
			2	2		
28	N	1	Total	O	0	0
			1	1		
28	O	2	Total	O	0	0
			2	2		
28	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

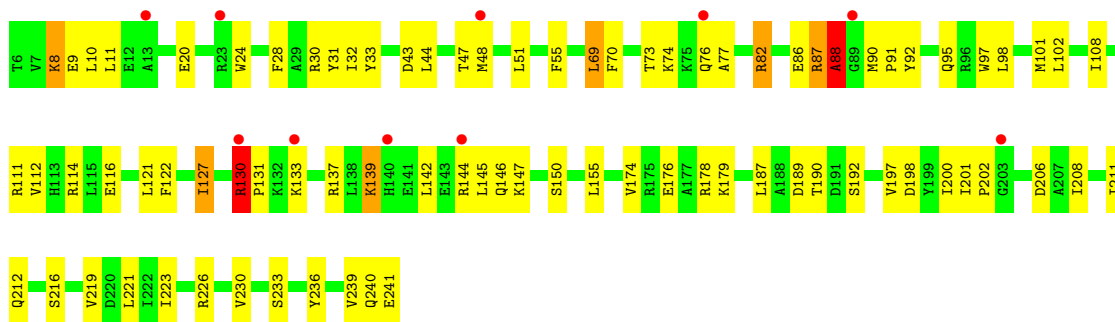
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S Ribosomal RNA rRNA

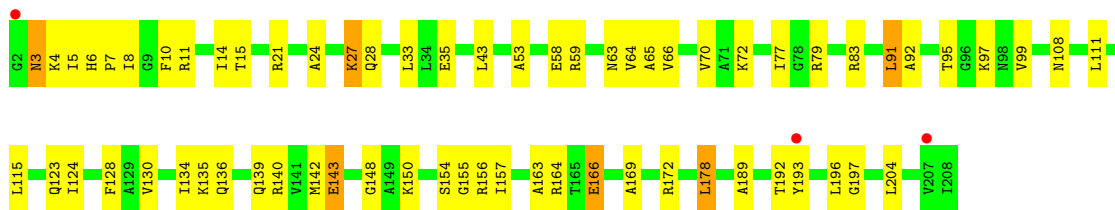




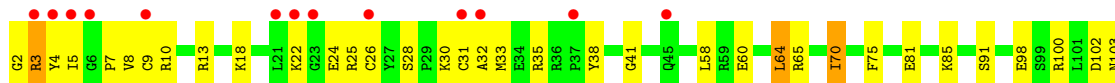
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

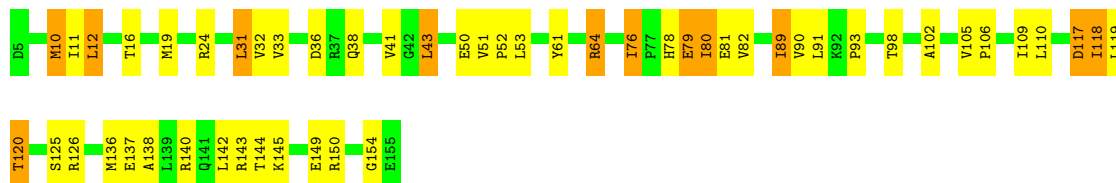


• Molecule 4: 30S ribosomal protein S4





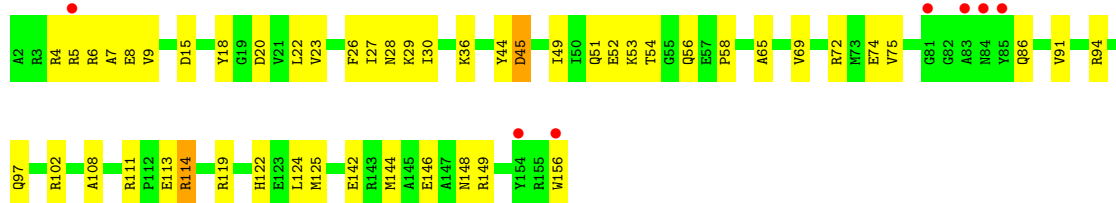
- Molecule 5: 30S ribosomal protein S5



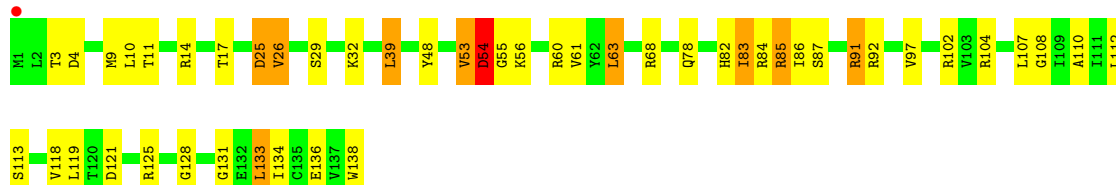
- Molecule 6: 30S ribosomal protein S6



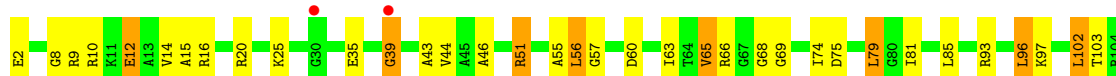
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

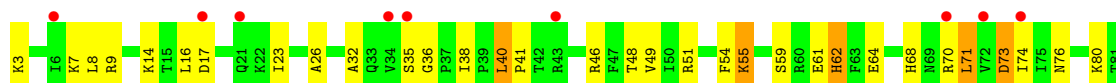


- Molecule 9: 30S ribosomal protein S9

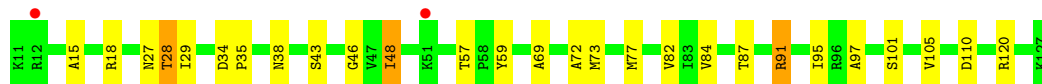
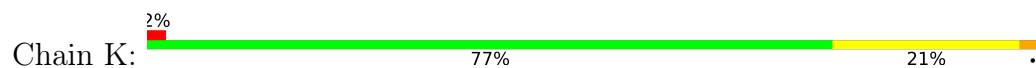




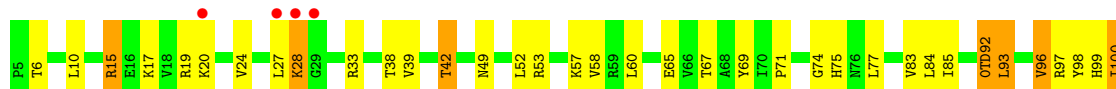
- Molecule 10: 30S ribosomal protein S10



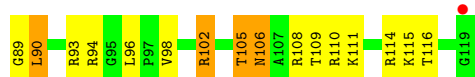
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

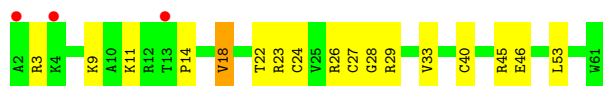


- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z





- Molecule 15: 30S ribosomal protein S15

Chain O: 69% 26% 5%



- Molecule 16: 30S ribosomal protein S16

Chain P: 65% 33% 2%



- Molecule 17: 30S ribosomal protein S17

Chain Q: 2% 67% 31%



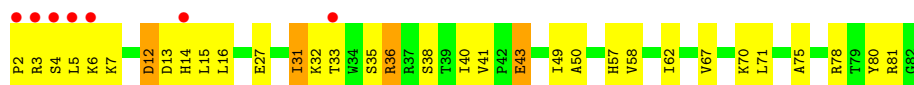
- Molecule 18: 30S ribosomal protein S18

Chain R: 67% 26% 7%



- Molecule 19: 30S ribosomal protein S19

Chain S: 9% 59% 36%



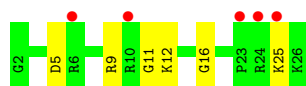
- Molecule 20: 30S ribosomal protein S20

Chain T: 3% 63% 27% 6%



- Molecule 21: 30S ribosomal protein Thx

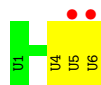
Chain U: 20% 76% 24%



- Molecule 22: RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3')



- Molecule 23: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.30Å 402.30Å 176.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 3.45 39.22 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.22-3.45) 99.8 (39.22-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.272 0.220 , 0.274	Depositor DCC
R_{free} test set	2000 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 135.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	52855	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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: MG, 0TD, 2MG, MA6, PSU, 5MC, ZN, 4OC, K, PAR, M2G, UR3, G7M

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	0.24	1/36037 (0.0%)	0.43	3/56239 (0.0%)
2	B	0.21	0/1909	0.48	0/2579
3	C	0.22	0/1637	0.44	0/2207
4	D	0.22	0/1733	0.47	0/2318
5	E	0.27	0/1163	0.48	0/1566
6	F	0.19	0/856	0.43	0/1154
7	G	0.22	0/1276	0.44	0/1709
8	H	0.28	0/1136	0.51	0/1527
9	I	0.22	0/1029	0.53	1/1379 (0.1%)
10	J	0.25	0/806	0.66	0/1084
11	K	0.25	0/888	0.45	0/1198
12	L	0.24	0/978	0.53	0/1308
13	M	0.23	0/947	0.49	0/1270
14	N	0.23	0/501	0.49	0/664
15	O	0.22	0/745	0.44	0/992
16	P	0.23	0/717	0.47	0/965
17	Q	0.25	0/836	0.49	0/1117
18	R	0.23	0/604	0.44	0/801
19	S	0.20	0/662	0.48	0/892
20	T	0.24	0/765	0.54	0/1007
21	U	0.17	0/213	0.43	0/279
22	W	0.19	0/357	0.36	0/555
23	Y	0.26	0/128	0.50	0/196
All	All	0.24	1/55923 (0.0%)	0.45	4/83006 (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	4
8	H	0	1
10	J	0	1
12	L	0	2
13	M	0	1
16	P	0	1
20	T	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.15	1.61	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-6.55	97.66	113.18
1	A	1301	U	C2'-C3'-O3'	5.38	117.58	109.50
1	A	1301	U	P-O3'-C3'	5.30	128.15	120.20
1	A	1498	UR3	P-O3'-C3'	5.10	125.82	119.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	ARG	Peptide
2	B	8	LYS	Peptide
2	B	87	ARG	Peptide
2	B	88	ALA	Peptide
8	H	53	VAL	Peptide
10	J	54	PHE	Peptide
12	L	104	VAL	Peptide
12	L	126	LYS	Peptide
13	M	105	THR	Peptide
16	P	19	ILE	Peptide
20	T	72	LEU	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	16433	399	0
2	B	1874	0	1887	46	0
3	C	1613	0	1677	48	0
4	D	1703	0	1763	52	0
5	E	1147	0	1207	37	0
6	F	843	0	857	17	0
7	G	1257	0	1296	34	0
8	H	1116	0	1177	31	0
9	I	1010	0	1037	34	0
10	J	793	0	835	27	0
11	K	873	0	894	17	0
12	L	973	0	1058	31	0
13	M	937	0	995	41	0
14	N	492	0	529	13	0
15	O	734	0	771	13	0
16	P	701	0	720	17	0
17	Q	823	0	891	20	0
18	R	598	0	670	21	0
19	S	648	0	673	24	0
20	T	763	0	861	32	0
21	U	209	0	221	2	0
22	W	319	0	164	6	0
23	Y	117	0	61	1	0
24	A	252	0	269	14	0
25	A	35	0	0	0	0
25	E	2	0	0	0	0
26	A	279	0	0	0	0
26	C	1	0	0	0	0
26	D	2	0	0	0	0
26	E	2	0	0	0	0
26	F	1	0	0	0	0
26	G	1	0	0	0	0
26	H	2	0	0	0	0
26	L	2	0	0	0	0
26	M	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	4	0	0	0	0
26	S	3	0	0	0	0
26	T	1	0	0	0	0
26	Y	1	0	0	0	0
27	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	N	1	0	0	0	0
28	A	199	0	0	4	0
28	D	2	0	0	0	0
28	E	5	0	0	0	0
28	I	1	0	0	0	0
28	K	1	0	0	0	0
28	L	2	0	0	0	0
28	N	1	0	0	0	0
28	O	2	0	0	0	0
28	T	1	0	0	0	0
All	All	52855	0	36946	846	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 10.

All (846) 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:664:G:H22	1:A:741:G:H1	1.15	0.93
24:A:1606:PAR:HN21	24:A:1606:PAR:H322	1.17	0.93
19:S:33:THR:HG22	19:S:35:SER:H	1.33	0.93
1:A:298:A:N6	28:A:2001:HOH:O	2.03	0.90
1:A:954:G:H21	1:A:1227:A:H62	1.25	0.84
1:A:659:U:OP2	15:O:8:LYS:NZ	2.13	0.82
20:T:10:LEU:HG	20:T:12:ALA:H	1.46	0.81
1:A:48:C:OP1	24:A:1603:PAR:N12	2.13	0.81
20:T:74:LYS:O	20:T:76:ALA:N	2.14	0.80
1:A:542:G:OP1	4:D:10:ARG:NH2	2.15	0.79
1:A:662:G:N7	24:A:1604:PAR:N12	2.28	0.79
10:J:51:ARG:HD2	10:J:59:SER:HB2	1.63	0.78
1:A:1502:A:H2	1:A:1505:G:H1	1.31	0.78
2:B:223:ILE:HD13	2:B:230:VAL:H	1.45	0.78
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.67	0.77
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.17	0.77
12:L:75:HIS:HA	12:L:102:ARG:HH22	1.49	0.77
1:A:559:A:OP1	5:E:126:ARG:NH2	2.18	0.77
1:A:501:C:OP1	12:L:117:ARG:NH2	2.17	0.76
1:A:132:C:O3'	20:T:74:LYS:NZ	2.18	0.75
18:R:32:ARG:HA	18:R:69:THR:HG21	1.68	0.75
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.68	0.75
1:A:235:C:N4	28:A:2002:HOH:O	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.20	0.75
19:S:5:LEU:HD21	19:S:70:LYS:HZ1	1.52	0.74
1:A:976:G:OP2	1:A:1358:U:O2'	2.06	0.73
8:H:85:ARG:NE	8:H:87:SER:O	2.21	0.73
11:K:15:ALA:HA	11:K:77:MET:HA	1.70	0.73
17:Q:9:VAL:HG21	17:Q:84:LEU:HD13	1.71	0.73
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.71	0.73
19:S:50:ALA:HA	19:S:58:VAL:O	1.88	0.72
2:B:8:LYS:O	2:B:10:LEU:N	2.23	0.71
3:C:156:ARG:H	3:C:163:ALA:HA	1.55	0.71
12:L:85:ILE:HG22	12:L:100:ILE:HG13	1.71	0.71
1:A:946:A:H2'	1:A:947:G:C8	2.26	0.70
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.54	0.70
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.72	0.70
3:C:27:LYS:HD3	3:C:27:LYS:H	1.55	0.70
1:A:1281:U:H5''	1:A:1282:C:H5	1.56	0.69
1:A:1124:G:N7	1:A:1145:C:O2'	2.21	0.69
1:A:625:G:O6	24:A:1605:PAR:N24	2.25	0.69
1:A:410:G:OP1	4:D:30:LYS:NZ	2.25	0.69
1:A:266:G:H5'	1:A:268:C:H41	1.57	0.68
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.76	0.68
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.73	0.68
1:A:677:U:H3	1:A:713:G:H22	1.41	0.68
1:A:1309:G:O2'	13:M:77:ASN:ND2	2.26	0.68
12:L:49:ASN:ND2	12:L:92:0TD:SB	2.66	0.68
13:M:86:CYS:SG	13:M:87:TYR:N	2.66	0.68
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.76	0.68
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.76	0.67
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.22	0.67
1:A:975:A:H4'	1:A:976:G:H5''	1.77	0.67
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.78	0.66
1:A:45:U:H2'	1:A:46:G:C8	2.30	0.66
14:N:9:LYS:HE2	14:N:23:ARG:HB2	1.75	0.66
20:T:75:ASN:OD1	20:T:75:ASN:N	2.27	0.66
1:A:670:G:OP2	24:A:1606:PAR:N24	2.29	0.66
1:A:1132:C:H2'	1:A:1133:G:H8	1.60	0.66
1:A:985:C:H2'	1:A:986:A:C8	2.31	0.66
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.29	0.66
4:D:18:LYS:NZ	4:D:31:CYS:SG	2.69	0.66
7:G:15:ASP:HB3	7:G:20:ASP:H	1.60	0.66
1:A:1266:G:N2	1:A:1269:A:OP2	2.22	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.77	0.65
1:A:1151:A:H5'	10:J:41:PRO:HA	1.79	0.65
7:G:72:ARG:NH2	7:G:142:GLU:OE2	2.30	0.65
1:A:983:A:O2'	1:A:1050:G:OP2	2.15	0.65
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.79	0.65
20:T:89:ARG:NH2	20:T:105:SER:O	2.30	0.65
1:A:1319:A:H5'	19:S:5:LEU:HD22	1.78	0.64
22:W:36:A:H2'	22:W:37:A:H8	1.62	0.64
1:A:277:C:H5''	17:Q:68:ARG:NH2	2.12	0.64
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.61	0.64
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.30	0.63
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.63
11:K:27:ASN:OD1	11:K:28:THR:N	2.31	0.63
1:A:1313:U:O4	19:S:4:SER:OG	2.13	0.63
1:A:1137:C:H4'	1:A:1138:G:C2	2.32	0.63
1:A:250:A:H4'	1:A:251:G:O5'	1.99	0.63
1:A:254:G:OP1	17:Q:66:SER:OG	2.17	0.63
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.80	0.63
1:A:1264:C:H2'	1:A:1265:G:H8	1.63	0.63
10:J:38:ILE:HD12	10:J:71:LEU:HD12	1.81	0.63
1:A:356:A:N3	1:A:368:U:O2'	2.30	0.62
1:A:811:C:O2'	1:A:901:A:N1	2.32	0.62
22:W:36:A:H2'	22:W:37:A:C8	2.35	0.62
1:A:1412:C:H2'	1:A:1413:A:C8	2.35	0.62
6:F:22:GLU:OE1	6:F:84:ASN:ND2	2.28	0.62
6:F:74:ASP:O	6:F:77:ARG:HB3	1.99	0.62
1:A:130:A:OP2	1:A:190(E):U:O2'	2.15	0.62
4:D:187:ARG:NH2	4:D:193:ASP:OD2	2.33	0.62
1:A:135:C:O2	16:P:1:MET:N	2.33	0.61
13:M:22:ILE:HB	13:M:25:ILE:HB	1.82	0.61
13:M:23:TYR:HB3	13:M:67:GLU:HG2	1.82	0.61
1:A:1062:U:H2'	1:A:1063:C:C6	2.35	0.61
1:A:1504:G:OP1	1:A:1507:A:H4'	1.99	0.61
3:C:59:ARG:HG2	3:C:64:VAL:HG22	1.82	0.61
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.82	0.61
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.83	0.61
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.82	0.61
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.34	0.61
5:E:98:THR:HB	5:E:117:ASP:HB3	1.82	0.61
20:T:53:LEU:HD13	20:T:102:GLY:H	1.65	0.61
1:A:1256:A:N6	1:A:1278:U:O4'	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:ASN:OD1	3:C:3:ASN:N	2.32	0.61
1:A:1301:U:O2'	1:A:1302:U:O5'	2.14	0.61
2:B:142:LEU:HD23	2:B:146:GLN:HG3	1.82	0.60
11:K:18:ARG:NH1	11:K:35:PRO:O	2.34	0.60
1:A:501:C:H1'	1:A:549:C:H1'	1.83	0.60
11:K:69:ALA:O	11:K:73:MET:HG2	2.00	0.60
1:A:241:C:H4'	12:L:19:ARG:HH22	1.67	0.60
7:G:23:VAL:O	7:G:27:ILE:HG12	2.02	0.60
11:K:87:THR:HA	11:K:91:ARG:HH12	1.66	0.60
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.84	0.60
1:A:35:G:H2'	1:A:36:C:C6	2.36	0.60
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.82	0.60
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.34	0.60
1:A:791:G:O6	1:A:792:A:N6	2.34	0.60
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.84	0.59
1:A:1190:G:OP1	3:C:5:ILE:HG13	2.03	0.59
16:P:38:TYR:OH	16:P:47:ASP:OD2	2.19	0.59
11:K:57:THR:HG22	11:K:59:TYR:H	1.67	0.59
1:A:1080:A:H5''	5:E:16:THR:HG21	1.85	0.59
1:A:1074:G:OP2	5:E:61:TYR:OH	2.18	0.59
1:A:537:G:OP1	12:L:113:ARG:NH2	2.36	0.59
1:A:1315:U:O2'	1:A:1360:A:N3	2.28	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.59
13:M:23:TYR:CD2	13:M:67:GLU:HA	2.38	0.59
17:Q:9:VAL:HG22	17:Q:56:VAL:HG22	1.85	0.59
1:A:390:C:O3'	16:P:28:ARG:NH2	2.36	0.59
3:C:6:HIS:HD2	3:C:8:ILE:H	1.51	0.59
19:S:31:ILE:HD13	19:S:32:LYS:H	1.68	0.59
1:A:376:G:H5''	16:P:5:ARG:HD2	1.84	0.58
1:A:1435:G:H2'	1:A:1436:U:C6	2.38	0.58
1:A:958:A:N3	1:A:985:C:O2'	2.34	0.58
2:B:8:LYS:O	2:B:11:LEU:N	2.32	0.58
24:A:1602:PAR:H23	24:A:1602:PAR:HN21	1.68	0.58
13:M:98:VAL:HG23	13:M:110:ARG:HH12	1.68	0.58
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.85	0.58
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.85	0.58
1:A:426:G:OP1	4:D:38:TYR:OH	2.19	0.58
1:A:835:U:OP1	18:R:64:ARG:NH2	2.29	0.58
1:A:1379:G:OP1	7:G:6:ARG:NH1	2.36	0.58
1:A:401:C:O2'	1:A:621:A:N3	2.34	0.58
7:G:122:HIS:HA	7:G:125:MET:HE2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:G:H5''	12:L:17:LYS:HE2	1.86	0.58
1:A:670:G:N7	24:A:1606:PAR:O44	2.36	0.58
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.85	0.58
1:A:279:A:OP1	1:A:280:C:O2'	2.19	0.58
1:A:509:A:N3	1:A:543:C:O2'	2.33	0.58
1:A:954:G:N2	1:A:1227:A:H62	1.98	0.57
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.86	0.57
1:A:1048:G:O3'	1:A:1049:U:H3'	2.03	0.57
4:D:3:ARG:CZ	4:D:5:ILE:HD11	2.34	0.57
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.86	0.57
12:L:42:THR:HG21	12:L:52:LEU:HD13	1.86	0.57
12:L:113:ARG:HH11	12:L:116:SER:H	1.53	0.57
1:A:539:A:H2'	1:A:540:G:C8	2.39	0.57
18:R:21:LYS:O	18:R:25:THR:OG1	2.22	0.57
12:L:104:VAL:HG12	12:L:105:TYR:H	1.69	0.57
15:O:5:LYS:H	15:O:5:LYS:HD2	1.68	0.57
7:G:51:GLN:C	7:G:53:LYS:H	2.13	0.57
1:A:1004:A:OP1	1:A:1025:U:N3	2.38	0.57
15:O:87:ILE:HG22	15:O:88:ARG:H	1.69	0.57
1:A:1301:U:HO2'	1:A:1302:U:C5'	2.16	0.57
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.85	0.57
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.86	0.57
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.20	0.57
20:T:56:MET:HE2	20:T:85:MET:HA	1.86	0.57
1:A:8:A:N7	4:D:208:SER:OG	2.33	0.57
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.87	0.56
4:D:150:GLU:CD	4:D:150:GLU:H	2.12	0.56
1:A:60:A:H4'	1:A:61:G:O5'	2.05	0.56
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.87	0.56
1:A:946:A:H2'	1:A:947:G:H8	1.70	0.56
1:A:1034:G:H2'	1:A:1035:A:C8	2.41	0.56
1:A:975:A:H5'	1:A:975:A:H8	1.71	0.56
20:T:73:HIS:O	20:T:74:LYS:O	2.24	0.56
1:A:949:A:OP2	13:M:106:ASN:ND2	2.39	0.56
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.86	0.56
18:R:31:LEU:HD22	18:R:66:LEU:HB2	1.86	0.56
1:A:413:G:H1'	1:A:428:G:N2	2.21	0.56
1:A:1250:A:H4'	9:I:68:GLY:N	2.20	0.56
13:M:23:TYR:HD2	13:M:67:GLU:HA	1.70	0.56
1:A:928:G:O2'	1:A:1533:C:OP1	2.24	0.56
16:P:26:ARG:HD2	16:P:31:LYS:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.88	0.56
1:A:436:C:H2'	1:A:437:U:C6	2.41	0.56
3:C:148:GLY:HA3	3:C:172:ARG:O	2.06	0.56
1:A:10:A:O2'	1:A:507:C:O2'	2.24	0.55
1:A:427:U:OP1	4:D:13:ARG:NH2	2.39	0.55
1:A:1054:C:N4	22:W:34:G:H1'	2.21	0.55
1:A:1057:G:H5''	3:C:154:SER:HB2	1.89	0.55
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	2.05	0.55
1:A:978:A:O2'	1:A:1322:C:N3	2.38	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.42	0.55
1:A:413:G:H1'	1:A:428:G:H21	1.71	0.55
12:L:93:LEU:HD13	12:L:96:VAL:HG21	1.88	0.55
13:M:89:GLY:O	13:M:93:ARG:HB2	2.07	0.55
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.40	0.55
5:E:80:ILE:HG23	8:H:104:ARG:HH22	1.72	0.55
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.40	0.55
1:A:1377:A:OP2	7:G:94:ARG:NE	2.40	0.54
9:I:25:LYS:N	9:I:60:ASP:OD1	2.30	0.54
10:J:86:MET:O	10:J:87:THR:OG1	2.20	0.54
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.38	0.54
1:A:976:G:H5'	1:A:1358:U:O2'	2.08	0.54
4:D:149:ALA:HB3	4:D:152:SER:HB2	1.89	0.54
5:E:11:ILE:HG21	5:E:105:VAL:HG13	1.89	0.54
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.47	0.54
4:D:65:ARG:HG3	4:D:75:PHE:CG	2.41	0.54
13:M:108:ARG:HD2	13:M:114:ARG:HE	1.72	0.54
1:A:1069:C:O2'	1:A:1192:C:H1'	2.08	0.54
1:A:1278:U:H5''	1:A:1279:A:C8	2.42	0.54
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.90	0.54
20:T:85:MET:HE2	20:T:104:LEU:HD23	1.89	0.54
1:A:956:U:C2	1:A:1225:A:C2	2.96	0.54
1:A:974:A:OP2	14:N:29:ARG:NH1	2.28	0.54
1:A:192:U:H1'	20:T:103:GLY:HA2	1.90	0.54
1:A:442:C:H42	1:A:492:G:H1	1.55	0.54
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.89	0.54
20:T:39:LYS:O	20:T:43:LEU:HG	2.08	0.54
1:A:664:G:N2	1:A:741:G:H1	1.94	0.54
1:A:1286:A:H2'	1:A:1287:A:H4'	1.90	0.54
4:D:159:ARG:O	4:D:163:GLU:HB2	2.08	0.54
19:S:36:ARG:NH2	19:S:75:ALA:O	2.39	0.54
5:E:79:GLU:O	8:H:104:ARG:NH1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:G:H1	1:A:1391:U:H3	1.54	0.54
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.90	0.54
10:J:48:THR:HA	10:J:62:HIS:HB3	1.90	0.54
1:A:456:C:O2	1:A:477:G:N2	2.41	0.53
16:P:9:PHE:CE1	16:P:18:ARG:HD2	2.42	0.53
1:A:8:A:N6	4:D:205:GLU:O	2.41	0.53
1:A:45:U:H2'	1:A:46:G:H8	1.71	0.53
1:A:1168:A:H2'	1:A:1169:A:C8	2.42	0.53
6:F:22:GLU:CD	6:F:84:ASN:HD22	2.14	0.53
1:A:110:C:H2'	1:A:111:G:O4'	2.08	0.53
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.90	0.53
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.90	0.53
1:A:1026:G:H3'	1:A:1027:C:H5''	1.89	0.53
1:A:1178:G:N2	1:A:1180:A:H3'	2.24	0.53
1:A:1443:G:H4'	1:A:1446:A:C5'	2.39	0.53
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.39	0.53
1:A:951:G:OP2	13:M:102:ARG:NH2	2.38	0.53
1:A:1159:U:O4'	1:A:1182:G:N2	2.41	0.53
1:A:1285:A:H4'	1:A:1286:A:O5'	2.08	0.53
20:T:31:SER:O	20:T:35:THR:OG1	2.27	0.53
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.90	0.53
13:M:96:LEU:O	13:M:110:ARG:NH1	2.42	0.53
5:E:90:VAL:O	5:E:120:THR:HA	2.09	0.53
2:B:47:THR:HA	2:B:202:PRO:HG2	1.90	0.52
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.74	0.52
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.91	0.52
8:H:53:VAL:O	8:H:55:GLY:N	2.42	0.52
10:J:26:ALA:O	10:J:84:GLN:NE2	2.42	0.52
1:A:41:G:H2'	1:A:42:G:C8	2.45	0.52
2:B:98:LEU:HG	2:B:101:MET:HE3	1.92	0.52
19:S:36:ARG:HA	19:S:71:LEU:HB2	1.91	0.52
1:A:1034:G:H2'	1:A:1035:A:H8	1.74	0.52
9:I:55:ALA:O	9:I:57:GLY:N	2.42	0.52
1:A:161:A:H2'	1:A:162:A:C8	2.44	0.52
1:A:325:A:H2'	1:A:326:G:O4'	2.10	0.52
16:P:53:VAL:HG12	16:P:57:ARG:HE	1.75	0.52
1:A:562:C:H1'	12:L:15:ARG:HG3	1.90	0.52
1:A:927:G:O2'	1:A:1503:A:N7	2.40	0.52
12:L:58:VAL:O	12:L:65:GLU:HA	2.09	0.52
1:A:372:C:H4'	1:A:373:A:O5'	2.10	0.52
1:A:974:A:OP1	1:A:974:A:H8	1.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.91	0.52
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.92	0.52
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.51
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.92	0.51
1:A:940:C:OP1	7:G:29:LYS:NZ	2.43	0.51
1:A:1475:G:H2'	1:A:1476:G:H8	1.74	0.51
1:A:1505:G:O2'	1:A:1506:U:OP2	2.26	0.51
2:B:122:PHE:HA	2:B:127:ILE:HG12	1.91	0.51
7:G:5:ARG:HG3	7:G:7:ALA:H	1.75	0.51
18:R:38:GLU:HA	18:R:41:LYS:HE3	1.91	0.51
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.51
10:J:51:ARG:NE	10:J:61:GLU:HB2	2.25	0.51
1:A:1347:G:O2'	1:A:1348:U:P	2.68	0.51
2:B:239:VAL:O	2:B:241:GLU:N	2.43	0.51
1:A:971:G:N2	1:A:1363:A:OP2	2.35	0.51
1:A:1131:G:H2'	1:A:1132:C:C6	2.45	0.51
3:C:124:ILE:HG12	3:C:130:VAL:HG22	1.92	0.51
9:I:16:ARG:O	9:I:63:ILE:HA	2.10	0.51
1:A:1251:A:H5'	9:I:12:GLU:HG2	1.92	0.51
9:I:81:ILE:O	9:I:85:LEU:HB2	2.10	0.51
1:A:160:A:H1'	1:A:344:A:N7	2.26	0.51
1:A:1127:G:N2	1:A:1146:A:H62	2.08	0.51
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.34	0.51
1:A:255:G:H2'	1:A:256:U:C6	2.46	0.51
1:A:1304:G:C6	1:A:1305:G:N1	2.78	0.51
2:B:95:GLN:HG3	2:B:147:LYS:HG2	1.93	0.51
12:L:83:VAL:HG21	12:L:100:ILE:HG12	1.92	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.45	0.51
1:A:737:A:H2'	1:A:738:C:C6	2.45	0.51
1:A:890:G:O2'	1:A:906:G:O6	2.24	0.51
1:A:821:G:N7	24:A:1602:PAR:O34	2.44	0.51
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.76	0.51
1:A:266:G:H5''	1:A:267:C:C5	2.46	0.50
2:B:133:LYS:O	2:B:137:ARG:HG3	2.11	0.50
2:B:189:ASP:O	2:B:192:SER:OG	2.26	0.50
2:B:88:ALA:HB1	2:B:226:ARG:HH21	1.75	0.50
1:A:1397:C:N4	23:Y:4:U:OP2	2.45	0.50
1:A:1455:G:OP1	20:T:35:THR:OG1	2.28	0.50
1:A:372:C:H1'	1:A:373:A:OP2	2.11	0.50
1:A:1306:A:N6	1:A:1331:G:H1'	2.26	0.50
4:D:100:ARG:NH2	4:D:136:PRO:HB2	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.91	0.50
13:M:15:VAL:HG23	13:M:43:THR:O	2.11	0.50
1:A:232:G:O2'	1:A:263:A:N1	2.44	0.50
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.93	0.50
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.94	0.50
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.11	0.50
1:A:149:A:H2'	1:A:150:C:C6	2.47	0.50
1:A:1086:U:H3	1:A:1099:G:H22	1.60	0.50
4:D:2:GLY:C	4:D:3:ARG:HG3	2.36	0.50
11:K:87:THR:HA	11:K:91:ARG:NH1	2.26	0.50
1:A:1228:C:H4'	13:M:116:THR:HA	1.93	0.50
1:A:1475:G:H2'	1:A:1476:G:C8	2.47	0.50
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.77	0.50
19:S:40:ILE:HG22	19:S:67:VAL:HA	1.94	0.49
1:A:593:G:H1	1:A:646:U:H3	1.60	0.49
1:A:673:G:H2'	1:A:674:G:C8	2.47	0.49
8:H:53:VAL:HG12	8:H:54:ASP:H	1.75	0.49
1:A:335:C:H2'	1:A:336:C:C6	2.47	0.49
1:A:1118:C:H1'	1:A:1179:A:C5	2.47	0.49
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.94	0.49
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.93	0.49
18:R:26:LEU:HD21	18:R:39:VAL:HG23	1.93	0.49
1:A:662:G:O2'	1:A:836:G:OP1	2.27	0.49
1:A:874:G:OP1	24:A:1602:PAR:O31	2.30	0.49
1:A:1296:C:H4'	1:A:1302:U:C5	2.48	0.49
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.95	0.49
1:A:524:G:H2'	1:A:525:C:C6	2.48	0.49
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.49
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.13	0.49
13:M:90:LEU:O	13:M:94:ARG:HG2	2.13	0.49
1:A:432:A:O2'	1:A:433:C:OP1	2.24	0.49
1:A:748:C:H4'	1:A:749:C:O5'	2.12	0.49
12:L:24:VAL:HG13	12:L:98:TYR:CE1	2.47	0.49
1:A:745:C:OP1	1:A:851:G:O2'	2.29	0.49
1:A:1273:G:H2'	1:A:1274:G:O4'	2.13	0.49
1:A:1280:A:H5'	10:J:40:LEU:HD22	1.95	0.49
1:A:1453:G:N2	1:A:1454:G:N7	2.61	0.49
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.27	0.49
7:G:54:THR:HG22	7:G:56:GLN:H	1.78	0.49
7:G:113:GLU:HB2	7:G:119:ARG:HG3	1.95	0.49
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:A:HO2'	1:A:1257:U:P	2.35	0.49
2:B:212:GLN:O	2:B:216:SER:OG	2.15	0.49
1:A:542:G:H5'	4:D:41:GLY:HA3	1.95	0.48
1:A:603:U:H2'	1:A:604:G:C8	2.48	0.48
1:A:1001:A:H2'	1:A:1002:G:C8	2.48	0.48
5:E:10:MET:HA	5:E:32:VAL:HA	1.95	0.48
7:G:45:ASP:O	7:G:49:ILE:HG13	2.13	0.48
13:M:12:ASN:H	13:M:45:VAL:HB	1.78	0.48
20:T:10:LEU:HD12	20:T:11:SER:H	1.78	0.48
20:T:81:LYS:O	20:T:85:MET:HG3	2.13	0.48
1:A:1427:U:H2'	1:A:1428:A:C8	2.48	0.48
14:N:23:ARG:NH1	14:N:28:GLY:O	2.47	0.48
1:A:109:A:C6	1:A:326:G:C6	3.01	0.48
1:A:316:G:OP2	1:A:351:G:O2'	2.31	0.48
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.29	0.48
1:A:1477:C:H2'	1:A:1478:C:C6	2.48	0.48
3:C:155:GLY:HA2	3:C:164:ARG:O	2.12	0.48
19:S:12:ASP:H	19:S:38:SER:HB3	1.77	0.48
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.31	0.48
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.95	0.48
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.96	0.48
18:R:25:THR:O	18:R:42:ARG:NH2	2.45	0.48
1:A:750:G:N3	15:O:23:GLY:HA3	2.28	0.48
1:A:1368:G:OP1	9:I:114:TYR:N	2.47	0.48
1:A:243:A:H4'	1:A:244:U:H5'	1.96	0.48
1:A:1074:G:O2'	1:A:1101:A:N1	2.42	0.48
3:C:135:LYS:NZ	5:E:50:GLU:HG2	2.28	0.48
1:A:384:G:H2'	1:A:385:C:C6	2.49	0.48
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.95	0.48
1:A:235:C:N4	28:A:2005:HOH:O	2.46	0.48
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.14	0.48
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.95	0.48
10:J:46:ARG:NH1	10:J:64:GLU:OE1	2.47	0.48
13:M:11:ARG:CZ	13:M:46:LYS:HB3	2.44	0.48
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.96	0.47
1:A:1288:A:N3	1:A:1352:C:O2'	2.38	0.47
4:D:152:SER:O	4:D:158:ILE:HD12	2.14	0.47
1:A:1239:A:H4'	1:A:1240:U:H5''	1.95	0.47
1:A:1298:C:N4	7:G:114:ARG:HG3	2.28	0.47
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.46	0.47
1:A:1502:A:H2	1:A:1505:G:N1	2.05	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:GLU:O	4:D:85:LYS:HG3	2.14	0.47
6:F:94:GLN:HB3	18:R:32:ARG:HH11	1.79	0.47
21:U:5:ASP:O	21:U:11:GLY:HA3	2.14	0.47
1:A:1054:C:H42	22:W:34:G:H1'	1.79	0.47
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.96	0.47
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.47	0.47
12:L:10:LEU:HB3	17:Q:32:TYR:CE2	2.50	0.47
1:A:137:C:O2'	16:P:61:SER:O	2.32	0.47
1:A:1179:A:O2'	1:A:1180:A:OP1	2.29	0.47
1:A:1311:G:N7	19:S:2:PRO:HA	2.30	0.47
2:B:51:LEU:HD21	2:B:201:ILE:HG23	1.96	0.47
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.95	0.47
1:A:161:A:N1	1:A:347:G:O2'	2.40	0.47
1:A:749:C:H2'	1:A:750:G:H8	1.79	0.47
1:A:1417:G:O2'	1:A:1483:A:N6	2.48	0.47
12:L:53:ARG:HH12	12:L:92:OTD:CG	2.22	0.47
15:O:5:LYS:O	15:O:9:GLN:HG2	2.14	0.47
1:A:1427:U:H2'	1:A:1428:A:H8	1.80	0.47
12:L:71:PRO:O	12:L:102:ARG:HD2	2.13	0.47
1:A:501:C:O2	1:A:549:C:O2'	2.28	0.47
1:A:579:G:H5'	1:A:728:A:H1'	1.95	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.50	0.47
1:A:1223:C:OP2	19:S:78:ARG:NH1	2.47	0.47
1:A:1268:A:N3	1:A:1326:C:O2'	2.48	0.47
1:A:1498:UR3:OP2	1:A:1542:U:O2'	2.28	0.47
3:C:63:ASN:HA	3:C:99:VAL:HG12	1.95	0.47
4:D:111:ALA:HB1	4:D:116:GLN:HB3	1.96	0.47
5:E:36:ASP:O	5:E:38:GLN:HG2	2.15	0.47
7:G:65:ALA:O	7:G:69:VAL:HG23	2.15	0.47
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.97	0.47
18:R:34:TYR:CE2	18:R:35:ARG:HG3	2.50	0.47
6:F:33:TYR:HB2	6:F:75:LEU:HD12	1.96	0.47
1:A:631:G:H5'	1:A:632:A:OP1	2.15	0.47
7:G:144:MET:O	7:G:148:ASN:ND2	2.48	0.47
12:L:117:ARG:HB3	12:L:122:THR:O	2.14	0.47
1:A:1027:C:N4	1:A:1035:A:H61	2.13	0.47
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.97	0.47
1:A:1399:C:C2	1:A:1401:G:C5	3.03	0.47
20:T:53:LEU:O	20:T:57:ARG:HD2	2.15	0.47
1:A:1352:C:H2'	1:A:1353:G:C8	2.51	0.46
4:D:31:CYS:C	4:D:33:MET:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LYS:HE3	9:I:117:HIS:O	2.15	0.46
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.74	0.46
1:A:413:G:N2	1:A:429:U:OP2	2.45	0.46
4:D:32:ALA:HA	4:D:35:ARG:HG2	1.97	0.46
8:H:17:THR:O	8:H:78:GLN:NE2	2.48	0.46
16:P:10:GLY:HA3	16:P:14:ASN:O	2.14	0.46
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.15	0.46
1:A:1376:U:H2'	1:A:1377:A:C8	2.50	0.46
24:A:1604:PAR:O53	24:A:1604:PAR:N21	2.44	0.46
1:A:462:G:H21	16:P:82:GLN:NE2	2.14	0.46
1:A:1128:C:H42	1:A:1143:G:H1	1.62	0.46
1:A:1392:G:N2	1:A:1502:A:H8	2.13	0.46
2:B:73:THR:HG23	2:B:95:GLN:O	2.14	0.46
6:F:25:ILE:HD13	6:F:82:ARG:HD2	1.97	0.46
7:G:15:ASP:CB	7:G:20:ASP:H	2.29	0.46
19:S:5:LEU:HD21	19:S:70:LYS:NZ	2.28	0.46
1:A:1413:A:H2	1:A:1487:G:H22	1.63	0.46
1:A:1498:UR3:O4'	1:A:1519:MA6:H2	2.15	0.46
3:C:70:VAL:HG12	3:C:72:LYS:H	1.79	0.46
3:C:77:ILE:O	3:C:83:ARG:HB3	2.15	0.46
1:A:629:G:H2'	1:A:630:G:O4'	2.16	0.46
1:A:718:G:O6	18:R:74:ARG:NH1	2.49	0.46
1:A:1071:C:H2'	1:A:1072:G:H8	1.80	0.46
1:A:178:C:OP2	20:T:65:LYS:NZ	2.40	0.46
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.78	0.46
1:A:6:G:H1	5:E:98:THR:HG1	1.61	0.46
1:A:62:U:OP1	1:A:385:C:O2'	2.32	0.46
1:A:932:C:H4'	7:G:4:ARG:NH2	2.31	0.46
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.96	0.46
1:A:560:U:H5'	1:A:566:G:N2	2.31	0.46
1:A:688:G:H5'	11:K:46:GLY:C	2.40	0.46
1:A:695:A:H61	1:A:797:C:H1'	1.81	0.46
1:A:838:G:N2	1:A:840:C:H5'	2.31	0.46
8:H:110:ALA:HB1	8:H:133:LEU:HD21	1.97	0.46
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.51	0.46
8:H:48:TYR:HA	8:H:60:ARG:O	2.16	0.46
1:A:580:U:H2'	1:A:581:G:O4'	2.16	0.45
1:A:591:U:H2'	1:A:592:G:C8	2.50	0.45
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.51	0.45
1:A:1343:G:H2'	1:A:1344:C:C6	2.51	0.45
1:A:1392:G:H21	1:A:1502:A:H8	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:VAL:O	2:B:178:ARG:HG2	2.15	0.45
6:F:4:TYR:CE2	6:F:92:LYS:HG2	2.51	0.45
6:F:33:TYR:HE1	6:F:74:ASP:HB3	1.80	0.45
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.81	0.45
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.98	0.45
8:H:25:ASP:OD1	8:H:25:ASP:N	2.47	0.45
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.97	0.45
4:D:4:TYR:OH	4:D:7:PRO:O	2.18	0.45
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.47	0.45
5:E:76:ILE:O	5:E:93:PRO:HB3	2.16	0.45
5:E:89:ILE:HD13	5:E:90:VAL:H	1.81	0.45
8:H:82:HIS:HE1	8:H:136:GLU:OE2	2.00	0.45
10:J:71:LEU:O	10:J:73:ASP:HB2	2.16	0.45
19:S:33:THR:HG22	19:S:35:SER:N	2.15	0.45
1:A:955:U:H2'	1:A:956:U:H6	1.81	0.45
4:D:70:ILE:HD12	4:D:70:ILE:HA	1.72	0.45
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.98	0.45
9:I:85:LEU:HD23	9:I:96:LEU:HD21	1.98	0.45
1:A:632:A:H2'	1:A:633:G:O4'	2.17	0.45
1:A:924:C:H2'	1:A:925:G:C8	2.52	0.45
1:A:1300:G:O2'	1:A:1301:U:P	2.75	0.45
2:B:70:PHE:O	2:B:92:TYR:HA	2.16	0.45
18:R:58:LEU:HD11	18:R:66:LEU:HD13	1.99	0.45
1:A:707:C:H2'	1:A:708:C:C6	2.52	0.45
1:A:775:G:H2'	1:A:776:G:O4'	2.17	0.45
1:A:851:G:H2'	1:A:852:G:C8	2.51	0.45
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.99	0.45
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.25	0.45
12:L:124:LYS:HG3	12:L:125:PRO:O	2.17	0.45
18:R:34:TYR:CD2	18:R:35:ARG:HG3	2.52	0.45
18:R:46:GLU:CD	18:R:46:GLU:H	2.24	0.45
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.45
1:A:1157:A:H4'	1:A:1158:C:O5'	2.17	0.45
1:A:1172:C:H2'	1:A:1173:G:H8	1.82	0.45
1:A:1331:G:O2'	1:A:1332:A:H8	2.00	0.45
4:D:9:CYS:SG	4:D:22:LYS:HD2	2.57	0.45
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.98	0.45
12:L:69:TYR:O	12:L:100:ILE:HB	2.16	0.45
13:M:2:ALA:HB3	13:M:53:VAL:HG11	1.98	0.45
20:T:74:LYS:C	20:T:76:ALA:H	2.25	0.45
1:A:390:C:H2'	1:A:391:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:U:H5'	1:A:566:G:C2	2.52	0.45
1:A:1264:C:H2'	1:A:1265:G:C8	2.47	0.45
2:B:112:VAL:O	2:B:116:GLU:HG2	2.17	0.45
9:I:55:ALA:C	9:I:57:GLY:H	2.25	0.45
15:O:70:LEU:HD21	15:O:77:ARG:HB2	1.99	0.45
1:A:26:A:N6	1:A:558:G:H1'	2.32	0.45
1:A:51:A:OP2	24:A:1603:PAR:N24	2.50	0.45
1:A:664:G:OP1	18:R:64:ARG:HD2	2.17	0.45
1:A:1065:U:H5''	1:A:1190:G:N2	2.32	0.45
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.99	0.45
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.98	0.45
20:T:62:LEU:HD22	20:T:62:LEU:HA	1.76	0.45
1:A:558:G:OP2	1:A:559:A:O2'	2.32	0.44
1:A:1127:G:H5'	9:I:66:ARG:HH22	1.81	0.44
1:A:1340:A:H2'	1:A:1341:U:O4'	2.16	0.44
1:A:1513:A:H2'	1:A:1514:C:C6	2.52	0.44
4:D:108:LEU:HD21	4:D:174:LEU:HD22	2.00	0.44
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.99	0.44
5:E:118:ILE:HG13	5:E:119:LEU:N	2.32	0.44
10:J:7:LYS:HD3	10:J:9:ARG:NH2	2.32	0.44
18:R:31:LEU:HD23	18:R:31:LEU:HA	1.76	0.44
1:A:299:G:N1	28:A:2001:HOH:O	2.36	0.44
1:A:375:U:C4	1:A:376:G:N7	2.85	0.44
1:A:994:A:N7	1:A:1216:G:H4'	2.32	0.44
2:B:48:MET:HA	2:B:51:LEU:HB2	1.99	0.44
3:C:139:GLN:O	3:C:143:GLU:HB2	2.17	0.44
14:N:24:CYS:SG	14:N:40:CYS:N	2.88	0.44
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.99	0.44
21:U:12:LYS:O	21:U:16:GLY:N	2.50	0.44
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.44
1:A:1399:C:C2	1:A:1502:A:N6	2.86	0.44
2:B:69:LEU:HG	2:B:155:LEU:HD11	1.98	0.44
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.98	0.44
4:D:4:TYR:O	4:D:4:TYR:CG	2.68	0.44
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.52	0.44
1:A:119:A:H4'	1:A:120:A:C8	2.53	0.44
1:A:1316:G:H4'	14:N:18:VAL:HG13	1.98	0.44
1:A:1410:G:H2'	1:A:1411:C:C6	2.53	0.44
2:B:48:MET:HA	2:B:51:LEU:HD12	1.98	0.44
4:D:151:LYS:H	4:D:151:LYS:HD2	1.82	0.44
1:A:114:U:H5''	24:A:1603:PAR:H52	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:A:O2'	1:A:564:C:N3	2.44	0.44
1:A:736:C:H2'	1:A:737:A:C8	2.52	0.44
1:A:812:C:H6	1:A:812:C:H2'	1.58	0.44
1:A:851:G:H2'	1:A:852:G:H8	1.82	0.44
1:A:1057:G:H5''	3:C:154:SER:CB	2.47	0.44
1:A:1375:A:H4'	7:G:29:LYS:HD3	1.99	0.44
10:J:3:LYS:O	10:J:101:VAL:N	2.51	0.44
1:A:266:G:O3'	17:Q:67:LYS:HB2	2.18	0.44
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.18	0.44
3:C:95:THR:C	3:C:97:LYS:H	2.25	0.44
9:I:118:LYS:C	9:I:120:ARG:H	2.25	0.44
11:K:84:VAL:CG2	11:K:95:ILE:HD11	2.46	0.44
19:S:12:ASP:OD2	19:S:35:SER:OG	2.32	0.44
1:A:1303:C:H2'	1:A:1304:G:H5'	1.99	0.44
3:C:35:GLU:HG2	3:C:59:ARG:HH22	1.83	0.44
3:C:157:ILE:HD13	3:C:166:GLU:HB2	2.00	0.44
5:E:142:LEU:O	5:E:143:ARG:NE	2.49	0.44
11:K:84:VAL:HG11	11:K:91:ARG:HE	1.83	0.44
1:A:779:C:O2'	11:K:120:ARG:HD3	2.18	0.44
1:A:1028:C:H2'	1:A:1029:C:C6	2.53	0.44
4:D:103:ASN:O	4:D:107:ARG:HG2	2.18	0.44
7:G:108:ALA:HA	7:G:111:ARG:HD2	2.00	0.44
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.65	0.44
13:M:98:VAL:HG23	13:M:110:ARG:NH1	2.32	0.44
1:A:755:G:OP2	15:O:65:ARG:HD2	2.17	0.44
1:A:1128:C:H42	1:A:1143:G:H22	1.65	0.44
8:H:86:ILE:HD12	8:H:133:LEU:HD22	2.00	0.44
13:M:49:THR:HG22	13:M:51:ALA:H	1.82	0.44
1:A:187:C:O2	20:T:105:SER:HB3	2.17	0.43
1:A:967:5MC:OP1	1:A:969:A:H5'	2.18	0.43
1:A:1494:G:OP1	24:A:1601:PAR:N32	2.43	0.43
4:D:102:ASP:OD1	4:D:102:ASP:N	2.48	0.43
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.91	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.17	0.43
1:A:1101:A:H4'	1:A:1102:A:O5'	2.18	0.43
2:B:88:ALA:O	2:B:90:MET:N	2.36	0.43
3:C:24:ALA:HB1	3:C:28:GLN:HB2	2.00	0.43
3:C:142:MET:HE3	3:C:142:MET:HB3	1.90	0.43
4:D:122:ARG:HE	4:D:122:ARG:HA	1.83	0.43
6:F:5:GLU:OE1	18:R:34:TYR:OH	2.30	0.43
13:M:65:LYS:O	13:M:66:LEU:HD23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.99	0.43
20:T:72:LEU:O	20:T:73:HIS:O	2.36	0.43
1:A:1029:C:H2'	1:A:1030:C:C6	2.54	0.43
4:D:13:ARG:HD2	4:D:38:TYR:O	2.17	0.43
4:D:60:GLU:HG2	4:D:202:LEU:HB2	2.00	0.43
4:D:108:LEU:HD23	4:D:174:LEU:HD13	2.00	0.43
10:J:51:ARG:NH2	10:J:61:GLU:HG3	2.33	0.43
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.82	0.43
1:A:269:C:H2'	1:A:270:A:H8	1.83	0.43
1:A:269:C:H2'	1:A:270:A:C8	2.53	0.43
1:A:833:U:H2'	1:A:834:C:H6	1.84	0.43
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.43
1:A:977:A:H1'	1:A:982:U:O4	2.17	0.43
2:B:144:ARG:HG3	2:B:145:LEU:N	2.34	0.43
20:T:54:LYS:HB3	20:T:54:LYS:HE2	1.76	0.43
1:A:1117:G:N2	1:A:1180:A:H1'	2.34	0.43
1:A:1320:C:O2	19:S:36:ARG:NH1	2.52	0.43
3:C:14:ILE:HG22	3:C:15:THR:HG23	2.00	0.43
4:D:24:GLU:C	4:D:26:CYS:H	2.26	0.43
5:E:64:ARG:HE	5:E:64:ARG:HB2	1.74	0.43
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.47	0.43
7:G:94:ARG:O	7:G:97:GLN:HB3	2.19	0.43
8:H:97:VAL:HG21	8:H:128:GLY:HA2	1.99	0.43
13:M:34:LEU:HD23	13:M:34:LEU:HA	1.87	0.43
17:Q:48:GLU:OE1	17:Q:50:LYS:HD2	2.18	0.43
1:A:653:A:C8	8:H:56:LYS:HG2	2.53	0.43
1:A:792:A:H4'	1:A:793:U:O5'	2.19	0.43
1:A:1107:C:C4	1:A:1108:G:C8	3.06	0.43
1:A:1217:C:H2'	1:A:1218:C:O4'	2.17	0.43
1:A:1247:U:O2'	1:A:1248:A:H5'	2.18	0.43
1:A:1256:A:O2'	1:A:1257:U:O5'	2.33	0.43
2:B:198:ASP:OD1	8:H:68:ARG:NH2	2.36	0.43
8:H:113:SER:O	8:H:131:GLY:HA3	2.19	0.43
17:Q:24:GLU:CD	17:Q:37:LYS:HD3	2.43	0.43
17:Q:60:ILE:HG12	17:Q:61:GLU:N	2.33	0.43
20:T:57:ARG:HE	20:T:102:GLY:HA2	1.83	0.43
1:A:133:U:P	20:T:74:LYS:HZ1	2.40	0.43
1:A:222:U:H2'	1:A:223:U:C6	2.53	0.43
1:A:745:C:H2'	1:A:746:A:C8	2.54	0.43
1:A:828:A:H5''	1:A:859:A:C2	2.54	0.43
1:A:1366:C:H2'	1:A:1367:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.54	0.43
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.54	0.43
13:M:8:GLU:CD	13:M:22:ILE:HA	2.44	0.43
13:M:34:LEU:HD13	13:M:41:PRO:HA	2.00	0.43
13:M:102:ARG:HD3	13:M:105:THR:OG1	2.18	0.43
1:A:939:G:H5''	7:G:102:ARG:NH2	2.34	0.43
1:A:1084:G:H5'	1:A:1102:A:OP2	2.19	0.43
3:C:123:GLN:O	3:C:128:PHE:HB2	2.19	0.43
12:L:74:GLY:O	12:L:102:ARG:NH1	2.43	0.43
14:N:11:LYS:O	14:N:14:PRO:HD3	2.18	0.43
1:A:17:U:H2'	1:A:18:C:C6	2.53	0.43
1:A:939:G:H5''	7:G:102:ARG:NH1	2.33	0.43
1:A:1126:U:H5'	1:A:1280:A:O2'	2.19	0.43
1:A:1143:G:H2'	1:A:1144:G:C8	2.54	0.43
1:A:1150:U:O3'	10:J:41:PRO:HB3	2.19	0.43
20:T:67:ALA:O	20:T:73:HIS:ND1	2.52	0.43
1:A:596:C:O5'	1:A:596:C:H6	2.02	0.43
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.19	0.43
8:H:29:SER:OG	8:H:32:LYS:HG3	2.19	0.43
9:I:10:ARG:HD3	9:I:105:ASP:HB3	2.00	0.43
10:J:32:ALA:HB2	10:J:76:ASN:HB2	2.01	0.43
11:K:72:ALA:HB1	11:K:77:MET:HE2	2.01	0.43
16:P:45:THR:OG1	16:P:47:ASP:O	2.37	0.43
1:A:327:A:O2'	1:A:328:C:H6	2.01	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.19	0.42
1:A:721:G:H4'	1:A:722:A:O4'	2.19	0.42
3:C:5:ILE:HG23	10:J:51:ARG:HH12	1.84	0.42
8:H:61:VAL:HG12	8:H:63:LEU:HD13	2.00	0.42
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.83	0.42
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.01	0.42
16:P:53:VAL:HG13	16:P:79:VAL:HG22	2.01	0.42
18:R:33:ASP:OD2	18:R:36:ASN:HB2	2.19	0.42
20:T:72:LEU:HD23	20:T:72:LEU:HA	1.85	0.42
1:A:129(A):G:N3	1:A:190(E):U:H3'	2.34	0.42
1:A:567:G:H2'	1:A:568:G:O4'	2.19	0.42
1:A:1182:G:H4'	1:A:1183:A:O5'	2.19	0.42
1:A:1319:A:H4'	1:A:1320:C:OP1	2.19	0.42
2:B:30:ARG:HG3	2:B:31:TYR:CD1	2.54	0.42
2:B:130:ARG:HD3	2:B:130:ARG:HA	1.49	0.42
10:J:14:LYS:HE2	10:J:14:LYS:HB3	1.63	0.42
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLN:O	2:B:150:SER:HB2	2.20	0.42
3:C:130:VAL:O	3:C:134:ILE:HG13	2.19	0.42
4:D:3:ARG:HE	4:D:3:ARG:HB2	1.57	0.42
16:P:17:TYR:HE2	16:P:41:PRO:HG3	1.84	0.42
19:S:6:LYS:HE3	19:S:6:LYS:HB2	1.83	0.42
1:A:713:G:H2'	1:A:714:G:C8	2.53	0.42
1:A:818:G:C3'	1:A:819:A:H5''	2.50	0.42
1:A:1172:C:H2'	1:A:1173:G:C8	2.54	0.42
1:A:1179:A:HO2'	1:A:1180:A:P	2.43	0.42
8:H:118:VAL:C	8:H:119:LEU:HD23	2.45	0.42
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	2.00	0.42
22:W:33:U:H5'	22:W:34:G:OP2	2.19	0.42
1:A:12:U:H4'	1:A:526:C:O2'	2.20	0.42
1:A:88:A:H2'	1:A:89:C:O4'	2.19	0.42
1:A:1316:G:H2'	1:A:1317:C:H5''	2.01	0.42
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.01	0.42
8:H:10:LEU:HD22	8:H:83:ILE:HD11	2.00	0.42
8:H:113:SER:HB2	8:H:134:ILE:HD11	2.01	0.42
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.00	0.42
15:O:4:THR:OG1	15:O:7:GLU:HG3	2.20	0.42
1:A:719:C:O2'	18:R:49:LYS:HB3	2.18	0.42
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.01	0.42
1:A:1014:A:C2	1:A:1219:U:H1'	2.54	0.42
2:B:82:ARG:O	2:B:86:GLU:HB2	2.19	0.42
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.34	0.42
4:D:25:ARG:NH1	4:D:30:LYS:O	2.53	0.42
6:F:44:GLY:HA2	6:F:59:TYR:CZ	2.53	0.42
8:H:121:ASP:N	8:H:121:ASP:OD1	2.53	0.42
11:K:34:ASP:OD1	11:K:38:ASN:N	2.52	0.42
1:A:187:C:OP1	20:T:82:SER:OG	2.37	0.42
1:A:1479:C:H2'	1:A:1480:G:H8	1.85	0.42
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.81	0.42
1:A:560:U:H4'	1:A:561:U:H5''	2.01	0.42
1:A:1148:U:H2'	1:A:1149:C:O4'	2.19	0.42
9:I:9:ARG:HG2	9:I:14:VAL:HG12	2.02	0.42
12:L:93:LEU:HD23	12:L:93:LEU:HA	1.87	0.42
13:M:66:LEU:HD23	13:M:66:LEU:HA	1.83	0.42
1:A:551:U:H2'	1:A:552:U:C6	2.55	0.42
1:A:1347:G:HO2'	1:A:1348:U:H6	1.65	0.42
1:A:1477:C:H2'	1:A:1478:C:H6	1.84	0.42
1:A:1527:C:O2'	1:A:1528:U:H5'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:VAL:HG12	3:C:72:LYS:N	2.35	0.42
3:C:136:GLN:O	3:C:140:ARG:HG3	2.20	0.42
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.53	0.42
8:H:39:LEU:HD13	8:H:39:LEU:HA	1.81	0.42
13:M:10:PRO:O	13:M:45:VAL:HG11	2.20	0.42
13:M:25:ILE:HD11	13:M:60:VAL:HG13	2.02	0.42
13:M:62:ASN:O	13:M:62:ASN:ND2	2.53	0.42
13:M:81:LEU:HD22	13:M:88:ARG:HB2	2.02	0.42
13:M:115:LYS:HB2	13:M:115:LYS:HE2	1.85	0.42
15:O:24:SER:O	15:O:28:GLN:HG3	2.20	0.42
1:A:476:G:H2'	1:A:477:G:C8	2.55	0.42
1:A:528:C:H41	12:L:49:ASN:CG	2.28	0.42
1:A:564:C:O2'	8:H:91:ARG:NH2	2.53	0.42
2:B:88:ALA:HB1	2:B:226:ARG:NH2	2.33	0.42
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.20	0.42
8:H:9:MET:HG3	8:H:26:VAL:HG11	2.01	0.42
1:A:539:A:H2'	1:A:540:G:H8	1.84	0.41
1:A:838:G:C2	1:A:840:C:H5'	2.55	0.41
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.55	0.41
4:D:25:ARG:HA	4:D:28:SER:HB2	2.01	0.41
5:E:50:GLU:HG3	5:E:52:PRO:CD	2.50	0.41
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.20	0.41
6:F:45:LEU:O	6:F:46:ARG:HG2	2.20	0.41
11:K:48:ILE:H	11:K:48:ILE:HG12	1.62	0.41
12:L:28:LYS:HZ2	12:L:28:LYS:HB3	1.85	0.41
20:T:74:LYS:H	20:T:74:LYS:HD2	1.84	0.41
1:A:262:A:C6	1:A:263:A:C6	3.08	0.41
1:A:474:G:H2'	1:A:475:G:H8	1.85	0.41
1:A:1404:5MC:H1'	1:A:1519:MA6:O2'	2.20	0.41
2:B:51:LEU:HD22	2:B:55:PHE:HE1	1.85	0.41
2:B:74:LYS:C	2:B:76:GLN:H	2.28	0.41
4:D:26:CYS:HA	4:D:31:CYS:HB2	2.01	0.41
5:E:145:LYS:O	5:E:149:GLU:HG2	2.20	0.41
10:J:84:GLN:O	10:J:88:LEU:HD12	2.20	0.41
15:O:15:PHE:CE2	15:O:84:LYS:HD2	2.55	0.41
1:A:909:A:O5'	1:A:909:A:H8	2.02	0.41
1:A:1229:A:OP2	13:M:114:ARG:HD3	2.20	0.41
3:C:64:VAL:HB	3:C:99:VAL:HG21	2.02	0.41
8:H:11:THR:OG1	8:H:14:ARG:NH1	2.47	0.41
1:A:440:A:H3'	1:A:442:C:H6	1.86	0.41
1:A:901:A:C5	1:A:902:G:H1'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:A:N3	1:A:1376:U:O2'	2.49	0.41
1:A:939:G:H5''	7:G:102:ARG:CZ	2.50	0.41
1:A:973:G:H3'	1:A:974:A:H5''	2.02	0.41
1:A:1233:G:H2'	1:A:1234:C:C6	2.56	0.41
1:A:1301:U:HO2'	1:A:1302:U:P	2.40	0.41
1:A:1407:5MC:HN42	24:A:1601:PAR:H23	1.85	0.41
3:C:91:LEU:HD23	3:C:92:ALA:N	2.35	0.41
1:A:922:G:H1'	5:E:19:MET:HB3	2.02	0.41
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.54	0.41
1:A:1235:U:H2'	1:A:1236:A:O4'	2.20	0.41
1:A:1331:G:O2'	1:A:1332:A:O5'	2.38	0.41
4:D:174:LEU:HD23	4:D:185:PHE:HA	2.01	0.41
5:E:10:MET:HE2	5:E:10:MET:HB3	2.00	0.41
6:F:46:ARG:HB2	6:F:60:PHE:CD2	2.55	0.41
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.78	0.41
13:M:4:ILE:HD11	13:M:56:LEU:HB3	2.01	0.41
1:A:186:C:H2'	1:A:187:C:C6	2.56	0.41
10:J:26:ALA:HB1	10:J:84:GLN:HB3	2.03	0.41
1:A:160:A:H2'	1:A:161:A:O4'	2.21	0.41
1:A:636:U:H2'	1:A:637:G:C8	2.55	0.41
1:A:707:C:H2'	1:A:708:C:H6	1.86	0.41
1:A:857:C:H2'	1:A:858:G:O4'	2.21	0.41
1:A:975:A:H5'	1:A:975:A:C8	2.55	0.41
1:A:1227:A:OP2	13:M:111:LYS:HE3	2.21	0.41
1:A:1298:C:H4'	1:A:1299:A:C4	2.56	0.41
3:C:154:SER:HG	3:C:197:GLY:H	1.62	0.41
5:E:80:ILE:HD13	5:E:138:ALA:HB1	2.03	0.41
1:A:19:C:H2'	1:A:20:U:H6	1.86	0.41
1:A:255:G:H2'	1:A:256:U:H6	1.84	0.41
1:A:620:C:N1	4:D:135:LEU:HD13	2.36	0.41
1:A:1128:C:OP1	9:I:66:ARG:NH1	2.54	0.41
1:A:1148:U:O2'	9:I:14:VAL:HG21	2.20	0.41
1:A:743:U:H2'	1:A:744:C:H6	1.86	0.41
1:A:861:G:O2'	1:A:874:G:O2'	2.39	0.41
1:A:1057:G:H2'	1:A:1058:G:O4'	2.21	0.41
1:A:1332:A:H2'	1:A:1333:A:C8	2.56	0.41
2:B:90:MET:HA	2:B:91:PRO:HD3	1.87	0.41
3:C:53:ALA:HB2	3:C:115:LEU:HG	2.03	0.41
3:C:108:ASN:ND2	3:C:111:LEU:HG	2.36	0.41
4:D:119:GLN:HE21	4:D:119:GLN:HB3	1.76	0.41
11:K:82:VAL:HG23	11:K:105:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:31:LYS:O	13:M:35:GLU:HB2	2.21	0.41
20:T:59:ALA:O	20:T:63:ILE:HG13	2.20	0.41
1:A:35:G:H2'	1:A:36:C:H6	1.84	0.41
1:A:518:C:H2'	1:A:530:G:N3	2.36	0.41
1:A:1054:C:C4	22:W:34:G:H1'	2.56	0.41
2:B:28:PHE:CD2	2:B:190:THR:HA	2.56	0.41
1:A:474:G:H5''	16:P:81:ARG:NH1	2.37	0.40
1:A:985:C:H2'	1:A:986:A:H8	1.80	0.40
1:A:1065:U:C5	1:A:1190:G:H1'	2.55	0.40
1:A:1202:G:H1'	14:N:29:ARG:HD2	2.02	0.40
3:C:65:ALA:O	3:C:66:VAL:C	2.64	0.40
6:F:76:ALA:O	6:F:80:ARG:HG3	2.21	0.40
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.21	0.40
7:G:20:ASP:OD2	7:G:22:LEU:HB3	2.20	0.40
20:T:10:LEU:HD12	20:T:11:SER:N	2.36	0.40
1:A:355:C:C4	1:A:356:A:N7	2.89	0.40
1:A:456:C:H2'	1:A:457:C:C6	2.57	0.40
2:B:101:MET:HA	2:B:108:ILE:HG13	2.02	0.40
10:J:16:LEU:HD12	10:J:68:HIS:HB2	2.03	0.40
11:K:97:ALA:O	11:K:101:SER:HB3	2.21	0.40
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.94	0.40
12:L:84:LEU:HB2	12:L:105:TYR:CE2	2.56	0.40
17:Q:85:VAL:O	17:Q:89:LEU:HG	2.21	0.40
19:S:27:GLU:H	19:S:27:GLU:CD	2.29	0.40
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.22	0.40
1:A:254:G:O2'	17:Q:16:GLN:O	2.39	0.40
1:A:488:C:H2'	1:A:489:C:C6	2.56	0.40
1:A:738:C:H6	1:A:738:C:O5'	2.03	0.40
1:A:895:G:H2'	1:A:896:C:C6	2.57	0.40
16:P:70:ALA:O	16:P:74:LEU:HG	2.21	0.40
1:A:731:G:OP1	1:A:766:A:H1'	2.22	0.40
1:A:951:G:O6	13:M:105:THR:HG21	2.20	0.40
1:A:1372:U:H2'	1:A:1373:G:O4'	2.22	0.40
3:C:7:PRO:CB	3:C:11:ARG:HH21	2.35	0.40
4:D:188:LEU:HD23	4:D:188:LEU:HA	1.98	0.40
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.85	0.40
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.04	0.40
9:I:51:ARG:HE	9:I:51:ARG:HB2	1.44	0.40
13:M:31:LYS:HE3	13:M:31:LYS:HB2	1.83	0.40
1:A:1191:A:H5''	3:C:4:LYS:HZ3	1.85	0.40
1:A:1200:C:O2'	1:A:1205:U:O4	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1403:C:H2'	1:A:1404:5MC:HM53	2.03	0.40
1:A:1418:A:N6	1:A:1482:G:O2'	2.53	0.40
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/236 (99%)	209 (89%)	20 (8%)	5 (2%)	5	31
3	C	205/207 (99%)	181 (88%)	24 (12%)	0	100	100
4	D	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	149/151 (99%)	143 (96%)	5 (3%)	1 (1%)	18	51
6	F	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	G	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	18	51
9	I	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	7	36
10	J	97/99 (98%)	76 (78%)	20 (21%)	1 (1%)	12	44
11	K	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
12	L	122/125 (98%)	115 (94%)	5 (4%)	2 (2%)	7	36
13	M	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
14	N	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
15	O	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
16	P	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
17	Q	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
18	R	71/73 (97%)	69 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	79/81 (98%)	70 (89%)	8 (10%)	1 (1%)	9	39
20	T	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	3	25
21	U	23/25 (92%)	22 (96%)	0	1 (4%)	2	18
All	All	2350/2391 (98%)	2164 (92%)	169 (7%)	17 (1%)	18	51

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
12	L	127	GLU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
2	B	88	ALA
2	B	131	PRO
2	B	240	GLN
9	I	56	LEU
21	U	25	LYS
8	H	54	ASP
10	J	55	LYS
19	S	81	ARG
9	I	119	ALA
12	L	126	LYS
2	B	130	ARG
5	E	154	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%)	180 (93%)	14 (7%)	13	39
3	C	160/161 (99%)	148 (92%)	12 (8%)	12	38
4	D	180/180 (100%)	170 (94%)	10 (6%)	19	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	115/116 (99%)	96 (84%)	19 (16%)	2	14
6	F	90/90 (100%)	83 (92%)	7 (8%)	11	37
7	G	126/126 (100%)	119 (94%)	7 (6%)	19	47
8	H	119/119 (100%)	106 (89%)	13 (11%)	6	27
9	I	98/98 (100%)	86 (88%)	12 (12%)	5	23
10	J	87/89 (98%)	73 (84%)	14 (16%)	2	14
11	K	89/89 (100%)	84 (94%)	5 (6%)	19	47
12	L	103/103 (100%)	86 (84%)	17 (16%)	2	14
13	M	94/94 (100%)	86 (92%)	8 (8%)	10	35
14	N	49/49 (100%)	46 (94%)	3 (6%)	17	44
15	O	79/79 (100%)	69 (87%)	10 (13%)	4	22
16	P	72/72 (100%)	68 (94%)	4 (6%)	19	47
17	Q	94/94 (100%)	85 (90%)	9 (10%)	8	31
18	R	64/64 (100%)	57 (89%)	7 (11%)	6	27
19	S	71/71 (100%)	63 (89%)	8 (11%)	5	25
20	T	76/76 (100%)	60 (79%)	16 (21%)	1	6
21	U	19/20 (95%)	18 (95%)	1 (5%)	20	48
All	All	1979/1994 (99%)	1783 (90%)	196 (10%)	7	30

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	20	GLU
2	B	44	LEU
2	B	69	LEU
2	B	82	ARG
2	B	114	ARG
2	B	121	LEU
2	B	127	ILE
2	B	139	LYS
2	B	179	LYS
2	B	187	LEU
2	B	206	ASP
2	B	208	ILE
2	B	221	LEU
2	B	236	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	3	ASN
3	C	21	ARG
3	C	27	LYS
3	C	43	LEU
3	C	79	ARG
3	C	91	LEU
3	C	143	GLU
3	C	166	GLU
3	C	178	LEU
3	C	192	THR
3	C	193	TYR
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	58	LEU
4	D	64	LEU
4	D	70	ILE
4	D	91	SER
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	175	SER
5	E	10	MET
5	E	12	LEU
5	E	24	ARG
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	64	ARG
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	89	ILE
5	E	117	ASP
5	E	118	ILE
5	E	120	THR
5	E	125	SER
5	E	144	THR
5	E	150	ARG
6	F	10	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	19	LEU
6	F	46	ARG
6	F	69	GLU
6	F	73	ASN
6	F	86	ARG
6	F	100	ASN
7	G	8	GLU
7	G	9	VAL
7	G	45	ASP
7	G	52	GLU
7	G	114	ARG
7	G	124	LEU
7	G	156	TRP
8	H	3	THR
8	H	25	ASP
8	H	26	VAL
8	H	39	LEU
8	H	54	ASP
8	H	63	LEU
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	102	ARG
8	H	133	LEU
9	I	2	GLU
9	I	12	GLU
9	I	20	ARG
9	I	35	GLU
9	I	51	ARG
9	I	65	VAL
9	I	79	LEU
9	I	96	LEU
9	I	102	LEU
9	I	103	THR
9	I	108	VAL
9	I	118	LYS
10	J	17	ASP
10	J	23	ILE
10	J	35	SER
10	J	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	49	VAL
10	J	55	LYS
10	J	62	HIS
10	J	71	LEU
10	J	73	ASP
10	J	74	ILE
10	J	80	LYS
10	J	83	GLU
10	J	86	MET
10	J	94	VAL
11	K	28	THR
11	K	29	ILE
11	K	43	SER
11	K	48	ILE
11	K	91	ARG
12	L	6	THR
12	L	15	ARG
12	L	20	LYS
12	L	27	LEU
12	L	28	LYS
12	L	33	ARG
12	L	38	THR
12	L	39	VAL
12	L	42	THR
12	L	93	LEU
12	L	96	VAL
12	L	97	ARG
12	L	99	HIS
12	L	100	ILE
12	L	111	LYS
12	L	113	ARG
12	L	127	GLU
13	M	4	ILE
13	M	56	LEU
13	M	58	GLU
13	M	64	TRP
13	M	90	LEU
13	M	102	ARG
13	M	106	ASN
13	M	109	THR
14	N	18	VAL
14	N	22	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	33	VAL
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	47	LYS
15	O	66	LEU
15	O	81	LEU
15	O	87	ILE
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	67	THR
17	Q	6	LEU
17	Q	38	ARG
17	Q	59	ILE
17	Q	60	ILE
17	Q	74	LEU
17	Q	78	GLU
17	Q	91	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	25	THR
18	R	26	LEU
18	R	41	LYS
18	R	42	ARG
18	R	47	THR
18	R	66	LEU
18	R	78	LEU
19	S	7	LYS
19	S	12	ASP
19	S	14	HIS
19	S	15	LEU
19	S	31	ILE
19	S	36	ARG
19	S	43	GLU
19	S	62	ILE
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	19	SER
20	T	35	THR
20	T	48	LYS
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	100	ILE
20	T	105	SER
21	U	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	74	GLN
5	E	78	HIS
6	F	73	ASN
6	F	94	GLN
7	G	109	ASN
7	G	148	ASN
8	H	70	GLN
9	I	3	GLN
9	I	73	GLN
10	J	76	ASN
10	J	78	ASN
11	K	78	GLN
13	M	62	ASN
13	M	106	ASN
16	P	82	GLN
19	S	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	228 (15%)	41 (2%)
22	W	14/15 (93%)	3 (21%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	Y	5/6 (83%)	2 (40%)	0
All	All	1529/1543 (99%)	233 (15%)	41 (2%)

All (233) 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	59	A
1	A	60	A
1	A	61	G
1	A	101	A
1	A	108	G
1	A	116	A
1	A	117	G
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	190(F)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	220	G
1	A	244	U
1	A	247	G
1	A	251	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	344	A
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
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	419	C
1	A	421	U
1	A	429	U
1	A	430	A
1	A	433	C
1	A	439	A
1	A	440	A
1	A	442	C
1	A	452	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
1	A	531	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	618	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A
1	A	703	G
1	A	721	G
1	A	722	A
1	A	731	G
1	A	748	C
1	A	749	C
1	A	755	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	876	G
1	A	902	G
1	A	914	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	966	M2G
1	A	967	5MC
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	982	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G
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	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	1108	G
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1158	C
1	A	1159	U
1	A	1171	G
1	A	1180	A
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1189	C
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	1225	A
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
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	1317	C
1	A	1320	C
1	A	1332	A
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1398	A
1	A	1405	G
1	A	1421	G
1	A	1442	G
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	1503	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
1	A	1531	A
22	W	30	G
22	W	33	U
22	W	34	G
23	Y	5	U
23	Y	6	U

All (41) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	429	U
1	A	432	A
1	A	484	G
1	A	496	A
1	A	509	A
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	965	A
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	1257	U
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 ⓘ

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
1	G7M	A	527	1	23,26,27	1.47	3 (13%)	34,39,42	1.88	7 (20%)
12	0TD	L	92	12	8,9,10	2.14	1 (12%)	6,11,13	1.71	1 (16%)
1	5MC	A	967	1	19,22,23	1.01	2 (10%)	26,32,35	0.97	2 (7%)
1	5MC	A	1400	1	19,22,23	1.20	2 (10%)	26,32,35	1.14	3 (11%)
1	MA6	A	1519	1	23,26,27	1.33	4 (17%)	33,38,41	0.92	1 (3%)
1	M2G	A	966	1	24,27,28	0.99	3 (12%)	33,40,43	0.82	0
1	2MG	A	1207	1	23,26,27	1.43	5 (21%)	33,38,41	1.17	4 (12%)
1	MA6	A	1518	1	23,26,27	1.03	2 (8%)	33,38,41	0.82	1 (3%)
1	PSU	A	1540	1	18,21,22	1.15	1 (5%)	21,30,33	1.91	4 (19%)
1	5MC	A	1407	1	19,22,23	1.06	1 (5%)	26,32,35	1.21	3 (11%)
1	PSU	A	516	26,1	18,21,22	1.17	1 (5%)	21,30,33	1.74	4 (19%)
1	5MC	A	1404	1	19,22,23	1.16	2 (10%)	26,32,35	1.14	4 (15%)
1	PSU	A	1541	1	18,21,22	1.16	1 (5%)	21,30,33	1.87	4 (19%)
1	UR3	A	1498	1	19,22,23	0.68	0	26,32,35	1.08	1 (3%)
1	4OC	A	1402	1	20,23,24	1.02	2 (10%)	25,32,35	0.77	0

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	G7M	A	527	1	-	2/7/25/26	0/3/3/3
12	0TD	L	92	12	-	3/7/12/14	-
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
1	M2G	A	966	1	-	3/11/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	2/11/29/30	0/3/3/3
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	26,1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	CB-CA	-5.09	1.53	1.54
1	A	527	G7M	C2-N2	4.59	1.44	1.34
1	A	516	PSU	C6-C5	4.00	1.39	1.35
1	A	1540	PSU	C6-C5	3.93	1.39	1.35
1	A	1541	PSU	C6-C5	3.89	1.39	1.35
1	A	1400	5MC	C2-N1	3.66	1.47	1.40
1	A	1404	5MC	C2-N1	3.48	1.47	1.40
1	A	1207	2MG	C2-N1	3.43	1.42	1.36
1	A	1207	2MG	C2-N2	3.37	1.40	1.33
1	A	527	G7M	C4-N3	3.31	1.41	1.34
1	A	527	G7M	CN7-N7	-3.12	1.41	1.46
1	A	1519	MA6	C8-N9	2.86	1.42	1.37
1	A	1519	MA6	C5-C4	2.81	1.44	1.39
1	A	1407	5MC	C2-N1	2.71	1.45	1.40
1	A	1518	MA6	C5-C4	2.66	1.43	1.39
1	A	1404	5MC	C2-N3	2.61	1.41	1.36
1	A	1402	4OC	C2-N3	2.55	1.41	1.36
1	A	1518	MA6	C8-N9	2.55	1.41	1.37
1	A	967	5MC	C2-N1	2.42	1.45	1.40
1	A	1207	2MG	C6-N1	2.38	1.43	1.38
1	A	1519	MA6	C5-N7	2.37	1.43	1.39
1	A	966	M2G	C4-N3	2.32	1.39	1.34
1	A	967	5MC	C2-N3	2.29	1.40	1.36
1	A	966	M2G	C6-N1	2.24	1.43	1.38
1	A	1400	5MC	C2-N3	2.22	1.40	1.36
1	A	1402	4OC	O2-C2	-2.20	1.19	1.23
1	A	1519	MA6	C4-N3	2.18	1.38	1.34
1	A	1207	2MG	C8-N9	2.15	1.42	1.37
1	A	966	M2G	C2-N2	2.15	1.39	1.35
1	A	1207	2MG	C4-N3	2.13	1.39	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	G7M	C2-N3-C4	4.92	120.78	112.30
1	A	1540	PSU	C4-N3-C2	-4.86	119.68	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	C4-N3-C2	-4.84	119.70	126.37
1	A	1540	PSU	N1-C2-N3	4.71	120.13	115.17
1	A	1541	PSU	N1-C2-N3	4.61	120.03	115.17
1	A	516	PSU	N1-C2-N3	4.48	119.90	115.17
1	A	516	PSU	C4-N3-C2	-4.36	120.36	126.37
1	A	527	G7M	C5-C4-N3	-4.06	120.47	128.15
1	A	527	G7M	C5-C6-N1	4.03	120.18	111.84
1	A	527	G7M	O6-C6-C5	-3.49	120.21	128.01
12	L	92	0TD	CSB-SB-CB	-3.33	96.38	102.36
1	A	527	G7M	N9-C4-N3	3.23	132.41	125.95
1	A	527	G7M	C6-C5-N7	3.18	136.16	132.17
1	A	1407	5MC	N4-C4-N3	-2.97	113.13	118.51
1	A	1498	UR3	C6-N1-C2	-2.83	119.48	121.80
1	A	527	G7M	C2-N1-C6	-2.83	119.98	125.11
1	A	516	PSU	C6-N1-C2	-2.80	120.09	122.69
1	A	1407	5MC	C5-C4-N3	2.74	124.57	121.75
1	A	1207	2MG	C5-C4-N3	-2.70	124.10	128.39
1	A	1540	PSU	O2-C2-N1	-2.67	120.03	122.79
1	A	1541	PSU	O2-C2-N1	-2.53	120.17	122.79
1	A	1400	5MC	O2-C2-N3	-2.44	118.49	122.33
1	A	1404	5MC	N4-C4-N3	-2.39	114.19	118.51
1	A	967	5MC	N4-C4-N3	-2.37	114.22	118.51
1	A	1400	5MC	N4-C4-N3	-2.37	114.22	118.51
1	A	1207	2MG	C2-N1-C6	-2.35	121.70	124.55
1	A	1207	2MG	O6-C6-N1	-2.26	115.86	120.11
1	A	1540	PSU	C6-N1-C2	-2.26	120.59	122.69
1	A	1541	PSU	C6-N1-C2	-2.25	120.60	122.69
1	A	967	5MC	C5-C4-N3	2.24	124.05	121.75
1	A	1207	2MG	N9-C4-N3	2.24	130.43	125.95
1	A	1404	5MC	C5-C4-N3	2.19	124.00	121.75
1	A	1404	5MC	O2-C2-N3	-2.09	119.04	122.33
1	A	1404	5MC	C1'-N1-C2	2.06	122.98	118.44
1	A	1519	MA6	C2-N1-C6	2.05	116.83	111.83
1	A	516	PSU	O2-C2-N1	-2.04	120.68	122.79
1	A	1407	5MC	O2-C2-N3	-2.03	119.14	122.33
1	A	1400	5MC	C5-C4-N3	2.02	123.83	121.75
1	A	1518	MA6	C2-N1-C6	2.00	116.72	111.83

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	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	1400	5MC	O4'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1404	5MC	O4'-C4'-C5'-O5'
1	A	1404	5MC	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1540	PSU	O4'-C1'-C5-C4
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	527	G7M	C3'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD2
1	A	1540	PSU	O4'-C1'-C5-C6
1	A	527	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	92	0TD	3	0
1	A	967	5MC	1	0
1	A	1400	5MC	1	0
1	A	1519	MA6	2	0
1	A	1518	MA6	1	0
1	A	1407	5MC	1	0
1	A	1404	5MC	2	0
1	A	1498	UR3	3	0
1	A	1402	4OC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 348 ligands modelled in this entry, 342 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PAR	A	1606	-	44,45,45	1.34	5 (11%)	63,67,67	1.66	12 (19%)
24	PAR	A	1602	-	44,45,45	1.44	8 (18%)	63,67,67	1.67	13 (20%)
24	PAR	A	1605	-	44,45,45	1.35	7 (15%)	63,67,67	1.61	12 (19%)
24	PAR	A	1604	-	44,45,45	1.25	6 (13%)	63,67,67	1.67	12 (19%)
24	PAR	A	1601	1	44,45,45	1.46	7 (15%)	63,67,67	1.62	11 (17%)
24	PAR	A	1603	-	44,45,45	1.47	6 (13%)	63,67,67	1.67	12 (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
24	PAR	A	1606	-	-	8/18/94/94	1/4/4/4
24	PAR	A	1602	-	-	7/18/94/94	0/4/4/4
24	PAR	A	1605	-	-	6/18/94/94	1/4/4/4
24	PAR	A	1604	-	-	4/18/94/94	1/4/4/4
24	PAR	A	1601	1	-	2/18/94/94	0/4/4/4
24	PAR	A	1603	-	-	7/18/94/94	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1603	PAR	C13-C23	4.78	1.59	1.52
24	A	1601	PAR	C34-C24	4.05	1.58	1.53
24	A	1601	PAR	C52-C42	3.82	1.60	1.52
24	A	1603	PAR	C52-C42	3.65	1.59	1.52
24	A	1606	PAR	C13-C23	3.44	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1602	PAR	C13-C23	3.39	1.57	1.52
24	A	1603	PAR	C34-C24	3.38	1.57	1.53
24	A	1606	PAR	C34-C24	3.29	1.57	1.53
24	A	1602	PAR	C34-C24	3.13	1.57	1.53
24	A	1605	PAR	C52-C42	3.07	1.58	1.52
24	A	1605	PAR	C13-C23	3.04	1.56	1.52
24	A	1606	PAR	C52-C42	3.03	1.58	1.52
24	A	1604	PAR	C52-C42	3.02	1.58	1.52
24	A	1601	PAR	C24-N24	3.00	1.51	1.47
24	A	1604	PAR	C34-C24	3.00	1.57	1.53
24	A	1603	PAR	O43-C13	2.99	1.47	1.41
24	A	1605	PAR	C34-C24	2.99	1.57	1.53
24	A	1601	PAR	C14-C24	2.96	1.58	1.52
24	A	1602	PAR	C31-C21	2.92	1.57	1.53
24	A	1604	PAR	C13-C23	2.81	1.56	1.52
24	A	1602	PAR	C33-C43	2.64	1.59	1.52
24	A	1606	PAR	C31-C21	2.64	1.56	1.53
24	A	1601	PAR	C33-C43	2.60	1.59	1.52
24	A	1602	PAR	C14-C24	2.59	1.57	1.52
24	A	1602	PAR	C11-C21	2.53	1.57	1.52
24	A	1605	PAR	C33-C43	2.50	1.59	1.52
24	A	1605	PAR	C14-C24	2.47	1.57	1.52
24	A	1601	PAR	C62-C52	2.42	1.58	1.52
24	A	1604	PAR	C33-C43	2.24	1.58	1.52
24	A	1605	PAR	O52-C52	2.21	1.49	1.43
24	A	1601	PAR	C13-C23	2.16	1.55	1.52
24	A	1602	PAR	O33-C14	2.14	1.47	1.41
24	A	1603	PAR	C14-C24	2.13	1.56	1.52
24	A	1603	PAR	C42-C32	2.12	1.57	1.53
24	A	1606	PAR	O43-C13	2.12	1.45	1.41
24	A	1604	PAR	C31-C21	2.11	1.56	1.53
24	A	1605	PAR	O43-C13	2.10	1.45	1.41
24	A	1602	PAR	O52-C52	2.09	1.49	1.43
24	A	1604	PAR	O43-C13	2.09	1.45	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1604	PAR	O33-C14-C24	6.71	119.07	108.08
24	A	1602	PAR	O33-C14-C24	6.69	119.02	108.08
24	A	1601	PAR	O33-C14-C24	6.62	118.91	108.08
24	A	1603	PAR	O33-C14-C24	6.60	118.88	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1606	PAR	O33-C14-C24	6.45	118.64	108.08
24	A	1605	PAR	O33-C14-C24	6.38	118.53	108.08
24	A	1603	PAR	C13-C23-C33	3.78	106.65	102.10
24	A	1606	PAR	C13-C23-C33	3.67	106.52	102.10
24	A	1604	PAR	C14-O33-C33	-3.16	110.49	117.98
24	A	1605	PAR	C34-C24-N24	-3.15	104.59	111.05
24	A	1602	PAR	O11-C11-O51	3.12	118.90	110.69
24	A	1604	PAR	C13-O52-C52	-3.08	110.68	117.98
24	A	1602	PAR	O34-C34-C44	-3.06	103.17	110.38
24	A	1602	PAR	C22-C12-C62	3.04	114.62	110.08
24	A	1604	PAR	C13-C23-C33	3.01	105.72	102.10
24	A	1602	PAR	C34-C24-N24	-3.00	104.91	111.05
24	A	1603	PAR	C14-O33-C33	-2.98	110.91	117.98
24	A	1603	PAR	O11-C11-O51	2.98	118.53	110.69
24	A	1606	PAR	C14-O33-C33	-2.96	110.96	117.98
24	A	1603	PAR	C34-C24-N24	-2.95	105.00	111.05
24	A	1604	PAR	O52-C13-O43	-2.95	108.36	111.37
24	A	1606	PAR	C34-C24-N24	-2.95	105.01	111.05
24	A	1604	PAR	O11-C11-O51	2.94	118.42	110.69
24	A	1604	PAR	O34-C34-C44	-2.93	103.46	110.38
24	A	1604	PAR	C34-C24-N24	-2.93	105.05	111.05
24	A	1601	PAR	O34-C34-C44	-2.93	103.48	110.38
24	A	1601	PAR	O11-C11-O51	2.91	118.36	110.69
24	A	1605	PAR	O11-C11-O51	2.90	118.32	110.69
24	A	1603	PAR	O34-C34-C44	-2.87	103.60	110.38
24	A	1606	PAR	O34-C34-C44	-2.87	103.61	110.38
24	A	1605	PAR	O34-C34-C44	-2.86	103.64	110.38
24	A	1601	PAR	C14-O33-C33	-2.82	111.30	117.98
24	A	1601	PAR	C13-O52-C52	-2.78	111.39	117.98
24	A	1606	PAR	O11-C11-O51	2.73	117.89	110.69
24	A	1606	PAR	C13-O52-C52	-2.68	111.62	117.98
24	A	1605	PAR	C14-O33-C33	-2.67	111.64	117.98
24	A	1602	PAR	C13-C23-C33	2.65	105.29	102.10
24	A	1606	PAR	O52-C13-O43	-2.55	108.77	111.37
24	A	1602	PAR	C14-O33-C33	-2.52	111.99	117.98
24	A	1603	PAR	C13-O52-C52	-2.51	112.03	117.98
24	A	1605	PAR	C13-O52-C52	-2.50	112.05	117.98
24	A	1601	PAR	C34-C24-N24	-2.46	106.00	111.05
24	A	1605	PAR	C13-C23-C33	2.45	105.04	102.10
24	A	1601	PAR	O43-C13-C23	-2.41	101.91	104.98
24	A	1602	PAR	O51-C51-C61	2.37	112.31	106.44
24	A	1603	PAR	O51-C51-C61	2.35	112.27	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1605	PAR	O51-C51-C61	2.35	112.27	106.44
24	A	1603	PAR	O52-C13-O43	-2.33	108.99	111.37
24	A	1602	PAR	C11-O51-C51	2.30	118.21	113.72
24	A	1606	PAR	O51-C51-C61	2.26	112.04	106.44
24	A	1602	PAR	C13-O52-C52	-2.24	112.67	117.98
24	A	1601	PAR	O51-C51-C61	2.24	111.98	106.44
24	A	1603	PAR	C22-C32-C42	2.21	114.93	109.50
24	A	1602	PAR	C32-C22-C12	2.21	114.81	111.02
24	A	1604	PAR	O51-C51-C61	2.19	111.87	106.44
24	A	1605	PAR	O52-C13-O43	-2.17	109.15	111.37
24	A	1601	PAR	O52-C13-O43	-2.16	109.16	111.37
24	A	1605	PAR	O54-C54-C44	2.16	113.59	109.70
24	A	1604	PAR	O52-C52-C42	2.15	112.88	107.42
24	A	1603	PAR	O54-C54-C44	2.13	113.54	109.70
24	A	1606	PAR	O54-C54-C44	2.12	113.51	109.70
24	A	1604	PAR	O54-C54-C44	2.11	113.50	109.70
24	A	1602	PAR	O43-C13-C23	-2.10	102.30	104.98
24	A	1603	PAR	C11-O51-C51	2.09	117.81	113.72
24	A	1604	PAR	C22-C12-C62	2.09	113.20	110.08
24	A	1601	PAR	C11-O51-C51	2.08	117.79	113.72
24	A	1605	PAR	O43-C13-C23	-2.08	102.33	104.98
24	A	1606	PAR	C22-C12-C62	2.08	113.19	110.08
24	A	1605	PAR	O52-C52-C42	2.04	112.59	107.42
24	A	1606	PAR	O52-C52-C42	2.03	112.58	107.42
24	A	1602	PAR	O43-C43-C53	2.02	113.48	109.22
24	A	1601	PAR	O33-C14-O54	-2.02	105.39	110.69

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	O54-C54-C64-N64
24	A	1602	PAR	C23-C13-O52-C52
24	A	1602	PAR	O43-C13-O52-C52
24	A	1604	PAR	C21-C11-O11-C42
24	A	1605	PAR	C21-C11-O11-C42
24	A	1605	PAR	C44-C54-C64-N64
24	A	1605	PAR	O54-C54-C64-N64
24	A	1606	PAR	O51-C11-O11-C42
24	A	1606	PAR	C23-C13-O52-C52
24	A	1606	PAR	O54-C54-C64-N64
24	A	1605	PAR	O51-C11-O11-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	1606	PAR	O54-C14-O33-C33
24	A	1602	PAR	O54-C14-O33-C33
24	A	1603	PAR	O43-C43-C53-O53
24	A	1603	PAR	O51-C11-O11-C42
24	A	1603	PAR	C41-C51-C61-O61
24	A	1604	PAR	O54-C14-O33-C33
24	A	1603	PAR	C33-C43-C53-O53
24	A	1602	PAR	C41-C51-C61-O61
24	A	1604	PAR	O43-C13-O52-C52
24	A	1603	PAR	O51-C51-C61-O61
24	A	1602	PAR	O43-C43-C53-O53
24	A	1605	PAR	O51-C51-C61-O61
24	A	1603	PAR	O54-C54-C64-N64
24	A	1606	PAR	O43-C43-C53-O53
24	A	1602	PAR	O51-C51-C61-O61
24	A	1606	PAR	O43-C13-O52-C52
24	A	1605	PAR	C62-C52-O52-C13
24	A	1606	PAR	C21-C11-O11-C42
24	A	1602	PAR	C43-C33-O33-C14
24	A	1603	PAR	C23-C33-O33-C14
24	A	1604	PAR	C43-C33-O33-C14
24	A	1606	PAR	C43-C33-O33-C14
24	A	1601	PAR	C52-C42-O11-C11

All (3) ring outliers are listed below:

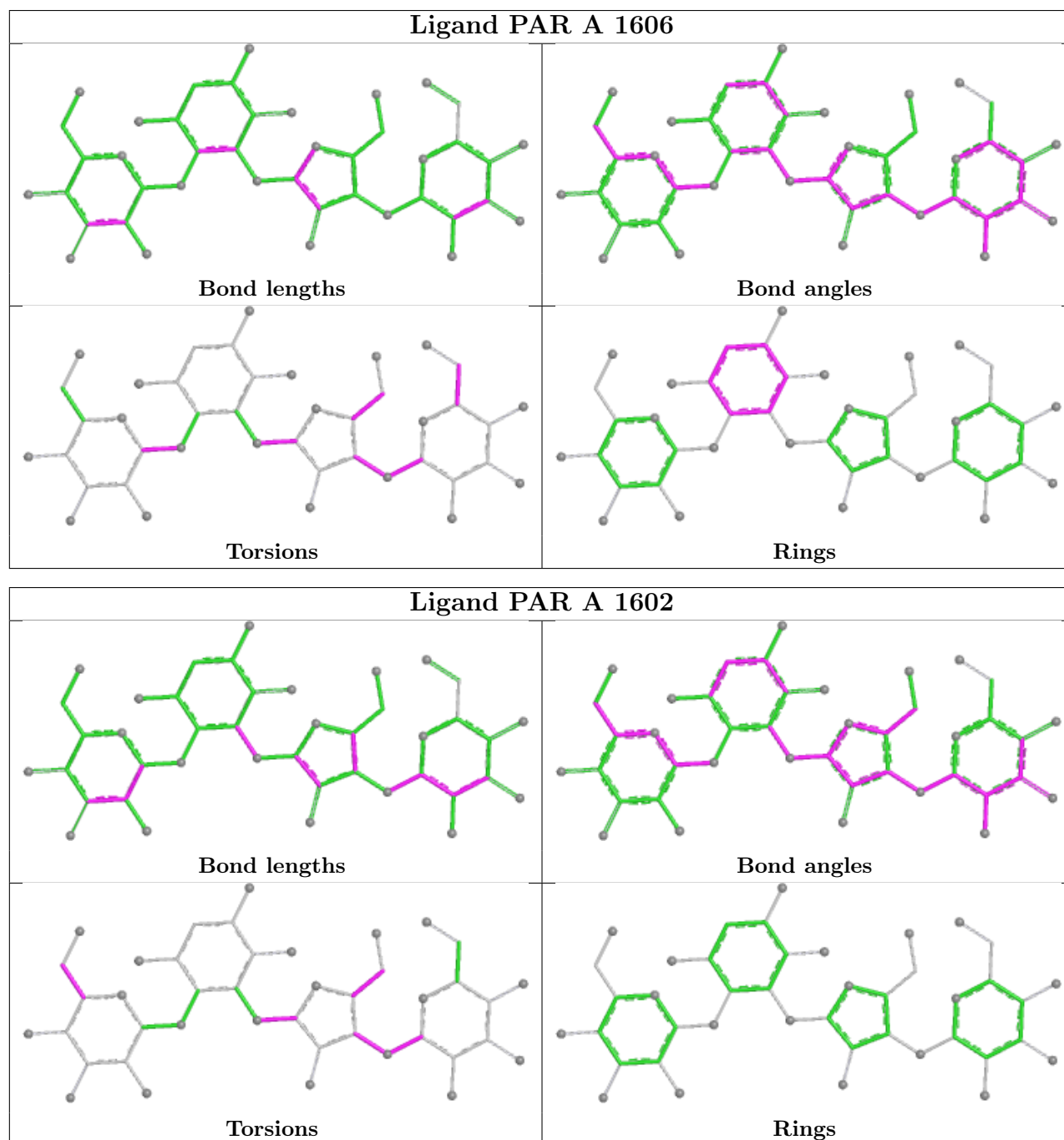
Mol	Chain	Res	Type	Atoms
24	A	1605	PAR	C12-C22-C32-C42-C52-C62
24	A	1606	PAR	C12-C22-C32-C42-C52-C62
24	A	1604	PAR	C12-C22-C32-C42-C52-C62

6 monomers are involved in 14 short contacts:

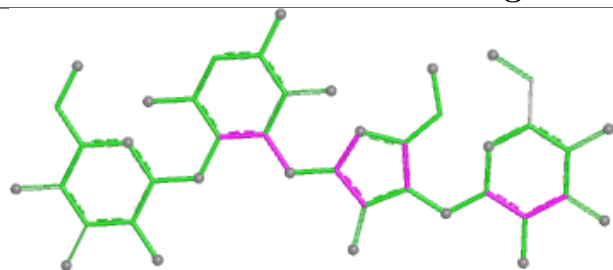
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1606	PAR	3	0
24	A	1602	PAR	3	0
24	A	1605	PAR	1	0
24	A	1604	PAR	2	0
24	A	1601	PAR	2	0
24	A	1603	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

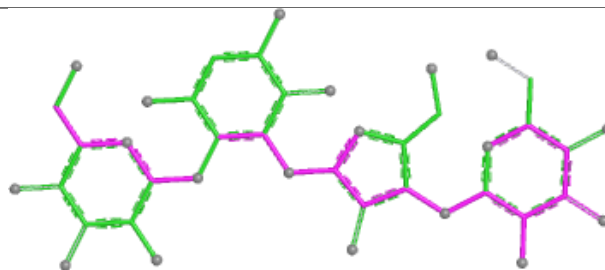
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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



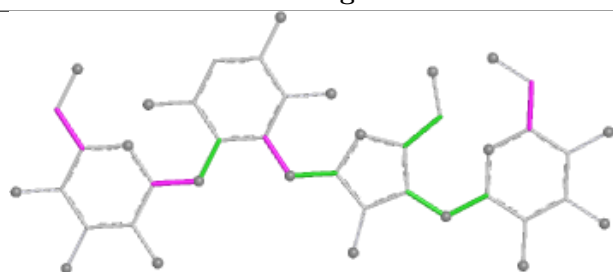
Ligand PAR A 1605



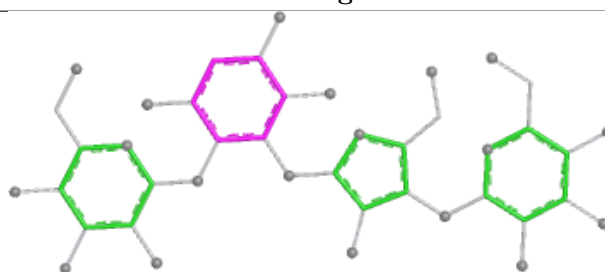
Bond lengths



Bond angles

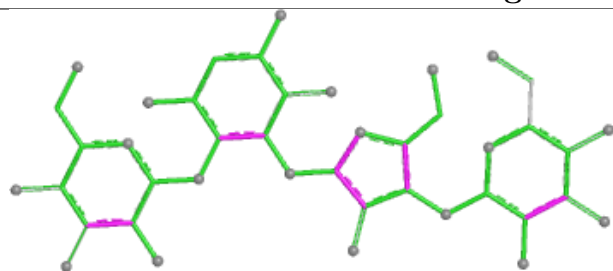


Torsions

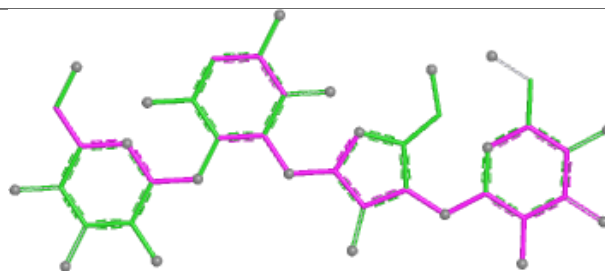


Rings

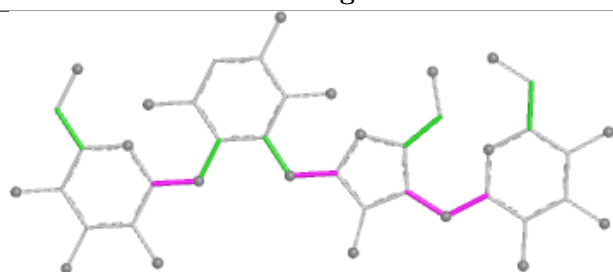
Ligand PAR A 1604



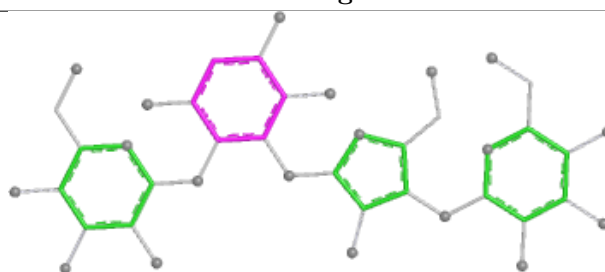
Bond lengths



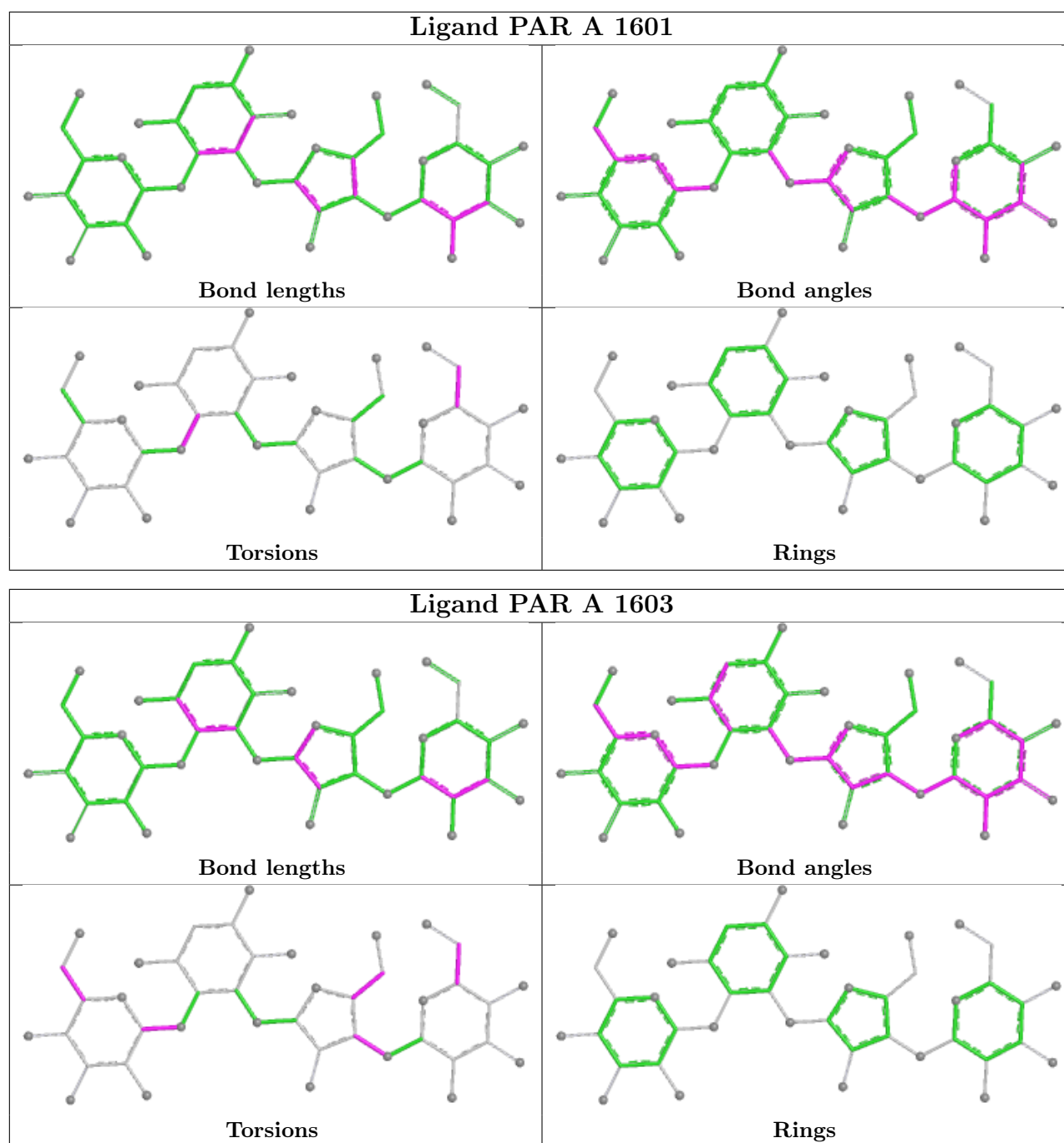
Bond angles



Torsions



Rings



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%)	-0.41	13 (0%) 81 58	43, 75, 152, 281	0
2	B	236/236 (100%)	0.18	10 (4%) 40 24	50, 105, 192, 246	0
3	C	207/207 (100%)	0.09	3 (1%) 73 49	17, 107, 144, 195	0
4	D	208/208 (100%)	0.19	14 (6%) 24 16	47, 83, 143, 184	0
5	E	151/151 (100%)	-0.32	0 100 100	39, 64, 97, 161	0
6	F	101/101 (100%)	-0.17	0 100 100	58, 97, 135, 153	0
7	G	155/155 (100%)	0.12	7 (4%) 38 22	57, 86, 177, 234	0
8	H	138/138 (100%)	-0.42	1 (0%) 84 64	34, 59, 92, 120	0
9	I	127/127 (100%)	0.30	4 (3%) 51 31	60, 101, 144, 163	0
10	J	99/99 (100%)	0.89	13 (13%) 7 6	38, 134, 197, 258	0
11	K	117/117 (100%)	-0.00	2 (1%) 69 44	45, 79, 113, 164	0
12	L	124/125 (99%)	0.11	5 (4%) 42 25	36, 71, 111, 250	0
13	M	118/118 (100%)	0.20	6 (5%) 33 20	66, 92, 136, 206	0
14	N	60/60 (100%)	0.33	3 (5%) 34 20	63, 85, 150, 255	0
15	O	88/88 (100%)	-0.13	0 100 100	37, 74, 120, 150	0
16	P	84/84 (100%)	-0.17	0 100 100	40, 68, 97, 201	0
17	Q	99/99 (100%)	-0.19	2 (2%) 65 41	34, 63, 104, 122	0
18	R	73/73 (100%)	-0.08	0 100 100	53, 82, 145, 173	0
19	S	81/81 (100%)	0.66	7 (8%) 16 12	32, 113, 164, 209	0
20	T	99/99 (100%)	0.01	3 (3%) 52 31	55, 71, 121, 157	0
21	U	25/25 (100%)	1.23	5 (20%) 3 3	35, 105, 164, 172	0
22	W	15/15 (100%)	0.39	0 100 100	80, 124, 197, 203	0
23	Y	6/6 (100%)	1.12	2 (33%) 1 1	92, 100, 173, 203	0
All	All	3909/3934 (99%)	-0.10	100 (2%) 57 34	17, 82, 152, 281	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	8.9
4	D	23	GLY	6.2
1	A	1129	C	5.8
19	S	2	PRO	5.7
7	G	5	ARG	5.4
21	U	25	LYS	4.8
12	L	29	GLY	4.7
12	L	28	LYS	4.1
10	J	43	ARG	4.1
3	C	2	GLY	4.0
10	J	17	ASP	3.8
21	U	6	ARG	3.7
4	D	9	CYS	3.6
4	D	37	PRO	3.6
2	B	140	HIS	3.5
1	A	1539	C	3.5
10	J	6	ILE	3.4
21	U	10	ARG	3.3
20	T	100	ILE	3.3
10	J	100	THR	3.2
14	N	13	THR	3.2
9	I	30	GLY	3.2
4	D	32	ALA	2.9
9	I	126	SER	2.9
7	G	83	ALA	2.9
10	J	35	SER	2.9
7	G	85	TYR	2.9
17	Q	92	ARG	2.8
1	A	202	U	2.7
4	D	26	CYS	2.7
10	J	34	VAL	2.7
1	A	1037	C	2.7
1	A	1533	C	2.7
10	J	72	VAL	2.7
19	S	6	LYS	2.6
2	B	203	GLY	2.6
2	B	144	ARG	2.6
10	J	21	GLN	2.6
1	A	298	A	2.6
1	A	412	A	2.6
4	D	6	GLY	2.6
12	L	27	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	U	24	ARG	2.6
10	J	90	LEU	2.6
7	G	156	TRP	2.5
1	A	723	U	2.5
4	D	5	ILE	2.5
7	G	81	GLY	2.5
1	A	1036	G	2.5
4	D	4	TYR	2.5
4	D	31	CYS	2.5
4	D	3	ARG	2.5
9	I	125	TYR	2.5
13	M	8	GLU	2.4
1	A	1003(A)	G	2.4
2	B	130	ARG	2.4
17	Q	100	LYS	2.4
21	U	23	PRO	2.4
11	K	12	ARG	2.4
11	K	51	LYS	2.3
13	M	5	ALA	2.3
1	A	532	A	2.3
2	B	133	LYS	2.3
9	I	39	GLY	2.3
3	C	207	VAL	2.3
23	Y	6	U	2.3
13	M	7	VAL	2.3
19	S	33	THR	2.2
7	G	154	TYR	2.2
10	J	70	ARG	2.2
3	C	193	TYR	2.2
4	D	22	LYS	2.2
20	T	73	HIS	2.2
10	J	74	ILE	2.1
10	J	98	ILE	2.1
23	Y	5	U	2.1
2	B	48	MET	2.1
19	S	4	SER	2.1
2	B	13	ALA	2.1
20	T	106	ALA	2.1
13	M	119	GLY	2.1
12	L	128	ALA	2.1
4	D	45	GLN	2.1
7	G	84	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	20	LYS	2.1
10	J	88	LEU	2.1
19	S	14	HIS	2.1
8	H	1	MET	2.1
2	B	76	GLN	2.1
4	D	209	ARG	2.0
13	M	9	ILE	2.0
19	S	5	LEU	2.0
14	N	2	ALA	2.0
2	B	23	ARG	2.0
13	M	80	ARG	2.0
1	A	1125	U	2.0
2	B	89	GLY	2.0
14	N	4	LYS	2.0
4	D	21	LEU	2.0
1	A	1054	C	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	0.83	0.22	248,254,267,267	0
1	PSU	A	1541	20/21	0.87	0.21	195,209,242,243	0
1	PSU	A	516	20/21	0.92	0.10	70,77,82,83	0
1	2MG	A	1207	24/25	0.95	0.09	88,93,104,109	0
1	5MC	A	1407	21/22	0.96	0.10	58,60,67,69	0
1	M2G	A	966	25/26	0.96	0.10	65,71,79,86	0
1	G7M	A	527	24/25	0.96	0.08	56,60,64,67	0
1	5MC	A	1404	21/22	0.97	0.08	53,54,56,58	0
1	5MC	A	967	21/22	0.97	0.08	62,71,77,80	0
1	UR3	A	1498	21/22	0.97	0.10	55,57,58,65	0
1	MA6	A	1518	24/25	0.97	0.09	55,59,65,72	0
1	MA6	A	1519	24/25	0.97	0.09	53,56,63,69	0
1	5MC	A	1400	21/22	0.97	0.08	55,58,66,76	0
1	4OC	A	1402	22/23	0.97	0.09	54,61,67,69	0
12	0TD	L	92	10/11	0.97	0.10	71,76,88,91	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
26	MG	A	1740	1/1	0.36	0.31	173,173,173,173	0
26	MG	A	1826	1/1	0.51	0.87	222,222,222,222	0
26	MG	A	1656	1/1	0.53	0.35	175,175,175,175	0
26	MG	A	1738	1/1	0.57	0.43	190,190,190,190	0
25	K	A	1621	1/1	0.69	0.16	119,119,119,119	0
25	K	A	1616	1/1	0.71	0.17	117,117,117,117	0
26	MG	S	103	1/1	0.73	0.13	97,97,97,97	0
26	MG	A	1834	1/1	0.75	0.34	188,188,188,188	0
26	MG	A	1731	1/1	0.75	0.47	128,128,128,128	0
25	K	A	1634	1/1	0.76	0.14	108,108,108,108	0
26	MG	A	1658	1/1	0.76	0.19	51,51,51,51	0
26	MG	A	1684	1/1	0.76	0.47	365,365,365,365	0
26	MG	A	1819	1/1	0.77	0.17	136,136,136,136	0
26	MG	A	1888	1/1	0.78	0.10	69,69,69,69	0
26	MG	A	1747	1/1	0.78	0.30	165,165,165,165	0
25	K	A	1629	1/1	0.79	0.13	144,144,144,144	0
25	K	A	1636	1/1	0.79	0.15	101,101,101,101	0
25	K	A	1625	1/1	0.80	0.10	68,68,68,68	0
26	MG	A	1673	1/1	0.80	0.24	135,135,135,135	0
25	K	A	1613	1/1	0.81	0.10	100,100,100,100	0
25	K	A	1628	1/1	0.81	0.14	99,99,99,99	0
25	K	A	1615	1/1	0.81	0.17	77,77,77,77	0
26	MG	A	1868	1/1	0.81	0.36	75,75,75,75	0
26	MG	A	1871	1/1	0.81	0.19	72,72,72,72	0
26	MG	A	1884	1/1	0.81	0.07	82,82,82,82	0
26	MG	A	1714	1/1	0.81	0.33	206,206,206,206	0
26	MG	A	1918	1/1	0.81	0.06	53,53,53,53	0
26	MG	A	1786	1/1	0.81	0.14	57,57,57,57	0
26	MG	D	302	1/1	0.82	0.15	94,94,94,94	0
26	MG	P	103	1/1	0.82	0.12	60,60,60,60	0
26	MG	A	1774	1/1	0.82	0.24	65,65,65,65	0
25	K	A	1608	1/1	0.83	0.08	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
26	MG	A	1654	1/1	0.83	0.31	158,158,158,158	0
26	MG	A	1757	1/1	0.83	0.15	74,74,74,74	0
25	K	A	1623	1/1	0.83	0.13	85,85,85,85	0
26	MG	A	1702	1/1	0.84	0.24	74,74,74,74	0
26	MG	A	1889	1/1	0.84	0.10	103,103,103,103	0
26	MG	A	1903	1/1	0.84	0.09	83,83,83,83	0
26	MG	A	1805	1/1	0.84	0.25	52,52,52,52	0
26	MG	A	1692	1/1	0.84	0.32	120,120,120,120	0
26	MG	A	1874	1/1	0.84	0.17	53,53,53,53	0
26	MG	A	1776	1/1	0.84	0.15	51,51,51,51	0
26	MG	A	1907	1/1	0.85	0.07	49,49,49,49	0
26	MG	A	1886	1/1	0.85	0.16	51,51,51,51	0
25	K	A	1607	1/1	0.85	0.12	113,113,113,113	0
25	K	A	1612	1/1	0.85	0.18	96,96,96,96	0
26	MG	A	1821	1/1	0.85	0.14	39,39,39,39	0
24	PAR	A	1605	42/42	0.86	0.25	120,149,155,158	0
26	MG	A	1724	1/1	0.86	0.09	64,64,64,64	0
26	MG	A	1675	1/1	0.86	0.42	125,125,125,125	0
26	MG	A	1678	1/1	0.86	0.16	120,120,120,120	0
26	MG	A	1806	1/1	0.86	0.16	62,62,62,62	0
25	K	A	1610	1/1	0.86	0.23	110,110,110,110	0
26	MG	A	1894	1/1	0.86	0.24	51,51,51,51	0
26	MG	A	1746	1/1	0.86	0.45	238,238,238,238	0
25	K	A	1631	1/1	0.86	0.11	102,102,102,102	0
26	MG	A	1827	1/1	0.86	0.09	77,77,77,77	0
25	K	A	1619	1/1	0.86	0.11	121,121,121,121	0
26	MG	A	1842	1/1	0.86	0.12	28,28,28,28	0
26	MG	A	1758	1/1	0.86	0.23	59,59,59,59	0
26	MG	C	301	1/1	0.87	0.11	57,57,57,57	0
26	MG	A	1707	1/1	0.87	0.20	99,99,99,99	0
25	K	A	1641	1/1	0.87	0.12	108,108,108,108	0
26	MG	A	1919	1/1	0.87	0.04	45,45,45,45	0
26	MG	A	1816	1/1	0.88	0.14	64,64,64,64	0
26	MG	A	1828	1/1	0.88	0.14	51,51,51,51	0
25	K	E	201	1/1	0.88	0.13	84,84,84,84	0
26	MG	A	1840	1/1	0.88	0.16	27,27,27,27	0
26	MG	A	1887	1/1	0.88	0.08	47,47,47,47	0
25	K	A	1633	1/1	0.88	0.09	102,102,102,102	0
26	MG	A	1867	1/1	0.88	0.15	35,35,35,35	0
26	MG	A	1742	1/1	0.88	0.30	172,172,172,172	0
26	MG	A	1648	1/1	0.89	0.21	58,58,58,58	0
26	MG	A	1883	1/1	0.89	0.12	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1659	1/1	0.89	0.25	70,70,70,70	0
26	MG	A	1649	1/1	0.89	0.19	128,128,128,128	0
26	MG	A	1823	1/1	0.89	0.10	50,50,50,50	0
26	MG	A	1748	1/1	0.89	0.10	41,41,41,41	0
26	MG	A	1715	1/1	0.89	0.09	38,38,38,38	0
26	MG	A	1652	1/1	0.89	0.33	377,377,377,377	0
26	MG	A	1829	1/1	0.89	0.16	41,41,41,41	0
26	MG	A	1773	1/1	0.89	0.14	55,55,55,55	0
26	MG	A	1909	1/1	0.89	0.16	60,60,60,60	0
26	MG	A	1914	1/1	0.89	0.09	60,60,60,60	0
26	MG	A	1725	1/1	0.89	0.11	64,64,64,64	0
26	MG	A	1726	1/1	0.89	0.10	46,46,46,46	0
26	MG	A	1844	1/1	0.89	0.34	63,63,63,63	0
24	PAR	A	1602	42/42	0.89	0.20	60,95,137,138	0
25	K	A	1618	1/1	0.89	0.10	109,109,109,109	0
26	MG	A	1657	1/1	0.89	0.23	91,91,91,91	0
26	MG	A	1762	1/1	0.90	0.10	41,41,41,41	0
26	MG	A	1857	1/1	0.90	0.10	62,62,62,62	0
26	MG	A	1896	1/1	0.90	0.08	56,56,56,56	0
26	MG	A	1772	1/1	0.90	0.09	43,43,43,43	0
26	MG	A	1663	1/1	0.90	0.10	57,57,57,57	0
26	MG	A	1668	1/1	0.90	0.10	30,30,30,30	0
26	MG	A	1670	1/1	0.90	0.15	54,54,54,54	0
26	MG	A	1878	1/1	0.90	0.08	38,38,38,38	0
25	K	A	1609	1/1	0.90	0.11	99,99,99,99	0
26	MG	A	1920	1/1	0.90	0.19	56,56,56,56	0
26	MG	A	1729	1/1	0.90	0.40	577,577,577,577	0
26	MG	A	1674	1/1	0.90	0.05	9,9,9,9	0
26	MG	D	303	1/1	0.90	0.07	50,50,50,50	0
26	MG	F	201	1/1	0.90	0.06	52,52,52,52	0
26	MG	A	1813	1/1	0.90	0.09	35,35,35,35	0
26	MG	S	102	1/1	0.90	0.05	61,61,61,61	0
25	K	A	1639	1/1	0.90	0.09	89,89,89,89	0
26	MG	A	1830	1/1	0.91	0.19	50,50,50,50	0
26	MG	A	1712	1/1	0.91	0.07	44,44,44,44	0
26	MG	A	1790	1/1	0.91	0.09	39,39,39,39	0
26	MG	A	1793	1/1	0.91	0.11	48,48,48,48	0
25	K	A	1617	1/1	0.91	0.16	112,112,112,112	0
26	MG	A	1734	1/1	0.91	0.19	47,47,47,47	0
26	MG	A	1912	1/1	0.91	0.06	37,37,37,37	0
26	MG	A	1695	1/1	0.91	0.27	107,107,107,107	0
26	MG	A	1768	1/1	0.91	0.05	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1869	1/1	0.91	0.07	17,17,17,17	0
26	MG	A	1817	1/1	0.91	0.10	74,74,74,74	0
26	MG	A	1717	1/1	0.91	0.06	61,61,61,61	0
26	MG	A	1696	1/1	0.91	0.17	61,61,61,61	0
26	MG	A	1645	1/1	0.91	0.13	90,90,90,90	0
25	K	A	1638	1/1	0.91	0.21	78,78,78,78	0
26	MG	A	1778	1/1	0.91	0.13	66,66,66,66	0
26	MG	A	1781	1/1	0.91	0.20	41,41,41,41	0
26	MG	A	1784	1/1	0.91	0.12	45,45,45,45	0
26	MG	A	1644	1/1	0.92	0.06	59,59,59,59	0
26	MG	A	1689	1/1	0.92	0.16	97,97,97,97	0
26	MG	A	1775	1/1	0.92	0.38	70,70,70,70	0
25	K	A	1640	1/1	0.92	0.16	113,113,113,113	0
24	PAR	A	1604	42/42	0.92	0.13	61,89,102,111	0
26	MG	A	1720	1/1	0.92	0.10	57,57,57,57	0
25	K	A	1611	1/1	0.92	0.08	101,101,101,101	0
26	MG	A	1701	1/1	0.92	0.09	18,18,18,18	0
26	MG	A	1898	1/1	0.92	0.06	63,63,63,63	0
26	MG	A	1835	1/1	0.92	0.12	62,62,62,62	0
26	MG	A	1904	1/1	0.92	0.07	34,34,34,34	0
25	K	E	202	1/1	0.92	0.06	82,82,82,82	0
26	MG	A	1759	1/1	0.92	0.09	61,61,61,61	0
26	MG	A	1843	1/1	0.92	0.09	35,35,35,35	0
26	MG	A	1913	1/1	0.92	0.16	55,55,55,55	0
26	MG	A	1706	1/1	0.92	0.12	48,48,48,48	0
26	MG	A	1849	1/1	0.92	0.12	66,66,66,66	0
26	MG	A	1766	1/1	0.92	0.07	29,29,29,29	0
26	MG	A	1860	1/1	0.92	0.11	44,44,44,44	0
26	MG	A	1807	1/1	0.92	0.11	57,57,57,57	0
26	MG	A	1653	1/1	0.92	0.15	112,112,112,112	0
26	MG	A	1815	1/1	0.92	0.16	35,35,35,35	0
26	MG	E	204	1/1	0.92	0.06	47,47,47,47	0
26	MG	A	1769	1/1	0.92	0.33	73,73,73,73	0
26	MG	P	102	1/1	0.92	0.07	53,53,53,53	0
26	MG	A	1770	1/1	0.92	0.12	31,31,31,31	0
26	MG	A	1708	1/1	0.92	0.16	80,80,80,80	0
26	MG	A	1882	1/1	0.92	0.11	46,46,46,46	0
26	MG	A	1744	1/1	0.93	0.08	60,60,60,60	0
25	K	A	1614	1/1	0.93	0.08	92,92,92,92	0
26	MG	A	1820	1/1	0.93	0.13	85,85,85,85	0
26	MG	A	1795	1/1	0.93	0.28	51,51,51,51	0
26	MG	A	1915	1/1	0.93	0.13	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1916	1/1	0.93	0.07	52,52,52,52	0
26	MG	A	1885	1/1	0.93	0.12	58,58,58,58	0
26	MG	A	1796	1/1	0.93	0.12	27,27,27,27	0
26	MG	A	1718	1/1	0.93	0.12	62,62,62,62	0
26	MG	A	1699	1/1	0.93	0.09	60,60,60,60	0
26	MG	A	1865	1/1	0.93	0.17	27,27,27,27	0
24	PAR	A	1603	42/42	0.93	0.15	34,78,97,101	0
26	MG	A	1812	1/1	0.93	0.13	48,48,48,48	0
25	K	A	1632	1/1	0.93	0.16	121,121,121,121	0
26	MG	L	202	1/1	0.93	0.04	58,58,58,58	0
26	MG	A	1785	1/1	0.93	0.10	59,59,59,59	0
26	MG	A	1681	1/1	0.93	0.06	41,41,41,41	0
26	MG	A	1905	1/1	0.93	0.24	65,65,65,65	0
26	MG	A	1877	1/1	0.93	0.08	48,48,48,48	0
26	MG	A	1750	1/1	0.94	0.12	61,61,61,61	0
26	MG	A	1895	1/1	0.94	0.15	65,65,65,65	0
26	MG	A	1850	1/1	0.94	0.18	59,59,59,59	0
26	MG	A	1854	1/1	0.94	0.09	50,50,50,50	0
26	MG	A	1900	1/1	0.94	0.18	41,41,41,41	0
26	MG	A	1756	1/1	0.94	0.12	35,35,35,35	0
26	MG	A	1728	1/1	0.94	0.08	23,23,23,23	0
24	PAR	A	1606	42/42	0.94	0.14	87,95,101,105	0
26	MG	A	1700	1/1	0.94	0.19	57,57,57,57	0
25	K	A	1622	1/1	0.94	0.10	97,97,97,97	0
26	MG	A	1911	1/1	0.94	0.10	67,67,67,67	0
26	MG	A	1765	1/1	0.94	0.10	47,47,47,47	0
26	MG	A	1736	1/1	0.94	0.22	108,108,108,108	0
26	MG	A	1686	1/1	0.94	0.16	111,111,111,111	0
26	MG	A	1876	1/1	0.94	0.06	55,55,55,55	0
25	K	A	1637	1/1	0.94	0.11	123,123,123,123	0
26	MG	A	1800	1/1	0.94	0.11	41,41,41,41	0
26	MG	A	1879	1/1	0.94	0.07	49,49,49,49	0
26	MG	A	1880	1/1	0.94	0.11	59,59,59,59	0
26	MG	A	1881	1/1	0.94	0.12	48,48,48,48	0
26	MG	A	1801	1/1	0.94	0.18	59,59,59,59	0
26	MG	A	1722	1/1	0.94	0.19	95,95,95,95	0
26	MG	A	1646	1/1	0.94	0.21	27,27,27,27	0
24	PAR	A	1601	42/42	0.94	0.11	35,58,77,81	0
26	MG	H	201	1/1	0.94	0.03	55,55,55,55	0
26	MG	L	201	1/1	0.94	0.05	69,69,69,69	0
26	MG	A	1841	1/1	0.94	0.13	26,26,26,26	0
26	MG	A	1810	1/1	0.94	0.11	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1679	1/1	0.94	0.14	80,80,80,80	0
26	MG	Q	201	1/1	0.94	0.10	51,51,51,51	0
26	MG	Q	203	1/1	0.94	0.04	44,44,44,44	0
26	MG	A	1727	1/1	0.94	0.19	105,105,105,105	0
26	MG	A	1891	1/1	0.94	0.15	57,57,57,57	0
26	MG	Y	101	1/1	0.94	0.27	74,74,74,74	0
26	MG	A	1783	1/1	0.95	0.07	32,32,32,32	0
26	MG	A	1908	1/1	0.95	0.17	87,87,87,87	0
25	K	A	1620	1/1	0.95	0.11	65,65,65,65	0
26	MG	A	1719	1/1	0.95	0.06	32,32,32,32	0
26	MG	A	1698	1/1	0.95	0.07	39,39,39,39	0
26	MG	A	1787	1/1	0.95	0.10	51,51,51,51	0
26	MG	A	1690	1/1	0.95	0.13	0,0,0,0	0
26	MG	A	1845	1/1	0.95	0.08	41,41,41,41	0
26	MG	A	1846	1/1	0.95	0.18	56,56,56,56	0
26	MG	A	1917	1/1	0.95	0.08	24,24,24,24	0
26	MG	A	1735	1/1	0.95	0.06	106,106,106,106	0
26	MG	A	1753	1/1	0.95	0.36	56,56,56,56	0
25	K	A	1624	1/1	0.95	0.12	97,97,97,97	0
26	MG	A	1855	1/1	0.95	0.12	54,54,54,54	0
26	MG	A	1799	1/1	0.95	0.10	46,46,46,46	0
26	MG	A	1694	1/1	0.95	0.09	35,35,35,35	0
26	MG	A	1890	1/1	0.95	0.04	53,53,53,53	0
26	MG	A	1651	1/1	0.95	0.09	30,30,30,30	0
26	MG	A	1892	1/1	0.95	0.09	33,33,33,33	0
26	MG	A	1866	1/1	0.95	0.17	39,39,39,39	0
26	MG	A	1803	1/1	0.95	0.05	18,18,18,18	0
26	MG	A	1705	1/1	0.95	0.04	49,49,49,49	0
26	MG	A	1760	1/1	0.95	0.06	28,28,28,28	0
26	MG	A	1899	1/1	0.95	0.10	29,29,29,29	0
26	MG	A	1833	1/1	0.95	0.20	146,146,146,146	0
26	MG	A	1872	1/1	0.95	0.10	35,35,35,35	0
26	MG	A	1743	1/1	0.95	0.11	77,77,77,77	0
26	MG	T	201	1/1	0.95	0.10	33,33,33,33	0
26	MG	A	1875	1/1	0.95	0.14	40,40,40,40	0
26	MG	A	1755	1/1	0.96	0.20	36,36,36,36	0
26	MG	A	1682	1/1	0.96	0.10	43,43,43,43	0
26	MG	A	1802	1/1	0.96	0.07	26,26,26,26	0
26	MG	A	1906	1/1	0.96	0.08	42,42,42,42	0
26	MG	A	1739	1/1	0.96	0.05	45,45,45,45	0
26	MG	A	1683	1/1	0.96	0.05	30,30,30,30	0
26	MG	A	1716	1/1	0.96	0.09	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1910	1/1	0.96	0.05	38,38,38,38	0
26	MG	A	1662	1/1	0.96	0.20	92,92,92,92	0
26	MG	A	1836	1/1	0.96	0.12	54,54,54,54	0
26	MG	A	1839	1/1	0.96	0.06	19,19,19,19	0
26	MG	A	1782	1/1	0.96	0.05	23,23,23,23	0
26	MG	A	1671	1/1	0.96	0.12	135,135,135,135	0
26	MG	A	1763	1/1	0.96	0.16	40,40,40,40	0
26	MG	A	1730	1/1	0.96	0.10	61,61,61,61	0
26	MG	A	1642	1/1	0.96	0.09	50,50,50,50	0
26	MG	A	1767	1/1	0.96	0.05	17,17,17,17	0
26	MG	A	1818	1/1	0.96	0.06	106,106,106,106	0
26	MG	A	1847	1/1	0.96	0.24	73,73,73,73	0
25	K	A	1630	1/1	0.96	0.10	84,84,84,84	0
26	MG	A	1710	1/1	0.96	0.07	50,50,50,50	0
26	MG	A	1851	1/1	0.96	0.16	46,46,46,46	0
26	MG	A	1853	1/1	0.96	0.05	25,25,25,25	0
26	MG	A	1751	1/1	0.96	0.18	45,45,45,45	0
26	MG	H	202	1/1	0.96	0.07	27,27,27,27	0
26	MG	A	1822	1/1	0.96	0.10	71,71,71,71	0
26	MG	A	1771	1/1	0.96	0.08	44,44,44,44	0
26	MG	A	1893	1/1	0.96	0.07	33,33,33,33	0
26	MG	A	1858	1/1	0.96	0.05	26,26,26,26	0
26	MG	A	1859	1/1	0.96	0.08	41,41,41,41	0
26	MG	Q	202	1/1	0.96	0.06	38,38,38,38	0
26	MG	A	1824	1/1	0.96	0.07	72,72,72,72	0
26	MG	A	1897	1/1	0.96	0.04	38,38,38,38	0
26	MG	A	1862	1/1	0.96	0.07	49,49,49,49	0
26	MG	A	1825	1/1	0.96	0.14	40,40,40,40	0
26	MG	A	1691	1/1	0.96	0.05	27,27,27,27	0
26	MG	A	1789	1/1	0.97	0.04	24,24,24,24	0
26	MG	A	1704	1/1	0.97	0.22	54,54,54,54	0
26	MG	A	1792	1/1	0.97	0.04	25,25,25,25	0
26	MG	A	1737	1/1	0.97	0.24	59,59,59,59	0
26	MG	A	1752	1/1	0.97	0.09	57,57,57,57	0
26	MG	A	1667	1/1	0.97	0.17	38,38,38,38	0
26	MG	A	1798	1/1	0.97	0.06	44,44,44,44	0
26	MG	A	1676	1/1	0.97	0.13	56,56,56,56	0
26	MG	A	1672	1/1	0.97	0.26	48,48,48,48	0
26	MG	A	1741	1/1	0.97	0.07	45,45,45,45	0
26	MG	A	1693	1/1	0.97	0.07	14,14,14,14	0
26	MG	A	1861	1/1	0.97	0.12	42,42,42,42	0
25	K	A	1626	1/1	0.97	0.14	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	E	203	1/1	0.97	0.06	96,96,96,96	0
26	MG	A	1864	1/1	0.97	0.14	26,26,26,26	0
26	MG	A	1832	1/1	0.97	0.12	49,49,49,49	0
26	MG	A	1711	1/1	0.97	0.17	68,68,68,68	0
26	MG	A	1780	1/1	0.97	0.09	46,46,46,46	0
26	MG	A	1761	1/1	0.97	0.06	31,31,31,31	0
26	MG	A	1745	1/1	0.97	0.12	18,18,18,18	0
26	MG	A	1837	1/1	0.97	0.11	31,31,31,31	0
26	MG	A	1811	1/1	0.97	0.11	40,40,40,40	0
26	MG	A	1732	1/1	0.97	0.07	23,23,23,23	0
26	MG	A	1764	1/1	0.97	0.09	61,61,61,61	0
26	MG	A	1814	1/1	0.97	0.06	11,11,11,11	0
26	MG	A	1647	1/1	0.97	0.12	68,68,68,68	0
26	MG	A	1713	1/1	0.97	0.16	47,47,47,47	0
26	MG	A	1749	1/1	0.97	0.05	45,45,45,45	0
26	MG	A	1788	1/1	0.97	0.06	39,39,39,39	0
26	MG	A	1848	1/1	0.98	0.06	34,34,34,34	0
26	MG	A	1688	1/1	0.98	0.07	43,43,43,43	0
26	MG	A	1666	1/1	0.98	0.06	9,9,9,9	0
25	K	A	1627	1/1	0.98	0.08	93,93,93,93	0
26	MG	A	1852	1/1	0.98	0.15	44,44,44,44	0
26	MG	A	1777	1/1	0.98	0.06	64,64,64,64	0
26	MG	A	1721	1/1	0.98	0.06	75,75,75,75	0
26	MG	A	1677	1/1	0.98	0.08	28,28,28,28	0
26	MG	A	1723	1/1	0.98	0.06	49,49,49,49	0
26	MG	A	1660	1/1	0.98	0.08	38,38,38,38	0
26	MG	A	1669	1/1	0.98	0.04	22,22,22,22	0
26	MG	A	1808	1/1	0.98	0.06	18,18,18,18	0
26	MG	A	1709	1/1	0.98	0.16	28,28,28,28	0
26	MG	A	1680	1/1	0.98	0.04	37,37,37,37	0
26	MG	A	1863	1/1	0.98	0.08	43,43,43,43	0
26	MG	A	1661	1/1	0.98	0.07	54,54,54,54	0
26	MG	A	1643	1/1	0.98	0.09	50,50,50,50	0
26	MG	A	1838	1/1	0.98	0.15	38,38,38,38	0
26	MG	A	1697	1/1	0.98	0.09	53,53,53,53	0
25	K	A	1635	1/1	0.98	0.10	67,67,67,67	0
26	MG	A	1664	1/1	0.98	0.13	7,7,7,7	0
26	MG	A	1870	1/1	0.98	0.10	32,32,32,32	0
26	MG	P	101	1/1	0.98	0.14	33,33,33,33	0
26	MG	A	1791	1/1	0.98	0.07	43,43,43,43	0
26	MG	A	1901	1/1	0.98	0.11	32,32,32,32	0
26	MG	A	1902	1/1	0.98	0.05	52,52,52,52	0

Continued on next page...

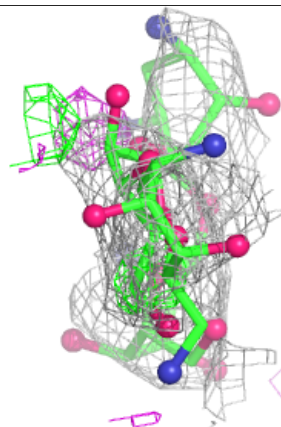
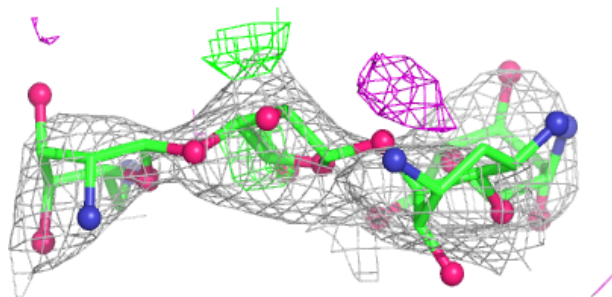
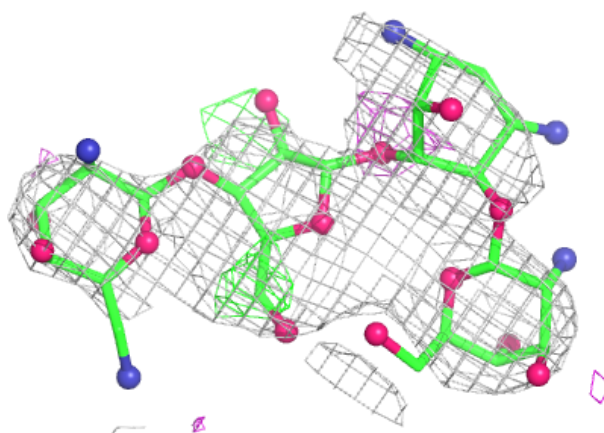
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1733	1/1	0.98	0.05	4,4,4,4	0
26	MG	A	1873	1/1	0.98	0.08	38,38,38,38	0
26	MG	A	1685	1/1	0.98	0.11	53,53,53,53	0
26	MG	A	1665	1/1	0.98	0.11	53,53,53,53	0
26	MG	A	1754	1/1	0.98	0.18	61,61,61,61	0
26	MG	A	1797	1/1	0.98	0.04	26,26,26,26	0
26	MG	A	1794	1/1	0.99	0.04	33,33,33,33	0
26	MG	M	201	1/1	0.99	0.04	32,32,32,32	0
26	MG	A	1779	1/1	0.99	0.16	26,26,26,26	0
26	MG	A	1809	1/1	0.99	0.04	28,28,28,28	0
26	MG	A	1703	1/1	0.99	0.03	26,26,26,26	0
26	MG	A	1655	1/1	0.99	0.04	55,55,55,55	0
26	MG	A	1804	1/1	0.99	0.06	23,23,23,23	0
26	MG	A	1856	1/1	0.99	0.04	43,43,43,43	0
26	MG	Q	204	1/1	0.99	0.04	46,46,46,46	0
26	MG	S	101	1/1	0.99	0.03	15,15,15,15	0
26	MG	G	201	1/1	0.99	0.05	41,41,41,41	0
26	MG	A	1650	1/1	0.99	0.06	49,49,49,49	0
26	MG	A	1687	1/1	0.99	0.19	76,76,76,76	0
26	MG	A	1831	1/1	0.99	0.05	44,44,44,44	0
27	ZN	D	301	1/1	0.99	0.11	69,69,69,69	0
27	ZN	N	101	1/1	0.99	0.03	101,101,101,101	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.

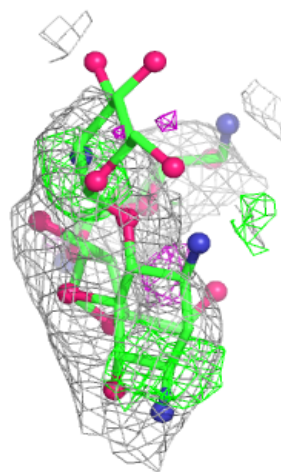
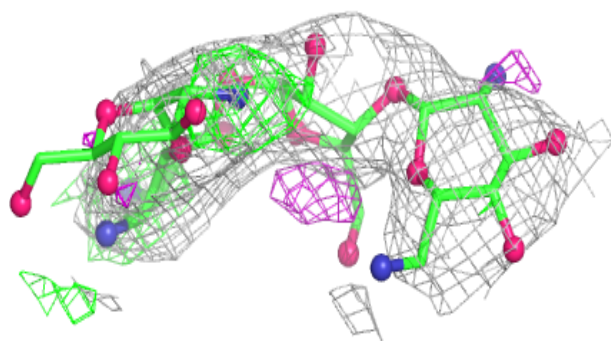
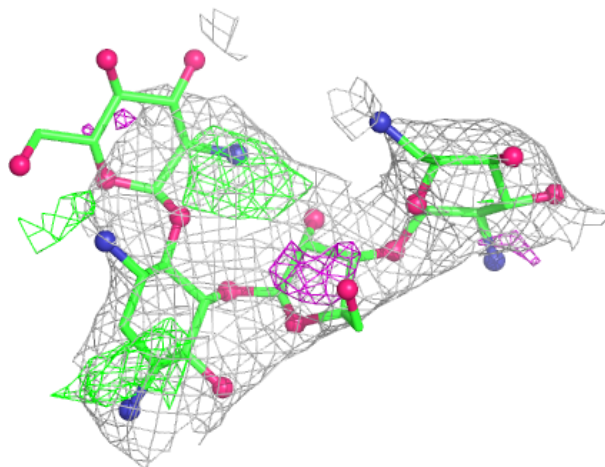
Electron density around PAR A 1605:

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



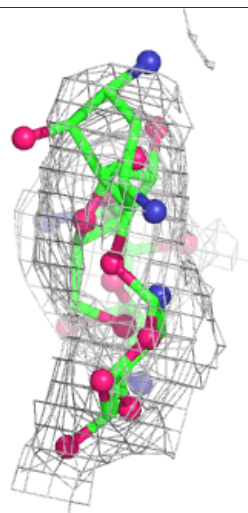
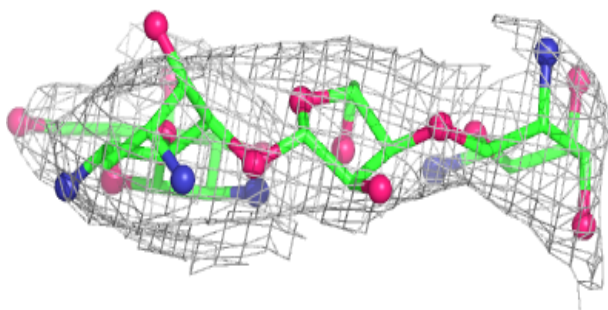
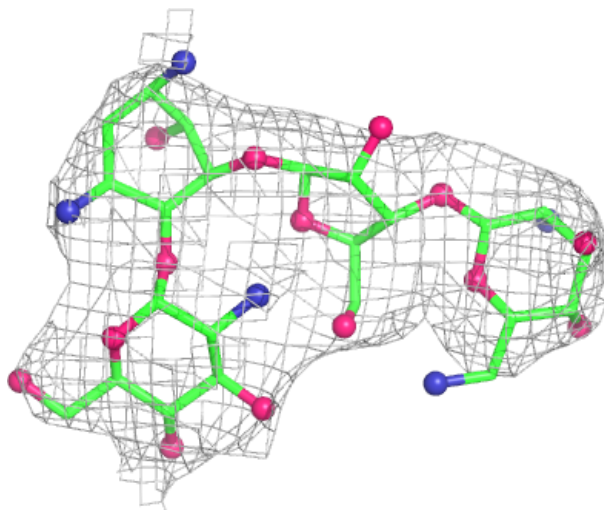
Electron density around PAR A 1602:

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



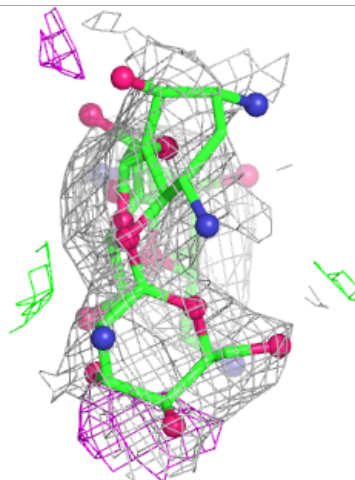
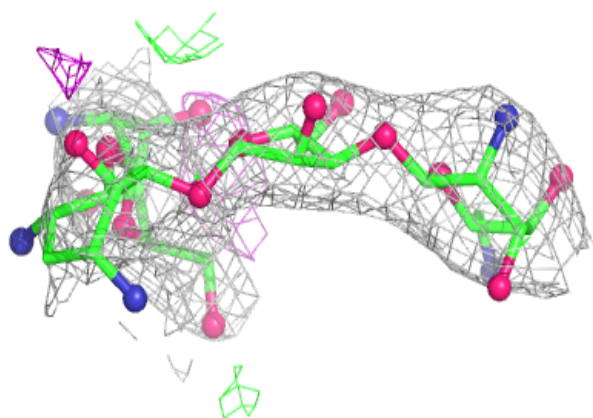
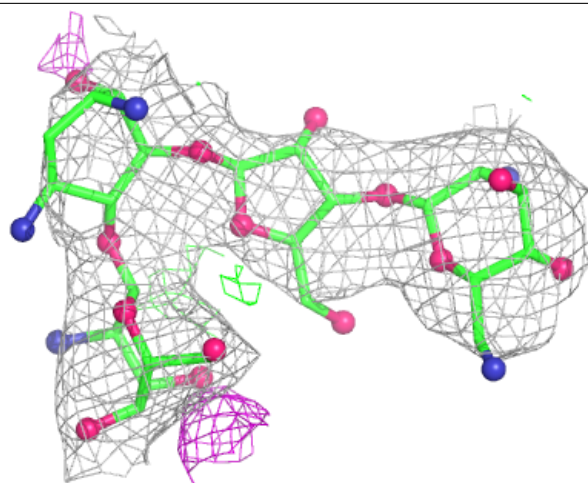
Electron density around PAR A 1604:

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



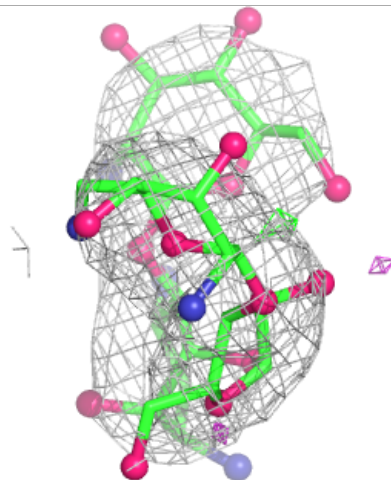
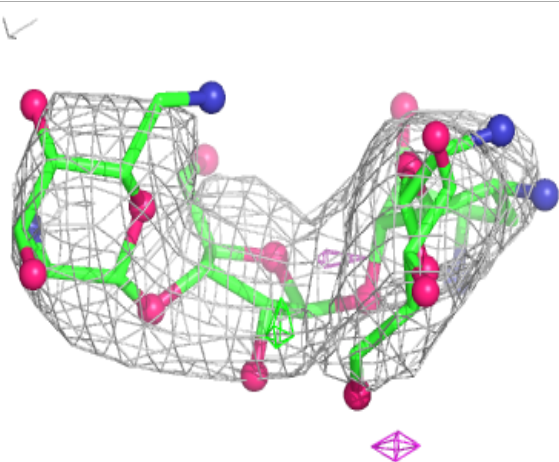
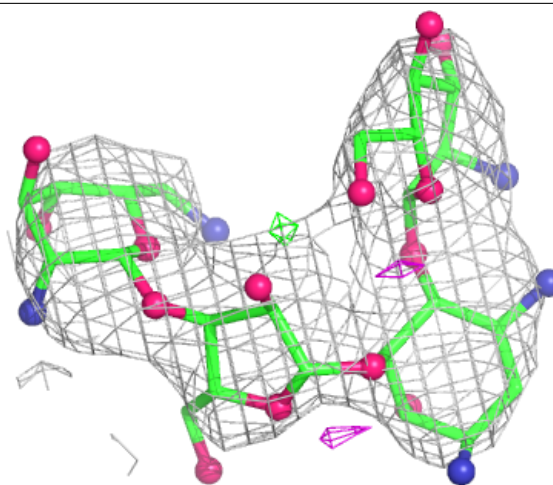
Electron density around PAR A 1603:

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



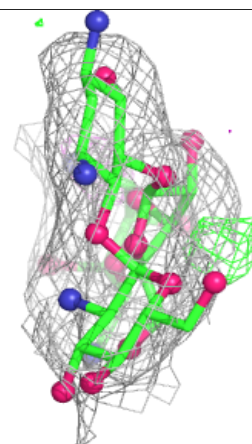
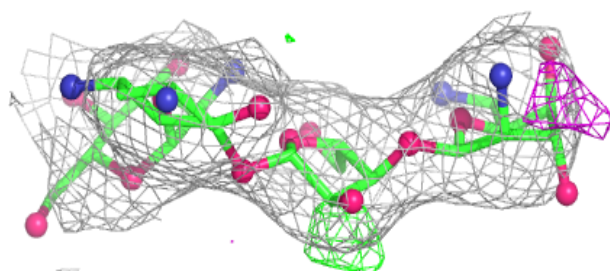
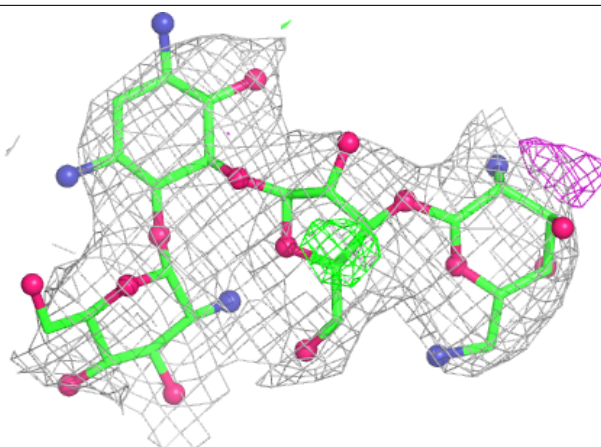
Electron density around PAR A 1606:

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



Electron density around PAR A 1601:

$2mF_o - DF_c$ (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.