



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 AM UTC

PDB ID : 3CC4 / pdb_00003cc4
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-24
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

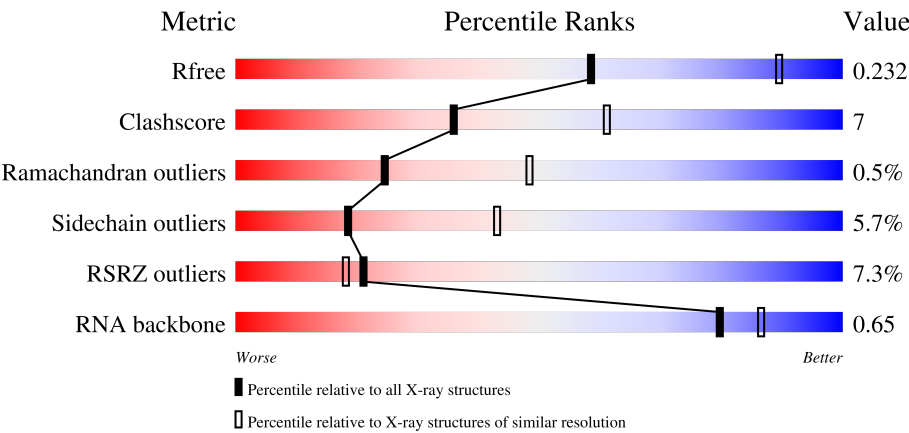
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	240	7% 80%16%..
2	B	338	4% 81%16%.
3	C	246	2% 80%17%.
4	D	177	47% 62%15%..21%

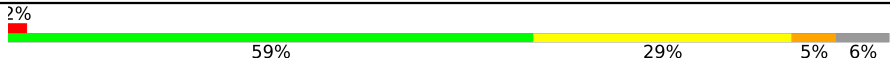
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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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
34	SR	0	8986	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8561	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99135 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	H	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	92	Total Sr 92 92	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	9	3	Total 3	Sr 3	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	J	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	0	66	Total 66	Na 66	0	0
35	9	2	Total 2	Na 2	0	0

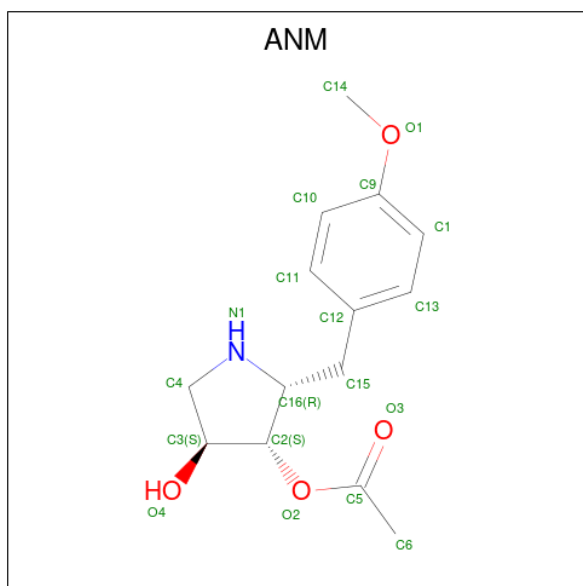
- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	1	Total C N O 19 14 1 4	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	110	Total O 110 110	0	0
39	B	140	Total O 140 140	0	0
39	C	163	Total O 163 163	0	0
39	D	46	Total O 46 46	0	0
39	E	44	Total O 44 44	0	0
39	F	26	Total O 26 26	0	0
39	G	17	Total O 17 17	0	0
39	H	67	Total O 67 67	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	I	6	Total 6	O 6	0	0
39	J	49	Total 49	O 49	0	0
39	K	56	Total 56	O 56	0	0
39	L	85	Total 85	O 85	0	0
39	M	121	Total 121	O 121	0	0
39	N	61	Total 61	O 61	0	0
39	O	44	Total 44	O 44	0	0
39	P	62	Total 62	O 62	0	0
39	Q	48	Total 48	O 48	0	0
39	R	78	Total 78	O 78	0	0
39	S	32	Total 32	O 32	0	0
39	T	39	Total 39	O 39	0	0
39	U	27	Total 27	O 27	0	0
39	V	13	Total 13	O 13	0	0
39	W	65	Total 65	O 65	0	0
39	X	23	Total 23	O 23	0	0
39	Y	92	Total 92	O 92	0	0
39	Z	31	Total 31	O 31	0	0
39	1	48	Total 48	O 48	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0

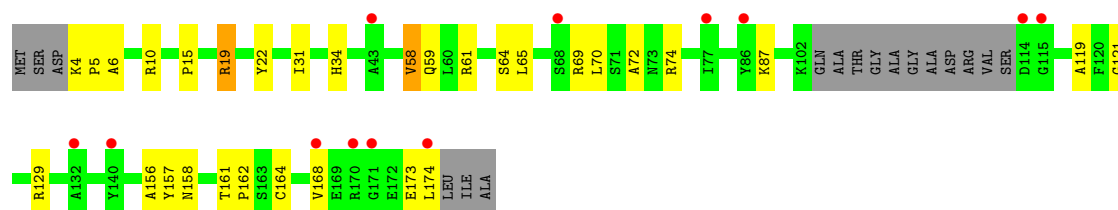
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5972	Total 5972	O 5972	0	0
39	9	147	Total 147	O 147	0	0

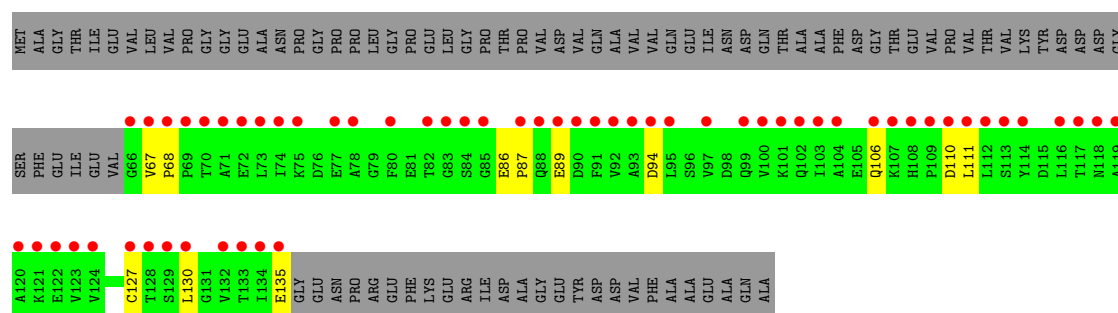
- Molecule 8: 50S ribosomal protein L10e

Chain H: 



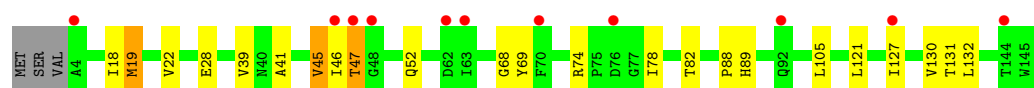
- Molecule 9: 50S ribosomal protein L11P

Chain I: 



- Molecule 10: 50S ribosomal protein L13P

Chain J: 



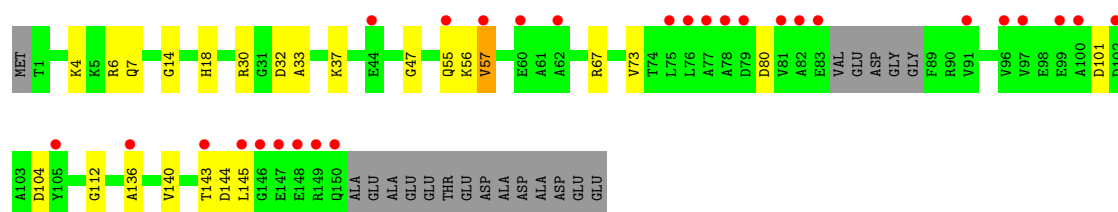
- Molecule 11: 50S ribosomal protein L14P

Chain K: 

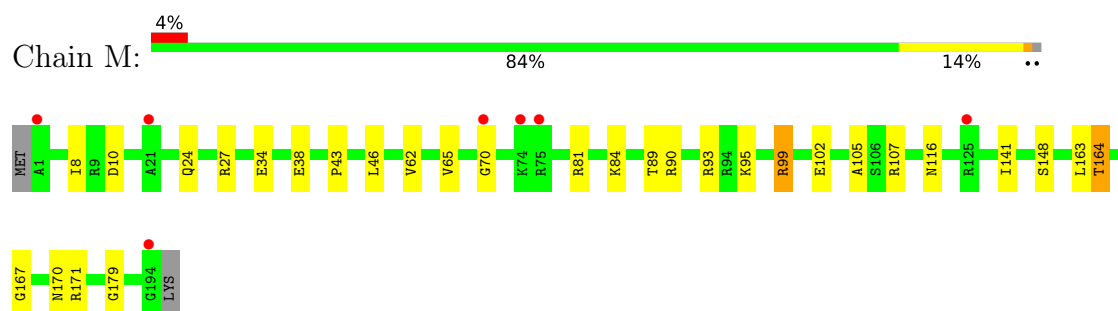


- Molecule 12: 50S ribosomal protein L15P

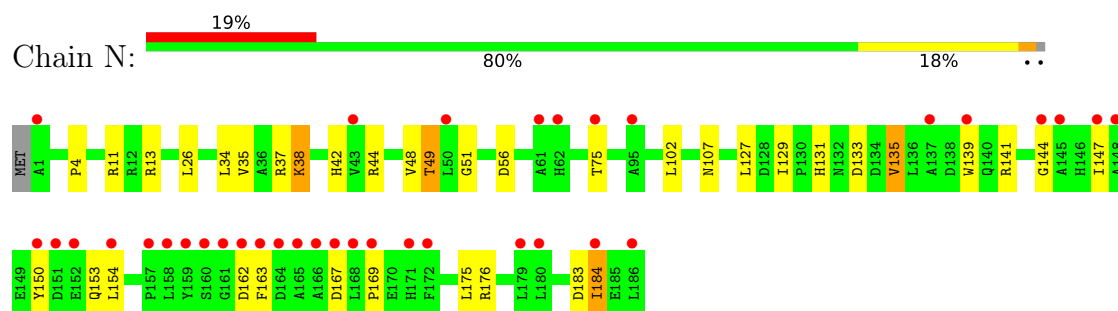
Chain L: 



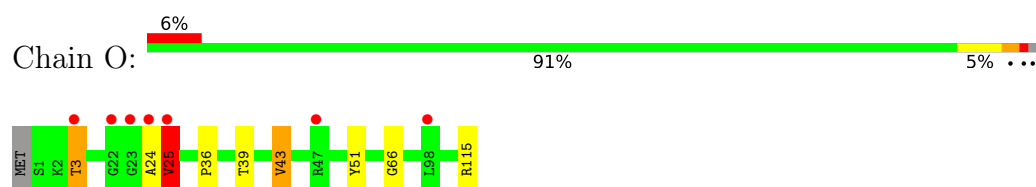
- Molecule 13: 50S ribosomal protein L15e



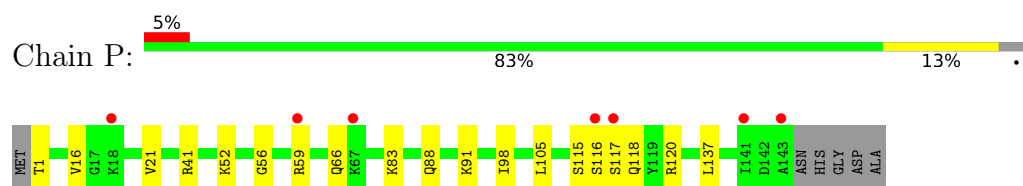
- Molecule 14: 50S ribosomal protein L18P



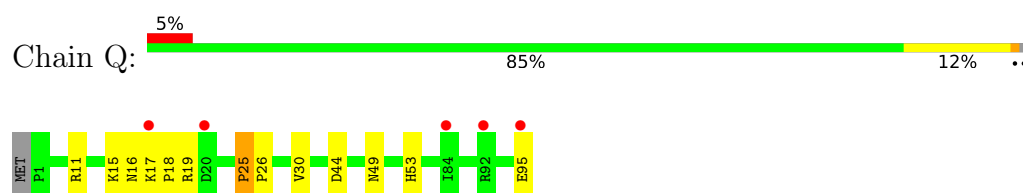
- Molecule 15: 50S ribosomal protein L18e



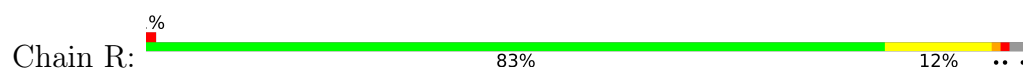
- Molecule 16: 50S ribosomal protein L19e



- Molecule 17: 50S ribosomal protein L21e

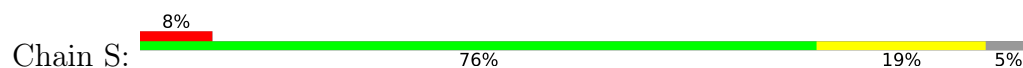


- Molecule 18: 50S ribosomal protein L22P

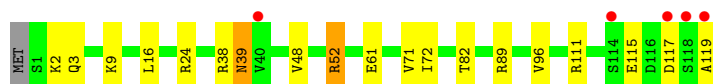
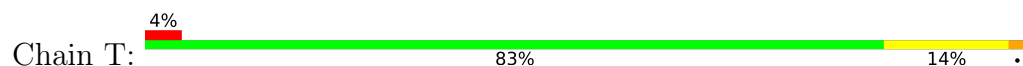




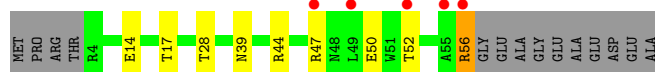
- Molecule 19: 50S ribosomal protein L23P



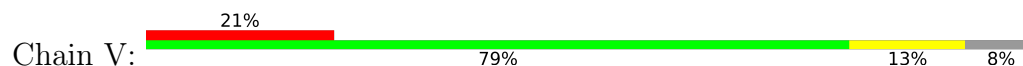
- Molecule 20: 50S ribosomal protein L24P



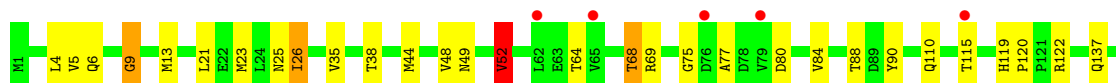
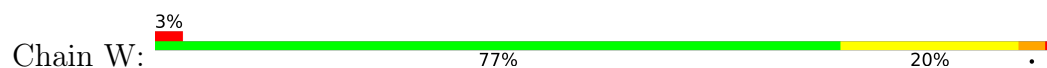
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



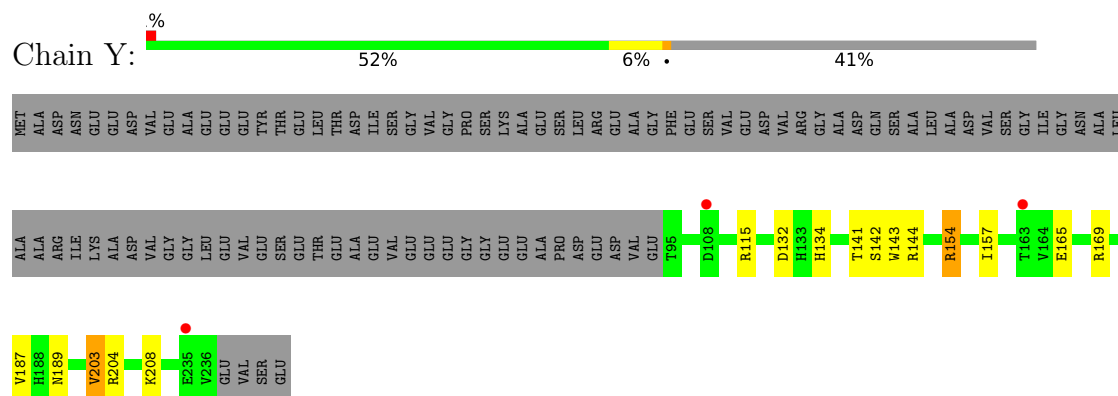
- Molecule 23: 50S ribosomal protein L30P



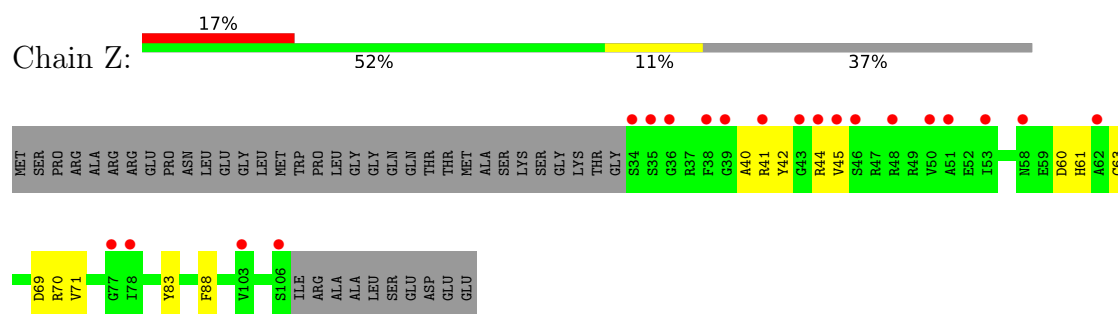
- Molecule 24: 50S ribosomal protein L31e



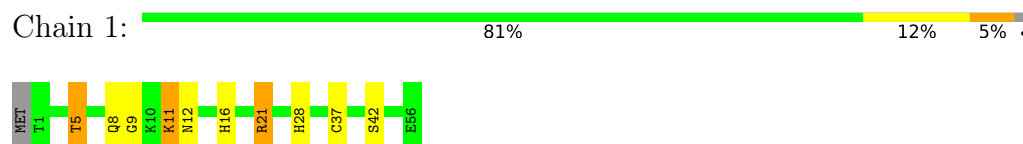
- Molecule 25: 50S ribosomal protein L32e



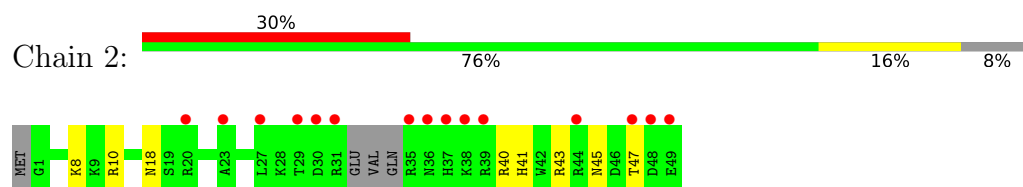
- Molecule 26: 50S ribosomal protein L37Ae



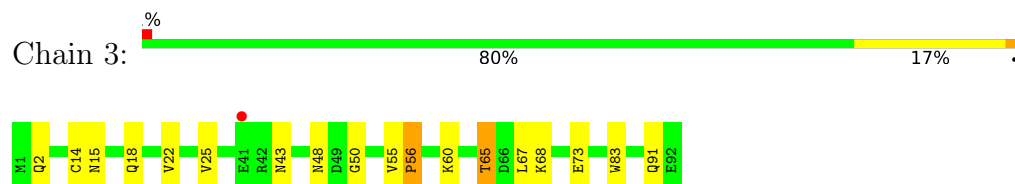
- Molecule 27: 50S ribosomal protein L37e



- Molecule 28: 50S ribosomal protein L39e

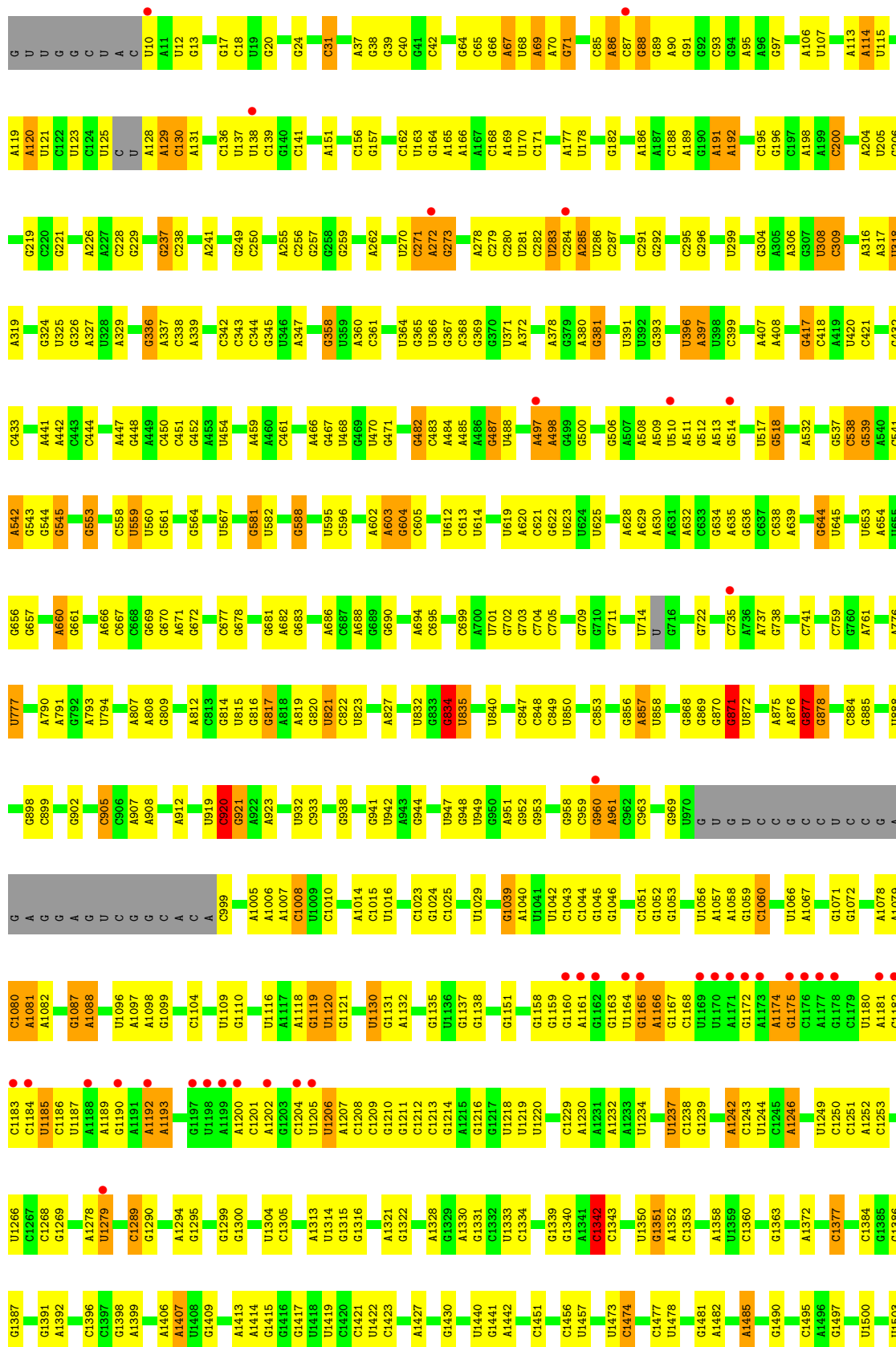


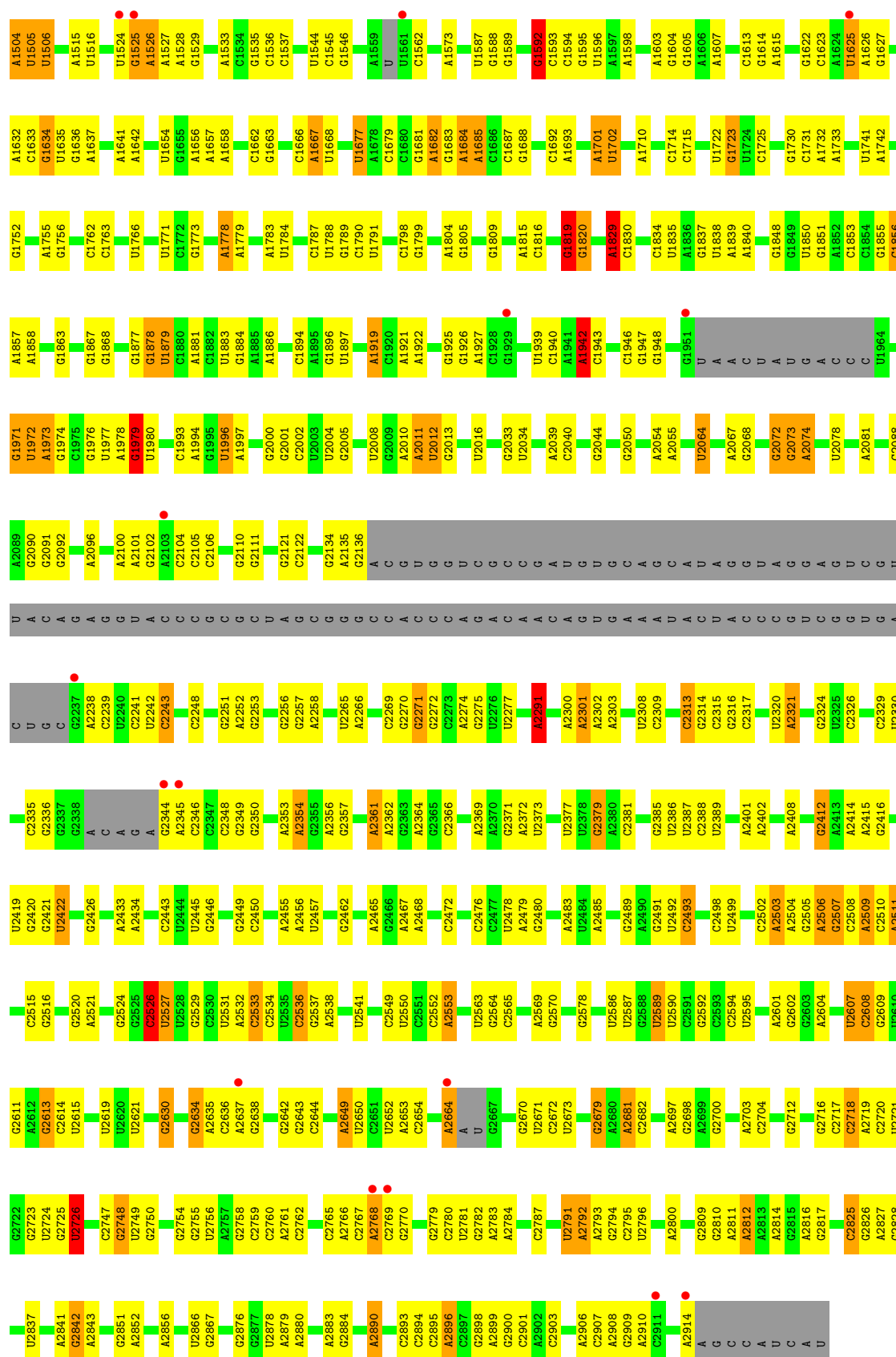
- Molecule 29: 50S ribosomal protein L44E

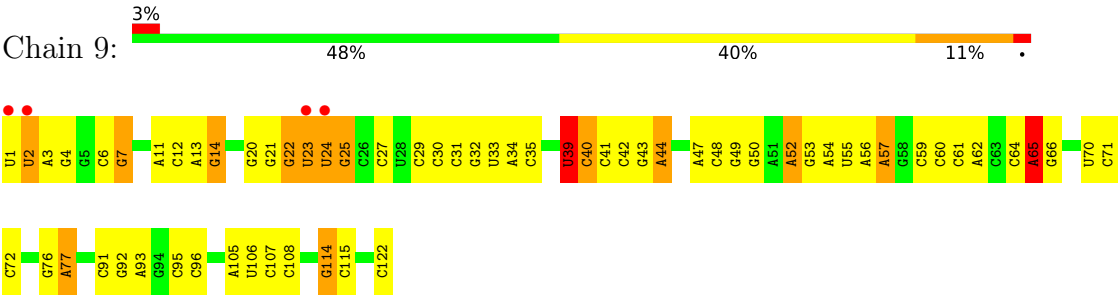


- Molecule 30: 23S ribosomal RNA









4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 299.08Å 573.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.70 49.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.70) 97.0 (49.85-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.244 0.192 , 0.232	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99135	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: OMG, SR, K, NA, CD, ANM, MG, UR3, CL, PSU, 1MA, OMU

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	0.64	0/1786	1.11	8/2408 (0.3%)
2	B	0.62	3/2690 (0.1%)	1.09	12/3652 (0.3%)
3	C	0.62	0/1885	1.10	8/2552 (0.3%)
4	D	0.74	2/1111 (0.2%)	1.10	6/1498 (0.4%)
5	E	0.67	0/1382	0.98	4/1880 (0.2%)
6	F	0.69	1/901 (0.1%)	1.14	2/1224 (0.2%)
7	G	0.61	0/241	1.03	0/324
8	H	0.64	0/1302	1.09	7/1743 (0.4%)
9	I	0.78	1/526 (0.2%)	1.13	5/716 (0.7%)
10	J	0.64	1/1136 (0.1%)	1.13	4/1530 (0.3%)
11	K	0.62	0/1004	1.09	2/1351 (0.1%)
12	L	0.56	0/1130	1.07	7/1509 (0.5%)
13	M	0.57	0/1582	1.04	4/2116 (0.2%)
14	N	0.61	0/1474	1.21	16/1999 (0.8%)
15	O	0.58	0/874	1.10	5/1181 (0.4%)
16	P	0.53	0/1147	1.04	1/1528 (0.1%)
17	Q	0.57	0/749	1.08	5/1005 (0.5%)
18	R	0.65	1/1172 (0.1%)	1.08	7/1578 (0.4%)
19	S	0.60	0/648	0.97	2/875 (0.2%)
20	T	0.54	0/958	1.11	5/1289 (0.4%)
21	U	0.58	0/417	1.07	1/562 (0.2%)
22	V	0.60	0/502	1.16	0/675
23	W	0.67	1/1219 (0.1%)	1.16	7/1655 (0.4%)
24	X	0.66	0/664	1.14	5/895 (0.6%)
25	Y	0.60	0/1146	1.08	3/1536 (0.2%)
26	Z	0.67	0/584	1.13	4/781 (0.5%)
27	1	0.54	0/438	1.03	3/578 (0.5%)
28	2	0.54	0/401	1.00	0/529
29	3	0.58	0/771	0.97	5/1024 (0.5%)
30	0	0.37	0/65958	0.60	18/102869 (0.0%)
31	9	0.36	0/2904	0.58	1/4526 (0.0%)
All	All	0.46	10/98702 (0.0%)	0.76	157/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	W	0	1
30	0	0	42
31	9	0	2
All	All	0	45

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	109	MET	SD-CE	-8.96	1.57	1.79
6	F	63	ILE	CA-CB	8.73	1.58	1.54
10	J	19	MET	SD-CE	-6.64	1.62	1.79
2	B	162	MET	SD-CE	-6.07	1.64	1.79
9	I	68	PRO	CA-C	5.99	1.55	1.51
2	B	79	MET	SD-CE	-5.55	1.65	1.79
4	D	23	VAL	CA-CB	5.49	1.60	1.54
23	W	153	MET	SD-CE	-5.33	1.66	1.79
4	D	25	MET	SD-CE	-5.30	1.66	1.79
2	B	251	VAL	CA-CB	5.10	1.60	1.53

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	163	PHE	N-CA-C	-10.66	98.50	112.68
4	D	170	TYR	N-CA-C	9.87	124.87	112.24
20	T	52	ARG	N-CA-C	9.37	125.64	113.18
23	W	75	GLY	N-CA-C	8.23	120.43	112.04
13	M	89	THR	N-CA-C	7.99	119.62	111.07
1	A	135	VAL	N-CA-C	7.36	119.35	108.45
25	Y	143	TRP	N-CA-C	7.35	121.05	110.10
30	0	1942	A	C5'-C4'-C3'	7.28	126.92	116.00
21	U	50	GLU	N-CA-C	7.27	120.07	111.71
2	B	222	LYS	N-CA-C	-7.22	99.83	110.52
3	C	205	ARG	N-CA-C	7.20	120.04	111.33
2	B	175	LEU	N-CA-C	-7.17	103.55	111.36
8	H	10	ARG	N-CA-C	7.11	119.89	111.71
9	I	127	CYS	N-CA-C	7.07	118.68	110.97
12	L	47	GLY	N-CA-C	7.04	119.31	111.85
8	H	119	ALA	N-CA-C	6.96	120.87	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	161	THR	N-CA-C	6.95	121.66	112.35
12	L	80	ASP	N-CA-C	6.88	120.46	110.42
25	Y	203	VAL	N-CA-C	6.88	118.50	108.53
17	Q	17	LYS	N-CA-C	-6.86	101.43	109.93
10	J	89	HIS	N-CA-C	6.68	121.02	112.34
20	T	3	GLN	CA-C-N	6.67	126.93	119.32
20	T	3	GLN	C-N-CA	6.67	126.93	119.32
14	N	51	GLY	CA-C-N	6.63	126.41	119.05
14	N	51	GLY	C-N-CA	6.63	126.41	119.05
8	H	58	VAL	N-CA-C	6.56	116.53	108.53
14	N	184	ILE	N-CA-C	6.45	122.76	109.34
30	0	1504	A	N9-C1'-C2'	6.45	121.68	112.00
23	W	35	VAL	N-CA-C	6.44	114.91	107.89
30	0	2726	U	N1-C1'-C2'	6.40	121.60	112.00
31	9	39	U	N1-C1'-C2'	6.39	121.59	112.00
18	R	106	GLY	N-CA-C	6.39	120.37	112.64
11	K	122	GLY	N-CA-C	6.38	119.91	112.50
14	N	169	PRO	N-CA-C	-6.35	106.41	114.35
3	C	236	THR	N-CA-C	-6.35	100.23	110.32
30	0	834	G	C2'-C3'-O3'	-6.34	104.19	113.70
24	X	79	GLU	N-CA-C	6.34	118.19	111.28
3	C	20	ASP	N-CA-C	6.32	118.98	111.33
14	N	153	GLN	N-CA-C	-6.27	101.96	110.68
20	T	16	LEU	N-CA-C	6.20	118.83	111.33
14	N	48	VAL	N-CA-C	6.13	116.75	108.17
30	0	1592	G	N9-C1'-C2'	6.09	121.14	112.00
2	B	103	ASP	N-CA-C	-6.09	105.76	113.43
12	L	73	VAL	N-CA-C	6.09	116.87	110.72
18	R	141	VAL	N-CA-C	6.07	117.34	108.53
26	Z	42	TYR	N-CA-C	6.06	123.71	110.80
3	C	215	ALA	N-CA-C	6.04	118.65	111.71
4	D	137	PRO	N-CA-C	6.01	124.85	112.47
24	X	25	ARG	N-CA-C	6.01	118.60	111.33
2	B	242	TRP	N-CA-C	-6.00	104.66	111.14
12	L	55	GLN	N-CA-C	5.99	119.42	111.75
14	N	13	ARG	N-CA-C	-5.98	105.64	113.12
9	I	67	VAL	CA-C-N	5.97	124.02	119.66
9	I	67	VAL	C-N-CA	5.97	124.02	119.66
2	B	213	GLY	CA-C-N	5.95	125.82	119.28
2	B	213	GLY	C-N-CA	5.95	125.82	119.28
18	R	13	THR	N-CA-C	5.93	118.20	109.24
29	3	55	VAL	CA-C-N	5.93	127.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3	55	VAL	C-N-CA	5.93	127.25	119.84
24	X	77	PHE	N-CA-C	5.93	115.92	108.45
15	O	66	GLY	N-CA-C	5.88	127.11	113.18
29	3	60	LYS	N-CA-C	-5.87	102.68	110.07
30	0	1819	G	C5'-C4'-C3'	5.86	124.78	116.00
27	1	5	THR	CA-C-N	-5.82	113.68	119.56
27	1	5	THR	C-N-CA	-5.82	113.68	119.56
24	X	22	ASN	N-CA-C	5.82	120.97	111.37
8	H	121	GLY	N-CA-C	5.80	119.97	112.54
26	Z	88	PHE	N-CA-C	5.78	117.76	109.14
30	0	871	G	C5'-C4'-O4'	-5.78	101.13	109.80
15	O	25	VAL	CB-CA-C	-5.77	104.46	112.02
12	L	7	GLN	N-CA-C	5.76	120.03	112.89
29	3	43	ASN	N-CA-C	5.72	119.88	113.01
29	3	67	LEU	N-CA-C	5.72	118.87	109.72
23	W	25	ASN	N-CA-C	5.71	119.83	112.86
30	0	2291	A	N9-C1'-C2'	5.71	120.56	112.00
2	B	265	LEU	N-CA-C	5.71	118.06	110.53
2	B	157	LYS	N-CA-C	-5.69	106.69	113.97
3	C	19	PRO	N-CA-C	5.67	120.14	111.34
1	A	166	ASP	N-CA-C	5.62	117.48	111.36
9	I	106	GLN	N-CA-C	5.61	117.48	111.36
13	M	8	ILE	N-CA-C	-5.60	104.90	111.00
27	1	11	LYS	N-CA-C	5.60	118.26	108.52
1	A	129	LEU	N-CA-C	5.59	119.53	111.02
2	B	83	ALA	N-CA-C	5.59	116.77	108.60
5	E	91	PHE	N-CA-C	5.57	116.98	109.24
30	0	1120	U	C5'-C4'-C3'	-5.56	107.66	116.00
30	0	1979	G	N9-C1'-C2'	5.56	120.34	112.00
24	X	60	ALA	N-CA-C	5.55	118.05	111.33
4	D	136	ARG	CA-C-N	5.55	126.78	119.84
4	D	136	ARG	C-N-CA	5.55	126.78	119.84
26	Z	63	CYS	N-CA-C	5.55	116.81	109.93
10	J	47	THR	N-CA-C	5.54	118.32	110.50
26	Z	45	VAL	N-CA-C	5.54	116.94	110.62
18	R	76	ASP	N-CA-C	5.54	119.71	112.13
2	B	323	LEU	N-CA-C	5.52	118.28	110.50
15	O	24	ALA	N-CA-C	-5.52	107.19	114.31
14	N	135	VAL	N-CA-C	-5.50	107.43	113.43
14	N	133	ASP	N-CA-C	5.50	117.27	111.28
30	0	1979	G	C4'-C3'-O3'	-5.48	104.78	113.00
30	0	2526	C	N1-C1'-C2'	5.48	120.22	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	62	HIS	N-CA-C	5.47	119.13	112.23
14	N	162	ASP	N-CA-C	5.46	117.14	108.67
23	W	9	GLY	N-CA-C	5.46	119.57	112.25
18	R	82	GLU	N-CA-C	5.45	117.30	111.36
18	R	63	ASN	N-CA-C	5.43	120.60	112.94
23	W	69	ARG	N-CA-C	5.42	120.77	113.72
5	E	11	VAL	N-CA-C	5.40	117.34	108.97
6	F	79	GLN	N-CA-C	5.40	118.29	109.59
3	C	177	GLY	N-CA-C	5.39	118.86	112.33
14	N	102	LEU	N-CA-C	5.38	117.50	109.59
14	N	42	HIS	N-CA-C	5.37	117.42	109.69
15	O	43	VAL	N-CA-C	5.35	115.66	108.17
25	Y	187	VAL	N-CA-C	5.35	115.60	108.11
2	B	22	GLU	N-CA-C	-5.34	106.27	112.89
1	A	111	SER	N-CA-C	-5.33	102.09	110.14
1	A	123	GLY	N-CA-C	5.32	122.44	115.47
13	M	70	GLY	N-CA-C	5.31	120.68	112.45
2	B	266	ASN	N-CA-C	5.31	118.65	111.17
17	Q	25	PRO	CA-C-N	5.30	125.11	119.28
17	Q	25	PRO	C-N-CA	5.30	125.11	119.28
8	H	164	CYS	N-CA-C	5.29	117.73	109.52
5	E	50	GLU	N-CA-C	5.29	117.23	109.24
10	J	68	GLY	N-CA-C	5.29	118.88	112.48
30	0	2301	A	N9-C1'-C2'	5.28	119.92	112.00
23	W	52	VAL	N-CA-C	5.28	116.31	108.65
12	L	57	VAL	N-CA-C	-5.28	107.16	112.17
30	0	877	G	C2'-C3'-O3'	-5.27	105.80	113.70
30	0	206	G	C5'-C4'-C3'	-5.26	108.10	116.00
14	N	75	THR	N-CA-C	5.26	120.36	112.94
1	A	162	GLY	N-CA-C	5.25	117.50	111.36
1	A	70	ALA	N-CA-C	5.23	118.90	109.44
15	O	51	TYR	N-CA-C	5.23	120.52	113.72
11	K	46	LYS	N-CA-C	5.22	118.74	109.96
30	0	920	C	C2'-C3'-O3'	-5.20	105.90	113.70
19	S	27	ALA	N-CA-C	-5.19	99.32	108.20
23	W	68	THR	N-CA-C	5.19	118.08	111.69
10	J	22	VAL	N-CA-C	-5.16	105.68	110.53
18	R	3	SER	N-CA-C	-5.16	101.45	109.24
12	L	145	LEU	N-CA-C	-5.16	105.73	112.23
20	T	72	ILE	N-CA-C	5.15	117.25	108.86
1	A	84	VAL	N-CA-C	5.15	115.36	110.42
30	0	2536	C	O4'-C4'-C3'	-5.12	100.98	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	89	ALA	N-CA-C	5.12	116.55	110.97
3	C	134	ASP	N-CA-C	-5.11	106.13	112.93
4	D	171	ASP	N-CA-C	5.10	115.27	108.38
16	P	56	GLY	N-CA-C	-5.10	101.08	113.18
8	H	34	HIS	N-CA-C	-5.10	107.72	114.04
5	E	13	ALA	N-CA-C	5.09	117.36	108.76
14	N	150	TYR	N-CA-C	-5.09	106.23	112.90
19	S	66	VAL	N-CA-C	5.08	115.41	107.99
14	N	131	HIS	N-CA-C	5.05	116.35	109.18
9	I	68	PRO	N-CA-C	5.04	115.31	110.47
30	0	2313	C	C5'-C4'-C3'	5.03	123.55	116.00
17	Q	44	ASP	N-CA-C	-5.03	102.25	109.24
4	D	100	ASP	N-CA-C	-5.02	106.67	112.89
17	Q	49	ASN	N-CA-C	5.01	117.94	110.52
13	M	148	SER	N-CA-C	5.01	118.88	112.87

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1342	C	Sidechain
30	0	1351	G	Sidechain
30	0	1417	G	Sidechain
30	0	1430	G	Sidechain
30	0	1677	U	Sidechain
30	0	1702	U	Sidechain
30	0	1809	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	1993	C	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2526	C	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	2679	G	Sidechain
30	0	270	U	Sidechain
30	0	2726	U	Sidechain
30	0	2842	G	Sidechain
30	0	391	U	Sidechain
30	0	396	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	888	U	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	21	0
2	B	2625	0	2533	30	0
3	C	1860	0	1813	23	0
4	D	1094	0	1085	11	0
5	E	1357	0	1266	10	0
6	F	890	0	843	8	0
7	G	240	0	231	0	0
8	H	1282	0	1292	18	0
9	I	519	0	500	5	0
10	J	1120	0	1098	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	994	0	1027	11	0
12	L	1118	0	1076	12	0
13	M	1558	0	1573	19	0
14	N	1445	0	1401	16	0
15	O	865	0	873	4	0
16	P	1136	0	1123	11	0
17	Q	735	0	729	6	0
18	R	1149	0	1122	11	0
19	S	641	0	605	6	0
20	T	950	0	924	8	0
21	U	410	0	364	3	0
22	V	499	0	511	4	0
23	W	1196	0	1137	24	0
24	X	654	0	653	12	0
25	Y	1130	0	1133	13	0
26	Z	573	0	532	6	0
27	1	431	0	426	9	0
28	2	396	0	413	5	0
29	3	755	0	729	7	0
30	0	59021	0	29812	847	0
31	9	2599	0	1325	64	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	1	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	19	0	19	5	0
39	0	5972	0	0	121	0
39	1	48	0	0	0	0
39	2	38	0	0	0	0
39	3	66	0	0	1	0
39	9	147	0	0	5	0
39	A	110	0	0	4	0
39	B	140	0	0	5	0
39	C	163	0	0	2	0
39	D	46	0	0	0	0
39	E	44	0	0	0	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	67	0	0	3	0
39	I	6	0	0	1	0
39	J	49	0	0	1	0
39	K	56	0	0	0	0
39	L	85	0	0	2	0
39	M	121	0	0	1	0
39	N	61	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	O	44	0	0	0	0
39	P	62	0	0	0	0
39	Q	48	0	0	0	0
39	R	78	0	0	0	0
39	S	32	0	0	0	0
39	T	39	0	0	0	0
39	U	27	0	0	0	0
39	V	13	0	0	0	0
39	W	65	0	0	2	0
39	X	23	0	0	1	0
39	Y	92	0	0	3	0
39	Z	31	0	0	1	0
All	All	99135	0	59934	1093	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 7.

All (1093) 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)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.22	1.16
31:9:76:G:H3'	31:9:77:A:H5''	1.34	1.02
15:O:3:THR:HG22	30:0:656:G:H5'	1.43	1.00
30:0:871:G:H5'	30:0:871:G:H8	1.27	0.98
30:0:871:G:H5'	30:0:871:G:C8	1.98	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.46	0.96
13:M:171:ARG:HD3	30:0:156:C:H5''	1.44	0.96
10:J:82:THR:HG23	30:0:1242:A:H5'	1.47	0.96
30:0:2717:C:C2'	30:0:2718:C:H5''	1.97	0.94
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.15	0.93
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.13	0.93
14:N:37:ARG:NH1	31:9:6:C:H5''	1.83	0.93
31:9:56:A:H2'	31:9:57:A:H5''	1.48	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.91
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.90
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.54	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.20	0.89
30:0:1474:C:H5'	30:0:1474:C:H6	1.37	0.89
30:0:2506:A:HO2'	30:0:2507:G:H8	0.90	0.88
30:0:1116:U:HO2'	30:0:1118:A:H2	0.87	0.87
30:0:1160:G:H5'	30:0:1161:A:C5'	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:C5'	30:0:1161:A:H5'	2.03	0.86
30:0:2812:A:H2	30:0:2814:A:H62	1.24	0.85
30:0:1667:A:H5'	30:0:1667:A:H8	1.42	0.85
30:0:1603:A:H5'	30:0:1605:G:O4'	1.75	0.85
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
30:0:1701:A:H4'	30:0:1702:U:H5''	1.56	0.84
11:K:10:GLN:H	11:K:10:GLN:HE21	1.25	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.21	0.83
39:N:8843:HOH:O	31:9:49:G:H5''	1.77	0.83
30:0:381:G:H5''	39:0:4352:HOH:O	1.77	0.83
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.83
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.61	0.82
30:0:541:C:H2'	30:0:542:A:H5''	1.61	0.82
30:0:559:U:H6	30:0:559:U:H5'	1.45	0.81
30:0:545:G:H5'	30:0:545:G:H8	1.44	0.81
30:0:2533:C:H6	30:0:2533:C:H5'	1.46	0.81
30:0:1979:G:H2'	39:0:3320:HOH:O	1.82	0.79
30:0:2291:A:C8	30:0:2309:C:H5'	2.18	0.78
30:0:871:G:H8	30:0:871:G:C5'	1.96	0.78
30:0:2908:A:H2'	30:0:2909:G:O4'	1.83	0.78
30:0:506:G:H22	30:0:509:A:C5'	1.97	0.78
38:0:2924:ANM:H151	38:0:2924:ANM:H63	1.63	0.78
30:0:1300:G:H1'	39:0:4716:HOH:O	1.82	0.77
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.85	0.77
30:0:1205:U:H2'	30:0:1206:U:H5''	1.66	0.77
30:0:506:G:H22	30:0:509:A:H5''	1.50	0.77
30:0:853:C:H3'	39:0:4586:HOH:O	1.83	0.77
30:0:541:C:C2'	30:0:542:A:H5''	2.15	0.76
30:0:1666:C:O2'	30:0:1667:A:H5''	1.86	0.75
28:2:41:HIS:H	28:2:45:ASN:HD22	1.34	0.75
31:9:29:C:H2'	31:9:30:C:H5'	1.68	0.75
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.75
3:C:27:ARG:NH2	30:0:657:G:OP1	2.20	0.75
30:0:1118:A:H3'	30:0:1118:A:C8	2.22	0.75
30:0:1118:A:H3'	30:0:1118:A:H8	1.51	0.75
30:0:2506:A:O2'	30:0:2507:G:H8	1.69	0.75
30:0:182:G:H5'	39:0:5189:HOH:O	1.86	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.51	0.74
30:0:1474:C:H5'	30:0:1474:C:C6	2.22	0.74
13:M:163:LEU:HD21	30:0:188:C:H5''	1.71	0.73
30:0:1120:U:H5'	30:0:1121:G:OP2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
18:R:98:ASN:HD21	30:0:500:G:H21	1.34	0.73
22:V:1:THR:HB	30:0:93:C:H5''	1.70	0.73
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.69	0.72
30:0:877:G:H5'	30:0:878:G:OP1	1.90	0.72
30:0:1166:A:H61	30:0:1180:U:H3	1.35	0.72
30:0:544:G:H2'	30:0:545:G:H5''	1.72	0.72
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72
31:9:56:A:C2'	31:9:57:A:H5''	2.20	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.37	0.71
30:0:1189:A:H1'	30:0:1209:C:O4'	1.90	0.71
30:0:1206:U:H6	30:0:1206:U:H5'	1.53	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.05	0.71
30:0:1878:G:H1'	39:0:6168:HOH:O	1.91	0.71
30:0:2491:G:H1'	39:0:6923:HOH:O	1.91	0.70
30:0:2534:C:H1'	39:0:3522:HOH:O	1.91	0.70
3:C:184:ARG:NH2	30:0:450:C:OP1	2.24	0.70
30:0:1741:U:H5'	30:0:1742:A:OP1	1.91	0.70
30:0:1183:C:H2'	39:0:6292:HOH:O	1.91	0.70
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.56	0.70
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.70
1:A:211:LYS:HB2	39:A:9075:HOH:O	1.91	0.69
30:0:1701:A:H5'	39:0:6332:HOH:O	1.92	0.69
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.69
30:0:823:U:H3'	39:0:4481:HOH:O	1.91	0.69
16:P:116:SER:O	30:0:1593:C:H5'	1.92	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.72	0.69
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.69
30:0:541:C:H2'	30:0:542:A:C5'	2.23	0.69
30:0:1159:G:H21	30:0:1189:A:H8	1.39	0.69
31:9:39:U:H1'	31:9:44:A:H61	1.57	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.21	0.68
30:0:1527:A:H1'	30:0:1528:A:C8	2.29	0.68
30:0:2533:C:H5'	30:0:2533:C:C6	2.27	0.68
30:0:12:U:H2'	30:0:13:G:H5'	1.75	0.68
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.58	0.68
3:C:139:VAL:HG13	39:C:8643:HOH:O	1.92	0.68
30:0:1119:G:N2	30:0:1246:A:C2	2.58	0.68
30:0:2769:C:C2'	30:0:2770:G:H5'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.75	0.67
30:0:603:A:H5''	30:0:604:G:OP1	1.94	0.67
30:0:681:G:N3	30:0:681:G:H5'	2.09	0.67
30:0:2783:A:H3'	39:0:5264:HOH:O	1.93	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.76	0.67
30:0:1205:U:H2'	30:0:1206:U:C5'	2.24	0.67
30:0:1666:C:C2'	30:0:1667:A:H5''	2.25	0.67
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.78	0.66
30:0:2538:A:H8	38:0:2924:ANM:H61	1.61	0.65
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.93	0.65
30:0:558:C:C2'	30:0:559:U:H5''	2.26	0.65
30:0:1701:A:H4'	30:0:1702:U:C5'	2.23	0.65
30:0:1377:C:H6	30:0:1377:C:H5'	1.61	0.65
30:0:1667:A:H5'	30:0:1667:A:C8	2.29	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.96	0.65
11:K:39:GLY:HA2	39:0:5253:HOH:O	1.97	0.65
10:J:52:GLN:HE22	30:0:1119:G:H8	1.43	0.65
12:L:136:ALA:HB3	39:L:8874:HOH:O	1.96	0.65
30:0:2073:G:H5''	39:0:3853:HOH:O	1.95	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
18:R:128:ARG:NH2	30:0:2054:A:N3	2.44	0.65
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.65
30:0:119:A:H2'	30:0:120:A:H5''	1.78	0.65
2:B:238:ASN:HD22	2:B:240:GLY:H	1.44	0.64
30:0:2005:G:OP2	30:0:2005:G:H3'	1.97	0.64
30:0:2766:A:H5'	39:0:9579:HOH:O	1.96	0.64
30:0:1183:C:N4	30:0:1184:C:H41	1.95	0.64
30:0:2578:G:H5'	30:0:2578:G:H8	1.62	0.64
30:0:2765:C:H4'	39:0:5557:HOH:O	1.98	0.64
30:0:542:A:H5'	30:0:542:A:C8	2.24	0.64
30:0:545:G:H5'	30:0:545:G:C8	2.29	0.64
2:B:212:GLN:HA	30:0:1733:A:H4'	1.80	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
30:0:1947:G:H2'	30:0:1948:G:H8	1.62	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.62	0.64
30:0:2637:A:H5'	39:0:9282:HOH:O	1.96	0.64
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.79	0.64
30:0:2635:A:O2'	30:0:2636:C:H5'	1.98	0.64
30:0:2756:U:H3	30:0:2896:A:H2	1.45	0.63
30:0:871:G:C8	30:0:871:G:C5'	2.73	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2878:U:H2'	30:0:2879:A:O4'	1.97	0.63
30:0:1189:A:H3'	39:0:7737:HOH:O	1.97	0.63
30:0:2502:C:C2'	30:0:2503:A:H5'	2.28	0.63
30:0:2717:C:O2'	30:0:2718:C:H5''	1.98	0.63
30:0:1116:U:O2'	30:0:1118:A:H2	1.70	0.63
30:0:544:G:C2'	30:0:545:G:H5''	2.28	0.63
4:D:154:LYS:H	4:D:154:LYS:HD2	1.63	0.62
30:0:2426:G:H1'	39:0:6139:HOH:O	1.97	0.62
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.62
30:0:1165:G:H4'	30:0:1174:A:O2'	1.99	0.62
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.15	0.62
30:0:90:A:H2'	30:0:91:G:O4'	1.98	0.62
30:0:1166:A:H1'	30:0:1192:A:C2	2.34	0.62
30:0:1205:U:C2'	30:0:1206:U:H5''	2.30	0.62
30:0:2004:U:H4'	39:0:5340:HOH:O	1.99	0.62
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.65	0.62
30:0:1666:C:H2'	30:0:1667:A:C5'	2.29	0.62
30:0:2679:G:H2'	30:0:2681:A:OP2	1.99	0.62
30:0:2896:A:H5''	39:0:6146:HOH:O	1.99	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.62
30:0:1184:C:H1'	39:0:7526:HOH:O	1.99	0.62
31:9:7:G:H5'	39:9:9098:HOH:O	2.00	0.62
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.62
30:0:832:U:OP2	39:0:7839:HOH:O	2.16	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.61
31:9:20:G:O2'	31:9:21:G:H5'	1.99	0.61
23:W:154:ARG:NH1	30:0:588:G:O6	2.33	0.61
30:0:1441:G:O2'	30:0:1442:A:H5'	1.99	0.61
30:0:123:U:H5'	39:0:6705:HOH:O	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:H	1.64	0.61
20:T:52:ARG:HD2	30:0:317:A:H5''	1.82	0.61
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.48	0.61
30:0:1666:C:H2'	30:0:1667:A:H5'	1.83	0.61
30:0:2768:A:H2'	30:0:2769:C:O4'	2.00	0.61
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.82	0.61
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.81	0.61
30:0:69:A:H5'	30:0:69:A:C8	2.36	0.61
30:0:282:C:O2'	30:0:283:U:H5'	2.00	0.61
30:0:2717:C:H2'	30:0:2718:C:C5'	2.26	0.61
11:K:87:ARG:NH2	30:0:2720:C:O2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.83	0.60
29:3:48:ASN:HD21	30:0:2468:A:H61	1.49	0.60
30:0:848:C:H5'	39:0:7329:HOH:O	2.00	0.60
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.83	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
30:0:558:C:O2'	30:0:559:U:H5''	2.02	0.60
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.60
30:0:2502:C:H2'	30:0:2503:A:H5'	1.83	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.84	0.60
31:9:39:U:H3'	31:9:40:C:H5''	1.84	0.60
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.99	0.60
30:0:905:C:H3'	39:0:5219:HOH:O	2.00	0.60
30:0:2241:C:O2'	30:0:2242:U:H5'	2.01	0.59
23:W:149:LEU:HG	23:W:153:MET:HE2	1.82	0.59
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.59
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.50	0.59
14:N:144:GLY:O	14:N:147:ILE:HG22	2.02	0.59
30:0:920:C:H5''	30:0:921:G:O5'	2.02	0.59
30:0:1372:A:H3'	39:0:7247:HOH:O	2.02	0.59
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.59
30:0:447:A:O2'	30:0:448:G:H5'	2.03	0.59
30:0:2507:G:H2'	30:0:2510:C:H42	1.67	0.59
30:0:2638:G:H5'	39:0:4962:HOH:O	2.02	0.59
30:0:2851:G:C2'	30:0:2852:A:H5'	2.32	0.58
30:0:2748:G:H5'	39:0:7599:HOH:O	2.02	0.58
30:0:969:G:H1	30:0:999:C:H42	1.50	0.58
30:0:69:A:H5'	30:0:69:A:H8	1.68	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.69	0.58
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.86	0.58
30:0:1681:G:H5''	30:0:1682:A:H5'	1.84	0.58
31:9:29:C:C2'	31:9:30:C:H5'	2.34	0.58
30:0:292:G:H2'	30:0:358:G:N2	2.19	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.36	0.58
30:0:2769:C:H2'	30:0:2770:G:H5'	1.85	0.57
30:0:2816:A:H5''	30:0:2817:G:H5'	1.86	0.57
31:9:71:C:H2'	31:9:72:C:H6	1.69	0.57
30:0:506:G:H22	30:0:509:A:H5'	1.70	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1201:C:H5''	39:0:6282:HOH:O	2.03	0.57
30:0:1632:A:H2'	30:0:1633:C:H5'	1.86	0.57
31:9:76:G:C3'	31:9:77:A:H5''	2.20	0.57
30:0:558:C:H2'	30:0:559:U:C5'	2.33	0.57
30:0:2372:A:H2'	30:0:2373:U:H6	1.69	0.57
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.85	0.57
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.70	0.57
30:0:1947:G:H2'	30:0:1948:G:C8	2.40	0.57
16:P:115:SER:H	16:P:118:GLN:NE2	1.98	0.57
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.05	0.57
30:0:2529:G:H3'	39:0:7241:HOH:O	2.05	0.57
30:0:2712:G:H5'	39:0:5253:HOH:O	2.05	0.57
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.56
30:0:2795:C:O2'	30:0:2796:U:H5'	2.05	0.56
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.87	0.56
30:0:2769:C:H2'	30:0:2770:G:O4'	2.05	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.34	0.56
30:0:317:A:H5'	39:0:3798:HOH:O	2.05	0.56
30:0:2301:A:H5''	30:0:2302:A:H5'	1.86	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.03	0.56
30:0:1080:C:H4'	30:0:1081:A:OP1	2.05	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.85	0.56
30:0:1835:U:C5	30:0:1840:A:N7	2.66	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.28	0.56
30:0:1116:U:O2'	30:0:1118:A:C2	2.52	0.56
30:0:2505:G:O2'	30:0:2506:A:H5'	2.05	0.56
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.53	0.56
30:0:1175:G:H1'	30:0:1193:A:H2'	1.86	0.56
30:0:1790:C:H2'	30:0:1791:U:H6	1.71	0.56
30:0:625:U:H5''	30:0:1044:C:N4	2.21	0.56
28:2:10:ARG:NH2	30:0:121:U:OP2	2.36	0.56
30:0:441:A:H1'	30:0:442:A:N7	2.21	0.56
30:0:711:G:H1'	39:0:7152:HOH:O	2.06	0.56
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.56
30:0:2700:G:H3'	39:0:3609:HOH:O	2.06	0.56
31:9:39:U:H1'	31:9:44:A:N6	2.20	0.56
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.21	0.55
30:0:1377:C:H5'	30:0:1377:C:C6	2.41	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
30:0:2748:G:H1'	39:0:7956:HOH:O	2.06	0.55
23:W:44:MET:HE2	30:0:944:G:H21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:644:G:N3	30:0:644:G:H5'	2.20	0.55
30:0:1187:U:O2'	30:0:1189:A:H2	1.89	0.55
30:0:2472:C:O2'	30:0:2634:G:H4'	2.07	0.55
30:0:2670:G:O2'	30:0:2671:U:H5'	2.06	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
30:0:907:A:H4'	30:0:1328:A:C2	2.41	0.55
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.87	0.55
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.22	0.55
30:0:2768:A:H5''	39:0:4460:HOH:O	2.06	0.55
30:0:138:U:H5''	30:0:139:C:OP2	2.07	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.06	0.55
30:0:2769:C:O2'	30:0:2770:G:H5'	2.07	0.55
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.88	0.55
29:3:2:GLN:HE21	29:3:91:GLN:HE21	1.54	0.55
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.22	0.54
30:0:2718:C:H5'	30:0:2718:C:H6	1.72	0.54
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.05	0.54
30:0:272:A:H3'	39:0:7588:HOH:O	2.07	0.54
30:0:595:U:H2'	30:0:596:C:H6	1.72	0.54
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.05	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.07	0.54
30:0:1625:U:H4'	39:0:4699:HOH:O	2.06	0.54
30:0:1666:C:C2'	30:0:1667:A:C5'	2.85	0.54
30:0:1682:A:H5''	39:0:9470:HOH:O	2.06	0.54
30:0:1174:A:C5	30:0:1201:C:H4'	2.43	0.54
30:0:1741:U:O2'	30:0:2723:G:H4'	2.07	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.07	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.07	0.54
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.23	0.54
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.22	0.53
30:0:1528:A:H2'	30:0:1529:G:O4'	2.08	0.53
30:0:1634:G:H3'	39:0:3923:HOH:O	2.06	0.53
30:0:2419:U:H5''	30:0:2420:G:H5'	1.90	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.38	0.53
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.89	0.53
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.89	0.53
23:W:84:VAL:HG12	39:W:6679:HOH:O	2.07	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1477:C:H5'	30:0:1868:G:C5'	2.38	0.53
30:0:2420:G:O2'	30:0:2421:G:H5'	2.08	0.53
31:9:54:A:O2'	31:9:55:U:H5'	2.08	0.53
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.91	0.53
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.43	0.53
14:N:37:ARG:NH1	31:9:6:C:C5'	2.67	0.53
29:3:48:ASN:ND2	29:3:50:GLY:H	2.06	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.74	0.53
30:0:1058:A:H2'	30:0:1060:C:H5''	1.89	0.53
31:9:39:U:HO2'	31:9:42:C:H5	1.54	0.53
30:0:380:A:H2'	39:0:7284:HOH:O	2.09	0.53
30:0:2265:U:H2'	30:0:2266:A:C8	2.44	0.53
30:0:2768:A:O2'	30:0:2769:C:H5'	2.08	0.53
30:0:272:A:H5'	30:0:273:G:OP2	2.09	0.53
30:0:671:A:O2'	30:0:672:G:H2'	2.09	0.53
30:0:899:C:H5'	39:0:3228:HOH:O	2.08	0.53
17:Q:95:GLU:HA	30:0:949:U:H4'	1.90	0.53
30:0:31:C:H2'	39:0:7745:HOH:O	2.08	0.53
30:0:1641:A:C2'	30:0:1642:A:H5'	2.39	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.90	0.53
30:0:2346:C:H6	30:0:2346:C:O5'	1.92	0.53
29:3:65:THR:HB	29:3:83:TRP:H	1.73	0.53
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.71	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:1456:C:H2'	30:0:1457:U:C6	2.44	0.53
30:0:2526:C:H5'	30:0:2526:C:C6	2.44	0.53
30:0:558:C:H2'	30:0:559:U:H5''	1.90	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.24	0.52
30:0:1279:U:H2'	30:0:1279:U:O2	2.08	0.52
30:0:2251:G:H2'	30:0:2252:A:C8	2.44	0.52
4:D:146:LYS:HZ1	14:N:38:LYS:HE2	1.75	0.52
30:0:17:G:H2'	30:0:18:C:C6	2.44	0.52
31:9:2:U:OP2	31:9:3:A:H5'	2.09	0.52
39:Z:8706:HOH:O	30:0:1886:A:H4'	2.10	0.52
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.52
30:0:849:C:H1'	39:0:6667:HOH:O	2.10	0.52
30:0:2787:C:H5	39:0:4665:HOH:O	1.92	0.52
39:I:1549:HOH:O	30:0:1180:U:H1'	2.08	0.52
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.52
30:0:814:G:H4'	39:0:3158:HOH:O	2.09	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.92	0.52
30:0:304:G:H1'	30:0:347:A:N6	2.24	0.52
30:0:343:C:O2'	30:0:344:C:H5'	2.08	0.52
30:0:1766:U:O2	30:0:1778:A:H5'	2.10	0.52
1:A:48:ASP:HB3	39:A:9064:HOH:O	2.08	0.52
3:C:76:ARG:HH22	30:0:1363:G:P	2.32	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.92	0.52
30:0:468:U:H3'	39:0:7628:HOH:O	2.10	0.52
30:0:1118:A:H8	30:0:1119:G:H5''	1.73	0.52
3:C:236:THR:HG22	3:C:239:ALA:H	1.75	0.52
12:L:6:ARG:HD3	30:0:1299:G:O6	2.09	0.52
15:O:3:THR:CG2	30:0:656:G:H5'	2.30	0.52
20:T:52:ARG:O	30:0:317:A:OP1	2.27	0.52
30:0:88:G:H2'	30:0:89:G:C8	2.44	0.52
30:0:1314:U:H2'	39:0:5916:HOH:O	2.08	0.52
30:0:2010:A:H2'	39:0:6002:HOH:O	2.09	0.52
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.75	0.52
30:0:1714:C:O2'	30:0:1715:C:H5'	2.10	0.52
30:0:2320:U:H4'	30:0:2321:A:O4'	2.10	0.52
30:0:2538:A:C8	38:0:2924:ANM:H61	2.44	0.52
30:0:1250:C:O2'	30:0:1251:C:H5'	2.10	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.74	0.51
30:0:280:C:H2'	30:0:281:U:O4'	2.10	0.51
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.51
30:0:2748:G:H2'	39:0:7599:HOH:O	2.10	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.10	0.51
30:0:2111:G:H1'	39:0:9050:HOH:O	2.10	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.94	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.98	0.51
30:0:2783:A:H2'	30:0:2784:A:C8	2.46	0.51
4:D:103:ASN:HD22	4:D:134:LEU:H	1.57	0.51
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.75	0.51
23:W:80:ASP:O	23:W:84:VAL:HG23	2.11	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
1:A:199:HIS:HD2	1:A:201:PHE:H	1.58	0.51
4:D:76:ARG:NE	31:9:44:A:O4'	2.42	0.51
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.51
30:0:1132:A:N6	30:0:1229:C:H2'	2.25	0.51
30:0:1189:A:O2'	30:0:1208:C:H2'	2.10	0.51
30:0:1268:C:O2'	30:0:1269:G:H5'	2.11	0.51
30:0:2604:A:H5'	39:0:5833:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:18:HIS:HD2	30:0:902:G:N7	2.09	0.51
12:L:143:THR:HG22	12:L:144:ASP:H	1.76	0.51
30:0:136:C:H2'	30:0:137:U:O4'	2.11	0.51
30:0:794:U:H3	30:0:819:A:H61	1.57	0.51
30:0:820:G:O2'	30:0:856:G:H4'	2.11	0.51
30:0:1249:U:H2'	30:0:1250:C:C6	2.45	0.51
30:0:2243:C:H5''	39:0:3776:HOH:O	2.11	0.51
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.91	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.25	0.51
31:9:54:A:H2	39:9:9064:HOH:O	1.93	0.51
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.43	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.10	0.51
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.57	0.50
18:R:117:HIS:HD2	30:0:20:G:H21	1.59	0.50
30:0:67:A:H5''	30:0:69:A:C8	2.46	0.50
30:0:182:G:H5''	39:0:3749:HOH:O	2.11	0.50
30:0:1211:G:O2'	30:0:1212:C:H5'	2.11	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.46	0.50
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.19	0.50
14:N:141:ARG:NH2	31:9:48:C:H4'	2.26	0.50
24:X:30:MET:HG2	30:0:1384:C:H5'	1.93	0.50
30:0:396:U:O2'	30:0:418:C:H4'	2.12	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.46	0.50
30:0:71:G:H5''	39:0:3940:HOH:O	2.10	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.46	0.50
30:0:1200:A:H3'	39:0:5796:HOH:O	2.10	0.50
30:0:407:A:H5'	39:0:6070:HOH:O	2.10	0.50
30:0:1940:C:H4'	39:0:7406:HOH:O	2.10	0.50
8:H:168:VAL:HG13	39:H:9008:HOH:O	2.11	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.92	0.50
14:N:11:ARG:HD3	31:9:114:G:O6	2.11	0.50
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.93	0.50
30:0:1172:G:H5''	39:0:7316:HOH:O	2.11	0.50
30:0:1596:U:H2'	30:0:1598:A:OP2	2.11	0.50
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.92	0.50
30:0:271:C:H41	30:0:378:A:H2	1.58	0.50
30:0:396:U:H1'	39:0:7686:HOH:O	2.09	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.93	0.50
30:0:125:U:H2'	39:0:3792:HOH:O	2.10	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1925:G:O2'	30:0:1926:G:H5'	2.12	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.46	0.50
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.50
30:0:485:A:N3	30:0:487:G:H5''	2.27	0.50
30:0:1819:G:H2'	30:0:1820:G:C5'	2.42	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.42	0.50
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
30:0:255:A:H2'	30:0:256:C:C6	2.46	0.50
30:0:559:U:H5'	30:0:559:U:C6	2.36	0.50
30:0:2104:C:O2	30:0:2485:A:N1	2.45	0.50
1:A:121:ALA:O	1:A:124:VAL:HG22	2.12	0.49
30:0:1562:C:H2'	30:0:1562:C:O2	2.12	0.49
1:A:192:VAL:HG12	39:A:9054:HOH:O	2.11	0.49
30:0:564:G:H1'	39:0:6359:HOH:O	2.12	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
12:L:14:GLY:O	30:0:1295:G:H5''	2.12	0.49
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.93	0.49
31:9:52:A:H2'	31:9:53:G:O4'	2.12	0.49
31:9:92:G:H2'	31:9:93:A:H8	1.76	0.49
8:H:31:ILE:HG23	39:H:9028:HOH:O	2.13	0.49
30:0:1350:U:H4'	39:0:5156:HOH:O	2.12	0.49
30:0:2256:G:O2'	30:0:2257:G:H5'	2.12	0.49
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.38	0.49
30:0:660:A:H4'	30:0:661:G:O5'	2.13	0.49
30:0:1181:A:N1	30:0:1192:A:O2'	2.44	0.49
30:0:249:G:O2'	30:0:250:C:H5'	2.13	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.47	0.49
30:0:1419:U:H2'	30:0:1685:A:C2	2.47	0.49
39:B:9096:HOH:O	30:0:2672:C:H1'	2.12	0.49
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.95	0.49
6:F:91:VAL:HG11	30:0:262:A:OP2	2.13	0.49
30:0:120:A:N3	30:0:120:A:H2'	2.28	0.49
30:0:1894:C:N4	30:0:1939:U:H2'	2.27	0.49
30:0:2508:C:H2'	39:0:6808:HOH:O	2.12	0.49
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.49
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.49
31:9:34:A:H2'	31:9:35:C:O4'	2.12	0.49
31:9:35:C:H5''	39:9:9077:HOH:O	2.12	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1135:G:H5'	39:0:5971:HOH:O	2.13	0.49
30:0:1838:U:O2'	30:0:2644:C:H5'	2.13	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
31:9:61:C:H2'	31:9:62:A:H8	1.77	0.49
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.49
30:0:459:A:H5''	39:0:9053:HOH:O	2.13	0.49
30:0:1046:G:N3	30:0:1082:A:H2	2.11	0.49
30:0:1632:A:C2'	30:0:1633:C:H5'	2.43	0.49
30:0:1919:A:H4'	39:0:4884:HOH:O	2.12	0.49
30:0:2248:C:H3'	39:0:5478:HOH:O	2.13	0.49
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.95	0.49
4:D:159:PRO:O	4:D:163:VAL:HG23	2.13	0.49
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.94	0.49
30:0:64:G:H2'	30:0:65:C:O4'	2.13	0.49
30:0:567:U:OP1	39:0:5320:HOH:O	2.19	0.49
30:0:1603:A:H5''	30:0:1605:G:H5'	1.95	0.49
5:E:137:ASP:O	5:E:141:VAL:HG23	2.12	0.48
8:H:70:LEU:O	8:H:74:ARG:HB2	2.13	0.48
30:0:1189:A:H1'	30:0:1209:C:H1'	1.94	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.48
2:B:16:ARG:NH1	39:B:9082:HOH:O	2.45	0.48
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.95	0.48
39:Y:8908:HOH:O	30:0:1330:A:H5''	2.12	0.48
30:0:1044:C:H5	39:0:6654:HOH:O	1.94	0.48
30:0:1946:C:H2'	30:0:1971:G:C8	2.48	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
13:M:164:THR:HG22	13:M:167:GLY:H	1.78	0.48
30:0:1441:G:H1'	39:0:7823:HOH:O	2.11	0.48
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.48
14:N:44:ARG:NH1	31:9:4:G:H21	2.11	0.48
30:0:324:G:O2'	30:0:325:U:H5'	2.13	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48
30:0:432:G:O2'	30:0:433:C:H5'	2.14	0.48
30:0:558:C:H2'	30:0:559:U:H5'	1.95	0.48
30:0:947:U:O2'	30:0:948:G:H5'	2.13	0.48
20:T:38:ARG:HH21	30:0:306:A:P	2.37	0.48
6:F:91:VAL:HG12	6:F:92:GLY:N	2.29	0.48
18:R:40:ALA:O	18:R:44:VAL:HG23	2.13	0.48
30:0:42:C:H1'	39:0:4709:HOH:O	2.13	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:932:U:H2'	30:0:933:C:C6	2.49	0.48
30:0:1819:G:H2'	30:0:1820:G:C4'	2.44	0.48
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.14	0.48
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.28	0.48
30:0:2011:A:H4'	30:0:2012:U:O5'	2.14	0.48
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.48
30:0:2608:C:H2'	39:0:7867:HOH:O	2.14	0.48
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.48
30:0:1066:U:H2'	30:0:1067:A:C8	2.49	0.48
30:0:1183:C:H42	30:0:1184:C:H41	1.61	0.48
30:0:2000:G:O2'	30:0:2001:G:H5'	2.14	0.48
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.78	0.47
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.14	0.47
16:P:41:ARG:HH22	30:0:1500:U:P	2.37	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.97	0.47
30:0:622:G:O2'	30:0:623:U:H5'	2.14	0.47
30:0:1087:G:H4'	30:0:1088:A:OP1	2.14	0.47
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.47
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
30:0:2135:A:O2'	30:0:2136:G:H5'	2.14	0.47
30:0:790:A:H1'	30:0:1710:A:H2'	1.96	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
1:A:51:ARG:NH1	1:A:120:ARG:O	2.47	0.47
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.27	0.47
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.95	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.29	0.47
30:0:635:A:H2'	30:0:636:G:H5''	1.95	0.47
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.47
30:0:2526:C:O2'	30:0:2527:U:H5'	2.14	0.47
30:0:2755:G:H1'	39:0:4715:HOH:O	2.14	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.28	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.97	0.47
21:U:14:GLU:O	21:U:17:THR:HB	2.15	0.47
30:0:961:A:H4'	39:0:6826:HOH:O	2.14	0.47
30:0:1166:A:OP1	30:0:1174:A:H4'	2.14	0.47
30:0:1926:G:H2'	30:0:1927:A:C8	2.50	0.47
30:0:2842:G:H2'	30:0:2843:A:H5'	1.95	0.47
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.47
30:0:1342:C:C2'	30:0:1343:C:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1603:A:H5'	30:0:1605:G:C4'	2.44	0.47
31:9:107:C:O2'	31:9:108:C:H5'	2.14	0.47
13:M:95:LYS:HE2	30:0:157:G:H4'	1.97	0.47
16:P:83:LYS:HG2	30:0:793:A:H5''	1.97	0.47
20:T:38:ARG:NH1	39:0:6736:HOH:O	2.47	0.47
23:W:23:MET:O	30:0:1025:C:H5'	2.15	0.47
29:3:15:ASN:O	30:0:2408:A:H4'	2.15	0.47
30:0:368:C:H2'	30:0:369:G:H5'	1.97	0.47
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
30:0:1829:A:H2'	30:0:1830:C:H5'	1.97	0.47
30:0:2064:U:H5'	30:0:2652:U:O3'	2.15	0.47
30:0:2105:C:H2'	30:0:2106:C:C6	2.49	0.47
27:1:16:HIS:HD2	30:0:470:U:O2'	1.97	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
30:0:714:U:H3'	39:0:6997:HOH:O	2.15	0.47
30:0:2414:A:H2'	30:0:2415:A:C8	2.50	0.47
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.47
30:0:653:U:H2'	30:0:654:A:C8	2.49	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
30:0:1016:U:H1'	39:0:3685:HOH:O	2.13	0.47
30:0:1588:G:C6	30:0:1589:G:N1	2.83	0.47
30:0:1662:C:H2'	30:0:1663:G:O4'	2.15	0.47
3:C:118:THR:O	3:C:136:VAL:HG13	2.15	0.47
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.49	0.47
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.97	0.47
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.97	0.47
30:0:255:A:H2'	30:0:256:C:H6	1.80	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
30:0:1595:G:O2'	30:0:1596:U:H5'	2.15	0.47
30:0:1815:A:H2'	30:0:1816:C:O4'	2.15	0.47
2:B:211:THR:HG21	39:0:7515:HOH:O	2.14	0.46
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
26:Z:40:ALA:HA	30:0:1773:G:C8	2.51	0.46
30:0:299:U:H5'	39:0:7395:HOH:O	2.16	0.46
30:0:2064:U:H4'	30:0:2653:A:OP1	2.14	0.46
17:Q:19:ARG:HH21	31:9:11:A:P	2.37	0.46
30:0:256:C:H2'	30:0:257:G:O4'	2.15	0.46
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.46
30:0:704:C:H2'	30:0:705:C:H6	1.80	0.46
30:0:951:A:O2'	30:0:952:G:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:960:G:C2'	30:0:960:G:N3	2.78	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.97	0.46
30:0:595:U:H2'	30:0:596:C:C6	2.49	0.46
30:0:834:G:H3'	30:0:835:U:H4'	1.98	0.46
30:0:1592:G:H2'	30:0:1593:C:C6	2.51	0.46
30:0:1603:A:C5'	30:0:1605:G:H5'	2.45	0.46
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.45	0.46
30:0:192:A:H5'	39:0:7700:HOH:O	2.16	0.46
30:0:1057:A:H1'	30:0:2492:U:O2'	2.15	0.46
30:0:2072:G:C6	30:0:2533:C:H1'	2.51	0.46
30:0:2909:G:H2'	30:0:2910:A:H8	1.80	0.46
19:S:33:SER:O	19:S:37:VAL:HG23	2.15	0.46
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.44	0.46
30:0:694:A:H2'	30:0:695:C:H5'	1.97	0.46
30:0:1137:G:H1'	39:0:3907:HOH:O	2.15	0.46
30:0:2781:U:C2'	30:0:2782:G:H5'	2.45	0.46
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.98	0.46
30:0:12:U:C2'	30:0:13:G:H5'	2.46	0.46
30:0:821:U:H3'	39:0:3796:HOH:O	2.15	0.46
30:0:1118:A:C8	30:0:1119:G:H5''	2.51	0.46
30:0:1973:A:H5'	30:0:1973:A:C8	2.42	0.46
30:0:645:U:O2	30:0:761:A:H2	1.98	0.46
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.16	0.46
30:0:1218:U:H2'	30:0:1219:U:C6	2.51	0.46
30:0:1804:A:H2'	30:0:1805:G:C8	2.50	0.46
30:0:2361:A:H5'	30:0:2361:A:H8	1.81	0.46
30:0:2531:U:O2'	30:0:2532:A:H5'	2.15	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.55	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46
30:0:1060:C:H6	30:0:1060:C:H5'	1.81	0.46
30:0:1614:G:H2'	39:0:4660:HOH:O	2.16	0.46
30:0:1771:U:O2'	30:0:1773:G:N7	2.48	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.50	0.46
30:0:2879:A:H2'	30:0:2880:A:O4'	2.16	0.46
30:0:2894:C:O2'	30:0:2895:C:H5'	2.15	0.46
30:0:2900:G:H2'	30:0:2901:C:O4'	2.16	0.46
2:B:238:ASN:HD22	2:B:240:GLY:N	2.11	0.46
30:0:113:A:OP2	30:0:114:A:H2'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:807:A:O2'	30:0:808:A:H5'	2.16	0.46
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.97	0.46
39:C:8656:HOH:O	30:0:2100:A:H5'	2.15	0.46
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.98	0.46
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.64	0.46
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.97	0.46
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.97	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
30:0:612:U:H2'	30:0:613:C:C6	2.51	0.46
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.97	0.45
30:0:876:A:H2'	30:0:876:A:N3	2.31	0.45
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.45
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.45
30:0:1972:U:H2'	30:0:1973:A:H5'	1.98	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.46	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	1.97	0.45
30:0:2852:A:H5''	39:0:5266:HOH:O	2.17	0.45
8:H:64:SER:OG	30:0:2520:G:H5'	2.16	0.45
30:0:95:A:H5''	30:0:97:G:O4'	2.16	0.45
30:0:319:A:H4'	30:0:338:C:C4	2.52	0.45
30:0:960:G:N3	30:0:960:G:H3'	2.31	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.16	0.45
30:0:1413:A:H2'	30:0:1414:A:O4'	2.16	0.45
30:0:2326:C:H4'	30:0:2412:G:C4'	2.47	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
11:K:55:VAL:HG12	11:K:56:SER:N	2.32	0.45
14:N:35:VAL:HG11	31:9:6:C:H4'	1.97	0.45
15:O:25:VAL:HG13	30:0:709:G:O2'	2.16	0.45
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.82	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.99	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.46	0.45
1:A:51:ARG:HB2	39:A:9064:HOH:O	2.17	0.45
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.53	0.45
18:R:39:THR:HG23	18:R:107:GLU:O	2.17	0.45
30:0:281:U:O2'	30:0:282:C:H5'	2.16	0.45
30:0:1485:A:H8	39:0:9975:HOH:O	1.99	0.45
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.45
30:0:1787:C:H4'	30:0:2883:A:O4'	2.17	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.45
30:0:2766:A:O2'	30:0:2767:C:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:2924:ANM:H62	38:0:2924:ANM:H2	1.87	0.45
31:9:13:A:O2'	31:9:14:G:H5''	2.17	0.45
31:9:24:U:H3'	31:9:25:G:H5'	1.97	0.45
8:H:69:ARG:HD3	39:H:9028:HOH:O	2.16	0.45
30:0:17:G:H2'	30:0:18:C:H6	1.81	0.45
30:0:812:A:H1'	39:0:3988:HOH:O	2.16	0.45
30:0:1304:U:H2'	30:0:1305:C:C6	2.52	0.45
30:0:1497:G:H4'	30:0:1627:G:O2'	2.16	0.45
30:0:2781:U:H2'	30:0:2782:G:H5'	1.98	0.45
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.45
30:0:777:U:H4'	30:0:777:U:OP2	2.16	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:2589:U:H2'	30:0:2590:U:C6	2.52	0.45
30:0:2758:G:H2'	30:0:2759:C:H6	1.82	0.45
31:9:49:G:H2'	31:9:50:G:O4'	2.17	0.45
3:C:88:SER:HB3	3:C:91:PRO:HB3	1.99	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45
30:0:1181:A:H2'	30:0:1182:C:H5'	1.98	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
30:0:2387:U:H2'	30:0:2388:C:C6	2.51	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.97	0.45
30:0:308:U:H5'	30:0:309:C:OP1	2.16	0.45
30:0:1015:C:H2'	30:0:1016:U:H6	1.80	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.52	0.45
2:B:94:GLN:O	30:0:2673:U:H4'	2.17	0.45
4:D:140:ARG:HB3	31:9:29:C:H5''	1.99	0.45
13:M:107:ARG:NH1	39:M:8871:HOH:O	2.49	0.45
30:0:168:C:H6	30:0:168:C:O5'	2.00	0.45
30:0:847:C:H4'	39:0:3779:HOH:O	2.16	0.45
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.45
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.45
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.82	0.45
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.97	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.32	0.45
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.45
30:0:2509:A:H2'	30:0:2510:C:O4'	2.17	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:O	1:A:38:ILE:N	2.44	0.44
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.44
2:B:254:GLN:HG2	2:B:255:GLY:N	2.32	0.44
19:S:11:THR:H	19:S:14:ALA:HB3	1.80	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.53	0.44
30:0:907:A:H2'	30:0:908:A:H8	1.80	0.44
30:0:2371:G:H5'	39:0:5043:HOH:O	2.17	0.44
30:0:2510:C:H5'	30:0:2511:A:OP2	2.18	0.44
30:0:2607:U:H4'	39:0:9455:HOH:O	2.16	0.44
31:9:22:G:H5'	31:9:23:U:OP1	2.17	0.44
23:W:44:MET:CE	30:0:944:G:H21	2.31	0.44
30:0:1204:C:H2'	30:0:1205:U:O4'	2.17	0.44
30:0:2866:U:H4'	30:0:2867:G:H5'	1.99	0.44
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.99	0.44
1:A:206:ARG:NH2	30:0:2630:G:O6	2.50	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.32	0.44
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.44
30:0:821:U:H2'	30:0:822:C:C6	2.53	0.44
30:0:1016:U:O2'	30:0:2303:A:N7	2.46	0.44
30:0:1167:G:H2'	30:0:1168:C:C6	2.51	0.44
30:0:1878:G:O2'	30:0:1879:U:C6	2.68	0.44
30:0:1942:A:H3'	39:0:7406:HOH:O	2.17	0.44
30:0:2524:G:H21	30:0:2526:C:N4	2.16	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
23:W:9:GLY:O	23:W:13:MET:HE3	2.16	0.44
30:0:168:C:H5'	30:0:2277:U:OP1	2.17	0.44
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.44
30:0:960:G:N3	30:0:960:G:H2'	2.31	0.44
30:0:1594:C:O2'	30:0:1607:A:H4'	2.17	0.44
30:0:1878:G:O2'	30:0:1879:U:P	2.74	0.44
12:L:30:ARG:NH2	39:L:8818:HOH:O	2.51	0.44
27:1:5:THR:HG23	30:0:1688:G:O2'	2.18	0.44
30:0:1996:U:O2'	30:0:1997:A:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
3:C:115:LEU:O	3:C:118:THR:HB	2.18	0.44
12:L:33:ALA:HB2	30:0:165:A:H5''	2.00	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
25:Y:165:GLU:HB3	39:Y:8889:HOH:O	2.17	0.44
29:3:73:GLU:HB3	39:3:9051:HOH:O	2.17	0.44
30:0:454:U:H5''	39:0:7834:HOH:O	2.17	0.44
30:0:2421:G:H3'	30:0:2422:U:H5''	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.44
1:A:132:ASP:HB3	1:A:135:VAL:H	1.82	0.44
4:D:146:LYS:HZ3	14:N:107:ASN:HD21	1.65	0.44
30:0:128:A:O2'	30:0:129:A:H5'	2.17	0.44
30:0:162:C:H2'	30:0:163:U:H5'	1.99	0.44
30:0:634:G:O2'	30:0:1358:A:OP1	2.34	0.44
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.44
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.44
30:0:1252:A:H2'	30:0:1253:C:O4'	2.18	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	2.00	0.44
30:0:1683:G:C2	30:0:1693:A:O4'	2.71	0.44
30:0:2092:G:H2'	30:0:2613:G:OP1	2.18	0.44
30:0:2256:G:C2'	30:0:2257:G:H5'	2.48	0.44
30:0:2899:A:O2'	30:0:2900:G:H5'	2.18	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
30:0:71:G:H8	39:0:3940:HOH:O	2.00	0.44
30:0:137:U:OP1	30:0:259:G:O2'	2.36	0.44
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.44
30:0:1165:G:H1'	30:0:1174:A:H1'	1.98	0.44
30:0:1172:G:H1'	39:0:5007:HOH:O	2.17	0.44
30:0:1422:U:H2'	30:0:1423:C:C6	2.52	0.44
30:0:2379:G:N7	30:0:2408:A:N1	2.65	0.44
30:0:2809:G:H2'	30:0:2810:G:O4'	2.18	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.00	0.44
30:0:920:C:H5'	30:0:921:G:C4	2.53	0.44
30:0:1130:U:H5'	39:0:7729:HOH:O	2.17	0.44
30:0:1592:G:H2'	30:0:1593:C:H6	1.83	0.44
30:0:2039:A:H2'	30:0:2040:C:C6	2.52	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.90	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.33	0.43
30:0:466:A:H2'	30:0:467:G:O4'	2.18	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.17	0.43
30:0:1790:C:H2'	30:0:1791:U:C6	2.52	0.43
30:0:2326:C:H4'	30:0:2412:G:H4'	2.00	0.43
30:0:2703:A:H2'	30:0:2704:C:H6	1.83	0.43
31:9:91:C:H2'	31:9:92:G:O4'	2.18	0.43
3:C:47:GLY:HA2	3:C:92:PRO:HB2	2.00	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:C2'	30:0:559:U:C5'	2.92	0.43
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:2533:C:H6	30:0:2533:C:C5'	2.24	0.43
30:0:2578:G:H5'	30:0:2578:G:C8	2.49	0.43
16:P:1:THR:O	30:0:1396:C:H1'	2.18	0.43
19:S:17:ASP:HB3	19:S:23:LYS:HB2	2.00	0.43
30:0:371:U:H2'	30:0:372:A:H8	1.83	0.43
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.43
13:M:171:ARG:CD	30:0:156:C:H5''	2.31	0.43
16:P:88:GLN:HE22	30:0:1799:G:H21	1.65	0.43
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.19	0.43
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.33	0.43
23:W:119:HIS:HE1	39:0:9570:HOH:O	2.01	0.43
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.16	0.43
30:0:603:A:H1'	30:0:605:C:C2	2.53	0.43
30:0:1377:C:H1'	39:0:9041:HOH:O	2.18	0.43
30:0:1504:A:H5'	39:0:4450:HOH:O	2.19	0.43
30:0:1544:U:H2'	30:0:1545:C:C6	2.54	0.43
30:0:1837:G:H3'	39:0:7851:HOH:O	2.18	0.43
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.43
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.88	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:417:G:P	39:0:7478:HOH:O	2.75	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43
30:0:1039:G:H2'	30:0:1040:A:O4'	2.19	0.43
30:0:1042:U:O2'	30:0:1043:C:H5'	2.18	0.43
30:0:1138:G:H4'	39:0:5749:HOH:O	2.18	0.43
30:0:1213:C:O2'	30:0:1214:G:H5'	2.18	0.43
30:0:1788:U:O2'	30:0:1789:G:H5'	2.19	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2274:A:O2'	30:0:2275:G:H5'	2.18	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
31:9:33:U:H2'	39:9:9068:HOH:O	2.19	0.43
12:L:37:LYS:NZ	30:0:919:U:O3'	2.50	0.43
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.52	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.99	0.43
30:0:271:C:H4'	30:0:272:A:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:364:U:H2'	30:0:365:G:O4'	2.19	0.43
30:0:407:A:H8	39:0:4495:HOH:O	2.00	0.43
30:0:497:A:H2'	30:0:498:A:C5'	2.49	0.43
30:0:1096:U:O2'	30:0:1097:A:H5'	2.18	0.43
2:B:297:VAL:HG23	39:B:9071:HOH:O	2.17	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.53	0.43
30:0:195:C:H2'	30:0:196:G:H5'	2.00	0.43
30:0:603:A:H4'	30:0:604:G:O5'	2.18	0.43
30:0:722:G:H22	30:0:938:G:P	2.41	0.43
30:0:1477:C:O2'	30:0:1478:U:H5'	2.18	0.43
30:0:1921:A:O2'	30:0:1922:A:H5'	2.19	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43
18:R:98:ASN:ND2	30:0:500:G:H21	2.10	0.43
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.43
30:0:488:U:H2'	39:0:4037:HOH:O	2.18	0.43
30:0:517:U:H1'	39:0:7636:HOH:O	2.19	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.18	0.43
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.43
30:0:2039:A:H4'	30:0:2760:C:O2'	2.19	0.43
31:9:47:A:C2	31:9:48:C:C2	3.07	0.43
2:B:36:PRO:HG3	2:B:169:GLY:H	1.83	0.43
10:J:52:GLN:NE2	30:0:1119:G:H8	2.13	0.43
30:0:1278:A:H4'	30:0:1279:U:N3	2.34	0.43
30:0:1481:G:H2'	30:0:1482:A:O4'	2.19	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.43
30:0:2001:G:O2'	30:0:2002:C:H5'	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:C5'	2.49	0.43
5:E:83:GLY:HA3	5:E:170:ARG:HE	1.83	0.43
22:V:39:ALA:N	22:V:40:PRO:HD2	2.34	0.43
25:Y:141:THR:HG23	39:Y:8884:HOH:O	2.18	0.43
30:0:65:C:O2'	30:0:66:G:H5'	2.19	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.19	0.43
30:0:285:A:H2'	30:0:286:U:O4'	2.19	0.43
30:0:1342:C:O2'	30:0:1343:C:H5'	2.19	0.43
30:0:1451:C:H5'	30:0:1505:U:C5	2.54	0.43
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.52	0.42
27:1:42:SER:HB3	30:0:1473:U:O4'	2.18	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.18	0.42
3:C:46:TYR:CE1	30:0:450:C:H4'	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.51	0.42
30:0:1490:G:H4'	30:0:1533:A:OP1	2.18	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:1834:C:H2'	30:0:1840:A:N6	2.34	0.42
30:0:2515:C:H2'	30:0:2516:G:O4'	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:C6	2.53	0.42
30:0:85:C:H5''	30:0:86:A:OP2	2.19	0.42
30:0:164:G:H3'	39:0:3671:HOH:O	2.18	0.42
30:0:204:A:C2'	30:0:205:U:H5'	2.49	0.42
30:0:255:A:H2'	30:0:256:C:O4'	2.19	0.42
30:0:1187:U:H2'	39:0:6950:HOH:O	2.18	0.42
30:0:2526:C:H5'	30:0:2526:C:H6	1.84	0.42
30:0:2793:A:H2'	30:0:2794:G:H5'	2.01	0.42
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.42
23:W:115:THR:HG23	39:W:5420:HOH:O	2.18	0.42
30:0:952:G:H4'	39:0:4063:HOH:O	2.18	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:2324:G:N2	30:0:2377:U:H1'	2.34	0.42
30:0:2433:A:H2'	30:0:2434:A:C8	2.54	0.42
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.42
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
25:Y:134:HIS:CD2	25:Y:134:HIS:H	2.37	0.42
30:0:661:G:C5	30:0:686:A:C2	3.08	0.42
30:0:1339:G:C6	30:0:1340:G:N1	2.87	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1850:U:H2'	30:0:1851:G:H8	1.84	0.42
30:0:1942:A:O2'	30:0:1943:C:H5'	2.20	0.42
30:0:2614:C:O2'	30:0:2615:U:H5'	2.20	0.42
3:C:149:LYS:NZ	30:0:327:A:OP1	2.47	0.42
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.55	0.42
30:0:1079:A:H4'	30:0:2078:U:H5'	2.02	0.42
30:0:1622:G:C2'	30:0:1623:C:H5'	2.49	0.42
30:0:1839:A:H5'	30:0:2643:G:H4'	2.01	0.42
31:9:56:A:C3'	31:9:57:A:H5''	2.49	0.42
30:0:129:A:O2'	30:0:131:A:OP1	2.37	0.42
30:0:204:A:H2'	30:0:205:U:H5'	2.01	0.42
30:0:278:A:H2'	30:0:279:C:O4'	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
30:0:1386:G:O2'	30:0:1387:G:H5'	2.19	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.42
10:J:41:ALA:HB3	39:J:5907:HOH:O	2.20	0.42
12:L:30:ARG:HD3	30:0:164:G:H4'	2.01	0.42
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.88	0.42
30:0:1525:G:H5'	30:0:1526:A:OP2	2.19	0.42
30:0:1682:A:H2'	39:0:9817:HOH:O	2.20	0.42
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.42
31:9:27:C:H1'	39:9:9053:HOH:O	2.17	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.38	0.42
30:0:816:G:C6	30:0:817:G:N1	2.88	0.42
30:0:1052:G:N3	30:0:1052:G:H2'	2.35	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.50	0.42
30:0:1186:C:H42	30:0:1190:G:H22	1.68	0.42
30:0:1243:C:H3'	39:0:4869:HOH:O	2.20	0.42
30:0:1537:C:H1'	39:0:6638:HOH:O	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:H6	1.85	0.42
3:C:79:ARG:O	3:C:87:ARG:HG2	2.20	0.42
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.28	0.42
9:I:87:PRO:C	9:I:89:GLU:H	2.28	0.42
10:J:74:ARG:NH1	10:J:105:LEU:HD11	2.35	0.42
10:J:82:THR:CG2	30:0:1242:A:H5'	2.34	0.42
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.02	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
30:0:200:C:H2'	39:0:3470:HOH:O	2.19	0.42
30:0:304:G:H1'	30:0:347:A:H61	1.84	0.42
30:0:567:U:H6	30:0:567:U:O5'	2.02	0.42
30:0:1023:C:O2'	30:0:1024:G:H5'	2.20	0.42
30:0:1406:A:H5'	30:0:1407:A:C8	2.55	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.49	0.42
30:0:1544:U:H2'	30:0:1545:C:H6	1.85	0.42
30:0:1883:U:H5'	30:0:2012:U:OP2	2.19	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2724:U:H2'	30:0:2725:G:O4'	2.19	0.42
18:R:80:TYR:O	30:0:2050:G:H5''	2.20	0.41
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.41
30:0:821:U:H5''	39:0:3074:HOH:O	2.20	0.41
30:0:1098:A:H2'	30:0:1099:G:O4'	2.20	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.20	0.41
30:0:1679:C:H5'	39:0:9335:HOH:O	2.20	0.41
30:0:1856:C:H5'	30:0:1858:A:O4'	2.20	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2134:G:N2	30:0:2242:U:C2	2.88	0.41
30:0:2335:C:H2'	30:0:2336:G:C8	2.55	0.41
30:0:2842:G:C2'	30:0:2843:A:H5'	2.50	0.41
31:9:60:C:O2'	31:9:61:C:H5'	2.19	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.20	0.41
4:D:103:ASN:ND2	4:D:134:LEU:H	2.17	0.41
24:X:10:VAL:HG23	24:X:72:VAL:HG12	2.03	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.41
30:0:68:U:O2'	30:0:69:A:H5''	2.20	0.41
30:0:177:A:H2'	30:0:178:U:O4'	2.20	0.41
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:2664:A:H8	30:0:2664:A:OP1	2.02	0.41
2:B:5:ARG:HE	2:B:5:ARG:HB3	1.69	0.41
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.96	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.28	0.41
24:X:25:ARG:HD2	39:X:5356:HOH:O	2.19	0.41
30:0:1615:A:H4'	39:0:5927:HOH:O	2.20	0.41
31:9:1:U:H5''	31:9:3:A:OP1	2.20	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.93	0.41
2:B:238:ASN:HD21	30:0:2609:G:N2	2.18	0.41
2:B:302:PRO:HA	30:0:2717:C:H5'	2.02	0.41
20:T:9:LYS:HD3	39:0:3781:HOH:O	2.20	0.41
23:W:122:ARG:HH12	23:W:154:ARG:N	2.19	0.41
30:0:308:U:C4	30:0:342:C:H1'	2.55	0.41
30:0:1315:G:H4'	30:0:1316:G:OP2	2.20	0.41
30:0:2073:G:C6	30:0:2489:G:H4'	2.55	0.41
30:0:2366:C:H6	30:0:2366:C:O5'	2.03	0.41
38:0:2924:ANM:H63	38:0:2924:ANM:C15	2.43	0.41
31:9:31:C:H2'	31:9:32:G:O4'	2.21	0.41
30:0:241:A:C2	30:0:378:A:H4'	2.55	0.41
30:0:932:U:H2'	30:0:933:C:H6	1.86	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
31:9:105:A:H2'	31:9:106:U:O4'	2.21	0.41
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.03	0.41
30:0:1205:U:C2'	30:0:1206:U:C5'	2.95	0.41
30:0:2379:G:H5'	30:0:2381:C:O4'	2.21	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:2672:C:O2'	30:0:2673:U:H5'	2.20	0.41
30:0:2781:U:H2'	30:0:2782:G:C5'	2.50	0.41
31:9:29:C:H2'	31:9:30:C:C5'	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:37:VAL:O	19:S:41:VAL:HG23	2.21	0.41
30:0:326:G:O2'	30:0:327:A:H5'	2.20	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.85	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.41
30:0:1603:A:H5''	30:0:1604:G:H3'	2.03	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
30:0:2349:G:O2'	30:0:2350:G:H5'	2.20	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
31:9:23:U:C2'	31:9:24:U:H4'	2.51	0.41
15:O:39:THR:O	15:O:115:ARG:NH2	2.54	0.41
26:Z:41:ARG:HH12	30:0:821:U:H4'	1.86	0.41
30:0:629:A:C2	30:0:2074:A:C2	3.09	0.41
30:0:1495:C:H1'	30:0:1573:A:H1'	2.03	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
31:9:39:U:H3'	31:9:40:C:C5'	2.50	0.41
1:A:171:LYS:HB2	30:0:820:G:C5	2.56	0.41
2:B:85:ARG:NH1	39:B:9096:HOH:O	2.53	0.41
2:B:254:GLN:NE2	39:B:9055:HOH:O	2.54	0.41
3:C:49:ASP:HB3	3:C:52:ALA:HB2	2.02	0.41
13:M:163:LEU:CD2	30:0:188:C:H5''	2.45	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
27:1:9:GLY:HA2	30:0:1687:C:O2	2.21	0.41
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
30:0:1829:A:C2'	30:0:1830:C:H5'	2.50	0.41
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.21	0.41
30:0:2271:G:H2'	30:0:2271:G:N3	2.36	0.41
30:0:2837:U:H2'	39:0:6892:HOH:O	2.21	0.41
30:0:2896:A:N3	30:0:2896:A:H2'	2.36	0.41
1:A:176:HIS:CD2	30:0:857:A:H4'	2.55	0.41
3:C:206:ASN:HB2	30:0:329:A:OP2	2.21	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.88	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.20	0.41
30:0:1398:G:O2'	30:0:1399:A:H5'	2.21	0.41
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
30:0:2016:U:H6	30:0:2016:U:O5'	2.03	0.41
30:0:2553:A:N3	30:0:2553:A:H2'	2.35	0.41
13:M:179:GLY:O	30:0:399:C:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:117:SER:HB3	30:0:1593:C:OP1	2.21	0.40
30:0:130:C:H2'	39:0:3186:HOH:O	2.21	0.40
30:0:226:A:H1'	30:0:393:G:C5	2.56	0.40
30:0:827:A:H1'	39:0:6263:HOH:O	2.20	0.40
30:0:2385:G:H2'	30:0:2386:U:H6	1.83	0.40
30:0:2493:C:H2'	30:0:2493:C:O2	2.21	0.40
30:0:2549:C:H2'	30:0:2550:U:O4'	2.22	0.40
30:0:2642:G:H2'	30:0:2643:G:O4'	2.21	0.40
9:I:110:ASP:O	30:0:1163:G:H5'	2.21	0.40
12:L:67:ARG:HB2	12:L:112:GLY:HA3	2.04	0.40
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.04	0.40
30:0:228:C:H2'	30:0:229:G:H5'	2.03	0.40
30:0:613:C:H2'	30:0:614:U:H6	1.87	0.40
30:0:912:A:C4	30:0:1294:A:C2	3.09	0.40
30:0:1185:U:H5'	39:0:7526:HOH:O	2.21	0.40
30:0:1268:C:H2'	30:0:1269:G:H8	1.86	0.40
30:0:1972:U:C2'	30:0:1973:A:C5'	2.99	0.40
30:0:2449:G:H2'	30:0:2450:C:O4'	2.21	0.40
30:0:2812:A:C2	30:0:2814:A:N6	2.75	0.40
6:F:30:LYS:HE2	6:F:99:THR:HG21	2.04	0.40
14:N:147:ILE:HD11	31:9:50:G:OP1	2.22	0.40
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.37	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.22	0.40
30:0:849:C:O2'	30:0:850:U:H5'	2.21	0.40
30:0:876:A:N3	30:0:876:A:C2'	2.85	0.40
30:0:2419:U:H5''	30:0:2420:G:C5'	2.51	0.40
3:C:1:MET:HG2	3:C:2:GLN:H	1.87	0.40
23:W:21:LEU:HD23	23:W:21:LEU:HA	1.86	0.40
27:1:16:HIS:CD2	30:0:470:U:O2'	2.73	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.22	0.40
30:0:441:A:O5'	30:0:441:A:H8	2.04	0.40
30:0:1080:C:H6	30:0:1080:C:O5'	2.04	0.40
30:0:1299:G:N2	39:0:4716:HOH:O	2.54	0.40
30:0:1545:C:H2'	30:0:1546:G:O4'	2.22	0.40
30:0:1762:C:O2'	30:0:1763:C:H5'	2.21	0.40
30:0:2291:A:N9	30:0:2309:C:H5'	2.35	0.40
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.56	0.40
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.36	0.40
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.55	0.40
30:0:396:U:HO2'	30:0:397:A:P	2.45	0.40
30:0:397:A:O2'	30:0:417:G:N3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:877:G:C5'	30:0:878:G:OP1	2.65	0.40
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.40
30:0:1119:G:C5	30:0:1243:C:C4	3.10	0.40
30:0:2478:U:O2'	30:0:2479:A:H5'	2.21	0.40
30:0:2893:C:O2'	30:0:2894:C:H5'	2.21	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	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	14	35
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	21	44
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	8	22
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100	100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	4	11
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	21	44
9	I	68/162 (42%)	60 (88%)	8 (12%)	0	100	100
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	16	37
12	L	141/165 (86%)	134 (95%)	7 (5%)	0	100	100
13	M	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
14	N	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	4	10
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	9	25
24	X	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	64 (90%)	6 (8%)	1 (1%)	9	23
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	11	29
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	24	48

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
14	N	154	LEU
14	N	184	ILE
14	N	183	ASP
1	A	27	LEU
4	D	56	ARG
8	H	19	ARG
14	N	139	TRP
14	N	167	ASP
23	W	77	ALA
2	B	2	GLN
6	F	100	ASP
6	F	101	ALA
11	K	127	ALA
2	B	185	GLY
4	D	137	PRO
23	W	49	ASN
26	Z	44	ARG

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Mol	Chain	Res	Type
6	F	61	MET
29	3	56	PRO

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	
1	A	179/182 (98%)	166 (93%)	13 (7%)	13	32
2	B	282/283 (100%)	262 (93%)	20 (7%)	13	33
3	C	193/193 (100%)	177 (92%)	16 (8%)	10	26
4	D	117/148 (79%)	103 (88%)	14 (12%)	5	12
5	E	152/156 (97%)	146 (96%)	6 (4%)	28	57
6	F	93/94 (99%)	89 (96%)	4 (4%)	26	54
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	59
8	H	134/145 (92%)	128 (96%)	6 (4%)	24	52
9	I	58/130 (45%)	56 (97%)	2 (3%)	32	62
10	J	118/121 (98%)	111 (94%)	7 (6%)	18	42
11	K	106/106 (100%)	101 (95%)	5 (5%)	23	51
12	L	113/127 (89%)	108 (96%)	5 (4%)	25	53
13	M	158/160 (99%)	149 (94%)	9 (6%)	18	43
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	51
15	O	93/94 (99%)	89 (96%)	4 (4%)	26	54
16	P	113/117 (97%)	108 (96%)	5 (4%)	25	53
17	Q	79/80 (99%)	76 (96%)	3 (4%)	29	58
18	R	117/122 (96%)	111 (95%)	6 (5%)	21	48
19	S	71/74 (96%)	68 (96%)	3 (4%)	26	55
20	T	105/106 (99%)	96 (91%)	9 (9%)	10	25
21	U	44/53 (83%)	40 (91%)	4 (9%)	9	22
22	V	51/57 (90%)	49 (96%)	2 (4%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	130/130 (100%)	123 (95%)	7 (5%)	20	45
24	X	66/74 (89%)	58 (88%)	8 (12%)	5	12
25	Y	120/196 (61%)	116 (97%)	4 (3%)	33	63
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	45	74
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	72
29	3	79/79 (100%)	74 (94%)	5 (6%)	16	39
All	All	3095/3646 (85%)	2918 (94%)	177 (6%)	18	43

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	68	ILE
1	A	69	LEU
1	A	85	SER
1	A	94	LEU
1	A	105	VAL
1	A	131	HIS
1	A	175	LYS
1	A	179	MET
1	A	192	VAL
1	A	200	PRO
1	A	217	ARG
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	53	LEU
2	B	66	GLU
2	B	71	VAL
2	B	84	LEU
2	B	97	LEU
2	B	98	THR
2	B	112	THR
2	B	162	MET
2	B	171	VAL
2	B	195	ARG
2	B	251	VAL

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Mol	Chain	Res	Type
2	B	254	GLN
2	B	257	THR
2	B	265	LEU
2	B	277	GLU
2	B	301	VAL
3	C	2	GLN
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	118	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	17	ARG
4	D	19	GLU
4	D	23	VAL
4	D	50	VAL
4	D	52	THR
4	D	58	VAL
4	D	69	ILE
4	D	101	THR
4	D	128	LEU
4	D	137	PRO
4	D	149	ARG
4	D	153	THR
4	D	161	ASP
4	D	172	VAL
5	E	36	PRO
5	E	102	VAL
5	E	108	LEU
5	E	126	ILE
5	E	131	LEU
5	E	156	ASP
6	F	12	LEU

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Mol	Chain	Res	Type
6	F	46	GLU
6	F	60	VAL
6	F	61	MET
7	G	12	ILE
8	H	58	VAL
8	H	65	LEU
8	H	87	LYS
8	H	157	TYR
8	H	162	PRO
8	H	173	GLU
9	I	94	ASP
9	I	135	GLU
10	J	28	GLU
10	J	39	VAL
10	J	45	VAL
10	J	46	ILE
10	J	47	THR
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	62	PRO
11	K	74	VAL
11	K	98	VAL
11	K	107	THR
12	L	4	LYS
12	L	32	ASP
12	L	101	ASP
12	L	104	ASP
12	L	140	VAL
13	M	10	ASP
13	M	46	LEU
13	M	81	ARG
13	M	84	LYS
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	141	ILE
13	M	164	THR
14	N	26	LEU
14	N	38	LYS
14	N	49	THR
14	N	127	LEU

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Mol	Chain	Res	Type
14	N	135	VAL
14	N	175	LEU
14	N	176	ARG
15	O	3	THR
15	O	25	VAL
15	O	36	PRO
15	O	43	VAL
16	P	16	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	18	PRO
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	123	GLN
18	R	143	VAL
19	S	10	VAL
19	S	44	GLN
19	S	81	ILE
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	71	VAL
20	T	82	THR
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	28	THR
21	U	47	ARG
21	U	52	THR
21	U	56	ARG
22	V	12	THR
22	V	13	PRO
23	W	4	LEU
23	W	26	ILE
23	W	38	THR

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Mol	Chain	Res	Type
23	W	52	VAL
23	W	120	PRO
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
24	X	88	GLU
25	Y	154	ARG
25	Y	157	ILE
25	Y	189	ASN
25	Y	203	VAL
27	1	21	ARG
28	2	18	ASN
29	3	14	CYS
29	3	18	GLN
29	3	22	VAL
29	3	56	PRO
29	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	127	GLN
2	B	221	GLN
2	B	230	GLN
2	B	238	ASN
2	B	243	ASN
2	B	260	HIS
2	B	266	ASN
2	B	332	ASN
3	C	67	GLN
3	C	73	GLN
3	C	129	HIS

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Mol	Chain	Res	Type
3	C	163	HIS
4	D	103	ASN
5	E	143	GLN
6	F	55	GLN
7	G	64	ASN
8	H	34	HIS
8	H	40	GLN
8	H	49	GLN
8	H	59	GLN
8	H	75	HIS
10	J	52	GLN
10	J	89	HIS
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
11	K	119	GLN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	22	GLN
14	N	107	ASN
14	N	132	ASN
14	N	140	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	89	ASN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	94	ASN
18	R	98	ASN
18	R	102	GLN
18	R	117	HIS
19	S	7	HIS
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN

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Mol	Chain	Res	Type
20	T	11	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	22	ASN
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	188	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	237 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	254 (8%)	29 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A

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Mol	Chain	Res	Type
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	285	A
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C

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Mol	Chain	Res	Type
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C

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Mol	Chain	Res	Type
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A

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Mol	Chain	Res	Type
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1857	A
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G

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Mol	Chain	Res	Type
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	G
30	0	2613	G
30	0	2634	G
30	0	2649	A

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Mol	Chain	Res	Type
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1684	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

5 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
30	OMG	0	2588	30	23,26,27	0.27	0	32,38,41	0.40	0
30	1MA	0	628	30,35	21,25,26	0.74	1 (4%)	30,37,40	0.82	1 (3%)
30	PSU	0	2621	30	18,21,22	1.43	2 (11%)	21,30,33	1.29	3 (14%)
30	UR3	0	2619	30	19,22,23	0.40	0	26,32,35	0.71	1 (3%)
30	OMU	0	2587	30	19,22,23	0.28	0	25,31,34	0.44	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
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	1MA	0	628	30,35	-	2/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.53	1.42	1.36
30	0	2621	PSU	C6-C5	2.91	1.38	1.35
30	0	628	1MA	C6-N6	2.61	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.11	120.28	118.17
30	0	2621	PSU	C6-N1-C2	-2.90	120.00	122.69
30	0	2621	PSU	O2-C2-N1	2.87	125.75	122.79
30	0	628	1MA	N1-C2-N3	2.84	129.37	126.00
30	0	2619	UR3	C4-N3-C2	2.73	126.78	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	ANM	0	2924	37	20,20,20	0.47	0	24,27,27	1.92	6 (25%)

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
38	ANM	0	2924	37	-	4/10/23/23	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	ANM	O2-C5-C6	5.40	120.72	111.09
38	0	2924	ANM	C4-C3-C2	-3.92	98.31	103.32
38	0	2924	ANM	C2-O2-C5	-3.73	111.92	117.72
38	0	2924	ANM	C3-C2-C16	-3.01	99.95	104.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	ANM	C14-O1-C9	-2.82	111.46	117.50
38	0	2924	ANM	O2-C5-O3	-2.15	118.84	122.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

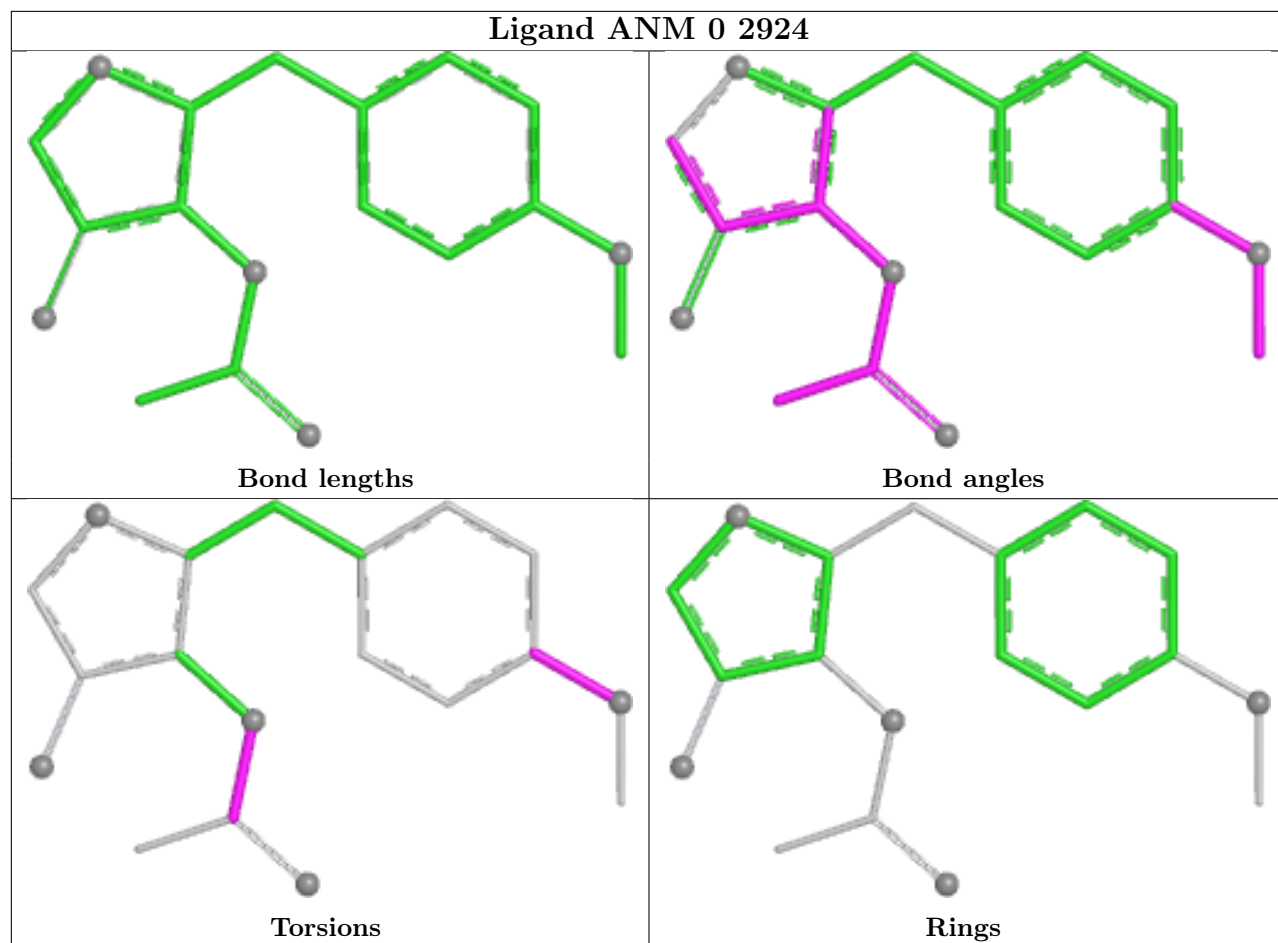
Mol	Chain	Res	Type	Atoms
38	0	2924	ANM	C6-C5-O2-C2
38	0	2924	ANM	O3-C5-O2-C2
38	0	2924	ANM	C10-C9-O1-C14
38	0	2924	ANM	C1-C9-O1-C14

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	ANM	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.51	17 (7%) 21 18	24, 49, 88, 107	0
2	B	337/338 (99%)	0.59	15 (4%) 38 34	27, 53, 82, 95	0
3	C	246/246 (100%)	0.39	6 (2%) 59 56	21, 42, 65, 78	0
4	D	140/177 (79%)	2.43	83 (59%) 0 0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.97	20 (11%) 9 8	44, 69, 88, 94	0
6	F	119/120 (99%)	1.16	19 (15%) 5 4	43, 69, 99, 114	0
7	G	29/348 (8%)	1.86	8 (27%) 1 1	77, 95, 103, 106	0
8	H	160/177 (90%)	0.72	12 (7%) 20 17	44, 61, 96, 101	0
9	I	70/162 (43%)	3.22	59 (84%) 0 0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.57	11 (7%) 19 17	35, 50, 71, 91	0
11	K	132/132 (100%)	0.36	1 (0%) 82 81	32, 49, 72, 77	0
12	L	145/165 (87%)	1.10	28 (19%) 3 3	25, 63, 109, 125	0
13	M	194/196 (98%)	0.25	7 (3%) 46 42	28, 40, 56, 62	0
14	N	186/187 (99%)	1.28	36 (19%) 3 2	42, 64, 112, 121	0
15	O	115/116 (99%)	0.71	7 (6%) 27 24	33, 53, 69, 80	0
16	P	143/149 (95%)	0.69	7 (4%) 35 31	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.37	5 (5%) 32 28	34, 45, 62, 73	0
18	R	150/155 (96%)	0.10	1 (0%) 84 83	30, 43, 63, 71	0
19	S	81/85 (95%)	0.59	7 (8%) 16 13	42, 56, 79, 90	0
20	T	119/120 (99%)	0.67	5 (4%) 40 37	35, 54, 84, 109	0
21	U	53/67 (79%)	0.70	5 (9%) 14 12	40, 56, 78, 84	0
22	V	65/71 (91%)	1.61	15 (23%) 2 2	52, 73, 117, 123	0
23	W	154/154 (100%)	0.57	5 (3%) 50 46	33, 49, 65, 75	0
24	X	82/92 (89%)	0.91	11 (13%) 7 6	43, 60, 85, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.25	3 (2%) 63 61	22, 41, 64, 89	0
26	Z	73/116 (62%)	1.62	20 (27%) 1 1	58, 76, 89, 100	0
27	1	56/57 (98%)	-0.29	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.37	15 (32%) 1 1	34, 60, 91, 101	0
29	3	92/92 (100%)	0.54	1 (1%) 78 76	36, 59, 72, 86	0
30	0	2749/2923 (94%)	-0.37	55 (2%) 65 62	18, 43, 87, 165	0
31	9	122/122 (100%)	0.22	4 (3%) 49 45	34, 65, 86, 145	0
All	All	6646/7517 (88%)	0.29	488 (7%) 21 18	18, 50, 99, 165	0

All (488) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	9.9
4	D	10	PHE	8.4
22	V	39	ALA	8.2
22	V	40	PRO	8.0
9	I	128	THR	7.9
14	N	166	ALA	7.2
22	V	43	PRO	7.0
4	D	63	ILE	6.3
31	9	1	U	6.2
22	V	2	VAL	6.1
9	I	97	VAL	6.0
9	I	120	ALA	6.0
4	D	174	VAL	5.8
4	D	44	ILE	5.8
26	Z	34	SER	5.6
9	I	134	ILE	5.6
4	D	55	LYS	5.6
9	I	74	ILE	5.5
28	2	49	GLU	5.3
14	N	154	LEU	5.3
14	N	168	LEU	5.3
7	G	71	LEU	5.3
4	D	90	LEU	5.2
9	I	100	VAL	5.2
1	A	37	VAL	5.2
4	D	107	GLY	5.1
26	Z	35	SER	5.1
26	Z	106	SER	5.0

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Mol	Chain	Res	Type	RSRZ
9	I	71	ALA	4.9
9	I	132	VAL	4.9
9	I	113	SER	4.9
4	D	40	ILE	4.9
7	G	12	ILE	4.8
28	2	38	LYS	4.8
9	I	112	LEU	4.8
4	D	35	ALA	4.7
5	E	154	ILE	4.7
25	Y	235	GLU	4.7
9	I	95	LEU	4.7
10	J	4	ALA	4.7
14	N	169	PRO	4.6
30	0	10	U	4.6
9	I	127	CYS	4.5
9	I	70	THR	4.5
9	I	130	LEU	4.5
4	D	135	VAL	4.5
30	0	1199	A	4.4
4	D	18	ILE	4.4
9	I	88	GLN	4.4
4	D	172	VAL	4.4
28	2	37	HIS	4.4
4	D	61	PHE	4.4
9	I	124	VAL	4.4
4	D	62	ASP	4.4
4	D	134	LEU	4.4
12	L	82	ALA	4.4
14	N	164	ASP	4.3
6	F	101	ALA	4.3
9	I	85	GLY	4.3
4	D	57	THR	4.3
5	E	53	GLU	4.3
9	I	119	ALA	4.2
10	J	70	PHE	4.2
19	S	81	ILE	4.2
22	V	36	ALA	4.2
6	F	102	GLY	4.2
9	I	116	LEU	4.2
24	X	85	VAL	4.1
24	X	88	GLU	4.1
12	L	145	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	4.0
12	L	60	GLU	4.0
9	I	104	ALA	4.0
30	0	735	C	4.0
4	D	104	PHE	4.0
9	I	80	PHE	4.0
12	L	99	GLU	4.0
26	Z	58	ASN	4.0
12	L	148	GLU	3.9
16	P	143	ALA	3.9
24	X	87	ALA	3.9
12	L	146	GLY	3.9
31	9	2	U	3.9
5	E	10	ASP	3.9
8	H	43	ALA	3.9
28	2	27	LEU	3.9
22	V	41	GLU	3.9
4	D	171	ASP	3.9
29	3	41	GLU	3.8
30	0	2637	A	3.8
22	V	37	GLY	3.8
1	A	32	VAL	3.8
4	D	154	LYS	3.8
30	0	1172	G	3.8
4	D	106	PHE	3.8
28	2	35	ARG	3.8
5	E	45	ASP	3.8
14	N	167	ASP	3.7
28	2	48	ASP	3.7
5	E	7	ILE	3.7
9	I	91	PHE	3.7
7	G	26	MET	3.7
9	I	73	LEU	3.7
4	D	37	ALA	3.7
4	D	11	HIS	3.6
12	L	75	LEU	3.6
4	D	69	ILE	3.6
14	N	145	ALA	3.6
26	Z	46	SER	3.6
6	F	99	THR	3.6
30	0	1198	U	3.6
1	A	237	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
9	I	133	THR	3.6
9	I	83	GLY	3.6
14	N	165	ALA	3.6
12	L	44	GLU	3.6
9	I	84	SER	3.6
14	N	158	LEU	3.6
9	I	72	GLU	3.5
28	2	20	ARG	3.5
4	D	75	LEU	3.5
9	I	67	VAL	3.5
12	L	149	ARG	3.5
4	D	53	LYS	3.5
20	T	119	ALA	3.5
14	N	163	PHE	3.5
14	N	160	SER	3.4
31	9	24	U	3.4
14	N	161	GLY	3.4
15	O	23	GLY	3.4
8	H	174	LEU	3.4
12	L	55	GLN	3.4
14	N	186	LEU	3.4
16	P	116	SER	3.4
9	I	66	GLY	3.4
4	D	128	LEU	3.4
30	0	2769	C	3.4
21	U	52	THR	3.4
30	0	1173	A	3.4
28	2	44	ARG	3.4
30	0	1279	U	3.3
14	N	148	ALA	3.3
14	N	152	GLU	3.3
4	D	26	GLY	3.3
8	H	171	GLY	3.3
24	X	83	ALA	3.3
1	A	211	LYS	3.3
9	I	101	LYS	3.3
4	D	89	PRO	3.3
9	I	106	GLN	3.3
4	D	58	VAL	3.3
4	D	19	GLU	3.3
16	P	18	LYS	3.2
4	D	66	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
7	G	27	ILE	3.2
5	E	172	PRO	3.2
4	D	59	GLY	3.2
12	L	105	TYR	3.2
30	0	2345	A	3.2
9	I	103	ILE	3.2
20	T	117	ASP	3.2
28	2	39	ARG	3.2
30	0	2237	G	3.2
14	N	159	TYR	3.2
12	L	97	VAL	3.2
1	A	36	ASP	3.2
12	L	78	ALA	3.2
30	0	1176	C	3.1
4	D	72	LYS	3.1
3	C	16	VAL	3.1
14	N	147	ILE	3.1
16	P	117	SER	3.1
20	T	118	SER	3.1
30	0	1561	U	3.1
30	0	1165	G	3.1
10	J	92	GLN	3.1
4	D	101	THR	3.1
9	I	123	VAL	3.1
9	I	118	ASN	3.1
5	E	156	ASP	3.1
25	Y	163	THR	3.1
12	L	77	ALA	3.1
22	V	46	ILE	3.1
21	U	47	ARG	3.1
5	E	6	GLU	3.0
4	D	56	ARG	3.0
24	X	84	ILE	3.0
30	0	87	C	3.0
22	V	38	GLY	3.0
12	L	96	VAL	3.0
8	H	114	ASP	3.0
9	I	90	ASP	3.0
10	J	127	ILE	3.0
4	D	91	ALA	3.0
6	F	22	VAL	3.0
4	D	65	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
9	I	107	LYS	2.9
14	N	157	PRO	2.9
8	H	132	ALA	2.9
4	D	23	VAL	2.9
30	O	1160	G	2.9
14	N	162	ASP	2.9
7	G	23	ILE	2.9
4	D	86	THR	2.9
6	F	17	LEU	2.9
30	O	1524	U	2.9
12	L	102	ASP	2.9
30	O	138	U	2.9
15	O	3	THR	2.9
4	D	85	GLN	2.8
10	J	46	ILE	2.8
15	O	22	GLY	2.8
14	N	1	ALA	2.8
5	E	11	VAL	2.8
6	F	49	PHE	2.8
4	D	68	PRO	2.8
21	U	56	ARG	2.8
9	I	111	LEU	2.8
6	F	26	THR	2.8
5	E	126	ILE	2.8
30	O	960	G	2.8
2	B	57	GLU	2.8
28	2	31	ARG	2.8
22	V	42	ASN	2.8
12	L	79	ASP	2.8
13	M	1	ALA	2.7
24	X	7	GLU	2.7
9	I	87	PRO	2.7
12	L	150	GLN	2.7
13	M	194	GLY	2.7
3	C	132	ASP	2.7
10	J	144	THR	2.7
26	Z	51	ALA	2.7
30	O	1161	A	2.7
1	A	68	ILE	2.7
4	D	142	ALA	2.7
5	E	13	ALA	2.7
6	F	104	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	94	ASP	2.7
14	N	184	ILE	2.7
12	L	83	GLU	2.7
4	D	21	VAL	2.7
4	D	153	THR	2.7
6	F	97	ALA	2.7
30	O	1175	G	2.6
3	C	139	VAL	2.6
22	V	35	ALA	2.6
5	E	100	ASP	2.6
4	D	25	MET	2.6
8	H	77	ILE	2.6
8	H	115	GLY	2.6
30	O	1171	A	2.6
4	D	130	VAL	2.6
12	L	91	VAL	2.6
6	F	75	ILE	2.6
30	O	1162	G	2.6
10	J	47	THR	2.6
30	O	2103	A	2.6
4	D	170	TYR	2.6
9	I	114	TYR	2.6
2	B	34	GLY	2.6
1	A	58	VAL	2.6
6	F	91	VAL	2.6
26	Z	45	VAL	2.6
28	2	36	ASN	2.6
20	T	114	SER	2.5
30	O	1192	A	2.5
26	Z	36	GLY	2.5
24	X	72	VAL	2.5
2	B	112	THR	2.5
9	I	117	THR	2.5
14	N	75	THR	2.5
4	D	99	ASP	2.5
30	O	2344	G	2.5
9	I	109	PRO	2.5
5	E	87	PHE	2.5
9	I	99	GLN	2.5
11	K	118	ALA	2.5
14	N	172	PHE	2.5
4	D	105	SER	2.5

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Mol	Chain	Res	Type	RSRZ
16	P	67	LYS	2.5
31	9	23	U	2.5
19	S	76	GLU	2.5
4	D	139	TYR	2.5
30	0	1190	G	2.5
15	O	24	ALA	2.5
4	D	36	ASN	2.5
4	D	52	THR	2.5
19	S	12	GLU	2.5
12	L	100	ALA	2.5
4	D	64	ARG	2.4
4	D	133	ASN	2.4
26	Z	44	ARG	2.4
30	0	497	A	2.4
30	0	1200	A	2.4
8	H	68	SER	2.4
30	0	514	G	2.4
14	N	62	HIS	2.4
1	A	35	GLY	2.4
9	I	68	PRO	2.4
4	D	169	THR	2.4
4	D	166	ILE	2.4
14	N	139	TRP	2.4
1	A	210	GLY	2.4
4	D	70	GLY	2.4
2	B	115	VAL	2.4
15	O	25	VAL	2.4
30	0	1184	C	2.4
1	A	65	ARG	2.4
4	D	54	ALA	2.4
21	U	55	ALA	2.4
26	Z	62	ALA	2.4
30	0	1625	U	2.4
6	F	103	GLU	2.4
7	G	73	ASP	2.4
10	J	62	ASP	2.4
6	F	1	PRO	2.4
9	I	75	LYS	2.4
22	V	44	GLY	2.4
26	Z	77	GLY	2.4
24	X	71	ARG	2.4
4	D	88	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	144	THR	2.4
4	D	131	THR	2.4
24	X	66	THR	2.4
14	N	171	HIS	2.4
9	I	77	GLU	2.4
9	I	129	SER	2.4
9	I	121	LYS	2.4
12	L	57	VAL	2.4
26	Z	103	VAL	2.4
4	D	165	PHE	2.4
30	0	1177	A	2.4
30	0	1181	A	2.4
30	0	2914	A	2.4
24	X	65	ASN	2.3
30	0	1197	G	2.3
30	0	1182	C	2.3
24	X	74	ALA	2.3
5	E	168	ILE	2.3
14	N	150	TYR	2.3
13	M	74	LYS	2.3
9	I	69	PRO	2.3
30	0	1178	G	2.3
30	0	1929	G	2.3
5	E	32	ARG	2.3
5	E	170	ARG	2.3
22	V	45	ARG	2.3
9	I	92	VAL	2.3
4	D	84	LEU	2.3
10	J	63	ILE	2.3
9	I	108	HIS	2.3
4	D	74	THR	2.3
8	H	140	TYR	2.3
2	B	108	GLU	2.3
2	B	183	GLU	2.3
9	I	122	GLU	2.3
12	L	147	GLU	2.3
30	0	1188	A	2.3
30	0	1202	A	2.3
10	J	48	GLY	2.3
26	Z	39	GLY	2.3
30	0	510	U	2.3
30	0	1169	U	2.3

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Mol	Chain	Res	Type	RSRZ
22	V	3	LEU	2.3
23	W	62	LEU	2.3
4	D	29	HIS	2.3
30	0	284	C	2.3
1	A	31	LYS	2.3
9	I	82	THR	2.3
12	L	143	THR	2.3
17	Q	95	GLU	2.3
13	M	75	ARG	2.3
5	E	108	LEU	2.3
6	F	118	LEU	2.3
12	L	81	VAL	2.3
23	W	65	VAL	2.3
1	A	99	ILE	2.2
4	D	13	MET	2.2
4	D	45	THR	2.2
8	H	86	TYR	2.2
30	0	1951	G	2.2
4	D	67	ASP	2.2
17	Q	20	ASP	2.2
2	B	171	VAL	2.2
12	L	76	LEU	2.2
21	U	49	LEU	2.2
26	Z	50	VAL	2.2
9	I	78	ALA	2.2
13	M	125	ARG	2.2
4	D	47	GLN	2.2
30	0	1183	C	2.2
26	Z	38	PHE	2.2
9	I	93	ALA	2.2
9	I	102	GLN	2.2
6	F	47	LEU	2.2
19	S	1	SER	2.2
5	E	3	VAL	2.2
5	E	97	VAL	2.2
7	G	24	VAL	2.2
14	N	43	VAL	2.2
6	F	111	ILE	2.2
12	L	136	ALA	2.2
4	D	43	GLU	2.2
2	B	257	THR	2.2
28	2	47	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	66	ARG	2.2
26	Z	41	ARG	2.2
19	S	44	GLN	2.2
4	D	41	LEU	2.2
14	N	50	LEU	2.2
14	N	179	LEU	2.2
4	D	77	ASP	2.2
9	I	110	ASP	2.2
23	W	76	ASP	2.2
25	Y	108	ASP	2.2
20	T	40	VAL	2.2
26	Z	53	ILE	2.2
12	L	62	ALA	2.1
13	M	21	ALA	2.1
14	N	95	ALA	2.1
14	N	137	ALA	2.1
15	O	98	LEU	2.1
30	0	272	A	2.1
2	B	119	HIS	2.1
4	D	163	VAL	2.1
8	H	168	VAL	2.1
16	P	141	ILE	2.1
23	W	79	VAL	2.1
30	0	1164	U	2.1
30	0	1170	U	2.1
4	D	83	PHE	2.1
3	C	135	GLU	2.1
4	D	156	ARG	2.1
1	A	67	LEU	2.1
4	D	138	GLY	2.1
13	M	70	GLY	2.1
4	D	22	VAL	2.1
10	J	76	ASP	2.1
6	F	112	ALA	2.1
28	2	23	ALA	2.1
26	Z	48	ARG	2.1
23	W	115	THR	2.1
28	2	29	THR	2.1
4	D	24	HIS	2.1
14	N	144	GLY	2.1
26	Z	43	GLY	2.1
30	0	2911	C	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	105	PHE	2.1
6	F	39	SER	2.1
4	D	15	GLU	2.1
4	D	17	ARG	2.1
6	F	90	GLU	2.1
8	H	170	ARG	2.1
16	P	59	ARG	2.1
19	S	2	TRP	2.1
30	O	1525	G	2.1
1	A	165	THR	2.1
2	B	98	THR	2.1
30	O	1205	U	2.1
30	O	2664	A	2.1
30	O	2768	A	2.1
14	N	180	LEU	2.1
1	A	45	ILE	2.1
17	Q	84	ILE	2.1
26	Z	78	ILE	2.1
2	B	4	SER	2.0
3	C	180	SER	2.0
4	D	96	SER	2.0
17	Q	17	LYS	2.0
30	O	1204	C	2.0
19	S	57	THR	2.0
7	G	13	PRO	2.0
3	C	8	LEU	2.0
4	D	157	LEU	2.0
4	D	12	GLU	2.0
4	D	100	ASP	2.0
5	E	39	ASP	2.0
9	I	89	GLU	2.0
9	I	135	GLU	2.0
14	N	61	ALA	2.0
14	N	151	ASP	2.0
18	R	73	ASP	2.0
28	2	30	ASP	2.0
1	A	88	ILE	2.0
2	B	168	GLY	2.0
15	O	47	ARG	2.0
17	Q	92	ARG	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
30	OMG	0	2588	24/25	0.97	0.06	27,30,33,35	0
30	UR3	0	2619	21/22	0.97	0.08	30,34,36,39	0
30	1MA	0	628	23/24	0.98	0.07	25,28,29,31	0
30	OMU	0	2587	21/22	0.98	0.06	31,33,35,37	0
30	PSU	0	2621	20/21	0.98	0.06	22,26,34,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	9	8572	1/1	0.53	0.29	76,76,76,76	0
34	SR	0	9001	1/1	0.56	0.20	169,169,169,169	0
34	SR	0	8983	1/1	0.56	0.22	164,164,164,164	0
32	MG	A	8051	1/1	0.58	0.17	81,81,81,81	0
35	NA	0	8557	1/1	0.61	0.27	67,67,67,67	0
34	SR	A	8977	1/1	0.61	0.12	172,172,172,172	0
35	NA	S	8510	1/1	0.62	0.25	79,79,79,79	0
34	SR	0	9006	1/1	0.63	0.29	200,200,200,200	0
35	NA	0	8546	1/1	0.63	0.48	95,95,95,95	0
35	NA	0	8571	1/1	0.65	0.30	83,83,83,83	0
34	SR	0	8991	1/1	0.65	0.22	191,191,191,191	0
34	SR	0	8919	1/1	0.66	0.23	178,178,178,178	0
34	SR	9	8980	1/1	0.68	0.17	182,182,182,182	0
34	SR	0	8944	1/1	0.69	0.25	185,185,185,185	0
35	NA	0	8561	1/1	0.70	0.53	74,74,74,74	0
32	MG	0	8063	1/1	0.70	0.30	72,72,72,72	0
34	SR	0	8959	1/1	0.70	0.11	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	9000	1/1	0.71	0.20	159,159,159,159	0
35	NA	0	8522	1/1	0.72	0.48	78,78,78,78	0
35	NA	0	8511	1/1	0.72	0.23	59,59,59,59	0
34	SR	0	8933	1/1	0.73	0.28	138,138,138,138	0
34	SR	0	8986	1/1	0.74	0.49	200,200,200,200	0
34	SR	9	9003	1/1	0.75	0.14	162,162,162,162	0
35	NA	0	8554	1/1	0.75	0.37	65,65,65,65	0
34	SR	0	8989	1/1	0.75	0.24	187,187,187,187	0
34	SR	0	8993	1/1	0.76	0.18	168,168,168,168	0
35	NA	0	8573	1/1	0.76	0.17	69,69,69,69	0
35	NA	9	8543	1/1	0.76	0.29	70,70,70,70	0
35	NA	0	8502	1/1	0.76	0.32	67,67,67,67	0
34	SR	9	8978	1/1	0.77	0.16	144,144,144,144	0
35	NA	0	8506	1/1	0.77	0.12	47,47,47,47	0
34	SR	0	8979	1/1	0.77	0.21	194,194,194,194	0
37	K	0	8401	1/1	0.77	0.35	81,81,81,81	0
34	SR	0	8951	1/1	0.78	0.11	146,146,146,146	0
34	SR	0	8997	1/1	0.78	0.28	184,184,184,184	0
34	SR	0	9002	1/1	0.78	0.22	184,184,184,184	0
35	NA	0	8520	1/1	0.79	0.28	54,54,54,54	0
35	NA	0	8509	1/1	0.79	0.28	64,64,64,64	0
35	NA	0	8525	1/1	0.79	0.25	69,69,69,69	0
34	SR	0	8922	1/1	0.79	0.24	159,159,159,159	0
35	NA	0	8501	1/1	0.80	0.17	39,39,39,39	0
35	NA	0	8560	1/1	0.80	0.23	69,69,69,69	0
34	SR	0	8956	1/1	0.80	0.17	142,142,142,142	0
34	SR	0	8947	1/1	0.80	0.26	200,200,200,200	0
35	NA	0	8531	1/1	0.80	0.14	40,40,40,40	0
34	SR	0	8994	1/1	0.80	0.29	190,190,190,190	0
32	MG	0	8039	1/1	0.80	0.28	69,69,69,69	0
35	NA	0	8555	1/1	0.80	0.32	54,54,54,54	0
34	SR	0	8967	1/1	0.81	0.15	133,133,133,133	0
34	SR	0	8976	1/1	0.81	0.22	186,186,186,186	0
32	MG	0	8040	1/1	0.81	0.22	83,83,83,83	0
34	SR	B	8987	1/1	0.81	0.36	200,200,200,200	0
35	NA	0	8548	1/1	0.81	0.32	57,57,57,57	0
35	NA	0	8533	1/1	0.82	0.26	63,63,63,63	0
32	MG	0	8017	1/1	0.82	0.15	56,56,56,56	0
34	SR	0	8957	1/1	0.82	0.32	200,200,200,200	0
34	SR	0	8982	1/1	0.82	0.48	180,180,180,180	0
35	NA	0	8567	1/1	0.82	0.41	78,78,78,78	0
34	SR	0	8939	1/1	0.83	0.18	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8924	1/1	0.83	0.18	145,145,145,145	0
34	SR	0	8990	1/1	0.83	0.16	118,118,118,118	0
35	NA	0	8575	1/1	0.83	0.47	94,94,94,94	0
34	SR	0	8996	1/1	0.83	0.25	200,200,200,200	0
34	SR	0	9004	1/1	0.83	0.34	200,200,200,200	0
35	NA	0	8519	1/1	0.83	0.17	39,39,39,39	0
35	NA	0	8514	1/1	0.84	0.16	42,42,42,42	0
34	SR	0	8942	1/1	0.84	0.16	121,121,121,121	0
34	SR	F	9005	1/1	0.84	0.12	136,136,136,136	0
35	NA	J	8538	1/1	0.85	0.15	56,56,56,56	0
34	SR	0	8988	1/1	0.85	0.10	163,163,163,163	0
34	SR	0	8971	1/1	0.85	0.17	170,170,170,170	0
35	NA	0	8556	1/1	0.85	0.24	44,44,44,44	0
34	SR	0	8949	1/1	0.85	0.17	110,110,110,110	0
35	NA	0	8544	1/1	0.85	0.33	64,64,64,64	0
34	SR	0	8920	1/1	0.85	0.16	124,124,124,124	0
34	SR	0	8953	1/1	0.86	0.19	160,160,160,160	0
34	SR	0	8995	1/1	0.86	0.15	136,136,136,136	0
34	SR	0	8955	1/1	0.86	0.28	200,200,200,200	0
35	NA	0	8574	1/1	0.86	0.36	53,53,53,53	0
32	MG	0	8092	1/1	0.86	0.17	61,61,61,61	0
34	SR	A	8930	1/1	0.86	0.11	116,116,116,116	0
34	SR	0	8938	1/1	0.86	0.14	159,159,159,159	0
34	SR	0	8960	1/1	0.86	0.10	145,145,145,145	0
35	NA	0	8559	1/1	0.87	0.32	75,75,75,75	0
32	MG	0	8031	1/1	0.87	0.12	61,61,61,61	0
34	SR	0	8958	1/1	0.87	0.12	108,108,108,108	0
35	NA	0	8562	1/1	0.87	0.44	69,69,69,69	0
35	NA	0	8564	1/1	0.87	0.19	65,65,65,65	0
32	MG	0	8069	1/1	0.87	0.19	47,47,47,47	0
34	SR	0	8916	1/1	0.87	0.16	118,118,118,118	0
34	SR	0	8927	1/1	0.87	0.23	167,167,167,167	0
35	NA	0	8512	1/1	0.87	0.24	43,43,43,43	0
34	SR	0	8970	1/1	0.87	0.11	131,131,131,131	0
32	MG	0	8071	1/1	0.87	0.25	55,55,55,55	0
35	NA	Q	8540	1/1	0.87	0.25	60,60,60,60	0
34	SR	0	8975	1/1	0.87	0.15	134,134,134,134	0
35	NA	0	8542	1/1	0.88	0.16	42,42,42,42	0
34	SR	0	8934	1/1	0.88	0.15	90,90,90,90	0
34	SR	0	8917	1/1	0.88	0.15	119,119,119,119	0
34	SR	0	8973	1/1	0.88	0.14	137,137,137,137	0
35	NA	0	8549	1/1	0.88	0.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8974	1/1	0.88	0.18	166,166,166,166	0
32	MG	0	8083	1/1	0.88	0.09	56,56,56,56	0
34	SR	B	8950	1/1	0.88	0.16	108,108,108,108	0
34	SR	0	8998	1/1	0.88	0.25	173,173,173,173	0
32	MG	0	8085	1/1	0.88	0.19	80,80,80,80	0
32	MG	0	8038	1/1	0.88	0.08	58,58,58,58	0
34	SR	0	8914	1/1	0.88	0.18	118,118,118,118	0
35	NA	0	8518	1/1	0.88	0.36	79,79,79,79	0
34	SR	0	8984	1/1	0.88	0.12	128,128,128,128	0
34	SR	0	8963	1/1	0.88	0.10	133,133,133,133	0
34	SR	0	9007	1/1	0.88	0.43	200,200,200,200	0
35	NA	0	8523	1/1	0.88	0.15	48,48,48,48	0
34	SR	0	8964	1/1	0.88	0.11	126,126,126,126	0
35	NA	0	8529	1/1	0.88	0.16	37,37,37,37	0
34	SR	0	8966	1/1	0.88	0.12	110,110,110,110	0
32	MG	0	8080	1/1	0.88	0.10	57,57,57,57	0
35	NA	0	8536	1/1	0.88	0.12	50,50,50,50	0
35	NA	0	8565	1/1	0.89	0.20	62,62,62,62	0
34	SR	0	8941	1/1	0.89	0.13	115,115,115,115	0
34	SR	0	8915	1/1	0.89	0.10	117,117,117,117	0
35	NA	B	8552	1/1	0.89	0.17	56,56,56,56	0
35	NA	0	8507	1/1	0.89	0.19	45,45,45,45	0
32	MG	0	8030	1/1	0.89	0.16	55,55,55,55	0
35	NA	M	8539	1/1	0.89	0.14	41,41,41,41	0
32	MG	0	8044	1/1	0.89	0.06	33,33,33,33	0
32	MG	0	8036	1/1	0.89	0.15	49,49,49,49	0
34	SR	0	8928	1/1	0.90	0.17	138,138,138,138	0
34	SR	0	8981	1/1	0.90	0.23	167,167,167,167	0
35	NA	0	8563	1/1	0.90	0.22	60,60,60,60	0
35	NA	0	8547	1/1	0.90	0.18	54,54,54,54	0
32	MG	0	8078	1/1	0.90	0.14	51,51,51,51	0
32	MG	0	8056	1/1	0.90	0.13	42,42,42,42	0
35	NA	0	8553	1/1	0.90	0.29	79,79,79,79	0
35	NA	R	8532	1/1	0.90	0.23	53,53,53,53	0
34	SR	0	8910	1/1	0.90	0.13	97,97,97,97	0
35	NA	0	8516	1/1	0.90	0.15	30,30,30,30	0
35	NA	0	8535	1/1	0.90	0.20	52,52,52,52	0
34	SR	0	8992	1/1	0.90	0.25	123,123,123,123	0
34	SR	0	8985	1/1	0.90	0.14	110,110,110,110	0
34	SR	0	8954	1/1	0.91	0.09	105,105,105,105	0
34	SR	0	8926	1/1	0.91	0.11	115,115,115,115	0
35	NA	C	8503	1/1	0.91	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8073	1/1	0.91	0.30	76,76,76,76	0
34	SR	0	8969	1/1	0.91	0.25	150,150,150,150	0
35	NA	0	8568	1/1	0.91	0.15	47,47,47,47	0
35	NA	0	8570	1/1	0.91	0.18	49,49,49,49	0
32	MG	0	8010	1/1	0.91	0.06	26,26,26,26	0
32	MG	0	8066	1/1	0.91	0.15	52,52,52,52	0
32	MG	T	8057	1/1	0.91	0.19	57,57,57,57	0
35	NA	0	8541	1/1	0.91	0.18	53,53,53,53	0
34	SR	0	8923	1/1	0.91	0.10	101,101,101,101	0
32	MG	0	8032	1/1	0.91	0.07	40,40,40,40	0
35	NA	0	8545	1/1	0.91	0.10	37,37,37,37	0
35	NA	0	8569	1/1	0.92	0.13	53,53,53,53	0
35	NA	0	8517	1/1	0.92	0.11	30,30,30,30	0
35	NA	0	8550	1/1	0.92	0.16	54,54,54,54	0
35	NA	0	8526	1/1	0.92	0.07	32,32,32,32	0
34	SR	S	8961	1/1	0.92	0.10	114,114,114,114	0
32	MG	0	8053	1/1	0.92	0.16	61,61,61,61	0
34	SR	0	8931	1/1	0.92	0.10	108,108,108,108	0
32	MG	0	8024	1/1	0.92	0.37	85,85,85,85	0
36	CD	O	8705	1/1	0.92	0.11	124,124,124,124	0
32	MG	0	8060	1/1	0.92	0.11	42,42,42,42	0
32	MG	0	8089	1/1	0.93	0.05	48,48,48,48	0
34	SR	0	8965	1/1	0.93	0.11	120,120,120,120	0
34	SR	0	8943	1/1	0.93	0.09	95,95,95,95	0
34	SR	H	8972	1/1	0.93	0.22	130,130,130,130	0
34	SR	0	8945	1/1	0.93	0.12	99,99,99,99	0
34	SR	0	8946	1/1	0.93	0.09	108,108,108,108	0
32	MG	0	8090	1/1	0.93	0.12	54,54,54,54	0
34	SR	0	8948	1/1	0.93	0.13	102,102,102,102	0
35	NA	0	8566	1/1	0.93	0.26	37,37,37,37	0
34	SR	1	8952	1/1	0.93	0.08	79,79,79,79	0
34	SR	3	8999	1/1	0.93	0.09	95,95,95,95	0
34	SR	0	8901	1/1	0.93	0.08	58,58,58,58	0
34	SR	0	8908	1/1	0.93	0.13	107,107,107,107	0
32	MG	0	8079	1/1	0.93	0.08	47,47,47,47	0
32	MG	9	8074	1/1	0.93	0.20	67,67,67,67	0
32	MG	0	8050	1/1	0.93	0.08	37,37,37,37	0
34	SR	0	8937	1/1	0.93	0.08	100,100,100,100	0
32	MG	0	8081	1/1	0.93	0.13	54,54,54,54	0
32	MG	0	8059	1/1	0.93	0.05	36,36,36,36	0
34	SR	0	8962	1/1	0.93	0.23	167,167,167,167	0
32	MG	0	8055	1/1	0.93	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8968	1/1	0.94	0.10	143,143,143,143	0
32	MG	0	8093	1/1	0.94	0.06	29,29,29,29	0
35	NA	0	8528	1/1	0.94	0.07	45,45,45,45	0
35	NA	0	8504	1/1	0.94	0.09	26,26,26,26	0
35	NA	0	8530	1/1	0.94	0.11	42,42,42,42	0
34	SR	0	8921	1/1	0.94	0.07	92,92,92,92	0
32	MG	B	8042	1/1	0.94	0.12	50,50,50,50	0
34	SR	0	9008	1/1	0.94	0.07	90,90,90,90	0
33	CL	J	8802	1/1	0.94	0.09	60,60,60,60	0
35	NA	0	8537	1/1	0.94	0.06	34,34,34,34	0
33	CL	0	8805	1/1	0.94	0.09	59,59,59,59	0
35	NA	0	8513	1/1	0.94	0.13	44,44,44,44	0
33	CL	0	8813	1/1	0.94	0.07	48,48,48,48	0
35	NA	0	8515	1/1	0.94	0.10	33,33,33,33	0
32	MG	0	8018	1/1	0.94	0.15	38,38,38,38	0
32	MG	0	8020	1/1	0.94	0.20	54,54,54,54	0
32	MG	0	8075	1/1	0.94	0.07	45,45,45,45	0
32	MG	0	8077	1/1	0.94	0.07	32,32,32,32	0
32	MG	0	8064	1/1	0.94	0.11	38,38,38,38	0
34	SR	0	8936	1/1	0.94	0.09	89,89,89,89	0
32	MG	0	8047	1/1	0.94	0.18	49,49,49,49	0
35	NA	0	8524	1/1	0.94	0.08	45,45,45,45	0
33	CL	J	8801	1/1	0.95	0.10	62,62,62,62	0
34	SR	0	8911	1/1	0.95	0.07	78,78,78,78	0
35	NA	0	8551	1/1	0.95	0.10	46,46,46,46	0
32	MG	0	8033	1/1	0.95	0.10	45,45,45,45	0
33	CL	J	8821	1/1	0.95	0.07	56,56,56,56	0
33	CL	N	8807	1/1	0.95	0.09	61,61,61,61	0
32	MG	0	8043	1/1	0.95	0.14	49,49,49,49	0
35	NA	0	8521	1/1	0.95	0.13	61,61,61,61	0
35	NA	0	8558	1/1	0.95	0.12	44,44,44,44	0
34	SR	0	8918	1/1	0.95	0.09	79,79,79,79	0
32	MG	0	8034	1/1	0.95	0.05	32,32,32,32	0
33	CL	0	8815	1/1	0.95	0.11	57,57,57,57	0
33	CL	0	8817	1/1	0.95	0.06	53,53,53,53	0
33	CL	0	8822	1/1	0.95	0.21	68,68,68,68	0
34	SR	A	8929	1/1	0.95	0.19	131,131,131,131	0
32	MG	0	8035	1/1	0.95	0.14	44,44,44,44	0
32	MG	0	8048	1/1	0.95	0.14	28,28,28,28	0
32	MG	0	8084	1/1	0.95	0.13	31,31,31,31	0
32	MG	0	8049	1/1	0.95	0.15	55,55,55,55	0
32	MG	K	8054	1/1	0.95	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8072	1/1	0.95	0.11	52,52,52,52	0
32	MG	0	8091	1/1	0.95	0.09	42,42,42,42	0
32	MG	0	8037	1/1	0.95	0.23	83,83,83,83	0
35	NA	0	8508	1/1	0.95	0.08	37,37,37,37	0
32	MG	0	8016	1/1	0.95	0.11	49,49,49,49	0
32	MG	0	8006	1/1	0.95	0.09	30,30,30,30	0
34	SR	0	8902	1/1	0.95	0.08	69,69,69,69	0
33	CL	A	8809	1/1	0.95	0.13	57,57,57,57	0
34	SR	0	8909	1/1	0.95	0.08	94,94,94,94	0
37	K	0	8402	1/1	0.95	0.12	64,64,64,64	0
38	ANM	0	2924	19/19	0.95	0.10	31,37,40,40	0
32	MG	0	8008	1/1	0.96	0.11	25,25,25,25	0
33	CL	L	8810	1/1	0.96	0.09	49,49,49,49	0
35	NA	0	8534	1/1	0.96	0.10	32,32,32,32	0
34	SR	0	8940	1/1	0.96	0.07	85,85,85,85	0
32	MG	0	8087	1/1	0.96	0.10	42,42,42,42	0
33	CL	Y	8820	1/1	0.96	0.06	38,38,38,38	0
34	SR	1	8913	1/1	0.96	0.09	85,85,85,85	0
33	CL	3	8804	1/1	0.96	0.06	54,54,54,54	0
32	MG	0	8027	1/1	0.96	0.07	34,34,34,34	0
32	MG	0	8062	1/1	0.96	0.07	34,34,34,34	0
34	SR	0	8925	1/1	0.96	0.09	90,90,90,90	0
32	MG	0	8001	1/1	0.96	0.06	25,25,25,25	0
33	CL	0	8816	1/1	0.96	0.15	60,60,60,60	0
32	MG	0	8041	1/1	0.96	0.13	24,24,24,24	0
32	MG	0	8011	1/1	0.96	0.09	23,23,23,23	0
32	MG	0	8067	1/1	0.96	0.11	34,34,34,34	0
32	MG	0	8068	1/1	0.96	0.10	47,47,47,47	0
35	NA	0	8505	1/1	0.96	0.27	39,39,39,39	0
35	NA	0	8527	1/1	0.96	0.11	52,52,52,52	0
34	SR	0	8935	1/1	0.96	0.08	79,79,79,79	0
32	MG	0	8015	1/1	0.96	0.09	27,27,27,27	0
32	MG	0	8045	1/1	0.96	0.11	32,32,32,32	0
32	MG	0	8082	1/1	0.97	0.12	48,48,48,48	0
32	MG	0	8029	1/1	0.97	0.14	39,39,39,39	0
32	MG	0	8076	1/1	0.97	0.06	35,35,35,35	0
32	MG	0	8061	1/1	0.97	0.17	37,37,37,37	0
32	MG	0	8022	1/1	0.97	0.13	29,29,29,29	0
34	SR	R	8912	1/1	0.97	0.07	84,84,84,84	0
32	MG	0	8088	1/1	0.97	0.08	37,37,37,37	0
32	MG	0	8019	1/1	0.97	0.13	24,24,24,24	0
32	MG	0	8058	1/1	0.97	0.08	23,23,23,23	0

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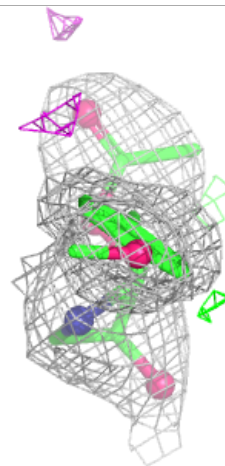
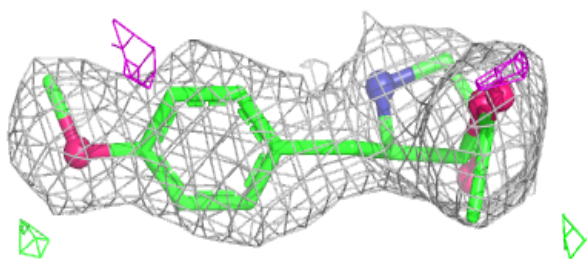
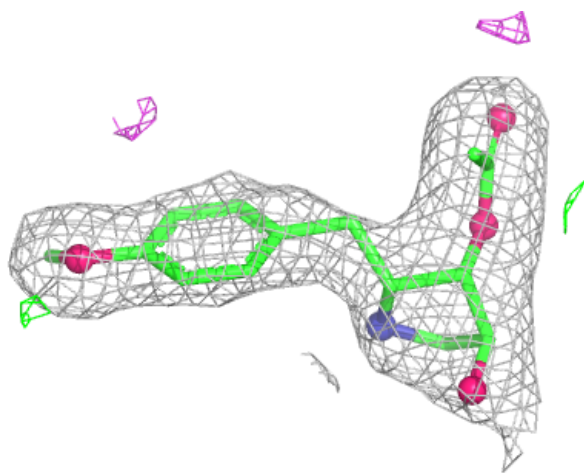
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	3	8932	1/1	0.97	0.05	73,73,73,73	0
32	MG	Y	8086	1/1	0.97	0.05	39,39,39,39	0
33	CL	O	8808	1/1	0.97	0.12	61,61,61,61	0
32	MG	0	8070	1/1	0.98	0.04	45,45,45,45	0
33	CL	0	8811	1/1	0.98	0.07	53,53,53,53	0
33	CL	0	8812	1/1	0.98	0.06	48,48,48,48	0
32	MG	0	8012	1/1	0.98	0.09	21,21,21,21	0
33	CL	0	8814	1/1	0.98	0.09	47,47,47,47	0
32	MG	0	8025	1/1	0.98	0.04	24,24,24,24	0
32	MG	0	8026	1/1	0.98	0.08	31,31,31,31	0
33	CL	M	8818	1/1	0.98	0.04	37,37,37,37	0
32	MG	0	8014	1/1	0.98	0.14	30,30,30,30	0
32	MG	0	8021	1/1	0.98	0.11	32,32,32,32	0
32	MG	0	8007	1/1	0.98	0.12	26,26,26,26	0
34	SR	0	8904	1/1	0.98	0.07	52,52,52,52	0
36	CD	Z	8703	1/1	0.98	0.04	81,81,81,81	0
34	SR	0	8906	1/1	0.98	0.07	56,56,56,56	0
32	MG	0	8052	1/1	0.98	0.05	40,40,40,40	0
33	CL	0	8803	1/1	0.98	0.08	46,46,46,46	0
32	MG	0	8004	1/1	0.99	0.09	25,25,25,25	0
32	MG	0	8009	1/1	0.99	0.11	21,21,21,21	0
32	MG	0	8005	1/1	0.99	0.13	26,26,26,26	0
33	CL	R	8806	1/1	0.99	0.03	43,43,43,43	0
32	MG	0	8065	1/1	0.99	0.07	33,33,33,33	0
32	MG	0	8046	1/1	0.99	0.06	28,28,28,28	0
33	CL	B	8819	1/1	0.99	0.09	46,46,46,46	0
32	MG	0	8023	1/1	0.99	0.07	22,22,22,22	0
32	MG	0	8002	1/1	0.99	0.05	22,22,22,22	0
34	SR	0	8903	1/1	0.99	0.12	53,53,53,53	0
32	MG	0	8003	1/1	0.99	0.08	30,30,30,30	0
36	CD	3	8704	1/1	0.99	0.03	66,66,66,66	0
34	SR	0	8905	1/1	0.99	0.14	57,57,57,57	0
32	MG	0	8013	1/1	0.99	0.08	26,26,26,26	0
34	SR	0	8907	1/1	0.99	0.20	76,76,76,76	0
32	MG	0	8028	1/1	1.00	0.11	22,22,22,22	0
36	CD	1	8702	1/1	1.00	0.04	57,57,57,57	0
36	CD	U	8701	1/1	1.00	0.04	58,58,58,58	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 ANM 0 2924:

$2mF_o-DF_c$ (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.