



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:48 PM GMT

PDB ID : 4V9F
Title : The re-refined crystal structure of the Haloarcula marismortui large ribosomal subunit at 2.4 Angstrom resolution: more complete structure of the L7/L12 and L1 stalk, L5 and LX proteins
Authors : Gabdulkhakov, A.
Deposited on : 2012-11-02
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

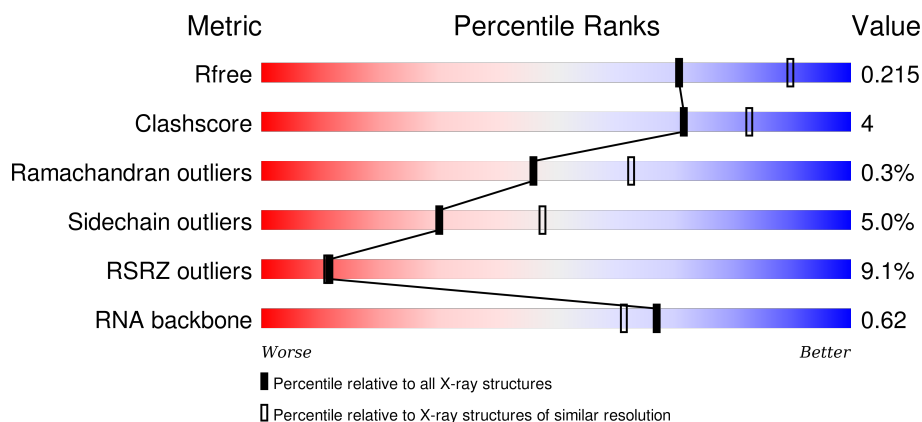
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)
RNA backbone	2183	1073 (2.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	0	2910	<div> <div>3%</div> <div>75% 18% . .</div> </div>
2	9	122	<div> <div>2%</div> <div>70% 25% 6%</div> </div>
3	A	240	<div> <div>6%</div> <div>85% 11% . .</div> </div>
4	B	338	<div> <div>2%</div> <div>87% 10% .</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	255	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	196	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	67	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	92	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	
32	4	70	
32	5	70	
33	6	56	

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	MG	0	8017	-	-	-	X
34	MG	0	8059	-	-	-	X
34	MG	0	8195	-	-	-	X
34	MG	0	8203	-	-	-	X
34	MG	0	8205	-	-	-	X
36	NA	0	8111	-	-	-	X
36	NA	0	8126	-	-	-	X
36	NA	0	8143	-	-	-	X
36	NA	0	8147	-	-	-	X
36	NA	0	8159	-	-	-	X
36	NA	0	8162	-	-	-	X
36	NA	0	8164	-	-	-	X
36	NA	0	8169	-	-	-	X
36	NA	0	8170	-	-	-	X
36	NA	0	8172	-	-	-	X
36	NA	0	8174	-	-	-	X
36	NA	9	202	-	-	-	X
36	NA	M	201	-	-	-	X
36	NA	R	202	-	-	-	X
37	CL	9	203	-	-	X	-
37	CL	B	402	-	-	-	X
38	ACY	0	8212	-	-	-	X
38	ACY	0	8213	-	-	X	-

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 103831 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2808	Total	C	N	O	P	0	0	0
			60186	26859	11069	19451	2807			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1130	345	383	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			1299	812	227	256	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	174	Total	C	N	O	S	0	0	0
			1376	850	230	292	4			

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			889	551	141	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	254	Total	C	N	O	S	0	0	0
			1805	1113	304	386	2			

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	165	Total	C	N	O	S	0	0	0
			1320	822	246	246	6			

- Molecule 11 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	145	Total	C	N	O	S	0	0	0
			1088	681	170	236	1			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	144	Total	C	N	O	S	0	0	0
			1132	704	201	224	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	149	Total	C	N	O	0	0	0
			1138	682	226	230			

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	195	Total	C	N	O	S	0	0	0
			1568	949	335	283	1			

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	144	Total	C	N	O	0	0	0
			1144	687	231	226			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O		0	0	0
			949	568	180	201				

- Molecule 23 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	56	Total	C	N	O	S	0	0	0
			435	259	81	90	5			

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	90	Total	C	N	O	S	0	0	0
			714	438	137	138	1			

- Molecule 27 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	144	Total	C	N	O		0	0	0
			1146	696	230	220				

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	83	Total	C	N	O	S	0	0	0
			645	387	127	126	5			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	49	Total	C	N	O	S	0	0	0
			421	254	93	73	1			

- Molecule 31 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	4	58	Total	C	N	O	0	0	0
			290	174	58	58			
32	5	56	Total	C	N	O	0	0	0
			280	168	56	56			

- Molecule 33 is a protein called 50S ribosomal protein LX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	6	55	Total	C	N	O	0	0	0
			441	271	78	92			

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	125	Total	Mg	0	0
			125	125		
34	Y	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	Mg 1	0	0
34	A	3	Total 3	Mg 3	0	0
34	T	1	Total 1	Mg 1	0	0
34	N	1	Total 1	Mg 1	0	0
34	9	1	Total 1	Mg 1	0	0
34	L	1	Total 1	Mg 1	0	0
34	3	1	Total 1	Mg 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total 2	K 2	0	0
35	O	1	Total 1	K 1	0	0

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	72	Total 72	Na 72	0	0
36	J	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	H	2	Total 2	Na 2	0	0
36	C	1	Total 1	Na 1	0	0
36	A	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0

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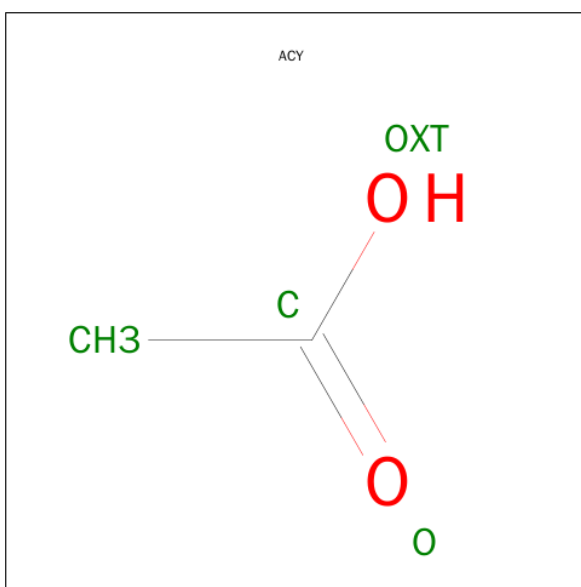
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	L	2	Total 2	Na 2	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	12	Total 12	Cl 12	0	0
37	G	1	Total 1	Cl 1	0	0
37	J	3	Total 3	Cl 3	0	0
37	Y	1	Total 1	Cl 1	0	0
37	B	2	Total 2	Cl 2	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	2	Total 2	Cl 2	0	0
37	R	2	Total 2	Cl 2	0	0
37	9	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	F	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	0	1	Total	C	O	0	0
			4	2	2		
38	0	1	Total	C	O	0	0
			4	2	2		
38	0	1	Total	C	O	0	0
			4	2	2		
38	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total	Cd	0	0
			1	1		
39	Z	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	3	1	Total	Cd	0	0
			1	1		
39	U	1	Total	Cd	0	0
			1	1		

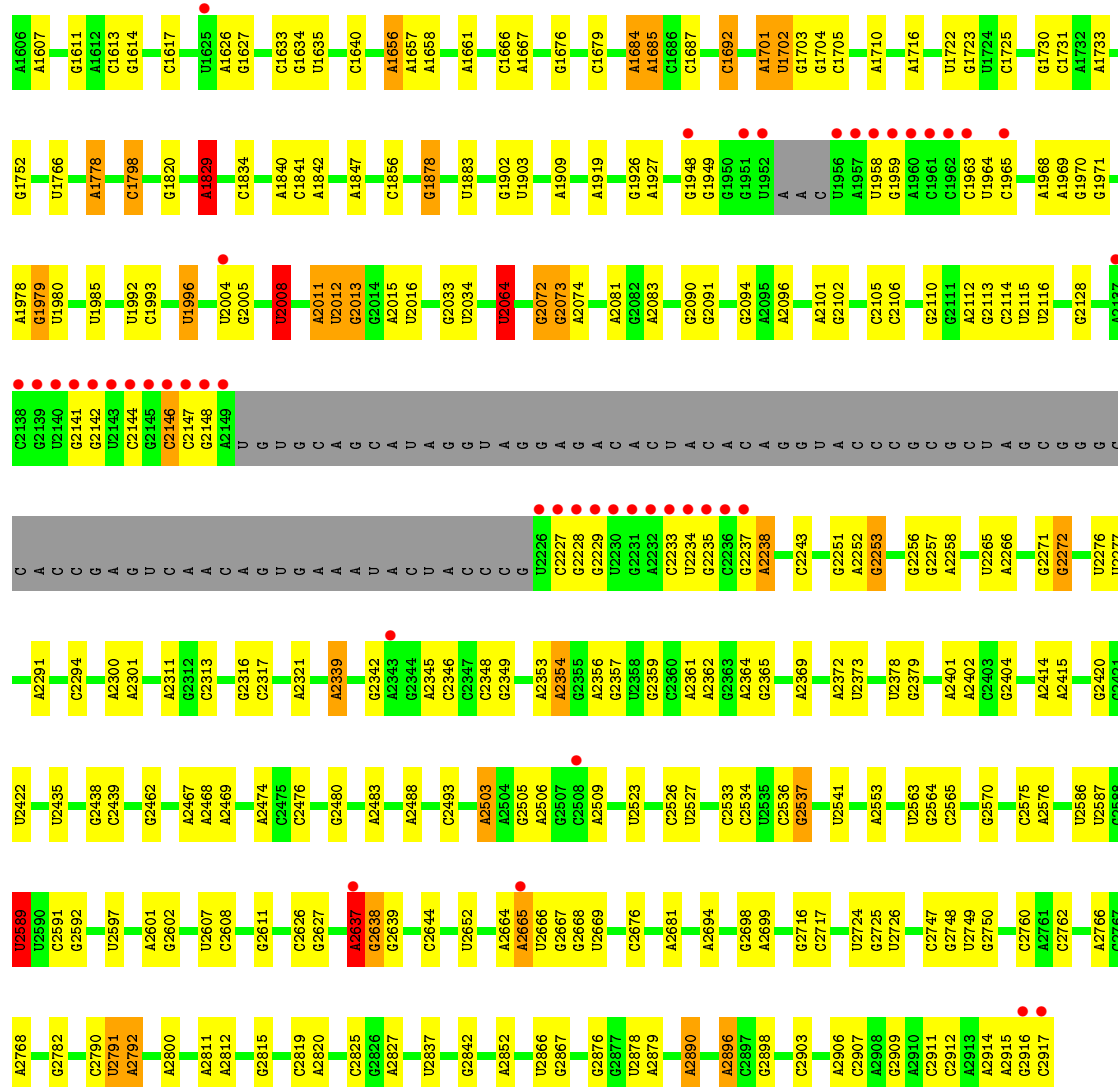
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5924	Total 5924	O 5924	0	0
40	9	153	Total 153	O 153	0	0
40	A	126	Total 126	O 126	0	0
40	B	151	Total 151	O 151	0	0
40	C	171	Total 171	O 171	0	0
40	D	9	Total 9	O 9	0	0
40	E	44	Total 44	O 44	0	0
40	F	22	Total 22	O 22	0	0
40	G	3	Total 3	O 3	0	0
40	H	58	Total 58	O 58	0	0
40	I	1	Total 1	O 1	0	0
40	J	54	Total 54	O 54	0	0
40	K	59	Total 59	O 59	0	0
40	L	67	Total 67	O 67	0	0
40	M	133	Total 133	O 133	0	0
40	N	59	Total 59	O 59	0	0
40	O	45	Total 45	O 45	0	0
40	P	63	Total 63	O 63	0	0
40	Q	54	Total 54	O 54	0	0
40	R	72	Total 72	O 72	0	0
40	S	34	Total 34	O 34	0	0
40	T	39	Total 39	O 39	0	0

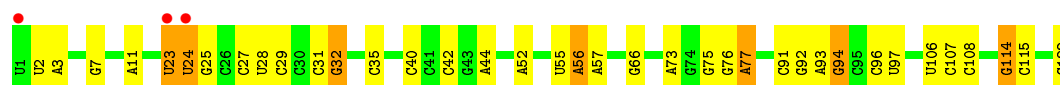
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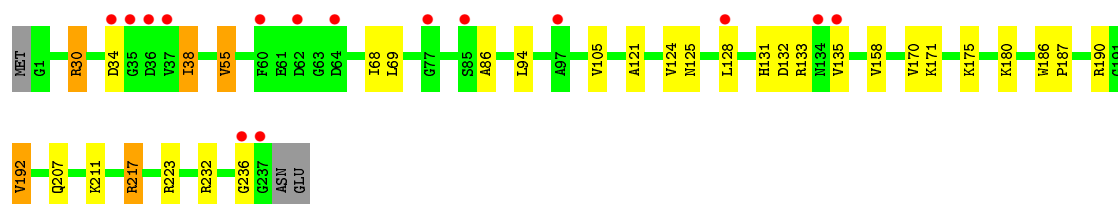
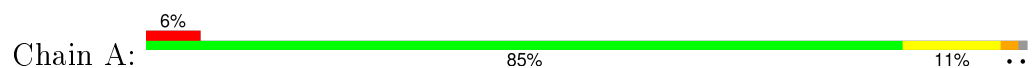
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	23	Total 23	O 23	0	0
40	V	12	Total 12	O 12	0	0
40	W	64	Total 64	O 64	0	0
40	X	20	Total 20	O 20	0	0
40	Y	104	Total 104	O 104	0	0
40	Z	28	Total 28	O 28	0	0
40	1	50	Total 50	O 50	0	0
40	2	39	Total 39	O 39	0	0
40	3	63	Total 63	O 63	0	0
40	6	1	Total 1	O 1	0	0



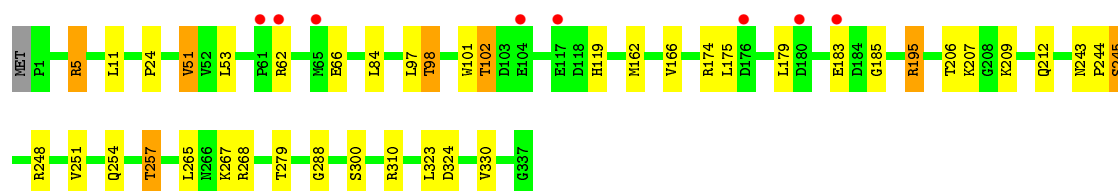
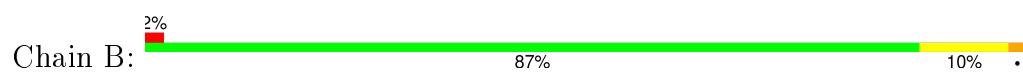
• Molecule 2: 5S Ribosomal RNA



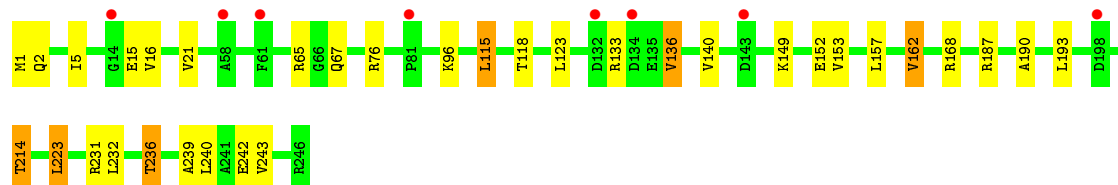
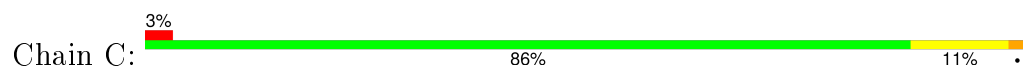
• Molecule 3: 50S ribosomal protein L2P



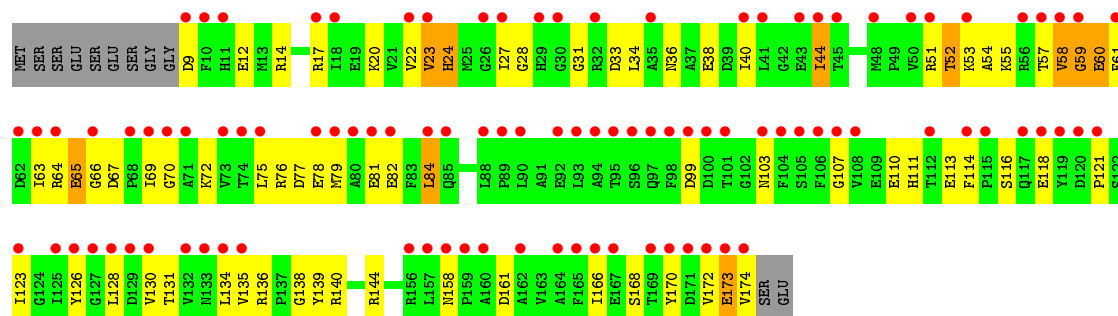
• Molecule 4: 50S ribosomal protein L3P



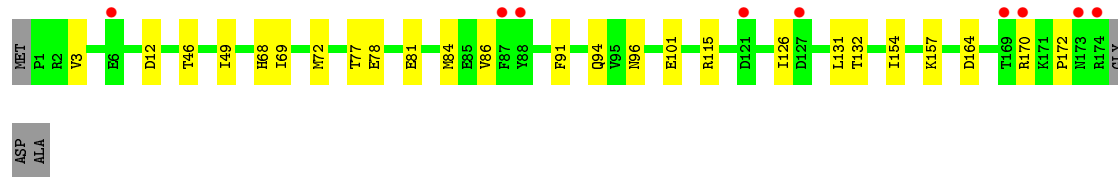
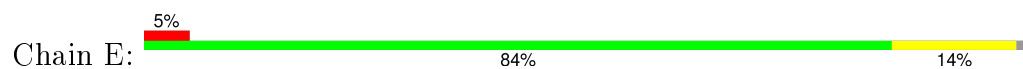
- Molecule 5: 50S ribosomal protein L4P



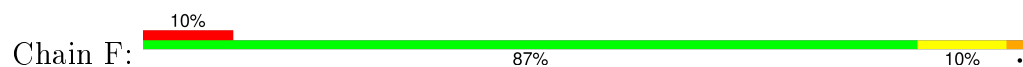
- Molecule 6: 50S ribosomal protein L5P



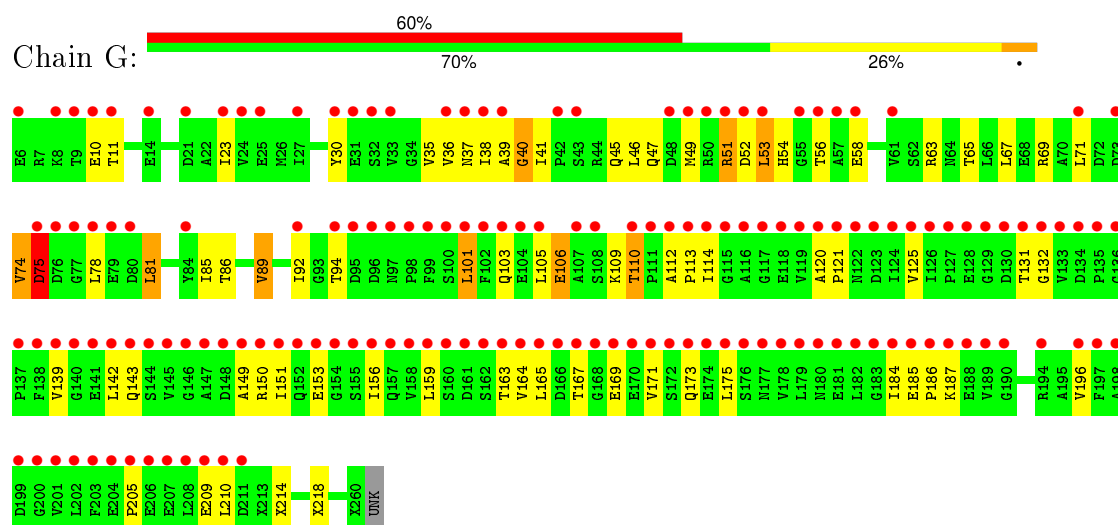
- Molecule 7: 50S ribosomal protein L6P



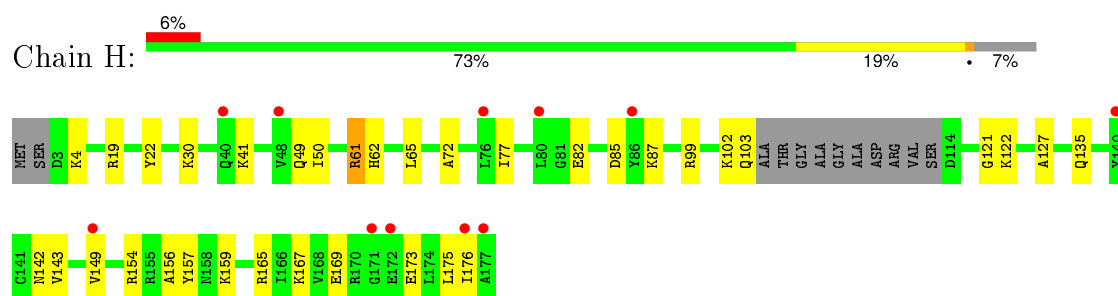
- Molecule 8: 50S ribosomal protein L7Ae



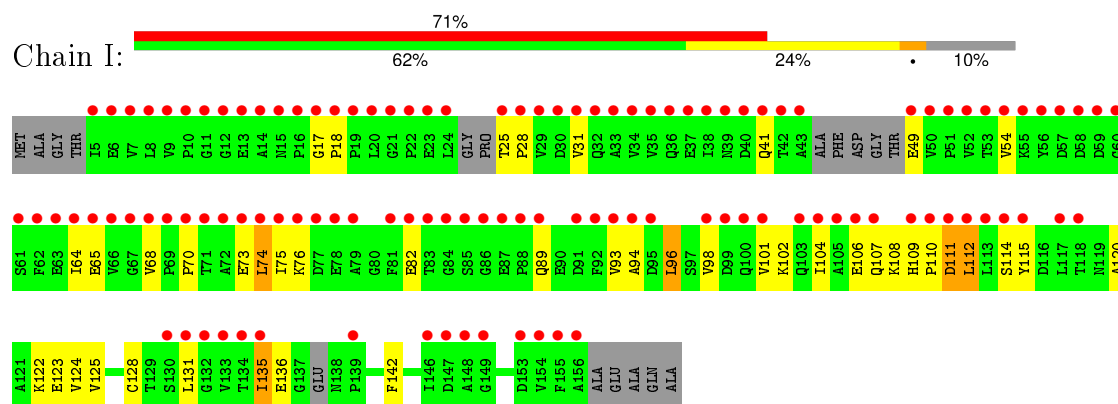
- Molecule 9: 50S ribosomal protein L10E



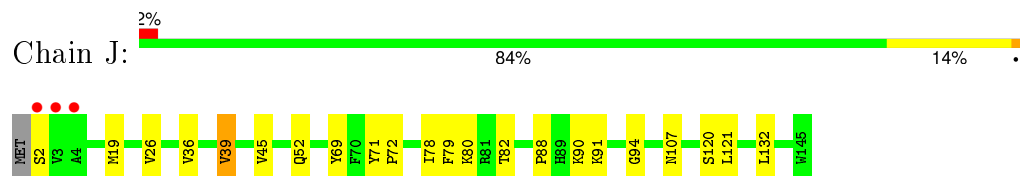
- Molecule 10: 50S ribosomal protein L10e



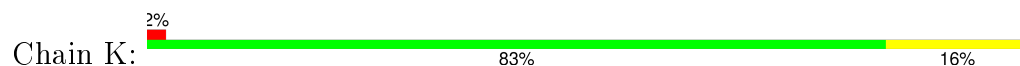
- Molecule 11: 50S ribosomal protein L11P



- Molecule 12: 50S ribosomal protein L13P

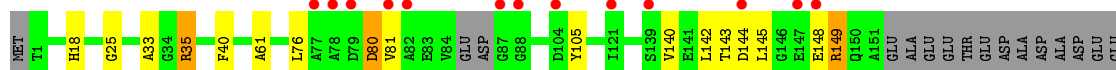
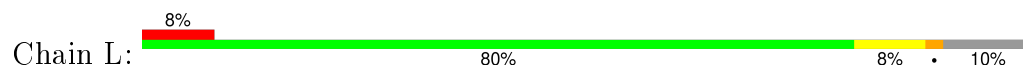


- Molecule 13: 50S ribosomal protein L14P

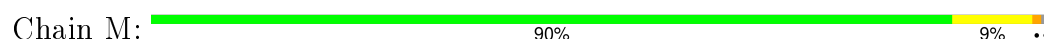




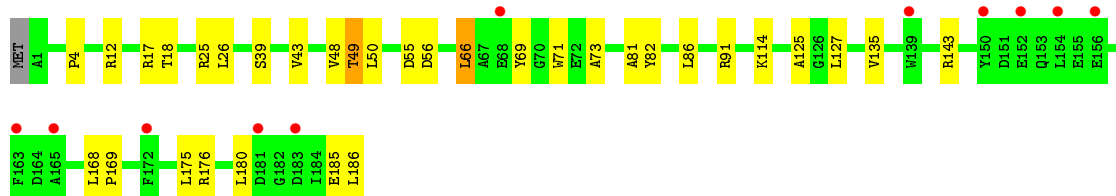
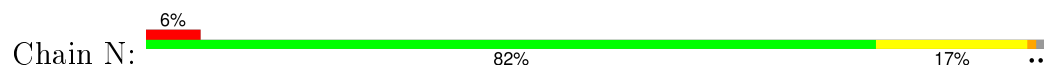
- Molecule 14: 50S ribosomal protein L15P



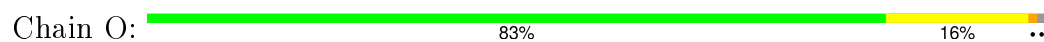
- Molecule 15: 50S ribosomal protein L15e



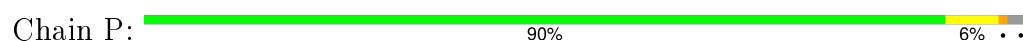
- Molecule 16: 50S ribosomal protein L18P



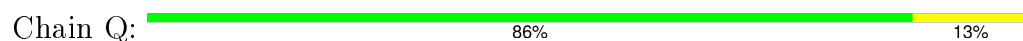
- Molecule 17: 50S ribosomal protein L18e




- Molecule 18: 50S ribosomal protein L19e



- Molecule 19: 50S ribosomal protein L21e




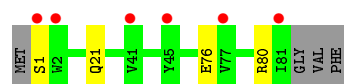
- Molecule 20: 50S ribosomal protein L22P

Chain R:  83% 14% ..




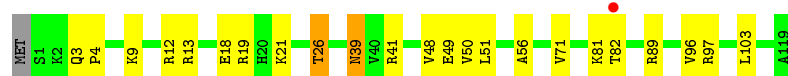
- Molecule 21: 50S ribosomal protein L23P

Chain S:  7% 91% 5% 5%



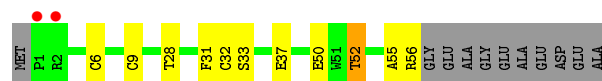
- Molecule 22: 50S ribosomal protein L24P

Chain T:  80% 18% ..




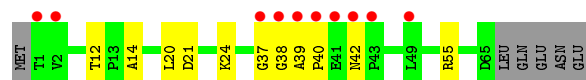
- Molecule 23: 50S ribosomal protein L24e

Chain U:  3% 67% 15% 16%




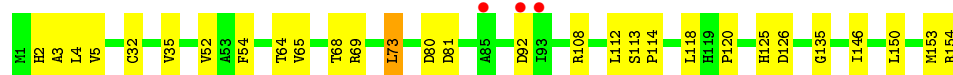
- Molecule 24: 50S ribosomal protein L29P

Chain V:  14% 76% 15% 8%




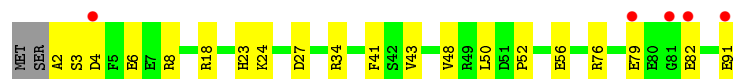
- Molecule 25: 50S ribosomal protein L30P

Chain W:  2% 81% 18% .

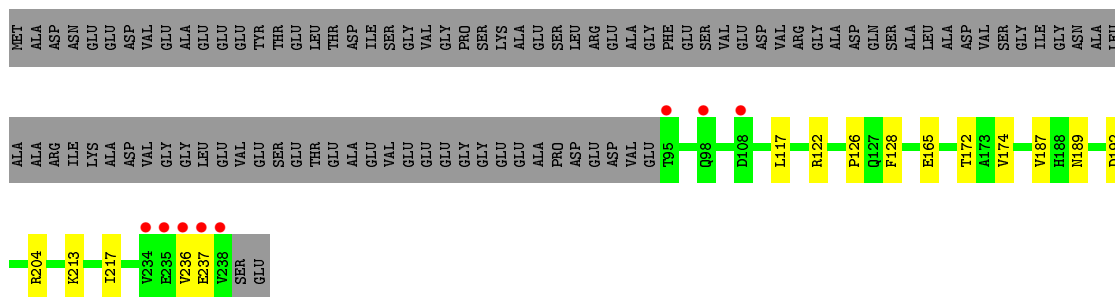


- Molecule 26: 50S ribosomal protein L31e

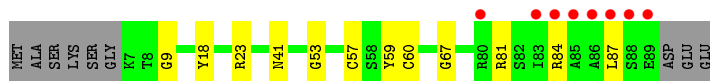
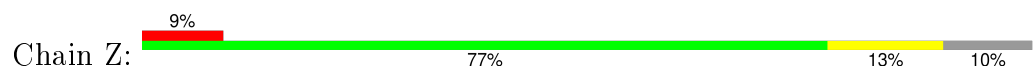
Chain X:  5% 76% 22% .



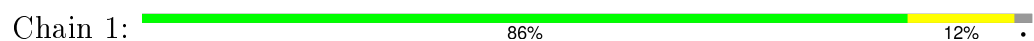
- Molecule 27: 50S ribosomal protein L32e



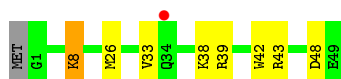
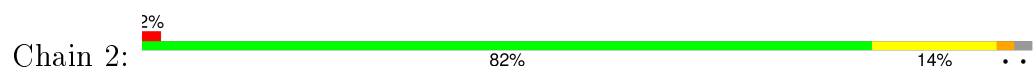
- Molecule 28: 50S ribosomal protein L37Ae



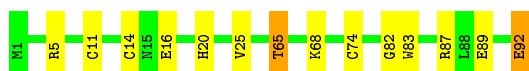
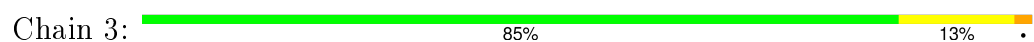
- Molecule 29: 50S ribosomal protein L37e



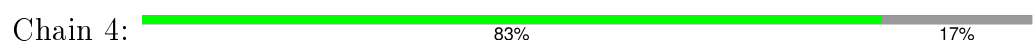
- Molecule 30: 50S ribosomal protein L39e



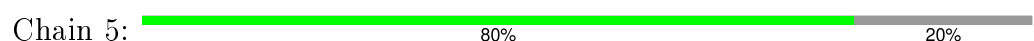
- Molecule 31: 50S ribosomal protein L44e



- Molecule 32: 50S ribosomal protein L12

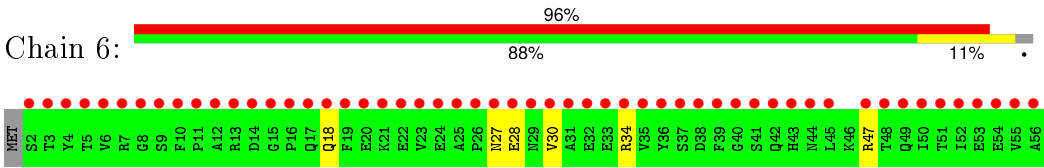


- Molecule 32: 50S ribosomal protein L12





● Molecule 33: 50S ribosomal protein LX



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.48 – 2.40 89.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (85.48-2.40) 95.5 (89.24-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.166 , 0.206 0.178 , 0.215	Depositor DCC
R_{free} test set	6956 reflections (1.05%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 701272 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	103831	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, CD, OMU, UR3, 1MA, ACY, PSU

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	0	0.55	3/67259 (0.0%)	1.00	67/104899 (0.1%)
2	9	0.47	0/2904	0.91	0/4526
3	A	0.41	0/1786	0.62	1/2408 (0.0%)
4	B	0.39	0/2690	0.58	0/3652
5	C	0.46	0/1884	0.64	0/2552
6	D	0.32	0/1324	0.55	0/1791
7	E	0.38	0/1401	0.53	0/1905
8	F	0.39	0/900	0.52	0/1224
9	G	0.30	0/1585	0.58	1/2156 (0.0%)
10	H	0.41	0/1340	0.59	0/1795
11	I	0.29	0/1107	0.53	0/1512
12	J	0.40	0/1148	0.57	0/1548
13	K	0.42	0/1003	0.61	0/1351
14	L	0.45	0/1150	0.62	0/1536
15	M	0.46	0/1592	0.63	0/2127
16	N	0.37	0/1473	0.58	0/1999
17	O	0.40	0/874	0.55	0/1181
18	P	0.39	0/1155	0.52	0/1539
19	Q	0.44	0/748	0.61	0/1005
20	R	0.43	0/1172	0.58	0/1578
21	S	0.40	0/648	0.52	0/875
22	T	0.39	0/957	0.60	0/1289
23	U	0.40	0/443	0.52	0/597
24	V	0.39	0/502	0.46	0/675
25	W	0.40	0/1219	0.61	0/1655
26	X	0.38	0/725	0.55	0/978
27	Y	0.43	0/1162	0.56	0/1558
28	Z	0.40	0/656	0.57	0/877
29	1	0.55	0/438	0.74	0/578
30	2	0.45	0/427	0.55	0/566
31	3	0.46	0/771	0.55	0/1024
33	6	0.32	0/449	0.45	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.51	3/102892 (0.0%)	0.90	69/153563 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	D	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	128	A	O3'-P	7.10	1.69	1.61
1	0	1656	A	O3'-P	-5.92	1.54	1.61
1	0	129	A	O3'-P	-5.40	1.54	1.61

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2013	G	O5'-P-OP1	-12.13	94.78	105.70
1	0	518	G	O4'-C1'-N9	10.81	116.85	108.20
1	0	777	U	O5'-P-OP1	-9.99	96.71	105.70
1	0	128	A	OP2-P-O3'	9.70	126.53	105.20
1	0	920	C	O5'-P-OP1	-8.82	97.76	105.70
1	0	1242	A	O5'-P-OP2	-8.76	97.82	105.70
1	0	1331	G	O5'-P-OP2	-8.61	97.95	105.70
1	0	1692	C	O5'-P-OP2	8.43	120.82	110.70
1	0	821	U	O5'-P-OP2	-8.02	98.48	105.70
1	0	2493	C	O4'-C1'-N1	8.02	114.62	108.20
1	0	2589	U	O5'-P-OP1	-7.91	98.58	105.70
1	0	777	U	O4'-C1'-N1	7.81	114.45	108.20
1	0	841	A	O4'-C1'-N9	7.72	114.38	108.20
1	0	331	A	O5'-P-OP2	-7.66	98.81	105.70
1	0	473	A	O5'-P-OP2	-7.65	98.82	105.70
1	0	777	U	N3-C2-O2	-7.33	117.07	122.20
1	0	308	U	O4'-C1'-N1	7.32	114.06	108.20
1	0	210	U	O5'-P-OP2	-7.30	99.13	105.70
1	0	1323	G	O5'-P-OP2	-7.08	99.33	105.70
1	0	331	A	O5'-P-OP1	6.79	118.84	110.70
1	0	2073	G	O5'-P-OP2	-6.65	99.72	105.70
1	0	2008	U	O5'-P-OP2	-6.59	99.77	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2607	U	N3-C2-O2	-6.55	117.61	122.20
1	0	2064	U	O5'-P-OP2	-6.50	99.85	105.70
1	0	1417	G	O4'-C1'-N9	6.45	113.36	108.20
1	0	2316	G	O4'-C1'-N9	6.45	113.36	108.20
1	0	237	G	O5'-P-OP2	-6.42	99.92	105.70
1	0	1970	G	O4'-C1'-N9	6.40	113.32	108.20
1	0	1692	C	O5'-P-OP1	-6.35	99.98	105.70
1	0	173	C	N1-C2-O2	-6.30	115.12	118.90
9	G	40	GLY	N-CA-C	-6.29	97.38	113.10
1	0	120	A	O5'-P-OP1	-6.16	100.16	105.70
1	0	920	C	O5'-P-OP2	6.10	118.02	110.70
1	0	1292	G	O5'-P-OP2	-5.91	100.38	105.70
1	0	1692	C	C6-N1-C2	5.91	122.66	120.30
1	0	1829	A	N9-C1'-C2'	-5.90	105.51	112.00
1	0	553	G	O5'-P-OP1	-5.81	100.47	105.70
1	0	2493	C	N1-C2-O2	5.80	122.38	118.90
1	0	821	U	O5'-P-OP1	5.70	117.54	110.70
1	0	270	U	O4'-C1'-N1	5.68	112.75	108.20
1	0	1430	G	O4'-C1'-N9	5.65	112.72	108.20
1	0	2607	U	N1-C1'-C2'	5.60	121.28	114.00
1	0	881	C	N3-C4-C5	-5.60	119.66	121.90
1	0	834	G	P-O3'-C3'	5.58	126.39	119.70
1	0	1407	A	O4'-C1'-N9	5.57	112.65	108.20
1	0	625	U	C2-N3-C4	-5.56	123.66	127.00
1	0	1841	C	C6-N1-C2	-5.53	118.09	120.30
1	0	196	G	O4'-C1'-N9	5.52	112.62	108.20
1	0	2503	A	O4'-C1'-N9	5.50	112.60	108.20
1	0	120	A	O5'-P-OP2	5.49	117.28	110.70
1	0	1036	G	N1-C6-O6	-5.49	116.61	119.90
1	0	2611	G	C8-N9-C4	5.46	108.58	106.40
1	0	2637	A	P-O3'-C3'	5.45	126.24	119.70
1	0	883	U	C2-N1-C1'	5.44	124.23	117.70
1	0	2114	C	N1-C2-O2	-5.44	115.64	118.90
1	0	868	G	O4'-C1'-N9	5.39	112.51	108.20
1	0	417	G	P-O3'-C3'	-5.37	113.25	119.70
1	0	1084	C	N1-C2-O2	-5.32	115.71	118.90
1	0	877	G	P-O3'-C3'	5.25	126.00	119.70
1	0	2644	C	N1-C2-O2	-5.25	115.75	118.90
1	0	915	C	C6-N1-C2	-5.22	118.21	120.30
1	0	71	G	N1-C6-O6	-5.21	116.78	119.90
1	0	1183	C	N1-C2-O2	5.18	122.01	118.90
1	0	134	U	O5'-P-OP2	-5.15	101.07	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	217	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	0	1054	G	O5'-P-OP2	-5.11	101.10	105.70
1	0	2842	G	O4'-C1'-N9	5.10	112.28	108.20
1	0	2364	A	O5'-P-OP2	-5.09	101.12	105.70
1	0	1244	U	O4'-C1'-N1	5.06	112.25	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	59	GLY	Peptide
6	D	65	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	60186	0	30379	291	0
2	9	2599	0	1325	23	0
3	A	1753	0	1766	17	0
4	B	2625	0	2533	27	0
5	C	1859	0	1813	23	0
6	D	1299	0	1263	48	0
7	E	1376	0	1285	15	0
8	F	889	0	843	6	0
9	G	1805	0	1560	47	0
10	H	1320	0	1331	22	0
11	I	1088	0	1029	27	0
12	J	1132	0	1112	15	0
13	K	993	0	1027	12	0
14	L	1138	0	1096	10	0
15	M	1568	0	1586	19	0
16	N	1444	0	1401	16	0
17	O	865	0	873	10	0
18	P	1144	0	1129	9	0
19	Q	734	0	729	9	0
20	R	1149	0	1122	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	S	641	0	605	2	0
22	T	949	0	924	14	0
23	U	435	0	394	6	0
24	V	499	0	511	6	0
25	W	1196	0	1137	20	0
26	X	714	0	700	11	0
27	Y	1146	0	1148	10	0
28	Z	645	0	610	6	0
29	1	431	0	426	5	0
30	2	421	0	437	8	0
31	3	755	0	728	7	0
32	4	290	0	60	0	0
32	5	280	0	59	0	0
33	6	441	0	411	4	0
34	0	125	0	0	0	0
34	3	1	0	0	0	0
34	9	1	0	0	0	0
34	A	3	0	0	0	0
34	K	1	0	0	0	0
34	L	1	0	0	0	0
34	N	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	4	0	0	0	0
35	0	2	0	0	0	0
35	O	1	0	0	0	0
36	0	72	0	0	0	0
36	9	1	0	0	0	0
36	A	1	0	0	0	0
36	C	1	0	0	0	0
36	H	2	0	0	0	0
36	J	1	0	0	0	0
36	L	2	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	12	0	0	1	0
37	3	1	0	0	0	0
37	9	1	0	0	3	0
37	A	1	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	2	0	0	1	0
37	R	2	0	0	0	0
37	Y	1	0	0	0	0
38	0	12	0	9	4	0
38	W	4	0	3	1	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5924	0	0	16	0
40	1	50	0	0	0	0
40	2	39	0	0	1	0
40	3	63	0	0	0	0
40	6	1	0	0	1	0
40	9	153	0	0	3	0
40	A	126	0	0	2	0
40	B	151	0	0	3	0
40	C	171	0	0	6	0
40	D	9	0	0	3	0
40	E	44	0	0	2	0
40	F	22	0	0	0	0
40	G	3	0	0	0	0
40	H	58	0	0	2	0
40	I	1	0	0	0	0
40	J	54	0	0	0	0
40	K	59	0	0	1	0
40	L	67	0	0	1	0
40	M	133	0	0	8	0
40	N	59	0	0	1	0
40	O	45	0	0	1	0
40	P	63	0	0	1	0
40	Q	54	0	0	2	0
40	R	72	0	0	1	0
40	S	34	0	0	0	0
40	T	39	0	0	0	0
40	U	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	V	12	0	0	0	0
40	W	64	0	0	1	0
40	X	20	0	0	2	0
40	Y	104	0	0	2	0
40	Z	28	0	0	1	0
All	All	103831	0	63364	679	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 4.

All (679) 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)
15:M:164:THR:HG22	15:M:167:GLY:H	1.28	0.97
5:C:236:THR:HG22	5:C:239:ALA:H	1.30	0.95
1:0:156:C:H5''	15:M:171:ARG:HD3	1.46	0.95
20:R:39:THR:HG22	20:R:42:GLU:H	1.33	0.94
1:0:1160:G:H5'	1:0:1161:A:H5'	1.58	0.85
1:0:2586:U:H3	1:0:2592:G:H22	1.22	0.85
2:9:75:G:H1	2:9:106:U:H3	1.25	0.84
1:0:2665:A:H62	1:0:2917:C:H41	1.29	0.81
2:9:76:G:H3'	2:9:77:A:H5''	1.63	0.81
17:O:32:ARG:HH21	17:O:35:LYS:HG3	1.45	0.81
37:0:8210:CL:CL	40:B:637:HOH:O	2.36	0.80
23:U:52:THR:HG22	23:U:55:ALA:H	1.46	0.80
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.81	0.80
1:0:1164:U:H3	1:0:1192:A:H2	1.29	0.79
1:0:1242:A:H5'	12:J:82:THR:HG23	1.66	0.77
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.69	0.74
7:E:101:GLU:OE1	7:E:115:ARG:NH1	2.20	0.73
4:B:195:ARG:NH1	4:B:324:ASP:OD1	2.21	0.73
1:0:929:A:N3	40:0:8652:HOH:O	2.21	0.73
1:0:2141:G:N2	1:0:2234:U:O2	2.21	0.72
1:0:1441:G:OP1	30:2:39:ARG:NH1	2.22	0.72
1:0:1165:G:N2	1:0:1173:A:OP1	2.22	0.72
9:G:110:THR:HG22	9:G:112:ALA:HB2	1.71	0.72
9:G:75:ASP:HA	9:G:78:LEU:H	1.55	0.71
1:0:2665:A:N6	1:0:2917:C:H41	1.88	0.71
1:0:967:U:H5''	38:0:8213:ACY:H3	1.72	0.71
37:9:203:CL:CL	40:9:447:HOH:O	2.45	0.71
11:I:108:LYS:HB2	11:I:111:ASP:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:102:LYS:HD2	10:H:122:LYS:HD3	1.71	0.70
1:O:1351:G:OP1	5:C:96:LYS:NZ	2.24	0.70
26:X:8:ARG:NH1	40:X:104:HOH:O	2.25	0.69
1:O:1160:G:H8	1:O:1207:A:H62	1.36	0.69
1:O:2349:G:OP1	6:D:20:LYS:NZ	2.25	0.69
4:B:102:THR:HG21	4:B:185:GLY:HA2	1.74	0.69
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.75	0.69
9:G:51:ARG:NH2	11:I:112:LEU:O	2.24	0.69
4:B:62:ARG:NH2	4:B:66:GLU:O	2.26	0.68
1:O:31:C:H4'	22:T:9:LYS:HD2	1.75	0.68
9:G:150:ARG:HE	9:G:159:LEU:HD22	1.59	0.67
5:C:1:MET:HG2	5:C:2:GLN:H	1.60	0.66
2:9:42:C:O2	6:D:76:ARG:NH1	2.28	0.66
1:O:966:U:C2	38:O:8213:ACY:H2	2.32	0.65
26:X:18:ARG:NH1	40:X:109:HOH:O	2.26	0.64
4:B:310:ARG:NH2	40:B:548:HOH:O	2.30	0.64
7:E:77:THR:OG1	7:E:78:GLU:N	2.31	0.64
5:C:133:ARG:NH1	40:C:511:HOH:O	2.21	0.63
1:O:2345:A:H2	6:D:28:GLY:HA3	1.63	0.63
9:G:125:VAL:HG13	9:G:163:THR:HA	1.79	0.63
26:X:41:PHE:O	26:X:76:ARG:NH1	2.32	0.63
5:C:236:THR:HG21	40:C:482:HOH:O	1.99	0.63
5:C:162:VAL:HG22	5:C:232:LEU:HD21	1.81	0.63
1:O:73:U:OP1	24:V:55:ARG:NH2	2.31	0.63
19:Q:4:ASN:ND2	40:Q:250:HOH:O	2.32	0.62
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.81	0.62
11:I:93:VAL:N	11:I:94:ALA:HA	2.13	0.62
11:I:98:VAL:HG13	11:I:135:ILE:HD11	1.81	0.62
2:9:73:A:H61	2:9:108:C:H42	1.47	0.62
3:A:192:VAL:HG13	3:A:207:GLN:HB3	1.81	0.62
1:O:1120:U:H6	1:O:1120:U:H5''	1.65	0.62
15:M:107:ARG:NH1	40:M:373:HOH:O	2.30	0.62
1:O:2488:A:H61	1:O:2534:C:H42	1.46	0.61
22:T:12:ARG:O	22:T:19:ARG:NH2	2.33	0.61
7:E:126:ILE:HG22	7:E:131:LEU:HG	1.81	0.61
15:M:5:TYR:HE1	15:M:46:LEU:HD13	1.65	0.61
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.83	0.61
1:O:2142:G:N2	1:O:2233:C:O2	2.33	0.61
2:9:40:C:N3	37:9:203:CL:CL	2.71	0.61
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.83	0.61
3:A:232:ARG:NH2	3:A:236:GLY:O	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2474:A:N3	40:0:9378:HOH:O	2.31	0.61
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.83	0.60
1:0:1666:C:H2'	1:0:1667:A:H8	1.66	0.60
1:0:1834:C:H2'	1:0:1840:A:N6	2.17	0.60
1:0:2353:A:H1'	19:Q:21:ARG:HH22	1.67	0.60
26:X:2:ALA:N	26:X:4:ASP:OD1	2.34	0.60
33:6:18:GLN:NE2	40:6:101:HOH:O	2.32	0.60
30:2:38:LYS:NZ	40:2:101:HOH:O	2.33	0.60
1:0:1964:U:H2'	1:0:1965:C:C6	2.36	0.60
9:G:184:ILE:HG22	9:G:186:PRO:HD3	1.83	0.60
5:C:118:THR:O	5:C:136:VAL:HG13	2.01	0.60
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.37	0.60
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.35	0.59
2:9:92:G:H2'	2:9:93:A:C8	2.37	0.59
5:C:5:ILE:HD11	5:C:16:VAL:HG13	1.85	0.59
1:0:1197:G:H21	1:0:1202:A:H2	1.49	0.59
1:0:327:A:OP1	5:C:149:LYS:NZ	2.20	0.59
7:E:170:ARG:NH1	40:E:209:HOH:O	2.35	0.59
1:0:2251:G:H2'	1:0:2252:A:C8	2.38	0.59
1:0:1676:G:OP1	30:2:8:LYS:NZ	2.36	0.59
6:D:52:THR:HG22	6:D:70:GLY:H	1.66	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:1025:C:P	25:W:108:ARG:HH12	2.26	0.58
15:M:164:THR:HG22	15:M:167:GLY:N	2.10	0.58
1:0:1197:G:O2'	1:0:1202:A:N6	2.35	0.58
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.85	0.58
26:X:3:SER:HB2	26:X:79:GLU:HG3	1.85	0.58
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.37	0.58
11:I:54:VAL:HG22	11:I:64:ILE:HG13	1.85	0.58
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.36	0.57
1:0:820:G:C6	3:A:171:LYS:HB2	2.39	0.57
1:0:2866:U:H4'	1:0:2867:G:H5'	1.86	0.57
1:0:969:G:H1	1:0:999:C:N4	2.03	0.57
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.40	0.57
11:I:114:SER:OG	11:I:123:GLU:OE1	2.22	0.56
1:0:2637:A:H2	1:0:2639:G:OP2	1.88	0.56
1:0:112:G:OP1	29:1:20:ARG:NH1	2.38	0.56
1:0:1008:C:H5''	10:H:19:ARG:HH12	1.69	0.56
6:D:38:GLU:OE2	6:D:51:ARG:NH1	2.38	0.56
1:0:969:G:H1	1:0:999:C:H42	1.52	0.56
4:B:162:MET:SD	4:B:310:ARG:HD3	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.88	0.56
9:G:75:ASP:HA	9:G:78:LEU:N	2.20	0.55
11:I:75:ILE:HD11	11:I:131:LEU:HD13	1.88	0.55
1:O:1500:U:P	18:P:41:ARG:HH22	2.29	0.55
9:G:171:VAL:HG23	9:G:175:LEU:HD23	1.88	0.55
9:G:214:UNK:O	9:G:218:UNK:N	2.39	0.55
3:A:30:ARG:HD3	3:A:38:ILE:HG21	1.88	0.55
9:G:71:LEU:HD13	9:G:81:LEU:HB3	1.88	0.55
1:O:2346:C:O2'	6:D:52:THR:HG21	2.06	0.55
1:O:1733:A:H4'	4:B:212:GLN:HA	1.88	0.55
1:O:92:G:H5'	24:V:42:ASN:HD22	1.72	0.55
1:O:588:G:O6	25:W:154:ARG:NH1	2.39	0.55
6:D:99:ASP:N	6:D:103:ASN:O	2.29	0.55
3:A:132:ASP:HB3	3:A:135:VAL:H	1.72	0.55
9:G:139:VAL:HG21	9:G:151:ILE:HD11	1.89	0.55
3:A:121:ALA:O	3:A:124:VAL:HG22	2.06	0.55
9:G:150:ARG:HH21	9:G:159:LEU:HD13	1.72	0.55
1:O:553:G:OP2	27:Y:204:ARG:NH2	2.30	0.55
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.89	0.54
1:O:1766:U:O2	1:O:1778:A:H5'	2.07	0.54
6:D:173:GLU:C	6:D:174:VAL:HG23	2.27	0.54
40:O:9667:HOH:O	10:H:61:ARG:HG2	2.06	0.54
2:9:28:U:H2'	2:9:29:C:C6	2.41	0.54
26:X:23:HIS:CE1	26:X:24:LYS:HG3	2.43	0.54
1:O:1494:A:O2'	1:O:1505:U:O2	2.25	0.54
1:O:1926:G:H2'	1:O:1927:A:C8	2.42	0.54
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.89	0.54
25:W:81:ASP:OD1	25:W:92:ASP:HB2	2.08	0.54
10:H:173:GLU:CD	10:H:173:GLU:H	2.10	0.54
15:M:169:ARG:NH2	40:M:351:HOH:O	2.40	0.54
9:G:65:THR:O	9:G:69:ARG:HG2	2.07	0.54
1:O:371:U:H2'	1:O:372:A:C8	2.43	0.54
10:H:85:ASP:OD2	10:H:142:ASN:ND2	2.37	0.54
1:O:1175:G:H8	1:O:1193:A:HO2'	1.56	0.53
1:O:2072:G:C6	1:O:2533:C:H1'	2.43	0.53
9:G:53:LEU:O	9:G:54:HIS:ND1	2.40	0.53
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.90	0.53
1:O:416:G:H5''	1:O:417:G:OP2	2.07	0.53
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.89	0.53
31:3:65:THR:HG21	31:3:83:TRP:CZ3	2.42	0.53
16:N:91:ARG:HG2	16:N:186:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:85:ILE:HG23	9:G:89:VAL:HG11	1.90	0.53
1:0:1120:U:C6	1:0:1120:U:H5''	2.44	0.53
10:H:61:ARG:HA	10:H:127:ALA:HA	1.91	0.53
23:U:33:SER:O	23:U:37:GLU:HG3	2.09	0.53
1:0:309:C:OP1	22:T:97:ARG:NH2	2.35	0.53
1:0:2666:U:H2'	1:0:2667:G:C8	2.44	0.53
1:0:1548:U:O2'	1:0:1798:C:O2	2.25	0.53
1:0:2637:A:H1'	1:0:2638:G:C5'	2.39	0.53
8:F:38:LYS:HE3	15:M:3:SER:HA	1.91	0.53
1:0:688:A:H61	1:0:698:A:H5''	1.73	0.53
3:A:211:LYS:HE3	40:A:484:HOH:O	2.09	0.52
16:N:71:TRP:CE2	16:N:73:ALA:HB3	2.44	0.52
30:2:26:MET:HG2	30:2:33:VAL:O	2.08	0.52
17:O:54:GLU:HG3	37:O:203:CL:CL	2.47	0.52
1:0:86:A:H4'	1:0:87:C:H5''	1.91	0.52
9:G:101:LEU:HD12	9:G:196:VAL:HG21	1.90	0.52
17:O:32:ARG:HG2	17:O:61:PRO:HB2	1.91	0.52
6:D:57:THR:HB	6:D:64:ARG:HG3	1.91	0.52
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.41	0.52
1:0:2911:C:H2'	1:0:2912:C:C6	2.45	0.52
24:V:12:THR:HG23	24:V:14:ALA:H	1.75	0.52
1:0:1181:A:N1	1:0:1192:A:O2'	2.41	0.52
1:0:1657:A:H2'	1:0:1658:A:C8	2.44	0.52
1:0:2878:U:H2'	1:0:2879:A:O4'	2.09	0.52
22:T:9:LYS:HG2	22:T:13:ARG:CZ	2.39	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.90	0.52
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.52
9:G:142:LEU:HD12	9:G:149:ALA:HB2	1.90	0.52
9:G:164:VAL:HG22	9:G:165:LEU:HG	1.90	0.52
9:G:45:GLN:O	9:G:49:MET:HG3	2.10	0.52
1:0:2815:G:H21	12:J:2:SER:HA	1.75	0.52
1:0:2716:G:H5''	4:B:206:THR:HG21	1.91	0.52
25:W:2:HIS:HE1	38:W:201:ACY:H1	1.74	0.52
18:P:80:ARG:HD2	18:P:87:ARG:NE	2.25	0.52
1:0:2064:U:H5'	1:0:2652:U:H4'	1.92	0.52
31:3:5:ARG:NE	31:3:92:GLU:OE1	2.28	0.52
1:0:966:U:H2'	38:0:8213:ACY:H2	1.92	0.51
1:0:2637:A:H1'	1:0:2638:G:H5''	1.92	0.51
9:G:151:ILE:HA	9:G:156:ILE:HA	1.91	0.51
1:0:2916:G:H2'	1:0:2917:C:H5''	1.93	0.51
19:Q:42:LYS:NZ	19:Q:57:ASP:OD2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:52:PRO:O	26:X:56:GLU:HG3	2.10	0.51
16:N:43:VAL:HG11	16:N:81:ALA:HA	1.92	0.51
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.11	0.51
1:0:1020:A:H1'	40:Q:203:HOH:O	2.10	0.51
22:T:49:GLU:OE2	22:T:97:ARG:NH1	2.35	0.51
1:0:564:G:N3	40:0:9147:HOH:O	2.34	0.51
1:0:1169:U:H3	1:0:1173:A:H2'	1.75	0.51
10:H:41:LYS:O	10:H:87:LYS:NZ	2.33	0.51
11:I:125:VAL:HG21	11:I:142:PHE:CD2	2.45	0.51
25:W:64:THR:O	25:W:68:THR:HG22	2.10	0.51
20:R:39:THR:HG23	20:R:107:GLU:O	2.11	0.51
9:G:30:TYR:HB3	9:G:94:THR:N	2.26	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
1:0:2256:G:H2'	1:0:2257:G:H5'	1.93	0.51
6:D:59:GLY:N	6:D:60:GLU:O	2.44	0.51
9:G:54:HIS:O	9:G:56:THR:N	2.44	0.50
1:0:1705:C:P	18:P:59:ARG:HH12	2.34	0.50
1:0:877:G:H5'	1:0:878:G:OP1	2.11	0.50
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.11	0.50
14:L:76:LEU:O	14:L:80:ASP:N	2.36	0.50
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.94	0.50
9:G:56:THR:O	9:G:94:THR:OG1	2.25	0.50
1:0:2339:A:H5''	6:D:107:GLY:HA3	1.92	0.50
1:0:1383:U:OP1	40:0:9192:HOH:O	2.20	0.50
1:0:1558:C:O2	1:0:1563:G:N2	2.39	0.50
1:0:2438:G:H2'	1:0:2439:C:O4'	2.12	0.50
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.92	0.50
3:A:186:TRP:CG	3:A:187:PRO:HA	2.47	0.50
6:D:140:ARG:O	6:D:144:ARG:HG2	2.12	0.50
1:0:1185:U:H2'	1:0:1186:C:C6	2.46	0.50
4:B:166:VAL:O	4:B:174:ARG:HD3	2.12	0.50
5:C:214:THR:HG23	40:C:532:HOH:O	2.11	0.50
1:0:2265:U:H2'	1:0:2266:A:C8	2.47	0.50
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.11	0.50
1:0:1184:C:H2'	1:0:1185:U:H6	1.76	0.50
11:I:125:VAL:HA	11:I:128:CYS:HB2	1.94	0.50
20:R:109:MET:HG2	20:R:148:GLU:C	2.31	0.49
1:0:2372:A:H2'	1:0:2373:U:C6	2.47	0.49
21:S:76:GLU:OE1	21:S:80:ARG:NH1	2.41	0.49
6:D:65:GLU:O	6:D:67:ASP:N	2.45	0.49
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:97:ARG:HD2	40:P:218:HOH:O	2.12	0.49
1:0:68:U:OP1	21:S:1:SER:OG	2.29	0.49
1:0:656:G:H5'	17:O:3:THR:OG1	2.12	0.49
1:0:1666:C:H2'	1:0:1667:A:C8	2.47	0.49
1:0:1992:U:OP2	13:K:66:ARG:HD3	2.13	0.49
1:0:1164:U:N3	1:0:1192:A:H2	2.03	0.49
6:D:20:LYS:HG2	6:D:22:VAL:HG23	1.95	0.49
1:0:1025:C:OP1	25:W:108:ARG:NH1	2.43	0.49
1:0:2359:G:N7	40:0:8507:HOH:O	2.35	0.49
10:H:135:GLN:NE2	10:H:169:GLU:OE2	2.45	0.49
1:0:2760:C:OP1	4:B:209:LYS:HE2	2.11	0.49
2:9:114:G:H2'	2:9:115:C:C6	2.48	0.49
4:B:51:VAL:HG22	4:B:330:VAL:HG22	1.94	0.49
8:F:60:VAL:HG22	8:F:63:ILE:HD12	1.94	0.49
5:C:168:ARG:NH2	5:C:190:ALA:O	2.46	0.49
1:0:1406:A:N6	1:0:1701:A:H5''	2.28	0.49
1:0:485:A:N3	1:0:487:G:H5''	2.28	0.49
1:0:2591:C:H2'	1:0:2592:G:O4'	2.13	0.48
27:Y:117:LEU:HA	27:Y:174:VAL:HG21	1.95	0.48
1:0:2361:A:H2'	1:0:2362:A:C8	2.48	0.48
1:0:2083:A:N6	12:J:90:LYS:HE2	2.27	0.48
1:0:166:A:N7	14:L:25:GLY:HA2	2.28	0.48
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.43	0.48
15:M:64:ARG:HD2	40:M:379:HOH:O	2.12	0.48
31:3:14:CYS:HB3	31:3:16:GLU:HG2	1.95	0.48
4:B:24:PRO:HG2	4:B:310:ARG:HG3	1.95	0.48
1:0:1528:A:H2'	1:0:1529:G:O4'	2.13	0.48
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.95	0.48
1:0:1209:C:H2'	1:0:1210:G:H8	1.77	0.48
1:0:1613:C:H2'	1:0:1614:G:O4'	2.13	0.48
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.95	0.48
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.96	0.48
6:D:9:ASP:N	6:D:9:ASP:OD1	2.47	0.48
9:G:40:GLY:O	9:G:41:ILE:HG13	2.13	0.48
1:0:2353:A:H4'	1:0:2354:A:O5'	2.13	0.48
1:0:1704:G:O3'	18:P:59:ARG:NH1	2.47	0.48
6:D:9:ASP:O	6:D:12:GLU:HG2	2.14	0.48
12:J:88:PRO:O	12:J:94:GLY:HA3	2.14	0.48
9:G:47:GLN:O	9:G:51:ARG:N	2.47	0.48
1:0:371:U:H2'	1:0:372:A:H8	1.78	0.48
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:H3'	1:0:1118:A:N3	2.29	0.48
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.94	0.48
9:G:164:VAL:HG13	9:G:165:LEU:H	1.79	0.47
1:0:1524:U:O2'	1:0:1525:G:OP2	2.24	0.47
1:0:834:G:H4'	1:0:835:U:OP2	2.14	0.47
17:O:32:ARG:NH2	17:O:35:LYS:HG3	2.23	0.47
2:9:107:C:H2'	2:9:108:C:C6	2.49	0.47
1:0:816:G:C6	1:0:817:G:N1	2.82	0.47
1:0:2146:C:N3	1:0:2147:C:N4	2.62	0.47
22:T:51:LEU:HD11	22:T:97:ARG:HB2	1.96	0.47
1:0:1304:U:H2'	1:0:1305:C:C6	2.50	0.47
10:H:72:ALA:HB2	10:H:156:ALA:HB2	1.96	0.47
15:M:169:ARG:NH1	40:M:369:HOH:O	2.48	0.47
27:Y:165:GLU:HG2	40:Y:477:HOH:O	2.14	0.47
6:D:111:HIS:CE1	6:D:126:TYR:H	2.33	0.47
27:Y:187:VAL:HG22	27:Y:192:ASP:HB3	1.97	0.47
14:L:149:ARG:HH11	14:L:149:ARG:HB3	1.80	0.47
1:0:1409:G:H5'	40:0:8530:HOH:O	2.13	0.47
2:9:56:A:OP2	40:9:393:HOH:O	2.21	0.47
5:C:153:VAL:O	5:C:157:LEU:HG	2.15	0.47
1:0:1588:G:C6	1:0:1589:G:N1	2.83	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.47
10:H:165:ARG:HH21	10:H:167:LYS:HD2	1.80	0.47
5:C:242:GLU:HB2	40:C:489:HOH:O	2.14	0.47
11:I:49:GLU:N	11:I:49:GLU:OE1	2.48	0.47
15:M:164:THR:HG23	40:M:426:HOH:O	2.15	0.47
7:E:68:HIS:O	7:E:72:MET:HG3	2.14	0.47
6:D:40:ILE:O	6:D:44:ILE:HG22	2.14	0.47
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.80	0.47
6:D:27:ILE:HB	6:D:69:ILE:O	2.15	0.47
6:D:110:GLU:O	6:D:113:GLU:HG2	2.14	0.47
1:0:1333:U:H2'	1:0:1334:C:C6	2.50	0.47
6:D:31:GLY:C	6:D:33:ASP:H	2.17	0.47
9:G:58:GLU:O	9:G:92:ILE:HD12	2.15	0.47
6:D:58:VAL:HB	6:D:60:GLU:O	2.14	0.46
1:0:2509:A:N7	40:0:9275:HOH:O	2.36	0.46
6:D:99:ASP:HB3	6:D:103:ASN:H	1.80	0.46
1:0:1097:A:H5''	25:W:125:HIS:CE1	2.51	0.46
14:L:80:ASP:N	14:L:80:ASP:OD1	2.49	0.46
1:0:2112:A:H2'	1:0:2113:G:C8	2.50	0.46
37:9:203:CL:CL	6:D:53:LYS:NZ	2.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:52:ASP:O	9:G:54:HIS:N	2.48	0.46
15:M:64:ARG:NH2	40:M:356:HOH:O	2.38	0.46
1:0:1842:A:C4	1:0:1979:G:C6	3.04	0.46
9:G:10:GLU:HG2	9:G:11:THR:H	1.80	0.46
5:C:193:LEU:HB2	5:C:231:ARG:HD3	1.96	0.46
4:B:51:VAL:CG1	4:B:53:LEU:HD13	2.46	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.46
40:0:8766:HOH:O	22:T:82:THR:HA	2.15	0.46
11:I:17:GLY:HA3	11:I:18:PRO:HD3	1.73	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.15	0.46
31:3:87:ARG:NH1	31:3:89:GLU:OE2	2.49	0.46
1:0:2237:G:O2'	1:0:2238:A:H8	1.99	0.46
1:0:2791:U:H1'	1:0:2792:A:H5''	1.98	0.46
6:D:135:VAL:CG2	40:D:209:HOH:O	2.63	0.46
1:0:1883:U:OP2	3:A:190:ARG:HD2	2.16	0.46
22:T:26:THR:HA	22:T:39:ASN:HB3	1.98	0.46
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.51	0.46
4:B:5:ARG:HD2	13:K:41:LYS:HD3	1.98	0.46
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.35	0.46
1:0:2666:U:O2'	1:0:2667:G:O4'	2.23	0.46
1:0:1948:G:H2'	1:0:1949:G:O4'	2.15	0.46
1:0:2348:C:H1'	6:D:131:THR:HG21	1.98	0.46
1:0:2115:U:H2'	1:0:2116:U:C6	2.51	0.46
1:0:2234:U:H2'	1:0:2235:G:H8	1.81	0.46
11:I:76:LYS:HD2	11:I:82:GLU:HA	1.98	0.46
26:X:34:ARG:NH1	26:X:48:VAL:O	2.43	0.46
1:0:1370:G:O5'	20:R:62:HIS:HB3	2.16	0.46
1:0:1574:C:H2'	1:0:1575:C:C6	2.51	0.46
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.80	0.46
1:0:1104:C:H4'	12:J:88:PRO:HD3	1.98	0.45
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.96	0.45
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.97	0.45
23:U:31:PHE:CG	23:U:37:GLU:HG2	2.51	0.45
1:0:2081:A:H4'	12:J:69:TYR:CE2	2.52	0.45
1:0:790:A:H2'	1:0:791:A:O4'	2.17	0.45
1:0:226:A:H1'	1:0:393:G:C5	2.51	0.45
7:E:96:ASN:HA	7:E:126:ILE:HD13	1.98	0.45
6:D:135:VAL:HG23	40:D:208:HOH:O	2.15	0.45
6:D:84:LEU:HA	6:D:84:LEU:HD22	1.80	0.45
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.98	0.45
7:E:69:ILE:HA	7:E:72:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:932:U:H2'	1:0:933:C:C6	2.52	0.45
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.51	0.45
1:0:1180:U:H2'	1:0:1181:A:O4'	2.16	0.45
1:0:1175:G:H1'	1:0:1193:A:H2'	1.98	0.45
11:I:109:HIS:HB3	11:I:110:PRO:HD3	1.98	0.45
1:0:138:U:H4'	1:0:139:C:OP2	2.16	0.45
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.98	0.45
1:0:397:A:O2'	1:0:417:G:N3	2.34	0.45
2:9:24:U:H2'	2:9:25:G:O4'	2.16	0.45
1:0:538:C:H5''	1:0:539:G:C8	2.52	0.45
15:M:5:TYR:CE1	15:M:46:LEU:HD13	2.49	0.45
17:O:57:THR:HB	17:O:111:VAL:HG12	1.97	0.45
14:L:144:ASP:O	14:L:148:GLU:HG3	2.17	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.52	0.45
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.99	0.45
1:0:2664:A:H8	1:0:2664:A:OP1	2.00	0.45
28:Z:81:ARG:HG2	28:Z:84:ARG:HH21	1.82	0.45
1:0:2866:U:C5	23:U:50:GLU:HB3	2.51	0.45
1:0:749:C:OP2	40:0:8806:HOH:O	2.21	0.45
4:B:248:ARG:O	4:B:251:VAL:HG13	2.16	0.45
29:1:26:SER:HB2	29:1:34:CYS:SG	2.57	0.45
1:0:2637:A:H4'	1:0:2638:G:OP1	2.15	0.45
10:H:165:ARG:HD3	40:H:342:HOH:O	2.17	0.45
9:G:35:VAL:HG22	9:G:89:VAL:HG22	1.99	0.44
9:G:120:ALA:HA	9:G:121:PRO:HD3	1.88	0.44
14:L:35:ARG:O	14:L:40:PHE:HA	2.18	0.44
1:0:1829:A:N6	28:Z:18:TYR:HA	2.32	0.44
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.99	0.44
1:0:88:G:H2'	1:0:89:G:C8	2.52	0.44
6:D:77:ASP:HB3	6:D:78:GLU:H	1.58	0.44
1:0:513:A:N3	40:0:8466:HOH:O	2.36	0.44
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.52	0.44
1:0:858:U:H2'	1:0:859:C:C6	2.52	0.44
10:H:143:VAL:HG13	10:H:175:LEU:HD23	1.99	0.44
19:Q:18:PRO:O	19:Q:21:ARG:HG2	2.17	0.44
6:D:168:SER:O	6:D:170:TYR:N	2.50	0.44
1:0:2820:A:OP1	4:B:98:THR:HG23	2.17	0.44
1:0:2563:U:H2'	1:0:2565:C:O5'	2.17	0.44
33:6:30:VAL:O	33:6:34:ARG:HG2	2.17	0.44
3:A:55:VAL:HG22	3:A:68:ILE:O	2.17	0.44
10:H:99:ARG:NH2	40:H:316:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:128:A:O2'	1:0:129:A:O4'	2.28	0.44
11:I:75:ILE:HG22	11:I:104:ILE:HD13	1.99	0.44
25:W:4:LEU:O	25:W:32:CYS:HA	2.17	0.44
1:0:291:C:H2'	1:0:292:G:O4'	2.17	0.44
5:C:152:GLU:HG3	40:C:515:HOH:O	2.17	0.44
15:M:164:THR:HB	40:M:325:HOH:O	2.17	0.44
9:G:74:VAL:O	9:G:75:ASP:HB3	2.17	0.44
2:9:73:A:N6	2:9:108:C:H42	2.14	0.44
31:3:65:THR:HG22	31:3:82:GLY:HA2	1.99	0.44
5:C:65:ARG:HB3	5:C:67:GLN:HE21	1.83	0.44
6:D:121:PRO:HB2	6:D:123:ILE:HG13	1.99	0.44
16:N:143:ARG:NH1	16:N:169:PRO:HB3	2.32	0.44
1:0:2015:A:H2'	1:0:2016:U:O4'	2.18	0.44
22:T:18:GLU:O	22:T:21:LYS:HG2	2.17	0.44
13:K:64:MET:O	13:K:67:GLN:HB2	2.17	0.44
7:E:81:GLU:O	7:E:172:PRO:HG3	2.18	0.44
20:R:125:ARG:NH2	40:R:369:HOH:O	2.42	0.44
1:0:1415:G:H5'	29:1:12:ASN:O	2.18	0.44
24:V:20:LEU:HG	24:V:24:LYS:HE3	1.99	0.44
22:T:103:LEU:HA	22:T:103:LEU:HD23	1.76	0.44
9:G:150:ARG:NE	9:G:159:LEU:HD22	2.30	0.44
11:I:122:LYS:HA	11:I:125:VAL:HG22	2.00	0.44
9:G:103:GLN:C	9:G:105:LEU:H	2.20	0.44
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.44	0.44
1:0:89:G:H2'	1:0:90:A:O4'	2.18	0.44
11:I:120:ALA:O	11:I:124:VAL:HG23	2.18	0.44
1:0:1339:G:C6	1:0:1340:G:N1	2.85	0.44
9:G:106:GLU:HA	9:G:109:LYS:HD3	2.00	0.44
1:0:278:A:H2'	1:0:279:C:O4'	2.18	0.44
5:C:123:LEU:HD23	5:C:123:LEU:HA	1.84	0.44
9:G:139:VAL:O	9:G:143:GLN:HG3	2.18	0.43
1:0:165:A:H5''	14:L:33:ALA:HB2	2.00	0.43
28:Z:23:ARG:NH1	40:Z:203:HOH:O	2.45	0.43
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.81	0.43
1:0:1181:A:C2	1:0:1192:A:C8	3.06	0.43
30:2:39:ARG:HA	30:2:39:ARG:HD2	1.67	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.18	0.43
2:9:31:C:H2'	2:9:32:G:O4'	2.18	0.43
1:0:484:A:N1	1:0:506:G:H4'	2.33	0.43
9:G:37:ASN:C	9:G:39:ALA:H	2.22	0.43
1:0:1221:G:N7	40:0:8631:HOH:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:116:SER:O	6:D:118:GLU:N	2.51	0.43
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.19	0.43
1:0:1546:G:H1'	1:0:1702:U:O2	2.18	0.43
1:0:23:G:C6	1:0:24:G:N1	2.86	0.43
1:0:1095:U:O2	25:W:120:PRO:HG2	2.18	0.43
16:N:66:LEU:HB3	16:N:71:TRP:CB	2.49	0.43
1:0:1006:A:N1	1:0:2311:A:H1'	2.32	0.43
5:C:65:ARG:HB3	5:C:67:GLN:NE2	2.33	0.43
1:0:776:A:H1'	1:0:779:U:O4	2.18	0.43
15:M:35:GLY:O	40:M:341:HOH:O	2.21	0.43
19:Q:10:THR:HB	19:Q:14:LEU:HG	2.00	0.43
1:0:1252:A:H4'	33:6:47:ARG:HD2	2.00	0.43
8:F:56:PRO:HA	37:F:201:CL:CL	2.55	0.43
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
6:D:36:ASN:O	6:D:40:ILE:HG12	2.19	0.43
17:O:73:ASP:HA	17:O:92:VAL:O	2.19	0.43
1:0:1968:A:H2'	1:0:1969:A:C8	2.54	0.43
25:W:65:VAL:HA	25:W:68:THR:HG22	2.00	0.43
12:J:90:LYS:HB2	37:J:203:CL:CL	2.55	0.43
6:D:31:GLY:O	6:D:33:ASP:N	2.52	0.43
4:B:267:LYS:NZ	4:B:300:SER:O	2.44	0.43
1:0:2094:G:H4'	4:B:245:SER:HB3	2.01	0.43
1:0:1198:U:O4	40:0:9554:HOH:O	2.21	0.43
25:W:118:LEU:HD12	25:W:153:MET:HE3	2.01	0.43
1:0:1130:U:O4	1:0:2523:U:H5''	2.19	0.43
6:D:54:ALA:HB2	6:D:69:ILE:HG13	2.01	0.43
31:3:25:VAL:HG22	31:3:68:LYS:HG3	2.00	0.43
33:6:27:ASN:OD1	33:6:28:GLU:N	2.49	0.43
25:W:150:LEU:HD23	25:W:150:LEU:HA	1.86	0.43
1:0:1527:A:H1'	1:0:1528:A:C8	2.54	0.43
11:I:73:GLU:HA	11:I:76:LYS:HG2	2.00	0.43
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.49	0.43
20:R:68:HIS:CD2	20:R:76:ASP:HB2	2.53	0.43
7:E:94:GLN:HG3	40:E:221:HOH:O	2.17	0.43
1:0:2782:G:O6	1:0:2790:C:H5''	2.19	0.43
1:0:1191:A:H3'	1:0:1192:A:H5''	2.01	0.43
11:I:108:LYS:HB3	11:I:108:LYS:HE2	1.91	0.43
5:C:2:GLN:HG2	5:C:15:GLU:OE2	2.18	0.43
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.34	0.43
1:0:653:U:H2'	1:0:654:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.54	0.43
1:0:2724:U:H2'	1:0:2725:G:O4'	2.19	0.43
11:I:68:VAL:HG11	11:I:108:LYS:HB3	2.01	0.42
22:T:9:LYS:HG2	22:T:13:ARG:NH1	2.34	0.42
1:0:2637:A:C2	1:0:2639:G:OP2	2.70	0.42
1:0:2911:C:H2'	1:0:2912:C:H6	1.81	0.42
1:0:1131:G:C6	1:0:1230:A:C4	3.07	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.42
1:0:1716:A:H4'	18:P:55:LYS:HD3	2.01	0.42
11:I:89:GLN:HB3	11:I:89:GLN:HE21	1.63	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.18	0.42
1:0:688:A:N6	1:0:698:A:H5"	2.34	0.42
1:0:401:C:H2'	1:0:402:U:C6	2.53	0.42
1:0:2276:U:H2'	1:0:2277:U:C6	2.54	0.42
16:N:69:TYR:OH	16:N:185:GLU:O	2.24	0.42
1:0:177:A:H2'	1:0:178:U:O4'	2.19	0.42
1:0:2415:A:C2	16:N:25:ARG:HB2	2.54	0.42
9:G:156:ILE:HG13	9:G:156:ILE:H	1.66	0.42
1:0:1123:A:C6	1:0:1238:C:H5'	2.54	0.42
15:M:30:GLU:O	15:M:34:GLU:HG3	2.19	0.42
1:0:1902:G:H2'	1:0:1903:U:O4'	2.19	0.42
14:L:142:LEU:HD12	14:L:142:LEU:HA	1.84	0.42
3:A:180:LYS:HE3	3:A:180:LYS:HB3	1.87	0.42
9:G:112:ALA:HB1	9:G:187:LYS:HE2	2.00	0.42
4:B:268:ARG:NE	40:B:592:HOH:O	2.52	0.42
1:0:1393:A:H2'	1:0:1394:C:C6	2.55	0.42
20:R:111:ILE:HG23	20:R:145:LEU:HD11	2.01	0.42
18:P:75:LYS:O	18:P:80:ARG:NH2	2.48	0.42
1:0:1184:C:H2'	1:0:1185:U:C6	2.54	0.42
5:C:115:LEU:HA	5:C:115:LEU:HD12	1.85	0.42
1:0:95:A:H5"	1:0:97:G:O4'	2.19	0.42
11:I:96:LEU:HD21	11:I:101:VAL:HG22	2.02	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.20	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.81	0.42
1:0:1014:A:H2'	1:0:1015:C:H5'	2.01	0.42
24:V:39:ALA:HA	24:V:40:PRO:HD3	1.81	0.42
11:I:74:LEU:HD11	11:I:107:GLN:HG2	2.01	0.42
13:K:120:ARG:HG2	13:K:121:PHE:CZ	2.54	0.42
1:0:1980:U:O2	1:0:2008:U:H4'	2.19	0.42
1:0:2898:G:H4'	4:B:288:GLY:HA2	2.01	0.42
26:X:79:GLU:O	26:X:82:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:70:PRO:HG2	11:I:73:GLU:HB2	2.02	0.42
1:0:2896:A:H2'	38:0:8212:ACY:H2	2.02	0.42
1:0:1687:C:O2	29:1:9:GLY:HA2	2.20	0.42
6:D:23:VAL:HB	6:D:130:VAL:HG22	2.00	0.42
1:0:2090:G:H2'	1:0:2091:G:C8	2.55	0.42
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.42
1:0:2570:G:H5''	40:0:9612:HOH:O	2.20	0.42
1:0:638:C:H2'	1:0:639:A:C8	2.54	0.42
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.20	0.42
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.60	0.42
1:0:417:G:OP1	1:0:417:G:H8	2.03	0.42
6:D:81:GLU:OE2	6:D:170:TYR:OH	2.24	0.42
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.42
1:0:1132:A:N6	1:0:1229:C:H2'	2.35	0.42
1:0:2356:A:H2'	1:0:2357:G:O4'	2.19	0.42
12:J:19:MET:CE	12:J:78:ILE:HG22	2.50	0.42
27:Y:122:ARG:NH1	40:Y:480:HOH:O	2.41	0.42
18:P:80:ARG:HD2	18:P:87:ARG:CZ	2.50	0.42
12:J:19:MET:HE1	12:J:78:ILE:HG22	2.02	0.42
25:W:3:ALA:O	25:W:54:PHE:HA	2.20	0.42
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.42
13:K:74:VAL:HB	13:K:113:ILE:HD12	2.02	0.42
1:0:2587:OMU:H2'	1:0:2589:U:H5''	2.01	0.42
1:0:1964:U:H2'	1:0:1965:C:H6	1.82	0.42
8:F:28:ALA:H	8:F:100:ASP:HB3	1.85	0.42
1:0:188:C:H5''	15:M:163:LEU:HD21	2.01	0.42
14:L:143:THR:HG21	40:L:327:HOH:O	2.20	0.42
1:0:1515:A:H2'	1:0:1516:U:C6	2.55	0.42
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.42
1:0:1449:G:C6	1:0:1450:C:N4	2.88	0.42
1:0:2141:G:N2	1:0:2235:G:C5	2.88	0.41
2:9:91:C:H2'	2:9:92:G:O4'	2.20	0.41
25:W:126:ASP:HB3	25:W:135:GLY:O	2.19	0.41
3:A:86:ALA:HB3	3:A:94:LEU:HG	2.01	0.41
17:O:32:ARG:O	17:O:35:LYS:HB2	2.20	0.41
4:B:209:LYS:HB2	4:B:257:THR:OG1	2.20	0.41
6:D:60:GLU:HG2	6:D:61:PHE:CD1	2.55	0.41
2:9:35:C:H5''	40:9:370:HOH:O	2.19	0.41
9:G:113:PRO:HG3	9:G:185:GLU:OE2	2.20	0.41
6:D:44:ILE:HD11	6:D:114:PHE:CZ	2.55	0.41
1:0:2668:G:H2'	1:0:2669:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:19:MET:HE2	12:J:132:LEU:HD11	2.01	0.41
25:W:113:SER:HA	25:W:114:PRO:HD3	1.86	0.41
17:O:22:GLY:O	40:O:325:HOH:O	2.21	0.41
9:G:205:PRO:O	9:G:209:GLU:HB2	2.20	0.41
1:O:486:A:OP2	22:T:81:LYS:NZ	2.46	0.41
13:K:27:ARG:NH2	40:K:334:HOH:O	2.38	0.41
1:O:1589:G:N2	1:O:1605:G:H1'	2.35	0.41
10:H:175:LEU:HD23	10:H:175:LEU:HA	1.79	0.41
10:H:99:ARG:HB3	10:H:121:GLY:HA3	2.02	0.41
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.03	0.41
10:H:77:ILE:HG23	10:H:82:GLU:HA	2.01	0.41
1:O:591:A:OP2	40:O:9919:HOH:O	2.21	0.41
1:O:2272:G:OP1	3:A:223:ARG:HD2	2.21	0.41
1:O:1257:C:H2'	1:O:1258:G:O4'	2.21	0.41
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.41
26:X:6:GLU:HG3	26:X:76:ARG:HB3	2.02	0.41
9:G:51:ARG:HG2	11:I:115:TYR:HE1	1.84	0.41
10:H:49:GLN:O	10:H:169:GLU:N	2.46	0.41
1:O:940:G:O2'	1:O:1032:A:N1	2.44	0.41
25:W:80:ASP:HB2	40:W:325:HOH:O	2.20	0.41
1:O:734:U:O2'	1:O:737:A:N6	2.53	0.41
29:1:25:LYS:HD2	30:2:48:ASP:HA	2.03	0.41
10:H:50:ILE:HD12	10:H:149:VAL:CG2	2.50	0.41
9:G:52:ASP:C	9:G:54:HIS:H	2.24	0.41
5:C:214:THR:HB	40:C:439:HOH:O	2.20	0.41
1:O:1684:A:O2'	1:O:1685:A:H5''	2.21	0.41
6:D:168:SER:C	6:D:170:TYR:H	2.24	0.41
1:O:1249:U:H2'	1:O:1250:C:C6	2.56	0.41
1:O:344:C:H2'	1:O:345:G:O4'	2.20	0.41
2:9:96:C:H2'	2:9:97:U:C6	2.56	0.41
1:O:644:G:H5'	1:O:644:G:N3	2.35	0.41
9:G:131:THR:OG1	9:G:132:GLY:N	2.54	0.41
6:D:135:VAL:HG23	40:D:209:HOH:O	2.20	0.41
2:9:92:G:C6	2:9:93:A:C6	3.09	0.41
11:I:64:ILE:HG12	11:I:65:GLU:N	2.36	0.41
2:9:28:U:OP2	16:N:39:SER:HB2	2.20	0.41
2:9:29:C:O3'	6:D:138:GLY:HA2	2.21	0.41
1:O:1006:A:H2'	1:O:1007:A:C8	2.56	0.41
1:O:858:U:H2'	1:O:859:C:H6	1.86	0.41
20:R:68:HIS:CG	20:R:76:ASP:HB2	2.55	0.41
8:F:18:GLU:O	8:F:22:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.21	0.41
1:0:797:A:H5'	28:Z:9:GLY:O	2.21	0.41
1:0:255:A:H2'	1:0:256:C:C6	2.55	0.41
1:0:821:U:H2'	1:0:822:C:H6	1.86	0.41
1:0:2365:G:H4'	19:Q:45:PRO:O	2.20	0.41
1:0:2597:U:OP2	40:0:8619:HOH:O	2.21	0.41
1:0:1066:U:H2'	1:0:1067:A:C8	2.56	0.41
6:D:14:ARG:HH21	6:D:136:ARG:CZ	2.33	0.41
11:I:102:LYS:O	11:I:106:GLU:HG2	2.20	0.41
1:0:1167:G:H4'	11:I:131:LEU:HG	2.02	0.41
2:9:27:C:H2'	2:9:28:U:O4'	2.20	0.41
1:0:1185:U:H2'	1:0:1186:C:H6	1.85	0.41
2:9:23:U:O2'	2:9:24:U:H5'	2.20	0.41
4:B:179:LEU:O	4:B:183:GLU:HG2	2.21	0.41
9:G:112:ALA:HB3	9:G:187:LYS:O	2.20	0.40
27:Y:117:LEU:CA	27:Y:174:VAL:HG21	2.51	0.40
1:0:1497:G:H4'	1:0:1627:G:O2'	2.21	0.40
2:9:93:A:C5	2:9:94:G:H1'	2.57	0.40
27:Y:126:PRO:HG2	27:Y:128:PHE:CE2	2.56	0.40
19:Q:42:LYS:HA	19:Q:42:LYS:HD2	1.98	0.40
3:A:175:LYS:HE2	40:A:475:HOH:O	2.20	0.40
1:0:615:G:OP1	12:J:91:LYS:HE3	2.22	0.40
24:V:37:GLY:N	24:V:38:GLY:HA3	2.37	0.40
1:0:625:U:H5''	1:0:1044:C:N4	2.37	0.40
16:N:114:LYS:NZ	40:N:353:HOH:O	2.53	0.40
1:0:2105:C:H2'	1:0:2106:C:C6	2.56	0.40
1:0:2575:C:H2'	1:0:2576:A:O4'	2.21	0.40
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.21	0.40
1:0:1422:U:H2'	1:0:1423:C:C6	2.56	0.40
1:0:2401:A:H2'	1:0:2402:A:C8	2.57	0.40
22:T:50:VAL:HG12	22:T:56:ALA:HA	2.03	0.40
1:0:2252:A:C5	1:0:2253:G:H1'	2.56	0.40
1:0:113:A:C8	1:0:114:A:C8	3.09	0.40
1:0:1596:U:H2'	1:0:1598:A:OP2	2.20	0.40
1:0:1385:G:H5'	26:X:50:LEU:O	2.20	0.40
1:0:1985:U:C2	1:0:1996:U:O4'	2.75	0.40
25:W:146:ILE:HA	25:W:146:ILE:HD12	1.93	0.40
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.94	0.40
1:0:2694:A:H4'	7:E:91:PHE:CE2	2.57	0.40
10:H:102:LYS:HG3	10:H:103:GLN:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:73:A:H61	2:9:108:C:N4	2.16	0.40
20:R:106:GLY:HA2	20:R:109:MET:CE	2.52	0.40
7:E:69:ILE:HA	7:E:72:MET:HE3	2.03	0.40
1:0:1993:C:H5''	13:K:66:ARG:NH1	2.37	0.40
6:D:44:ILE:HD11	6:D:114:PHE:CE1	2.57	0.40
1:0:2819:C:H2'	1:0:2820:A:C8	2.56	0.40
10:H:30:LYS:HG3	10:H:62:HIS:CE1	2.57	0.40
12:J:39:VAL:HG22	12:J:107:ASN:HA	2.04	0.40
16:N:180:LEU:HD23	16:N:180:LEU:HA	1.92	0.40
1:0:2698:G:H2'	1:0:2699:A:C8	2.57	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	
3	A	235/240 (98%)	223 (95%)	11 (5%)	1 (0%)	39	56
4	B	335/338 (99%)	327 (98%)	8 (2%)	0	100	100
5	C	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
6	D	164/177 (93%)	143 (87%)	18 (11%)	3 (2%)	11	13
7	E	172/178 (97%)	168 (98%)	4 (2%)	0	100	100
8	F	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
9	G	204/255 (80%)	171 (84%)	28 (14%)	5 (2%)	7	7
10	H	161/177 (91%)	156 (97%)	4 (2%)	1 (1%)	30	43
11	I	141/162 (87%)	122 (86%)	17 (12%)	2 (1%)	14	19
12	J	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
13	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
14	L	145/165 (88%)	139 (96%)	5 (3%)	1 (1%)	26	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	M	193/196 (98%)	189 (98%)	4 (2%)	0	100	100
16	N	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
17	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
18	P	142/149 (95%)	142 (100%)	0	0	100	100
19	Q	93/96 (97%)	93 (100%)	0	0	100	100
20	R	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
21	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
22	T	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
23	U	54/67 (81%)	53 (98%)	1 (2%)	0	100	100
24	V	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
25	W	152/154 (99%)	152 (100%)	0	0	100	100
26	X	88/92 (96%)	83 (94%)	5 (6%)	0	100	100
27	Y	142/241 (59%)	142 (100%)	0	0	100	100
28	Z	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	47/50 (94%)	46 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
33	6	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
All	All	4083/4411 (93%)	3924 (96%)	146 (4%)	13 (0%)	46	63

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	G	38	ILE
6	D	173	GLU
9	G	74	VAL
9	G	53	LEU
9	G	75	ASP
10	H	176	ILE
11	I	25	THR
11	I	28	PRO
3	A	170	VAL
14	L	81	VAL
6	D	63	ILE
6	D	66	GLY
9	G	114	ILE

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	
3	A	179/182 (98%)	170 (95%)	9 (5%)	30	48
4	B	282/283 (100%)	268 (95%)	14 (5%)	30	48
5	C	193/193 (100%)	182 (94%)	11 (6%)	25	40
6	D	139/148 (94%)	124 (89%)	15 (11%)	8	11
7	E	154/156 (99%)	148 (96%)	6 (4%)	39	59
8	F	93/94 (99%)	85 (91%)	8 (9%)	13	19
9	G	174/174 (100%)	159 (91%)	15 (9%)	13	19
10	H	138/145 (95%)	133 (96%)	5 (4%)	42	63
11	I	120/130 (92%)	112 (93%)	8 (7%)	20	31
12	J	120/121 (99%)	115 (96%)	5 (4%)	36	56
13	K	106/106 (100%)	102 (96%)	4 (4%)	40	60
14	L	114/127 (90%)	108 (95%)	6 (5%)	28	44
15	M	159/160 (99%)	154 (97%)	5 (3%)	47	69
16	N	149/150 (99%)	140 (94%)	9 (6%)	24	37
17	O	93/94 (99%)	85 (91%)	8 (9%)	13	19
18	P	114/117 (97%)	110 (96%)	4 (4%)	43	64
19	Q	79/80 (99%)	77 (98%)	2 (2%)	55	76
20	R	117/122 (96%)	112 (96%)	5 (4%)	35	55
21	S	71/74 (96%)	70 (99%)	1 (1%)	74	88
22	T	105/106 (99%)	98 (93%)	7 (7%)	20	31
23	U	47/53 (89%)	44 (94%)	3 (6%)	22	34
24	V	51/57 (90%)	50 (98%)	1 (2%)	63	81
25	W	130/130 (100%)	126 (97%)	4 (3%)	47	69
26	X	72/74 (97%)	69 (96%)	3 (4%)	36	56
27	Y	122/196 (62%)	119 (98%)	3 (2%)	55	76
28	Z	67/74 (90%)	64 (96%)	3 (4%)	34	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	1	46/47 (98%)	45 (98%)	1 (2%)	60	79
30	2	45/46 (98%)	44 (98%)	1 (2%)	60	79
31	3	79/79 (100%)	76 (96%)	3 (4%)	40	60
33	6	48/49 (98%)	48 (100%)	0	100	100
All	All	3406/3567 (96%)	3237 (95%)	169 (5%)	30	48

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	30	ARG
3	A	34	ASP
3	A	38	ILE
3	A	55	VAL
3	A	69	LEU
3	A	105	VAL
3	A	133	ARG
3	A	192	VAL
3	A	217	ARG
4	B	5	ARG
4	B	11	LEU
4	B	51	VAL
4	B	84	LEU
4	B	97	LEU
4	B	98	THR
4	B	102	THR
4	B	175	LEU
4	B	195	ARG
4	B	245	SER
4	B	254	GLN
4	B	257	THR
4	B	265	LEU
4	B	279	THR
5	C	21	VAL
5	C	115	LEU
5	C	136	VAL
5	C	140	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	223	LEU
5	C	236	THR

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Mol	Chain	Res	Type
5	C	240	LEU
5	C	243	VAL
6	D	17	ARG
6	D	23	VAL
6	D	24	HIS
6	D	34	LEU
6	D	44	ILE
6	D	52	THR
6	D	55	LYS
6	D	58	VAL
6	D	60	GLU
6	D	82	GLU
6	D	84	LEU
6	D	128	LEU
6	D	158	ASN
6	D	161	ASP
6	D	172	VAL
7	E	12	ASP
7	E	46	THR
7	E	86	VAL
7	E	132	THR
7	E	154	ILE
7	E	164	ASP
8	F	1	PRO
8	F	12	LEU
8	F	22	VAL
8	F	38	LYS
8	F	60	VAL
8	F	65	GLU
8	F	99	THR
8	F	118	LEU
9	G	36	VAL
9	G	46	LEU
9	G	51	ARG
9	G	75	ASP
9	G	81	LEU
9	G	86	THR
9	G	89	VAL
9	G	101	LEU
9	G	106	GLU
9	G	110	THR
9	G	153	GLU

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Mol	Chain	Res	Type
9	G	167	THR
9	G	169	GLU
9	G	173	GLN
9	G	210	LEU
10	H	4	LYS
10	H	61	ARG
10	H	65	LEU
10	H	157	TYR
10	H	159	LYS
11	I	31	VAL
11	I	41	GLN
11	I	74	LEU
11	I	96	LEU
11	I	111	ASP
11	I	112	LEU
11	I	135	ILE
11	I	136	GLU
12	J	39	VAL
12	J	52	GLN
12	J	79	PHE
12	J	80	LYS
12	J	120	SER
13	K	55	VAL
13	K	63	GLU
13	K	98	VAL
13	K	115	ARG
14	L	18	HIS
14	L	35	ARG
14	L	80	ASP
14	L	140	VAL
14	L	145	LEU
14	L	149	ARG
15	M	22	GLU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	49	THR
16	N	50	LEU
16	N	66	LEU

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Mol	Chain	Res	Type
16	N	127	LEU
16	N	135	VAL
16	N	168	LEU
16	N	175	LEU
17	O	21	SER
17	O	25	VAL
17	O	28	ASP
17	O	32	ARG
17	O	42	GLU
17	O	47	ARG
17	O	96	VAL
17	O	98	LEU
18	P	16	VAL
18	P	52	LYS
18	P	80	ARG
18	P	91	LYS
19	Q	20	ASP
19	Q	64	GLU
20	R	39	THR
20	R	55	GLN
20	R	82	GLU
20	R	119	VAL
20	R	143	VAL
21	S	21	GLN
22	T	26	THR
22	T	39	ASN
22	T	41	ARG
22	T	48	VAL
22	T	71	VAL
22	T	89	ARG
22	T	96	VAL
23	U	9	CYS
23	U	28	THR
23	U	52	THR
24	V	21	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	112	LEU
26	X	27	ASP
26	X	43	VAL
26	X	91	GLU

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Mol	Chain	Res	Type
27	Y	172	THR
27	Y	236	VAL
27	Y	237	GLU
28	Z	41	ASN
28	Z	60	CYS
28	Z	87	LEU
29	1	37	CYS
30	2	8	LYS
31	3	65	THR
31	3	74	CYS
31	3	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
19	Q	4	ASN
20	R	123	GLN
25	W	2	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2804/2910 (96%)	263 (9%)	23 (0%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2925/3032 (96%)	279 (9%)	24 (0%)

All (279) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	9	C
1	0	17	G
1	0	31	C
1	0	67	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	92	G
1	0	113	A
1	0	114	A
1	0	115	U

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Mol	Chain	Res	Type
1	0	120	A
1	0	126	C
1	0	127	U
1	0	128	A
1	0	138	U
1	0	140	G
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	210	U
1	0	219	G
1	0	237	G
1	0	256	C
1	0	271	C
1	0	273	G
1	0	308	U
1	0	309	C
1	0	331	A
1	0	337	A
1	0	338	C
1	0	345	G
1	0	358	G
1	0	396	U
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	487	G
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	553	G
1	0	581	G
1	0	588	G

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Mol	Chain	Res	Type
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	698	A
1	0	699	C
1	0	700	A
1	0	701	U
1	0	702	G
1	0	715	U
1	0	716	G
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	925	C
1	0	961	A
1	0	998	U
1	0	1003	U
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1052	G

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Mol	Chain	Res	Type
1	0	1059	G
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1120	U
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1166	A
1	0	1173	A
1	0	1174	A
1	0	1175	G
1	0	1176	C
1	0	1187	U
1	0	1192	A
1	0	1193	A
1	0	1194	A
1	0	1202	A
1	0	1216	G
1	0	1226	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1252	A
1	0	1279	U
1	0	1280	A
1	0	1289	C
1	0	1299	G
1	0	1342	C
1	0	1360	C
1	0	1380	U
1	0	1386	G
1	0	1406	A
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1477	C

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Mol	Chain	Res	Type
1	0	1485	A
1	0	1492	A
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1592	G
1	0	1611	G
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1635	U
1	0	1640	C
1	0	1656	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1702	U
1	0	1703	G
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1878	G
1	0	1919	A
1	0	1958	U
1	0	1959	G
1	0	1963	C
1	0	1971	G
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2005	G

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Mol	Chain	Res	Type
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2144	C
1	0	2146	C
1	0	2148	G
1	0	2227	C
1	0	2228	G
1	0	2229	G
1	0	2238	A
1	0	2243	C
1	0	2253	G
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2294	C
1	0	2313	C
1	0	2317	C
1	0	2321	A
1	0	2339	A
1	0	2342	G
1	0	2354	A
1	0	2369	A
1	0	2378	U
1	0	2379	G
1	0	2404	G
1	0	2420	G
1	0	2422	U
1	0	2462	G
1	0	2467	A

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Mol	Chain	Res	Type
1	0	2468	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2505	G
1	0	2527	U
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2637	A
1	0	2638	G
1	0	2665	A
1	0	2676	C
1	0	2681	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2827	A
1	0	2837	U
1	0	2852	A
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2909	G
1	0	2914	A
1	0	2915	A

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Mol	Chain	Res	Type
2	9	3	A
2	9	7	G
2	9	11	A
2	9	23	U
2	9	24	U
2	9	32	G
2	9	44	A
2	9	52	A
2	9	55	U
2	9	56	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	94	G
2	9	114	G
2	9	122	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	8	A
1	0	169	A
1	0	417	G
1	0	509	A
1	0	699	C
1	0	715	U
1	0	716	G
1	0	834	G
1	0	857	A
1	0	877	G
1	0	1080	C
1	0	1246	A
1	0	1504	A
1	0	1524	U
1	0	1684	A
1	0	1692	C
1	0	1856	C
1	0	1979	G
1	0	2467	A
1	0	2536	C
1	0	2553	A
1	0	2637	A

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Mol	Chain	Res	Type
1	0	2791	U
2	9	2	U

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

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$
1	OMU	0	2587	1	12,22,23	0.46	0	19,31,34	1.62	1 (5%)
1	OMG	0	2588	1	17,26,27	1.21	2 (11%)	21,38,41	2.07	6 (28%)
1	UR3	0	2619	1	12,22,23	0.78	0	16,32,35	0.82	1 (6%)
1	PSU	0	2621	1	13,21,22	1.03	1 (7%)	18,30,33	3.79	6 (33%)
1	1MA	0	628	1,36	14,25,26	1.74	4 (28%)	15,37,40	1.53	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-2.82	1.49	1.52
1	0	628	1MA	C2-N3	2.03	1.34	1.30
1	0	628	1MA	C5-C4	2.85	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2588	OMG	C5-C4	3.11	1.47	1.40
1	0	2588	OMG	C6-C5	3.41	1.48	1.41
1	0	628	1MA	C6-N6	3.63	1.35	1.29
1	0	628	1MA	C6-C5	3.85	1.48	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-12.39	120.43	128.33
1	0	2588	OMG	C5-C6-N1	-4.34	117.66	123.59
1	0	2588	OMG	C6-C5-C4	-3.48	116.74	120.90
1	0	628	1MA	C4-C5-N7	-3.41	106.35	109.48
1	0	2588	OMG	C4-C5-N7	-3.19	106.54	109.48
1	0	2588	OMG	N3-C2-N1	-3.08	122.75	127.44
1	0	628	1MA	C1'-N9-C4	-3.03	122.37	126.94
1	0	2621	PSU	C5-C1'-C2'	-2.90	110.36	115.52
1	0	2588	OMG	C1'-N9-C4	-2.65	122.94	126.94
1	0	2621	PSU	C5-C6-N1	-2.56	120.77	124.39
1	0	2619	UR3	C3U-N3-C4	2.08	121.08	118.19
1	0	2621	PSU	O4'-C1'-C2'	2.11	106.88	104.73
1	0	628	1MA	C2-N3-C4	3.37	121.63	116.40
1	0	2621	PSU	C6-N1-C2	4.02	121.93	115.47
1	0	2588	OMG	C6-N1-C2	4.99	122.86	115.94
1	0	2587	OMU	C4-N3-C2	6.49	120.57	114.14
1	0	2621	PSU	C4-N3-C2	7.87	122.05	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 265 ligands modelled in this entry, 261 are monoatomic - leaving 4 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	ACY	0	8212	-	1,3,3	1.18	0	0,3,3	0.00	-
38	ACY	0	8213	-	1,3,3	0.19	0	0,3,3	0.00	-
38	ACY	0	8214	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
38	ACY	W	201	-	1,3,3	1.75	0	0,3,3	0.00	-

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	ACY	0	8212	-	-	0/0/0/0	0/0/0/0
38	ACY	0	8213	-	-	0/0/0/0	0/0/0/0
38	ACY	0	8214	-	-	0/0/0/0	0/0/0/0
38	ACY	W	201	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	8214	ACY	CH3-C	2.30	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	8212	ACY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	8213	ACY	3	0
38	W	201	ACY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	211:ASP	C	213:UNK	N	3.25

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	0	2803/2910 (96%)	-0.06	84 (2%) 54 53	9, 28, 77, 221	0
2	9	122/122 (100%)	-0.37	3 (2%) 61 60	24, 44, 61, 127	0
3	A	237/240 (98%)	0.37	15 (6%) 23 24	12, 30, 63, 98	0
4	B	337/338 (99%)	0.26	8 (2%) 62 61	14, 35, 60, 72	0
5	C	246/246 (100%)	0.32	8 (3%) 50 50	10, 27, 48, 58	0
6	D	166/177 (93%)	2.51	99 (59%) 0 0	33, 81, 106, 113	0
7	E	174/178 (97%)	0.33	9 (5%) 31 31	30, 47, 64, 83	0
8	F	119/120 (99%)	0.71	12 (10%) 9 8	27, 46, 72, 78	0
9	G	206/255 (80%)	4.91	154 (74%) 0 0	57, 105, 173, 186	0
10	H	165/177 (93%)	0.44	11 (6%) 21 21	22, 37, 70, 94	0
11	I	145/162 (89%)	4.50	115 (79%) 0 0	81, 115, 155, 179	0
12	J	144/145 (99%)	0.09	3 (2%) 67 66	23, 33, 55, 82	0
13	K	132/132 (100%)	0.14	3 (2%) 64 63	19, 32, 49, 63	0
14	L	149/165 (90%)	0.80	13 (8%) 13 12	12, 41, 80, 88	0
15	M	195/196 (99%)	-0.05	0 100 100	14, 22, 34, 47	0
16	N	186/187 (99%)	0.36	11 (5%) 26 26	25, 41, 76, 101	0
17	O	115/116 (99%)	-0.19	0 100 100	23, 34, 50, 55	0
18	P	144/149 (96%)	-0.07	0 100 100	23, 34, 48, 60	0
19	Q	95/96 (98%)	0.05	0 100 100	19, 26, 41, 50	0
20	R	150/155 (96%)	0.07	0 100 100	16, 26, 45, 56	0
21	S	81/85 (95%)	0.39	6 (7%) 17 17	23, 36, 54, 63	0
22	T	119/120 (99%)	0.22	1 (0%) 87 87	21, 36, 55, 76	0
23	U	56/67 (83%)	0.30	2 (3%) 46 47	28, 36, 60, 103	0
24	V	65/71 (91%)	1.22	10 (15%) 3 3	30, 46, 78, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.21	3 (1%) 70 69	22, 32, 47, 56	0
26	X	90/92 (97%)	0.28	5 (5%) 28 28	26, 39, 101, 111	0
27	Y	144/241 (59%)	0.11	8 (5%) 28 28	15, 28, 53, 104	0
28	Z	83/92 (90%)	0.47	8 (9%) 10 10	25, 39, 85, 108	0
29	1	56/57 (98%)	0.53	0 100 100	11, 16, 23, 24	0
30	2	49/50 (98%)	0.35	1 (2%) 68 68	20, 37, 64, 73	0
31	3	92/92 (100%)	0.05	0 100 100	16, 32, 46, 52	0
32	4	0/70	-	-	-	-
32	5	0/70	-	-	-	-
33	6	55/56 (98%)	5.33	54 (98%) 0 0	56, 98, 117, 122	0
All	All	7074/7583 (93%)	0.44	646 (9%) 11 11	9, 33, 102, 221	0

All (646) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	G	133	VAL	16.0
9	G	136	GLY	15.6
9	G	119	VAL	13.5
9	G	139	VAL	13.3
9	G	208	LEU	13.2
6	D	174	VAL	13.2
11	I	50	VAL	13.0
9	G	138	PHE	12.8
9	G	167	THR	12.8
9	G	123	ASP	12.3
9	G	124	ILE	12.0
9	G	137	PRO	11.9
9	G	134	ASP	11.8
1	0	2148	G	11.8
9	G	132	GLY	11.8
9	G	166	ASP	11.8
11	I	59	ASP	11.8
33	6	25	ALA	11.6
11	I	9	VAL	10.9
1	0	2147	C	10.9
9	G	189	VAL	10.9
11	I	60	GLY	10.8
11	I	62	PHE	10.8
9	G	149	ALA	10.8

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Mol	Chain	Res	Type	RSRZ
9	G	143	GLN	10.5
11	I	38	ILE	10.4
11	I	11	GLY	10.4
11	I	5	ILE	10.3
9	G	122	ASN	10.2
9	G	144	SER	10.2
9	G	131	THR	10.2
1	0	2146	C	10.0
9	G	145	VAL	9.9
9	G	127	PRO	9.9
9	G	114	ILE	9.7
9	G	171	VAL	9.7
11	I	61	SER	9.6
9	G	126	ILE	9.6
11	I	18	PRO	9.6
33	6	3	THR	9.5
1	0	2149	A	9.5
9	G	165	LEU	9.4
9	G	168	GLY	9.4
33	6	4	TYR	9.3
9	G	141	GLU	9.2
27	Y	238	VAL	9.2
9	G	152	GLN	9.1
9	G	53	LEU	9.0
9	G	184	ILE	9.0
1	0	997	C	9.0
9	G	147	ALA	9.0
9	G	170	GLU	8.9
9	G	112	ALA	8.9
9	G	77	GLY	8.8
9	G	140	GLY	8.8
9	G	121	PRO	8.8
33	6	15	GLY	8.6
11	I	58	ASP	8.6
11	I	64	ILE	8.5
11	I	29	VAL	8.4
9	G	154	GLY	8.4
11	I	105	ALA	8.3
9	G	156	ILE	8.2
9	G	130	ASP	8.2
11	I	31	VAL	8.1
9	G	180	ASN	8.1

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Mol	Chain	Res	Type	RSRZ
9	G	178	VAL	8.1
11	I	6	GLU	8.0
9	G	135	PRO	8.0
6	D	173	GLU	8.0
1	0	2145	G	8.0
11	I	49	GLU	7.9
9	G	163	THR	7.9
1	0	2144	C	7.9
9	G	110	THR	7.9
9	G	150	ARG	7.9
9	G	155	SER	7.8
9	G	176	SER	7.8
9	G	142	LEU	7.8
33	6	23	VAL	7.7
24	V	39	ALA	7.7
33	6	24	GLU	7.7
11	I	16	PRO	7.6
9	G	125	VAL	7.6
33	6	2	SER	7.6
9	G	116	ALA	7.6
11	I	14	ALA	7.6
9	G	183	GLY	7.5
11	I	52	VAL	7.5
11	I	8	LEU	7.5
9	G	162	SER	7.4
11	I	66	VAL	7.4
11	I	51	PRO	7.3
1	0	2231	G	7.3
6	D	69	ILE	7.3
11	I	10	PRO	7.3
9	G	159	LEU	7.2
9	G	105	LEU	7.2
33	6	5	THR	7.2
33	6	29	ASN	7.2
9	G	157	GLN	7.2
1	0	715	U	7.1
3	A	237	GLY	7.1
14	L	87	GLY	7.1
33	6	31	ALA	7.1
1	0	2229	G	7.1
11	I	34	VAL	7.1
9	G	153	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
9	G	115	GLY	7.1
11	I	56	TYR	7.1
33	6	50	ILE	7.1
33	6	26	PRO	7.1
9	G	101	LEU	7.0
9	G	151	ILE	7.0
1	0	2141	G	7.0
9	G	182	LEU	6.9
11	I	101	VAL	6.9
9	G	146	GLY	6.8
6	D	32	ARG	6.8
33	6	56	ALA	6.8
9	G	117	GLY	6.8
11	I	43	ALA	6.8
1	0	2228	G	6.8
11	I	131	LEU	6.7
9	G	210	LEU	6.6
11	I	133	VAL	6.6
9	G	169	GLU	6.6
11	I	7	VAL	6.6
9	G	203	PHE	6.6
33	6	14	ASP	6.5
12	J	2	SER	6.5
11	I	71	THR	6.5
33	6	27	ASN	6.5
11	I	93	VAL	6.5
33	6	9	SER	6.4
6	D	119	TYR	6.4
12	J	3	VAL	6.4
11	I	15	ASN	6.4
9	G	57	ALA	6.4
1	0	2230	U	6.3
33	6	28	GLU	6.3
10	H	176	ILE	6.3
11	I	113	LEU	6.3
9	G	118	GLU	6.2
28	Z	87	LEU	6.2
33	6	10	PHE	6.2
9	G	128	GLU	6.2
9	G	79	GLU	6.2
9	G	148	ASP	6.2
11	I	77	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
33	6	6	VAL	6.2
33	6	19	PHE	6.1
9	G	129	GLY	6.1
33	6	13	ARG	6.1
11	I	42	THR	6.1
9	G	177	ASN	6.1
33	6	35	VAL	6.1
9	G	173	GLN	6.1
33	6	52	ILE	6.0
9	G	107	ALA	6.0
9	G	174	GLU	6.0
6	D	18	ILE	5.9
11	I	39	ASN	5.9
1	0	972	U	5.9
9	G	95	ASP	5.9
33	6	55	VAL	5.9
11	I	109	HIS	5.9
33	6	30	VAL	5.9
23	U	2	ARG	5.8
11	I	107	GLN	5.8
11	I	81	PHE	5.8
33	6	39	PHE	5.8
11	I	32	GLN	5.8
1	0	2227	C	5.8
11	I	35	VAL	5.8
9	G	158	VAL	5.7
9	G	120	ALA	5.7
21	S	81	ILE	5.7
11	I	79	ALA	5.6
11	I	57	ASP	5.6
9	G	164	VAL	5.6
1	0	1952	U	5.6
11	I	91	ASP	5.6
6	D	170	TYR	5.5
1	0	2142	G	5.5
11	I	110	PRO	5.5
12	J	4	ALA	5.5
9	G	108	SER	5.5
1	0	971	G	5.5
9	G	172	SER	5.5
33	6	51	THR	5.5
27	Y	237	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	0	127	U	5.4
6	D	10	PHE	5.4
11	I	65	GLU	5.3
9	G	179	LEU	5.3
3	A	35	GLY	5.3
33	6	54	GLU	5.3
9	G	160	SER	5.3
6	D	169	THR	5.3
9	G	200	GLY	5.3
11	I	20	LEU	5.2
16	N	154	LEU	5.2
9	G	181	GLU	5.2
9	G	175	LEU	5.2
6	D	166	ILE	5.2
11	I	75	ILE	5.2
11	I	53	THR	5.2
24	V	1	THR	5.2
11	I	92	PHE	5.2
9	G	201	VAL	5.2
1	0	2235	G	5.1
11	I	40	ASP	5.1
9	G	94	THR	5.0
6	D	117	GLN	5.0
24	V	41	GLU	5.0
11	I	28	PRO	5.0
11	I	13	GLU	4.9
11	I	73	GLU	4.9
33	6	43	HIS	4.9
9	G	111	PRO	4.9
6	D	85	GLN	4.8
11	I	117	LEU	4.8
26	X	91	GLU	4.8
11	I	36	GLN	4.8
6	D	64	ARG	4.8
9	G	207	GLU	4.8
6	D	165	PHE	4.8
9	G	211	ASP	4.8
26	X	81	GLY	4.8
33	6	20	GLU	4.8
9	G	113	PRO	4.7
10	H	177	ALA	4.7
9	G	199	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
33	6	18	GLN	4.7
1	0	2143	U	4.7
6	D	118	GLU	4.7
9	G	190	GLY	4.7
11	I	153	ASP	4.7
9	G	76	ASP	4.6
9	G	80	ASP	4.6
9	G	98	PRO	4.6
33	6	34	ARG	4.6
9	G	198	ALA	4.6
33	6	7	ARG	4.6
9	G	33	VAL	4.6
11	I	130	SER	4.6
33	6	44	ASN	4.6
6	D	75	LEU	4.5
1	0	1202	A	4.5
9	G	104	GLU	4.5
11	I	155	PHE	4.5
11	I	88	PRO	4.5
6	D	84	LEU	4.5
11	I	17	GLY	4.5
33	6	11	PRO	4.5
11	I	24	LEU	4.5
6	D	95	THR	4.5
1	0	1171	A	4.5
1	0	1198	U	4.4
11	I	54	VAL	4.4
11	I	37	GLU	4.4
9	G	37	ASN	4.4
11	I	156	ALA	4.4
1	0	2233	C	4.3
6	D	94	ALA	4.3
14	L	82	ALA	4.3
6	D	123	ILE	4.3
33	6	53	GLU	4.3
28	Z	83	ILE	4.3
9	G	206	GLU	4.3
1	0	2140	U	4.3
6	D	92	GLU	4.3
9	G	202	LEU	4.3
11	I	89	GLN	4.3
6	D	35	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	0	2226	U	4.3
9	G	99	PHE	4.2
11	I	22	PRO	4.2
11	I	70	PRO	4.2
11	I	103	GLN	4.2
11	I	83	THR	4.2
33	6	42	GLN	4.1
6	D	9	ASP	4.1
9	G	187	LYS	4.1
33	6	40	GLY	4.1
6	D	104	PHE	4.1
11	I	41	GLN	4.1
11	I	146	ILE	4.1
1	0	126	C	4.1
11	I	69	PRO	4.1
9	G	185	GLU	4.1
6	D	108	VAL	4.1
1	0	1956	U	4.1
9	G	161	ASP	4.1
6	D	61	PHE	4.1
24	V	38	GLY	4.1
11	I	100	GLN	4.0
6	D	62	ASP	4.0
11	I	82	GLU	4.0
11	I	118	THR	4.0
26	X	82	GLU	4.0
1	0	1959	G	4.0
33	6	33	GLU	4.0
9	G	55	GLY	4.0
11	I	68	VAL	4.0
6	D	121	PRO	4.0
1	0	2236	C	3.9
6	D	81	GLU	3.9
1	0	1960	A	3.9
7	E	174	ARG	3.9
33	6	22	GLU	3.9
11	I	111	ASP	3.9
6	D	63	ILE	3.9
11	I	33	ALA	3.9
24	V	37	GLY	3.9
9	G	30	TYR	3.9
11	I	25	THR	3.8

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Mol	Chain	Res	Type	RSRZ
7	E	87	PHE	3.8
9	G	186	PRO	3.8
1	0	1962	C	3.8
7	E	173	ASN	3.8
1	0	996	C	3.8
11	I	23	GLU	3.8
11	I	74	LEU	3.8
33	6	21	LYS	3.8
1	0	1951	G	3.8
1	0	1957	A	3.7
6	D	120	ASP	3.7
9	G	209	GLU	3.7
6	D	125	ILE	3.7
6	D	57	THR	3.7
9	G	196	VAL	3.7
14	L	79	ASP	3.7
24	V	43	PRO	3.7
11	I	72	ALA	3.7
6	D	98	PHE	3.7
11	I	55	LYS	3.7
6	D	11	HIS	3.6
6	D	58	VAL	3.6
11	I	84	GLY	3.6
6	D	26	GLY	3.6
1	0	1172	G	3.6
11	I	134	THR	3.6
14	L	81	VAL	3.6
33	6	38	ASP	3.6
9	G	96	ASP	3.5
33	6	8	GLY	3.5
9	G	100	SER	3.5
28	Z	89	GLU	3.5
33	6	32	GLU	3.5
6	D	56	ARG	3.5
9	G	8	LYS	3.5
1	0	1199	A	3.5
10	H	40	GLN	3.5
9	G	23	ILE	3.5
11	I	104	ILE	3.5
11	I	76	LYS	3.5
1	0	8	A	3.5
3	A	85	SER	3.5

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Mol	Chain	Res	Type	RSRZ
9	G	97	ASN	3.5
11	I	21	GLY	3.5
9	G	205	PRO	3.5
6	D	134	LEU	3.5
6	D	162	ALA	3.5
8	F	115	VAL	3.5
6	D	128	LEU	3.5
7	E	169	THR	3.4
33	6	41	SER	3.4
11	I	63	GLU	3.4
11	I	154	VAL	3.4
27	Y	95	THR	3.4
14	L	78	ALA	3.4
9	G	24	VAL	3.4
6	D	79	MET	3.4
11	I	19	PRO	3.4
11	I	139	PRO	3.4
3	A	62	ASP	3.4
1	0	2234	U	3.3
1	0	1961	C	3.3
6	D	105	SER	3.3
6	D	29	HIS	3.3
28	Z	84	ARG	3.3
1	0	282	C	3.3
1	0	1963	C	3.3
11	I	94	ALA	3.3
33	6	45	LEU	3.3
6	D	101	THR	3.3
23	U	1	PRO	3.2
6	D	80	ALA	3.2
11	I	112	LEU	3.2
6	D	50	VAL	3.2
9	G	56	THR	3.2
8	F	119	ARG	3.2
9	G	71	LEU	3.2
1	0	2917	C	3.2
16	N	183	ASP	3.2
2	9	24	U	3.2
6	D	158	ASN	3.2
6	D	66	GLY	3.2
11	I	86	GLY	3.2
33	6	36	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
21	S	2	TRP	3.2
6	D	114	PHE	3.2
9	G	102	PHE	3.2
9	G	194	ARG	3.2
11	I	99	ASP	3.2
1	0	2138	C	3.2
33	6	12	ALA	3.1
1	0	1169	U	3.1
11	I	147	ASP	3.1
1	0	2237	G	3.1
6	D	78	GLU	3.1
9	G	73	ASP	3.1
22	T	82	THR	3.1
4	B	183	GLU	3.1
11	I	87	GLU	3.1
1	0	1177	A	3.1
16	N	152	GLU	3.1
27	Y	108	ASP	3.1
27	Y	235	GLU	3.1
6	D	112	THR	3.0
11	I	30	ASP	3.0
6	D	40	ILE	3.0
6	D	127	GLY	3.0
6	D	30	GLY	3.0
11	I	98	VAL	3.0
26	X	79	GLU	3.0
9	G	38	ILE	3.0
11	I	12	GLY	3.0
1	0	1174	A	3.0
6	D	48	MET	2.9
30	2	34	GLN	2.9
9	G	39	ALA	2.9
16	N	165	ALA	2.9
6	D	171	ASP	2.9
11	I	95	ASP	2.9
9	G	31	GLU	2.9
6	D	44	ILE	2.9
6	D	107	GLY	2.9
9	G	52	ASP	2.9
6	D	167	GLU	2.9
14	L	147	GLU	2.9
3	A	64	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
14	L	88	GLY	2.9
33	6	48	THR	2.9
21	S	1	SER	2.9
1	0	1200	A	2.9
1	0	735	C	2.9
33	6	16	PRO	2.8
21	S	45	TYR	2.8
14	L	77	ALA	2.8
2	9	23	U	2.8
9	G	84	TYR	2.8
6	D	93	LEU	2.8
6	D	17	ARG	2.8
1	0	1525	G	2.8
1	0	2343	A	2.8
9	G	75	ASP	2.8
6	D	22	VAL	2.8
6	D	106	PHE	2.8
14	L	148	GLU	2.8
28	Z	80	ARG	2.8
11	I	67	GLY	2.8
6	D	99	ASP	2.8
1	0	2004	U	2.7
6	D	88	LEU	2.7
10	H	171	GLY	2.7
1	0	2139	G	2.7
3	A	37	VAL	2.7
4	B	180	ASP	2.7
8	F	29	VAL	2.7
33	6	49	GLN	2.7
1	0	2232	A	2.7
9	G	25	GLU	2.7
13	K	129	THR	2.7
6	D	97	GLN	2.7
1	0	1625	U	2.7
5	C	198	ASP	2.7
28	Z	88	SER	2.7
1	0	736	A	2.7
9	G	188	GLU	2.7
6	D	51	ARG	2.6
9	G	92	ILE	2.6
11	I	114	SER	2.6
3	A	97	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	100	ASP	2.6
1	0	1175	G	2.6
9	G	197	PHE	2.6
7	E	170	ARG	2.6
10	H	140	TYR	2.6
9	G	48	ASP	2.6
16	N	181	ASP	2.6
6	D	172	VAL	2.6
9	G	36	VAL	2.6
10	H	48	VAL	2.6
4	B	61	PRO	2.6
6	D	115	PRO	2.6
11	I	135	ILE	2.6
6	D	133	ASN	2.6
8	F	110	ASP	2.6
11	I	149	GLY	2.6
1	0	1181	A	2.6
1	0	283	U	2.6
2	9	1	U	2.6
26	X	4	ASP	2.5
1	0	1179	C	2.5
1	0	2137	A	2.5
8	F	117	GLU	2.5
6	D	126	TYR	2.5
13	K	119	GLN	2.5
1	0	1948	G	2.5
1	0	128	A	2.5
3	A	36	ASP	2.5
6	D	96	SER	2.5
6	D	132	VAL	2.5
1	0	1201	C	2.5
11	I	115	TYR	2.5
7	E	121	ASP	2.5
3	A	60	PHE	2.5
16	N	163	PHE	2.5
10	H	86	TYR	2.5
6	D	160	ALA	2.5
14	L	139	SER	2.5
6	D	73	VAL	2.5
6	D	82	GLU	2.5
8	F	11	ASP	2.4
33	6	47	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
6	D	27	ILE	2.4
6	D	53	LYS	2.4
6	D	159	PRO	2.4
3	A	135	VAL	2.4
6	D	23	VAL	2.4
11	I	106	GLU	2.4
3	A	77	GLY	2.4
6	D	157	LEU	2.4
6	D	164	ALA	2.4
28	Z	86	ALA	2.4
9	G	103	GLN	2.4
1	0	1170	U	2.4
27	Y	236	VAL	2.4
33	6	37	SER	2.4
24	V	2	VAL	2.4
33	6	17	GLN	2.4
11	I	132	GLY	2.4
8	F	25	ASP	2.4
25	W	93	ILE	2.4
7	E	88	TYR	2.3
21	S	77	VAL	2.3
1	0	1195	G	2.3
13	K	101	ASN	2.3
6	D	68	PRO	2.3
8	F	15	ASP	2.3
11	I	78	GLU	2.3
6	D	90	LEU	2.3
24	V	49	LEU	2.3
8	F	16	ALA	2.3
28	Z	85	ALA	2.3
16	N	172	PHE	2.3
7	E	6	GLU	2.3
5	C	132	ASP	2.3
9	G	11	THR	2.3
1	0	998	U	2.3
9	G	10	GLU	2.3
16	N	68	GLU	2.3
6	D	41	LEU	2.3
21	S	41	VAL	2.3
9	G	204	GLU	2.2
1	0	1180	U	2.2
4	B	176	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
9	G	9	THR	2.2
9	G	6	GLU	2.2
6	D	71	ALA	2.2
9	G	43	SER	2.2
5	C	61	PHE	2.2
5	C	14	GLY	2.2
8	F	18	GLU	2.2
6	D	135	VAL	2.2
24	V	40	PRO	2.2
5	C	58	ALA	2.2
11	I	148	ALA	2.2
14	L	121	ILE	2.2
6	D	103	ASN	2.2
11	I	85	SER	2.2
14	L	104	ASP	2.2
1	0	1965	C	2.2
27	Y	98	GLN	2.2
4	B	65	MET	2.2
1	0	2508	C	2.2
1	0	2916	G	2.2
5	C	143	ASP	2.2
9	G	50	ARG	2.2
25	W	85	ALA	2.2
1	0	1178	G	2.2
6	D	156	ARG	2.2
4	B	62	ARG	2.1
5	C	134	ASP	2.1
9	G	21	ASP	2.1
1	0	970	U	2.1
10	H	172	GLU	2.1
9	G	32	SER	2.1
1	0	284	C	2.1
10	H	80	LEU	2.1
1	0	2665	A	2.1
1	0	960	G	2.1
6	D	130	VAL	2.1
9	G	51	ARG	2.1
1	0	9	C	2.1
1	0	575	A	2.1
1	0	2637	A	2.1
3	A	236	GLY	2.1
6	D	59	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
16	N	139	TRP	2.1
10	H	149	VAL	2.1
3	A	34	ASP	2.1
8	F	14	ASP	2.1
16	N	156	GLU	2.1
3	A	128	LEU	2.1
9	G	78	LEU	2.1
6	D	74	THR	2.1
1	0	1192	A	2.1
4	B	117	GLU	2.1
9	G	14	GLU	2.1
9	G	49	MET	2.1
9	G	27	ILE	2.1
5	C	81	PRO	2.1
9	G	42	PRO	2.1
10	H	76	LEU	2.1
1	0	1958	U	2.1
6	D	43	GLU	2.1
9	G	58	GLU	2.1
24	V	42	ASN	2.1
6	D	70	GLY	2.1
8	F	118	LEU	2.1
14	L	144	ASP	2.1
4	B	104	GLU	2.0
27	Y	234	VAL	2.0
9	G	61	VAL	2.0
6	D	89	PRO	2.0
6	D	129	ASP	2.0
3	A	134	ASN	2.0
1	0	1203	G	2.0
7	E	127	ASP	2.0
25	W	92	ASP	2.0
6	D	45	THR	2.0
16	N	150	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	OMU	0	2587	21/22	0.99	0.13	-	15,18,20,22	0
1	OMG	0	2588	24/25	0.98	0.14	-	15,17,20,22	0
1	PSU	0	2621	20/21	0.99	0.18	-	14,17,20,21	0
1	1MA	0	628	23/24	0.99	0.18	-	13,15,17,18	0
1	UR3	0	2619	21/22	0.98	0.15	-	16,18,21,26	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8172	1/1	0.89	0.28	14.24	33,33,33,33	0
37	CL	B	402	1/1	0.92	0.47	13.12	62,62,62,62	0
36	NA	0	8162	1/1	0.96	0.36	11.49	25,25,25,25	0
36	NA	0	8164	1/1	0.96	0.23	11.47	39,39,39,39	0
36	NA	0	8147	1/1	0.97	0.23	10.87	23,23,23,23	0
36	NA	0	8174	1/1	0.94	0.30	9.90	28,28,28,28	0
36	NA	0	8126	1/1	0.98	0.28	9.87	23,23,23,23	0
36	NA	R	202	1/1	0.77	0.38	8.91	48,48,48,48	0
38	ACY	0	8212	4/4	0.91	0.33	8.42	35,39,41,43	0
36	NA	0	8170	1/1	0.94	0.26	5.67	38,38,38,38	0
34	MG	0	8195	1/1	0.90	0.19	5.44	45,45,45,45	0
34	MG	0	8059	1/1	0.99	0.24	4.81	21,21,21,21	0
34	MG	0	8205	1/1	0.92	0.23	4.31	43,43,43,43	0
36	NA	9	202	1/1	0.90	0.21	3.75	42,42,42,42	0
34	MG	0	8203	1/1	0.55	0.26	3.38	43,43,43,43	0
34	MG	0	8017	1/1	0.98	0.25	3.34	11,11,11,11	0
36	NA	M	201	1/1	0.97	0.21	3.30	15,15,15,15	0
36	NA	0	8143	1/1	0.97	0.23	2.82	13,13,13,13	0
36	NA	0	8159	1/1	0.98	0.22	2.60	26,26,26,26	0
36	NA	0	8169	1/1	0.95	0.17	2.49	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8111	1/1	0.96	0.17	2.13	25,25,25,25	0
36	NA	0	8136	1/1	0.98	0.20	1.96	20,20,20,20	0
34	MG	0	8063	1/1	0.96	0.20	1.60	19,19,19,19	0
34	MG	0	8054	1/1	0.97	0.21	1.17	10,10,10,10	0
36	NA	0	8137	1/1	0.99	0.17	1.02	21,21,21,21	0
36	NA	H	201	1/1	0.98	0.15	0.85	19,19,19,19	0
36	NA	0	8167	1/1	0.92	0.18	0.78	29,29,29,29	0
36	NA	0	8130	1/1	0.93	0.20	0.78	31,31,31,31	0
36	NA	0	8127	1/1	0.97	0.20	0.72	22,22,22,22	0
36	NA	0	8123	1/1	0.97	0.19	0.67	23,23,23,23	0
34	MG	0	8004	1/1	0.99	0.20	0.29	13,13,13,13	0
36	NA	0	8117	1/1	0.95	0.14	0.19	24,24,24,24	0
34	MG	0	8015	1/1	0.98	0.21	0.13	15,15,15,15	0
36	NA	0	8151	1/1	0.99	0.19	0.07	11,11,11,11	0
39	CD	Z	101	1/1	0.99	0.16	-0.01	38,38,38,38	0
36	NA	C	301	1/1	0.93	0.16	-0.35	20,20,20,20	0
34	MG	0	8038	1/1	0.99	0.17	-0.39	13,13,13,13	0
34	MG	Y	305	1/1	0.98	0.13	-0.47	33,33,33,33	0
34	MG	0	8001	1/1	0.96	0.17	-0.48	16,16,16,16	0
37	CL	0	8210	1/1	0.97	0.16	-0.51	49,49,49,49	0
34	MG	0	8013	1/1	0.94	0.17	-0.52	16,16,16,16	0
34	MG	0	8010	1/1	0.99	0.18	-0.56	14,14,14,14	0
36	NA	0	8120	1/1	0.98	0.19	-0.59	21,21,21,21	0
36	NA	0	8140	1/1	0.98	0.17	-0.72	21,21,21,21	0
39	CD	U	8401	1/1	0.99	0.12	-0.79	39,39,39,39	0
37	CL	0	8188	1/1	0.99	0.13	-0.87	30,30,30,30	0
39	CD	3	102	1/1	0.98	0.13	-0.92	39,39,39,39	0
34	MG	0	8007	1/1	0.95	0.16	-0.93	18,18,18,18	0
36	NA	0	8171	1/1	0.94	0.12	-1.00	39,39,39,39	0
34	MG	0	8012	1/1	0.99	0.13	-1.09	23,23,23,23	0
37	CL	0	8187	1/1	0.99	0.12	-1.18	38,38,38,38	0
37	CL	M	202	1/1	0.98	0.14	-1.23	21,21,21,21	0
36	NA	0	8139	1/1	0.97	0.12	-1.27	29,29,29,29	0
34	MG	0	8100	1/1	0.85	0.14	-1.31	42,42,42,42	0
36	NA	L	201	1/1	0.95	0.18	-1.58	24,24,24,24	0
37	CL	F	201	1/1	0.98	0.10	-1.59	33,33,33,33	0
34	MG	0	8064	1/1	0.94	0.12	-1.70	20,20,20,20	0
36	NA	0	8132	1/1	0.92	0.14	-1.72	23,23,23,23	0
36	NA	0	8112	1/1	0.98	0.16	-1.74	19,19,19,19	0
34	MG	0	8069	1/1	0.93	0.09	-1.81	29,29,29,29	0
34	MG	0	8056	1/1	0.96	0.13	-1.83	25,25,25,25	0
37	CL	R	204	1/1	0.98	0.11	-1.83	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
39	CD	1	101	1/1	1.00	0.11	-2.30	37,37,37,37	0
36	NA	0	8157	1/1	0.98	0.18	-2.31	24,24,24,24	0
36	NA	J	201	1/1	0.98	0.12	-2.40	27,27,27,27	0
34	MG	Y	301	1/1	0.98	0.12	-2.43	19,19,19,19	0
36	NA	0	8131	1/1	0.95	0.12	-2.51	28,28,28,28	0
37	CL	J	204	1/1	0.98	0.12	-2.54	36,36,36,36	0
36	NA	0	8154	1/1	0.96	0.14	-2.58	24,24,24,24	0
36	NA	0	8163	1/1	0.97	0.13	-2.64	18,18,18,18	0
34	MG	0	8080	1/1	0.96	0.04	-2.70	31,31,31,31	0
34	MG	N	202	1/1	0.95	0.13	-2.71	58,58,58,58	0
36	NA	0	8129	1/1	0.98	0.12	-2.72	37,37,37,37	0
34	MG	0	8032	1/1	0.96	0.14	-2.75	17,17,17,17	0
36	NA	A	304	1/1	0.96	0.09	-2.81	28,28,28,28	0
36	NA	0	8166	1/1	0.95	0.11	-2.82	38,38,38,38	0
34	MG	0	8003	1/1	0.98	0.12	-2.93	12,12,12,12	0
36	NA	0	8138	1/1	0.97	0.10	-2.94	20,20,20,20	0
34	MG	0	8020	1/1	0.98	0.11	-2.95	17,17,17,17	0
34	MG	Y	304	1/1	0.93	0.09	-2.96	33,33,33,33	0
34	MG	T	201	1/1	0.98	0.07	-2.97	47,47,47,47	0
37	CL	0	8184	1/1	0.99	0.10	-2.99	26,26,26,26	0
34	MG	0	8191	1/1	0.93	0.11	-3.03	31,31,31,31	0
36	NA	Q	101	1/1	0.98	0.07	-3.24	25,25,25,25	0
34	MG	0	8055	1/1	0.99	0.07	-3.27	31,31,31,31	0
36	NA	L	202	1/1	0.98	0.15	-3.31	24,24,24,24	0
34	MG	0	8199	1/1	0.97	0.10	-3.32	55,55,55,55	0
34	MG	A	302	1/1	0.98	0.12	-3.36	20,20,20,20	0
37	CL	B	401	1/1	0.99	0.14	-3.43	24,24,24,24	0
37	CL	0	8182	1/1	0.98	0.09	-3.48	26,26,26,26	0
34	MG	0	8035	1/1	0.98	0.10	-3.51	27,27,27,27	0
34	MG	0	8072	1/1	0.91	0.15	-3.51	15,15,15,15	0
36	NA	R	201	1/1	0.96	0.09	-3.53	29,29,29,29	0
34	MG	0	8022	1/1	0.92	0.16	-3.58	23,23,23,23	0
37	CL	O	202	1/1	0.99	0.07	-3.66	36,36,36,36	0
34	MG	0	8018	1/1	0.97	0.12	-3.70	22,22,22,22	0
34	MG	0	8008	1/1	0.99	0.13	-3.71	13,13,13,13	0
34	MG	0	8014	1/1	0.94	0.15	-3.75	19,19,19,19	0
34	MG	0	8105	1/1	0.96	0.09	-3.88	23,23,23,23	0
34	MG	3	101	1/1	0.90	0.10	-4.40	27,27,27,27	0
36	NA	0	8113	1/1	0.99	0.14	-4.51	19,19,19,19	0
34	MG	0	8002	1/1	0.97	0.15	-4.52	19,19,19,19	0
34	MG	0	8033	1/1	0.97	0.10	-4.52	16,16,16,16	0
36	NA	0	8192	1/1	0.98	0.09	-4.64	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8021	1/1	0.99	0.12	-4.64	17,17,17,17	0
34	MG	L	204	1/1	0.95	0.10	-4.73	26,26,26,26	0
36	NA	0	8128	1/1	0.97	0.14	-4.80	19,19,19,19	0
34	MG	0	8044	1/1	0.98	0.11	-4.97	21,21,21,21	0
34	MG	0	8074	1/1	0.94	0.10	-5.27	30,30,30,30	0
34	MG	0	8103	1/1	0.99	0.08	-5.62	15,15,15,15	0
35	K	0	8109	1/1	0.92	0.10	-5.63	44,44,44,44	0
34	MG	0	8101	1/1	0.98	0.12	-5.70	19,19,19,19	0
34	MG	0	8078	1/1	0.95	0.09	-5.73	27,27,27,27	0
34	MG	0	8006	1/1	0.91	0.10	-5.94	22,22,22,22	0
36	NA	0	8142	1/1	0.99	0.06	-6.12	28,28,28,28	0
34	MG	0	8057	1/1	0.97	0.06	-6.39	23,23,23,23	0
36	NA	0	8160	1/1	0.97	0.17	-6.42	26,26,26,26	0
34	MG	0	8061	1/1	0.85	0.07	-6.43	30,30,30,30	0
34	MG	0	8085	1/1	0.94	0.07	-6.56	28,28,28,28	0
34	MG	0	8019	1/1	0.96	0.08	-6.76	23,23,23,23	0
34	MG	0	8039	1/1	0.98	0.07	-7.07	27,27,27,27	0
34	MG	0	8089	1/1	0.96	0.08	-7.90	23,23,23,23	0
34	MG	0	8066	1/1	0.96	0.09	-8.49	27,27,27,27	0
34	MG	0	8099	1/1	0.98	0.07	-9.29	26,26,26,26	0
34	MG	0	8208	1/1	0.83	0.08	-9.65	45,45,45,45	0
34	MG	0	8053	1/1	0.98	0.09	-14.24	22,22,22,22	0
37	CL	3	103	1/1	0.98	0.06	-16.21	33,33,33,33	0
34	MG	0	8052	1/1	0.90	0.04	-19.36	36,36,36,36	0
34	MG	0	8193	1/1	0.99	0.13	-22.45	14,14,14,14	0
34	MG	0	8049	1/1	0.96	0.09	-	36,36,36,36	0
34	MG	0	8102	1/1	0.99	0.15	-	24,24,24,24	0
37	CL	0	8186	1/1	0.98	0.16	-	25,25,25,25	0
38	ACY	W	201	4/4	0.96	0.29	-	46,47,48,49	0
34	MG	0	8040	1/1	0.93	0.11	-	26,26,26,26	0
36	NA	0	8165	1/1	0.96	0.20	-	29,29,29,29	0
34	MG	0	8204	1/1	0.91	0.12	-	33,33,33,33	0
34	MG	A	303	1/1	0.97	0.15	-	23,23,23,23	0
34	MG	0	8042	1/1	0.98	0.07	-	28,28,28,28	0
34	MG	0	8207	1/1	0.91	0.09	-	33,33,33,33	0
37	CL	0	8185	1/1	0.99	0.11	-	32,32,32,32	0
34	MG	0	8082	1/1	0.97	0.18	-	17,17,17,17	0
36	NA	0	8149	1/1	0.94	0.38	-	28,28,28,28	0
34	MG	0	8076	1/1	0.92	0.12	-	38,38,38,38	0
34	MG	0	8011	1/1	0.99	0.14	-	16,16,16,16	0
34	MG	0	8009	1/1	0.99	0.19	-	15,15,15,15	0
34	MG	0	8106	1/1	0.95	0.12	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8121	1/1	0.94	0.21	-	20,20,20,20	0
36	NA	0	8144	1/1	0.88	0.22	-	37,37,37,37	0
34	MG	0	8005	1/1	0.99	0.19	-	13,13,13,13	0
34	MG	A	301	1/1	0.89	0.11	-	42,42,42,42	0
36	NA	0	8148	1/1	0.92	0.15	-	21,21,21,21	0
34	MG	0	8060	1/1	0.97	0.14	-	22,22,22,22	0
36	NA	0	8114	1/1	0.98	0.15	-	19,19,19,19	0
37	CL	0	8181	1/1	0.97	0.16	-	29,29,29,29	0
37	CL	0	8189	1/1	0.98	0.08	-	35,35,35,35	0
36	NA	0	8116	1/1	0.98	0.16	-	29,29,29,29	0
36	NA	0	8134	1/1	0.90	0.17	-	46,46,46,46	0
37	CL	9	203	1/1	0.90	0.07	-	59,59,59,59	0
38	ACY	0	8213	4/4	0.85	0.38	-	34,39,40,49	0
34	MG	0	8094	1/1	0.89	0.18	-	32,32,32,32	0
37	CL	J	203	1/1	0.95	0.10	-	42,42,42,42	0
36	NA	0	8155	1/1	0.98	0.09	-	34,34,34,34	0
34	MG	0	8070	1/1	0.99	0.07	-	22,22,22,22	0
34	MG	0	8202	1/1	0.92	0.14	-	33,33,33,33	0
37	CL	J	202	1/1	0.97	0.10	-	34,34,34,34	0
34	MG	0	8031	1/1	0.96	0.15	-	15,15,15,15	0
39	CD	O	201	1/1	0.99	0.07	-	58,58,58,58	0
34	MG	0	8034	1/1	0.90	0.10	-	25,25,25,25	0
36	NA	0	8158	1/1	0.97	0.14	-	28,28,28,28	0
34	MG	0	8093	1/1	0.97	0.21	-	42,42,42,42	0
34	MG	0	8030	1/1	0.99	0.10	-	17,17,17,17	0
36	NA	0	8125	1/1	0.97	0.19	-	19,19,19,19	0
34	MG	0	8026	1/1	0.94	0.17	-	19,19,19,19	0
34	MG	0	8086	1/1	0.88	0.10	-	38,38,38,38	0
34	MG	0	8098	1/1	0.92	0.06	-	33,33,33,33	0
34	MG	0	8198	1/1	0.94	0.16	-	39,39,39,39	0
34	MG	0	8027	1/1	0.95	0.09	-	30,30,30,30	0
36	NA	0	8153	1/1	0.98	0.29	-	29,29,29,29	0
36	NA	0	8110	1/1	0.94	0.17	-	26,26,26,26	0
36	NA	0	8173	1/1	0.97	0.21	-	25,25,25,25	0
34	MG	0	8041	1/1	0.97	0.13	-	25,25,25,25	0
34	MG	K	201	1/1	0.98	0.10	-	25,25,25,25	0
36	NA	0	8141	1/1	0.92	0.08	-	30,30,30,30	0
34	MG	0	8062	1/1	0.96	0.08	-	35,35,35,35	0
34	MG	0	8083	1/1	0.96	0.08	-	34,34,34,34	0
36	NA	0	8124	1/1	0.95	0.26	-	32,32,32,32	0
37	CL	G	301	1/1	0.91	0.11	-	58,58,58,58	0
34	MG	0	8045	1/1	0.95	0.05	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8037	1/1	0.93	0.08	-	29,29,29,29	0
37	CL	0	8209	1/1	0.88	0.10	-	54,54,54,54	0
34	MG	0	8046	1/1	0.94	0.11	-	37,37,37,37	0
37	CL	N	201	1/1	0.98	0.10	-	36,36,36,36	0
36	NA	0	8176	1/1	0.97	0.29	-	37,37,37,37	0
36	NA	H	202	1/1	0.93	0.24	-	39,39,39,39	0
34	MG	0	8087	1/1	0.87	0.11	-	22,22,22,22	0
34	MG	0	8096	1/1	0.90	0.19	-	43,43,43,43	0
38	ACY	0	8214	4/4	0.86	0.27	-	28,35,37,39	0
36	NA	0	8118	1/1	0.87	0.17	-	41,41,41,41	0
36	NA	0	8115	1/1	0.96	0.12	-	32,32,32,32	0
34	MG	0	8206	1/1	0.94	0.21	-	33,33,33,33	0
36	NA	0	8146	1/1	0.96	0.19	-	22,22,22,22	0
34	MG	0	8197	1/1	0.93	0.17	-	31,31,31,31	0
34	MG	0	8029	1/1	0.98	0.10	-	22,22,22,22	0
36	NA	0	8119	1/1	0.94	0.21	-	32,32,32,32	0
37	CL	R	203	1/1	0.98	0.13	-	30,30,30,30	0
36	NA	0	8179	1/1	0.89	0.09	-	43,43,43,43	0
34	MG	0	8194	1/1	0.97	0.13	-	35,35,35,35	0
34	MG	0	8065	1/1	0.86	0.05	-	40,40,40,40	0
34	MG	0	8036	1/1	0.95	0.11	-	21,21,21,21	0
34	MG	0	8043	1/1	0.93	0.06	-	29,29,29,29	0
36	NA	0	8135	1/1	0.97	0.09	-	29,29,29,29	0
34	MG	0	8050	1/1	0.81	0.55	-	73,73,73,73	0
36	NA	0	8178	1/1	0.87	0.19	-	60,60,60,60	0
34	MG	0	8048	1/1	0.99	0.07	-	33,33,33,33	0
34	MG	0	8028	1/1	0.97	0.09	-	21,21,21,21	0
35	K	0	8211	1/1	0.94	0.14	-	51,51,51,51	0
37	CL	0	8190	1/1	0.99	0.19	-	31,31,31,31	0
34	MG	0	8196	1/1	0.91	0.14	-	39,39,39,39	0
34	MG	0	8200	1/1	0.97	0.20	-	37,37,37,37	0
34	MG	0	8108	1/1	0.95	0.05	-	20,20,20,20	0
36	NA	0	8175	1/1	0.95	0.18	-	30,30,30,30	0
36	NA	0	8150	1/1	0.97	0.11	-	36,36,36,36	0
34	MG	0	8107	1/1	0.97	0.06	-	32,32,32,32	0
34	MG	0	8023	1/1	0.94	0.17	-	20,20,20,20	0
34	MG	0	8090	1/1	0.95	0.09	-	19,19,19,19	0
36	NA	0	8180	1/1	0.94	0.26	-	37,37,37,37	0
34	MG	0	8088	1/1	0.96	0.06	-	40,40,40,40	0
36	NA	S	101	1/1	0.97	0.14	-	25,25,25,25	0
34	MG	Y	303	1/1	0.97	0.28	-	38,38,38,38	0
36	NA	0	8177	1/1	0.97	0.15	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	CL	L	203	1/1	0.97	0.10	-	29,29,29,29	0
36	NA	0	8156	1/1	0.92	0.43	-	33,33,33,33	0
34	MG	0	8079	1/1	0.90	0.09	-	27,27,27,27	0
37	CL	O	203	1/1	0.85	0.16	-	56,56,56,56	0
36	NA	0	8122	1/1	0.98	0.25	-	16,16,16,16	0
34	MG	0	8025	1/1	0.98	0.08	-	25,25,25,25	0
34	MG	0	8067	1/1	0.98	0.12	-	33,33,33,33	0
34	MG	0	8051	1/1	0.97	0.07	-	32,32,32,32	0
34	MG	0	8092	1/1	0.94	0.21	-	25,25,25,25	0
34	MG	0	8058	1/1	0.95	0.09	-	18,18,18,18	0
34	MG	0	8091	1/1	0.92	0.12	-	20,20,20,20	0
34	MG	0	8016	1/1	0.97	0.12	-	20,20,20,20	0
34	MG	0	8201	1/1	0.89	0.25	-	42,42,42,42	0
34	MG	0	8024	1/1	0.99	0.23	-	17,17,17,17	0
34	MG	0	8075	1/1	0.94	0.14	-	28,28,28,28	0
34	MG	0	8071	1/1	0.93	0.06	-	37,37,37,37	0
36	NA	0	8161	1/1	0.94	0.26	-	29,29,29,29	0
34	MG	0	8068	1/1	0.81	0.08	-	34,34,34,34	0
37	CL	0	8183	1/1	0.99	0.10	-	25,25,25,25	0
34	MG	0	8097	1/1	0.94	0.12	-	34,34,34,34	0
34	MG	0	8104	1/1	0.92	0.12	-	26,26,26,26	0
34	MG	0	8077	1/1	0.96	0.11	-	24,24,24,24	0
34	MG	0	8084	1/1	0.74	0.30	-	37,37,37,37	0
37	CL	Y	302	1/1	0.98	0.12	-	26,26,26,26	0
34	MG	0	8073	1/1	0.96	0.20	-	10,10,10,10	0
36	NA	0	8145	1/1	0.97	0.09	-	31,31,31,31	0
36	NA	0	8133	1/1	0.99	0.20	-	28,28,28,28	0
34	MG	0	8081	1/1	0.96	0.14	-	42,42,42,42	0
36	NA	0	8152	1/1	0.98	0.21	-	17,17,17,17	0
37	CL	A	305	1/1	0.98	0.10	-	35,35,35,35	0
34	MG	0	8095	1/1	0.96	0.16	-	34,34,34,34	0
34	MG	0	8047	1/1	0.88	0.14	-	49,49,49,49	0
34	MG	9	201	1/1	0.97	0.07	-	54,54,54,54	0
36	NA	0	8168	1/1	0.89	0.30	-	43,43,43,43	0
35	K	O	204	1/1	0.92	0.18	-	77,77,77,77	0

6.5 Other polymers

There are no such residues in this entry.