



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 08:35 am BST

PDB ID : 6ZXH / pdb_00006zxh
EMDB ID : EMD-11521
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - State H2
Authors : Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.;
Kutay, U.; Beckmann, R.
Deposited on : 2020-07-29
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

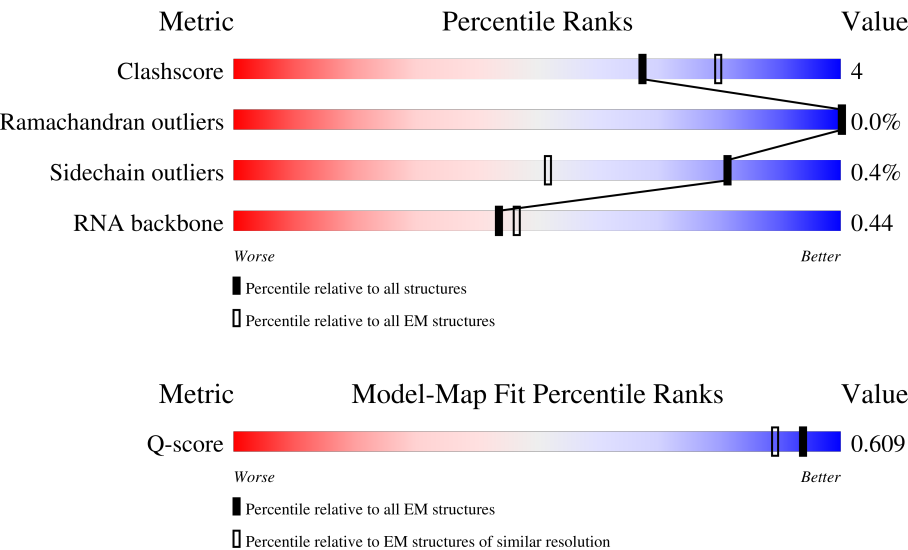
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1869	7% 57% 26% 12%
2	A	295	6% 65% 7% 27%
3	B	264	6% 71% 9% 20%

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Mol	Chain	Length	Quality of chain
4	C	293	
5	h	115	
6	E	263	
7	D	243	
8	G	249	
9	H	194	
10	I	208	
11	J	194	
12	F	204	
13	L	158	
14	K	165	
15	N	151	
16	O	151	
17	M	132	
18	P	145	
19	R	135	
20	Q	146	
21	S	152	
22	T	145	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	U	119	
28	Z	125	

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Mol	Chain	Length	Quality of chain
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	
34	g	317	
35	j	165	
36	z	568	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 76979 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1651	Total	C	N	O	P	0	0
			35310	15787	6344	11528	1651		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	216	Total	C	N	O	S	0	0
			1674	1085	287	292	10		

- Molecule 5 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	255	Total	C	N	O	S	0	0
			2031	1299	377	347	8		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	223	Total	C	N	O	S	0	0
			1802	1128	358	309	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	179	Total	C	N	O	S	0	0
			1446	927	264	254	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	199	Total	C	N	O	S	0	0
			1638	1027	322	284	5		

- Molecule 11 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	176	Total	C	N	O	S	0	0
			1465	934	295	234	2		

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	136	Total	C	N	O	S	0	0
			1127	719	212	190	6		

- Molecule 14 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	126	Total	C	N	O	S	0	0
			947	580	188	173	6		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

- Molecule 18 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	132	Total	C	N	O	S	0	0
			1077	685	202	183	7		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 21 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	141	Total	C	N	O	S	0	0
			1162	731	232	198	1		

- Molecule 22 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	122	Total	C	N	O	S	0	0
			987	624	193	165	5		

- Molecule 27 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	98	Total	C	N	O	S	0	0
			774	486	145	139	4		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	82	Total	C	N	O	S	0	0
			638	410	117	110	1		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	77	Total	C	N	O	S	0	0
			611	386	113	107	5		

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	54	Total	C	N	O	S	0	0
			450	282	93	70	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	50	Total	C	N	O	S	0	0
			398	244	90	63	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	295	Total	C	N	O	S	0	0
			2306	1460	403	431	12		

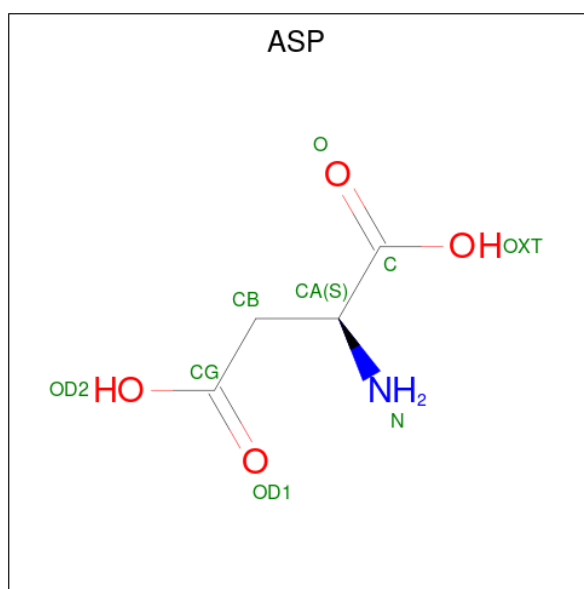
- Molecule 35 is a protein called Probable RNA-binding protein EIF1AD.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	116	Total	C	N	O	S	0	0
			934	593	167	172	2		

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	349	Total	C	N	O	S	0	0
			2803	1757	515	511	20		

- Molecule 37 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				AltConf
37	2	1	Total	C	N	O	0
			8	4	1	3	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	124	Total	Mg	0
			124	124	
38	h	1	Total	Mg	0
			1	1	
38	G	1	Total	Mg	0
			1	1	
38	F	1	Total	Mg	0
			1	1	

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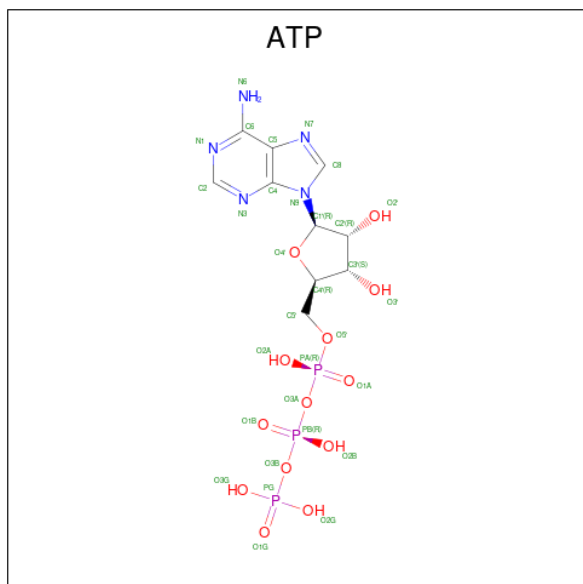
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Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Mg	0
			1	1	
38	d	1	Total	Mg	0
			1	1	
38	z	2	Total	Mg	0
			2	2	

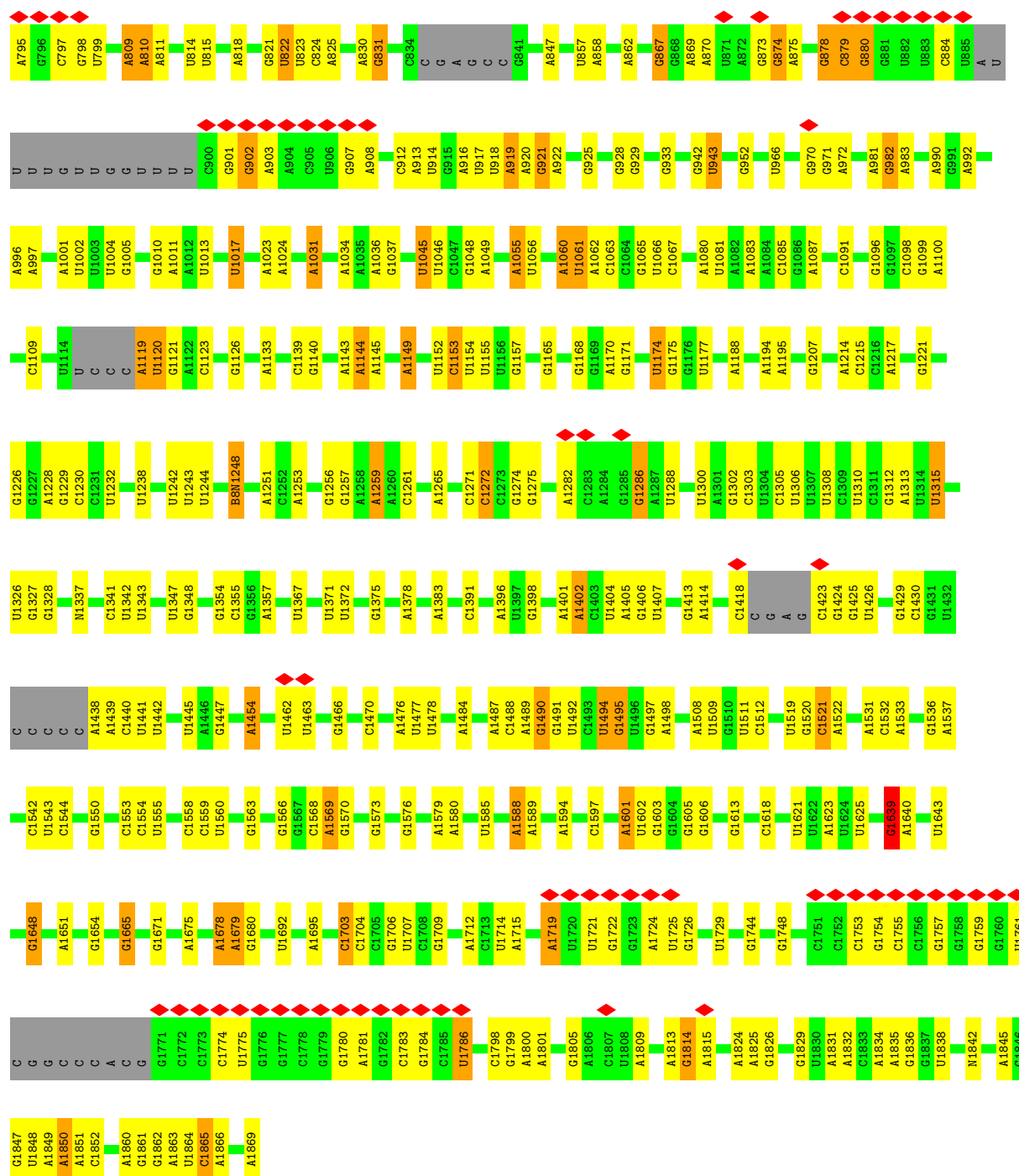
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	h	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

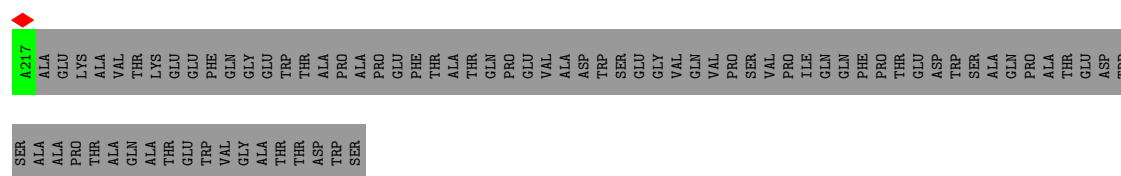


Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	N	O	P	0
			31	10	5	13	3	



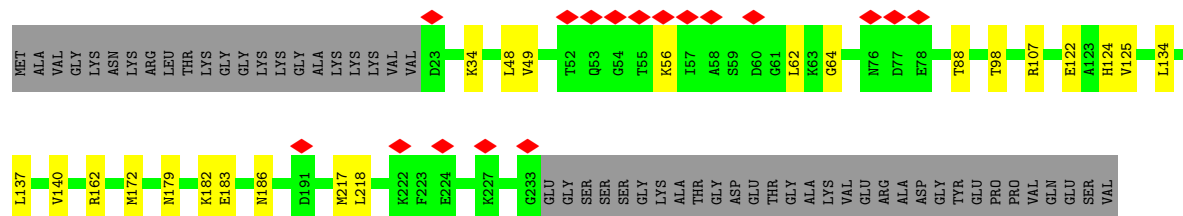
• Molecule 2: 40S ribosomal protein SA





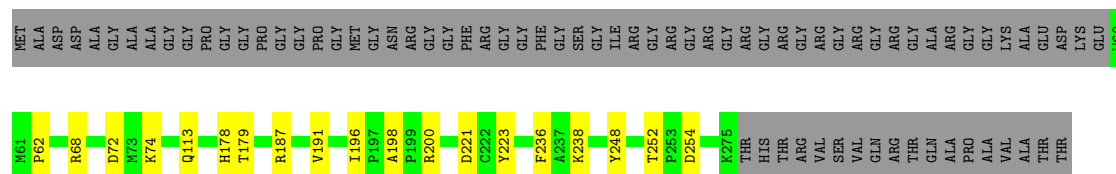
- Molecule 3: 40S ribosomal protein S3a

Chain B:



- Molecule 4: 40S ribosomal protein S2

Chain C:



- Molecule 5: 40S ribosomal protein S26

Chain h:



- Molecule 6: 40S ribosomal protein S4, X isoform

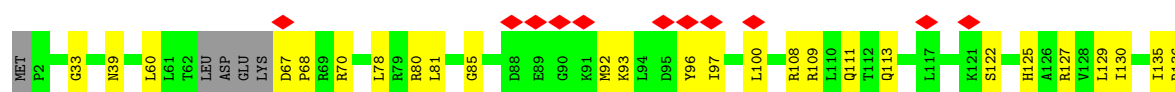
Chain E:

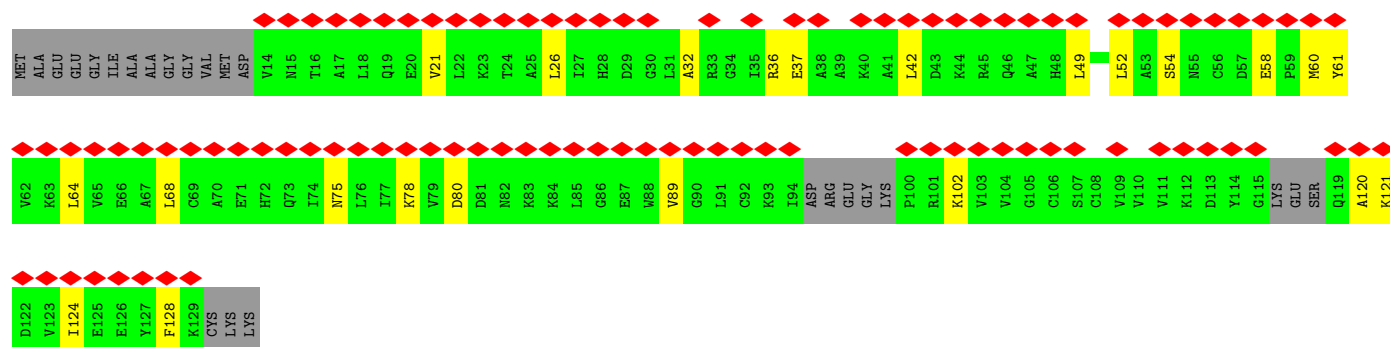


- Molecule 7: 40S ribosomal protein S3

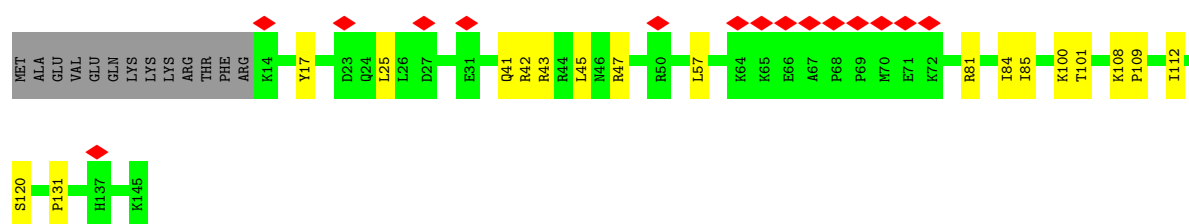
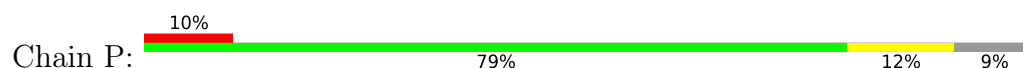
Chain D:



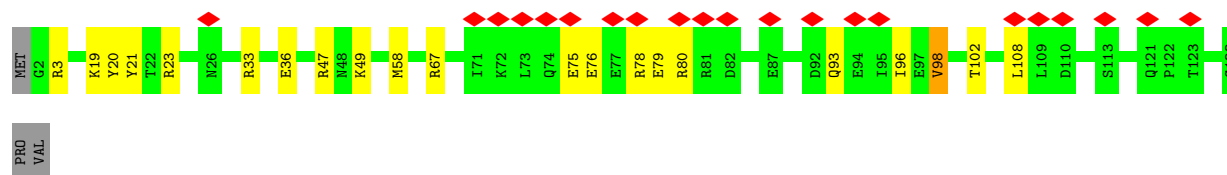
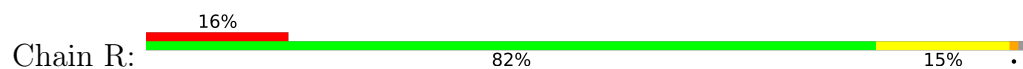




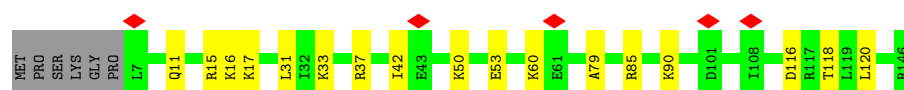
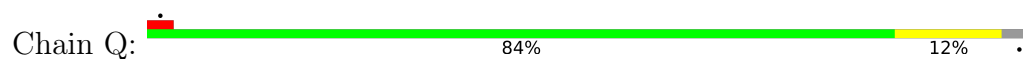
• Molecule 18: 40S ribosomal protein S15



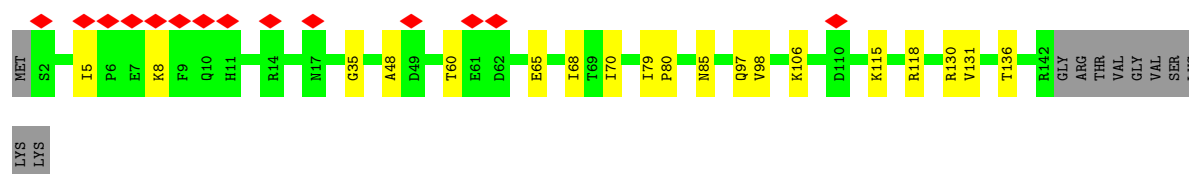
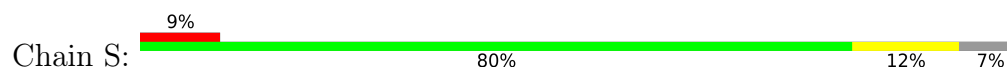
• Molecule 19: 40S ribosomal protein S17



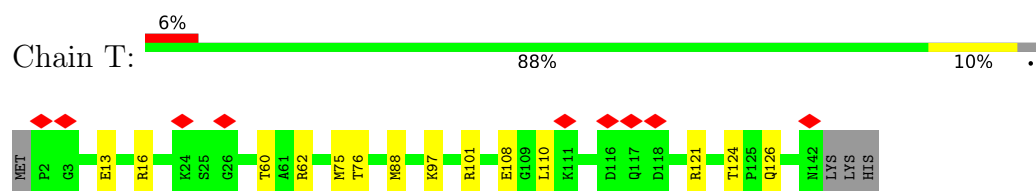
• Molecule 20: 40S ribosomal protein S16



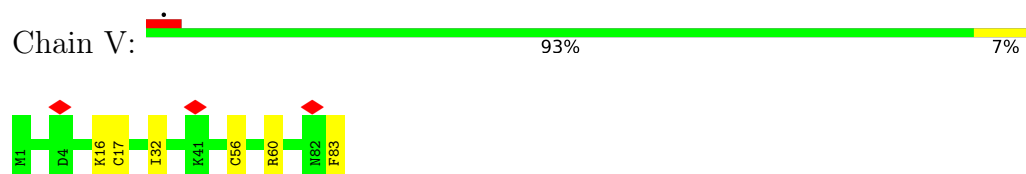
• Molecule 21: 40S ribosomal protein S18



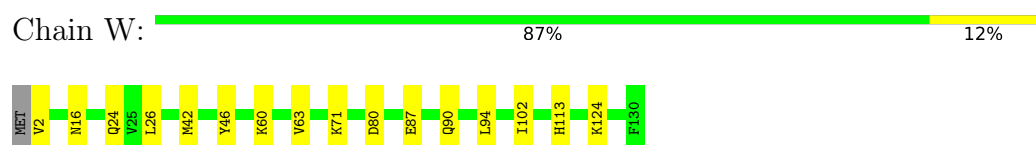
- Molecule 22: 40S ribosomal protein S19



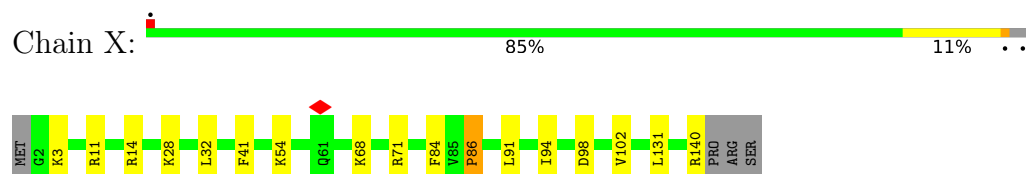
- Molecule 23: 40S ribosomal protein S21



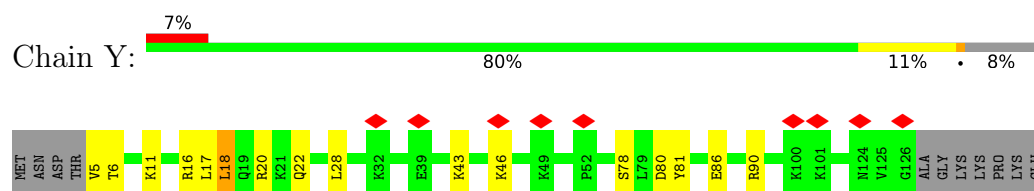
- Molecule 24: 40S ribosomal protein S15a



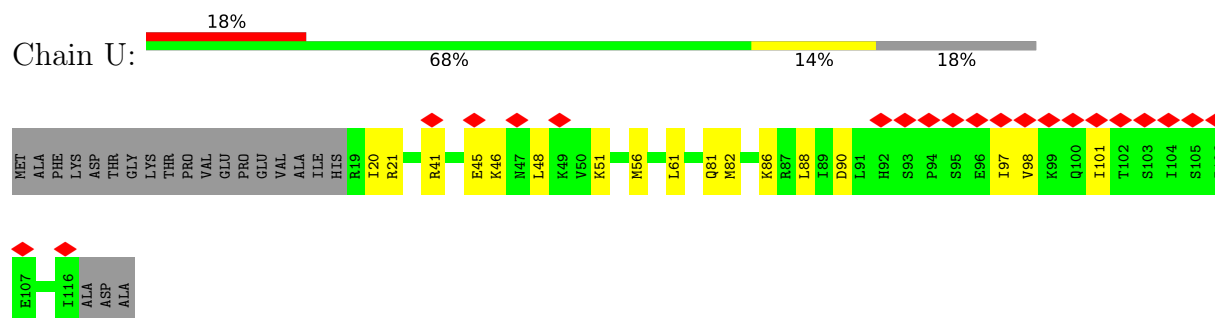
- Molecule 25: 40S ribosomal protein S23



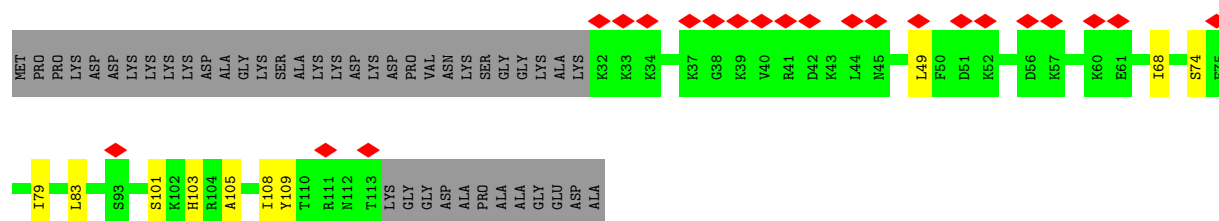
- Molecule 26: 40S ribosomal protein S24



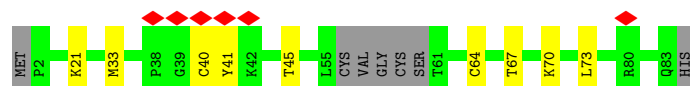
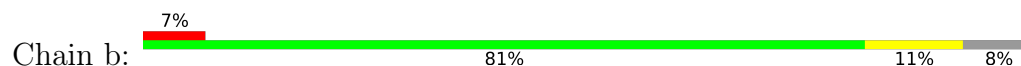
- Molecule 27: 40S ribosomal protein S20



- Molecule 28: 40S ribosomal protein S25



- Molecule 29: 40S ribosomal protein S27



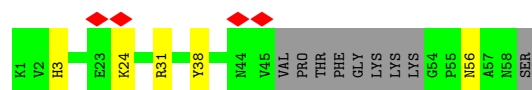
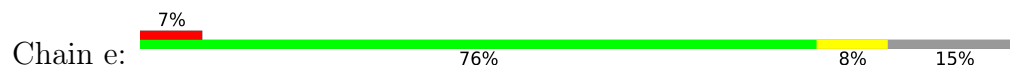
- Molecule 30: 40S ribosomal protein S28



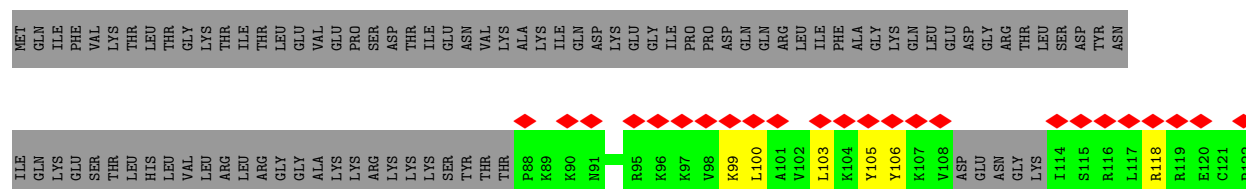
- Molecule 31: 40S ribosomal protein S29

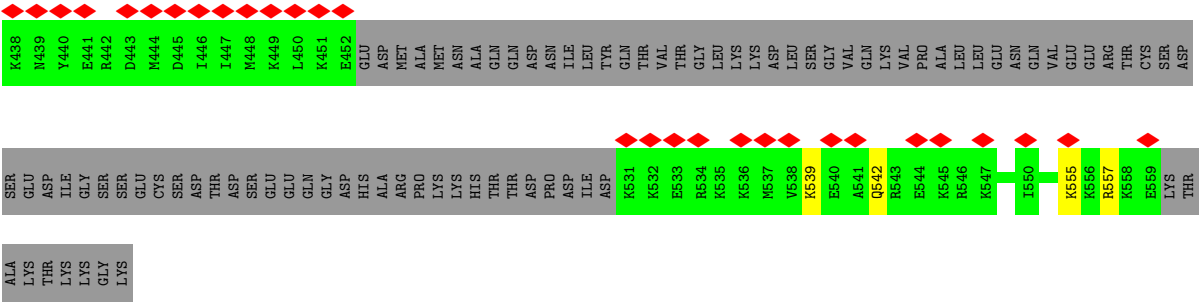


- Molecule 32: 40S ribosomal protein S30



- Molecule 33: Ubiquitin-40S ribosomal protein S27a





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.868	Depositor
Minimum map value	-0.424	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, PSU, B8N, MA6, OMC, 7MG, ATP, 4AC, OMG, ZN, OMU, MG, A2M

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	2	0.48	0/37709	0.62	31/58755 (0.1%)
2	A	0.39	0/1742	0.55	0/2367
3	B	0.34	0/1742	0.55	0/2330
4	C	0.42	0/1710	0.57	0/2310
5	h	0.45	0/805	0.60	0/1079
6	E	0.37	0/2073	0.53	0/2791
7	D	0.35	0/1773	0.57	0/2387
8	G	0.30	0/1825	0.55	0/2431
9	H	0.32	0/1466	0.55	0/1959
10	I	0.34	0/1666	0.57	0/2223
11	J	0.34	0/1489	0.59	0/1987
12	F	0.34	0/1481	0.59	0/1988
13	L	0.40	0/1147	0.51	0/1535
14	K	0.31	0/823	0.52	0/1111
15	N	0.36	0/1226	0.51	0/1649
16	O	0.38	0/959	0.56	0/1286
17	M	0.25	0/845	0.61	0/1134
18	P	0.33	0/1099	0.54	0/1471
19	R	0.33	0/1080	0.61	0/1449
20	Q	0.36	0/1133	0.58	0/1517
21	S	0.35	0/1180	0.63	0/1582
22	T	0.38	0/1113	0.55	0/1493
23	V	0.37	0/643	0.50	0/860
24	W	0.44	0/1051	0.62	2/1406 (0.1%)
25	X	0.42	0/1097	0.59	0/1464
26	Y	0.33	0/1004	0.54	0/1337
27	U	0.36	0/783	0.60	0/1052
28	Z	0.27	0/646	0.56	0/869
29	b	0.37	0/623	0.54	0/834
30	c	0.30	0/481	0.60	0/643
31	d	0.42	0/461	0.70	0/612
32	e	0.32	0/401	0.64	0/526

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.26	0/474	0.57	0/626
34	g	0.29	0/2360	0.63	1/3207 (0.0%)
35	j	0.29	0/952	0.55	0/1282
36	z	0.34	0/2848	0.59	0/3816
All	All	0.42	0/79910	0.60	34/115368 (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
16	O	0	2
20	Q	0	2
All	All	0	4

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	668	A2M	P-O3'-C3'	33.01	159.31	119.70
1	2	166	A2M	P-O3'-C3'	28.31	153.67	119.70
1	2	166	A2M	OP1-P-O3'	25.32	160.89	105.20
1	2	99	A2M	OP1-P-O3'	-24.29	51.77	105.20
1	2	1031	A2M	P-O3'-C3'	23.05	147.35	119.70
1	2	159	A2M	P-O3'-C3'	22.60	146.82	119.70
1	2	99	A2M	P-O3'-C3'	-20.91	94.60	119.70
1	2	1678	A2M	O3'-P-O5'	19.92	141.84	104.00
1	2	27	A2M	P-O3'-C3'	19.87	143.54	119.70
1	2	576	A2M	OP1-P-O3'	-19.52	62.26	105.20
1	2	1031	A2M	OP1-P-O3'	18.79	146.53	105.20
1	2	576	A2M	OP2-P-O3'	18.48	145.85	105.20
1	2	512	A2M	OP1-P-O3'	-18.09	65.41	105.20
1	2	166	A2M	OP2-P-O3'	-17.75	66.16	105.20
1	2	668	A2M	OP1-P-O3'	17.33	143.32	105.20
1	2	1031	A2M	OP2-P-O3'	-15.51	71.08	105.20
1	2	576	A2M	P-O3'-C3'	-12.56	104.62	119.70
1	2	668	A2M	OP2-P-O3'	-12.24	78.26	105.20
1	2	1678	A2M	OP1-P-O3'	-11.86	79.11	105.20
1	2	99	A2M	OP2-P-O3'	11.80	131.16	105.20
1	2	1383	A2M	P-O3'-C3'	11.24	133.18	119.70
1	2	512	A2M	OP2-P-O3'	11.06	129.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	27	A2M	OP1-P-O3'	10.89	129.16	105.20
1	2	166	A2M	O3'-P-O5'	-9.56	85.83	104.00
1	2	99	A2M	O3'-P-O5'	8.88	120.87	104.00
1	2	27	A2M	OP2-P-O3'	-8.56	86.36	105.20
1	2	512	A2M	O3'-P-O5'	7.44	118.14	104.00
1	2	484	A2M	P-O3'-C3'	6.27	127.22	119.70
24	W	46	TYR	CA-C-N	-6.11	116.68	123.16
24	W	46	TYR	C-N-CA	-6.11	116.68	123.16
1	2	484	A2M	OP1-P-O3'	5.99	118.38	105.20
34	g	249	CYS	CA-CB-SG	5.80	127.75	114.40
1	2	159	A2M	OP2-P-O3'	5.79	117.94	105.20
1	2	468	A2M	P-O3'-C3'	5.39	126.17	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	O	137	SER	Peptide
16	O	138	ASP	Peptide
20	Q	15	ARG	Peptide
20	Q	42	ILE	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	2	35310	0	17882	173	0
2	A	1705	0	1706	14	0
3	B	1715	0	1785	13	0
4	C	1674	0	1764	11	0
5	h	792	0	841	7	0
6	E	2031	0	2133	17	0
7	D	1745	0	1839	19	0
8	G	1802	0	1953	26	0
9	H	1446	0	1540	10	0
10	I	1638	0	1710	19	0
11	J	1465	0	1583	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	F	1461	0	1511	6	0
13	L	1127	0	1190	13	0
14	K	799	0	823	15	0
15	N	1202	0	1289	7	0
16	O	947	0	976	9	0
17	M	837	0	870	16	0
18	P	1077	0	1123	11	0
19	R	1066	0	1116	15	0
20	Q	1116	0	1185	10	0
21	S	1162	0	1215	12	0
22	T	1094	0	1120	11	0
23	V	636	0	637	4	0
24	W	1034	0	1080	11	0
25	X	1080	0	1147	13	0
26	Y	987	0	1038	11	0
27	U	774	0	839	13	0
28	Z	638	0	679	6	0
29	b	611	0	637	5	0
30	c	479	0	507	7	0
31	d	450	0	445	2	0
32	e	398	0	439	5	0
33	f	465	0	481	8	0
34	g	2306	0	2266	36	0
35	j	934	0	928	5	0
36	z	2803	0	2799	26	0
37	2	8	0	3	0	0
38	2	124	0	0	0	0
38	F	1	0	0	0	0
38	G	1	0	0	0	0
38	O	1	0	0	0	0
38	d	1	0	0	0	0
38	h	1	0	0	0	0
38	z	2	0	0	0	0
39	d	1	0	0	0	0
39	f	1	0	0	0	0
39	h	1	0	0	0	0
40	z	31	0	12	0	0
All	All	76979	0	61091	513	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 (513) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:878:G:H1	1:2:908:A:N6	1.65	0.95
1:2:878:G:H1	1:2:908:A:H61	0.87	0.76
1:2:1748:G:H1	1:2:1786:U:H3	1.33	0.73
1:2:952:G:H21	16:O:52:THR:HG21	1.55	0.71
11:J:113:GLN:HE21	11:J:154:GLN:HE22	1.39	0.70
3:B:107:ARG:NH1	16:O:133:THR:O	2.24	0.69
17:M:61:TYR:HB3	33:f:103:LEU:HD21	1.76	0.67
18:P:100:LYS:HG3	18:P:101:THR:HG23	1.76	0.66
18:P:81:ARG:NH2	18:P:120:SER:O	2.28	0.66
7:D:148:LYS:NZ	36:z:143:GLU:OE1	2.27	0.66
1:2:1719:A:N6	1:2:1814:G:O2'	2.30	0.65
1:2:1153:C:OP2	24:W:71:LYS:NZ	2.29	0.65
1:2:1170:A:OP2	36:z:557:ARG:NH1	2.29	0.65
3:B:122:GLU:HG2	3:B:140:VAL:HG12	1.79	0.65
8:G:154:ARG:HH21	8:G:179:LEU:HD21	1.61	0.65
1:2:1651:A:H1'	12:F:83:ASN:HD22	1.62	0.64
1:2:928:G:H1	1:2:1013:U:H3	1.45	0.64
1:2:167:G:H21	8:G:132:ARG:HD3	1.63	0.64
1:2:1639:7MG:H4'	36:z:363:ASN:HD21	1.62	0.64
2:A:128:ARG:NH2	2:A:151:ASP:O	2.30	0.64
13:L:20:LYS:O	13:L:22:ARG:NH1	2.31	0.64
8:G:69:THR:HG22	8:G:71:GLY:H	1.62	0.64
17:M:52:LEU:O	17:M:78:LYS:HA	1.98	0.63
11:J:93:LYS:HB2	11:J:96:TYR:HD2	1.62	0.63
1:2:563:G:N7	11:J:172:ARG:NH2	2.46	0.63
1:2:818:A:OP1	11:J:80:ARG:NH2	2.31	0.63
1:2:1847:G:O6	36:z:555:LYS:NZ	2.32	0.62
1:2:1566:G:N7	22:T:101:ARG:NH2	2.47	0.62
27:U:20:ILE:HG21	27:U:98:VAL:HG11	1.82	0.61
1:2:317:C:OP2	8:G:183:ARG:NH2	2.30	0.61
11:J:109:ARG:NH1	11:J:111:GLN:OE1	2.34	0.61
1:2:1678:A2M:H2'	1:2:1679:A:C8	2.36	0.61
8:G:44:GLU:HB2	8:G:119:LYS:HG2	1.83	0.61
1:2:925:G:H1	1:2:1017:U:H3	1.47	0.61
14:K:15:LEU:HD22	14:K:49:MET:HE1	1.84	0.60
9:H:53:VAL:HG11	9:H:172:THR:HA	1.84	0.60
36:z:210:TYR:OH	36:z:250:GLU:OE1	2.20	0.60
2:A:206:ASP:OD1	2:A:206:ASP:N	2.34	0.60
27:U:56:MET:HB2	27:U:86:LYS:HB3	1.84	0.60
1:2:1055:A:N1	1:2:1063:C:N4	2.49	0.60
27:U:61:LEU:O	27:U:81:GLN:HA	2.02	0.59
1:2:1228:A:H2'	1:2:1229:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:509:OMG:H5'	6:E:26:VAL:HG21	1.84	0.59
1:2:1091:C:HO2'	24:W:2:VAL:N	2.00	0.59
6:E:64:ILE:HD11	26:Y:18:LEU:HD22	1.84	0.59
1:2:1354:G:N2	1:2:1357:A:OP2	2.29	0.59
1:2:1259:A:N6	1:2:1519:U:OP1	2.34	0.59
11:J:81:LEU:HD13	11:J:97:ILE:HG12	1.85	0.59
34:g:68:ASP:HB3	34:g:111:VAL:HG22	1.83	0.59
25:X:28:LYS:HE2	25:X:32:LEU:HD22	1.85	0.59
33:f:99:LYS:HG2	33:f:100:LEU:HD12	1.85	0.59
34:g:255:SER:HB3	34:g:271:LYS:HE3	1.84	0.59
10:I:82:VAL:O	10:I:205:ARG:NH1	2.36	0.58
15:N:55:ARG:NH1	15:N:56:ASP:OD1	2.36	0.58
1:2:1310:U:OP2	17:M:36:ARG:NH2	2.36	0.58
1:2:640:A:H2'	1:2:641:A:C8	2.39	0.58
1:2:1143:A:OP2	4:C:187:ARG:NH2	2.36	0.58
22:T:60:THR:HG23	22:T:75:MET:HE2	1.84	0.58
7:D:75:LYS:NZ	14:K:34:GLU:OE1	2.36	0.58
24:W:102:ILE:H	24:W:113:HIS:HD2	1.50	0.58
36:z:129:ASP:O	36:z:133:ASN:ND2	2.36	0.57
1:2:1024:A:OP2	15:N:124:ARG:NH2	2.32	0.57
7:D:224:SER:OG	7:D:225:GLU:N	2.36	0.57
1:2:1729:U:O2	1:2:1805:G:O6	2.21	0.57
11:J:85:GLY:HA3	11:J:108:ARG:HE	1.69	0.57
19:R:75:GLU:OE1	19:R:78:ARG:NH2	2.37	0.57
34:g:133:ASN:HB3	34:g:139:LYS:HE2	1.85	0.57
1:2:878:G:N2	1:2:908:A:N1	2.40	0.57
34:g:174:VAL:HB	34:g:188:HIS:HB2	1.86	0.57
7:D:172:VAL:HG22	7:D:185:LYS:HG2	1.86	0.57
25:X:54:LYS:NZ	25:X:91:LEU:O	2.37	0.57
1:2:11:A:H5'	4:C:113:GLN:HE21	1.71	0.56
1:2:1230:C:OP1	21:S:130:ARG:NH2	2.39	0.56
4:C:196:ILE:HB	4:C:223:TYR:HB2	1.87	0.56
5:h:44:ILE:O	16:O:113:GLN:NE2	2.30	0.56
4:C:178:HIS:CE1	4:C:200:ARG:HG2	2.41	0.56
11:J:137:VAL:HG22	11:J:157:ILE:HG12	1.88	0.56
20:Q:90:LYS:HG2	20:Q:120:LEU:HD23	1.88	0.56
1:2:527:C:OP1	11:J:122:SER:OG	2.19	0.56
6:E:49:ARG:HH21	6:E:50:ASN:HD21	1.55	0.55
7:D:113:LEU:HD22	7:D:118:ALA:HB2	1.88	0.55
1:2:1639:7MG:H2'	1:2:1640:A:C8	2.40	0.55
36:z:403:MET:O	36:z:407:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:5:ILE:HG23	28:Z:49:LEU:HB2	1.87	0.55
1:2:1563:G:OP1	22:T:121:ARG:NH1	2.38	0.55
22:T:13:GLU:HA	22:T:16:ARG:HH11	1.72	0.54
13:L:75:GLY:HA3	13:L:88:ILE:HD12	1.89	0.54
35:j:51:VAL:HG12	35:j:82:ALA:HB3	1.90	0.54
1:2:1470:C:OP2	12:F:59:LYS:NZ	2.38	0.54
1:2:1454:A:OP1	19:R:49:LYS:NZ	2.40	0.54
1:2:17:C:O2'	1:2:1194:A:N1	2.40	0.54
7:D:32:ASP:OD2	7:D:65:ARG:NH1	2.41	0.54
33:f:105:TYR:HE1	33:f:118:ARG:HB2	1.72	0.54
8:G:162:LEU:HD11	8:G:172:LYS:HG3	1.89	0.54
9:H:60:ILE:HB	9:H:92:VAL:HG12	1.89	0.54
9:H:138:GLU:OE1	15:N:19:ARG:NH1	2.33	0.54
1:2:1005:G:OP2	3:B:162:ARG:NH2	2.41	0.54
1:2:943:U:O2'	16:O:135:ILE:O	2.23	0.53
8:G:142:ARG:HG2	8:G:147:LEU:HB2	1.90	0.53
1:2:996:A:H2'	1:2:997:A:C8	2.44	0.53
11:J:111:GLN:HE21	11:J:127:ARG:HB2	1.73	0.53
1:2:449:A:OP1	10:I:23:LYS:NZ	2.30	0.53
4:C:252:THR:OG1	4:C:254:ASP:OD1	2.22	0.53
6:E:160:ILE:HG23	6:E:169:ILE:HG23	1.89	0.53
26:Y:5:VAL:N	26:Y:28:LEU:O	2.42	0.53
1:2:594:A:H61	1:2:643:A:H5''	1.72	0.53
34:g:212:LYS:HA	34:g:235:ILE:HG13	1.90	0.53
1:2:380:G:OP1	10:I:31:ARG:NH1	2.37	0.53
3:B:34:LYS:O	3:B:98:THR:OG1	2.25	0.53
30:c:40:ARG:HH22	30:c:62:GLU:HA	1.73	0.53
17:M:49:LEU:HD22	17:M:124:ILE:HD12	1.90	0.52
14:K:52:LEU:HD23	14:K:55:ARG:HH21	1.75	0.52
1:2:1060:A:H4'	1:2:1061:U:H5'	1.92	0.52
3:B:64:GLY:H	3:B:88:THR:HG23	1.75	0.52
18:P:108:LYS:HG2	18:P:109:PRO:HD2	1.91	0.52
30:c:36:ASP:OD1	30:c:38:THR:OG1	2.20	0.52
6:E:54:TYR:OH	6:E:97:GLU:OE2	2.22	0.52
14:K:29:MET:HB3	14:K:42:ASN:HB2	1.91	0.52
1:2:145:G:O6	8:G:178:ARG:NH2	2.43	0.52
11:J:97:ILE:HA	11:J:100:LEU:HD23	1.92	0.52
1:2:1588:A:H2'	1:2:1589:A:C8	2.45	0.52
2:A:76:VAL:HG12	2:A:123:VAL:HB	1.92	0.51
1:2:1407:U:H3	1:2:1439:A:H62	1.58	0.51
6:E:152:PRO:HD2	8:G:216:ARG:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:76:VAL:HG12	13:L:125:ILE:HG13	1.92	0.51
28:Z:68:ILE:HB	28:Z:109:TYR:HB2	1.91	0.51
1:2:637:U:O2	32:e:56:ASN:ND2	2.40	0.51
25:X:68:LYS:HB3	25:X:91:LEU:HD22	1.93	0.51
30:c:34:PHE:HB2	30:c:38:THR:HB	1.93	0.51
1:2:1550:G:H3'	1:2:1579:A:H61	1.76	0.51
10:I:84:ASN:HD22	10:I:87:ASN:H	1.58	0.51
7:D:158:ILE:HG12	7:D:189:MET:HE3	1.91	0.51
21:S:65:GLU:HA	21:S:68:ILE:HG12	1.92	0.51
25:X:54:LYS:NZ	25:X:94:ILE:O	2.40	0.51
34:g:302:TYR:HE2	34:g:308:ARG:HB2	1.76	0.51
1:2:857:U:H2'	1:2:858:A:C8	2.45	0.51
24:W:80:ASP:OD1	24:W:124:LYS:NZ	2.43	0.51
1:2:525:A:O3'	32:e:31:ARG:NH2	2.44	0.51
1:2:1512:C:O2'	31:d:7:TYR:O	2.20	0.51
4:C:62:PRO:HG2	4:C:68:ARG:HG3	1.91	0.51
8:G:82:SER:O	8:G:82:SER:OG	2.29	0.51
2:A:6:ASP:HA	2:A:9:GLN:HG2	1.93	0.51
27:U:51:LYS:HB2	27:U:90:ASP:HB2	1.93	0.51
34:g:87:LEU:HB2	34:g:101:PHE:HB2	1.93	0.51
8:G:194:LEU:HD23	8:G:197:GLN:HE21	1.76	0.51
18:P:41:GLN:HG3	18:P:84:ILE:HD13	1.92	0.51
14:K:90:VAL:HG23	14:K:95:ARG:HH11	1.76	0.50
17:M:42:LEU:HD13	17:M:68:LEU:HB3	1.92	0.50
1:2:526:A:O2'	11:J:125:HIS:ND1	2.31	0.50
1:2:634:A:H2'	1:2:635:G:C8	2.46	0.50
1:2:874:G:H2'	1:2:875:A:H8	1.77	0.50
23:V:32:ILE:HG12	23:V:60:ARG:HD2	1.92	0.50
1:2:1261:C:O2	31:d:10:HIS:NE2	2.36	0.50
4:C:179:THR:HG22	4:C:221:ASP:HB2	1.94	0.50
17:M:54:SER:HB3	17:M:80:ASP:HA	1.93	0.50
1:2:1139:C:H5	1:2:1149:A:H62	1.60	0.50
1:2:792:C:H2'	1:2:793:G:C8	2.47	0.50
1:2:1282:A:OP2	17:M:102:LYS:NZ	2.40	0.50
1:2:1286:G:N2	1:2:1312:G:O2'	2.45	0.50
6:E:102:ILE:HD12	6:E:239:PRO:HD3	1.93	0.50
36:z:261:GLU:O	36:z:313:ARG:NH2	2.45	0.50
8:G:159:ARG:NH1	8:G:171:THR:OG1	2.43	0.50
8:G:50:VAL:HG12	8:G:113:ILE:HD13	1.93	0.50
11:J:33:GLY:HA3	32:e:38:TYR:CG	2.47	0.50
1:2:493:A:H1'	1:2:574:A:H5''	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:634:A:H2'	1:2:635:G:H8	1.76	0.50
34:g:168:CYS:HB3	34:g:198:VAL:HG13	1.93	0.50
19:R:93:GLN:HE21	19:R:96:ILE:HG12	1.77	0.49
26:Y:86:GLU:OE2	26:Y:90:ARG:NH1	2.38	0.49
1:2:1532:C:O2'	1:2:1601:A:N1	2.44	0.49
8:G:136:LYS:NZ	8:G:175:LYS:O	2.42	0.49
5:h:24:THR:HG21	5:h:71:LEU:HD22	1.95	0.49
1:2:1315:U:H4'	14:K:2:LEU:HG	1.94	0.49
7:D:109:LEU:HD12	7:D:184:ILE:HD11	1.95	0.49
18:P:131:PRO:HB2	36:z:184:GLY:HA3	1.93	0.49
19:R:36:GLU:HB3	19:R:47:ARG:HD2	1.93	0.49
25:X:98:ASP:OD1	25:X:140:ARG:NH2	2.46	0.49
1:2:584:A:OP1	11:J:169:ARG:NH2	2.46	0.49
1:2:1714:U:OP1	25:X:71:ARG:NH1	2.46	0.49
8:G:85:ARG:O	8:G:87:ARG:NH1	2.46	0.49
8:G:26:THR:HG21	8:G:40:ALA:HB3	1.95	0.49
1:2:1798:C:H2'	1:2:1799:G:O4'	2.13	0.48
20:Q:16:LYS:HD3	20:Q:79:ALA:HA	1.95	0.48
26:Y:20:ARG:HE	26:Y:22:GLN:HE21	1.60	0.48
27:U:20:ILE:HG13	27:U:98:VAL:HG21	1.94	0.48
34:g:72:SER:OG	34:g:73:SER:N	2.45	0.48
1:2:544:G:H2'	1:2:545:A:H8	1.78	0.48
9:H:170:VAL:O	9:H:173:PHE:HB2	2.13	0.48
36:z:190:LYS:HD2	36:z:217:PHE:HB2	1.94	0.48
1:2:902:G:H2'	1:2:903:A:H8	1.77	0.48
6:E:153:LEU:HD13	8:G:216:ARG:HD2	1.96	0.48
9:H:51:ILE:HG21	9:H:179:LYS:HG2	1.94	0.48
20:Q:31:LEU:HD13	20:Q:33:LYS:HG2	1.95	0.48
1:2:1413:G:H2'	1:2:1414:A:H8	1.77	0.48
21:S:98:VAL:HG11	21:S:106:LYS:HG3	1.95	0.48
34:g:176:VAL:HB	34:g:186:THR:HG22	1.95	0.48
1:2:116:OMU:H6	1:2:116:OMU:O5'	2.14	0.48
1:2:554:A:H4'	1:2:555:A:C5	2.48	0.48
1:2:1536:G:H2'	1:2:1537:A:C8	2.48	0.48
6:E:95:THR:HG22	26:Y:16:ARG:HB2	1.94	0.48
36:z:379:ARG:O	36:z:383:GLU:HG2	2.13	0.48
6:E:64:ILE:HD12	26:Y:17:LEU:HB3	1.96	0.48
15:N:87:ASP:OD1	15:N:87:ASP:N	2.43	0.48
3:B:179:ASN:HB3	3:B:183:GLU:HB2	1.95	0.48
26:Y:43:LYS:HA	26:Y:46:LYS:HE3	1.95	0.48
29:b:67:THR:OG1	29:b:70:LYS:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:z:312:ARG:NH1	36:z:384:PHE:O	2.43	0.48
1:2:1226:G:N1	1:2:1639:7MG:OP2	2.46	0.48
1:2:429:C:OP1	6:E:10:LYS:NZ	2.39	0.47
1:2:1098:C:H2'	1:2:1099:G:C8	2.48	0.47
4:C:191:VAL:HG11	4:C:236:PHE:HA	1.95	0.47
24:W:102:ILE:H	24:W:113:HIS:CD2	2.30	0.47
13:L:104:LYS:O	25:X:11:ARG:NH2	2.47	0.47
1:2:318:A:H61	8:G:186:GLN:HE22	1.62	0.47
1:2:1010:G:H2'	1:2:1011:A:C8	2.50	0.47
3:B:124:HIS:HA	3:B:137:LEU:O	2.14	0.47
1:2:1454:A:H5''	19:R:3:ARG:HD3	1.97	0.47
11:J:136:ARG:NE	11:J:159:PHE:O	2.41	0.47
16:O:67:ASP:O	16:O:70:SER:OG	2.28	0.47
17:M:60:MET:HB2	33:f:103:LEU:HD13	1.96	0.47
34:g:35:SER:OG	34:g:36:ARG:N	2.47	0.47
1:2:617:G:OP2	25:X:68:LYS:NZ	2.47	0.47
1:2:1152:U:O2'	24:W:16:ASN:ND2	2.40	0.47
1:2:1597:C:H4'	1:2:1603:G:C6	2.50	0.47
10:I:4:SER:HB2	10:I:24:LYS:HD3	1.96	0.47
34:g:227:LEU:HD12	34:g:228:TYR:HB2	1.96	0.47
1:2:532:C:H2'	1:2:533:A:C8	2.50	0.47
1:2:562:U:H2'	1:2:563:G:C8	2.50	0.47
1:2:919:A:OP2	15:N:64:ARG:NH1	2.47	0.47
10:I:11:ARG:NH1	10:I:15:GLY:O	2.46	0.47
1:2:1272:OMC:HM23	1:2:1272:OMC:H1'	1.63	0.47
1:2:1568:C:H2'	1:2:1569:A:C8	2.50	0.47
1:2:981:A:H2'	1:2:982:G:C8	2.50	0.47
1:2:1866:A:N6	5:h:84:VAL:HG22	2.29	0.47
12:F:195:GLU:HG3	36:z:423:GLU:HG2	1.97	0.47
34:g:172:LYS:HD3	34:g:193:GLY:H	1.80	0.47
20:Q:53:GLU:OE1	20:Q:85:ARG:NH2	2.42	0.46
34:g:73:SER:OG	34:g:117:ASN:ND2	2.49	0.46
1:2:101:U:H5''	10:I:19:LYS:HD2	1.96	0.46
1:2:164:A:H3'	1:2:165:G:H21	1.80	0.46
1:2:867:OMG:H1'	1:2:867:OMG:HM23	1.68	0.46
1:2:1543:U:P	22:T:62:ARG:HH22	2.39	0.46
7:D:64:ARG:O	7:D:67:ARG:HB2	2.14	0.46
11:J:172:ARG:O	11:J:176:LYS:HB2	2.14	0.46
21:S:8:LYS:HE2	21:S:60:THR:HG22	1.97	0.46
6:E:154:ILE:HG21	6:E:160:ILE:HD11	1.97	0.46
35:j:11:VAL:HA	35:j:14:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:8:LYS:HG2	27:U:61:LEU:HD21	1.98	0.46
9:H:80:VAL:HG22	9:H:92:VAL:HG23	1.98	0.46
1:2:63:U:O2'	1:2:170:A:N3	2.40	0.46
1:2:1703:OMC:H2'	1:2:1704:C:O4'	2.15	0.46
11:J:60:LEU:HD22	11:J:70:ARG:HA	1.97	0.46
20:Q:116:ASP:OD2	20:Q:118:THR:OG1	2.33	0.46
35:j:31:LEU:HD11	35:j:42:GLU:HB2	1.97	0.46
2:A:182:VAL:O	2:A:186:ARG:HB2	2.14	0.46
30:c:10:LYS:HE3	30:c:10:LYS:HB2	1.78	0.46
34:g:29:ASP:HA	34:g:45:LEU:HB2	1.97	0.46
2:A:80:ARG:NH2	2:A:165:ASN:O	2.35	0.46
25:X:84:PHE:CE2	25:X:86:PRO:HA	2.51	0.46
36:z:137:GLU:OE1	36:z:140:ARG:NH2	2.40	0.46
1:2:367:U:H4'	1:2:371:A:C8	2.50	0.46
1:2:643:A:OP1	11:J:39:ASN:ND2	2.49	0.46
3:B:134:LEU:HG	3:B:218:LEU:HD12	1.97	0.46
5:h:60:ASP:N	5:h:60:ASP:OD1	2.45	0.46
14:K:53:LYS:HG3	14:K:60:GLU:HB2	1.98	0.46
16:O:59:GLY:HA2	16:O:68:GLU:HG2	1.98	0.46
24:W:42:MET:HB3	24:W:42:MET:HE2	1.78	0.46
1:2:942:G:H2'	1:2:943:U:C6	2.50	0.46
1:2:952:G:OP1	3:B:56:LYS:NZ	2.49	0.46
2:A:39:TYR:HE1	19:R:108:LEU:HD21	1.80	0.46
34:g:191:HIS:CG	34:g:195:LEU:HD21	2.50	0.46
1:2:385:G:H3'	13:L:136:LYS:HB2	1.99	0.45
3:B:49:VAL:HB	3:B:62:LEU:HD13	1.98	0.45
3:B:182:LYS:O	3:B:186:ASN:ND2	2.50	0.45
4:C:179:THR:HG21	4:C:198:ALA:O	2.16	0.45
21:S:48:ALA:HB2	21:S:70:ILE:HD12	1.97	0.45
27:U:61:LEU:HD12	27:U:82:MET:HE2	1.97	0.45
1:2:527:C:H2'	1:2:528:A:C8	2.52	0.45
1:2:907:G:H2'	1:2:908:A:C8	2.51	0.45
6:E:154:ILE:HD13	6:E:160:ILE:HD11	1.97	0.45
10:I:3:ILE:O	10:I:30:GLY:N	2.47	0.45
13:L:33:LEU:HD12	13:L:34:PRO:HD2	1.98	0.45
36:z:305:LEU:HD11	36:z:399:LEU:HD13	1.98	0.45
36:z:350:HIS:HB3	36:z:353:ALA:HB2	1.97	0.45
2:A:200:ASP:N	2:A:200:ASP:OD1	2.50	0.45
1:2:1315:U:OP1	14:K:1:MET:N	2.35	0.45
1:2:1639:7MG:H4'	36:z:363:ASN:ND2	2.29	0.45
5:h:23:CYS:O	16:O:142:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:91:HIS:HD2	9:H:172:THR:HG21	1.82	0.45
19:R:76:GLU:O	19:R:80:ARG:HB2	2.17	0.45
27:U:97:ILE:O	27:U:101:ILE:HG12	2.16	0.45
1:2:1542:C:OP1	22:T:62:ARG:NH1	2.50	0.45
6:E:124:CYS:HA	6:E:142:HIS:CE1	2.52	0.45
14:K:32:HIS:CD2	14:K:34:GLU:H	2.34	0.45
1:2:636:C:OP1	32:e:24:LYS:NZ	2.49	0.45
1:2:1648:G:N7	20:Q:17:LYS:HE2	2.32	0.45
9:H:63:PHE:HA	9:H:95:ILE:O	2.17	0.45
16:O:96:LYS:HD2	16:O:132:VAL:HG11	1.99	0.45
19:R:98:VAL:HG22	19:R:102:THR:HB	1.99	0.45
21:S:35:GLY:O	21:S:97:GLN:NE2	2.42	0.45
29:b:40:CYS:SG	29:b:41:TYR:N	2.90	0.45
1:2:563:G:H2'	1:2:564:A:H8	1.81	0.45
1:2:1407:U:O2'	20:Q:11:GLN:NE2	2.34	0.45
6:E:46:ILE:HA	6:E:50:ASN:HD22	1.82	0.45
36:z:186:ILE:HD11	36:z:196:HIS:HB2	1.99	0.45
1:2:1144:A:H2'	1:2:1145:A:C8	2.52	0.44
13:L:114:SER:OG	13:L:116:CYS:SG	2.73	0.44
27:U:46:LYS:HB2	27:U:48:LEU:HG	1.99	0.44
34:g:107:ASP:OD2	34:g:125:ARG:NH1	2.48	0.44
10:I:13:LYS:HE3	13:L:137:THR:HG21	2.00	0.44
24:W:87:GLU:HA	24:W:90:GLN:HG2	2.00	0.44
1:2:203:G:N2	1:2:204:G:N7	2.66	0.44
1:2:1396:A:O2'	1:2:1398:G:N7	2.46	0.44
3:B:125:VAL:HG22	3:B:172:MET:HE3	2.00	0.44
3:B:217:MET:HE2	3:B:217:MET:HB2	1.87	0.44
6:E:71:LYS:HB2	6:E:91:SER:HB2	1.99	0.44
1:2:115:U:O2'	1:2:381:C:O2	2.29	0.44
1:2:1494:U:H4'	1:2:1495:G:H5''	1.98	0.44
34:g:30:MET:HA	34:g:43:TRP:O	2.18	0.44
36:z:399:LEU:O	36:z:403:MET:HB2	2.18	0.44
36:z:539:LYS:HD2	36:z:542:GLN:HE21	1.81	0.44
1:2:532:C:H2'	1:2:533:A:H8	1.83	0.44
8:G:37:ALA:HA	8:G:49:VAL:HG22	1.99	0.44
26:Y:6:THR:HG23	26:Y:28:LEU:HB2	2.00	0.44
34:g:289:LEU:HD22	34:g:298:LEU:HD11	1.98	0.44
1:2:1406:G:H2'	1:2:1407:U:C6	2.53	0.44
5:h:44:ILE:HG12	5:h:67:LEU:HG	1.99	0.44
14:K:19:GLY:HA2	14:K:71:LEU:HD12	1.99	0.44
14:K:47:LYS:HA	14:K:47:LYS:HD3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:43:ARG:O	18:P:47:ARG:HG2	2.18	0.44
28:Z:79:ILE:HB	28:Z:83:LEU:HD23	1.99	0.44
1:2:1543:U:OP1	20:Q:37:ARG:NH2	2.42	0.44
11:J:163:SER:O	11:J:167:GLY:N	2.50	0.44
13:L:144:LYS:HB3	13:L:144:LYS:HE2	1.84	0.44
25:X:11:ARG:HA	25:X:14:ARG:HG2	2.00	0.44
1:2:928:G:H2'	1:2:929:G:C8	2.53	0.44
7:D:66:ILE:HA	7:D:69:LEU:HD12	2.00	0.44
10:I:4:SER:OG	10:I:6:ASP:OD2	2.35	0.44
11:J:78:LEU:HD22	11:J:92:MET:HA	2.00	0.44
22:T:76:THR:HG21	22:T:97:LYS:HG2	2.00	0.44
34:g:295:GLY:N	34:g:296:GLN:OE1	2.51	0.44
14:K:38:LYS:HB2	14:K:40:VAL:HG23	2.00	0.44
17:M:32:ALA:HB1	17:M:37:GLU:HB3	1.98	0.44
19:R:21:TYR:CD1	19:R:58:MET:HE1	2.52	0.44
36:z:254:LEU:HD23	36:z:254:LEU:HA	1.86	0.44
1:2:545:A:H2'	1:2:546:G:C8	2.53	0.43
8:G:56:ASN:HB2	8:G:108:VAL:HG12	1.99	0.43
36:z:369:MET:HE3	36:z:369:MET:HB3	1.80	0.43
1:2:809:A:H2'	1:2:810:A:O4'	2.18	0.43
1:2:1404:U:C5	27:U:88:LEU:HD21	2.53	0.43
1:2:115:U:H2'	1:2:116:OMU:C6	2.48	0.43
1:2:145:G:H2'	1:2:146:G:C8	2.53	0.43
1:2:1554:C:H3'	1:2:1555:U:H2'	2.00	0.43
2:A:134:LEU:HD22	2:A:144:THR:HG21	2.00	0.43
7:D:225:GLU:HB2	34:g:187:ASN:HB2	2.00	0.43
8:G:58:LYS:HA	8:G:107:SER:HB2	1.99	0.43
34:g:101:PHE:CD2	34:g:136:GLY:HA2	2.53	0.43
34:g:256:ILE:HB	34:g:270:LEU:HB2	2.01	0.43
34:g:164:ILE:HD11	34:g:221:LEU:HD13	2.01	0.43
1:2:121:OMU:HM22	1:2:122:G:O4'	2.18	0.43
2:A:190:SER:OG	2:A:192:GLU:OE1	2.36	0.43
8:G:200:LYS:O	8:G:204:GLU:HG2	2.19	0.43
17:M:58:GLU:HB2	17:M:61:TYR:HE1	1.84	0.43
18:P:17:TYR:HB3	18:P:25:LEU:HD11	2.01	0.43
36:z:319:ARG:HA	36:z:319:ARG:HD3	1.79	0.43
8:G:164:LYS:HE2	8:G:164:LYS:HB3	1.89	0.43
12:F:28:VAL:O	12:F:42:LYS:NZ	2.41	0.43
14:K:15:LEU:HD23	14:K:79:LEU:HD11	2.00	0.43
17:M:75:ASN:HB3	17:M:128:PHE:CZ	2.54	0.43
30:c:44:ARG:HA	30:c:65:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:918:U:O3'	15:N:20:ARG:NH2	2.51	0.43
16:O:34:PHE:HB3	16:O:41:PHE:HB2	2.01	0.43
2:A:53:ARG:HE	23:V:83:PHE:C	2.27	0.43
13:L:111:VAL:HG12	13:L:140:PHE:HB2	2.01	0.43
34:g:47:ARG:NH1	34:g:52:TYR:OH	2.51	0.43
10:I:160:SER:HA	10:I:163:GLU:HG2	2.01	0.43
11:J:130:ILE:HG12	11:J:135:ILE:HG13	2.01	0.43
11:J:153:SER:O	11:J:153:SER:OG	2.35	0.43
17:M:121:LYS:HA	17:M:124:ILE:HG12	2.00	0.43
25:X:41:PHE:HZ	25:X:102:VAL:HG12	1.83	0.43
33:f:135:HIS:HE1	33:f:140:TYR:HD2	1.66	0.43
34:g:254:PRO:HB2	34:g:271:LYS:HE2	2.00	0.43
1:2:520:A:O2'	1:2:825:A:N3	2.51	0.42
1:2:588:G:OP2	1:2:588:G:N2	2.37	0.42
10:I:119:LEU:HD21	10:I:153:LYS:HE3	2.00	0.42
1:2:750:C:H2'	1:2:751:G:C8	2.54	0.42
1:2:792:C:H2'	1:2:793:G:H8	1.82	0.42
10:I:76:THR:HG22	10:I:108:PRO:HG2	2.01	0.42
21:S:85:ASN:HB2	21:S:97:GLN:CD	2.44	0.42
1:2:1375:G:H5'	19:R:67:ARG:HH12	1.85	0.42
1:2:1521:C:OP2	21:S:136:THR:OG1	2.25	0.42
7:D:225:GLU:O	34:g:186:THR:OG1	2.31	0.42
1:2:831:G:O6	26:Y:11:LYS:NZ	2.44	0.42
11:J:170:PRO:HB2	11:J:174:LYS:HB2	2.02	0.42
10:I:143:LYS:NZ	10:I:147:LYS:HE3	2.35	0.42
12:F:103:LEU:HD23	12:F:103:LEU:HA	1.88	0.42
13:L:93:LEU:HD23	13:L:104:LYS:HG3	2.01	0.42
27:U:41:ARG:O	27:U:45:GLU:HG2	2.19	0.42
1:2:223:C:H2'	1:2:224:A:C8	2.55	0.42
1:2:1554:C:OP2	1:2:1555:U:O2'	2.28	0.42
2:A:42:LYS:HD2	2:A:48:ILE:HD11	2.02	0.42
29:b:33:MET:O	29:b:45:THR:HA	2.20	0.42
30:c:17:VAL:HG12	30:c:30:VAL:HG12	2.00	0.42
1:2:874:G:H2'	1:2:875:A:C8	2.54	0.42
19:R:20:TYR:HD1	19:R:23:ARG:HD2	1.84	0.42
22:T:108:GLU:OE2	22:T:121:ARG:NE	2.53	0.42
22:T:110:LEU:HD23	22:T:110:LEU:HA	1.87	0.42
1:2:921:G:OP2	29:b:21:LYS:NZ	2.53	0.42
1:2:1265:A:O2'	1:2:1327:G:OP2	2.34	0.42
1:2:1404:U:OP1	27:U:21:ARG:NH2	2.37	0.42
1:2:1531:A:H2'	1:2:1532:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:ILE:HD12	2:A:47:TYR:HB3	2.01	0.42
28:Z:103:HIS:CD2	28:Z:105:ALA:H	2.38	0.42
36:z:142:LYS:HA	36:z:142:LYS:HD3	1.84	0.42
1:2:29:G:H2'	1:2:30:C:C6	2.55	0.42
10:I:114:GLU:OE2	10:I:123:ARG:NE	2.53	0.42
19:R:76:GLU:HA	19:R:79:GLU:HG3	2.02	0.42
8:G:77:LEU:HD13	8:G:95:LYS:HB2	2.00	0.42
11:J:125:HIS:O	11:J:129:LEU:HB2	2.20	0.42
25:X:131:LEU:HD12	25:X:131:LEU:HA	1.84	0.42
30:c:18:LEU:N	30:c:29:GLN:O	2.40	0.42
1:2:661:U:OP2	25:X:3:LYS:NZ	2.50	0.41
1:2:1119:A:H2'	1:2:1120:U:C6	2.55	0.41
1:2:1174:PSU:H2'	1:2:1175:G:C8	2.55	0.41
1:2:1865:C:O2	5:h:92:ARG:HB3	2.19	0.41
9:H:107:LYS:HB2	9:H:107:LYS:HE3	1.87	0.41
14:K:86:PRO:HA	14:K:87:PRO:HD3	1.82	0.41
15:N:132:LYS:HA	15:N:132:LYS:HD3	1.93	0.41
18:P:85:ILE:HB	18:P:112:ILE:HA	2.00	0.41
19:R:19:LYS:HG3	19:R:20:TYR:CD2	2.55	0.41
21:S:106:LYS:HD3	21:S:106:LYS:HA	1.89	0.41
27:U:56:MET:HE3	27:U:88:LEU:HD22	2.02	0.41
34:g:33:SER:OG	34:g:43:TRP:NE1	2.40	0.41
1:2:1665:G:C8	22:T:88:MET:HE3	2.55	0.41
17:M:26:LEU:HD22	17:M:89:VAL:O	2.20	0.41
17:M:64:LEU:HD11	33:f:106:TYR:HB2	2.01	0.41
24:W:24:GLN:HA	24:W:63:VAL:O	2.20	0.41
1:2:184:G:H2'	1:2:185:G:H8	1.85	0.41
1:2:354:OMU:HM22	1:2:355:G:O4'	2.20	0.41
1:2:1536:G:H2'	1:2:1537:A:H8	1.84	0.41
7:D:197:LYS:HD3	7:D:197:LYS:HA	1.94	0.41
26:Y:80:ASP:OD1	26:Y:81:TYR:N	2.53	0.41
34:g:5:MET:HB3	34:g:312:VAL:HG12	2.03	0.41
1:2:1423:C:H2'	1:2:1424:G:O4'	2.20	0.41
19:R:33:ARG:HA	19:R:36:GLU:HG2	2.03	0.41
34:g:188:HIS:HB3	34:g:219:TRP:CZ2	2.56	0.41
7:D:142:LEU:HD12	7:D:148:LYS:HB2	2.03	0.41
13:L:79:LYS:HE3	13:L:79:LYS:HB2	1.87	0.41
14:K:85:LEU:HD23	14:K:85:LEU:HA	1.86	0.41
21:S:115:LYS:O	21:S:118:ARG:NH1	2.53	0.41
34:g:145:GLU:HG3	34:g:177:TRP:HZ3	1.85	0.41
2:A:39:TYR:CE1	19:R:108:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:3:ASP:OD1	13:L:3:ASP:N	2.53	0.41
17:M:21:VAL:HG23	17:M:120:ALA:HB3	2.02	0.41
20:Q:60:LYS:HE2	20:Q:60:LYS:HB2	1.94	0.41
28:Z:74:SER:OG	28:Z:79:ILE:O	2.33	0.41
29:b:64:CYS:HB3	29:b:73:LEU:HD23	2.03	0.41
1:2:667:U:H5''	1:2:1087:A:C5	2.55	0.41
1:2:1037:G:H4'	1:2:1845:A:H4'	2.03	0.41
1:2:1214:A:H2'	1:2:1217:A:N7	2.36	0.41
1:2:1425:G:H2'	1:2:1426:U:C6	2.56	0.41
1:2:1753:C:H2'	1:2:1754:G:H8	1.85	0.41
4:C:72:ASP:O	4:C:74:LYS:N	2.53	0.41
7:D:80:PRO:O	7:D:83:SER:OG	2.33	0.41
7:D:173:ARG:HD3	7:D:173:ARG:HA	1.89	0.41
21:S:79:ILE:HA	21:S:80:PRO:HD3	1.93	0.41
1:2:99:A2M:HM'3	1:2:99:A2M:H1'	1.85	0.41
1:2:102:A:H4'	1:2:104:A:C8	2.56	0.41
1:2:377:G:H5'	10:I:98:LYS:HB3	2.03	0.41
1:2:1401:A:H2'	1:2:1402:A:C8	2.56	0.41
8:G:77:LEU:HD23	8:G:81:HIS:HB3	2.02	0.41
1:2:750:C:H2'	1:2:751:G:H8	1.85	0.41
1:2:879:C:H2'	1:2:880:G:O4'	2.21	0.41
1:2:1139:C:H2'	1:2:1140:G:O4'	2.21	0.41
1:2:1511:U:H2'	1:2:1512:C:C6	2.56	0.41
6:E:10:LYS:HA	6:E:10:LYS:HD3	1.87	0.41
10:I:81:VAL:HG12	10:I:91:VAL:HG13	2.03	0.41
11:J:67:ASP:HA	11:J:68:PRO:HD3	1.90	0.41
12:F:49:LEU:HD12	20:Q:50:LYS:HG2	2.03	0.41
17:M:64:LEU:HD11	33:f:106:TYR:HD2	1.85	0.41
35:j:28:VAL:HB	35:j:41:VAL:HB	2.02	0.41
1:2:318:A:H61	8:G:186:GLN:NE2	2.19	0.41
1:2:344:U:H2'	1:2:345:U:C6	2.55	0.41
1:2:1413:G:H2'	1:2:1414:A:C8	2.56	0.41
34:g:206:LEU:HD21	34:g:261:LEU:HD23	2.03	0.41
34:g:244:ASN:OD1	34:g:295:GLY:N	2.54	0.41
1:2:1678:A2M:H1'	1:2:1678:A2M:HM'3	1.50	0.40
7:D:61:GLU:O	7:D:64:ARG:HB3	2.21	0.40
18:P:45:LEU:HD23	18:P:45:LEU:HA	1.94	0.40
23:V:16:LYS:HE3	23:V:16:LYS:HB2	1.80	0.40
26:Y:78:SER:OG	26:Y:80:ASP:OD1	2.36	0.40
36:z:312:ARG:NH2	36:z:387:ASP:O	2.43	0.40
1:2:194:C:H1'	1:2:206:G:N2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:134:VAL:HG12	9:H:173:PHE:CE2	2.56	0.40
18:P:57:LEU:HD23	18:P:57:LEU:HA	1.96	0.40
24:W:90:GLN:HB2	24:W:94:LEU:HD12	2.02	0.40
34:g:206:LEU:HG	34:g:218:LEU:HD12	2.03	0.40
34:g:214:GLY:HA2	34:g:236:ILE:HG13	2.02	0.40
36:z:301:ARG:HG2	36:z:373:VAL:HG22	2.03	0.40
1:2:554:A:H4'	1:2:555:A:N7	2.36	0.40
1:2:1491:G:H2'	1:2:1492:U:C6	2.56	0.40
23:V:17:CYS:HB2	23:V:56:CYS:HB3	2.03	0.40
34:g:218:LEU:HD23	34:g:230:LEU:HD23	2.03	0.40
1:2:1355:C:O3'	4:C:238:LYS:NZ	2.54	0.40
1:2:1613:G:OP1	18:P:42:ARG:NH2	2.49	0.40
7:D:221:THR:HA	7:D:222:PRO:HD3	1.98	0.40
24:W:26:LEU:HD11	24:W:60:LYS:HD3	2.04	0.40
28:Z:101:SER:HB3	28:Z:108:ILE:HD12	2.04	0.40
32:e:3:HIS:NE2	35:j:36:ASN:O	2.55	0.40
10:I:172:LEU:HB3	10:I:190:LEU:HD12	2.04	0.40
10:I:197:PHE:CZ	10:I:201:LYS:HE3	2.57	0.40
22:T:124:THR:HG22	22:T:126:GLN:H	1.86	0.40
33:f:140:TYR:CZ	33:f:142:GLY:HA2	2.56	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	214/295 (72%)	207 (97%)	6 (3%)	1 (0%)	24	48
3	B	209/264 (79%)	207 (99%)	2 (1%)	0	100	100
4	C	214/293 (73%)	207 (97%)	7 (3%)	0	100	100
5	h	97/115 (84%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	253/263 (96%)	245 (97%)	8 (3%)	0	100	100
7	D	222/243 (91%)	219 (99%)	3 (1%)	0	100	100
8	G	221/249 (89%)	213 (96%)	8 (4%)	0	100	100
9	H	171/194 (88%)	165 (96%)	6 (4%)	0	100	100
10	I	195/208 (94%)	187 (96%)	8 (4%)	0	100	100
11	J	172/194 (89%)	165 (96%)	7 (4%)	0	100	100
12	F	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
13	L	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
14	K	93/165 (56%)	88 (95%)	5 (5%)	0	100	100
15	N	147/151 (97%)	147 (100%)	0	0	100	100
16	O	124/151 (82%)	120 (97%)	4 (3%)	0	100	100
17	M	102/132 (77%)	98 (96%)	4 (4%)	0	100	100
18	P	130/145 (90%)	122 (94%)	8 (6%)	0	100	100
19	R	130/135 (96%)	117 (90%)	13 (10%)	0	100	100
20	Q	138/146 (94%)	129 (94%)	9 (6%)	0	100	100
21	S	139/152 (91%)	132 (95%)	7 (5%)	0	100	100
22	T	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
23	V	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
24	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
25	X	137/143 (96%)	132 (96%)	4 (3%)	1 (1%)	18	41
26	Y	120/133 (90%)	116 (97%)	4 (3%)	0	100	100
27	U	96/119 (81%)	91 (95%)	5 (5%)	0	100	100
28	Z	80/125 (64%)	75 (94%)	5 (6%)	0	100	100
29	b	73/84 (87%)	68 (93%)	5 (7%)	0	100	100
30	c	59/69 (86%)	57 (97%)	2 (3%)	0	100	100
31	d	52/56 (93%)	48 (92%)	4 (8%)	0	100	100
32	e	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
33	f	53/156 (34%)	49 (92%)	4 (8%)	0	100	100
34	g	287/317 (90%)	266 (93%)	21 (7%)	0	100	100
35	j	112/165 (68%)	108 (96%)	4 (4%)	0	100	100
36	z	343/568 (60%)	319 (93%)	24 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5088/6209 (82%)	4877 (96%)	209 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	6	ASP
25	X	86	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/243 (74%)	177 (98%)	3 (2%)	53	79
3	B	192/231 (83%)	191 (100%)	1 (0%)	81	92
4	C	182/225 (81%)	181 (100%)	1 (0%)	81	92
5	h	86/98 (88%)	85 (99%)	1 (1%)	63	84
6	E	220/225 (98%)	220 (100%)	0	100	100
7	D	188/202 (93%)	188 (100%)	0	100	100
8	G	194/218 (89%)	191 (98%)	3 (2%)	57	81
9	H	160/174 (92%)	159 (99%)	1 (1%)	78	91
10	I	174/180 (97%)	174 (100%)	0	100	100
11	J	156/168 (93%)	156 (100%)	0	100	100
12	F	156/170 (92%)	155 (99%)	1 (1%)	78	91
13	L	126/142 (89%)	126 (100%)	0	100	100
14	K	86/136 (63%)	86 (100%)	0	100	100
15	N	130/131 (99%)	130 (100%)	0	100	100
16	O	99/119 (83%)	99 (100%)	0	100	100
17	M	91/108 (84%)	91 (100%)	0	100	100
18	P	117/130 (90%)	117 (100%)	0	100	100
19	R	118/122 (97%)	117 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Q	116/121 (96%)	116 (100%)	0	100	100
21	S	122/132 (92%)	121 (99%)	1 (1%)	73	88
22	T	111/115 (96%)	111 (100%)	0	100	100
23	V	67/67 (100%)	67 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	111/115 (96%)	111 (100%)	0	100	100
26	Y	103/115 (90%)	102 (99%)	1 (1%)	68	86
27	U	90/107 (84%)	90 (100%)	0	100	100
28	Z	67/103 (65%)	67 (100%)	0	100	100
29	b	70/76 (92%)	70 (100%)	0	100	100
30	c	54/62 (87%)	53 (98%)	1 (2%)	50	77
31	d	47/49 (96%)	47 (100%)	0	100	100
32	e	40/48 (83%)	40 (100%)	0	100	100
33	f	51/140 (36%)	51 (100%)	0	100	100
34	g	255/275 (93%)	253 (99%)	2 (1%)	73	88
35	j	103/150 (69%)	102 (99%)	1 (1%)	68	86
36	z	299/512 (58%)	297 (99%)	2 (1%)	76	90
All	All	4473/5322 (84%)	4453 (100%)	20 (0%)	81	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	124	VAL
2	A	200	ASP
2	A	206	ASP
3	B	48	LEU
4	C	248	TYR
5	h	84	VAL
8	G	13	GLN
8	G	105	ASN
8	G	192	ILE
9	H	9	VAL
12	F	41	VAL
19	R	98	VAL
21	S	131	VAL
26	Y	18	LEU

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Mol	Chain	Res	Type
30	c	46	VAL
34	g	107	ASP
34	g	291	TRP
35	j	76	GLU
36	z	346	VAL
36	z	424	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	50	ASN
2	A	84	GLN
2	A	131	HIS
3	B	76	ASN
3	B	101	HIS
4	C	113	GLN
6	E	8	HIS
6	E	17	HIS
6	E	50	ASN
6	E	98	ASN
6	E	157	ASN
6	E	216	ASN
6	E	224	ASN
8	G	56	ASN
8	G	65	GLN
8	G	155	GLN
9	H	73	GLN
9	H	91	HIS
9	H	97	GLN
9	H	157	HIS
9	H	165	ASN
9	H	193	GLN
10	I	84	ASN
10	I	165	GLN
10	I	167	GLN
10	I	168	GLN
11	J	75	ASN
11	J	113	GLN
11	J	132	GLN
12	F	79	HIS
12	F	83	ASN
13	L	11	GLN

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Mol	Chain	Res	Type
13	L	108	ASN
14	K	32	HIS
15	N	62	GLN
15	N	123	HIS
16	O	38	ASN
17	M	15	ASN
17	M	46	GLN
18	P	53	GLN
18	P	79	HIS
19	R	74	GLN
19	R	83	ASN
19	R	93	GLN
19	R	116	ASN
20	Q	35	ASN
20	Q	80	GLN
20	Q	86	GLN
21	S	42	HIS
21	S	120	HIS
21	S	135	HIS
22	T	91	HIS
23	V	29	HIS
24	W	15	ASN
24	W	16	ASN
24	W	113	HIS
25	X	23	HIS
25	X	73	GLN
26	Y	22	GLN
28	Z	45	ASN
28	Z	103	HIS
29	b	26	GLN
31	d	45	GLN
32	e	15	GLN
33	f	135	HIS
34	g	51	ASN
34	g	64	HIS
34	g	117	ASN
34	g	222	ASN
34	g	237	ASN
34	g	272	GLN
34	g	285	GLN
35	j	60	ASN
36	z	306	GLN

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Mol	Chain	Res	Type
36	z	316	GLN
36	z	348	HIS
36	z	363	ASN
36	z	365	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1641/1869 (87%)	364 (22%)	14 (0%)

All (364) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	17	C
1	2	33	G
1	2	41	G
1	2	44	U
1	2	46	A
1	2	49	C
1	2	56	G
1	2	58	C
1	2	59	U
1	2	64	A
1	2	67	C
1	2	68	A
1	2	72	C
1	2	99	A2M
1	2	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	127	C
1	2	129	C
1	2	130	G
1	2	142	C
1	2	143	U
1	2	147	A
1	2	155	G
1	2	159	A2M

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Mol	Chain	Res	Type
1	2	160	U
1	2	161	U
1	2	168	C
1	2	171	A
1	2	172	OMU
1	2	177	G
1	2	178	C
1	2	182	C
1	2	184	G
1	2	192	C
1	2	195	C
1	2	198	U
1	2	199	C
1	2	201	C
1	2	202	G
1	2	203	G
1	2	204	G
1	2	205	G
1	2	214	U
1	2	291	G
1	2	292	A
1	2	302	A
1	2	305	U
1	2	306	C
1	2	307	G
1	2	308	G
1	2	310	C
1	2	312	G
1	2	320	G
1	2	331	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	351	G
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	381	C
1	2	382	C
1	2	385	G
1	2	386	C

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Mol	Chain	Res	Type
1	2	388	U
1	2	407	G
1	2	408	A
1	2	409	C
1	2	428	OMU
1	2	436	OMG
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	455	A
1	2	465	A
1	2	467	G
1	2	470	G
1	2	471	G
1	2	472	C
1	2	474	G
1	2	482	G
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	493	A
1	2	508	A
1	2	509	OMG
1	2	512	A2M
1	2	516	A
1	2	525	A
1	2	529	A
1	2	539	C
1	2	540	U
1	2	541	U
1	2	542	U
1	2	544	G
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A

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Mol	Chain	Res	Type
1	2	561	A
1	2	563	G
1	2	564	A
1	2	568	C
1	2	574	A
1	2	588	G
1	2	590	A
1	2	591	U
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	623	G
1	2	626	G
1	2	629	A
1	2	632	C
1	2	639	C
1	2	640	A
1	2	643	A
1	2	644	OMG
1	2	655	A
1	2	663	C
1	2	664	A
1	2	666	U
1	2	668	A2M
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	684	G
1	2	687	C
1	2	749	U
1	2	750	C
1	2	792	C
1	2	793	G
1	2	795	A
1	2	797	C
1	2	798	G
1	2	799	U
1	2	810	A
1	2	811	A

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Mol	Chain	Res	Type
1	2	821	G
1	2	822	PSU
1	2	823	U
1	2	824	C
1	2	830	A
1	2	831	G
1	2	847	A
1	2	862	A
1	2	869	A
1	2	870	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	879	C
1	2	880	G
1	2	884	C
1	2	901	G
1	2	902	G
1	2	913	A
1	2	914	U
1	2	916	A
1	2	917	U
1	2	919	A
1	2	920	A
1	2	921	G
1	2	922	A
1	2	933	G
1	2	943	U
1	2	970	G
1	2	971	G
1	2	972	A
1	2	982	G
1	2	983	A
1	2	990	A
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1031	A2M
1	2	1034	A
1	2	1036	A

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Mol	Chain	Res	Type
1	2	1045	PSU
1	2	1048	G
1	2	1049	A
1	2	1055	A
1	2	1060	A
1	2	1061	U
1	2	1062	A
1	2	1066	U
1	2	1067	C
1	2	1080	A
1	2	1083	A
1	2	1085	C
1	2	1096	G
1	2	1100	A
1	2	1109	C
1	2	1120	U
1	2	1121	G
1	2	1123	C
1	2	1126	G
1	2	1133	A
1	2	1144	A
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1168	G
1	2	1171	G
1	2	1188	A
1	2	1195	A
1	2	1207	G
1	2	1215	C
1	2	1221	G
1	2	1242	U
1	2	1243	U
1	2	1248	B8N
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1271	C

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Mol	Chain	Res	Type
1	2	1274	G
1	2	1275	G
1	2	1286	G
1	2	1300	U
1	2	1302	G
1	2	1303	C
1	2	1305	C
1	2	1306	U
1	2	1308	U
1	2	1313	A
1	2	1315	U
1	2	1341	C
1	2	1342	U
1	2	1343	U
1	2	1348	G
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1402	A
1	2	1405	A
1	2	1418	C
1	2	1429	G
1	2	1430	C
1	2	1438	A
1	2	1440	C
1	2	1441	U
1	2	1447	G
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1466	G
1	2	1476	A
1	2	1477	U
1	2	1478	U
1	2	1484	A
1	2	1487	A
1	2	1488	C
1	2	1489	A
1	2	1490	OMG
1	2	1494	U
1	2	1495	G
1	2	1497	G

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Mol	Chain	Res	Type
1	2	1498	A
1	2	1508	A
1	2	1509	U
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1544	C
1	2	1553	C
1	2	1558	C
1	2	1559	C
1	2	1560	U
1	2	1569	A
1	2	1570	G
1	2	1573	G
1	2	1576	G
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1594	A
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1639	7MG
1	2	1648	G
1	2	1654	G
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1679	A
1	2	1680	G
1	2	1695	A
1	2	1706	G
1	2	1707	U
1	2	1709	G
1	2	1712	A
1	2	1715	A
1	2	1719	A
1	2	1721	U

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Mol	Chain	Res	Type
1	2	1722	G
1	2	1724	A
1	2	1725	U
1	2	1726	G
1	2	1744	G
1	2	1755	C
1	2	1757	G
1	2	1759	G
1	2	1761	U
1	2	1774	C
1	2	1775	U
1	2	1780	G
1	2	1781	A
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1809	A
1	2	1813	A
1	2	1814	G
1	2	1815	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1834	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1848	U
1	2	1849	A
1	2	1850	MA6
1	2	1852	C
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1869	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	291	G
1	2	381	C
1	2	435	A
1	2	683	OMG
1	2	791	C
1	2	809	A
1	2	912	C
1	2	1060	A
1	2	1065	G
1	2	1119	A
1	2	1165	G
1	2	1440	C
1	2	1605	G
1	2	1814	G

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

74 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	PSU	2	651	1	18,21,22	1.15	2 (11%)	22,30,33	1.68	3 (13%)
1	PSU	2	36	1	18,21,22	1.09	2 (11%)	22,30,33	1.80	3 (13%)
1	A2M	2	484	1	22,25,26	3.44	9 (40%)	31,36,39	2.28	9 (29%)
1	PSU	2	105	1	18,21,22	1.11	1 (5%)	22,30,33	1.69	4 (18%)
1	PSU	2	572	1	18,21,22	1.04	3 (16%)	22,30,33	1.77	4 (18%)
1	PSU	2	109	1	18,21,22	1.09	1 (5%)	22,30,33	1.89	4 (18%)
1	PSU	2	34	1	18,21,22	1.01	1 (5%)	22,30,33	1.97	4 (18%)
1	OMG	2	644	1	23,26,27	2.40	6 (26%)	33,38,41	1.87	9 (27%)
1	OMU	2	116	1	19,22,23	3.00	8 (42%)	26,31,34	1.76	7 (26%)
1	PSU	2	1232	1	18,21,22	1.09	1 (5%)	22,30,33	1.76	3 (13%)
1	OMG	2	1490	38,1	23,26,27	2.39	6 (26%)	33,38,41	1.79	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2	814	1	18,21,22	0.95	1 (5%)	22,30,33	1.73	3 (13%)
1	A2M	2	1031	1	22,25,26	3.45	9 (40%)	31,36,39	2.09	9 (29%)
1	B8N	2	1248	1	24,29,30	2.30	10 (41%)	29,42,45	1.64	5 (17%)
1	PSU	2	815	1	18,21,22	0.95	1 (5%)	22,30,33	1.80	3 (13%)
1	A2M	2	668	38,1	22,25,26	3.45	9 (40%)	31,36,39	2.34	9 (29%)
1	OMC	2	517	1	19,22,23	2.35	7 (36%)	26,31,34	0.75	1 (3%)
1	PSU	2	1367	1	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
1	PSU	2	119	1	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
1	PSU	2	1625	1	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	2	1347	1	18,21,22	1.04	1 (5%)	22,30,33	1.76	3 (13%)
1	OMC	2	1391	1	19,22,23	2.28	6 (31%)	26,31,34	0.83	1 (3%)
1	PSU	2	1177	1	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
1	OMG	2	436	1	23,26,27	2.42	6 (26%)	33,38,41	1.96	10 (30%)
1	OMU	2	1326	38,1	19,22,23	2.90	7 (36%)	26,31,34	1.90	4 (15%)
1	OMU	2	354	1	19,22,23	2.94	8 (42%)	26,31,34	1.92	5 (19%)
1	A2M	2	468	1	22,25,26	3.42	8 (36%)	31,36,39	2.35	12 (38%)
1	OMC	2	1703	1	19,22,23	2.33	7 (36%)	26,31,34	0.87	1 (3%)
1	PSU	2	1004	1	18,21,22	1.08	1 (5%)	22,30,33	1.90	4 (18%)
1	4AC	2	1842	38,1	21,24,25	1.92	6 (28%)	29,34,37	1.61	5 (17%)
1	OMC	2	174	1	19,22,23	2.31	7 (36%)	26,31,34	0.80	0
1	OMG	2	1328	1	23,26,27	2.41	6 (26%)	33,38,41	1.83	9 (27%)
1	PSU	2	93	1	18,21,22	1.21	1 (5%)	22,30,33	1.78	4 (18%)
1	PSU	2	1643	38,1	18,21,22	1.04	1 (5%)	22,30,33	1.62	4 (18%)
1	MA6	2	1850	1	23,26,27	1.17	3 (13%)	34,38,41	2.16	9 (26%)
1	PSU	2	686	1	18,21,22	1.00	1 (5%)	22,30,33	1.76	4 (18%)
1	PSU	2	681	1	18,21,22	1.13	1 (5%)	22,30,33	1.83	4 (18%)
1	PSU	2	1056	1	18,21,22	1.05	1 (5%)	22,30,33	1.73	3 (13%)
1	A2M	2	1383	1	22,25,26	3.39	8 (36%)	31,36,39	2.32	10 (32%)
1	PSU	2	649	1	18,21,22	1.25	1 (5%)	22,30,33	1.79	4 (18%)
1	OMG	2	867	1	23,26,27	2.37	6 (26%)	33,38,41	1.97	10 (30%)
1	OMG	2	509	38,1	23,26,27	2.34	6 (26%)	33,38,41	2.01	7 (21%)
1	OMC	2	1272	1	19,22,23	2.28	6 (31%)	26,31,34	0.91	1 (3%)
1	PSU	2	966	1	18,21,22	0.94	1 (5%)	22,30,33	1.65	3 (13%)
1	PSU	2	218	1	18,21,22	0.94	1 (5%)	22,30,33	1.75	4 (18%)
1	OMU	2	428	1	19,22,23	2.93	7 (36%)	26,31,34	2.06	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2	406	1	18,21,22	1.01	1 (5%)	22,30,33	2.00	3 (13%)
1	A2M	2	99	38,1	22,25,26	3.47	8 (36%)	31,36,39	2.24	7 (22%)
1	A2M	2	27	38,1	22,25,26	3.49	9 (40%)	31,36,39	2.16	9 (29%)
1	PSU	2	1244	1	18,21,22	1.06	1 (5%)	22,30,33	1.91	5 (22%)
1	OMU	2	1288	1	19,22,23	2.89	7 (36%)	26,31,34	1.76	5 (19%)
1	OMG	2	601	1	23,26,27	2.35	6 (26%)	33,38,41	1.93	8 (24%)
1	PSU	2	1238	1	18,21,22	1.07	1 (5%)	22,30,33	1.77	3 (13%)
1	4AC	2	1337	1	21,24,25	1.90	6 (28%)	29,34,37	1.12	1 (3%)
1	A2M	2	512	1	22,25,26	3.43	9 (40%)	31,36,39	2.32	11 (35%)
1	OMG	2	683	1	23,26,27	2.39	6 (26%)	33,38,41	2.29	14 (42%)
1	OMC	2	462	1	19,22,23	2.29	5 (26%)	26,31,34	0.82	1 (3%)
1	PSU	2	1692	1	18,21,22	1.19	1 (5%)	22,30,33	1.98	5 (22%)
1	OMU	2	1442	38,1	19,22,23	3.00	7 (36%)	26,31,34	1.73	6 (23%)
1	6MZ	2	1832	38,1	22,25,26	3.22	2 (9%)	30,36,39	2.25	9 (30%)
1	MA6	2	1851	1	23,26,27	1.35	4 (17%)	34,38,41	1.96	8 (23%)
1	7MG	2	1639	1	22,26,27	5.49	6 (27%)	29,39,42	2.41	9 (31%)
1	A2M	2	1678	1	22,25,26	3.45	9 (40%)	31,36,39	2.27	9 (29%)
1	OMU	2	121	1	19,22,23	3.02	7 (36%)	26,31,34	1.76	5 (19%)
1	PSU	2	822	1	18,21,22	1.02	1 (5%)	22,30,33	1.90	5 (22%)
1	PSU	2	1045	1	18,21,22	1.06	1 (5%)	22,30,33	1.62	4 (18%)
1	PSU	2	1445	1	18,21,22	1.11	1 (5%)	22,30,33	1.98	5 (22%)
1	A2M	2	166	1	22,25,26	3.41	8 (36%)	31,36,39	2.35	9 (29%)
1	PSU	2	1081	1	18,21,22	1.10	2 (11%)	22,30,33	1.86	4 (18%)
1	PSU	2	1174	38,1	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
1	OMU	2	172	1	19,22,23	2.97	7 (36%)	26,31,34	1.78	5 (19%)
1	A2M	2	159	1	22,25,26	3.41	8 (36%)	31,36,39	2.34	9 (29%)
1	PSU	2	1046	1	18,21,22	1.02	1 (5%)	22,30,33	1.77	3 (13%)
1	A2M	2	576	1	22,25,26	3.41	8 (36%)	31,36,39	2.14	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	651	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	36	1	-	0/7/25/26	0/2/2/2
1	A2M	2	484	1	-	0/9/27/28	0/3/3/3
1	PSU	2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	2	572	1	-	0/7/25/26	0/2/2/2
1	PSU	2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	2	34	1	-	0/7/25/26	0/2/2/2
1	OMG	2	644	1	-	3/9/27/28	0/3/3/3
1	OMU	2	116	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1232	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1490	38,1	-	2/9/27/28	0/3/3/3
1	PSU	2	814	1	-	0/7/25/26	0/2/2/2
1	A2M	2	1031	1	-	1/9/27/28	0/3/3/3
1	B8N	2	1248	1	-	7/16/34/35	0/2/2/2
1	PSU	2	815	1	-	0/7/25/26	0/2/2/2
1	A2M	2	668	38,1	-	3/9/27/28	0/3/3/3
1	OMC	2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1367	1	-	0/7/25/26	0/2/2/2
1	PSU	2	119	1	-	2/7/25/26	0/2/2/2
1	PSU	2	1625	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1347	1	-	0/7/25/26	0/2/2/2
1	OMC	2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1177	1	-	0/7/25/26	0/2/2/2
1	OMG	2	436	1	-	0/9/27/28	0/3/3/3
1	OMU	2	1326	38,1	-	0/9/27/28	0/2/2/2
1	OMU	2	354	1	-	0/9/27/28	0/2/2/2
1	A2M	2	468	1	-	3/9/27/28	0/3/3/3
1	OMC	2	1703	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1004	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1842	38,1	-	2/11/29/30	0/2/2/2
1	OMC	2	174	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1328	1	-	0/9/27/28	0/3/3/3
1	PSU	2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1643	38,1	-	0/7/25/26	0/2/2/2
1	MA6	2	1850	1	-	2/11/29/30	0/3/3/3
1	PSU	2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	2	681	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1056	1	-	0/7/25/26	0/2/2/2
1	A2M	2	1383	1	-	0/9/27/28	0/3/3/3
1	PSU	2	649	1	-	2/7/25/26	0/2/2/2
1	OMG	2	867	1	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	509	38,1	-	3/9/27/28	0/3/3/3
1	OMC	2	1272	1	-	1/9/27/28	0/2/2/2
1	PSU	2	966	1	-	0/7/25/26	0/2/2/2
1	PSU	2	218	1	-	0/7/25/26	0/2/2/2
1	OMU	2	428	1	-	5/9/27/28	0/2/2/2
1	PSU	2	406	1	-	0/7/25/26	0/2/2/2
1	A2M	2	99	38,1	-	2/9/27/28	0/3/3/3
1	A2M	2	27	38,1	-	0/9/27/28	0/3/3/3
1	PSU	2	1244	1	-	0/7/25/26	0/2/2/2
1	OMU	2	1288	1	-	0/9/27/28	0/2/2/2
1	OMG	2	601	1	-	0/9/27/28	0/3/3/3
1	PSU	2	1238	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1337	1	-	0/11/29/30	0/2/2/2
1	A2M	2	512	1	-	0/9/27/28	0/3/3/3
1	OMG	2	683	1	-	2/9/27/28	0/3/3/3
1	OMC	2	462	1	-	1/9/27/28	0/2/2/2
1	PSU	2	1692	1	-	2/7/25/26	0/2/2/2
1	OMU	2	1442	38,1	-	0/9/27/28	0/2/2/2
1	6MZ	2	1832	38,1	-	0/9/27/28	0/3/3/3
1	MA6	2	1851	1	-	1/11/29/30	0/3/3/3
1	7MG	2	1639	1	-	0/7/37/38	0/3/3/3
1	A2M	2	1678	1	-	1/9/27/28	0/3/3/3
1	OMU	2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	2	822	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1045	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1445	1	-	0/7/25/26	0/2/2/2
1	A2M	2	166	1	-	0/9/27/28	0/3/3/3
1	PSU	2	1081	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1174	38,1	-	0/7/25/26	0/2/2/2
1	OMU	2	172	1	-	2/9/27/28	0/2/2/2
1	A2M	2	159	1	-	0/9/27/28	0/3/3/3
1	PSU	2	1046	1	-	0/7/25/26	0/2/2/2
1	A2M	2	576	1	-	0/9/27/28	0/3/3/3

All (321) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	7MG	C8-N9	-22.93	1.33	1.46
1	2	1832	6MZ	C6-N6	14.41	1.49	1.34
1	2	1678	A2M	C2'-C1'	-9.13	1.29	1.53
1	2	27	A2M	C2'-C1'	-9.08	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	7MG	O6-C6	9.04	1.40	1.23
1	2	468	A2M	C2'-C1'	-9.02	1.29	1.53
1	2	1031	A2M	C2'-C1'	-8.96	1.30	1.53
1	2	159	A2M	C2'-C1'	-8.92	1.30	1.53
1	2	99	A2M	C2'-C1'	-8.85	1.30	1.53
1	2	166	A2M	C2'-C1'	-8.83	1.30	1.53
1	2	484	A2M	C2'-C1'	-8.78	1.30	1.53
1	2	576	A2M	C2'-C1'	-8.72	1.30	1.53
1	2	512	A2M	C2'-C1'	-8.70	1.30	1.53
1	2	668	A2M	C2'-C1'	-8.68	1.30	1.53
1	2	468	A2M	O4'-C1'	8.64	1.62	1.42
1	2	1383	A2M	O4'-C1'	8.63	1.62	1.42
1	2	99	A2M	O4'-C1'	8.62	1.62	1.42
1	2	1288	OMU	O4-C4	8.59	1.41	1.24
1	2	1383	A2M	C2'-C1'	-8.54	1.31	1.53
1	2	166	A2M	O4'-C1'	8.54	1.62	1.42
1	2	867	OMG	O6-C6	8.51	1.39	1.23
1	2	27	A2M	O4'-C1'	8.50	1.62	1.42
1	2	436	OMG	O6-C6	8.48	1.39	1.23
1	2	159	A2M	O4'-C1'	8.44	1.62	1.42
1	2	512	A2M	O4'-C1'	8.44	1.62	1.42
1	2	683	OMG	O6-C6	8.43	1.39	1.23
1	2	1442	OMU	O4-C4	8.42	1.40	1.24
1	2	1031	A2M	O4'-C1'	8.42	1.61	1.42
1	2	172	OMU	O4-C4	8.34	1.40	1.24
1	2	644	OMG	O6-C6	8.30	1.39	1.23
1	2	1328	OMG	O6-C6	8.28	1.39	1.23
1	2	116	OMU	O4-C4	8.26	1.40	1.24
1	2	1326	OMU	O4-C4	8.23	1.40	1.24
1	2	1678	A2M	O4'-C1'	8.20	1.61	1.42
1	2	121	OMU	O4-C4	8.18	1.40	1.24
1	2	484	A2M	O4'-C1'	8.17	1.61	1.42
1	2	576	A2M	O4'-C1'	8.15	1.61	1.42
1	2	428	OMU	O4-C4	8.11	1.40	1.24
1	2	1490	OMG	O6-C6	8.03	1.38	1.23
1	2	354	OMU	O4-C4	8.00	1.40	1.24
1	2	509	OMG	O6-C6	7.92	1.38	1.23
1	2	601	OMG	O6-C6	7.90	1.38	1.23
1	2	668	A2M	O4'-C1'	7.71	1.60	1.42
1	2	668	A2M	O4'-C4'	-7.48	1.28	1.45
1	2	484	A2M	O4'-C4'	-6.89	1.29	1.45
1	2	1678	A2M	O4'-C4'	-6.67	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	576	A2M	O4'-C4'	-6.50	1.30	1.45
1	2	27	A2M	O4'-C4'	-6.48	1.30	1.45
1	2	1031	A2M	O4'-C4'	-6.47	1.30	1.45
1	2	99	A2M	O4'-C4'	-6.43	1.30	1.45
1	2	166	A2M	O4'-C4'	-6.43	1.30	1.45
1	2	159	A2M	O4'-C4'	-6.37	1.30	1.45
1	2	512	A2M	O4'-C4'	-6.34	1.30	1.45
1	2	468	A2M	O4'-C4'	-6.27	1.31	1.45
1	2	1383	A2M	O4'-C4'	-6.23	1.31	1.45
1	2	462	OMC	C4-N4	6.15	1.48	1.33
1	2	1272	OMC	C4-N4	6.08	1.48	1.33
1	2	354	OMU	C4-N3	-6.02	1.27	1.38
1	2	428	OMU	C4-N3	-5.92	1.28	1.38
1	2	121	OMU	C4-N3	-5.91	1.28	1.38
1	2	1391	OMC	C4-N4	5.91	1.47	1.33
1	2	174	OMC	C4-N4	5.88	1.47	1.33
1	2	1248	B8N	O4-C4	5.87	1.35	1.23
1	2	172	OMU	C4-N3	-5.85	1.28	1.38
1	2	116	OMU	C4-N3	-5.83	1.28	1.38
1	2	1703	OMC	C4-N4	5.81	1.47	1.33
1	2	517	OMC	C4-N4	5.72	1.47	1.33
1	2	1442	OMU	C4-N3	-5.66	1.28	1.38
1	2	1703	OMC	O2-C2	-5.64	1.13	1.23
1	2	517	OMC	O2-C2	-5.61	1.13	1.23
1	2	1326	OMU	C4-N3	-5.45	1.28	1.38
1	2	1288	OMU	C4-N3	-5.35	1.29	1.38
1	2	1272	OMC	O2-C2	-5.25	1.14	1.23
1	2	1391	OMC	O2-C2	-5.18	1.14	1.23
1	2	174	OMC	O2-C2	-5.11	1.14	1.23
1	2	462	OMC	O2-C2	-5.05	1.14	1.23
1	2	121	OMU	C2-N1	-5.04	1.30	1.38
1	2	1248	B8N	C4-N3	-4.97	1.31	1.40
1	2	1842	4AC	C4-N4	4.83	1.46	1.39
1	2	1337	4AC	C4-N4	4.81	1.46	1.39
1	2	116	OMU	C2-N1	-4.74	1.30	1.38
1	2	1639	7MG	C2-N2	4.71	1.45	1.34
1	2	1442	OMU	C2-N1	-4.63	1.31	1.38
1	2	867	OMG	C2-N2	4.57	1.45	1.34
1	2	172	OMU	C2-N1	-4.46	1.31	1.38
1	2	1248	B8N	C2-N3	-4.40	1.31	1.38
1	2	354	OMU	C2-N3	-4.38	1.30	1.38
1	2	159	A2M	C6-N6	4.33	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	172	OMU	C2-N3	-4.31	1.30	1.38
1	2	1326	OMU	C2-N1	-4.31	1.31	1.38
1	2	601	OMG	C6-N1	-4.28	1.30	1.38
1	2	428	OMU	C2-N3	-4.27	1.30	1.38
1	2	121	OMU	C2-N3	-4.26	1.30	1.38
1	2	436	OMG	C2-N2	4.25	1.44	1.34
1	2	166	A2M	C6-N6	4.23	1.44	1.34
1	2	1678	A2M	C6-N6	4.23	1.44	1.34
1	2	1442	OMU	C2-N3	-4.21	1.30	1.38
1	2	576	A2M	C6-N6	4.20	1.44	1.34
1	2	683	OMG	C2-N2	4.18	1.44	1.34
1	2	116	OMU	C2-N3	-4.18	1.30	1.38
1	2	1328	OMG	C2-N2	4.16	1.44	1.34
1	2	1326	OMU	C2-N3	-4.14	1.30	1.38
1	2	509	OMG	C6-N1	-4.12	1.31	1.38
1	2	468	A2M	C6-N6	4.12	1.44	1.34
1	2	644	OMG	C2-N2	4.12	1.44	1.34
1	2	1490	OMG	C6-N1	-4.11	1.31	1.38
1	2	1288	OMU	C2-N3	-4.11	1.30	1.38
1	2	1328	OMG	C6-N1	-4.11	1.31	1.38
1	2	512	A2M	C6-N6	4.10	1.44	1.34
1	2	1383	A2M	C6-N6	4.08	1.44	1.34
1	2	428	OMU	C2-N1	-4.08	1.31	1.38
1	2	1031	A2M	C6-N6	4.07	1.44	1.34
1	2	1288	OMU	C2-N1	-4.06	1.31	1.38
1	2	484	A2M	C6-N6	4.05	1.44	1.34
1	2	601	OMG	C2-N2	4.03	1.43	1.34
1	2	354	OMU	C2-N1	-4.03	1.32	1.38
1	2	99	A2M	C6-N6	4.02	1.44	1.34
1	2	27	A2M	C6-N6	4.01	1.44	1.34
1	2	668	A2M	C6-N6	4.00	1.44	1.34
1	2	1490	OMG	C2-N2	3.90	1.43	1.34
1	2	509	OMG	C2-N2	3.90	1.43	1.34
1	2	683	OMG	C6-N1	-3.87	1.31	1.38
1	2	644	OMG	C6-N1	-3.85	1.31	1.38
1	2	1337	4AC	O2-C2	-3.77	1.16	1.23
1	2	93	PSU	C6-C5	3.73	1.39	1.35
1	2	1639	7MG	C6-N1	-3.70	1.32	1.38
1	2	436	OMG	C6-N1	-3.70	1.32	1.38
1	2	867	OMG	C6-N1	-3.63	1.32	1.38
1	2	484	A2M	C8-N9	-3.62	1.31	1.37
1	2	1842	4AC	C2-N1	-3.59	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	576	A2M	C8-N9	-3.53	1.31	1.37
1	2	668	A2M	C8-N9	-3.53	1.31	1.37
1	2	1842	4AC	O2-C2	-3.52	1.17	1.23
1	2	99	A2M	C8-N9	-3.49	1.31	1.37
1	2	517	OMC	C2-N1	-3.44	1.32	1.40
1	2	174	OMC	C2-N1	-3.41	1.32	1.40
1	2	1678	A2M	C8-N9	-3.35	1.31	1.37
1	2	105	PSU	C6-C5	3.33	1.39	1.35
1	2	1851	MA6	C8-N9	-3.31	1.31	1.37
1	2	99	A2M	C5-N7	-3.29	1.32	1.39
1	2	1031	A2M	C8-N9	-3.28	1.31	1.37
1	2	1842	4AC	C7-N4	3.27	1.43	1.37
1	2	1326	OMU	C6-N1	-3.24	1.30	1.38
1	2	1625	PSU	C6-C5	3.23	1.39	1.35
1	2	1337	4AC	C2-N1	-3.23	1.33	1.40
1	2	27	A2M	O3'-C3'	-3.23	1.35	1.43
1	2	159	A2M	C8-N9	-3.22	1.31	1.37
1	2	1391	OMC	C2-N1	-3.20	1.33	1.40
1	2	27	A2M	C8-N9	-3.20	1.31	1.37
1	2	649	PSU	C6-C5	3.19	1.39	1.35
1	2	512	A2M	C8-N9	-3.18	1.31	1.37
1	2	1383	A2M	C8-N9	-3.17	1.31	1.37
1	2	468	A2M	O3'-C3'	-3.15	1.35	1.43
1	2	1004	PSU	C6-C5	3.14	1.39	1.35
1	2	1031	A2M	C5-N7	-3.14	1.33	1.39
1	2	1445	PSU	C6-C5	3.13	1.39	1.35
1	2	576	A2M	C5-N7	-3.12	1.33	1.39
1	2	354	OMU	C6-N1	-3.12	1.30	1.38
1	2	166	A2M	C8-N9	-3.11	1.31	1.37
1	2	1850	MA6	C8-N9	-3.11	1.31	1.37
1	2	668	A2M	C5-N7	-3.10	1.33	1.39
1	2	1045	PSU	C6-C5	3.10	1.38	1.35
1	2	121	OMU	C6-N1	-3.10	1.30	1.38
1	2	116	OMU	C6-N1	-3.09	1.30	1.38
1	2	1639	7MG	C4-N9	-3.08	1.34	1.37
1	2	576	A2M	O3'-C3'	-3.06	1.35	1.43
1	2	1490	OMG	C5-N7	-3.05	1.33	1.39
1	2	512	A2M	O3'-C3'	-3.04	1.35	1.43
1	2	462	OMC	C2-N1	-3.04	1.33	1.40
1	2	172	OMU	C6-N1	-3.03	1.30	1.38
1	2	1272	OMC	C2-N1	-3.02	1.33	1.40
1	2	119	PSU	C6-C5	3.02	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	644	OMG	C5-N7	-3.02	1.33	1.39
1	2	1442	OMU	C6-N1	-3.00	1.30	1.38
1	2	159	A2M	O3'-C3'	-3.00	1.35	1.43
1	2	462	OMC	C6-C5	2.99	1.42	1.35
1	2	484	A2M	C5-N7	-2.98	1.33	1.39
1	2	484	A2M	O3'-C3'	-2.97	1.36	1.43
1	2	1703	OMC	C6-N1	-2.96	1.30	1.38
1	2	27	A2M	C5-N7	-2.93	1.33	1.39
1	2	468	A2M	C5-N7	-2.92	1.33	1.39
1	2	668	A2M	O2'-C2'	2.92	1.50	1.42
1	2	174	OMC	C6-N1	-2.91	1.30	1.38
1	2	1337	4AC	C7-N4	2.90	1.42	1.37
1	2	1238	PSU	C6-C5	2.89	1.38	1.35
1	2	1832	6MZ	C8-N9	-2.88	1.32	1.37
1	2	1174	PSU	C6-C5	2.88	1.38	1.35
1	2	1703	OMC	C2-N1	-2.88	1.33	1.40
1	2	822	PSU	C6-C5	2.88	1.38	1.35
1	2	436	OMG	C5-N7	-2.88	1.33	1.39
1	2	166	A2M	O3'-C3'	-2.86	1.36	1.43
1	2	1490	OMG	C2-N1	-2.86	1.30	1.37
1	2	166	A2M	C5-N7	-2.85	1.33	1.39
1	2	1391	OMC	C6-C5	2.85	1.41	1.35
1	2	1232	PSU	C6-C5	2.84	1.38	1.35
1	2	509	OMG	C2-N1	-2.84	1.30	1.37
1	2	462	OMC	C6-N1	-2.84	1.31	1.38
1	2	512	A2M	C5-N7	-2.83	1.33	1.39
1	2	681	PSU	C6-C5	2.83	1.38	1.35
1	2	815	PSU	C6-C5	2.82	1.38	1.35
1	2	99	A2M	O3'-C3'	-2.82	1.36	1.43
1	2	484	A2M	O2'-C2'	2.82	1.49	1.42
1	2	1490	OMG	C8-N9	-2.82	1.31	1.37
1	2	1383	A2M	C5-N7	-2.81	1.33	1.39
1	2	1328	OMG	C5-N7	-2.81	1.33	1.39
1	2	601	OMG	C5-N7	-2.80	1.33	1.39
1	2	34	PSU	C6-C5	2.79	1.38	1.35
1	2	1031	A2M	O2'-C2'	2.79	1.49	1.42
1	2	428	OMU	C6-N1	-2.78	1.31	1.38
1	2	1272	OMC	C6-N1	-2.78	1.31	1.38
1	2	1678	A2M	O3'-C3'	-2.77	1.36	1.43
1	2	1347	PSU	C6-C5	2.77	1.38	1.35
1	2	683	OMG	C8-N9	-2.77	1.31	1.37
1	2	116	OMU	O2-C2	-2.76	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1692	PSU	C6-C5	2.76	1.38	1.35
1	2	428	OMU	O2-C2	-2.76	1.18	1.23
1	2	644	OMG	C8-N9	-2.75	1.31	1.37
1	2	1442	OMU	O2-C2	-2.75	1.18	1.23
1	2	572	PSU	C6-C5	2.75	1.38	1.35
1	2	1031	A2M	O3'-C3'	-2.75	1.36	1.43
1	2	99	A2M	O2'-C2'	2.75	1.49	1.42
1	2	1244	PSU	C6-C5	2.75	1.38	1.35
1	2	1678	A2M	C5-N7	-2.74	1.33	1.39
1	2	1383	A2M	O3'-C3'	-2.73	1.36	1.43
1	2	354	OMU	O2-C2	-2.73	1.18	1.23
1	2	172	OMU	O2-C2	-2.72	1.18	1.23
1	2	509	OMG	C8-N9	-2.71	1.31	1.37
1	2	159	A2M	O2'-C2'	2.70	1.49	1.42
1	2	1703	OMC	C6-C5	2.70	1.41	1.35
1	2	159	A2M	C5-N7	-2.69	1.33	1.39
1	2	121	OMU	O2-C2	-2.69	1.18	1.23
1	2	517	OMC	C6-N1	-2.68	1.31	1.38
1	2	1288	OMU	C6-N1	-2.68	1.31	1.38
1	2	517	OMC	C6-C5	2.68	1.41	1.35
1	2	1328	OMG	C2-N1	-2.68	1.31	1.37
1	2	166	A2M	O2'-C2'	2.67	1.49	1.42
1	2	683	OMG	C5-N7	-2.67	1.33	1.39
1	2	966	PSU	C6-C5	2.67	1.38	1.35
1	2	644	OMG	C2-N1	-2.66	1.31	1.37
1	2	1056	PSU	C6-C5	2.65	1.38	1.35
1	2	1248	B8N	C6-C5	2.65	1.38	1.34
1	2	27	A2M	O2'-C2'	2.64	1.49	1.42
1	2	468	A2M	C8-N9	-2.64	1.32	1.37
1	2	1383	A2M	O2'-C2'	2.64	1.49	1.42
1	2	174	OMC	C6-C5	2.63	1.41	1.35
1	2	512	A2M	O2'-C2'	2.63	1.49	1.42
1	2	1678	A2M	O2'-C2'	2.60	1.49	1.42
1	2	1272	OMC	C6-C5	2.59	1.41	1.35
1	2	686	PSU	C6-C5	2.58	1.38	1.35
1	2	36	PSU	C6-C5	2.58	1.38	1.35
1	2	509	OMG	C5-N7	-2.58	1.34	1.39
1	2	109	PSU	C6-C5	2.56	1.38	1.35
1	2	436	OMG	C8-N9	-2.56	1.31	1.37
1	2	1391	OMC	C6-N1	-2.56	1.31	1.38
1	2	406	PSU	C6-C5	2.55	1.38	1.35
1	2	1177	PSU	C6-C5	2.55	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	601	OMG	C8-N9	-2.55	1.31	1.37
1	2	576	A2M	O2'-C2'	2.53	1.49	1.42
1	2	651	PSU	C6-C5	2.53	1.38	1.35
1	2	1337	4AC	C2-N3	-2.53	1.31	1.36
1	2	668	A2M	O3'-C3'	-2.52	1.37	1.43
1	2	436	OMG	C2-N1	-2.50	1.31	1.37
1	2	1328	OMG	C8-N9	-2.50	1.32	1.37
1	2	601	OMG	C2-N1	-2.49	1.31	1.37
1	2	1643	PSU	C6-C5	2.49	1.38	1.35
1	2	867	OMG	C8-N9	-2.49	1.32	1.37
1	2	683	OMG	C2-N1	-2.48	1.31	1.37
1	2	1288	OMU	O2-C2	-2.48	1.18	1.23
1	2	1248	B8N	C1'-C5	2.46	1.55	1.50
1	2	1367	PSU	C6-C5	2.46	1.38	1.35
1	2	218	PSU	C6-C5	2.46	1.38	1.35
1	2	1337	4AC	C6-C5	2.45	1.40	1.35
1	2	517	OMC	C5-C4	-2.45	1.37	1.42
1	2	1850	MA6	C6-N6	2.44	1.44	1.36
1	2	174	OMC	C5-C4	-2.43	1.37	1.42
1	2	1081	PSU	O4'-C1'	-2.41	1.40	1.43
1	2	1851	MA6	C10-N6	2.38	1.51	1.45
1	2	1850	MA6	C10-N6	2.37	1.51	1.45
1	2	867	OMG	C5-N7	-2.37	1.34	1.39
1	2	1326	OMU	O2'-CM2	-2.36	1.34	1.42
1	2	1442	OMU	O2'-CM2	-2.34	1.34	1.42
1	2	668	A2M	O5'-C5'	-2.34	1.39	1.44
1	2	1851	MA6	C6-N6	2.33	1.43	1.36
1	2	1851	MA6	C5-N7	-2.32	1.34	1.39
1	2	1326	OMU	O2-C2	-2.32	1.18	1.23
1	2	468	A2M	O2'-C2'	2.30	1.48	1.42
1	2	1081	PSU	C6-C5	2.30	1.38	1.35
1	2	354	OMU	O2'-CM2	-2.29	1.34	1.42
1	2	121	OMU	O2'-CM2	-2.28	1.34	1.42
1	2	1842	4AC	C6-C5	2.28	1.40	1.35
1	2	867	OMG	C2-N1	-2.28	1.32	1.37
1	2	428	OMU	O2'-CM2	-2.27	1.34	1.42
1	2	512	A2M	O5'-C5'	-2.24	1.39	1.44
1	2	1046	PSU	C6-C5	2.24	1.37	1.35
1	2	116	OMU	O2'-CM2	-2.21	1.34	1.42
1	2	116	OMU	C5-C4	-2.17	1.38	1.43
1	2	172	OMU	O2'-CM2	-2.16	1.34	1.42
1	2	1288	OMU	O2'-CM2	-2.16	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1703	OMC	C2-N3	-2.16	1.32	1.36
1	2	1703	OMC	C5-C4	-2.15	1.38	1.42
1	2	1248	B8N	O4'-C1'	-2.14	1.40	1.43
1	2	354	OMU	C5-C4	-2.13	1.38	1.43
1	2	174	OMC	C2-N3	-2.13	1.32	1.36
1	2	1639	7MG	C2-N1	-2.13	1.32	1.37
1	2	517	OMC	C2-N3	-2.12	1.32	1.36
1	2	814	PSU	C6-C5	2.11	1.37	1.35
1	2	1842	4AC	C2-N3	-2.11	1.32	1.36
1	2	1272	OMC	C5-C4	-2.11	1.38	1.42
1	2	36	PSU	C4-C5	-2.10	1.38	1.44
1	2	1391	OMC	C5-C4	-2.10	1.38	1.42
1	2	1031	A2M	O5'-C5'	-2.07	1.39	1.44
1	2	651	PSU	O4'-C1'	-2.06	1.41	1.43
1	2	27	A2M	O5'-C5'	-2.06	1.39	1.44
1	2	484	A2M	O5'-C5'	-2.05	1.39	1.44
1	2	572	PSU	O4'-C1'	-2.05	1.41	1.43
1	2	1678	A2M	O5'-C5'	-2.04	1.39	1.44
1	2	1248	B8N	C32-C31	2.03	1.56	1.52
1	2	1248	B8N	O2-C2	-2.03	1.18	1.22
1	2	572	PSU	C4-C5	-2.03	1.38	1.44
1	2	1248	B8N	C6-N1	-2.02	1.32	1.36
1	2	1248	B8N	C2-N1	-2.02	1.32	1.39

All (407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	99	A2M	C5-C4-N3	-6.92	117.72	126.75
1	2	509	OMG	C5-C4-N3	-6.10	118.56	128.46
1	2	683	OMG	C5-C4-N3	-6.04	118.66	128.46
1	2	668	A2M	C5-C4-N3	-5.99	118.93	126.75
1	2	166	A2M	C5-C4-N3	-5.97	118.96	126.75
1	2	159	A2M	C5-C4-N3	-5.94	119.00	126.75
1	2	484	A2M	C5-C4-N3	-5.93	119.01	126.75
1	2	867	OMG	C5-C4-N3	-5.82	119.02	128.46
1	2	1383	A2M	C5-C4-N3	-5.82	119.16	126.75
1	2	27	A2M	C5-C4-N3	-5.76	119.24	126.75
1	2	601	OMG	C5-C4-N3	-5.74	119.15	128.46
1	2	1639	7MG	C5-C6-N1	5.64	120.93	110.99
1	2	1850	MA6	C5-C4-N3	-5.59	119.45	126.75
1	2	576	A2M	C5-C4-N3	-5.57	119.48	126.75
1	2	1842	4AC	CM7-C7-N4	5.57	124.92	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	683	OMG	C2-N3-C4	5.56	122.21	112.30
1	2	1490	OMG	C5-C4-N3	-5.51	119.52	128.46
1	2	1678	A2M	C5-C4-N3	-5.48	119.60	126.75
1	2	34	PSU	N1-C2-N3	5.45	121.30	115.13
1	2	436	OMG	C5-C4-N3	-5.41	119.69	128.46
1	2	1692	PSU	C4-N3-C2	-5.38	118.58	126.34
1	2	644	OMG	C5-C4-N3	-5.37	119.75	128.46
1	2	512	A2M	C5-C4-N3	-5.37	119.74	126.75
1	2	468	A2M	C5-C4-N3	-5.34	119.78	126.75
1	2	1031	A2M	C5-C4-N3	-5.26	119.89	126.75
1	2	1832	6MZ	C5-C4-N3	-5.25	119.90	126.75
1	2	1639	7MG	N9-C4-N3	5.22	133.28	125.47
1	2	406	PSU	C4-N3-C2	-5.21	118.84	126.34
1	2	1445	PSU	N1-C2-N3	5.20	121.02	115.13
1	2	1004	PSU	N1-C2-N3	5.12	120.93	115.13
1	2	109	PSU	N1-C2-N3	5.10	120.91	115.13
1	2	99	A2M	N3-C4-N9	5.10	135.48	127.08
1	2	1328	OMG	C5-C4-N3	-5.10	120.19	128.46
1	2	1639	7MG	C2-N3-C4	5.07	121.34	112.30
1	2	1850	MA6	N1-C2-N3	-5.07	120.67	128.60
1	2	1244	PSU	N1-C2-N3	5.05	120.86	115.13
1	2	406	PSU	N1-C2-N3	5.04	120.83	115.13
1	2	172	OMU	N3-C2-N1	5.02	121.56	114.89
1	2	34	PSU	C4-N3-C2	-5.02	119.11	126.34
1	2	1445	PSU	C4-N3-C2	-5.01	119.11	126.34
1	2	681	PSU	N1-C2-N3	5.01	120.81	115.13
1	2	1177	PSU	N1-C2-N3	5.00	120.79	115.13
1	2	601	OMG	C2-N3-C4	4.98	121.17	112.30
1	2	1367	PSU	N1-C2-N3	4.97	120.76	115.13
1	2	1081	PSU	N1-C2-N3	4.96	120.75	115.13
1	2	1692	PSU	N1-C2-N3	4.94	120.73	115.13
1	2	436	OMG	C2-N3-C4	4.93	121.08	112.30
1	2	1851	MA6	C5-C4-N3	-4.92	120.33	126.75
1	2	509	OMG	C2-N3-C4	4.92	121.06	112.30
1	2	93	PSU	N1-C2-N3	4.92	120.70	115.13
1	2	867	OMG	C2-N3-C4	4.90	121.03	112.30
1	2	815	PSU	C4-N3-C2	-4.89	119.29	126.34
1	2	36	PSU	N1-C2-N3	4.89	120.67	115.13
1	2	1367	PSU	C4-N3-C2	-4.86	119.34	126.34
1	2	822	PSU	N1-C2-N3	4.84	120.61	115.13
1	2	428	OMU	N3-C2-N1	4.83	121.30	114.89
1	2	27	A2M	N3-C2-N1	-4.83	121.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	354	OMU	N3-C2-N1	4.82	121.29	114.89
1	2	1625	PSU	N1-C2-N3	4.81	120.58	115.13
1	2	509	OMG	N9-C4-N3	4.81	135.59	125.94
1	2	512	A2M	N3-C2-N1	-4.78	121.13	128.60
1	2	1056	PSU	C4-N3-C2	-4.75	119.49	126.34
1	2	1174	PSU	N1-C2-N3	4.75	120.51	115.13
1	2	1347	PSU	N1-C2-N3	4.75	120.51	115.13
1	2	1046	PSU	C4-N3-C2	-4.75	119.50	126.34
1	2	572	PSU	C4-N3-C2	-4.72	119.54	126.34
1	2	1232	PSU	C4-N3-C2	-4.71	119.55	126.34
1	2	1238	PSU	C4-N3-C2	-4.70	119.56	126.34
1	2	1639	7MG	C5-C4-N3	-4.69	119.20	128.13
1	2	1177	PSU	C4-N3-C2	-4.68	119.60	126.34
1	2	1639	7MG	N9-C8-N7	4.68	110.07	103.38
1	2	1326	OMU	C4-N3-C2	-4.67	120.41	126.58
1	2	1326	OMU	N3-C2-N1	4.66	121.08	114.89
1	2	681	PSU	C4-N3-C2	-4.65	119.63	126.34
1	2	649	PSU	C4-N3-C2	-4.65	119.64	126.34
1	2	815	PSU	N1-C2-N3	4.64	120.39	115.13
1	2	1442	OMU	N3-C2-N1	4.63	121.04	114.89
1	2	1244	PSU	C4-N3-C2	-4.63	119.67	126.34
1	2	109	PSU	C4-N3-C2	-4.63	119.67	126.34
1	2	686	PSU	N1-C2-N3	4.62	120.37	115.13
1	2	1248	B8N	C4-N3-C2	-4.62	119.62	125.46
1	2	116	OMU	N3-C2-N1	4.62	121.02	114.89
1	2	651	PSU	C4-N3-C2	-4.62	119.69	126.34
1	2	814	PSU	C4-N3-C2	-4.61	119.69	126.34
1	2	644	OMG	C2-N3-C4	4.61	120.51	112.30
1	2	966	PSU	C4-N3-C2	-4.59	119.73	126.34
1	2	572	PSU	N1-C2-N3	4.58	120.32	115.13
1	2	822	PSU	C4-N3-C2	-4.57	119.75	126.34
1	2	121	OMU	N3-C2-N1	4.57	120.95	114.89
1	2	218	PSU	C4-N3-C2	-4.55	119.78	126.34
1	2	1056	PSU	N1-C2-N3	4.55	120.29	115.13
1	2	354	OMU	C4-N3-C2	-4.54	120.59	126.58
1	2	1174	PSU	C4-N3-C2	-4.54	119.80	126.34
1	2	1232	PSU	N1-C2-N3	4.54	120.27	115.13
1	2	218	PSU	N1-C2-N3	4.53	120.27	115.13
1	2	1328	OMG	C2-N3-C4	4.51	120.34	112.30
1	2	1490	OMG	C2-N3-C4	4.51	120.34	112.30
1	2	814	PSU	N1-C2-N3	4.51	120.24	115.13
1	2	105	PSU	N1-C2-N3	4.50	120.23	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1288	OMU	N3-C2-N1	4.48	120.84	114.89
1	2	668	A2M	C5-N7-C8	4.47	109.86	103.51
1	2	1081	PSU	C4-N3-C2	-4.47	119.90	126.34
1	2	166	A2M	N3-C2-N1	-4.47	121.62	128.60
1	2	1046	PSU	N1-C2-N3	4.46	120.19	115.13
1	2	1031	A2M	N3-C2-N1	-4.46	121.63	128.60
1	2	1832	6MZ	C6-C5-N7	4.45	137.20	132.39
1	2	166	A2M	N3-C4-N9	4.45	134.41	127.08
1	2	1851	MA6	N1-C2-N3	-4.45	121.65	128.60
1	2	1347	PSU	C4-N3-C2	-4.44	119.94	126.34
1	2	1625	PSU	C4-N3-C2	-4.44	119.94	126.34
1	2	668	A2M	N3-C4-N9	4.43	134.38	127.08
1	2	686	PSU	C4-N3-C2	-4.42	119.98	126.34
1	2	1238	PSU	N1-C2-N3	4.41	120.13	115.13
1	2	1004	PSU	C4-N3-C2	-4.41	119.99	126.34
1	2	428	OMU	C4-N3-C2	-4.38	120.80	126.58
1	2	1383	A2M	N3-C2-N1	-4.38	121.75	128.60
1	2	1248	B8N	N3-C2-N1	4.37	122.94	116.76
1	2	1678	A2M	N3-C2-N1	-4.37	121.76	128.60
1	2	93	PSU	C4-N3-C2	-4.36	120.05	126.34
1	2	484	A2M	C5-N7-C8	4.35	109.69	103.51
1	2	172	OMU	C4-N3-C2	-4.33	120.87	126.58
1	2	668	A2M	N3-C2-N1	-4.32	121.84	128.60
1	2	159	A2M	N3-C4-N9	4.29	134.15	127.08
1	2	1643	PSU	C4-N3-C2	-4.28	120.17	126.34
1	2	651	PSU	N1-C2-N3	4.28	119.98	115.13
1	2	468	A2M	N3-C2-N1	-4.27	121.93	128.60
1	2	468	A2M	C2'-C1'-N9	-4.27	106.35	113.53
1	2	119	PSU	N1-C2-N3	4.26	119.96	115.13
1	2	1851	MA6	C2-N1-C6	4.25	121.79	111.75
1	2	105	PSU	C4-N3-C2	-4.25	120.22	126.34
1	2	484	A2M	N3-C2-N1	-4.22	122.01	128.60
1	2	576	A2M	N3-C2-N1	-4.21	122.02	128.60
1	2	1045	PSU	C4-N3-C2	-4.20	120.29	126.34
1	2	159	A2M	C5-N7-C8	4.20	109.47	103.51
1	2	1850	MA6	C2-N3-C4	4.19	121.66	111.75
1	2	166	A2M	C5-N7-C8	4.18	109.45	103.51
1	2	36	PSU	C4-N3-C2	-4.18	120.31	126.34
1	2	1383	A2M	N3-C4-N9	4.17	133.96	127.08
1	2	159	A2M	N3-C2-N1	-4.17	122.09	128.60
1	2	649	PSU	N1-C2-N3	4.16	119.84	115.13
1	2	1832	6MZ	N1-C2-N3	-4.16	122.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	966	PSU	N1-C2-N3	4.16	119.84	115.13
1	2	121	OMU	C4-N3-C2	-4.15	121.11	126.58
1	2	1643	PSU	N1-C2-N3	4.14	119.82	115.13
1	2	27	A2M	N3-C4-N9	4.14	133.90	127.08
1	2	1383	A2M	C5-N7-C8	4.14	109.39	103.51
1	2	867	OMG	N9-C4-N3	4.13	134.24	125.94
1	2	1678	A2M	C5-N7-C8	4.11	109.36	103.51
1	2	1045	PSU	N1-C2-N3	4.11	119.79	115.13
1	2	576	A2M	N3-C4-N9	4.11	133.85	127.08
1	2	166	A2M	N9-C8-N7	-4.09	108.31	113.91
1	2	1678	A2M	N9-C8-N7	-4.09	108.32	113.91
1	2	159	A2M	N9-C8-N7	-4.08	108.34	113.91
1	2	1850	MA6	C2-N1-C6	4.07	121.37	111.75
1	2	484	A2M	C4-C5-N7	-4.05	105.68	110.62
1	2	1288	OMU	C4-N3-C2	-4.05	121.24	126.58
1	2	512	A2M	N3-C4-N9	4.03	133.72	127.08
1	2	484	A2M	N3-C4-N9	4.03	133.72	127.08
1	2	1678	A2M	N3-C4-N9	4.03	133.72	127.08
1	2	27	A2M	C2-N3-C4	4.02	121.26	111.75
1	2	668	A2M	N9-C8-N7	-4.01	108.42	113.91
1	2	1832	6MZ	C5-N7-C8	4.00	109.19	103.51
1	2	468	A2M	N3-C4-N9	4.00	133.67	127.08
1	2	99	A2M	C2-N3-C4	4.00	121.19	111.75
1	2	119	PSU	C4-N3-C2	-3.99	120.58	126.34
1	2	512	A2M	N9-C8-N7	-3.99	108.45	113.91
1	2	601	OMG	N9-C4-N3	3.97	133.92	125.94
1	2	484	A2M	C2-N3-C4	3.96	121.10	111.75
1	2	1383	A2M	N9-C8-N7	-3.96	108.50	113.91
1	2	1442	OMU	C4-N3-C2	-3.95	121.36	126.58
1	2	1031	A2M	N3-C4-N9	3.95	133.59	127.08
1	2	668	A2M	C2-N3-C4	3.92	121.02	111.75
1	2	166	A2M	C2-N3-C4	3.91	120.98	111.75
1	2	683	OMG	N9-C4-N3	3.90	133.77	125.94
1	2	512	A2M	C2'-C1'-N9	-3.90	106.97	113.53
1	2	512	A2M	C2-N3-C4	3.89	120.93	111.75
1	2	1832	6MZ	C4-C5-N7	-3.87	105.90	110.62
1	2	1383	A2M	C2-N3-C4	3.85	120.85	111.75
1	2	159	A2M	C2-N3-C4	3.85	120.85	111.75
1	2	468	A2M	O4'-C1'-N9	3.84	115.62	108.06
1	2	354	OMU	C5-C4-N3	3.82	120.56	114.84
1	2	116	OMU	C4-N3-C2	-3.81	121.56	126.58
1	2	1832	6MZ	C2-N3-C4	3.78	120.69	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	512	A2M	C5-N7-C8	3.78	108.88	103.51
1	2	1678	A2M	C2-N3-C4	3.77	120.67	111.75
1	2	1850	MA6	N3-C4-N9	3.77	133.29	127.08
1	2	99	A2M	N3-C2-N1	-3.72	122.78	128.60
1	2	576	A2M	C5-N7-C8	3.70	108.77	103.51
1	2	428	OMU	C5-C4-N3	3.69	120.37	114.84
1	2	1326	OMU	C5-C4-N3	3.67	120.34	114.84
1	2	1490	OMG	N9-C4-N3	3.66	133.29	125.94
1	2	668	A2M	C4-C5-N7	-3.65	106.17	110.62
1	2	406	PSU	O2-C2-N1	-3.65	118.78	122.79
1	2	576	A2M	N9-C8-N7	-3.64	108.94	113.91
1	2	576	A2M	C2-N3-C4	3.63	120.32	111.75
1	2	484	A2M	N9-C8-N7	-3.62	108.96	113.91
1	2	468	A2M	C2-N3-C4	3.62	120.29	111.75
1	2	1031	A2M	C2-N3-C4	3.61	120.29	111.75
1	2	822	PSU	O2-C2-N1	-3.60	118.83	122.79
1	2	1031	A2M	C5-N7-C8	3.59	108.61	103.51
1	2	1832	6MZ	N9-C8-N7	-3.59	109.00	113.91
1	2	1851	MA6	C2-N3-C4	3.58	120.22	111.75
1	2	159	A2M	C4-C5-N7	-3.56	106.28	110.62
1	2	1850	MA6	C5-N7-C8	3.53	108.53	103.51
1	2	428	OMU	C1'-N1-C2	3.53	123.95	117.57
1	2	1288	OMU	C5-C4-N3	3.50	120.07	114.84
1	2	109	PSU	O2-C2-N1	-3.49	118.94	122.79
1	2	99	A2M	C5-N7-C8	3.49	108.47	103.51
1	2	1383	A2M	C4-C5-N7	-3.48	106.38	110.62
1	2	1678	A2M	C4-C5-N7	-3.44	106.42	110.62
1	2	121	OMU	C5-C4-N3	3.44	119.98	114.84
1	2	172	OMU	C5-C4-N3	3.44	119.98	114.84
1	2	1851	MA6	C4-C5-N7	-3.43	106.44	110.62
1	2	1337	4AC	O2-C2-N3	-3.43	116.75	122.33
1	2	1850	MA6	C4-C5-N7	-3.42	106.45	110.62
1	2	1328	OMG	C6-C5-N7	3.42	136.61	130.25
1	2	1832	6MZ	N3-C4-N9	3.39	132.67	127.08
1	2	1326	OMU	O4-C4-C5	-3.38	119.22	125.16
1	2	116	OMU	C5-C4-N3	3.36	119.87	114.84
1	2	683	OMG	O3'-C3'-C4'	3.32	120.65	111.05
1	2	166	A2M	C4-C5-N7	-3.31	106.59	110.62
1	2	683	OMG	C2'-C1'-N9	-3.29	107.83	114.22
1	2	1046	PSU	O2-C2-N1	-3.29	119.17	122.79
1	2	27	A2M	C5-N7-C8	3.27	108.16	103.51
1	2	1031	A2M	N9-C8-N7	-3.27	109.44	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	644	OMG	C6-C5-N7	3.26	136.30	130.25
1	2	644	OMG	N9-C4-N3	3.25	132.47	125.94
1	2	436	OMG	N9-C4-N3	3.23	132.43	125.94
1	2	1678	A2M	C4-N9-C8	3.21	109.20	105.73
1	2	1442	OMU	C5-C4-N3	3.20	119.64	114.84
1	2	436	OMG	C6-C5-N7	3.20	136.20	130.25
1	2	36	PSU	C6-N1-C2	-3.19	119.42	122.68
1	2	468	A2M	N9-C8-N7	-3.18	109.57	113.91
1	2	576	A2M	C4-C5-N7	-3.17	106.75	110.62
1	2	1851	MA6	C5-N7-C8	3.16	107.99	103.51
1	2	1850	MA6	N9-C8-N7	-3.14	109.61	113.91
1	2	683	OMG	C6-C5-N7	3.13	136.06	130.25
1	2	512	A2M	C4-N9-C8	3.11	109.10	105.73
1	2	1004	PSU	C6-N1-C2	-3.11	119.50	122.68
1	2	468	A2M	C5-N7-C8	3.10	107.92	103.51
1	2	1639	7MG	C2-N1-C6	-3.08	119.48	125.10
1	2	159	A2M	C2'-C1'-N9	-3.08	108.34	113.53
1	2	159	A2M	C4-N9-C8	3.07	109.06	105.73
1	2	686	PSU	O2-C2-N1	-3.07	119.41	122.79
1	2	1004	PSU	O2-C2-N1	-3.06	119.43	122.79
1	2	1692	PSU	O4-C4-N3	-3.05	114.26	120.12
1	2	116	OMU	O4-C4-C5	-3.05	119.79	125.16
1	2	121	OMU	O4-C4-C5	-3.04	119.81	125.16
1	2	166	A2M	C4-N9-C8	3.03	109.01	105.73
1	2	1442	OMU	O4-C4-C5	-3.03	119.83	125.16
1	2	27	A2M	N9-C8-N7	-3.01	109.80	113.91
1	2	99	A2M	C4-C5-N7	-3.00	106.97	110.62
1	2	1842	4AC	O2-C2-N3	-2.99	117.47	122.33
1	2	1031	A2M	C4-C5-N7	-2.97	107.00	110.62
1	2	1328	OMG	N9-C4-N3	2.95	131.87	125.94
1	2	354	OMU	O4-C4-C5	-2.95	119.97	125.16
1	2	1851	MA6	N3-C4-N9	2.94	131.93	127.08
1	2	512	A2M	C4-C5-N7	-2.94	107.03	110.62
1	2	1445	PSU	O2-C2-N1	-2.93	119.56	122.79
1	2	1288	OMU	O4-C4-C5	-2.93	120.01	125.16
1	2	576	A2M	C4-N9-C8	2.91	108.88	105.73
1	2	509	OMG	C5-C6-N1	2.90	120.57	113.19
1	2	649	PSU	O4-C4-N3	-2.89	114.57	120.12
1	2	668	A2M	C4-N9-C8	2.88	108.85	105.73
1	2	1383	A2M	C4-N9-C8	2.88	108.85	105.73
1	2	1639	7MG	O6-C6-C5	-2.88	120.48	127.54
1	2	815	PSU	O2-C2-N1	-2.87	119.63	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	601	OMG	C5-C6-N1	2.86	120.46	113.19
1	2	93	PSU	C6-N1-C2	-2.86	119.76	122.68
1	2	644	OMG	C4-C5-N7	-2.85	106.20	110.72
1	2	27	A2M	C4-C5-N7	-2.84	107.16	110.62
1	2	1842	4AC	O7-C7-N4	-2.83	117.23	121.82
1	2	99	A2M	N9-C8-N7	-2.83	110.05	113.91
1	2	1238	PSU	O2-C2-N1	-2.79	119.72	122.79
1	2	436	OMG	C4-C5-N7	-2.79	106.31	110.72
1	2	683	OMG	C4-C5-N7	-2.78	106.33	110.72
1	2	468	A2M	O4'-C4'-C3'	-2.77	99.64	105.11
1	2	1232	PSU	O2-C2-N1	-2.76	119.75	122.79
1	2	109	PSU	C6-N1-C2	-2.76	119.86	122.68
1	2	1639	7MG	C6-C5-C4	-2.74	116.98	122.62
1	2	1244	PSU	O2-C2-N1	-2.72	119.80	122.79
1	2	1851	MA6	N9-C8-N7	-2.72	110.20	113.91
1	2	1328	OMG	C4-C5-N7	-2.71	106.42	110.72
1	2	34	PSU	O2-C2-N1	-2.71	119.81	122.79
1	2	601	OMG	C2-N1-C6	-2.70	120.17	125.10
1	2	1383	A2M	C2'-C1'-N9	-2.70	108.98	113.53
1	2	166	A2M	C2'-C1'-N9	-2.69	109.00	113.53
1	2	1625	PSU	O2-C2-N1	-2.69	119.83	122.79
1	2	428	OMU	O2-C2-N3	-2.67	116.53	121.50
1	2	683	OMG	C5-C6-N1	2.66	119.95	113.19
1	2	1490	OMG	C6-C5-N7	2.66	135.20	130.25
1	2	651	PSU	O2-C2-N1	-2.65	119.88	122.79
1	2	1328	OMG	C5-C6-N1	2.64	119.89	113.19
1	2	1174	PSU	O2-C2-N1	-2.63	119.89	122.79
1	2	218	PSU	O2-C2-N1	-2.63	119.90	122.79
1	2	1703	OMC	O2-C2-N3	-2.61	118.08	122.33
1	2	601	OMG	C6-C5-N7	2.60	135.09	130.25
1	2	172	OMU	O4-C4-C5	-2.60	120.59	125.16
1	2	1639	7MG	C6-C5-N7	2.60	136.00	131.91
1	2	1391	OMC	O2-C2-N3	-2.60	118.11	122.33
1	2	867	OMG	O6-C6-C5	-2.60	119.71	126.60
1	2	1367	PSU	O2-C2-N1	-2.59	119.94	122.79
1	2	1288	OMU	C1'-N1-C2	2.58	122.25	117.57
1	2	681	PSU	C6-N1-C2	-2.58	120.04	122.68
1	2	428	OMU	C1'-N1-C6	-2.58	115.22	120.84
1	2	119	PSU	O4-C4-N3	-2.57	115.20	120.12
1	2	1625	PSU	C6-N1-C2	-2.56	120.06	122.68
1	2	867	OMG	C5-C6-N1	2.56	119.70	113.19
1	2	1842	4AC	C5-C4-N3	-2.56	118.48	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1174	PSU	C6-N1-C2	-2.55	120.07	122.68
1	2	509	OMG	C2-N1-C6	-2.54	120.46	125.10
1	2	822	PSU	C6-N1-C2	-2.54	120.08	122.68
1	2	683	OMG	C8-N7-C5	2.54	108.84	104.24
1	2	867	OMG	C6-C5-N7	2.53	134.96	130.25
1	2	468	A2M	C4-C5-N7	-2.53	107.53	110.62
1	2	1832	6MZ	C4-N9-C8	2.53	108.47	105.73
1	2	1347	PSU	C6-N1-C2	-2.53	120.10	122.68
1	2	1328	OMG	C2-N1-C6	-2.51	120.53	125.10
1	2	105	PSU	C6-N1-C2	-2.50	120.13	122.68
1	2	468	A2M	C4'-O4'-C1'	-2.50	103.96	109.47
1	2	468	A2M	C4-N9-C8	2.49	108.43	105.73
1	2	1031	A2M	C4-N9-C8	2.49	108.43	105.73
1	2	601	OMG	O6-C6-C5	-2.49	120.00	126.60
1	2	34	PSU	C6-N1-C2	-2.47	120.15	122.68
1	2	428	OMU	O4-C4-C5	-2.47	120.82	125.16
1	2	484	A2M	C4-N9-C8	2.46	108.40	105.73
1	2	1045	PSU	C6-N1-C2	-2.46	120.17	122.68
1	2	1244	PSU	C6-N1-C2	-2.46	120.17	122.68
1	2	509	OMG	O6-C6-C5	-2.46	120.08	126.60
1	2	484	A2M	C6-C5-N7	2.46	136.60	132.02
1	2	105	PSU	O2-C2-N1	-2.45	120.09	122.79
1	2	27	A2M	O4'-C1'-N9	2.45	112.89	108.06
1	2	644	OMG	C8-N7-C5	2.45	108.68	104.24
1	2	814	PSU	O2-C2-N1	-2.45	120.10	122.79
1	2	1177	PSU	C6-N1-C2	-2.45	120.18	122.68
1	2	1177	PSU	O2-C2-N1	-2.42	120.12	122.79
1	2	436	OMG	C8-N7-C5	2.39	108.57	104.24
1	2	683	OMG	C2-N1-C6	-2.39	120.74	125.10
1	2	436	OMG	C5-C6-N1	2.39	119.26	113.19
1	2	512	A2M	C5'-C4'-C3'	-2.39	106.23	115.18
1	2	1045	PSU	O2-C2-N1	-2.39	120.16	122.79
1	2	572	PSU	O2-C2-N1	-2.38	120.17	122.79
1	2	867	OMG	C2-N1-C6	-2.38	120.77	125.10
1	2	867	OMG	C4-C5-N7	-2.37	106.96	110.72
1	2	1248	B8N	C31-N3-C2	2.37	121.23	117.67
1	2	1490	OMG	C5-C6-N1	2.37	119.21	113.19
1	2	436	OMG	O6-C6-C5	-2.37	120.32	126.60
1	2	116	OMU	O2-C2-N1	-2.35	119.66	122.79
1	2	1490	OMG	C2-N1-C6	-2.35	120.82	125.10
1	2	93	PSU	O2-C2-N1	-2.35	120.21	122.79
1	2	644	OMG	C5-C6-N1	2.35	119.15	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1692	PSU	C5-C4-N3	2.34	121.87	116.58
1	2	686	PSU	C6-N1-C2	-2.33	120.31	122.68
1	2	1272	OMC	O2-C2-N3	-2.32	118.56	122.33
1	2	649	PSU	C5-C4-N3	2.32	121.83	116.58
1	2	867	OMG	C8-N7-C5	2.31	108.43	104.24
1	2	1081	PSU	C6-N1-C2	-2.30	120.33	122.68
1	2	1328	OMG	C8-N7-C5	2.28	108.37	104.24
1	2	121	OMU	O2-C2-N1	-2.28	119.76	122.79
1	2	1490	OMG	C4-C5-N7	-2.27	107.12	110.72
1	2	428	OMU	O2'-C2'-C1'	2.27	113.51	109.08
1	2	1248	B8N	O2-C2-N3	-2.27	118.83	121.99
1	2	1445	PSU	C6-N1-C2	-2.27	120.36	122.68
1	2	1842	4AC	O7-C7-CM7	-2.27	117.84	122.06
1	2	683	OMG	O3'-C3'-C2'	2.27	117.61	111.17
1	2	822	PSU	O4'-C1'-C2'	2.27	108.34	105.14
1	2	644	OMG	C2-N1-C6	-2.27	120.96	125.10
1	2	1643	PSU	C6-N1-C2	-2.25	120.39	122.68
1	2	1383	A2M	C6-C5-N7	2.24	136.20	132.02
1	2	462	OMC	O2-C2-N3	-2.24	118.69	122.33
1	2	509	OMG	C6-C5-N7	2.24	134.42	130.25
1	2	683	OMG	O6-C6-C5	-2.24	120.66	126.60
1	2	1850	MA6	C4-N9-C8	2.23	108.15	105.73
1	2	1367	PSU	C6-N1-C2	-2.23	120.40	122.68
1	2	116	OMU	C1'-N1-C2	2.22	121.60	117.57
1	2	867	OMG	N9-C8-N7	-2.22	109.21	113.39
1	2	1490	OMG	O6-C6-C5	-2.21	120.73	126.60
1	2	116	OMU	C6-C5-C4	-2.20	116.51	119.52
1	2	119	PSU	C6-N1-C2	-2.19	120.44	122.68
1	2	517	OMC	O2-C2-N3	-2.19	118.77	122.33
1	2	1445	PSU	C6-C5-C4	2.18	119.72	118.20
1	2	436	OMG	N9-C8-N7	-2.18	109.29	113.39
1	2	572	PSU	C6-N1-C2	-2.17	120.46	122.68
1	2	966	PSU	O2-C2-N1	-2.17	120.40	122.79
1	2	1031	A2M	C2'-C1'-N9	-2.17	109.88	113.53
1	2	683	OMG	C3'-C2'-C1'	-2.16	98.83	102.89
1	2	683	OMG	N9-C8-N7	-2.16	109.33	113.39
1	2	172	OMU	O2-C2-N1	-2.15	119.92	122.79
1	2	1692	PSU	O2-C2-N3	-2.15	117.76	121.82
1	2	668	A2M	C6-C5-N7	2.14	136.02	132.02
1	2	1248	B8N	C5-C4-N3	2.14	120.13	116.17
1	2	681	PSU	O2-C2-N1	-2.13	120.44	122.79
1	2	354	OMU	C1'-N1-C2	2.13	121.43	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1328	OMG	N9-C8-N7	-2.13	109.39	113.39
1	2	1244	PSU	C6-C5-C4	2.12	119.68	118.20
1	2	1081	PSU	O4'-C1'-C2'	2.12	108.13	105.14
1	2	1442	OMU	O2-C2-N1	-2.12	119.97	122.79
1	2	27	A2M	C4-N9-C8	2.11	108.02	105.73
1	2	436	OMG	C2-N1-C6	-2.09	121.28	125.10
1	2	1056	PSU	C6-N1-C2	-2.08	120.55	122.68
1	2	1678	A2M	C6-C5-N7	2.08	135.90	132.02
1	2	601	OMG	C4-C5-N7	-2.07	107.44	110.72
1	2	512	A2M	C6-C5-N7	2.06	135.85	132.02
1	2	644	OMG	N9-C8-N7	-2.05	109.53	113.39
1	2	1643	PSU	O2-C2-N1	-2.05	120.54	122.79
1	2	1442	OMU	C1'-N1-C2	2.03	121.24	117.57
1	2	218	PSU	C6-N1-C2	-2.03	120.61	122.68

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	428	OMU	C3'-C4'-C5'-O5'
1	2	428	OMU	O4'-C4'-C5'-O5'
1	2	468	A2M	O4'-C1'-N9-C8
1	2	468	A2M	O4'-C1'-N9-C4
1	2	509	OMG	O4'-C4'-C5'-O5'
1	2	509	OMG	C3'-C4'-C5'-O5'
1	2	644	OMG	O4'-C4'-C5'-O5'
1	2	644	OMG	C3'-C4'-C5'-O5'
1	2	649	PSU	O4'-C1'-C5-C4
1	2	649	PSU	O4'-C1'-C5-C6
1	2	668	A2M	C3'-C4'-C5'-O5'
1	2	867	OMG	C1'-C2'-O2'-CM2
1	2	1248	B8N	O4'-C4'-C5'-O5'
1	2	1248	B8N	C3'-C4'-C5'-O5'
1	2	1248	B8N	N34-C33-C34-O35
1	2	1248	B8N	N3-C31-C32-C33
1	2	1248	B8N	C31-C32-C33-N34
1	2	1272	OMC	C1'-C2'-O2'-CM2
1	2	1678	A2M	C1'-C2'-O2'-CM'
1	2	1692	PSU	O4'-C1'-C5-C4
1	2	1692	PSU	O4'-C1'-C5-C6
1	2	99	A2M	O4'-C4'-C5'-O5'
1	2	172	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	668	A2M	O4'-C4'-C5'-O5'
1	2	172	OMU	C3'-C4'-C5'-O5'
1	2	683	OMG	C3'-C4'-C5'-O5'
1	2	1248	B8N	N34-C33-C34-O36
1	2	99	A2M	C3'-C4'-C5'-O5'
1	2	119	PSU	C3'-C4'-C5'-O5'
1	2	683	OMG	O4'-C4'-C5'-O5'
1	2	1850	MA6	O4'-C4'-C5'-O5'
1	2	468	A2M	O4'-C4'-C5'-O5'
1	2	1842	4AC	O7-C7-N4-C4
1	2	1842	4AC	CM7-C7-N4-C4
1	2	428	OMU	O4'-C1'-N1-C6
1	2	867	OMG	O4'-C4'-C5'-O5'
1	2	1248	B8N	C31-C32-C33-C34
1	2	509	OMG	C4'-C5'-O5'-P
1	2	1490	OMG	C4'-C5'-O5'-P
1	2	119	PSU	O4'-C4'-C5'-O5'
1	2	1490	OMG	O4'-C4'-C5'-O5'
1	2	644	OMG	C4'-C5'-O5'-P
1	2	1850	MA6	C3'-C4'-C5'-O5'
1	2	428	OMU	O4'-C1'-N1-C2
1	2	1031	A2M	O4'-C4'-C5'-O5'
1	2	462	OMC	C1'-C2'-O2'-CM2
1	2	428	OMU	C2'-C1'-N1-C2
1	2	867	OMG	C3'-C4'-C5'-O5'
1	2	1851	MA6	C3'-C4'-C5'-O5'
1	2	668	A2M	C2'-C1'-N9-C8

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	116	OMU	2	0
1	2	354	OMU	1	0
1	2	1703	OMC	1	0
1	2	867	OMG	1	0
1	2	509	OMG	1	0
1	2	1272	OMC	1	0
1	2	99	A2M	1	0
1	2	1639	7MG	4	0
1	2	1678	A2M	2	0
1	2	121	OMU	1	0

Continued on next page...

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1174	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 134 are monoatomic - leaving 2 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	$\# Z > 2$
37	ASP	2	1901	-	6,7,8	0.86	0	5,8,10	1.07	0
40	ATP	z	602	38	29,33,33	1.35	4 (13%)	44,52,52	1.87	10 (22%)

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
37	ASP	2	1901	-	-	2/5/6/8	-
40	ATP	z	602	38	-	1/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	z	602	ATP	C5-C4	4.17	1.46	1.39
40	z	602	ATP	C5-N7	-2.67	1.34	1.39
40	z	602	ATP	C5-C6	2.44	1.47	1.41
40	z	602	ATP	C4-N9	-2.12	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	z	602	ATP	C5-C4-N3	-6.01	118.90	126.75
40	z	602	ATP	N3-C4-N9	4.97	135.28	127.08
40	z	602	ATP	C2-N3-C4	3.74	120.58	111.75
40	z	602	ATP	C4-C5-N7	-3.03	106.93	110.62
40	z	602	ATP	N3-C2-N1	-2.95	123.98	128.60
40	z	602	ATP	C4-N9-C8	2.79	108.76	105.73
40	z	602	ATP	C5-N7-C8	2.68	107.32	103.51
40	z	602	ATP	PA-O3A-PB	-2.54	124.10	132.83
40	z	602	ATP	C6-C5-N7	2.10	135.93	132.02
40	z	602	ATP	N9-C8-N7	-2.01	111.17	113.91

There are no chirality outliers.

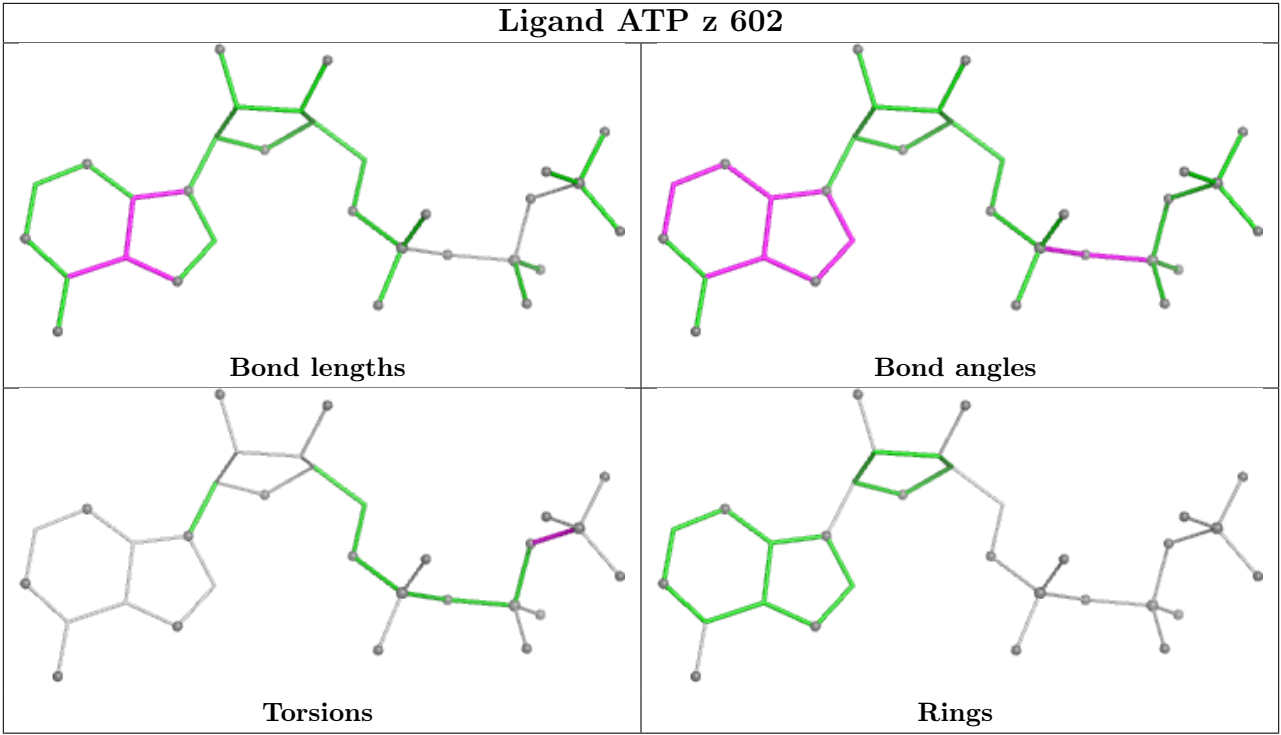
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1901	ASP	C-CA-CB-CG
40	z	602	ATP	PB-O3B-PG-O3G
37	2	1901	ASP	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	563:G	O3'	564:A	P	3.12

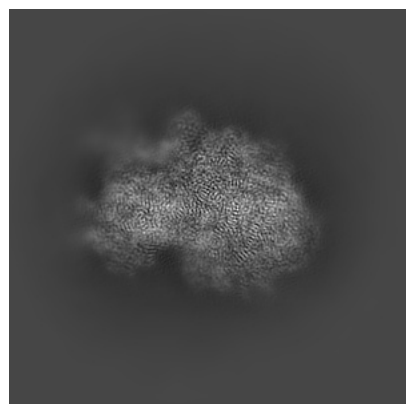
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11521. These allow visual inspection of the internal detail of the map and identification of artifacts.

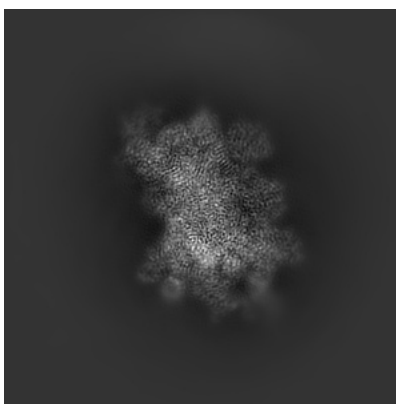
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

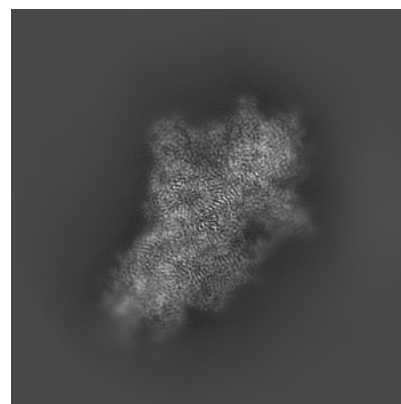
6.1.1 Primary map



X

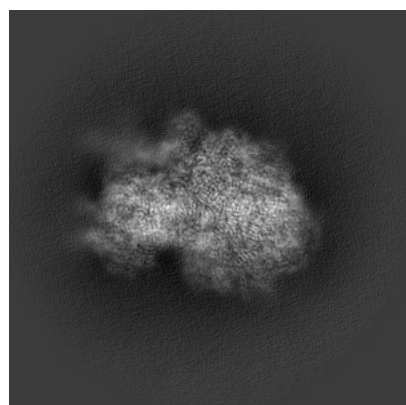


Y

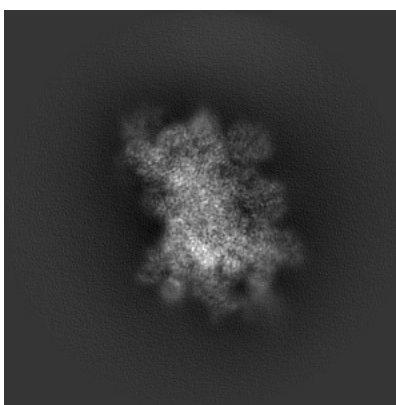


Z

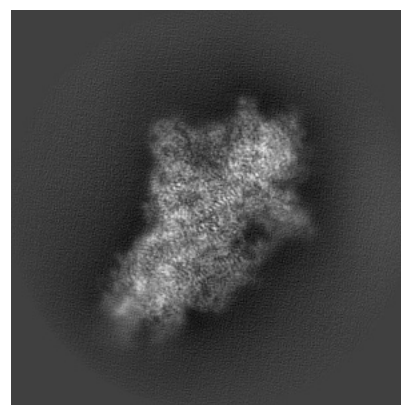
6.1.2 Raw map



X



Y

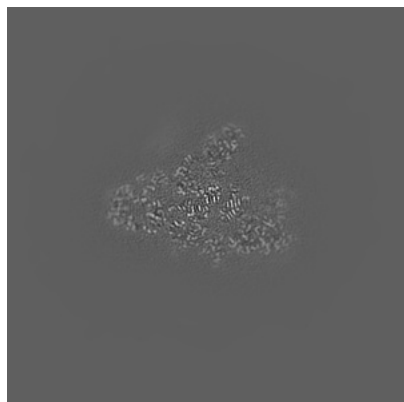


Z

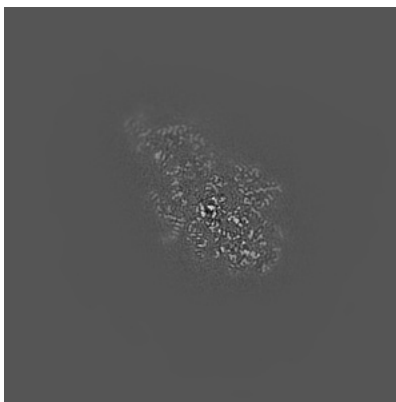
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

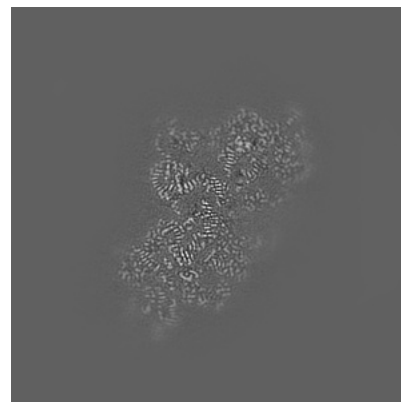
6.2.1 Primary map



X Index: 180

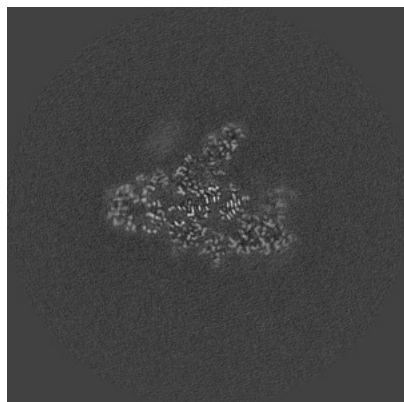


Y Index: 180

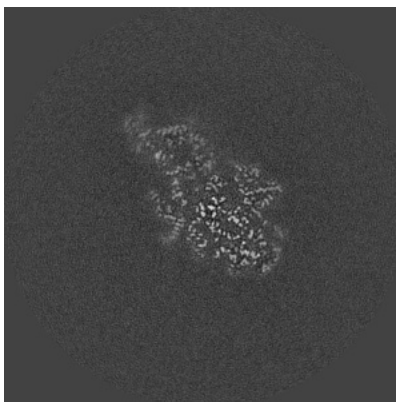


Z Index: 180

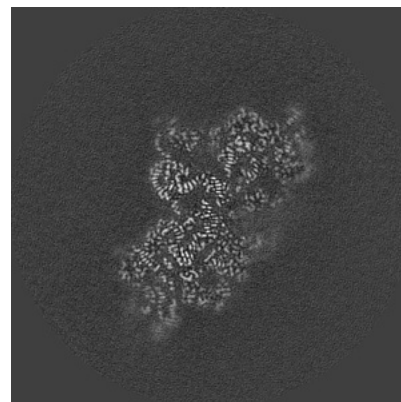
6.2.2 Raw map



X Index: 180



Y Index: 180

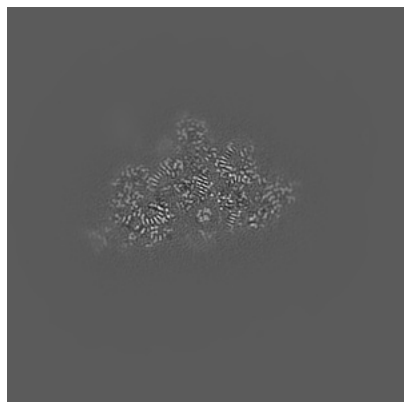


Z Index: 180

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

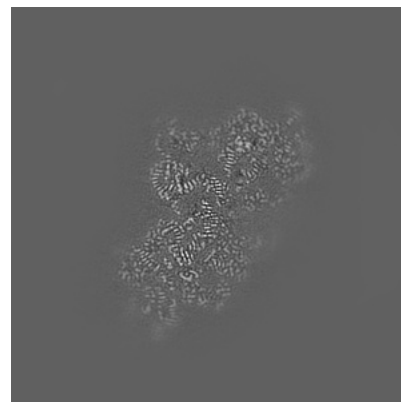
6.3.1 Primary map



X Index: 155

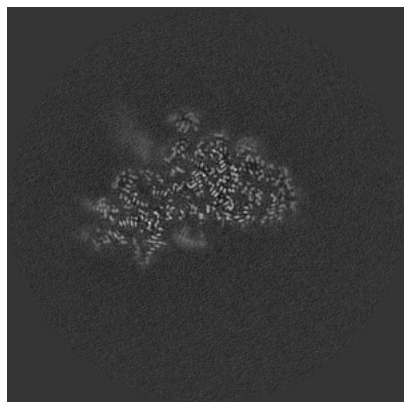


Y Index: 199

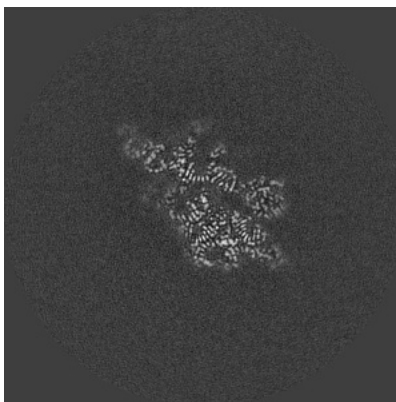


Z Index: 180

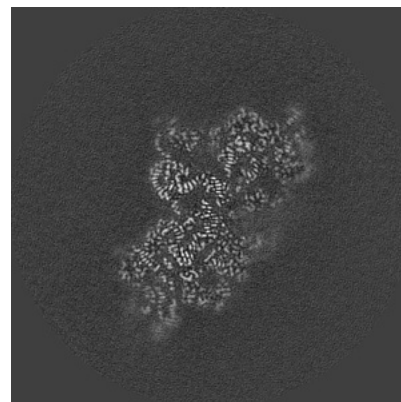
6.3.2 Raw map



X Index: 145



Y Index: 199

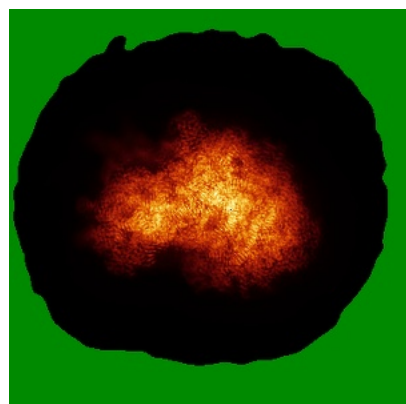


Z Index: 180

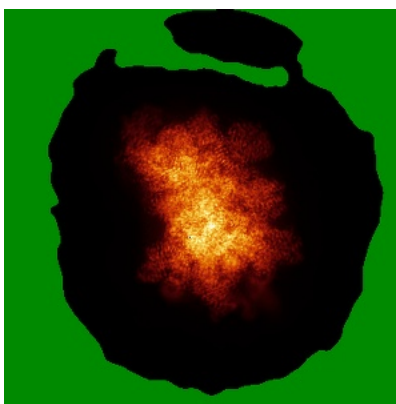
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

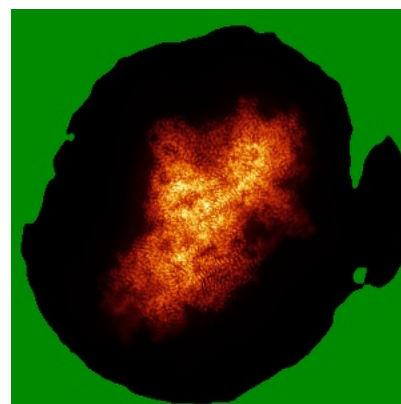
6.4.1 Primary map



X

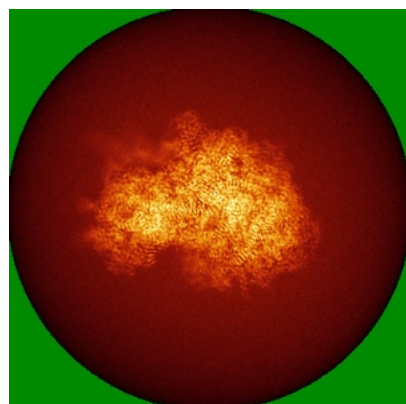


Y

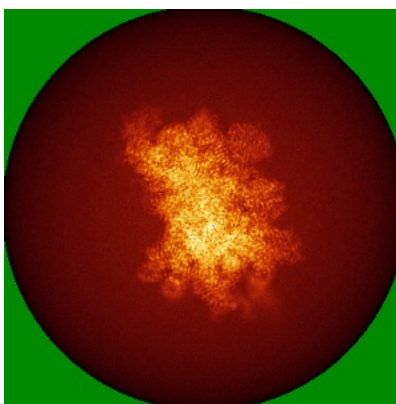


Z

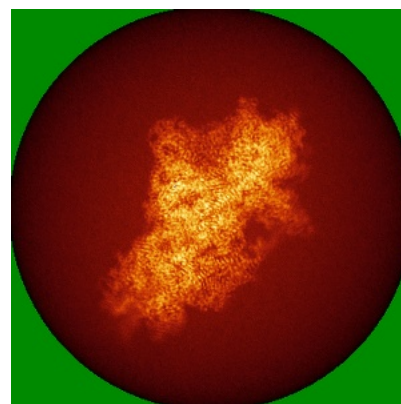
6.4.2 Raw map



X



Y

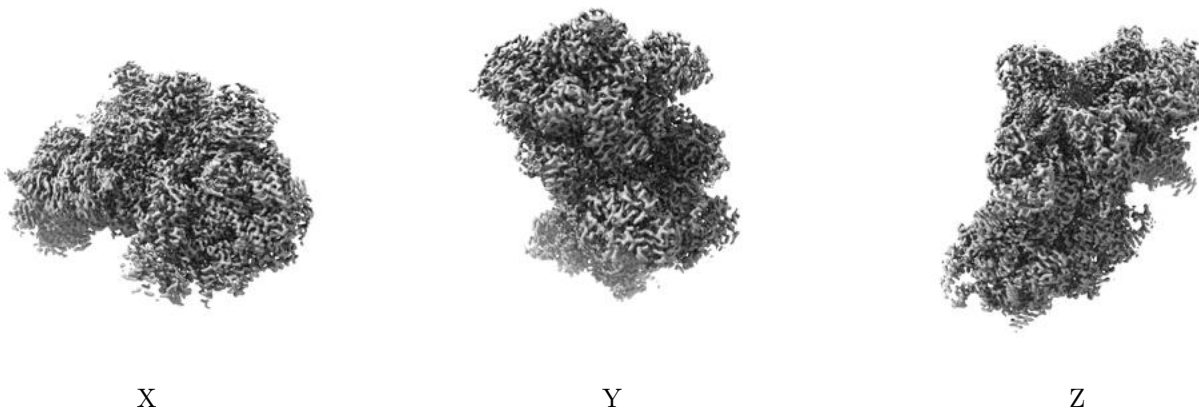


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

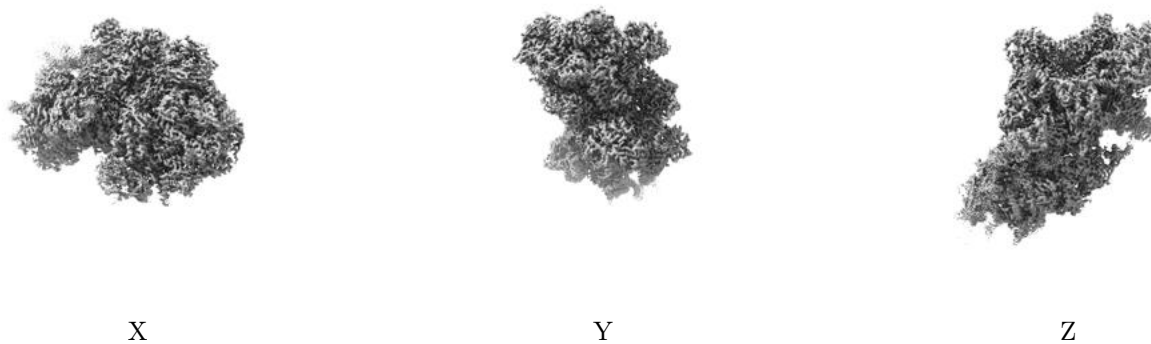
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

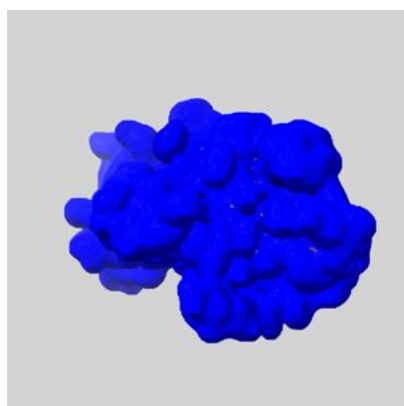
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

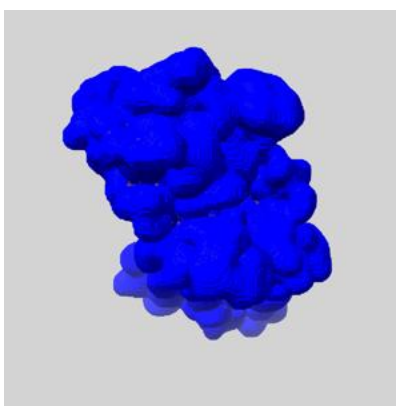
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

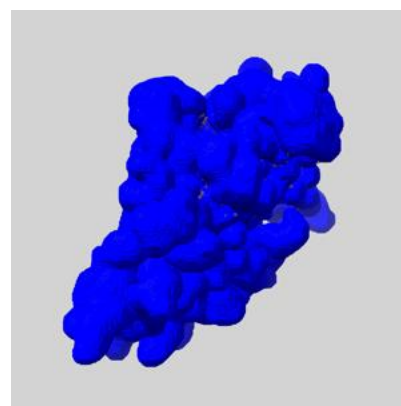
6.6.1 emd_11521_msk_1.map [i](#)



X



Y

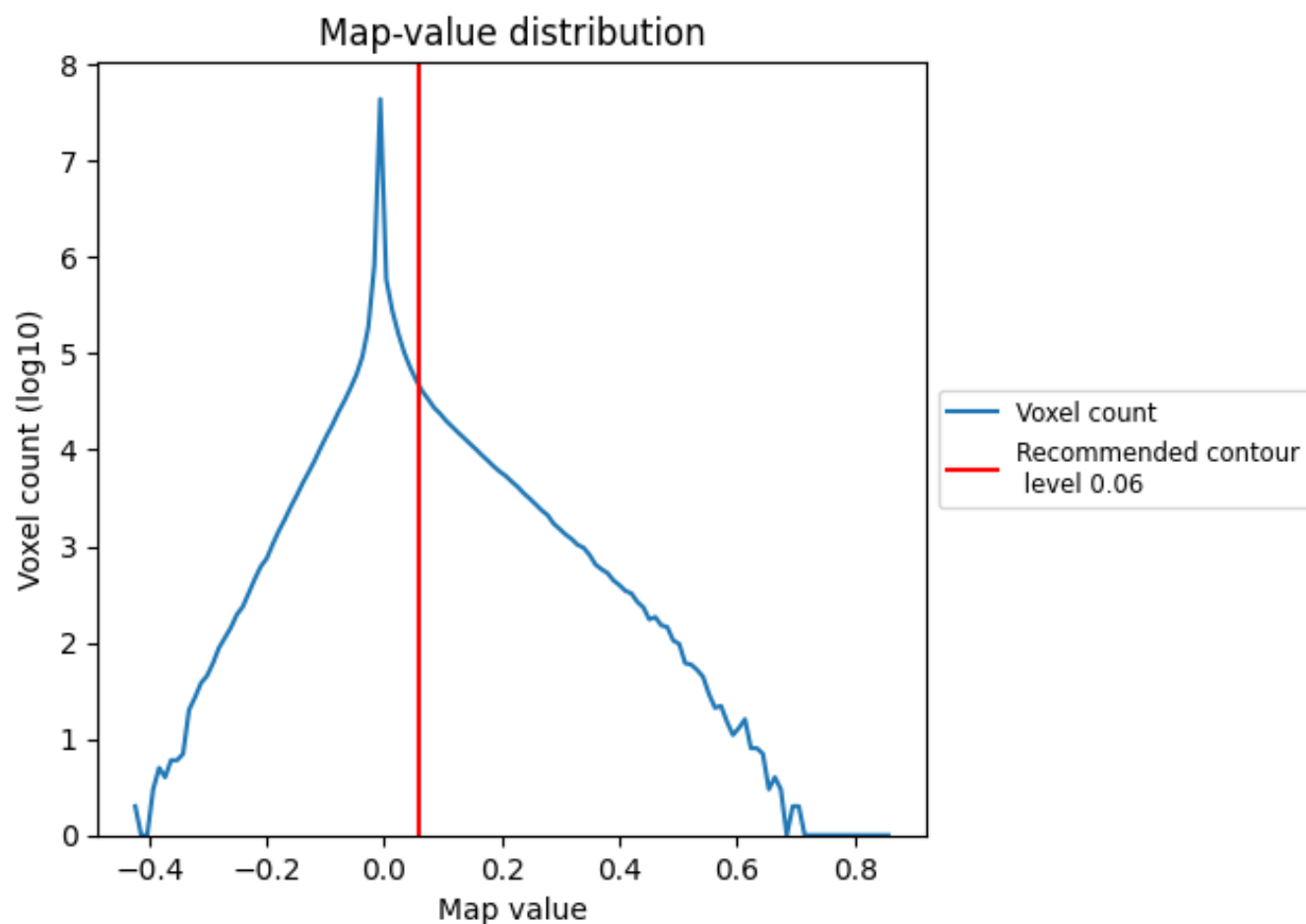


Z

7 Map analysis [i](#)

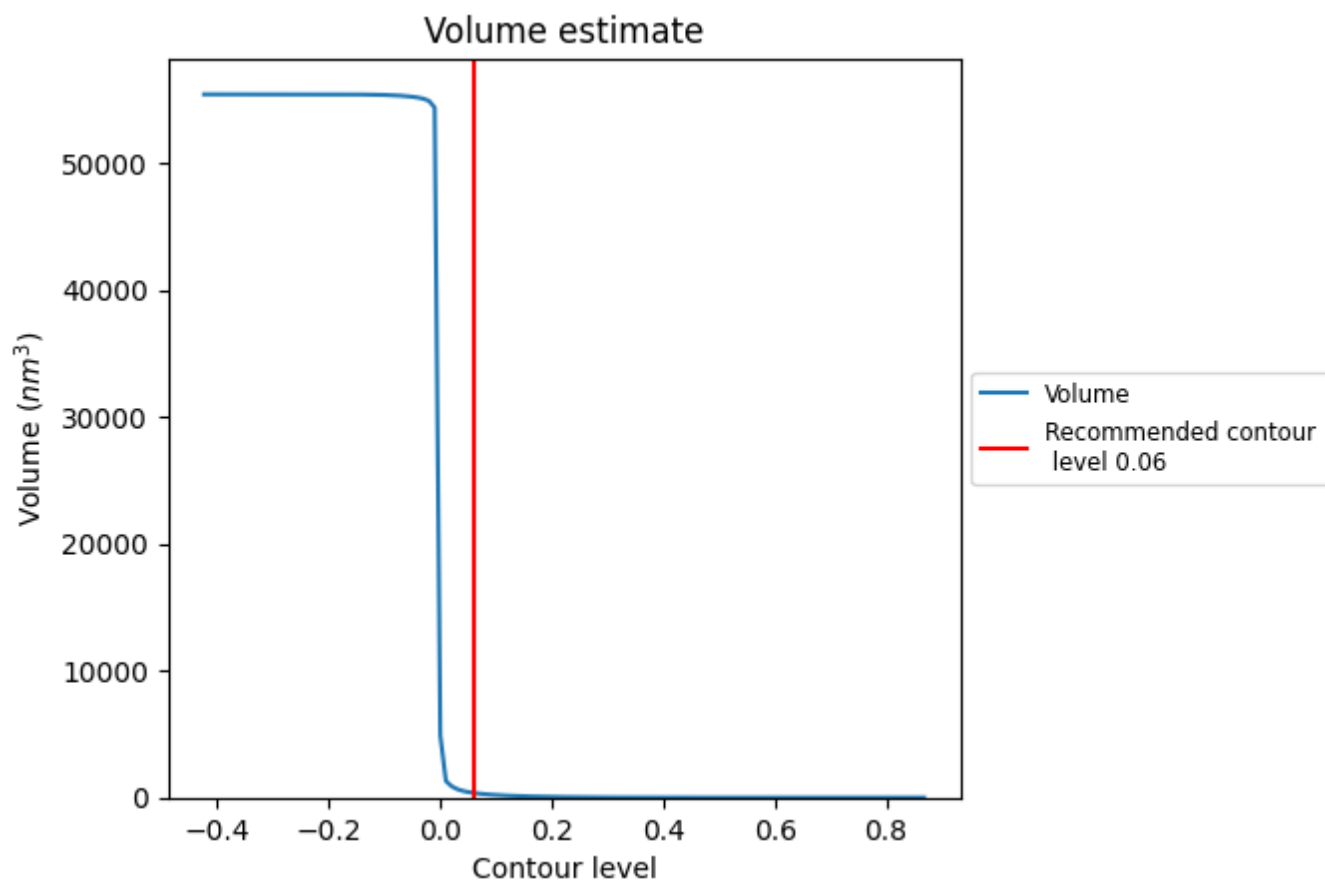
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

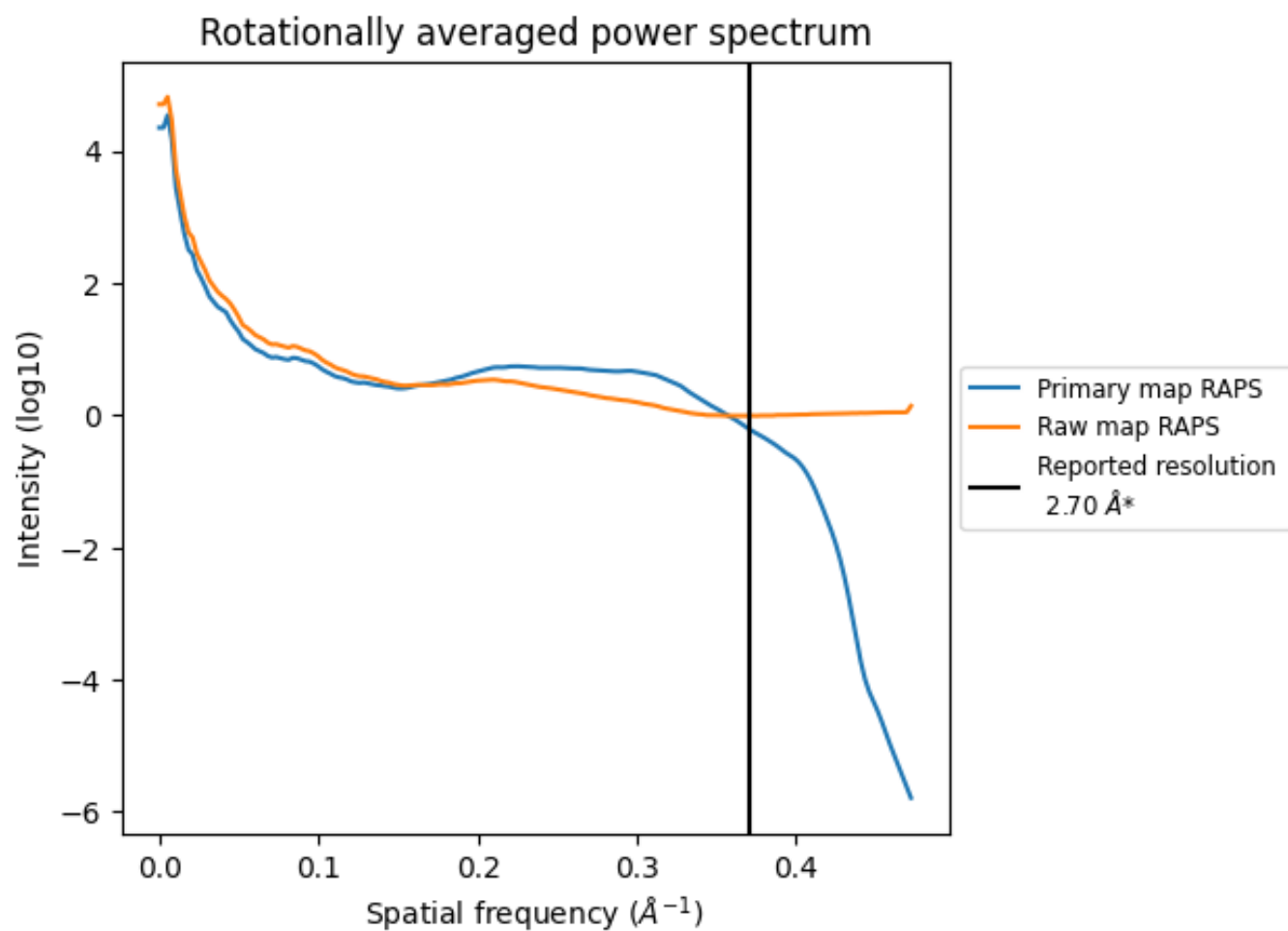
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm^3 ; this corresponds to an approximate mass of 328 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

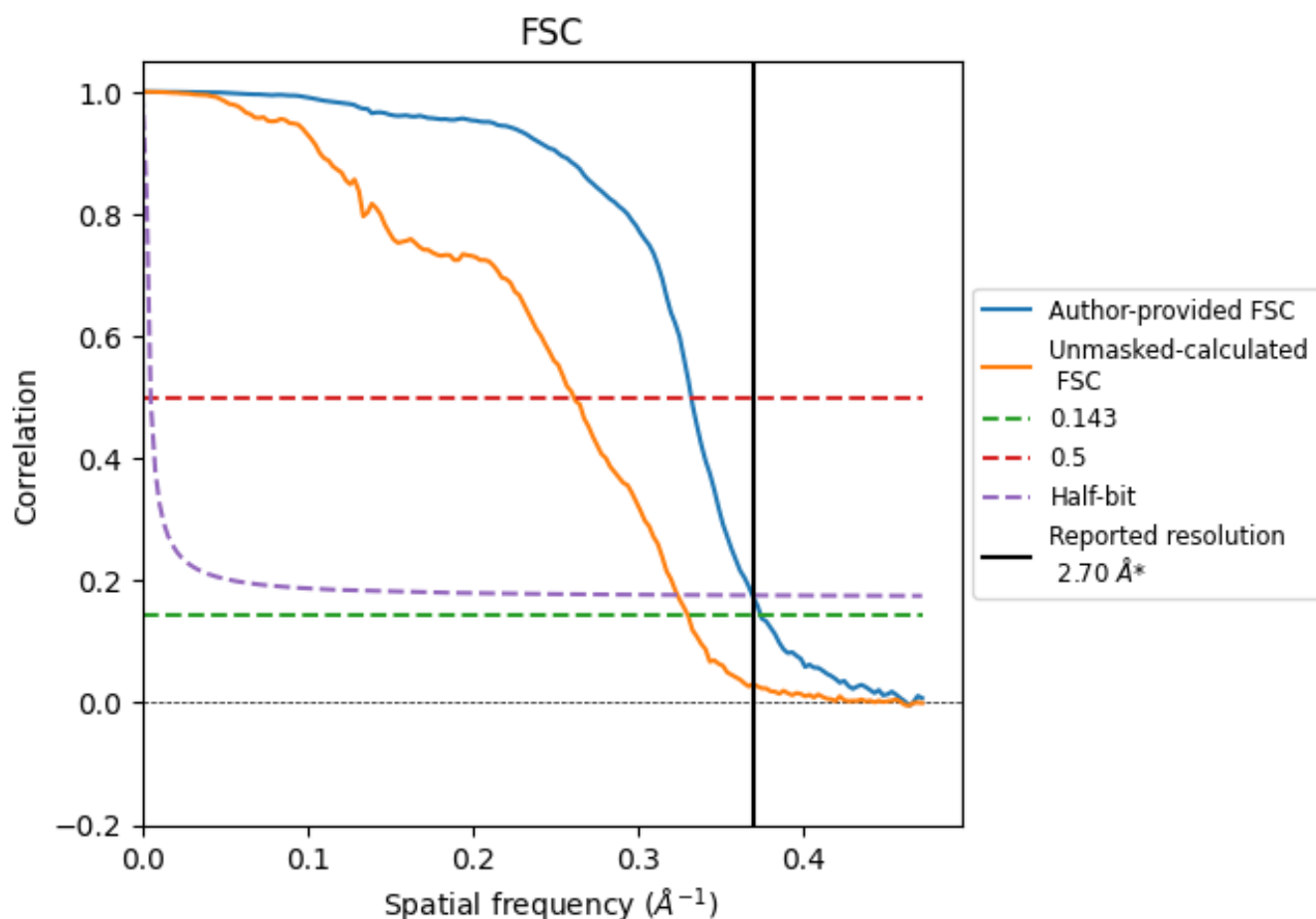


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

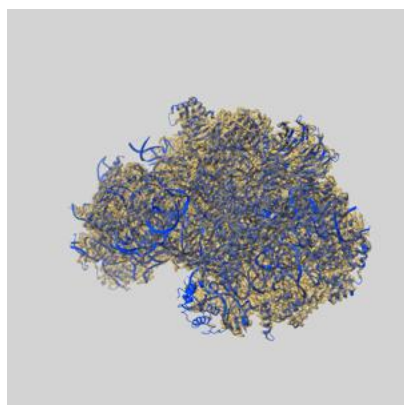
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.01	2.71
Unmasked-calculated*	3.03	3.83	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.7 by more than 10 %

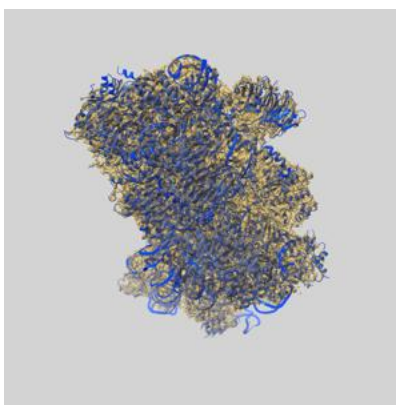
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11521 and PDB model 6ZXH. Per-residue inclusion information can be found in section 3 on page 12.

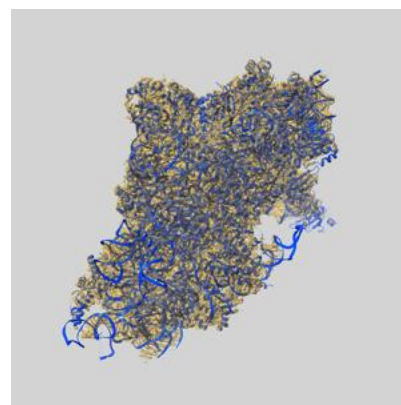
9.1 Map-model overlay [i](#)



X



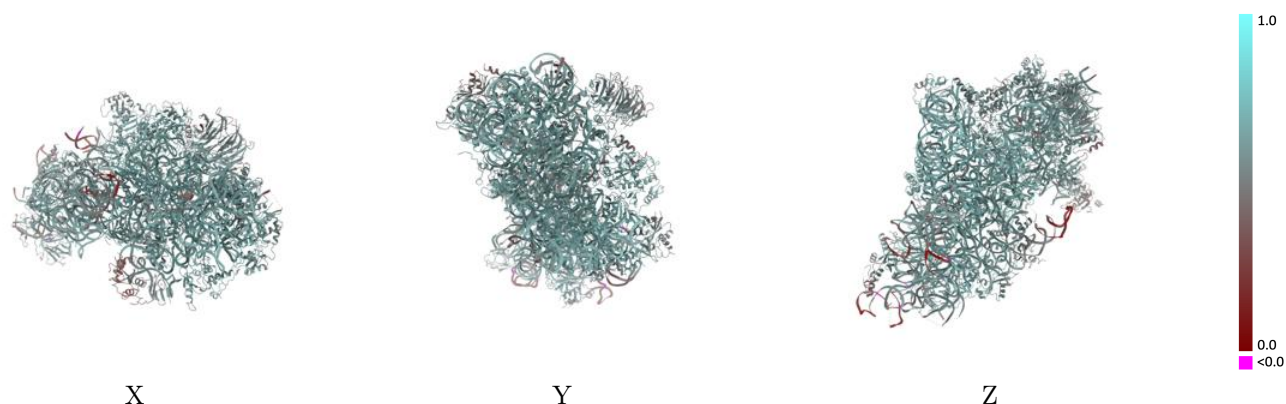
Y



Z

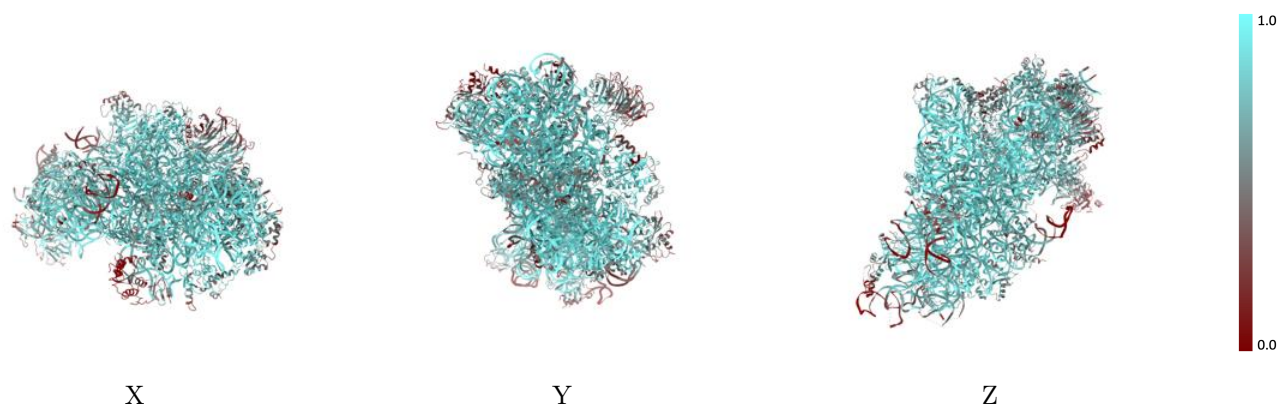
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



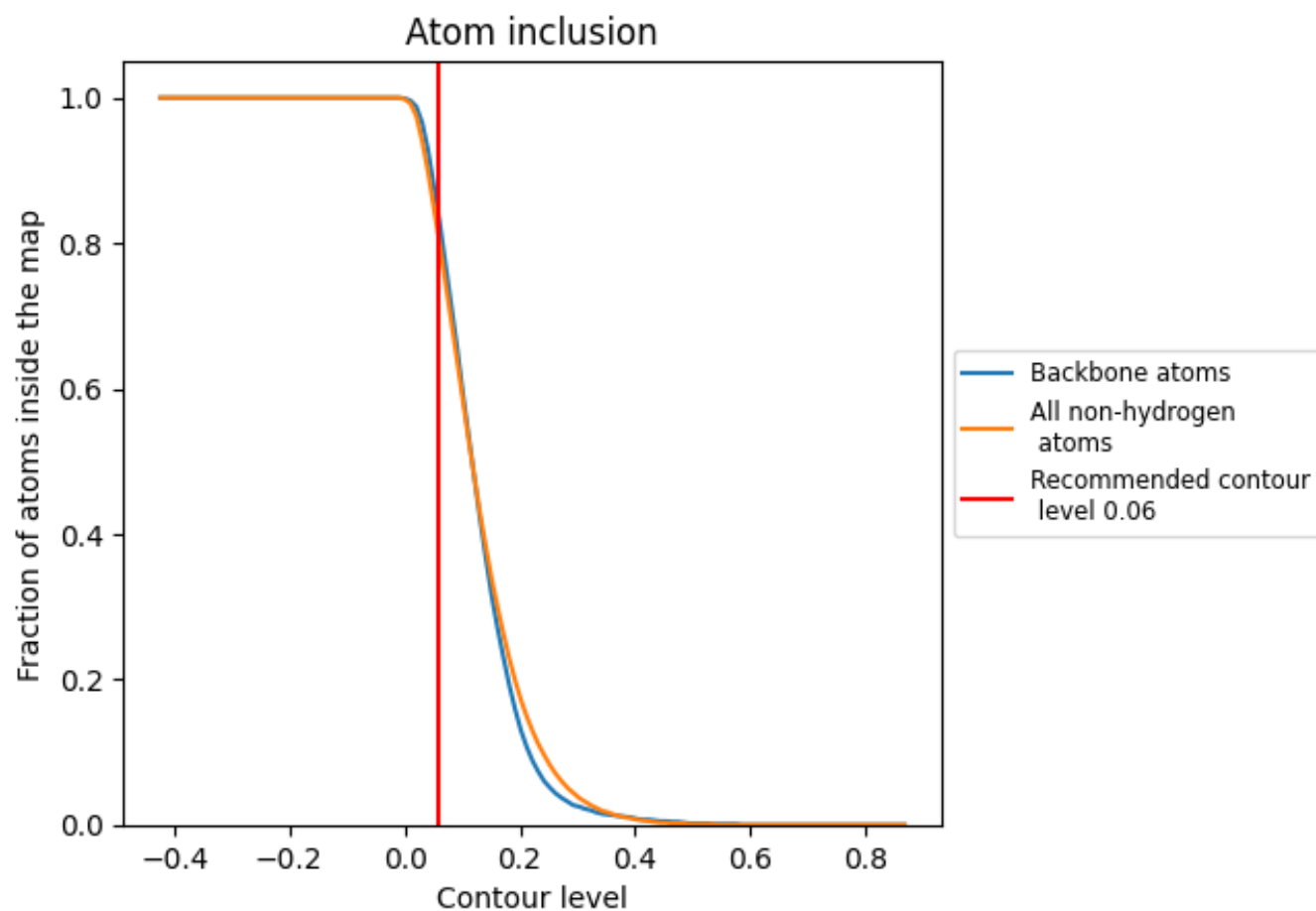
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.6090
2	 0.8820	 0.6210
A	 0.8600	 0.6310
B	 0.7690	 0.6170
C	 0.9050	 0.6580
D	 0.7270	 0.5980
E	 0.8400	 0.6310
F	 0.7690	 0.5910
G	 0.6090	 0.5490
H	 0.6080	 0.5590
I	 0.7190	 0.5920
J	 0.7050	 0.5460
K	 0.7170	 0.5920
L	 0.8760	 0.6380
M	 0.1140	 0.3940
N	 0.8640	 0.6400
O	 0.8560	 0.6310
P	 0.7420	 0.6070
Q	 0.8300	 0.6250
R	 0.7060	 0.5890
S	 0.7150	 0.6060
T	 0.8100	 0.6280
U	 0.6640	 0.5790
V	 0.8540	 0.6410
W	 0.9450	 0.6720
X	 0.9170	 0.6610
Y	 0.7700	 0.5940
Z	 0.5660	 0.5690
b	 0.7750	 0.6250
c	 0.5360	 0.5460
d	 0.9330	 0.6640
e	 0.7650	 0.5970
f	 0.3050	 0.4810
g	 0.5090	 0.5380
h	 0.8560	 0.6530



Continued on next page...

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Chain	Atom inclusion	Q-score
j	 0.6660	 0.5890
z	 0.7110	 0.5990