



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 04:23 am BST

PDB ID : 8AUV / pdb_00008auv
EMDB ID : EMD-15674
Title : Cryo-EM structure of the plant 40S subunit
Authors : Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.;
Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.
Deposited on : 2022-08-25
Resolution : 2.38 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:

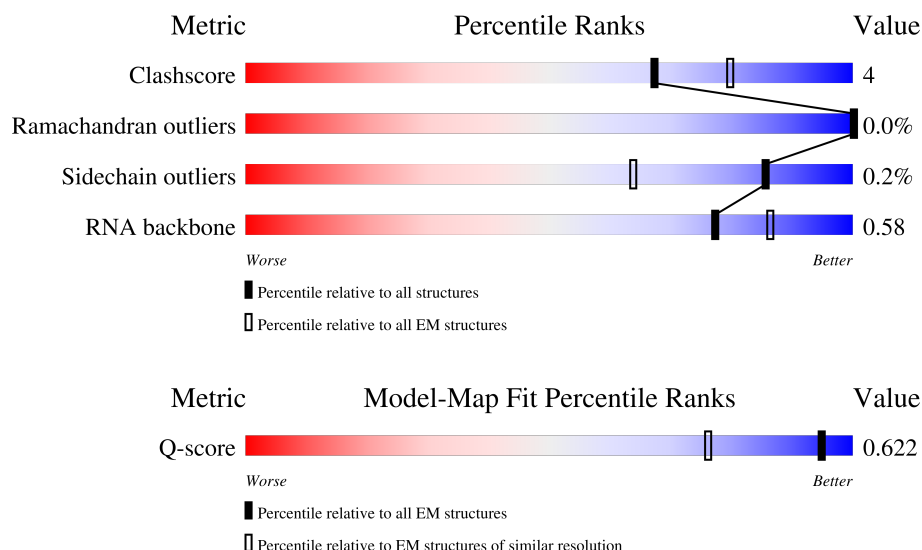
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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

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

The reported resolution of this entry is 2.38 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	4811 (1.88 - 2.88)

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	A	264	
2	k	249	
3	h	1808	

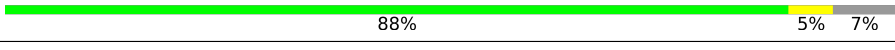
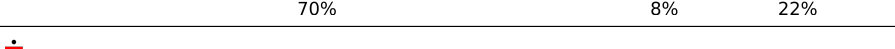
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Mol	Chain	Length	Quality of chain
4	I	208	
5	C	144	
6	D	149	
7	E	143	
8	F	261	
9	G	83	
10	H	133	
11	I	107	
12	J	127	
13	K	86	
14	L	65	
15	M	62	
16	N	156	
17	O	191	
18	P	224	
19	Q	328	
20	R	122	
21	S	150	
22	T	142	
23	U	152	
24	V	56	
25	W	151	
26	X	159	
27	Y	152	
28	Z	336	

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Mol	Chain	Length	Quality of chain
29	a	248	
30	b	197	
31	c	280	
32	d	210	
33	e	130	
34	f	147	
35	B	12	

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 132938 atoms, of which 57333 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 protein called eS4 (40S ribosomal protein S4).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	259	Total	C	H	N	O	S	0	0
			4254	1323	2180	387	357	7		

- Molecule 2 is a protein called eS6 (40S ribosomal protein S6).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	k	230	Total	C	H	N	O	S	0	0
			3816	1156	1965	361	326	8		

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	h	1626	Total	C	H	N	O	P	0	0
			52301	15549	17560	6195	11371	1626		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	603	UY1	U	modified residue	GB HQ384692
h	1194	B8N	U	modified residue	GB HQ384692
h	1283	4AC	C	modified residue	GB HQ384692

- Molecule 4 is a protein called eS10 (40S ribosomal protein S10).

Mol	Chain	Residues	Atoms						AltConf	Trace
4	l	91	Total	C	H	N	O	S	0	0
			1549	508	776	125	136	4		

- Molecule 5 is a protein called eS12 (40S ribosomal protein S12).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	117	Total	C	H	N	O	S	0	0
			1778	553	900	153	165	7		

- Molecule 6 is a protein called eS17 (40S ribosomal protein S17).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	D	119	Total	C	H	N	O	S	0	0
			1989	604	1026	178	177	4		

- Molecule 7 is a protein called eS19 (40S ribosomal protein S19).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	E	136	Total	C	H	N	O	S	0	0
			2172	676	1091	211	190	4		

- Molecule 8 is a protein called eS1 (40S ribosomal protein S3a).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	F	216	Total	C	H	N	O	S	0	0
			3578	1118	1818	314	320	8		

- Molecule 9 is a protein called eS21 (40S ribosomal protein S21).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	G	83	Total	C	H	N	O	S	0	0
			1295	404	643	120	125	3		

- Molecule 10 is a protein called eS24 (40S ribosomal protein S24).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	H	127	Total	C	H	N	O	S	0	0
			2145	657	1111	200	174	3		

- Molecule 11 is a protein called eS25 (40S ribosomal protein S25).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	74	Total	C	H	N	O	S	0	0
			1204	365	621	109	106	3		

- Molecule 12 is a protein called eS26 (40S ribosomal protein S26).

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	98	Total	C	H	N	O	S	0	0
			1610	491	818	161	132	8		

- Molecule 13 is a protein called eS27 (40S ribosomal protein S27).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K	84	Total	C	H	N	O	S	0	0
			1307	404	656	122	118	7		

- Molecule 14 is a protein called eS28 (40S ribosomal protein S28).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L	61	Total	C	H	N	O	S	0	0
			1018	303	525	102	86	2		

- Molecule 15 is a protein called eS30 (40S ribosomal protein S30).

Mol	Chain	Residues	Atoms						AltConf	Trace
15	M	52	Total	C	H	N	O	S	0	0
			851	249	442	94	65	1		

- Molecule 16 is a protein called eS31 (ubiquitin-40S ribosomal protein S27a).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	N	69	Total	C	H	N	O	S	0	0
			1143	360	581	103	94	5		

- Molecule 17 is a protein called eS7 (40S ribosomal protein S7).

Mol	Chain	Residues	Atoms						AltConf	Trace
17	O	188	Total	C	H	N	O	S	0	0
			3125	972	1591	281	279	2		

- Molecule 18 is a protein called eS8 (40S ribosomal protein S8).

Mol	Chain	Residues	Atoms						AltConf	Trace
18	P	186	Total	C	H	N	O	S	0	0
			3081	944	1570	300	263	4		

- Molecule 19 is a protein called RACK1 (guanine nucleotide-binding protein subunit beta-like protein).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Q	309	Total	C	H	N	O	S	0	0
			4756	1512	2362	414	456	12		

- Molecule 20 is a protein called uS10 (40S ribosomal protein S20).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	R	102	Total	C	H	N	O	S	0	0
			1668	505	864	151	145	3		

- Molecule 21 is a protein called uS11 (40S ribosomal protein S14).

Mol	Chain	Residues	Atoms						AltConf	Trace
21	S	132	Total	C	H	N	O	S	0	0
			2026	611	1028	197	185	5		

- Molecule 22 is a protein called uS12 (40S ribosomal protein S23).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	T	141	Total	C	H	N	O	S	0	0
			2264	695	1164	215	187	3		

- Molecule 23 is a protein called uS13 (40S ribosomal protein S18).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	U	142	Total	C	H	N	O	S	0	0
			2337	718	1184	227	202	6		

- Molecule 24 is a protein called uS14 (40S ribosomal protein S29).

Mol	Chain	Residues	Atoms						AltConf	Trace
24	V	55	Total	C	H	N	O	S	0	0
			871	274	430	90	71	6		

- Molecule 25 is a protein called uS15 (40S ribosomal protein S13).

Mol	Chain	Residues	Atoms						AltConf	Trace
25	W	149	Total	C	H	N	O	S	0	0
			2467	762	1278	223	202	2		

- Molecule 26 is a protein called uS17 (40S ribosomal protein S11).

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X	145	Total	C	H	N	O	S	0	0
			2362	734	1207	222	194	5		

- Molecule 27 is a protein called uS19 (40S ribosomal protein S15).

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Y	131	Total	C	H	N	O	S	0	0
			2193	681	1132	199	176	5		

- Molecule 28 is a protein called uS2 (40S ribosomal protein SA).

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Z	202	Total	C	H	N	O	S	0	0
			3233	1023	1623	289	288	10		

- Molecule 29 is a protein called uS3 (40S ribosomal protein S3).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	a	211	Total	C	H	N	O	S	0	0
			3413	1052	1752	306	295	8		

- Molecule 30 is a protein called uS4 (40S ribosomal protein S9).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	b	183	Total	C	H	N	O	S	0	0
			3118	964	1595	301	253	5		

- Molecule 31 is a protein called uS5 (40S ribosomal protein S2).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	c	217	Total	C	H	N	O	S	0	0
			3472	1089	1786	300	289	8		

- Molecule 32 is a protein called uS7 (40S ribosomal protein S5).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	d	194	Total	C	H	N	O	S	0	0
			3103	953	1572	290	280	8		

- Molecule 33 is a protein called uS8 (40S ribosomal protein S15a).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	e	129	Total	C	H	N	O	S	0	0
			2100	659	1068	188	180	5		

- Molecule 34 is a protein called uS9 (40S ribosomal protein S16).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	f	141	Total	C	H	N	O	S	0	0
			2332	722	1197	221	188	4		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	B	12	Total	C	H	N	O	P	0	0
			360	108	120	24	96	12		

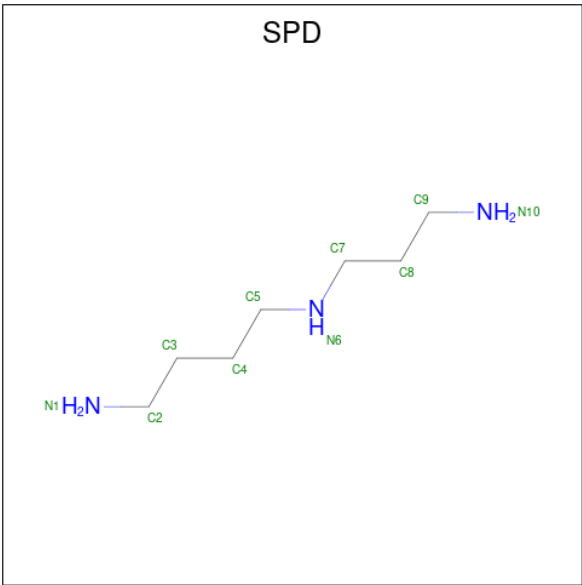
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	h	73	Total	Mg	0
			73	73	
36	J	1	Total	Mg	0
			1	1	
36	U	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	

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

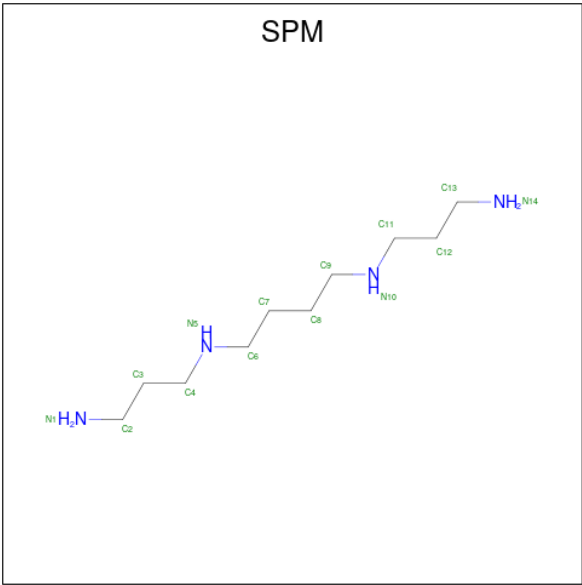
Mol	Chain	Residues	Atoms		AltConf
37	h	41	Total	K	0
			41	41	
37	S	1	Total	K	0
			1	1	
37	T	1	Total	K	0
			1	1	
37	U	1	Total	K	0
			1	1	
37	V	1	Total	K	0
			1	1	
37	W	1	Total	K	0
			1	1	
37	d	1	Total	K	0
			1	1	

- Molecule 38 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
38	h	1	29	7	19	3	0

- Molecule 39 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
39	h	1	40	10	26	4	0
39	h	1	40	10	26	4	0
39	h	1	40	10	26	4	0

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	J	1	Total 1	Zn 1	0
40	N	1	Total 1	Zn 1	0
40	V	1	Total 1	Zn 1	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	10	Total 10	O 10	0
41	k	6	Total 6	O 6	0
41	h	2050	Total 2050	O 2050	0
41	E	10	Total 10	O 10	0
41	F	11	Total 11	O 11	0
41	I	1	Total 1	O 1	0
41	J	29	Total 29	O 29	0
41	K	5	Total 5	O 5	0
41	M	1	Total 1	O 1	0
41	O	1	Total 1	O 1	0
41	P	18	Total 18	O 18	0
41	R	11	Total 11	O 11	0
41	S	26	Total 26	O 26	0
41	T	43	Total 43	O 43	0
41	U	8	Total 8	O 8	0
41	V	5	Total 5	O 5	0

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Mol	Chain	Residues	Atoms		AltConf
41	W	27	Total 27	O 27	0
41	X	22	Total 22	O 22	0
41	Y	6	Total 6	O 6	0
41	Z	1	Total 1	O 1	0
41	a	1	Total 1	O 1	0
41	b	11	Total 11	O 11	0
41	c	11	Total 11	O 11	0
41	d	11	Total 11	O 11	0
41	e	16	Total 16	O 16	0
41	f	15	Total 15	O 15	0
41	B	16	Total 16	O 16	0

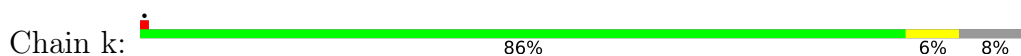
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: eS4 (40S ribosomal protein S4)



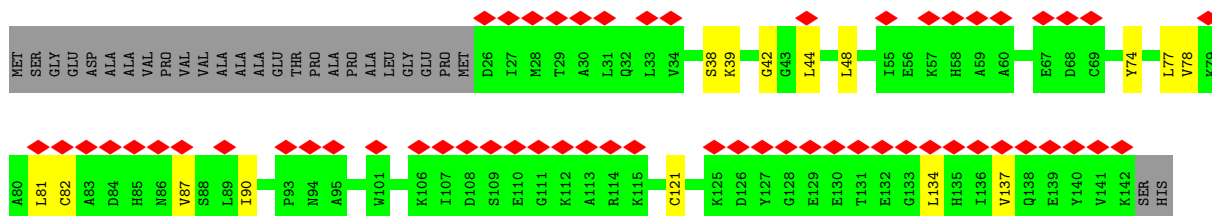
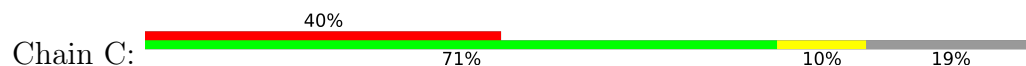
- Molecule 2: eS6 (40S ribosomal protein S6)



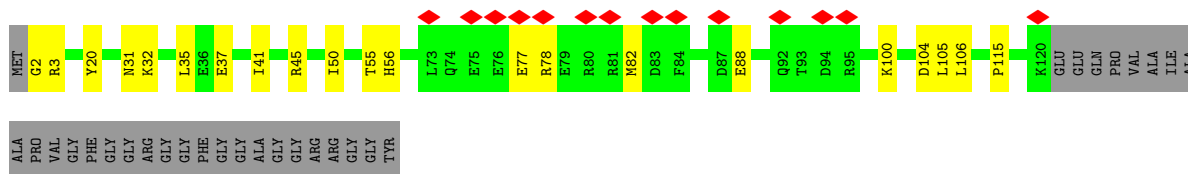
- Molecule 3: 18S rRNA



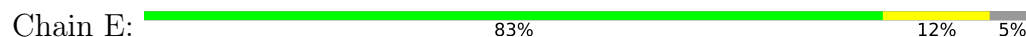
- Molecule 5: eS12 (40S ribosomal protein S12)



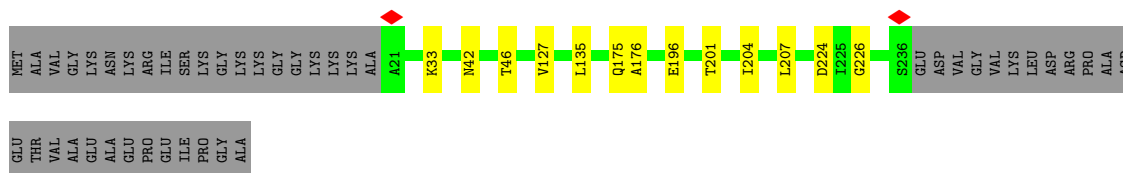
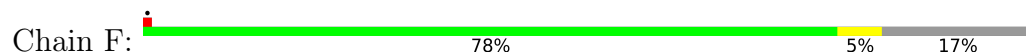
- Molecule 6: eS17 (40S ribosomal protein S17)



- Molecule 7: eS19 (40S ribosomal protein S19)



- Molecule 8: eS1 (40S ribosomal protein S3a)



- Molecule 9: eS21 (40S ribosomal protein S21)



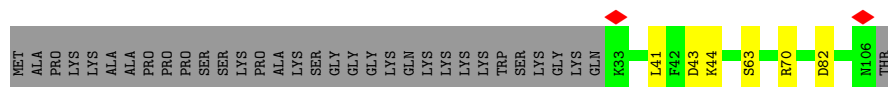
- Molecule 10: eS24 (40S ribosomal protein S24)

Chain H:  92% 5%



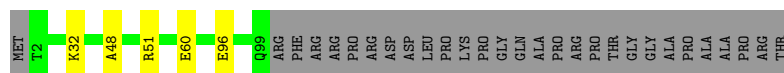
- Molecule 11: eS25 (40S ribosomal protein S25)

Chain I:  64% 6% 31%



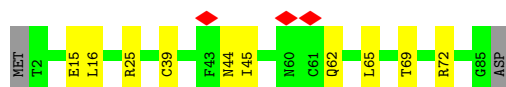
- Molecule 12: eS26 (40S ribosomal protein S26)

Chain J:  73% 23%



- Molecule 13: eS27 (40S ribosomal protein S27)

Chain K:  86% 12%



- Molecule 14: eS28 (40S ribosomal protein S28)

Chain L:  83% 11% 6%



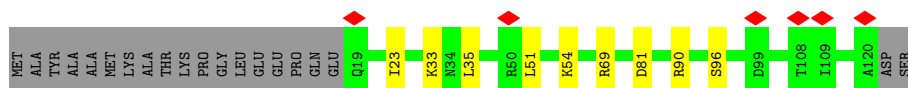
- Molecule 15: eS30 (40S ribosomal protein S30)

Chain M:  74% 10% 16%

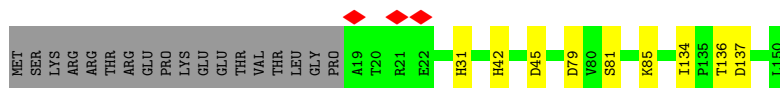
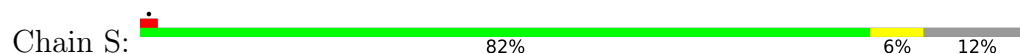


- Molecule 16: eS31 (ubiquitin-40S ribosomal protein S27a)

Chain N:  15% 40% 56%



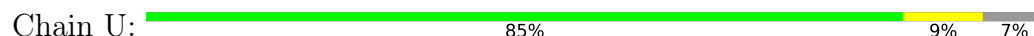
- Molecule 21: uS11 (40S ribosomal protein S14)



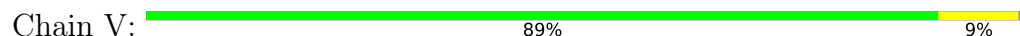
- Molecule 22: uS12 (40S ribosomal protein S23)



- Molecule 23: uS13 (40S ribosomal protein S18)



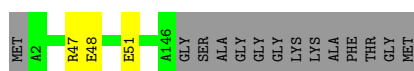
- Molecule 24: uS14 (40S ribosomal protein S29)



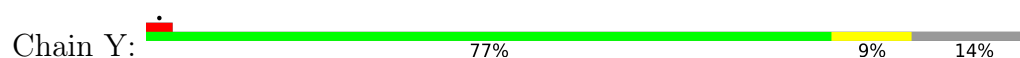
- Molecule 25: uS15 (40S ribosomal protein S13)

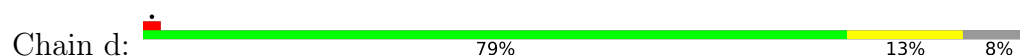


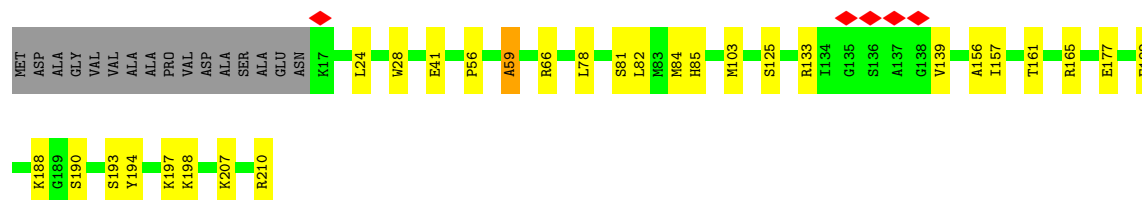
- Molecule 26: uS17 (40S ribosomal protein S11)



- Molecule 27: uS19 (40S ribosomal protein S15)







- Molecule 33: uS8 (40S ribosomal protein S15a)

Chain e: 93% 6% .



- Molecule 34: uS9 (40S ribosomal protein S16)

Chain f: 88% 8% .



- Molecule 35: mRNA

Chain B: 67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.349	Depositor
Minimum map value	-6.212	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.189	Depositor
Recommended contour level	0.426	Depositor
Map size ($\text{\AA}$)	381.6, 381.6, 381.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 6MZ, MA6, SPM, OMG, K, UY1, OMC, A2M, 4AC, ZN, OMU, MG, PSU, SPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.13	0/2114	0.26	0/2837
2	k	0.11	0/1875	0.25	0/2494
3	h	0.17	2/36945 (0.0%)	0.26	0/57563
4	l	0.11	0/794	0.23	0/1074
5	C	0.09	0/889	0.21	0/1198
6	D	0.14	0/973	0.29	0/1299
7	E	0.11	0/1103	0.22	0/1480
8	F	0.11	0/1790	0.23	0/2402
9	G	0.10	0/662	0.21	0/891
10	H	0.11	0/1049	0.22	0/1391
11	I	0.14	0/589	0.29	0/789
12	J	0.13	0/805	0.24	0/1076
13	K	0.15	0/662	0.29	0/892
14	L	0.12	0/496	0.22	0/661
15	M	0.16	0/414	0.23	0/544
16	N	0.11	0/574	0.21	0/763
17	O	0.11	0/1560	0.23	0/2097
18	P	0.12	0/1535	0.22	0/2050
19	Q	0.09	0/2446	0.23	0/3324
20	R	0.14	0/813	0.25	0/1095
21	S	0.12	0/1010	0.25	0/1352
22	T	0.13	0/1119	0.25	0/1487
23	U	0.11	0/1170	0.23	0/1562
24	V	0.15	0/453	0.23	0/605
25	W	0.13	0/1214	0.23	0/1632
26	X	0.13	0/1180	0.25	0/1579
27	Y	0.12	0/1084	0.24	0/1450
28	Z	0.12	0/1644	0.24	0/2223
29	a	0.10	0/1684	0.23	0/2257
30	b	0.11	0/1550	0.25	0/2073
31	c	0.12	0/1721	0.25	0/2320
32	d	0.14	0/1553	0.46	2/2095 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.12	0/1050	0.25	0/1405
34	f	0.16	0/1154	0.26	0/1542
35	B	0.11	0/263	0.21	0/404
All	All	0.14	2/75937 (0.0%)	0.25	2/109906 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1272	OMU	O3'-P	5.17	1.61	1.56
3	h	622	A2M	O3'-P	5.01	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	59	ALA	CA-C-N	10.58	133.97	120.64
32	d	59	ALA	C-N-CA	10.58	133.97	120.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2074	2180	2181	10	0
2	k	1851	1965	1969	11	0
3	h	34741	17560	17528	224	0
4	l	773	776	776	4	0
5	C	878	900	905	12	0
6	D	963	1026	1025	22	0
7	E	1081	1091	1091	12	0
8	F	1760	1818	1820	8	0
9	G	652	643	645	1	0
10	H	1034	1111	1110	3	0
11	I	583	621	620	5	0
12	J	792	818	820	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	651	656	661	6	0
14	L	493	525	524	6	0
15	M	409	442	440	6	0
16	N	562	581	580	8	0
17	O	1534	1591	1590	14	0
18	P	1511	1570	1570	11	0
19	Q	2394	2362	2368	37	0
20	R	804	864	865	7	0
21	S	998	1028	1028	8	0
22	T	1100	1164	1165	2	0
23	U	1153	1184	1184	8	0
24	V	441	430	430	4	0
25	W	1189	1278	1277	6	0
26	X	1155	1207	1210	2	0
27	Y	1061	1132	1131	9	0
28	Z	1610	1623	1624	16	0
29	a	1661	1752	1754	25	0
30	b	1523	1595	1595	7	0
31	c	1686	1786	1789	15	0
32	d	1531	1572	1573	28	0
33	e	1032	1068	1068	8	0
34	f	1135	1197	1198	8	0
35	B	240	120	121	3	0
36	B	1	0	0	0	0
36	J	1	0	0	0	0
36	U	1	0	0	0	0
36	h	73	0	0	0	0
37	S	1	0	0	0	0
37	T	1	0	0	0	0
37	U	1	0	0	0	0
37	V	1	0	0	0	0
37	W	1	0	0	0	0
37	d	1	0	0	0	0
37	h	41	0	0	0	0
38	h	10	19	19	1	0
39	h	42	78	78	2	0
40	J	1	0	0	0	0
40	N	1	0	0	0	0
40	V	1	0	0	0	0
41	A	10	0	0	0	0
41	B	16	0	0	2	0
41	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	F	11	0	0	0	0
41	I	1	0	0	0	0
41	J	29	0	0	0	0
41	K	5	0	0	1	0
41	M	1	0	0	0	0
41	O	1	0	0	0	0
41	P	18	0	0	1	0
41	R	11	0	0	1	0
41	S	26	0	0	1	0
41	T	43	0	0	0	0
41	U	8	0	0	0	0
41	V	5	0	0	0	0
41	W	27	0	0	0	0
41	X	22	0	0	0	0
41	Y	6	0	0	0	0
41	Z	1	0	0	0	0
41	a	1	0	0	0	0
41	b	11	0	0	0	0
41	c	11	0	0	0	0
41	d	11	0	0	0	0
41	e	16	0	0	1	0
41	f	15	0	0	0	0
41	h	2050	0	0	49	0
41	k	6	0	0	0	0
All	All	75605	57333	57332	490	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 (490) 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)
29:a:178:ILE:CD1	29:a:187:ILE:HD12	1.48	1.44
29:a:178:ILE:CD1	29:a:187:ILE:CD1	2.22	1.17
31:c:147:ILE:HD13	31:c:229:MET:HG2	1.28	1.11
19:Q:165:PRO:HB2	19:Q:181:LEU:HD23	1.36	1.06
29:a:178:ILE:HD11	29:a:187:ILE:HD12	1.11	1.04
19:Q:84:TRP:O	19:Q:108:ASP:OD1	1.77	1.01
31:c:147:ILE:CD1	31:c:229:MET:HG2	1.93	0.96
32:d:194:TYR:CE2	32:d:198:LYS:HE3	2.00	0.96
3:h:76:C:O2'	3:h:77:A:O4'	1.86	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:236:THR:OG1	31:c:238:ASP:OD1	1.85	0.94
29:a:112:LEU:HD12	29:a:187:ILE:HD11	1.48	0.93
3:h:392:OMG:OP2	3:h:427:G:O2'	1.89	0.90
29:a:178:ILE:HD12	29:a:187:ILE:HD12	1.55	0.89
32:d:194:TYR:CZ	32:d:198:LYS:HE3	2.07	0.89
32:d:194:TYR:CE2	32:d:198:LYS:CE	2.55	0.88
29:a:178:ILE:HD11	29:a:187:ILE:CD1	1.97	0.88
31:c:147:ILE:HD13	31:c:229:MET:CG	2.06	0.85
3:h:392:OMG:OP1	41:h:2101:HOH:O	1.95	0.84
26:X:48:GLU:N	26:X:48:GLU:OE1	2.10	0.84
32:d:125:SER:OG	32:d:156:ALA:HB1	1.78	0.82
21:S:137:ASP:O	41:S:301:HOH:O	1.98	0.82
32:d:24:LEU:HD23	32:d:103:MET:HE1	1.61	0.81
34:f:57:GLU:OE1	34:f:89:ARG:NH1	2.13	0.81
19:Q:75:ASP:OD2	19:Q:77:MET:HE3	1.81	0.80
3:h:1205:A:N7	41:h:2146:HOH:O	2.13	0.80
3:h:782:C:O2'	3:h:783:U:O5'	2.01	0.79
3:h:514:A:OP2	30:b:178:ASN:ND2	2.15	0.79
29:a:178:ILE:HD13	29:a:187:ILE:CD1	2.11	0.79
3:h:47:A:OP2	41:h:2102:HOH:O	2.00	0.79
3:h:943:A:OP1	41:h:2104:HOH:O	2.01	0.78
35:B:24:U:OP2	41:B:201:HOH:O	1.98	0.78
3:h:1376:G:O2'	3:h:1379:A:OP2	2.00	0.78
3:h:1488:A:N3	3:h:1613:G:O2'	2.17	0.77
6:D:82:MET:SD	28:Z:85:ARG:CZ	2.73	0.77
3:h:1775:G:OP1	41:h:2106:HOH:O	2.04	0.76
3:h:648:U:O2	3:h:688:G:O6	2.03	0.76
3:h:630:C:OP1	41:h:2105:HOH:O	2.04	0.76
19:Q:165:PRO:CB	19:Q:181:LEU:HD23	2.15	0.76
19:Q:165:PRO:HB2	19:Q:181:LEU:CD2	2.13	0.75
19:Q:75:ASP:OD2	19:Q:77:MET:CE	2.35	0.75
3:h:996:A:N6	3:h:1014:C:O2	2.20	0.75
3:h:387:G:O6	41:h:2109:HOH:O	2.05	0.74
3:h:1196:A:OP1	41:h:2108:HOH:O	2.05	0.74
3:h:1273:G:OP1	41:h:2113:HOH:O	2.06	0.74
3:h:1559:G:O2'	24:V:14:TYR:OH	2.05	0.74
3:h:308:U:OP1	41:h:2115:HOH:O	2.06	0.73
6:D:82:MET:SD	28:Z:85:ARG:NH1	2.61	0.73
3:h:1048:C:OP1	41:h:2110:HOH:O	2.06	0.73
31:c:147:ILE:CD1	31:c:229:MET:CG	2.62	0.73
3:h:1548:G:OP2	41:h:2112:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:OG1	1:A:143:ASP:OD1	2.04	0.73
3:h:994:G:OP2	41:h:2114:HOH:O	2.06	0.72
6:D:105:LEU:HD11	28:Z:50:ASN:HA	1.71	0.72
2:k:165:ASN:OD1	2:k:175:SER:HB3	1.89	0.72
32:d:81:SER:O	32:d:161:THR:HG21	1.90	0.71
3:h:774:A:OP2	41:h:2117:HOH:O	2.06	0.71
7:E:7:VAL:HG22	7:E:15:PHE:CE1	2.25	0.71
29:a:112:LEU:CD1	29:a:187:ILE:HD11	2.21	0.71
3:h:938:U:O2	41:h:2121:HOH:O	2.07	0.70
29:a:178:ILE:HD13	29:a:187:ILE:HD11	1.71	0.70
3:h:100:C:OP2	41:h:2123:HOH:O	2.08	0.70
26:X:47:ARG:NH1	26:X:51:GLU:OE2	2.24	0.70
3:h:116:G:OP2	41:h:2128:HOH:O	2.10	0.70
3:h:996:A:OP2	41:h:2127:HOH:O	2.10	0.70
3:h:1076:G:OP1	41:h:2122:HOH:O	2.08	0.70
23:U:88:LYS:O	27:Y:25:ARG:NH1	2.25	0.70
3:h:1095:A:O2'	41:h:2124:HOH:O	2.09	0.70
29:a:149:ARG:NH1	35:B:29:U:O2'	2.25	0.69
3:h:603:UY1:OP1	41:h:2125:HOH:O	2.09	0.69
3:h:1334:A:OP1	6:D:45:ARG:NH2	2.24	0.69
32:d:194:TYR:CE2	32:d:198:LYS:HE2	2.26	0.69
35:B:27:U:O2'	41:B:202:HOH:O	2.11	0.69
3:h:945:G:OP2	41:h:2131:HOH:O	2.10	0.68
3:h:1612:C:OP1	41:h:2129:HOH:O	2.10	0.68
33:e:107:SER:OG	41:e:202:HOH:O	2.08	0.68
3:h:610:G:OP1	41:h:2134:HOH:O	2.11	0.68
3:h:21:U:OP1	41:h:2133:HOH:O	2.10	0.68
3:h:275:C:HO2'	3:h:276:G:H8	1.42	0.68
3:h:1342:C:O2'	3:h:1344:G:N7	2.26	0.68
3:h:598:OMG:OP2	41:h:2139:HOH:O	2.12	0.68
34:f:66:ARG:NH2	34:f:111:GLU:OE1	2.28	0.67
3:h:993:C:OP2	41:h:2136:HOH:O	2.11	0.67
13:K:25:ARG:O	41:K:101:HOH:O	2.13	0.67
3:h:880:G:OP1	41:h:2138:HOH:O	2.12	0.67
3:h:620:U:OP1	41:h:2143:HOH:O	2.12	0.67
3:h:1298:G:O6	41:h:2126:HOH:O	2.10	0.67
3:h:1361:A:O2'	7:E:133:ASP:OD2	2.10	0.67
3:h:1234:OMU:O4	16:N:95:LYS:NZ	2.27	0.67
3:h:1780:C:OP2	41:h:2140:HOH:O	2.12	0.67
11:I:43:ASP:OD1	11:I:44:LYS:N	2.28	0.67
3:h:17:C:O2'	3:h:1140:A:N1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:251:CYS:SG	19:Q:260:ILE:HG12	2.35	0.66
3:h:1790:MA6:OP2	41:h:2145:HOH:O	2.13	0.66
3:h:1176:C:OP1	23:U:130:ARG:NH2	2.27	0.66
3:h:983:G:OP2	41:h:2149:HOH:O	2.14	0.66
3:h:338:G:OP1	41:h:2142:HOH:O	2.12	0.66
13:K:69:THR:OG1	13:K:72:ARG:O	2.13	0.65
3:h:556:G:OP2	41:h:2147:HOH:O	2.14	0.65
3:h:9:U:OP2	41:h:2148:HOH:O	2.14	0.65
3:h:1332:A:OP1	41:h:2150:HOH:O	2.14	0.65
3:h:1546:G:OP2	41:h:2151:HOH:O	2.14	0.65
3:h:1789:MA6:H92	3:h:1790:MA6:H93	1.79	0.64
31:c:153:TYR:OH	31:c:159:GLY:O	2.16	0.64
3:h:96:G:HO2'	3:h:464:A:HO2'	1.43	0.64
11:I:70:ARG:O	11:I:70:ARG:HG2	1.98	0.64
19:Q:20:THR:OG1	19:Q:35:SER:OG	2.15	0.64
3:h:1278:A:O2'	29:a:148:GLN:O	2.15	0.64
3:h:533:C:O2	10:H:63:ARG:NH1	2.31	0.63
6:D:82:MET:HG2	28:Z:85:ARG:CZ	2.28	0.62
19:Q:111:SER:HB3	19:Q:124:ALA:HB3	1.81	0.62
19:Q:12:MET:HE1	19:Q:32:ILE:HD11	1.80	0.62
23:U:16:GLN:NE2	23:U:100:SER:OG	2.32	0.61
4:l:95:LEU:HD21	4:l:103:LEU:HD12	1.82	0.61
3:h:476:U:O2'	3:h:773:A:N3	2.32	0.60
28:Z:90:PHE:O	28:Z:94:THR:OG1	2.16	0.60
29:a:116:LEU:HD23	29:a:121:ALA:HB2	1.84	0.60
3:h:261:C:O2	18:P:193:ARG:NH1	2.33	0.60
6:D:106:LEU:HD21	28:Z:19:LEU:HD11	1.84	0.60
3:h:275:C:O2'	3:h:276:G:O4'	2.19	0.60
3:h:96:G:O2'	3:h:464:A:O2'	2.19	0.59
20:R:69:ARG:O	41:R:201:HOH:O	2.16	0.59
3:h:1613:G:OP2	38:h:2015:SPD:N1	2.36	0.58
3:h:385:C:O2'	3:h:759:A:N1	2.34	0.58
32:d:161:THR:HG22	32:d:165:ARG:NH2	2.19	0.58
2:k:57:ASP:OD1	2:k:61:PHE:N	2.36	0.58
3:h:1806:U:O2	3:h:1808:G:O2'	2.21	0.58
3:h:1275:U:O2'	3:h:1278:A:OP2	2.11	0.58
7:E:115:ASP:CG	7:E:116:PHE:H	2.12	0.58
29:a:112:LEU:HD12	29:a:187:ILE:CD1	2.28	0.58
12:J:48:ALA:HB2	14:L:60:GLU:OE2	2.03	0.58
19:Q:251:CYS:SG	19:Q:260:ILE:HD13	2.44	0.57
3:h:874:A:H2'	3:h:875:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:971:U:OP1	3:h:1036:C:O2'	2.22	0.57
3:h:888:G:H2'	3:h:889:U:C6	2.39	0.57
3:h:1477:C:OP1	41:h:2153:HOH:O	2.16	0.57
20:R:81:ASP:OD1	24:V:54:LYS:NZ	2.31	0.57
29:a:170:TYR:OH	29:a:205:THR:O	2.13	0.57
3:h:538:A:OP2	30:b:170:ARG:NH2	2.36	0.57
13:K:39:CYS:SG	13:K:65:LEU:HD21	2.45	0.57
3:h:889:U:O2'	21:S:134:ILE:O	2.24	0.56
6:D:31:ASN:ND2	6:D:55:THR:OG1	2.39	0.56
6:D:82:MET:HG2	28:Z:85:ARG:NH2	2.21	0.56
13:K:44:ASN:OD1	13:K:45:ILE:N	2.39	0.56
17:O:171:SER:OG	17:O:182:VAL:O	2.21	0.56
31:c:48:THR:OG1	31:c:74:GLU:OE1	2.20	0.55
3:h:96:G:O6	41:h:2152:HOH:O	2.15	0.55
3:h:1530:A:N3	3:h:1596:G:O2'	2.33	0.55
3:h:503:C:O2'	3:h:504:U:P	2.66	0.54
3:h:1205:A:C8	41:h:2146:HOH:O	2.57	0.54
5:C:77:LEU:HD23	5:C:81:LEU:HD23	1.89	0.54
18:P:12:ARG:NH2	41:P:303:HOH:O	2.41	0.54
3:h:782:C:HO2'	3:h:783:U:P	2.27	0.54
32:d:82:LEU:HD23	32:d:161:THR:HG23	1.88	0.54
3:h:1030:A:OP1	3:h:1797:G:O2'	2.22	0.53
3:h:1067:G:O2'	8:F:204:ILE:O	2.25	0.53
3:h:1586:C:OP2	41:h:2158:HOH:O	2.19	0.53
3:h:81:U:O2'	3:h:82:G:OP1	2.23	0.53
32:d:125:SER:OG	32:d:156:ALA:CB	2.55	0.53
19:Q:251:CYS:SG	19:Q:260:ILE:CD1	2.97	0.53
30:b:114:LEU:O	30:b:118:THR:HG23	2.07	0.53
3:h:465:G:OP1	30:b:2:VAL:N	2.42	0.53
17:O:145:VAL:HG23	33:e:49:GLU:HG2	1.91	0.53
19:Q:242:CYS:HG	19:Q:305:TRP:CD1	2.26	0.53
2:k:181:GLN:NE2	3:h:65:A:OP1	2.40	0.53
3:h:1614:U:OP1	34:f:22:THR:OG1	2.22	0.53
15:M:4:VAL:HG12	15:M:10:ARG:NH2	2.25	0.52
3:h:1644:G:OP1	41:h:2154:HOH:O	2.18	0.52
19:Q:260:ILE:O	19:Q:269:VAL:N	2.39	0.52
19:Q:251:CYS:SG	19:Q:260:ILE:HG23	2.50	0.52
32:d:194:TYR:OH	32:d:198:LYS:HE3	2.10	0.52
14:L:32:ASP:OD1	14:L:33:ASP:N	2.42	0.52
19:Q:251:CYS:SG	19:Q:260:ILE:CG1	2.97	0.52
3:h:185:G:O2'	3:h:195:A:N6	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:995:A:OP1	39:h:2018:SPM:N14	2.43	0.52
3:h:1101:U:OP1	31:c:169:THR:OG1	2.21	0.52
8:F:127:VAL:HG21	8:F:176:ALA:CB	2.40	0.52
19:Q:30:ASP:O	19:Q:46:LEU:HD12	2.09	0.52
19:Q:171:SER:OG	19:Q:172:TRP:N	2.43	0.52
3:h:77:A:O2'	3:h:78:G:O4'	2.28	0.52
3:h:100:C:OP2	3:h:382:A:O2'	2.26	0.51
11:I:82:ASP:OD1	11:I:82:ASP:C	2.52	0.51
19:Q:88:LEU:O	19:Q:102:PHE:N	2.36	0.51
32:d:193:SER:O	32:d:197:LYS:NZ	2.44	0.51
31:c:54:VAL:HG21	31:c:77:ILE:HG23	1.91	0.51
3:h:139:U:H4'	3:h:140:OMC:O5'	2.10	0.51
3:h:1424:G:O4'	24:V:56:ARG:HA	2.11	0.51
6:D:115:PRO:O	28:Z:16:GLN:NE2	2.44	0.51
3:h:1173:G:C2	3:h:1174:A:C8	2.98	0.51
3:h:1789:MA6:C9	3:h:1790:MA6:H93	2.40	0.51
7:E:54:TYR:OH	7:E:103:ASN:OD1	2.21	0.51
32:d:24:LEU:CD2	32:d:103:MET:HE1	2.35	0.51
11:I:41:LEU:HD11	23:U:58:GLU:OE2	2.11	0.50
3:h:1419:U:OP1	6:D:2:GLY:N	2.44	0.50
6:D:82:MET:CG	28:Z:85:ARG:CZ	2.89	0.50
3:h:1471:G:O2'	3:h:1608:C:OP1	2.30	0.50
3:h:542:G:OP2	3:h:542:G:N2	2.38	0.50
3:h:1025:C:O2'	3:h:1128:A:N1	2.45	0.50
8:F:201:THR:OG1	8:F:207:LEU:HD12	2.12	0.50
17:O:30:MET:HE1	17:O:87:LYS:HD2	1.92	0.50
27:Y:44:PHE:O	27:Y:49:ARG:NH2	2.44	0.50
32:d:133:ARG:NH2	32:d:139:VAL:O	2.45	0.50
3:h:370:A:OP1	3:h:762:PSU:O2'	2.15	0.50
3:h:192:G:N7	18:P:156:ARG:NH2	2.59	0.50
31:c:175:VAL:HG11	31:c:220:PHE:HA	1.93	0.50
6:D:105:LEU:HD12	28:Z:39:PHE:CG	2.47	0.49
2:k:20:ASP:OD1	2:k:22:GLN:N	2.45	0.49
3:h:390:G:OP2	41:h:2155:HOH:O	2.18	0.49
29:a:142:SER:HG	29:a:152:SER:HG	1.60	0.49
3:h:1476:A:H2	3:h:1479:G:N3	2.11	0.49
3:h:204:U:O2	18:P:193:ARG:NH2	2.46	0.49
3:h:933:A:OP1	12:J:32:LYS:NZ	2.30	0.49
8:F:33:LYS:NZ	8:F:42:ASN:OD1	2.44	0.49
13:K:62:GLN:OE1	13:K:62:GLN:O	2.31	0.49
23:U:21:ASP:OD1	23:U:23:LYS:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:142:SER:OG	29:a:152:SER:OG	2.28	0.49
30:b:31:LYS:NZ	30:b:35:GLU:OE1	2.46	0.49
33:e:105:THR:HG23	33:e:105:THR:O	2.13	0.49
41:h:3435:HOH:O	27:Y:145:SER:HB3	2.12	0.49
3:h:12:U:H2'	3:h:13:C:C6	2.48	0.48
3:h:1344:G:C2	3:h:1345:C:C6	3.01	0.48
3:h:1348:A:H5'	20:R:54:LYS:HD2	1.95	0.48
7:E:43:LEU:HD23	7:E:43:LEU:H	1.78	0.48
8:F:46:THR:OG1	21:S:45:ASP:OD2	2.31	0.48
3:h:129:U:H3'	3:h:130:A:H5'	1.95	0.48
3:h:1389:A:OP1	20:R:33:LYS:NZ	2.43	0.48
28:Z:168:LYS:NZ	28:Z:204:TYR:O	2.40	0.48
5:C:48:LEU:HD12	5:C:74:TYR:CE1	2.47	0.48
10:H:119:VAL:HG21	10:H:127:ALA:HB1	1.96	0.48
32:d:41:GLU:C	32:d:41:GLU:OE2	2.56	0.48
3:h:193:G:O2'	3:h:194:A:OP2	2.26	0.48
27:Y:117:GLU:OE1	27:Y:117:GLU:N	2.47	0.48
30:b:65:ASP:OD1	30:b:66:GLU:N	2.46	0.48
7:E:109:GLN:HG3	7:E:114:VAL:HG23	1.95	0.48
7:E:115:ASP:CG	7:E:116:PHE:N	2.71	0.48
3:h:17:C:OP1	39:h:2016:SPM:N1	2.47	0.48
3:h:857:U:O4	3:h:858:A:N6	2.47	0.48
5:C:38:SER:O	5:C:42:GLY:N	2.46	0.48
9:G:55:LEU:HD11	9:G:69:LEU:HD12	1.95	0.48
19:Q:180:ASN:O	19:Q:184:CYS:N	2.44	0.48
32:d:194:TYR:O	32:d:198:LYS:HG2	2.13	0.48
3:h:399:U:H2'	3:h:400:G:O4'	2.13	0.48
3:h:1044:G:H2'	3:h:1045:G:C8	2.49	0.48
16:N:133:ALA:N	16:N:140:TYR:O	2.43	0.48
7:E:136:ALA:HA	7:E:139:ILE:HD12	1.95	0.48
19:Q:75:ASP:OD2	19:Q:77:MET:HE2	2.10	0.47
7:E:37:ILE:HD13	23:U:43:ILE:HD13	1.97	0.47
3:h:936:A:OP2	41:h:2162:HOH:O	2.20	0.47
17:O:5:ARG:NH1	17:O:21:GLU:OE1	2.48	0.47
19:Q:119:ARG:HB2	19:Q:119:ARG:CZ	2.44	0.47
3:h:325:C:N4	3:h:1673:G:OP1	2.47	0.47
6:D:88:GLU:OE2	6:D:88:GLU:N	2.45	0.47
3:h:202:C:C2	3:h:203:A:C8	3.02	0.47
3:h:1110:G:O2'	3:h:1111:G:H5'	2.14	0.47
3:h:1249:C:O2'	16:N:92:LYS:NZ	2.47	0.47
3:h:1419:U:OP2	6:D:3:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:1621:C:OP1	32:d:66:ARG:NH2	2.47	0.47
3:h:319:A:C2	3:h:357:A:C5	3.03	0.47
18:P:171:ILE:HD11	18:P:200:GLU:HG2	1.96	0.47
3:h:814:U:O2	17:O:112:GLN:NE2	2.48	0.47
3:h:959:U:OP1	3:h:1075:C:O2'	2.32	0.47
3:h:1034:U:H4'	3:h:1035:G:OP2	2.15	0.47
3:h:1414:G:N1	3:h:1417:G:OP2	2.48	0.47
29:a:116:LEU:HD11	29:a:120:ARG:HD3	1.97	0.47
29:a:178:ILE:HD12	29:a:187:ILE:CD1	2.25	0.47
3:h:1590:G:O2'	3:h:1616:G:O6	2.28	0.46
3:h:628:C:H2'	3:h:629:U:C6	2.51	0.46
5:C:48:LEU:HD23	16:N:102:VAL:HG21	1.98	0.46
17:O:11:ASP:C	17:O:11:ASP:OD1	2.58	0.46
17:O:25:GLN:O	17:O:29:ASP:OD1	2.32	0.46
3:h:1117:G:O2'	3:h:1133:G:O6	2.30	0.46
4:l:43:PHE:HB2	4:l:103:LEU:HD13	1.98	0.46
8:F:224:ASP:OD1	8:F:226:GLY:N	2.48	0.46
12:J:48:ALA:CB	14:L:60:GLU:OE2	2.62	0.46
3:h:1174:A:H2'	3:h:1175:G:C8	2.50	0.46
3:h:127:G:H3'	3:h:128:G:H5'	1.98	0.46
3:h:194:A:HO2'	3:h:195:A:H8	1.63	0.46
8:F:175:GLN:NE2	8:F:196:GLU:OE1	2.48	0.46
17:O:75:LYS:HG3	17:O:76:ILE:HG23	1.98	0.46
3:h:187:C:H2'	3:h:188:U:O4'	2.15	0.46
3:h:1543:A:H2'	3:h:1543:A:N3	2.30	0.46
6:D:100:LYS:O	6:D:104:ASP:OD1	2.33	0.46
17:O:7:LYS:NZ	17:O:41:LEU:O	2.48	0.46
32:d:207:LYS:HD2	32:d:210:ARG:HH21	1.81	0.46
3:h:1237:A:N3	16:N:140:TYR:OH	2.43	0.46
29:a:165:GLN:N	29:a:166:PRO:HD2	2.31	0.45
6:D:35:LEU:HD21	6:D:50:ILE:HG22	1.98	0.45
3:h:411:A:H2'	3:h:412:C:C6	2.51	0.45
3:h:1392:G:OP1	6:D:32:LYS:NZ	2.35	0.45
2:k:152:GLU:OE1	2:k:152:GLU:N	2.47	0.45
12:J:60:GLU:CD	12:J:60:GLU:H	2.24	0.45
3:h:204:U:O2	18:P:193:ARG:NH1	2.49	0.45
12:J:96:GLU:OE1	12:J:96:GLU:HA	2.17	0.45
3:h:1621:C:OP1	14:L:16:ARG:NH2	2.49	0.45
3:h:1623:U:H2'	3:h:1624:C:C6	2.52	0.45
5:C:48:LEU:HD22	16:N:102:VAL:HG11	1.98	0.45
3:h:397:C:H2'	3:h:398:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:516:U:H2'	3:h:517:G:C8	2.52	0.45
3:h:759:A:H2'	3:h:760:A:O4'	2.16	0.45
3:h:1737:U:H2'	3:h:1738:G:O4'	2.15	0.45
1:A:104:ASP:OD1	1:A:104:ASP:C	2.60	0.45
3:h:757:A:H2'	3:h:758:G:O4'	2.16	0.45
18:P:169:PRO:O	18:P:173:GLU:HG3	2.17	0.45
3:h:615:U:OP2	3:h:616:G:O2'	2.33	0.45
7:E:15:PHE:HA	7:E:139:ILE:HD11	1.98	0.45
28:Z:54:THR:OG1	28:Z:162:PRO:O	2.29	0.45
3:h:970:A:OP2	25:W:124:ARG:NH2	2.39	0.45
6:D:37:GLU:OE1	6:D:37:GLU:HA	2.17	0.45
3:h:1406:A:OP1	6:D:56:HIS:NE2	2.46	0.44
4:l:47:VAL:HG21	29:a:74:SER:OG	2.17	0.44
34:f:35:LEU:HD12	34:f:35:LEU:C	2.42	0.44
19:Q:303:LEU:O	19:Q:303:LEU:HD12	2.17	0.44
28:Z:44:ASP:OD1	28:Z:44:ASP:C	2.60	0.44
3:h:864:U:H2'	3:h:865:A:O4'	2.17	0.44
27:Y:113:GLU:OE2	27:Y:115:LYS:NZ	2.50	0.44
2:k:128:ASP:OD1	2:k:128:ASP:N	2.50	0.44
3:h:141:G:H2'	3:h:142:G:C8	2.52	0.44
3:h:1491:G:O6	3:h:1529:G:N2	2.51	0.44
1:A:59:ARG:NH1	10:H:87:TYR:O	2.50	0.44
2:k:122:ASP:OD1	2:k:122:ASP:C	2.59	0.44
3:h:648:U:O2	3:h:688:G:C6	2.70	0.44
3:h:1382:U:O2	3:h:1384:C:N4	2.44	0.44
32:d:194:TYR:CZ	32:d:198:LYS:CE	2.90	0.44
3:h:616:G:H4'	3:h:617:C:OP1	2.17	0.44
5:C:39:LYS:HA	5:C:44:LEU:HD22	2.00	0.44
18:P:36:THR:OG1	18:P:58:ALA:O	2.29	0.44
19:Q:69:ASP:HB3	19:Q:112:VAL:HG12	1.99	0.44
32:d:188:LYS:O	32:d:190:SER:N	2.50	0.44
1:A:22:LYS:N	3:h:777:C:OP1	2.51	0.44
3:h:81:U:H4'	3:h:82:G:OP2	2.16	0.44
5:C:82:CYS:HA	5:C:87:VAL:HG12	2.00	0.44
19:Q:111:SER:HB2	19:Q:155:CYS:HA	2.00	0.44
22:T:7:MET:HE1	33:e:79:PHE:HA	2.00	0.44
23:U:54:LYS:HB3	23:U:58:GLU:OE1	2.18	0.44
25:W:87:ASP:OD1	25:W:88:LEU:N	2.51	0.44
29:a:45:THR:OG1	29:a:48:ARG:O	2.26	0.44
1:A:181:VAL:HG12	1:A:227:THR:HA	2.00	0.43
3:h:137:A:N6	3:h:173:G:O2'	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:594:A:H2'	3:h:595:A:C8	2.53	0.43
3:h:1733:C:H2'	3:h:1734:C:C6	2.53	0.43
29:a:194:ASP:OD1	29:a:195:TRP:N	2.50	0.43
31:c:193:VAL:HB	31:c:194:PRO:HD3	2.00	0.43
3:h:130:A:N6	3:h:268:G:OP1	2.50	0.43
3:h:927:A:H2'	3:h:928:G:C8	2.53	0.43
3:h:1345:C:C2	3:h:1346:U:C5	3.05	0.43
4:l:79:LYS:HG3	4:l:81:TYR:CE2	2.53	0.43
5:C:74:TYR:O	5:C:78:VAL:HG23	2.18	0.43
19:Q:243:PHE:CE2	19:Q:250:LEU:HD23	2.53	0.43
21:S:79:ASP:C	21:S:79:ASP:OD1	2.60	0.43
29:a:81:LYS:CD	29:a:81:LYS:N	2.81	0.43
3:h:931:G:H4'	21:S:137:ASP:OD2	2.18	0.43
3:h:1781:4AC:O5'	3:h:1781:4AC:H6	2.18	0.43
5:C:48:LEU:HD22	16:N:102:VAL:CG1	2.49	0.43
19:Q:306:SER:OG	19:Q:307:ALA:N	2.50	0.43
3:h:541:A:H5'	3:h:546:C:H41	1.83	0.43
28:Z:147:PHE:O	28:Z:165:ASN:ND2	2.50	0.43
3:h:437:C:H2'	3:h:438:G:O4'	2.19	0.43
3:h:971:U:H2'	3:h:972:C:O4'	2.18	0.43
32:d:24:LEU:HD11	32:d:56:PRO:HD3	2.00	0.43
32:d:84:MET:O	32:d:85:HIS:HB2	2.19	0.43
3:h:337:A:OP2	18:P:55:LYS:NZ	2.52	0.43
19:Q:232:LEU:N	19:Q:232:LEU:HD12	2.33	0.43
3:h:871:G:H1	3:h:963:U:H3	1.67	0.43
28:Z:201:LEU:O	28:Z:205:ARG:NH2	2.52	0.43
3:h:628:C:O2'	3:h:942:A:N3	2.52	0.43
17:O:162:ASN:OD1	17:O:162:ASN:N	2.52	0.43
27:Y:60:PRO:O	27:Y:64:ILE:HG13	2.19	0.43
3:h:932:A:C8	21:S:136:THR:O	2.71	0.43
30:b:60:MET:SD	30:b:60:MET:C	3.02	0.43
1:A:10:LYS:NZ	3:h:97:G:OP1	2.48	0.42
7:E:14:GLU:OE2	7:E:17:LYS:NZ	2.52	0.42
12:J:51:ARG:NH1	14:L:35:ASN:O	2.52	0.42
3:h:761:A:C5	3:h:762:PSU:C6	3.07	0.42
3:h:1061:U:H3	3:h:1065:A:H62	1.67	0.42
3:h:1742:C:N3	3:h:1743:U:C5	2.87	0.42
3:h:889:U:C2	3:h:890:A:C8	3.07	0.42
5:C:78:VAL:HG21	5:C:121:CYS:SG	2.59	0.42
6:D:77:GLU:OE2	6:D:78:ARG:N	2.52	0.42
8:F:224:ASP:OD1	8:F:224:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:4:VAL:HG12	15:M:4:VAL:O	2.19	0.42
18:P:213:LYS:HE2	18:P:213:LYS:HA	2.00	0.42
19:Q:60:LEU:HD13	19:Q:91:TRP:CE3	2.54	0.42
3:h:1476:A:N3	3:h:1476:A:H2'	2.34	0.42
6:D:20:TYR:OH	29:a:214:HIS:O	2.22	0.42
22:T:130:LEU:HD21	22:T:134:LYS:HE3	2.00	0.42
1:A:139:LEU:C	1:A:139:LEU:HD12	2.44	0.42
3:h:587:C:OP2	41:h:2166:HOH:O	2.22	0.42
3:h:1446:C:H2'	3:h:1447:OMU:H6	2.02	0.42
28:Z:21:ALA:HB2	28:Z:173:VAL:HG21	2.01	0.42
3:h:2:A:O4'	3:h:374:A:C8	2.72	0.42
3:h:503:C:O2'	3:h:504:U:OP1	2.37	0.42
3:h:942:A:H2'	3:h:943:A:C8	2.54	0.42
3:h:1136:A:H2'	3:h:1137:C:O4'	2.20	0.42
3:h:1479:G:H2'	3:h:1480:A:C8	2.54	0.42
5:C:90:ILE:HD11	5:C:137:VAL:HG13	2.01	0.42
6:D:41:ILE:HD12	6:D:41:ILE:N	2.35	0.42
15:M:7:SER:OG	15:M:10:ARG:NH2	2.51	0.42
19:Q:262:ASP:O	19:Q:266:LYS:N	2.48	0.42
21:S:81:SER:OG	21:S:85:LYS:NZ	2.53	0.42
32:d:28:TRP:CD1	32:d:103:MET:HE2	2.54	0.42
32:d:161:THR:CG2	32:d:165:ARG:NH2	2.82	0.42
3:h:86:A:N3	3:h:146:A:O2'	2.49	0.42
3:h:1594:G:H1	3:h:1614:U:H3	1.68	0.42
7:E:128:GLY:O	7:E:132:LEU:HD12	2.20	0.42
13:K:15:GLU:OE2	13:K:16:LEU:N	2.53	0.42
19:Q:31:MET:SD	19:Q:31:MET:C	3.02	0.42
32:d:182:GLU:OE2	32:d:194:TYR:N	2.52	0.42
2:k:165:ASN:OD1	2:k:175:SER:CB	2.63	0.42
3:h:806:G:H21	33:e:107:SER:HB3	1.85	0.42
3:h:1100:U:O4	31:c:211:ARG:HD2	2.20	0.42
11:I:63:SER:OG	32:d:177:GLU:OE1	2.35	0.42
18:P:11:ARG:NH1	18:P:15:GLY:O	2.51	0.42
25:W:110:ASP:O	25:W:114:ARG:HG2	2.20	0.42
29:a:94:VAL:O	29:a:94:VAL:HG13	2.20	0.42
34:f:104:VAL:HG12	34:f:105:ASP:N	2.34	0.42
3:h:139:U:H1'	3:h:140:OMC:OP2	2.20	0.42
3:h:1455:U:H2'	3:h:1456:C:H6	1.84	0.42
3:h:1548:G:O2'	3:h:1549:A:OP2	2.36	0.42
3:h:1383:OMU:HM21	34:f:17:PHE:HB3	2.02	0.41
16:N:135:HIS:O	16:N:150:TYR:OH	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:114:VAL:HA	27:Y:118:MET:HE2	2.02	0.41
31:c:255:ASP:N	31:c:255:ASP:OD1	2.52	0.41
3:h:983:G:H4'	3:h:1784:A:H4'	2.01	0.41
3:h:1488:A:H2'	3:h:1489:A:C8	2.55	0.41
3:h:1561:A:OP1	27:Y:54:ARG:NE	2.44	0.41
19:Q:49:ASP:N	19:Q:49:ASP:OD1	2.50	0.41
25:W:66:VAL:HG23	25:W:67:THR:N	2.35	0.41
27:Y:47:ARG:HB3	27:Y:48:PRO:HD3	2.02	0.41
3:h:308:U:H2'	3:h:309:C:C6	2.55	0.41
3:h:866:A:OP1	33:e:57:ARG:NE	2.49	0.41
19:Q:41:LEU:HD21	19:Q:67:VAL:HG11	2.03	0.41
1:A:129:VAL:HG12	1:A:139:LEU:HB3	2.01	0.41
2:k:32:ILE:O	2:k:52:ILE:O	2.39	0.41
3:h:16:G:H2'	3:h:17:C:C6	2.56	0.41
3:h:595:A:H2'	3:h:596:U:O4'	2.21	0.41
3:h:1493:G:O2'	3:h:1501:C:O2	2.35	0.41
3:h:1676:G:O2'	3:h:1739:A:N6	2.49	0.41
5:C:134:LEU:HD23	5:C:134:LEU:C	2.45	0.41
15:M:4:VAL:HG12	15:M:10:ARG:HH22	1.86	0.41
20:R:51:LEU:HD22	20:R:96:SER:HB3	2.01	0.41
24:V:22:ARG:NH1	24:V:36:LEU:O	2.51	0.41
31:c:189:VAL:O	31:c:208:THR:OG1	2.31	0.41
2:k:58:LYS:HA	2:k:109:SER:HB2	2.03	0.41
3:h:30:G:H2'	3:h:31:C:C6	2.56	0.41
3:h:503:C:O2'	3:h:504:U:O5'	2.36	0.41
3:h:637:G:H5'	33:e:4:VAL:HG13	2.02	0.41
3:h:1147:U:H2'	3:h:1148:U:C6	2.55	0.41
3:h:1553:A:H2'	3:h:1554:U:O4'	2.21	0.41
19:Q:197:VAL:HG23	19:Q:212:GLY:O	2.21	0.41
1:A:163:ASP:O	1:A:167:ASN:N	2.52	0.41
17:O:150:ILE:HD11	17:O:183:VAL:HG13	2.02	0.41
25:W:138:VAL:O	25:W:138:VAL:HG22	2.20	0.41
3:h:1741:C:H2'	3:h:1742:C:H6	1.86	0.41
17:O:11:ASP:OD1	17:O:11:ASP:O	2.39	0.41
20:R:35:LEU:HD21	20:R:90:ARG:HG2	2.03	0.41
21:S:31:HIS:N	21:S:42:HIS:O	2.50	0.41
3:h:94:A:H4'	3:h:95:PSU:OP2	2.21	0.41
3:h:117:U:H2'	3:h:118:U:C6	2.56	0.41
3:h:601:U:O2'	41:h:2137:HOH:O	2.11	0.41
3:h:1177:C:O2'	3:h:1199:A:N6	2.53	0.41
15:M:30:PRO:HB2	15:M:34:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:82:ARG:HH11	17:O:82:ARG:HB2	1.85	0.41
19:Q:82:GLY:HA2	19:Q:88:LEU:HD23	2.03	0.41
19:Q:297:ILE:HG23	19:Q:297:ILE:O	2.21	0.41
25:W:63:VAL:HG21	25:W:71:ILE:HD11	2.02	0.41
32:d:161:THR:HG22	32:d:165:ARG:HH22	1.85	0.41
34:f:110:LYS:NZ	34:f:114:ASP:OD2	2.43	0.41
3:h:569:C:H4'	15:M:5:HIS:O	2.21	0.41
3:h:763:PSU:C4	3:h:764:A:C8	3.09	0.41
3:h:1530:A:H2'	3:h:1531:A:C8	2.56	0.41
17:O:131:VAL:O	17:O:134:ALA:N	2.54	0.41
19:Q:81:SER:O	19:Q:88:LEU:HD23	2.21	0.41
23:U:89:ASP:OD1	23:U:90:TYR:N	2.54	0.41
2:k:3:PHE:N	2:k:16:LEU:O	2.52	0.40
3:h:604:A:H2'	3:h:605:PSU:O4'	2.21	0.40
20:R:23:ILE:N	20:R:23:ILE:HD13	2.37	0.40
32:d:78:LEU:HD12	32:d:157:ILE:HG23	2.02	0.40
3:h:109:A:H2'	3:h:110:G:C8	2.56	0.40
3:h:193:G:H1'	3:h:194:A:H5'	2.01	0.40
3:h:1266:G:H2'	3:h:1267:G:O4'	2.21	0.40
3:h:1434:G:H2'	3:h:1435:U:C6	2.56	0.40
3:h:1520:G:O2'	3:h:1522:A:N3	2.47	0.40
3:h:19:A:N7	41:h:2295:HOH:O	2.37	0.40
3:h:44:U:OP2	3:h:441:A:N6	2.48	0.40
3:h:1644:G:H2'	3:h:1645:OMC:O4'	2.21	0.40
31:c:225:PHE:O	31:c:229:MET:HG3	2.21	0.40
33:e:55:ASP:OD2	33:e:60:LYS:NZ	2.54	0.40
34:f:62:LEU:O	34:f:66:ARG:HD2	2.21	0.40
1:A:21:ASP:N	1:A:21:ASP:OD1	2.53	0.40
3:h:965:C:H2'	3:h:966:A:O4'	2.22	0.40
14:L:10:VAL:HG22	14:L:28:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	257/264 (97%)	253 (98%)	4 (2%)	0	100	100
2	k	228/249 (92%)	228 (100%)	0	0	100	100
4	l	89/208 (43%)	88 (99%)	1 (1%)	0	100	100
5	C	115/144 (80%)	115 (100%)	0	0	100	100
6	D	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
7	E	134/143 (94%)	132 (98%)	2 (2%)	0	100	100
8	F	214/261 (82%)	212 (99%)	2 (1%)	0	100	100
9	G	81/83 (98%)	81 (100%)	0	0	100	100
10	H	125/133 (94%)	122 (98%)	3 (2%)	0	100	100
11	I	72/107 (67%)	72 (100%)	0	0	100	100
12	J	96/127 (76%)	95 (99%)	1 (1%)	0	100	100
13	K	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
14	L	59/65 (91%)	59 (100%)	0	0	100	100
15	M	48/62 (77%)	44 (92%)	4 (8%)	0	100	100
16	N	67/156 (43%)	67 (100%)	0	0	100	100
17	O	186/191 (97%)	182 (98%)	4 (2%)	0	100	100
18	P	182/224 (81%)	180 (99%)	2 (1%)	0	100	100
19	Q	305/328 (93%)	298 (98%)	7 (2%)	0	100	100
20	R	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
21	S	130/150 (87%)	128 (98%)	2 (2%)	0	100	100
22	T	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
23	U	140/152 (92%)	138 (99%)	2 (1%)	0	100	100
24	V	53/56 (95%)	53 (100%)	0	0	100	100
25	W	147/151 (97%)	147 (100%)	0	0	100	100
26	X	143/159 (90%)	140 (98%)	3 (2%)	0	100	100
27	Y	129/152 (85%)	125 (97%)	4 (3%)	0	100	100
28	Z	200/336 (60%)	198 (99%)	2 (1%)	0	100	100
29	a	209/248 (84%)	203 (97%)	6 (3%)	0	100	100
30	b	181/197 (92%)	179 (99%)	2 (1%)	0	100	100
31	c	215/280 (77%)	213 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	192/210 (91%)	184 (96%)	7 (4%)	1 (0%)	24	34
33	e	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
34	f	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
All	All	4701/5612 (84%)	4628 (98%)	72 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	d	59	ALA

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	
1	A	225/228 (99%)	224 (100%)	1 (0%)	84	91
2	k	199/213 (93%)	199 (100%)	0	100	100
4	l	85/169 (50%)	85 (100%)	0	100	100
5	C	94/112 (84%)	94 (100%)	0	100	100
6	D	109/124 (88%)	109 (100%)	0	100	100
7	E	111/114 (97%)	111 (100%)	0	100	100
8	F	195/228 (86%)	194 (100%)	1 (0%)	81	90
9	G	70/70 (100%)	69 (99%)	1 (1%)	59	77
10	H	108/113 (96%)	108 (100%)	0	100	100
11	I	64/89 (72%)	64 (100%)	0	100	100
12	J	87/109 (80%)	87 (100%)	0	100	100
13	K	76/78 (97%)	76 (100%)	0	100	100
14	L	54/57 (95%)	54 (100%)	0	100	100
15	M	41/49 (84%)	41 (100%)	0	100	100
16	N	60/134 (45%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	169/171 (99%)	169 (100%)	0	100	100
18	P	158/178 (89%)	157 (99%)	1 (1%)	78	88
19	Q	266/279 (95%)	264 (99%)	2 (1%)	73	85
20	R	93/108 (86%)	93 (100%)	0	100	100
21	S	103/120 (86%)	103 (100%)	0	100	100
22	T	113/114 (99%)	113 (100%)	0	100	100
23	U	122/131 (93%)	120 (98%)	2 (2%)	55	74
24	V	46/47 (98%)	46 (100%)	0	100	100
25	W	130/131 (99%)	130 (100%)	0	100	100
26	X	124/131 (95%)	124 (100%)	0	100	100
27	Y	115/130 (88%)	115 (100%)	0	100	100
28	Z	171/256 (67%)	171 (100%)	0	100	100
29	a	179/215 (83%)	179 (100%)	0	100	100
30	b	161/171 (94%)	161 (100%)	0	100	100
31	c	184/226 (81%)	183 (100%)	1 (0%)	81	90
32	d	165/175 (94%)	165 (100%)	0	100	100
33	e	111/112 (99%)	111 (100%)	0	100	100
34	f	116/120 (97%)	116 (100%)	0	100	100
All	All	4104/4702 (87%)	4095 (100%)	9 (0%)	85	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
8	F	135	LEU
9	G	44	LEU
18	P	210	LYS
19	Q	114	PHE
19	Q	133	TRP
23	U	13	LEU
23	U	59	LEU
31	c	205	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
2	k	91	ASN
4	l	44	GLN
7	E	22	HIS
7	E	107	GLN
8	F	174	ASN
8	F	175	GLN
12	J	13	HIS
12	J	43	ASN
12	J	72	GLN
13	K	11	ASN
13	K	53	GLN
13	K	62	GLN
15	M	24	GLN
19	Q	149	HIS
23	U	16	GLN
23	U	73	ASN
23	U	119	ASN
24	V	3	HIS
24	V	28	HIS
25	W	78	HIS
27	Y	144	HIS
28	Z	132	GLN
28	Z	169	HIS
31	c	99	GLN
31	c	104	GLN
32	d	209	ASN
33	e	42	GLN
34	f	15	GLN
34	f	65	HIS
34	f	81	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	h	1617/1808 (89%)	225 (13%)	0
35	B	11/12 (91%)	1 (9%)	0
All	All	1628/1820 (89%)	226 (13%)	0

All (226) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	h	2	A
3	h	17	C
3	h	25	C
3	h	26	A
3	h	34	G
3	h	42	G
3	h	45	U
3	h	47	A
3	h	56	U
3	h	68	A
3	h	82	G
3	h	84	G
3	h	105	A
3	h	115	A
3	h	123	OMU
3	h	128	G
3	h	129	U
3	h	130	A
3	h	132	C
3	h	133	U
3	h	135	C
3	h	136	U
3	h	139	U
3	h	140	OMC
3	h	144	U
3	h	150	U
3	h	151	A
3	h	158	C
3	h	164	C
3	h	174	C
3	h	186	A
3	h	189	U
3	h	190	C
3	h	191	U
3	h	192	G
3	h	193	G
3	h	194	A
3	h	213	U
3	h	214	A
3	h	252	U
3	h	253	C
3	h	260	A
3	h	274	A

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Mol	Chain	Res	Type
3	h	277	G
3	h	278	C
3	h	318	C
3	h	320	A
3	h	324	U
3	h	326	G
3	h	341	G
3	h	342	C
3	h	363	G
3	h	365	C
3	h	382	A
3	h	384	U
3	h	392	OMG
3	h	394	G
3	h	404	A
3	h	405	A
3	h	406	C
3	h	415	C
3	h	420	A
3	h	427	G
3	h	428	C
3	h	429	A
3	h	430	G
3	h	432	A
3	h	438	G
3	h	443	U
3	h	448	C
3	h	449	A
3	h	472	A
3	h	481	A
3	h	489	C
3	h	490	G
3	h	504	U
3	h	505	G
3	h	510	U
3	h	513	G
3	h	518	A
3	h	522	C
3	h	541	A
3	h	544	A2M
3	h	545	U
3	h	552	G

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Mol	Chain	Res	Type
3	h	558	A
3	h	560	G
3	h	568	C
3	h	581	OMU
3	h	582	A
3	h	584	PSU
3	h	585	U
3	h	586	C
3	h	597	A
3	h	598	OMG
3	h	609	A
3	h	614	OMU
3	h	620	U
3	h	622	A2M
3	h	623	A
3	h	625	A
3	h	626	A
3	h	642	U
3	h	647	A
3	h	759	A
3	h	769	G
3	h	770	C
3	h	775	A
3	h	779	A
3	h	783	U
3	h	784	A
3	h	785	C
3	h	786	G
3	h	790	U
3	h	793	A
3	h	816	A
3	h	832	A
3	h	834	U
3	h	866	A
3	h	915	U
3	h	931	G
3	h	936	A
3	h	938	U
3	h	945	G
3	h	954	A
3	h	963	U
3	h	991	C

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Mol	Chain	Res	Type
3	h	1006	A
3	h	1007	U
3	h	1008	A
3	h	1029	A
3	h	1031	C
3	h	1042	A
3	h	1059	G
3	h	1060	C
3	h	1085	U
3	h	1090	A
3	h	1095	A
3	h	1100	U
3	h	1141	A
3	h	1153	G
3	h	1161	C
3	h	1166	A
3	h	1170	G
3	h	1188	U
3	h	1197	A
3	h	1199	A
3	h	1202	G
3	h	1203	G
3	h	1204	G
3	h	1205	A
3	h	1220	A
3	h	1221	G
3	h	1234	OMU
3	h	1246	G
3	h	1247	A
3	h	1248	G
3	h	1249	C
3	h	1268	G
3	h	1272	OMU
3	h	1274	OMG
3	h	1302	G
3	h	1317	U
3	h	1318	U
3	h	1324	A
3	h	1328	A
3	h	1364	U
3	h	1365	A
3	h	1366	U

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Mol	Chain	Res	Type
3	h	1375	G
3	h	1383	OMU
3	h	1395	U
3	h	1396	A
3	h	1403	U
3	h	1404	U
3	h	1418	U
3	h	1420	U
3	h	1432	A
3	h	1433	OMG
3	h	1437	U
3	h	1440	G
3	h	1451	A
3	h	1464	C
3	h	1465	A
3	h	1476	A
3	h	1495	U
3	h	1503	U
3	h	1518	G
3	h	1523	A
3	h	1524	PSU
3	h	1528	U
3	h	1530	A
3	h	1543	A
3	h	1548	G
3	h	1563	U
3	h	1565	G
3	h	1579	A2M
3	h	1581	G
3	h	1596	G
3	h	1606	A
3	h	1607	G
3	h	1617	A
3	h	1637	A
3	h	1640	C
3	h	1646	C
3	h	1657	A
3	h	1663	U
3	h	1664	G
3	h	1686	G
3	h	1763	A
3	h	1765	G

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Mol	Chain	Res	Type
3	h	1774	A
3	h	1775	G
3	h	1777	U
3	h	1787	PSU
3	h	1788	G
3	h	1790	MA6
3	h	1791	C
3	h	1800	G
3	h	1801	G
3	h	1802	A
3	h	1803	U
3	h	1804	C
3	h	1807	U
3	h	1808	G
35	B	19	U

There are no RNA pucker outliers to report.

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

81 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	$\# Z > 2$
3	PSU	h	1634	3	18,21,22	4.61	8 (44%)	22,30,33	1.80	5 (22%)
3	PSU	h	1535	3	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
3	OMG	h	246	37,3	23,26,27	2.56	8 (34%)	33,38,41	2.24	10 (30%)
3	A2M	h	544	3	22,25,26	3.90	9 (40%)	31,36,39	2.97	14 (45%)
3	PSU	h	607	3	18,21,22	4.60	8 (44%)	22,30,33	1.87	6 (27%)
3	PSU	h	809	3	18,21,22	4.59	8 (44%)	22,30,33	1.83	6 (27%)
3	6MZ	h	1771	37,3,36	22,25,26	2.72	4 (18%)	30,36,39	2.47	11 (36%)
3	PSU	h	95	3	18,21,22	4.62	8 (44%)	22,30,33	1.84	5 (22%)
3	PSU	h	1567	3	18,21,22	4.62	8 (44%)	22,30,33	1.84	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	h	753	3	18,21,22	4.62	8 (44%)	22,30,33	1.82	5 (22%)
3	MA6	h	1790	3	23,26,27	1.27	4 (17%)	34,38,41	2.83	15 (44%)
3	PSU	h	1002	3	18,21,22	4.60	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	h	306	3	18,21,22	4.55	8 (44%)	22,30,33	1.78	5 (22%)
3	A2M	h	977	3	22,25,26	3.91	9 (40%)	31,36,39	2.97	12 (38%)
3	PSU	h	1485	3	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
3	OMU	h	886	3	19,22,23	3.21	8 (42%)	26,31,34	1.82	5 (19%)
3	PSU	h	1106	3	18,21,22	4.56	8 (44%)	22,30,33	1.82	5 (22%)
3	PSU	h	470	3	18,21,22	4.61	8 (44%)	22,30,33	1.86	5 (22%)
3	OMC	h	473	3	19,22,23	3.24	8 (42%)	26,31,34	0.69	0
3	B8N	h	1194	3	24,29,30	3.01	7 (29%)	29,42,45	1.72	7 (24%)
3	PSU	h	1304	3	18,21,22	4.59	8 (44%)	22,30,33	1.85	5 (22%)
3	OMG	h	598	3	23,26,27	2.53	8 (34%)	33,38,41	2.22	11 (33%)
3	OMU	h	123	3	19,22,23	3.21	8 (42%)	26,31,34	1.66	4 (15%)
3	OMC	h	418	3	19,22,23	3.27	8 (42%)	26,31,34	0.90	1 (3%)
3	OMG	h	392	3	23,26,27	2.55	9 (39%)	33,38,41	2.19	13 (39%)
3	PSU	h	339	37,3	18,21,22	4.63	8 (44%)	22,30,33	1.86	6 (27%)
3	PSU	h	1178	3	18,21,22	4.57	8 (44%)	22,30,33	1.83	5 (22%)
3	OMU	h	1447	3	19,22,23	3.18	8 (42%)	26,31,34	1.66	4 (15%)
3	OMC	h	1645	3	19,22,23	3.25	8 (42%)	26,31,34	0.75	0
3	PSU	h	1615	3	18,21,22	4.61	8 (44%)	22,30,33	1.80	5 (22%)
3	OMG	h	1274	37,3	23,26,27	2.55	8 (34%)	33,38,41	2.20	11 (33%)
3	PSU	h	362	3	18,21,22	4.58	8 (44%)	22,30,33	1.84	5 (22%)
3	4AC	h	1781	3	21,24,25	3.17	11 (52%)	29,34,37	1.56	4 (13%)
3	OMU	h	1234	3	19,22,23	3.19	8 (42%)	26,31,34	1.66	4 (15%)
3	A2M	h	162	3	22,25,26	3.94	9 (40%)	31,36,39	2.94	12 (38%)
3	A2M	h	28	3,36	22,25,26	3.94	9 (40%)	31,36,39	2.98	12 (38%)
3	A2M	h	440	3	22,25,26	3.92	9 (40%)	31,36,39	3.05	12 (38%)
3	OMC	h	38	3	19,22,23	3.28	8 (42%)	26,31,34	0.69	0
3	A2M	h	1758	3	22,25,26	3.96	10 (45%)	31,36,39	2.98	13 (41%)
3	UY1	h	603	3	19,22,23	4.13	7 (36%)	22,31,34	1.80	5 (22%)
3	PSU	h	762	3	18,21,22	4.57	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	h	121	3,36	18,21,22	4.62	8 (44%)	22,30,33	1.79	5 (22%)
3	PSU	h	605	3	18,21,22	4.57	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	h	417	3	18,21,22	4.57	8 (44%)	22,30,33	1.75	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	h	961	37,3	18,21,22	4.61	8 (44%)	22,30,33	1.91	5 (22%)
3	MA6	h	1789	3	23,26,27	1.25	3 (13%)	34,38,41	2.75	14 (41%)
3	OMU	h	581	37,3	19,22,23	3.20	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	h	1293	3	18,21,22	4.62	8 (44%)	22,30,33	1.82	5 (22%)
3	A2M	h	622	3,36	22,25,26	3.91	10 (45%)	31,36,39	3.15	14 (45%)
3	PSU	h	1524	3	18,21,22	4.68	8 (44%)	22,30,33	1.75	5 (22%)
3	A2M	h	468	3	22,25,26	3.96	9 (40%)	31,36,39	3.02	13 (41%)
3	4AC	h	1283	3	21,24,25	3.14	11 (52%)	29,34,37	1.15	3 (10%)
3	PSU	h	584	3	18,21,22	5.19	10 (55%)	22,30,33	4.36	6 (27%)
3	PSU	h	1217	3	18,21,22	4.62	8 (44%)	22,30,33	1.79	5 (22%)
3	PSU	h	1190	3	18,21,22	4.62	8 (44%)	22,30,33	1.86	5 (22%)
3	OMU	h	373	3	19,22,23	3.19	8 (42%)	26,31,34	1.67	4 (15%)
3	PSU	h	606	3	18,21,22	4.59	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	h	763	3	18,21,22	4.57	8 (44%)	22,30,33	1.79	5 (22%)
3	PSU	h	950	3	18,21,22	4.59	8 (44%)	22,30,33	1.80	5 (22%)
3	PSU	h	1210	3	18,21,22	4.61	8 (44%)	22,30,33	1.89	5 (22%)
3	PSU	h	1787	3	18,21,22	4.63	8 (44%)	22,30,33	1.91	5 (22%)
3	A2M	h	800	3	22,25,26	3.93	9 (40%)	31,36,39	3.00	12 (38%)
3	PSU	h	1184	3	18,21,22	4.60	8 (44%)	22,30,33	1.90	5 (22%)
3	PSU	h	258	3	18,21,22	4.63	8 (44%)	22,30,33	1.79	5 (22%)
3	PSU	h	1120	3	18,21,22	4.55	8 (44%)	22,30,33	1.85	5 (22%)
3	PSU	h	451	37,3	18,21,22	4.58	8 (44%)	22,30,33	1.83	6 (27%)
3	OMU	h	614	3	19,22,23	3.19	8 (42%)	26,31,34	1.65	4 (15%)
3	OMU	h	1272	3	19,22,23	3.20	8 (42%)	26,31,34	1.67	4 (15%)
3	OMU	h	1383	3,36	19,22,23	3.19	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	h	103	37,3	18,21,22	4.58	8 (44%)	22,30,33	1.83	5 (22%)
3	OMG	h	1433	3,36	23,26,27	2.54	9 (39%)	33,38,41	2.15	11 (33%)
3	A2M	h	1329	3	22,25,26	3.93	9 (40%)	31,36,39	3.00	13 (41%)
3	PSU	h	1308	3	18,21,22	4.58	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	h	1027	3	18,21,22	4.62	9 (50%)	22,30,33	1.86	5 (22%)
3	PSU	h	635	3	18,21,22	4.58	8 (44%)	22,30,33	1.82	5 (22%)
3	A2M	h	424	3	22,25,26	3.96	9 (40%)	31,36,39	3.00	13 (41%)
3	OMC	h	1218	3	19,22,23	3.30	8 (42%)	26,31,34	0.79	0
3	OMU	h	1012	3	19,22,23	3.17	8 (42%)	26,31,34	1.69	4 (15%)
3	A2M	h	1579	3	22,25,26	3.95	9 (40%)	31,36,39	3.04	12 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	h	140	3	19,22,23	3.29	8 (42%)	26,31,34	0.73	0
3	PSU	h	310	3	18,21,22	4.61	8 (44%)	22,30,33	1.84	5 (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
3	PSU	h	1634	3	-	0/7/25/26	0/2/2/2
3	PSU	h	1535	3	-	0/7/25/26	0/2/2/2
3	OMG	h	246	37,3	-	0/9/27/28	0/3/3/3
3	A2M	h	544	3	-	2/9/27/28	0/3/3/3
3	PSU	h	607	3	-	0/7/25/26	0/2/2/2
3	PSU	h	809	3	-	0/7/25/26	0/2/2/2
3	6MZ	h	1771	37,3,36	-	0/9/27/28	0/3/3/3
3	PSU	h	95	3	-	0/7/25/26	0/2/2/2
3	PSU	h	1567	3	-	0/7/25/26	0/2/2/2
3	PSU	h	753	3	-	0/7/25/26	0/2/2/2
3	MA6	h	1790	3	-	3/11/29/30	0/3/3/3
3	PSU	h	1002	3	-	0/7/25/26	0/2/2/2
3	PSU	h	306	3	-	0/7/25/26	0/2/2/2
3	A2M	h	977	3	-	0/9/27/28	0/3/3/3
3	PSU	h	1485	3	-	0/7/25/26	0/2/2/2
3	OMU	h	886	3	-	3/9/27/28	0/2/2/2
3	PSU	h	1106	3	-	0/7/25/26	0/2/2/2
3	PSU	h	470	3	-	0/7/25/26	0/2/2/2
3	OMC	h	473	3	-	0/9/27/28	0/2/2/2
3	B8N	h	1194	3	-	2/16/34/35	0/2/2/2
3	PSU	h	1304	3	-	1/7/25/26	0/2/2/2
3	OMG	h	598	3	-	3/9/27/28	0/3/3/3
3	OMU	h	123	3	-	2/9/27/28	0/2/2/2
3	OMC	h	418	3	-	2/9/27/28	0/2/2/2
3	OMG	h	392	3	-	2/9/27/28	0/3/3/3
3	PSU	h	339	37,3	-	0/7/25/26	0/2/2/2
3	PSU	h	1178	3	-	0/7/25/26	0/2/2/2
3	OMU	h	1447	3	-	0/9/27/28	0/2/2/2
3	OMC	h	1645	3	-	0/9/27/28	0/2/2/2
3	PSU	h	1615	3	-	0/7/25/26	0/2/2/2
3	OMG	h	1274	37,3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	h	362	3	-	0/7/25/26	0/2/2/2
3	4AC	h	1781	3	-	0/11/29/30	0/2/2/2
3	OMU	h	1234	3	-	2/9/27/28	0/2/2/2
3	A2M	h	162	3	-	0/9/27/28	0/3/3/3
3	A2M	h	28	3,36	-	0/9/27/28	0/3/3/3
3	A2M	h	440	3	-	0/9/27/28	0/3/3/3
3	OMC	h	38	3	-	0/9/27/28	0/2/2/2
3	A2M	h	1758	3	-	0/9/27/28	0/3/3/3
3	UY1	h	603	3	-	0/9/27/28	0/2/2/2
3	PSU	h	762	3	-	0/7/25/26	0/2/2/2
3	PSU	h	121	3,36	-	0/7/25/26	0/2/2/2
3	PSU	h	605	3	-	0/7/25/26	0/2/2/2
3	PSU	h	417	3	-	0/7/25/26	0/2/2/2
3	PSU	h	961	37,3	-	2/7/25/26	0/2/2/2
3	MA6	h	1789	3	-	0/11/29/30	0/3/3/3
3	OMU	h	581	37,3	-	2/9/27/28	0/2/2/2
3	PSU	h	1293	3	-	0/7/25/26	0/2/2/2
3	A2M	h	622	3,36	-	5/9/27/28	0/3/3/3
3	PSU	h	1524	3	-	2/7/25/26	0/2/2/2
3	A2M	h	468	3	-	0/9/27/28	0/3/3/3
3	4AC	h	1283	3	-	0/11/29/30	0/2/2/2
3	PSU	h	584	3	-	5/7/25/26	0/2/2/2
3	PSU	h	1217	3	-	0/7/25/26	0/2/2/2
3	PSU	h	1190	3	-	0/7/25/26	0/2/2/2
3	OMU	h	373	3	-	0/9/27/28	0/2/2/2
3	PSU	h	606	3	-	0/7/25/26	0/2/2/2
3	PSU	h	763	3	-	0/7/25/26	0/2/2/2
3	PSU	h	950	3	-	0/7/25/26	0/2/2/2
3	PSU	h	1210	3	-	0/7/25/26	0/2/2/2
3	PSU	h	1787	3	-	2/7/25/26	0/2/2/2
3	A2M	h	800	3	-	0/9/27/28	0/3/3/3
3	PSU	h	1184	3	-	0/7/25/26	0/2/2/2
3	PSU	h	258	3	-	2/7/25/26	0/2/2/2
3	PSU	h	1120	3	-	0/7/25/26	0/2/2/2
3	PSU	h	451	37,3	-	0/7/25/26	0/2/2/2
3	OMU	h	614	3	-	1/9/27/28	0/2/2/2
3	OMU	h	1272	3	-	1/9/27/28	0/2/2/2
3	OMU	h	1383	3,36	-	0/9/27/28	0/2/2/2
3	PSU	h	103	37,3	-	0/7/25/26	0/2/2/2
3	OMG	h	1433	3,36	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	h	1329	3	-	0/9/27/28	0/3/3/3
3	PSU	h	1308	3	-	2/7/25/26	0/2/2/2
3	PSU	h	1027	3	-	0/7/25/26	0/2/2/2
3	PSU	h	635	3	-	0/7/25/26	0/2/2/2
3	A2M	h	424	3	-	0/9/27/28	0/3/3/3
3	OMC	h	1218	3	-	0/9/27/28	0/2/2/2
3	OMU	h	1012	3	-	0/9/27/28	0/2/2/2
3	A2M	h	1579	3	-	2/9/27/28	0/3/3/3
3	OMC	h	140	3	-	2/9/27/28	0/2/2/2
3	PSU	h	310	3	-	0/7/25/26	0/2/2/2

All (658) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1524	PSU	C6-C5	12.31	1.49	1.35
3	h	1485	PSU	C6-C5	12.20	1.49	1.35
3	h	1787	PSU	C6-C5	12.20	1.49	1.35
3	h	1535	PSU	C6-C5	12.19	1.49	1.35
3	h	470	PSU	C6-C5	12.16	1.49	1.35
3	h	1615	PSU	C6-C5	12.13	1.49	1.35
3	h	339	PSU	C6-C5	12.11	1.49	1.35
3	h	121	PSU	C6-C5	12.11	1.49	1.35
3	h	1190	PSU	C6-C5	12.11	1.49	1.35
3	h	258	PSU	C6-C5	12.10	1.49	1.35
3	h	753	PSU	C6-C5	12.09	1.49	1.35
3	h	950	PSU	C6-C5	12.09	1.49	1.35
3	h	961	PSU	C6-C5	12.09	1.49	1.35
3	h	1293	PSU	C6-C5	12.09	1.49	1.35
3	h	95	PSU	C6-C5	12.08	1.49	1.35
3	h	1634	PSU	C6-C5	12.07	1.49	1.35
3	h	1184	PSU	C6-C5	12.07	1.49	1.35
3	h	310	PSU	C6-C5	12.07	1.49	1.35
3	h	1027	PSU	C6-C5	12.06	1.49	1.35
3	h	1002	PSU	C6-C5	12.04	1.49	1.35
3	h	1217	PSU	C6-C5	12.04	1.49	1.35
3	h	451	PSU	C6-C5	12.04	1.49	1.35
3	h	1567	PSU	C6-C5	12.01	1.49	1.35
3	h	635	PSU	C6-C5	12.00	1.49	1.35
3	h	1304	PSU	C6-C5	11.97	1.49	1.35
3	h	1210	PSU	C6-C5	11.97	1.49	1.35
3	h	1178	PSU	C6-C5	11.97	1.49	1.35
3	h	362	PSU	C6-C5	11.97	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	607	PSU	C6-C5	11.96	1.49	1.35
3	h	103	PSU	C6-C5	11.95	1.49	1.35
3	h	605	PSU	C6-C5	11.94	1.49	1.35
3	h	1120	PSU	C6-C5	11.94	1.49	1.35
3	h	606	PSU	C6-C5	11.93	1.49	1.35
3	h	306	PSU	C6-C5	11.93	1.49	1.35
3	h	809	PSU	C6-C5	11.91	1.49	1.35
3	h	762	PSU	C6-C5	11.87	1.49	1.35
3	h	417	PSU	C6-C5	11.87	1.49	1.35
3	h	1308	PSU	C6-C5	11.86	1.49	1.35
3	h	1106	PSU	C6-C5	11.84	1.49	1.35
3	h	584	PSU	C2-N1	11.84	1.52	1.36
3	h	763	PSU	C6-C5	11.81	1.49	1.35
3	h	1771	6MZ	C6-N6	11.35	1.46	1.34
3	h	603	UY1	C6-C5	11.17	1.48	1.35
3	h	584	PSU	C6-C5	10.99	1.48	1.35
3	h	584	PSU	C2-N3	10.58	1.55	1.37
3	h	544	A2M	C3'-C4'	-9.92	1.27	1.53
3	h	162	A2M	C3'-C4'	-9.88	1.27	1.53
3	h	1758	A2M	C3'-C4'	-9.85	1.27	1.53
3	h	622	A2M	C3'-C4'	-9.83	1.27	1.53
3	h	1579	A2M	C2'-C1'	-9.82	1.27	1.53
3	h	424	A2M	C3'-C4'	-9.81	1.27	1.53
3	h	1758	A2M	C2'-C1'	-9.79	1.27	1.53
3	h	1329	A2M	C3'-C4'	-9.79	1.28	1.53
3	h	424	A2M	C2'-C1'	-9.78	1.27	1.53
3	h	468	A2M	C3'-C4'	-9.78	1.28	1.53
3	h	28	A2M	C3'-C4'	-9.76	1.28	1.53
3	h	468	A2M	C2'-C1'	-9.74	1.28	1.53
3	h	800	A2M	C3'-C4'	-9.74	1.28	1.53
3	h	977	A2M	C2'-C1'	-9.69	1.28	1.53
3	h	1579	A2M	C3'-C4'	-9.68	1.28	1.53
3	h	162	A2M	C2'-C1'	-9.66	1.28	1.53
3	h	977	A2M	C3'-C4'	-9.65	1.28	1.53
3	h	440	A2M	C3'-C4'	-9.64	1.28	1.53
3	h	28	A2M	C2'-C1'	-9.58	1.28	1.53
3	h	1329	A2M	C2'-C1'	-9.58	1.28	1.53
3	h	1524	PSU	C2-N1	9.56	1.49	1.36
3	h	800	A2M	C2'-C1'	-9.55	1.28	1.53
3	h	440	A2M	C2'-C1'	-9.54	1.28	1.53
3	h	95	PSU	C2-N1	9.53	1.49	1.36
3	h	1535	PSU	C2-N1	9.51	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1190	PSU	C2-N1	9.48	1.49	1.36
3	h	339	PSU	C2-N1	9.48	1.49	1.36
3	h	606	PSU	C2-N1	9.48	1.49	1.36
3	h	753	PSU	C2-N1	9.47	1.49	1.36
3	h	1567	PSU	C2-N1	9.46	1.49	1.36
3	h	1027	PSU	C2-N1	9.46	1.49	1.36
3	h	1184	PSU	C2-N1	9.46	1.49	1.36
3	h	1634	PSU	C2-N1	9.45	1.49	1.36
3	h	809	PSU	C2-N1	9.45	1.49	1.36
3	h	607	PSU	C2-N1	9.45	1.49	1.36
3	h	1217	PSU	C2-N1	9.44	1.49	1.36
3	h	1308	PSU	C2-N1	9.44	1.49	1.36
3	h	121	PSU	C2-N1	9.43	1.49	1.36
3	h	258	PSU	C2-N1	9.43	1.49	1.36
3	h	1210	PSU	C2-N1	9.42	1.49	1.36
3	h	622	A2M	C2'-C1'	-9.42	1.28	1.53
3	h	310	PSU	C2-N1	9.41	1.49	1.36
3	h	1787	PSU	C2-N1	9.40	1.49	1.36
3	h	470	PSU	C2-N1	9.40	1.49	1.36
3	h	1002	PSU	C2-N1	9.40	1.49	1.36
3	h	763	PSU	C2-N1	9.40	1.49	1.36
3	h	635	PSU	C2-N1	9.39	1.49	1.36
3	h	417	PSU	C2-N1	9.39	1.49	1.36
3	h	1485	PSU	C2-N1	9.37	1.49	1.36
3	h	961	PSU	C2-N1	9.37	1.49	1.36
3	h	1615	PSU	C2-N1	9.36	1.49	1.36
3	h	362	PSU	C2-N1	9.36	1.49	1.36
3	h	1293	PSU	C2-N1	9.35	1.49	1.36
3	h	603	UY1	C2-N1	9.34	1.49	1.36
3	h	103	PSU	C2-N1	9.32	1.49	1.36
3	h	605	PSU	C2-N1	9.32	1.49	1.36
3	h	1304	PSU	C2-N1	9.30	1.49	1.36
3	h	762	PSU	C2-N1	9.29	1.49	1.36
3	h	1178	PSU	C2-N1	9.27	1.49	1.36
3	h	950	PSU	C2-N1	9.25	1.49	1.36
3	h	451	PSU	C2-N1	9.25	1.49	1.36
3	h	1106	PSU	C2-N1	9.24	1.49	1.36
3	h	306	PSU	C2-N1	9.22	1.49	1.36
3	h	1120	PSU	C2-N1	9.22	1.49	1.36
3	h	544	A2M	C2'-C1'	-9.20	1.29	1.53
3	h	1524	PSU	C2-N3	8.28	1.51	1.37
3	h	1485	PSU	C2-N3	8.23	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	753	PSU	C2-N3	8.22	1.51	1.37
3	h	1567	PSU	C2-N3	8.20	1.51	1.37
3	h	1293	PSU	C2-N3	8.19	1.51	1.37
3	h	258	PSU	C2-N3	8.19	1.51	1.37
3	h	1027	PSU	C2-N3	8.18	1.51	1.37
3	h	1535	PSU	C2-N3	8.17	1.51	1.37
3	h	1615	PSU	C2-N3	8.17	1.51	1.37
3	h	310	PSU	C2-N3	8.16	1.51	1.37
3	h	1210	PSU	C2-N3	8.15	1.51	1.37
3	h	1634	PSU	C2-N3	8.15	1.51	1.37
3	h	339	PSU	C2-N3	8.15	1.51	1.37
3	h	950	PSU	C2-N3	8.14	1.51	1.37
3	h	1106	PSU	C2-N3	8.14	1.51	1.37
3	h	763	PSU	C2-N3	8.14	1.51	1.37
3	h	762	PSU	C2-N3	8.14	1.51	1.37
3	h	1308	PSU	C2-N3	8.13	1.51	1.37
3	h	1304	PSU	C2-N3	8.13	1.51	1.37
3	h	1190	PSU	C2-N3	8.12	1.51	1.37
3	h	362	PSU	C2-N3	8.11	1.51	1.37
3	h	103	PSU	C2-N3	8.11	1.51	1.37
3	h	1184	PSU	C2-N3	8.11	1.51	1.37
3	h	1217	PSU	C2-N3	8.10	1.51	1.37
3	h	121	PSU	C2-N3	8.10	1.51	1.37
3	h	95	PSU	C2-N3	8.09	1.51	1.37
3	h	809	PSU	C2-N3	8.08	1.51	1.37
3	h	417	PSU	C2-N3	8.08	1.51	1.37
3	h	470	PSU	C2-N3	8.07	1.51	1.37
3	h	1120	PSU	C2-N3	8.07	1.51	1.37
3	h	607	PSU	C2-N3	8.07	1.51	1.37
3	h	1002	PSU	C2-N3	8.06	1.51	1.37
3	h	1178	PSU	C2-N3	8.06	1.51	1.37
3	h	635	PSU	C2-N3	8.05	1.51	1.37
3	h	605	PSU	C2-N3	8.03	1.51	1.37
3	h	961	PSU	C2-N3	8.03	1.51	1.37
3	h	1787	PSU	C2-N3	8.02	1.51	1.37
3	h	606	PSU	C2-N3	8.02	1.51	1.37
3	h	451	PSU	C2-N3	8.01	1.51	1.37
3	h	306	PSU	C2-N3	7.95	1.51	1.37
3	h	1194	B8N	C4-N3	-7.76	1.26	1.40
3	h	1194	B8N	C6-N1	7.47	1.55	1.36
3	h	603	UY1	C2-N3	7.26	1.49	1.37
3	h	1781	4AC	C4-N3	7.08	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1218	OMC	C2-N3	7.03	1.50	1.36
3	h	581	OMU	C2-N3	7.02	1.50	1.38
3	h	140	OMC	C2-N3	6.98	1.50	1.36
3	h	123	OMU	C2-N3	6.96	1.50	1.38
3	h	1447	OMU	C2-N3	6.95	1.50	1.38
3	h	418	OMC	C2-N3	6.94	1.50	1.36
3	h	614	OMU	C2-N3	6.93	1.50	1.38
3	h	886	OMU	C2-N3	6.92	1.50	1.38
3	h	373	OMU	C2-N3	6.91	1.50	1.38
3	h	1272	OMU	C2-N3	6.90	1.50	1.38
3	h	1383	OMU	C2-N3	6.88	1.50	1.38
3	h	38	OMC	C2-N3	6.87	1.50	1.36
3	h	1645	OMC	C2-N3	6.85	1.50	1.36
3	h	1012	OMU	C2-N3	6.84	1.50	1.38
3	h	1234	OMU	C2-N3	6.81	1.50	1.38
3	h	1283	4AC	C4-N3	6.78	1.44	1.32
3	h	473	OMC	C2-N3	6.76	1.50	1.36
3	h	886	OMU	C2-N1	6.59	1.49	1.38
3	h	123	OMU	C2-N1	6.59	1.49	1.38
3	h	584	PSU	C4-N3	6.58	1.51	1.38
3	h	614	OMU	C2-N1	6.53	1.48	1.38
3	h	246	OMG	C4-N3	6.52	1.49	1.34
3	h	1433	OMG	C4-N3	6.51	1.49	1.34
3	h	1272	OMU	C2-N1	6.50	1.48	1.38
3	h	1234	OMU	C2-N1	6.50	1.48	1.38
3	h	373	OMU	C2-N1	6.49	1.48	1.38
3	h	581	OMU	C2-N1	6.47	1.48	1.38
3	h	1447	OMU	C2-N1	6.45	1.48	1.38
3	h	1012	OMU	C2-N1	6.45	1.48	1.38
3	h	1383	OMU	C2-N1	6.45	1.48	1.38
3	h	1274	OMG	C4-N3	6.42	1.49	1.34
3	h	392	OMG	C4-N3	6.39	1.49	1.34
3	h	598	OMG	C4-N3	6.35	1.49	1.34
3	h	1283	4AC	C6-C5	6.31	1.49	1.35
3	h	1781	4AC	C2-N3	6.30	1.49	1.36
3	h	418	OMC	C6-C5	6.15	1.49	1.35
3	h	473	OMC	C6-C5	6.14	1.49	1.35
3	h	622	A2M	C3'-C2'	6.13	1.66	1.52
3	h	1218	OMC	C6-C5	6.12	1.49	1.35
3	h	38	OMC	C6-C5	6.11	1.49	1.35
3	h	544	A2M	C3'-C2'	6.10	1.66	1.52
3	h	140	OMC	C6-C5	6.08	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1645	OMC	C6-C5	6.07	1.49	1.35
3	h	440	A2M	C3'-C2'	6.04	1.66	1.52
3	h	468	A2M	O4'-C1'	6.03	1.56	1.42
3	h	162	A2M	O4'-C1'	6.01	1.56	1.42
3	h	800	A2M	O4'-C1'	5.95	1.56	1.42
3	h	544	A2M	O4'-C1'	5.95	1.56	1.42
3	h	28	A2M	O4'-C1'	5.94	1.56	1.42
3	h	1579	A2M	C3'-C2'	5.93	1.66	1.52
3	h	424	A2M	O4'-C1'	5.93	1.56	1.42
3	h	1283	4AC	C2-N3	5.92	1.48	1.36
3	h	1329	A2M	C3'-C2'	5.91	1.66	1.52
3	h	1329	A2M	O4'-C1'	5.91	1.56	1.42
3	h	1758	A2M	O4'-C1'	5.89	1.56	1.42
3	h	1781	4AC	C6-C5	5.89	1.48	1.35
3	h	440	A2M	O4'-C1'	5.86	1.55	1.42
3	h	977	A2M	O4'-C1'	5.85	1.55	1.42
3	h	246	OMG	C2-N3	5.83	1.47	1.33
3	h	1579	A2M	O4'-C1'	5.81	1.55	1.42
3	h	28	A2M	C3'-C2'	5.81	1.65	1.52
3	h	1758	A2M	C3'-C2'	5.81	1.65	1.52
3	h	258	PSU	C6-N1	5.78	1.45	1.36
3	h	468	A2M	C3'-C2'	5.78	1.65	1.52
3	h	1524	PSU	C6-N1	5.77	1.45	1.36
3	h	162	A2M	C3'-C2'	5.76	1.65	1.52
3	h	424	A2M	C3'-C2'	5.76	1.65	1.52
3	h	1293	PSU	C6-N1	5.76	1.45	1.36
3	h	1308	PSU	C6-N1	5.75	1.45	1.36
3	h	800	A2M	C3'-C2'	5.75	1.65	1.52
3	h	417	PSU	C6-N1	5.74	1.45	1.36
3	h	1535	PSU	C6-N1	5.74	1.45	1.36
3	h	1567	PSU	C6-N1	5.72	1.45	1.36
3	h	961	PSU	C6-N1	5.72	1.45	1.36
3	h	1787	PSU	C6-N1	5.72	1.45	1.36
3	h	977	A2M	C3'-C2'	5.72	1.65	1.52
3	h	95	PSU	C6-N1	5.72	1.45	1.36
3	h	1217	PSU	C6-N1	5.71	1.45	1.36
3	h	762	PSU	C6-N1	5.70	1.45	1.36
3	h	763	PSU	C6-N1	5.69	1.45	1.36
3	h	1002	PSU	C6-N1	5.69	1.45	1.36
3	h	1304	PSU	C6-N1	5.69	1.45	1.36
3	h	470	PSU	C6-N1	5.68	1.45	1.36
3	h	1485	PSU	C6-N1	5.68	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	121	PSU	C6-N1	5.68	1.45	1.36
3	h	622	A2M	O4'-C1'	5.68	1.55	1.42
3	h	1210	PSU	C6-N1	5.68	1.45	1.36
3	h	598	OMG	C2-N3	5.67	1.46	1.33
3	h	1274	OMG	C2-N3	5.67	1.46	1.33
3	h	1190	PSU	C6-N1	5.66	1.45	1.36
3	h	310	PSU	C6-N1	5.66	1.45	1.36
3	h	1615	PSU	C6-N1	5.64	1.45	1.36
3	h	606	PSU	C6-N1	5.63	1.45	1.36
3	h	605	PSU	C6-N1	5.63	1.45	1.36
3	h	339	PSU	C6-N1	5.63	1.45	1.36
3	h	1433	OMG	C2-N3	5.63	1.46	1.33
3	h	1106	PSU	C6-N1	5.62	1.45	1.36
3	h	451	PSU	C6-N1	5.62	1.45	1.36
3	h	1184	PSU	C6-N1	5.62	1.45	1.36
3	h	753	PSU	C6-N1	5.61	1.45	1.36
3	h	950	PSU	C6-N1	5.60	1.45	1.36
3	h	392	OMG	C2-N3	5.60	1.46	1.33
3	h	306	PSU	C6-N1	5.60	1.45	1.36
3	h	1634	PSU	C6-N1	5.59	1.45	1.36
3	h	809	PSU	C6-N1	5.59	1.45	1.36
3	h	1027	PSU	C6-N1	5.59	1.45	1.36
3	h	607	PSU	C6-N1	5.58	1.45	1.36
3	h	1178	PSU	C6-N1	5.58	1.45	1.36
3	h	362	PSU	C6-N1	5.57	1.45	1.36
3	h	103	PSU	C6-N1	5.56	1.45	1.36
3	h	1234	OMU	C6-C5	5.55	1.47	1.35
3	h	1120	PSU	C6-N1	5.53	1.45	1.36
3	h	635	PSU	C6-N1	5.53	1.45	1.36
3	h	1194	B8N	C2-N1	5.52	1.55	1.39
3	h	1194	B8N	C6-C5	5.50	1.42	1.34
3	h	38	OMC	C4-N3	5.49	1.45	1.34
3	h	140	OMC	C4-N3	5.48	1.45	1.34
3	h	373	OMU	C6-C5	5.48	1.47	1.35
3	h	418	OMC	C4-N3	5.48	1.45	1.34
3	h	1383	OMU	C6-C5	5.46	1.47	1.35
3	h	123	OMU	C6-C5	5.45	1.47	1.35
3	h	581	OMU	C6-C5	5.45	1.47	1.35
3	h	1272	OMU	C6-C5	5.44	1.47	1.35
3	h	1218	OMC	C4-N3	5.44	1.45	1.34
3	h	886	OMU	C6-C5	5.43	1.47	1.35
3	h	1012	OMU	C6-C5	5.40	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1447	OMU	C6-C5	5.39	1.47	1.35
3	h	614	OMU	C6-C5	5.38	1.47	1.35
3	h	392	OMG	C2-N2	5.36	1.46	1.34
3	h	1645	OMC	C4-N3	5.35	1.45	1.34
3	h	1433	OMG	C2-N2	5.33	1.46	1.34
3	h	246	OMG	C2-N2	5.33	1.46	1.34
3	h	473	OMC	C4-N3	5.32	1.45	1.34
3	h	1274	OMG	C2-N2	5.32	1.46	1.34
3	h	598	OMG	C2-N2	5.32	1.46	1.34
3	h	418	OMC	C4-N4	5.21	1.46	1.33
3	h	140	OMC	C4-N4	5.21	1.46	1.33
3	h	1218	OMC	C4-N4	5.18	1.46	1.33
3	h	38	OMC	C4-N4	5.16	1.46	1.33
3	h	468	A2M	O4'-C4'	5.12	1.56	1.45
3	h	800	A2M	O4'-C4'	5.11	1.56	1.45
3	h	1645	OMC	C4-N4	5.07	1.45	1.33
3	h	584	PSU	C6-N1	5.07	1.44	1.36
3	h	424	A2M	O4'-C4'	5.04	1.56	1.45
3	h	473	OMC	C4-N4	5.04	1.45	1.33
3	h	1579	A2M	O4'-C4'	5.03	1.56	1.45
3	h	28	A2M	O4'-C4'	5.03	1.56	1.45
3	h	1758	A2M	O4'-C4'	5.02	1.56	1.45
3	h	977	A2M	O4'-C4'	5.02	1.56	1.45
3	h	603	UY1	C6-N1	4.98	1.44	1.36
3	h	440	A2M	O4'-C4'	4.97	1.56	1.45
3	h	1329	A2M	O4'-C4'	4.96	1.56	1.45
3	h	162	A2M	O4'-C4'	4.93	1.56	1.45
3	h	544	A2M	O4'-C4'	4.73	1.55	1.45
3	h	622	A2M	O4'-C4'	4.65	1.55	1.45
3	h	373	OMU	C4-N3	4.60	1.46	1.38
3	h	1383	OMU	C4-N3	4.60	1.46	1.38
3	h	614	OMU	O4-C4	-4.59	1.15	1.24
3	h	1234	OMU	C4-N3	4.59	1.46	1.38
3	h	886	OMU	C4-N3	4.58	1.46	1.38
3	h	544	A2M	C6-N6	4.58	1.45	1.34
3	h	1758	A2M	C6-N6	4.55	1.45	1.34
3	h	1272	OMU	C4-N3	4.55	1.46	1.38
3	h	1579	A2M	C6-N6	4.55	1.45	1.34
3	h	1272	OMU	O4-C4	-4.54	1.15	1.24
3	h	581	OMU	C4-N3	4.53	1.46	1.38
3	h	1447	OMU	C4-N3	4.53	1.46	1.38
3	h	886	OMU	O4-C4	-4.52	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1012	OMU	O4-C4	-4.52	1.15	1.24
3	h	28	A2M	C6-N6	4.52	1.45	1.34
3	h	440	A2M	C6-N6	4.51	1.45	1.34
3	h	140	OMC	C2-N1	4.51	1.49	1.40
3	h	123	OMU	O4-C4	-4.51	1.15	1.24
3	h	1383	OMU	O4-C4	-4.51	1.15	1.24
3	h	1012	OMU	C4-N3	4.50	1.46	1.38
3	h	162	A2M	C6-N6	4.50	1.45	1.34
3	h	1645	OMC	C2-N1	4.49	1.49	1.40
3	h	800	A2M	C6-N6	4.49	1.45	1.34
3	h	1329	A2M	C6-N6	4.49	1.45	1.34
3	h	1447	OMU	O4-C4	-4.49	1.15	1.24
3	h	977	A2M	C6-N6	4.48	1.45	1.34
3	h	468	A2M	C6-N6	4.48	1.45	1.34
3	h	424	A2M	C6-N6	4.47	1.45	1.34
3	h	622	A2M	C6-N6	4.46	1.45	1.34
3	h	123	OMU	C4-N3	4.45	1.46	1.38
3	h	1218	OMC	C2-N1	4.45	1.49	1.40
3	h	581	OMU	O4-C4	-4.44	1.15	1.24
3	h	1234	OMU	O4-C4	-4.43	1.15	1.24
3	h	373	OMU	O4-C4	-4.42	1.15	1.24
3	h	1194	B8N	C1'-C5	-4.41	1.40	1.50
3	h	614	OMU	C4-N3	4.41	1.46	1.38
3	h	38	OMC	O2-C2	-4.39	1.15	1.23
3	h	1485	PSU	C4-N3	4.38	1.47	1.38
3	h	473	OMC	C2-N1	4.38	1.49	1.40
3	h	1293	PSU	C4-N3	4.37	1.47	1.38
3	h	121	PSU	C4-N3	4.37	1.46	1.38
3	h	339	PSU	C4-N3	4.35	1.46	1.38
3	h	1524	PSU	C4-N3	4.34	1.46	1.38
3	h	809	PSU	C4-N3	4.34	1.46	1.38
3	h	961	PSU	C4-N3	4.33	1.46	1.38
3	h	38	OMC	C2-N1	4.33	1.49	1.40
3	h	1190	PSU	C4-N3	4.33	1.46	1.38
3	h	418	OMC	C2-N1	4.32	1.49	1.40
3	h	1217	PSU	C4-N3	4.32	1.46	1.38
3	h	103	PSU	C4-N3	4.31	1.46	1.38
3	h	762	PSU	C4-N3	4.31	1.46	1.38
3	h	1645	OMC	O2-C2	-4.31	1.15	1.23
3	h	763	PSU	C4-N3	4.30	1.46	1.38
3	h	950	PSU	C4-N3	4.30	1.46	1.38
3	h	1535	PSU	C4-N3	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	607	PSU	C4-N3	4.29	1.46	1.38
3	h	1218	OMC	O2-C2	-4.29	1.15	1.23
3	h	140	OMC	O2-C2	-4.29	1.15	1.23
3	h	473	OMC	O2-C2	-4.29	1.15	1.23
3	h	1567	PSU	C4-N3	4.28	1.46	1.38
3	h	258	PSU	C4-N3	4.28	1.46	1.38
3	h	753	PSU	C4-N3	4.28	1.46	1.38
3	h	1210	PSU	C4-N3	4.27	1.46	1.38
3	h	1178	PSU	C4-N3	4.24	1.46	1.38
3	h	1184	PSU	C4-N3	4.24	1.46	1.38
3	h	1304	PSU	C4-N3	4.24	1.46	1.38
3	h	1002	PSU	C4-N3	4.24	1.46	1.38
3	h	1308	PSU	C4-N3	4.24	1.46	1.38
3	h	1615	PSU	C4-N3	4.24	1.46	1.38
3	h	1787	PSU	C4-N3	4.24	1.46	1.38
3	h	95	PSU	C4-N3	4.23	1.46	1.38
3	h	1106	PSU	C4-N3	4.22	1.46	1.38
3	h	310	PSU	C4-N3	4.22	1.46	1.38
3	h	417	PSU	C4-N3	4.21	1.46	1.38
3	h	418	OMC	O2-C2	-4.21	1.15	1.23
3	h	635	PSU	C4-N3	4.21	1.46	1.38
3	h	306	PSU	C4-N3	4.21	1.46	1.38
3	h	1781	4AC	C2-N1	4.20	1.49	1.40
3	h	470	PSU	C4-N3	4.20	1.46	1.38
3	h	1634	PSU	C4-N3	4.20	1.46	1.38
3	h	606	PSU	C4-N3	4.19	1.46	1.38
3	h	1120	PSU	C4-N3	4.19	1.46	1.38
3	h	605	PSU	C4-N3	4.18	1.46	1.38
3	h	451	PSU	C4-N3	4.18	1.46	1.38
3	h	1027	PSU	C4-N3	4.14	1.46	1.38
3	h	362	PSU	C4-N3	4.12	1.46	1.38
3	h	1283	4AC	C5-C4	3.99	1.49	1.40
3	h	1283	4AC	C2-N1	3.96	1.48	1.40
3	h	1218	OMC	C6-N1	3.87	1.47	1.38
3	h	1781	4AC	C5-C4	3.83	1.49	1.40
3	h	38	OMC	C6-N1	3.82	1.47	1.38
3	h	473	OMC	C6-N1	3.82	1.47	1.38
3	h	603	UY1	C4-N3	3.82	1.45	1.38
3	h	1645	OMC	C6-N1	3.80	1.47	1.38
3	h	418	OMC	C6-N1	3.80	1.47	1.38
3	h	140	OMC	C6-N1	3.74	1.47	1.38
3	h	1781	4AC	C7-N4	3.71	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	581	OMU	C6-N1	3.69	1.46	1.38
3	h	1272	OMU	C6-N1	3.69	1.46	1.38
3	h	1283	4AC	C7-N4	3.67	1.44	1.37
3	h	614	OMU	O2-C2	-3.67	1.16	1.23
3	h	373	OMU	C6-N1	3.66	1.46	1.38
3	h	614	OMU	C6-N1	3.66	1.46	1.38
3	h	1012	OMU	O2-C2	-3.66	1.16	1.23
3	h	123	OMU	C6-N1	3.65	1.46	1.38
3	h	1012	OMU	C6-N1	3.64	1.46	1.38
3	h	1234	OMU	C6-N1	3.64	1.46	1.38
3	h	1383	OMU	C6-N1	3.64	1.46	1.38
3	h	581	OMU	O2-C2	-3.63	1.16	1.23
3	h	886	OMU	C6-N1	3.62	1.46	1.38
3	h	1272	OMU	O2-C2	-3.60	1.16	1.23
3	h	123	OMU	O2-C2	-3.60	1.16	1.23
3	h	1447	OMU	O2-C2	-3.58	1.16	1.23
3	h	1447	OMU	C6-N1	3.57	1.46	1.38
3	h	1781	4AC	O2-C2	-3.56	1.17	1.23
3	h	373	OMU	O2-C2	-3.56	1.16	1.23
3	h	1383	OMU	O2-C2	-3.56	1.16	1.23
3	h	1234	OMU	O2-C2	-3.55	1.16	1.23
3	h	886	OMU	O2-C2	-3.54	1.16	1.23
3	h	635	PSU	O4-C4	-3.46	1.17	1.23
3	h	1283	4AC	O2-C2	-3.43	1.17	1.23
3	h	310	PSU	O4-C4	-3.35	1.17	1.23
3	h	306	PSU	O4-C4	-3.33	1.17	1.23
3	h	1210	PSU	O4-C4	-3.32	1.17	1.23
3	h	1787	PSU	O4-C4	-3.32	1.17	1.23
3	h	606	PSU	O4-C4	-3.32	1.17	1.23
3	h	451	PSU	O4-C4	-3.31	1.17	1.23
3	h	1106	PSU	O4-C4	-3.31	1.17	1.23
3	h	1304	PSU	O4-C4	-3.30	1.17	1.23
3	h	1002	PSU	O4-C4	-3.29	1.17	1.23
3	h	1178	PSU	O4-C4	-3.29	1.17	1.23
3	h	1120	PSU	O4-C4	-3.29	1.17	1.23
3	h	362	PSU	O4-C4	-3.28	1.17	1.23
3	h	950	PSU	O4-C4	-3.27	1.17	1.23
3	h	607	PSU	O4-C4	-3.27	1.17	1.23
3	h	470	PSU	O4-C4	-3.27	1.17	1.23
3	h	1634	PSU	O4-C4	-3.27	1.17	1.23
3	h	339	PSU	O4-C4	-3.26	1.17	1.23
3	h	809	PSU	O4-C4	-3.26	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1535	PSU	O4-C4	-3.25	1.17	1.23
3	h	1293	PSU	O4-C4	-3.25	1.17	1.23
3	h	1190	PSU	O4-C4	-3.25	1.17	1.23
3	h	103	PSU	O4-C4	-3.24	1.17	1.23
3	h	95	PSU	O4-C4	-3.24	1.17	1.23
3	h	753	PSU	O4-C4	-3.24	1.17	1.23
3	h	1184	PSU	O4-C4	-3.24	1.17	1.23
3	h	1308	PSU	O4-C4	-3.23	1.17	1.23
3	h	605	PSU	O4-C4	-3.23	1.17	1.23
3	h	1567	PSU	O4-C4	-3.22	1.17	1.23
3	h	258	PSU	O4-C4	-3.22	1.17	1.23
3	h	763	PSU	O4-C4	-3.22	1.17	1.23
3	h	961	PSU	O4-C4	-3.22	1.17	1.23
3	h	1027	PSU	O4-C4	-3.22	1.17	1.23
3	h	417	PSU	O4-C4	-3.21	1.17	1.23
3	h	1283	4AC	C6-N1	3.21	1.45	1.38
3	h	1524	PSU	O4-C4	-3.20	1.17	1.23
3	h	1615	PSU	O4-C4	-3.20	1.17	1.23
3	h	121	PSU	O4-C4	-3.19	1.17	1.23
3	h	762	PSU	O4-C4	-3.17	1.17	1.23
3	h	1485	PSU	O4-C4	-3.17	1.17	1.23
3	h	1217	PSU	O4-C4	-3.17	1.17	1.23
3	h	584	PSU	O4-C4	-3.17	1.17	1.23
3	h	1790	MA6	C5-C4	-3.12	1.33	1.39
3	h	246	OMG	C2-N1	3.02	1.45	1.37
3	h	392	OMG	C2-N1	3.02	1.45	1.37
3	h	1274	OMG	C2-N1	3.01	1.45	1.37
3	h	1781	4AC	C4-N4	3.00	1.44	1.39
3	h	584	PSU	O4'-C1'	-2.99	1.39	1.43
3	h	1283	4AC	C4-N4	2.99	1.44	1.39
3	h	598	OMG	C2-N1	2.97	1.45	1.37
3	h	1781	4AC	C6-N1	2.96	1.45	1.38
3	h	1433	OMG	O6-C6	-2.94	1.18	1.23
3	h	392	OMG	C5-C6	2.92	1.55	1.44
3	h	1789	MA6	C5-C4	-2.92	1.33	1.39
3	h	584	PSU	C1'-C5	2.91	1.56	1.50
3	h	1274	OMG	C5-C6	2.90	1.55	1.44
3	h	1524	PSU	C1'-C5	2.90	1.56	1.50
3	h	1217	PSU	C1'-C5	2.89	1.56	1.50
3	h	598	OMG	C5-C6	2.88	1.55	1.44
3	h	1433	OMG	C2-N1	2.88	1.44	1.37
3	h	246	OMG	C5-C6	2.87	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	622	A2M	C5-C4	-2.87	1.33	1.39
3	h	451	PSU	C1'-C5	2.86	1.56	1.50
3	h	606	PSU	C1'-C5	2.85	1.56	1.50
3	h	809	PSU	C1'-C5	2.85	1.56	1.50
3	h	38	OMC	C5-C4	2.85	1.49	1.42
3	h	392	OMG	O6-C6	-2.83	1.18	1.23
3	h	162	A2M	C5-C4	-2.83	1.33	1.39
3	h	1274	OMG	O6-C6	-2.83	1.18	1.23
3	h	1790	MA6	C6-N6	2.83	1.45	1.36
3	h	28	A2M	C5-C4	-2.82	1.33	1.39
3	h	1218	OMC	C5-C4	2.82	1.49	1.42
3	h	1789	MA6	C6-N6	2.81	1.45	1.36
3	h	598	OMG	O6-C6	-2.81	1.18	1.23
3	h	800	A2M	C5-C4	-2.80	1.33	1.39
3	h	306	PSU	C1'-C5	2.80	1.56	1.50
3	h	140	OMC	C5-C4	2.80	1.49	1.42
3	h	468	A2M	C5-C4	-2.79	1.33	1.39
3	h	424	A2M	C5-C4	-2.79	1.33	1.39
3	h	473	OMC	C5-C4	2.79	1.49	1.42
3	h	28	A2M	C5-N7	-2.79	1.33	1.39
3	h	121	PSU	C1'-C5	2.79	1.56	1.50
3	h	1579	A2M	C5-C4	-2.78	1.33	1.39
3	h	392	OMG	C6-N1	2.78	1.44	1.38
3	h	440	A2M	C5-C4	-2.78	1.33	1.39
3	h	1002	PSU	C1'-C5	2.78	1.56	1.50
3	h	246	OMG	O6-C6	-2.77	1.18	1.23
3	h	1485	PSU	C1'-C5	2.77	1.56	1.50
3	h	362	PSU	O2-C2	-2.77	1.17	1.23
3	h	753	PSU	C1'-C5	2.77	1.56	1.50
3	h	605	PSU	C1'-C5	2.77	1.56	1.50
3	h	1329	A2M	C5-C4	-2.77	1.33	1.39
3	h	1433	OMG	C5-C6	2.77	1.54	1.44
3	h	1190	PSU	C1'-C5	2.76	1.56	1.50
3	h	1758	A2M	C5-C4	-2.76	1.33	1.39
3	h	1304	PSU	O2-C2	-2.75	1.17	1.23
3	h	258	PSU	C1'-C5	2.75	1.56	1.50
3	h	961	PSU	O2-C2	-2.75	1.17	1.23
3	h	1106	PSU	O2-C2	-2.75	1.17	1.23
3	h	1027	PSU	C1'-C5	2.75	1.56	1.50
3	h	310	PSU	O2-C2	-2.75	1.17	1.23
3	h	451	PSU	O2-C2	-2.75	1.17	1.23
3	h	1771	6MZ	C5-N7	-2.75	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	1645	OMC	C5-C4	2.74	1.49	1.42
3	h	1787	PSU	O2-C2	-2.74	1.17	1.23
3	h	1274	OMG	C6-N1	2.73	1.43	1.38
3	h	1210	PSU	O2-C2	-2.73	1.17	1.23
3	h	598	OMG	C6-N1	2.73	1.43	1.38
3	h	1106	PSU	C1'-C5	2.72	1.56	1.50
3	h	763	PSU	O2-C2	-2.72	1.17	1.23
3	h	607	PSU	O2-C2	-2.72	1.17	1.23
3	h	977	A2M	C5-C4	-2.72	1.33	1.39
3	h	607	PSU	C1'-C5	2.72	1.56	1.50
3	h	440	A2M	C5-N7	-2.72	1.33	1.39
3	h	1535	PSU	C1'-C5	2.72	1.56	1.50
3	h	1634	PSU	O2-C2	-2.72	1.17	1.23
3	h	1293	PSU	C1'-C5	2.72	1.56	1.50
3	h	418	OMC	C5-C4	2.71	1.49	1.42
3	h	362	PSU	C1'-C5	2.71	1.56	1.50
3	h	103	PSU	O2-C2	-2.71	1.17	1.23
3	h	1758	A2M	C5-N7	-2.71	1.33	1.39
3	h	1567	PSU	C1'-C5	2.71	1.56	1.50
3	h	1178	PSU	O2-C2	-2.71	1.17	1.23
3	h	950	PSU	C1'-C5	2.70	1.56	1.50
3	h	635	PSU	O2-C2	-2.70	1.17	1.23
3	h	1615	PSU	O2-C2	-2.70	1.17	1.23
3	h	470	PSU	C1'-C5	2.69	1.56	1.50
3	h	800	A2M	C5-N7	-2.69	1.33	1.39
3	h	103	PSU	C1'-C5	2.69	1.56	1.50
3	h	246	OMG	C6-N1	2.69	1.43	1.38
3	h	1634	PSU	C1'-C5	2.69	1.56	1.50
3	h	544	A2M	C5-N7	-2.69	1.33	1.39
3	h	1308	PSU	O2-C2	-2.69	1.17	1.23
3	h	762	PSU	O2-C2	-2.69	1.17	1.23
3	h	339	PSU	C1'-C5	2.68	1.56	1.50
3	h	762	PSU	C1'-C5	2.68	1.56	1.50
3	h	1120	PSU	O2-C2	-2.68	1.17	1.23
3	h	1027	PSU	O2-C2	-2.68	1.17	1.23
3	h	1787	PSU	C1'-C5	2.68	1.56	1.50
3	h	809	PSU	O2-C2	-2.68	1.17	1.23
3	h	306	PSU	O2-C2	-2.68	1.17	1.23
3	h	635	PSU	C1'-C5	2.67	1.56	1.50
3	h	606	PSU	O2-C2	-2.67	1.17	1.23
3	h	417	PSU	C1'-C5	2.67	1.56	1.50
3	h	763	PSU	C1'-C5	2.67	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	961	PSU	C1'-C5	2.67	1.56	1.50
3	h	605	PSU	O2-C2	-2.67	1.17	1.23
3	h	603	UY1	O4-C4	-2.66	1.18	1.23
3	h	121	PSU	O2-C2	-2.66	1.17	1.23
3	h	424	A2M	C5-N7	-2.66	1.34	1.39
3	h	1304	PSU	C1'-C5	2.66	1.56	1.50
3	h	1184	PSU	C1'-C5	2.65	1.56	1.50
3	h	1120	PSU	C1'-C5	2.65	1.56	1.50
3	h	753	PSU	O2-C2	-2.65	1.17	1.23
3	h	1485	PSU	O2-C2	-2.65	1.17	1.23
3	h	1308	PSU	C1'-C5	2.65	1.56	1.50
3	h	468	A2M	C5-N7	-2.65	1.34	1.39
3	h	584	PSU	C4-C5	2.65	1.51	1.44
3	h	1615	PSU	C1'-C5	2.65	1.56	1.50
3	h	339	PSU	O2-C2	-2.65	1.17	1.23
3	h	1178	PSU	C1'-C5	2.64	1.56	1.50
3	h	95	PSU	C1'-C5	2.64	1.56	1.50
3	h	1002	PSU	O2-C2	-2.64	1.17	1.23
3	h	258	PSU	O2-C2	-2.63	1.17	1.23
3	h	1567	PSU	O2-C2	-2.63	1.17	1.23
3	h	470	PSU	O2-C2	-2.63	1.17	1.23
3	h	1184	PSU	O2-C2	-2.62	1.17	1.23
3	h	950	PSU	O2-C2	-2.62	1.17	1.23
3	h	1210	PSU	C1'-C5	2.61	1.56	1.50
3	h	1190	PSU	O2-C2	-2.61	1.17	1.23
3	h	162	A2M	C5-N7	-2.61	1.34	1.39
3	h	310	PSU	C1'-C5	2.61	1.56	1.50
3	h	1293	PSU	O2-C2	-2.61	1.17	1.23
3	h	1535	PSU	O2-C2	-2.60	1.17	1.23
3	h	977	A2M	C5-N7	-2.60	1.34	1.39
3	h	544	A2M	C5-C4	-2.60	1.34	1.39
3	h	1217	PSU	O2-C2	-2.59	1.18	1.23
3	h	1524	PSU	O2-C2	-2.59	1.18	1.23
3	h	95	PSU	O2-C2	-2.59	1.18	1.23
3	h	622	A2M	C5-N7	-2.57	1.34	1.39
3	h	1579	A2M	C5-N7	-2.57	1.34	1.39
3	h	417	PSU	O2-C2	-2.56	1.18	1.23
3	h	1329	A2M	C5-N7	-2.51	1.34	1.39
3	h	1433	OMG	C5-N7	-2.51	1.34	1.39
3	h	584	PSU	O2-C2	-2.50	1.18	1.23
3	h	1433	OMG	C6-N1	2.47	1.43	1.38
3	h	246	OMG	C5-N7	-2.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	598	OMG	C5-N7	-2.41	1.34	1.39
3	h	1234	OMU	C5-C4	2.39	1.48	1.43
3	h	1789	MA6	C5-N7	-2.38	1.34	1.39
3	h	1274	OMG	C5-N7	-2.36	1.34	1.39
3	h	392	OMG	C5-N7	-2.35	1.34	1.39
3	h	373	OMU	C5-C4	2.33	1.48	1.43
3	h	1383	OMU	C5-C4	2.33	1.48	1.43
3	h	603	UY1	O2-C2	-2.31	1.18	1.23
3	h	614	OMU	C5-C4	2.31	1.48	1.43
3	h	886	OMU	C5-C4	2.31	1.48	1.43
3	h	1194	B8N	O4-C4	-2.31	1.18	1.23
3	h	581	OMU	C5-C4	2.30	1.48	1.43
3	h	1771	6MZ	C5-C4	-2.30	1.34	1.39
3	h	123	OMU	C5-C4	2.27	1.48	1.43
3	h	1272	OMU	C5-C4	2.27	1.48	1.43
3	h	1027	PSU	O4'-C1'	-2.27	1.40	1.43
3	h	1012	OMU	C5-C4	2.20	1.48	1.43
3	h	1790	MA6	C5-N7	-2.20	1.34	1.39
3	h	800	A2M	C8-N9	-2.20	1.33	1.37
3	h	1447	OMU	C5-C4	2.19	1.48	1.43
3	h	1771	6MZ	C6-N1	-2.19	1.31	1.35
3	h	622	A2M	C8-N9	-2.19	1.33	1.37
3	h	1194	B8N	O2-C2	-2.16	1.18	1.22
3	h	1781	4AC	O7-C7	-2.14	1.18	1.23
3	h	1283	4AC	CM7-C7	2.12	1.54	1.50
3	h	424	A2M	C8-N9	-2.11	1.33	1.37
3	h	1329	A2M	C8-N9	-2.10	1.33	1.37
3	h	1758	A2M	C8-N9	-2.09	1.33	1.37
3	h	1283	4AC	O7-C7	-2.08	1.18	1.23
3	h	468	A2M	C8-N9	-2.07	1.33	1.37
3	h	977	A2M	C8-N9	-2.07	1.33	1.37
3	h	1758	A2M	O5'-C5'	-2.07	1.39	1.44
3	h	544	A2M	C8-N9	-2.07	1.33	1.37
3	h	28	A2M	C8-N9	-2.05	1.33	1.37
3	h	1790	MA6	C8-N9	-2.05	1.33	1.37
3	h	1579	A2M	C8-N9	-2.05	1.33	1.37
3	h	622	A2M	O5'-C5'	-2.03	1.39	1.44
3	h	440	A2M	C8-N9	-2.02	1.33	1.37
3	h	1433	OMG	C4-N9	-2.02	1.32	1.38
3	h	1781	4AC	CM7-C7	2.01	1.54	1.50
3	h	162	A2M	C8-N9	-2.01	1.33	1.37
3	h	392	OMG	C4-N9	-2.01	1.32	1.38

All (519) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	584	PSU	C6-N1-C2	-12.08	110.33	122.68
3	h	584	PSU	C6-C5-C4	-10.84	110.62	118.20
3	h	584	PSU	C5-C6-N1	9.88	136.90	122.11
3	h	1790	MA6	N1-C6-N6	-9.19	107.03	117.08
3	h	1789	MA6	N1-C6-N6	-7.95	108.39	117.08
3	h	622	A2M	N6-C6-N1	-6.88	103.28	118.35
3	h	468	A2M	N6-C6-N1	-6.85	103.34	118.35
3	h	800	A2M	N6-C6-N1	-6.85	103.36	118.35
3	h	424	A2M	N6-C6-N1	-6.79	103.47	118.35
3	h	440	A2M	N6-C6-N1	-6.79	103.47	118.35
3	h	1329	A2M	N6-C6-N1	-6.78	103.50	118.35
3	h	544	A2M	N6-C6-N1	-6.74	103.59	118.35
3	h	977	A2M	N6-C6-N1	-6.74	103.59	118.35
3	h	1579	A2M	N6-C6-N1	-6.74	103.60	118.35
3	h	162	A2M	N6-C6-N1	-6.73	103.61	118.35
3	h	1758	A2M	N6-C6-N1	-6.68	103.72	118.35
3	h	28	A2M	N6-C6-N1	-6.66	103.78	118.35
3	h	622	A2M	C4-N9-C1'	-6.41	111.31	126.59
3	h	544	A2M	C5-C4-N3	-6.17	118.69	126.75
3	h	800	A2M	C5-C6-N6	6.10	136.71	123.43
3	h	468	A2M	C5-C6-N6	6.09	136.68	123.43
3	h	622	A2M	C5-C6-N6	6.08	136.66	123.43
3	h	440	A2M	C5-C6-N6	6.05	136.60	123.43
3	h	424	A2M	C5-C6-N6	6.04	136.58	123.43
3	h	977	A2M	C5-C6-N6	6.03	136.56	123.43
3	h	1329	A2M	C5-C6-N6	5.99	136.47	123.43
3	h	622	A2M	C1'-N9-C8	5.99	140.66	127.14
3	h	1579	A2M	C5-C6-N6	5.94	136.36	123.43
3	h	544	A2M	C5-C6-N6	5.91	136.29	123.43
3	h	162	A2M	C5-C6-N6	5.91	136.28	123.43
3	h	28	A2M	C5-C6-N6	5.91	136.28	123.43
3	h	246	OMG	C1'-N9-C8	-5.90	109.89	126.70
3	h	1758	A2M	C5-C6-N6	5.89	136.25	123.43
3	h	468	A2M	C4-N9-C1'	-5.75	112.88	126.59
3	h	440	A2M	C4-N9-C1'	-5.72	112.96	126.59
3	h	424	A2M	C4-N9-C1'	-5.71	112.99	126.59
3	h	1579	A2M	C4-N9-C1'	-5.70	113.00	126.59
3	h	1433	OMG	C1'-N9-C8	-5.65	110.61	126.70
3	h	598	OMG	C1'-N9-C8	-5.64	110.63	126.70
3	h	1790	MA6	N1-C2-N3	-5.60	119.84	128.60
3	h	28	A2M	C4-N9-C1'	-5.59	113.27	126.59
3	h	1329	A2M	C4-N9-C1'	-5.58	113.29	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	440	A2M	C5-C4-N3	-5.58	119.47	126.75
3	h	800	A2M	C4-N9-C1'	-5.57	113.31	126.59
3	h	424	A2M	N3-C2-N1	-5.57	119.89	128.60
3	h	622	A2M	N3-C2-N1	-5.57	119.89	128.60
3	h	1758	A2M	C5-C4-N3	-5.53	119.54	126.75
3	h	1274	OMG	C1'-N9-C8	-5.49	111.06	126.70
3	h	440	A2M	C1'-N9-C8	5.47	139.49	127.14
3	h	1579	A2M	N3-C2-N1	-5.47	120.05	128.60
3	h	977	A2M	C4-N9-C1'	-5.47	113.56	126.59
3	h	1789	MA6	N1-C2-N3	-5.47	120.05	128.60
3	h	468	A2M	N3-C2-N1	-5.45	120.08	128.60
3	h	1579	A2M	C5-C4-N3	-5.45	119.65	126.75
3	h	1758	A2M	N3-C2-N1	-5.44	120.10	128.60
3	h	1771	6MZ	N1-C2-N3	-5.44	120.10	128.60
3	h	28	A2M	N3-C2-N1	-5.44	120.10	128.60
3	h	1329	A2M	C5-C4-N3	-5.43	119.67	126.75
3	h	28	A2M	C5-C4-N3	-5.42	119.68	126.75
3	h	440	A2M	N3-C2-N1	-5.41	120.13	128.60
3	h	162	A2M	C5-C4-N3	-5.41	119.69	126.75
3	h	977	A2M	C5-C4-N3	-5.41	119.69	126.75
3	h	800	A2M	N3-C2-N1	-5.40	120.15	128.60
3	h	1329	A2M	N3-C2-N1	-5.40	120.16	128.60
3	h	468	A2M	C1'-N9-C8	5.40	139.32	127.14
3	h	162	A2M	N3-C2-N1	-5.38	120.19	128.60
3	h	392	OMG	C1'-N9-C8	-5.37	111.40	126.70
3	h	977	A2M	N3-C2-N1	-5.37	120.20	128.60
3	h	544	A2M	N3-C2-N1	-5.35	120.23	128.60
3	h	1771	6MZ	C5-C4-N3	-5.35	119.78	126.75
3	h	162	A2M	C4-N9-C1'	-5.32	113.91	126.59
3	h	800	A2M	C5-C4-N3	-5.31	119.83	126.75
3	h	28	A2M	C1'-N9-C8	5.30	139.11	127.14
3	h	1579	A2M	C1'-N9-C8	5.30	139.10	127.14
3	h	468	A2M	C5-C4-N3	-5.29	119.85	126.75
3	h	1758	A2M	C4-N9-C1'	-5.28	114.01	126.59
3	h	424	A2M	C1'-N9-C8	5.28	139.05	127.14
3	h	424	A2M	C5-C4-N3	-5.27	119.87	126.75
3	h	622	A2M	C5-C4-N3	-5.26	119.88	126.75
3	h	800	A2M	C1'-N9-C8	5.22	138.93	127.14
3	h	886	OMU	C4-N3-C2	-5.17	119.77	126.58
3	h	1329	A2M	C1'-N9-C8	5.16	138.79	127.14
3	h	1383	OMU	C4-N3-C2	-5.16	119.78	126.58
3	h	581	OMU	C4-N3-C2	-5.16	119.78	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	373	OMU	C4-N3-C2	-5.14	119.80	126.58
3	h	1012	OMU	C4-N3-C2	-5.12	119.83	126.58
3	h	1272	OMU	C4-N3-C2	-5.11	119.84	126.58
3	h	1194	B8N	C5-C4-N3	5.11	125.63	116.17
3	h	1234	OMU	C4-N3-C2	-5.09	119.87	126.58
3	h	977	A2M	C1'-N9-C8	5.05	138.54	127.14
3	h	123	OMU	C4-N3-C2	-4.98	120.00	126.58
3	h	614	OMU	C4-N3-C2	-4.97	120.02	126.58
3	h	1447	OMU	C4-N3-C2	-4.93	120.07	126.58
3	h	1781	4AC	N4-C4-N3	4.93	122.13	113.85
3	h	162	A2M	C1'-N9-C8	4.92	138.25	127.14
3	h	1758	A2M	C1'-N9-C8	4.89	138.18	127.14
3	h	246	OMG	C1'-N9-C4	4.84	140.86	126.50
3	h	1789	MA6	C5-C4-N3	-4.81	120.47	126.75
3	h	1787	PSU	C4-N3-C2	-4.71	119.55	126.34
3	h	1304	PSU	C4-N3-C2	-4.71	119.56	126.34
3	h	1790	MA6	C5-C4-N3	-4.70	120.61	126.75
3	h	1210	PSU	C4-N3-C2	-4.68	119.59	126.34
3	h	584	PSU	N1-C2-N3	4.67	120.42	115.13
3	h	1790	MA6	N9-C8-N7	-4.67	107.53	113.91
3	h	95	PSU	C4-N3-C2	-4.66	119.63	126.34
3	h	1184	PSU	C4-N3-C2	-4.65	119.64	126.34
3	h	961	PSU	C4-N3-C2	-4.62	119.69	126.34
3	h	1308	PSU	C4-N3-C2	-4.61	119.69	126.34
3	h	1217	PSU	C4-N3-C2	-4.61	119.69	126.34
3	h	310	PSU	C4-N3-C2	-4.61	119.70	126.34
3	h	246	OMG	C5-C4-N3	-4.61	120.99	128.46
3	h	362	PSU	C4-N3-C2	-4.60	119.71	126.34
3	h	605	PSU	C4-N3-C2	-4.60	119.71	126.34
3	h	1106	PSU	C4-N3-C2	-4.60	119.71	126.34
3	h	1190	PSU	C4-N3-C2	-4.60	119.71	126.34
3	h	1789	MA6	C1'-N9-C8	-4.59	116.76	127.14
3	h	103	PSU	C4-N3-C2	-4.59	119.72	126.34
3	h	1293	PSU	C4-N3-C2	-4.59	119.73	126.34
3	h	1485	PSU	C4-N3-C2	-4.59	119.73	126.34
3	h	1567	PSU	C4-N3-C2	-4.59	119.73	126.34
3	h	598	OMG	C1'-N9-C4	4.58	140.11	126.50
3	h	635	PSU	C4-N3-C2	-4.58	119.74	126.34
3	h	1535	PSU	C4-N3-C2	-4.58	119.75	126.34
3	h	470	PSU	C4-N3-C2	-4.57	119.75	126.34
3	h	121	PSU	C4-N3-C2	-4.57	119.76	126.34
3	h	1027	PSU	C4-N3-C2	-4.56	119.77	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1634	PSU	C4-N3-C2	-4.56	119.77	126.34
3	h	1120	PSU	C4-N3-C2	-4.55	119.78	126.34
3	h	607	PSU	C4-N3-C2	-4.55	119.78	126.34
3	h	762	PSU	C4-N3-C2	-4.55	119.78	126.34
3	h	339	PSU	C4-N3-C2	-4.54	119.80	126.34
3	h	763	PSU	C4-N3-C2	-4.54	119.80	126.34
3	h	1178	PSU	C4-N3-C2	-4.54	119.80	126.34
3	h	809	PSU	C4-N3-C2	-4.54	119.80	126.34
3	h	1524	PSU	C4-N3-C2	-4.52	119.82	126.34
3	h	1433	OMG	C1'-N9-C4	4.52	139.93	126.50
3	h	1787	PSU	N1-C2-N3	4.52	120.25	115.13
3	h	753	PSU	C4-N3-C2	-4.52	119.83	126.34
3	h	451	PSU	C4-N3-C2	-4.51	119.84	126.34
3	h	603	UY1	C4-N3-C2	-4.50	119.86	126.34
3	h	1789	MA6	N9-C8-N7	-4.49	107.77	113.91
3	h	1790	MA6	C5-C6-N6	4.48	133.11	125.30
3	h	950	PSU	C4-N3-C2	-4.48	119.89	126.34
3	h	1274	OMG	C1'-N9-C4	4.45	139.72	126.50
3	h	1615	PSU	C4-N3-C2	-4.44	119.94	126.34
3	h	1274	OMG	C5-C4-N3	-4.43	121.27	128.46
3	h	258	PSU	C4-N3-C2	-4.43	119.96	126.34
3	h	306	PSU	C4-N3-C2	-4.42	119.97	126.34
3	h	961	PSU	N1-C2-N3	4.42	120.14	115.13
3	h	1002	PSU	C4-N3-C2	-4.40	119.99	126.34
3	h	598	OMG	C5-C4-N3	-4.40	121.32	128.46
3	h	606	PSU	C4-N3-C2	-4.35	120.07	126.34
3	h	1210	PSU	N1-C2-N3	4.35	120.06	115.13
3	h	1184	PSU	N1-C2-N3	4.33	120.03	115.13
3	h	622	A2M	N9-C8-N7	-4.30	108.03	113.91
3	h	1274	OMG	C2-N3-C4	4.28	119.92	112.30
3	h	392	OMG	C5-C4-N3	-4.27	121.53	128.46
3	h	392	OMG	C1'-N9-C4	4.27	139.18	126.50
3	h	392	OMG	C2-N3-C4	4.26	119.90	112.30
3	h	417	PSU	C4-N3-C2	-4.26	120.20	126.34
3	h	598	OMG	C2-N3-C4	4.25	119.88	112.30
3	h	1304	PSU	N1-C2-N3	4.25	119.94	115.13
3	h	1178	PSU	N1-C2-N3	4.23	119.92	115.13
3	h	470	PSU	N1-C2-N3	4.23	119.92	115.13
3	h	246	OMG	C2-N3-C4	4.22	119.82	112.30
3	h	1433	OMG	C5-C4-N3	-4.22	121.62	128.46
3	h	1120	PSU	N1-C2-N3	4.22	119.91	115.13
3	h	339	PSU	N1-C2-N3	4.21	119.90	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1190	PSU	N1-C2-N3	4.20	119.89	115.13
3	h	1194	B8N	C4-N3-C2	-4.19	120.16	125.46
3	h	1535	PSU	N1-C2-N3	4.19	119.88	115.13
3	h	1771	6MZ	C4-C5-C6	4.19	120.06	116.81
3	h	1567	PSU	N1-C2-N3	4.19	119.87	115.13
3	h	1579	A2M	N9-C8-N7	-4.18	108.20	113.91
3	h	1308	PSU	N1-C2-N3	4.17	119.86	115.13
3	h	607	PSU	N1-C2-N3	4.17	119.86	115.13
3	h	362	PSU	N1-C2-N3	4.17	119.86	115.13
3	h	1329	A2M	N9-C8-N7	-4.17	108.22	113.91
3	h	1771	6MZ	N9-C8-N7	-4.16	108.23	113.91
3	h	605	PSU	N1-C2-N3	4.16	119.84	115.13
3	h	1027	PSU	N1-C2-N3	4.15	119.83	115.13
3	h	95	PSU	N1-C2-N3	4.15	119.83	115.13
3	h	424	A2M	N9-C8-N7	-4.15	108.24	113.91
3	h	451	PSU	N1-C2-N3	4.15	119.83	115.13
3	h	635	PSU	N1-C2-N3	4.15	119.83	115.13
3	h	103	PSU	N1-C2-N3	4.14	119.83	115.13
3	h	1217	PSU	N1-C2-N3	4.14	119.82	115.13
3	h	977	A2M	N9-C8-N7	-4.13	108.26	113.91
3	h	1293	PSU	N1-C2-N3	4.12	119.80	115.13
3	h	162	A2M	N9-C8-N7	-4.12	108.27	113.91
3	h	1485	PSU	N1-C2-N3	4.12	119.80	115.13
3	h	603	UY1	N1-C2-N3	4.11	119.79	115.13
3	h	809	PSU	N1-C2-N3	4.10	119.78	115.13
3	h	121	PSU	N1-C2-N3	4.10	119.78	115.13
3	h	468	A2M	N9-C8-N7	-4.10	108.31	113.91
3	h	950	PSU	N1-C2-N3	4.10	119.77	115.13
3	h	1106	PSU	N1-C2-N3	4.09	119.77	115.13
3	h	753	PSU	N1-C2-N3	4.09	119.76	115.13
3	h	1758	A2M	N9-C8-N7	-4.09	108.33	113.91
3	h	1634	PSU	N1-C2-N3	4.08	119.75	115.13
3	h	310	PSU	N1-C2-N3	4.07	119.75	115.13
3	h	800	A2M	N9-C8-N7	-4.07	108.34	113.91
3	h	1433	OMG	C2-N3-C4	4.07	119.55	112.30
3	h	1524	PSU	N1-C2-N3	4.04	119.71	115.13
3	h	306	PSU	N1-C2-N3	4.04	119.71	115.13
3	h	28	A2M	N9-C8-N7	-4.04	108.39	113.91
3	h	1615	PSU	N1-C2-N3	4.04	119.70	115.13
3	h	258	PSU	N1-C2-N3	4.04	119.70	115.13
3	h	440	A2M	N9-C8-N7	-4.03	108.40	113.91
3	h	762	PSU	N1-C2-N3	4.03	119.69	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	763	PSU	N1-C2-N3	4.01	119.67	115.13
3	h	544	A2M	C4-N9-C1'	-3.98	117.10	126.59
3	h	606	PSU	N1-C2-N3	3.98	119.64	115.13
3	h	1002	PSU	N1-C2-N3	3.95	119.60	115.13
3	h	1771	6MZ	C9-N6-C6	-3.92	119.50	122.87
3	h	584	PSU	C4-N3-C2	-3.90	120.72	126.34
3	h	417	PSU	N1-C2-N3	3.89	119.53	115.13
3	h	1789	MA6	C5-C6-N6	3.88	132.06	125.30
3	h	544	A2M	N3-C4-N9	3.87	133.46	127.08
3	h	1272	OMU	N3-C2-N1	3.82	119.96	114.89
3	h	581	OMU	N3-C2-N1	3.80	119.94	114.89
3	h	1771	6MZ	C4-N9-C1'	-3.80	117.54	126.59
3	h	1234	OMU	N3-C2-N1	3.79	119.92	114.89
3	h	1383	OMU	N3-C2-N1	3.78	119.90	114.89
3	h	544	A2M	C1'-N9-C8	3.77	135.65	127.14
3	h	544	A2M	C2-N3-C4	3.77	120.65	111.75
3	h	1012	OMU	N3-C2-N1	3.72	119.83	114.89
3	h	886	OMU	N3-C2-N1	3.72	119.82	114.89
3	h	544	A2M	C4'-O4'-C1'	-3.71	101.30	109.47
3	h	544	A2M	N9-C8-N7	-3.71	108.85	113.91
3	h	1789	MA6	C2-N1-C6	3.70	120.48	111.75
3	h	1790	MA6	C2-N1-C6	3.69	120.46	111.75
3	h	373	OMU	N3-C2-N1	3.67	119.77	114.89
3	h	614	OMU	N3-C2-N1	3.67	119.76	114.89
3	h	392	OMG	N9-C8-N7	-3.66	106.50	113.39
3	h	1447	OMU	N3-C2-N1	3.66	119.74	114.89
3	h	123	OMU	N3-C2-N1	3.63	119.71	114.89
3	h	440	A2M	C2-N3-C4	3.60	120.25	111.75
3	h	1781	4AC	CM7-C7-N4	3.60	121.52	115.29
3	h	598	OMG	N9-C8-N7	-3.59	106.63	113.39
3	h	1758	A2M	C2-N3-C4	3.58	120.22	111.75
3	h	1579	A2M	C2-N3-C4	3.58	120.22	111.75
3	h	622	A2M	C2-N3-C4	3.58	120.20	111.75
3	h	1274	OMG	N9-C8-N7	-3.56	106.68	113.39
3	h	1329	A2M	C2-N3-C4	3.56	120.16	111.75
3	h	162	A2M	C2-N3-C4	3.55	120.15	111.75
3	h	1789	MA6	C4-C5-C6	3.53	119.84	115.88
3	h	468	A2M	C2-N3-C4	3.53	120.10	111.75
3	h	977	A2M	C2-N3-C4	3.53	120.09	111.75
3	h	28	A2M	C2-N3-C4	3.53	120.09	111.75
3	h	424	A2M	C2-N3-C4	3.52	120.06	111.75
3	h	1433	OMG	N9-C8-N7	-3.51	106.79	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	246	OMG	N9-C8-N7	-3.50	106.81	113.39
3	h	1771	6MZ	C2-N3-C4	3.49	120.00	111.75
3	h	800	A2M	C2-N3-C4	3.49	120.00	111.75
3	h	1210	PSU	C6-C5-C4	3.47	120.62	118.20
3	h	1790	MA6	C1'-N9-C8	-3.46	119.32	127.14
3	h	1790	MA6	C2-N3-C4	3.46	119.92	111.75
3	h	1789	MA6	C4-N9-C1'	3.46	134.83	126.59
3	h	1771	6MZ	N3-C4-N9	3.46	132.78	127.08
3	h	1758	A2M	N3-C4-N9	3.39	132.67	127.08
3	h	1012	OMU	C5-C4-N3	3.38	119.90	114.84
3	h	1308	PSU	C6-C5-C4	3.38	120.56	118.20
3	h	886	OMU	C5-C4-N3	3.36	119.87	114.84
3	h	1790	MA6	C5-N7-C8	3.36	108.28	103.51
3	h	1184	PSU	C6-C5-C4	3.36	120.54	118.20
3	h	373	OMU	C5-C4-N3	3.35	119.85	114.84
3	h	1789	MA6	C2-N3-C4	3.33	119.61	111.75
3	h	1383	OMU	C5-C4-N3	3.33	119.82	114.84
3	h	961	PSU	C6-C5-C4	3.32	120.52	118.20
3	h	1283	4AC	N4-C4-N3	3.31	119.41	113.85
3	h	1272	OMU	C5-C4-N3	3.31	119.79	114.84
3	h	581	OMU	C5-C4-N3	3.30	119.78	114.84
3	h	123	OMU	C5-C4-N3	3.30	119.77	114.84
3	h	162	A2M	N3-C4-N9	3.29	132.50	127.08
3	h	440	A2M	N3-C4-N9	3.28	132.49	127.08
3	h	614	OMU	C5-C4-N3	3.28	119.74	114.84
3	h	1234	OMU	C5-C4-N3	3.27	119.73	114.84
3	h	1447	OMU	C5-C4-N3	3.27	119.72	114.84
3	h	1579	A2M	N3-C4-N9	3.26	132.45	127.08
3	h	977	A2M	N3-C4-N9	3.25	132.44	127.08
3	h	1789	MA6	C5-N7-C8	3.24	108.11	103.51
3	h	622	A2M	C5-N7-C8	3.23	108.11	103.51
3	h	1329	A2M	N3-C4-N9	3.23	132.40	127.08
3	h	28	A2M	N3-C4-N9	3.23	132.40	127.08
3	h	424	A2M	N3-C4-N9	3.22	132.38	127.08
3	h	470	PSU	C6-C5-C4	3.21	120.44	118.20
3	h	1190	PSU	C6-C5-C4	3.21	120.44	118.20
3	h	1771	6MZ	C1'-N9-C8	3.20	134.37	127.14
3	h	886	OMU	CM2-O2'-C2'	3.20	122.92	114.52
3	h	1027	PSU	C6-C5-C4	3.18	120.42	118.20
3	h	800	A2M	N3-C4-N9	3.15	132.28	127.08
3	h	440	A2M	C5-N7-C8	3.14	107.97	103.51
3	h	339	PSU	C6-C5-C4	3.14	120.39	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1579	A2M	C5-N7-C8	3.14	107.97	103.51
3	h	1329	A2M	C5-N7-C8	3.13	107.96	103.51
3	h	468	A2M	N3-C4-N9	3.12	132.22	127.08
3	h	800	A2M	C5-N7-C8	3.12	107.94	103.51
3	h	961	PSU	C6-N1-C2	-3.12	119.50	122.68
3	h	1787	PSU	C6-C5-C4	3.11	120.37	118.20
3	h	977	A2M	C5-N7-C8	3.11	107.92	103.51
3	h	28	A2M	C5-N7-C8	3.10	107.92	103.51
3	h	310	PSU	C6-C5-C4	3.10	120.36	118.20
3	h	1120	PSU	C6-C5-C4	3.09	120.36	118.20
3	h	1304	PSU	C6-C5-C4	3.09	120.36	118.20
3	h	1787	PSU	C6-N1-C2	-3.09	119.52	122.68
3	h	544	A2M	C5-N7-C8	3.09	107.89	103.51
3	h	162	A2M	C5-N7-C8	3.08	107.89	103.51
3	h	1567	PSU	C6-C5-C4	3.07	120.34	118.20
3	h	1790	MA6	C4-C5-C6	3.07	119.31	115.88
3	h	1485	PSU	C6-C5-C4	3.07	120.34	118.20
3	h	622	A2M	N3-C4-N9	3.06	132.13	127.08
3	h	606	PSU	C6-N1-C2	-3.06	119.55	122.68
3	h	1758	A2M	C5-N7-C8	3.05	107.84	103.51
3	h	468	A2M	C5-N7-C8	3.05	107.84	103.51
3	h	362	PSU	C6-C5-C4	3.04	120.32	118.20
3	h	424	A2M	C5-N7-C8	3.04	107.82	103.51
3	h	950	PSU	C6-N1-C2	-3.02	119.59	122.68
3	h	339	PSU	C6-N1-C2	-3.01	119.60	122.68
3	h	1535	PSU	C6-C5-C4	2.99	120.29	118.20
3	h	1210	PSU	C6-N1-C2	-2.99	119.62	122.68
3	h	1771	6MZ	C5-N7-C8	2.99	107.76	103.51
3	h	417	PSU	C6-N1-C2	-2.98	119.63	122.68
3	h	607	PSU	C6-N1-C2	-2.97	119.65	122.68
3	h	753	PSU	C6-N1-C2	-2.97	119.65	122.68
3	h	451	PSU	C6-C5-C4	2.96	120.27	118.20
3	h	607	PSU	C6-C5-C4	2.96	120.27	118.20
3	h	1634	PSU	C6-C5-C4	2.96	120.27	118.20
3	h	1535	PSU	C6-N1-C2	-2.96	119.65	122.68
3	h	1178	PSU	C6-C5-C4	2.96	120.27	118.20
3	h	1178	PSU	C6-N1-C2	-2.95	119.66	122.68
3	h	1524	PSU	C6-N1-C2	-2.95	119.66	122.68
3	h	95	PSU	C6-C5-C4	2.95	120.26	118.20
3	h	1567	PSU	C6-N1-C2	-2.95	119.67	122.68
3	h	1615	PSU	C6-N1-C2	-2.95	119.67	122.68
3	h	1447	OMU	O4-C4-C5	-2.95	119.98	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	605	PSU	C6-C5-C4	2.94	120.26	118.20
3	h	809	PSU	C6-N1-C2	-2.94	119.68	122.68
3	h	1789	MA6	N3-C4-N9	2.94	131.92	127.08
3	h	1184	PSU	C6-N1-C2	-2.93	119.68	122.68
3	h	246	OMG	C2-N1-C6	-2.93	119.76	125.10
3	h	1272	OMU	O4-C4-C5	-2.93	120.01	125.16
3	h	103	PSU	C6-C5-C4	2.92	120.24	118.20
3	h	1274	OMG	C2-N1-C6	-2.92	119.77	125.10
3	h	1002	PSU	C6-C5-C4	2.92	120.24	118.20
3	h	598	OMG	C2-N1-C6	-2.92	119.77	125.10
3	h	1383	OMU	O4-C4-C5	-2.92	120.02	125.16
3	h	306	PSU	C6-N1-C2	-2.92	119.70	122.68
3	h	1194	B8N	N3-C2-N1	2.91	120.87	116.76
3	h	635	PSU	C6-N1-C2	-2.91	119.71	122.68
3	h	1781	4AC	C5-C4-N4	-2.91	117.87	122.92
3	h	603	UY1	C6-N1-C2	-2.91	119.71	122.68
3	h	258	PSU	C6-N1-C2	-2.91	119.71	122.68
3	h	753	PSU	C6-C5-C4	2.90	120.22	118.20
3	h	258	PSU	C6-C5-C4	2.90	120.22	118.20
3	h	1308	PSU	C6-N1-C2	-2.89	119.72	122.68
3	h	1615	PSU	C6-C5-C4	2.89	120.22	118.20
3	h	1120	PSU	C6-N1-C2	-2.89	119.72	122.68
3	h	886	OMU	O4-C4-C5	-2.89	120.08	125.16
3	h	373	OMU	O4-C4-C5	-2.89	120.08	125.16
3	h	1012	OMU	O4-C4-C5	-2.89	120.08	125.16
3	h	123	OMU	O4-C4-C5	-2.88	120.09	125.16
3	h	470	PSU	C6-N1-C2	-2.88	119.74	122.68
3	h	809	PSU	C6-C5-C4	2.88	120.21	118.20
3	h	763	PSU	C6-N1-C2	-2.87	119.74	122.68
3	h	1190	PSU	C6-N1-C2	-2.87	119.75	122.68
3	h	635	PSU	C6-C5-C4	2.87	120.20	118.20
3	h	451	PSU	C6-N1-C2	-2.86	119.76	122.68
3	h	1217	PSU	C6-N1-C2	-2.85	119.76	122.68
3	h	417	PSU	C6-C5-C4	2.85	120.19	118.20
3	h	392	OMG	C2-N1-C6	-2.85	119.90	125.10
3	h	762	PSU	C6-N1-C2	-2.84	119.78	122.68
3	h	614	OMU	O4-C4-C5	-2.84	120.17	125.16
3	h	121	PSU	C6-N1-C2	-2.84	119.78	122.68
3	h	1106	PSU	C6-N1-C2	-2.83	119.79	122.68
3	h	362	PSU	C6-N1-C2	-2.83	119.79	122.68
3	h	1485	PSU	C6-N1-C2	-2.83	119.79	122.68
3	h	581	OMU	O4-C4-C5	-2.82	120.20	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1027	PSU	C6-N1-C2	-2.82	119.80	122.68
3	h	605	PSU	C6-N1-C2	-2.81	119.81	122.68
3	h	1293	PSU	C6-C5-C4	2.80	120.15	118.20
3	h	103	PSU	C6-N1-C2	-2.80	119.83	122.68
3	h	1234	OMU	O4-C4-C5	-2.79	120.25	125.16
3	h	1293	PSU	C6-N1-C2	-2.79	119.83	122.68
3	h	95	PSU	C6-N1-C2	-2.79	119.83	122.68
3	h	246	OMG	N9-C4-N3	2.77	131.50	125.94
3	h	1304	PSU	C6-N1-C2	-2.77	119.85	122.68
3	h	1002	PSU	C6-N1-C2	-2.77	119.85	122.68
3	h	1106	PSU	C6-C5-C4	2.76	120.13	118.20
3	h	950	PSU	C6-C5-C4	2.75	120.12	118.20
3	h	1634	PSU	C6-N1-C2	-2.75	119.87	122.68
3	h	306	PSU	C6-C5-C4	2.73	120.11	118.20
3	h	310	PSU	C6-N1-C2	-2.73	119.89	122.68
3	h	1210	PSU	O2-C2-N1	-2.72	119.79	122.79
3	h	1120	PSU	O2-C2-N1	-2.72	119.80	122.79
3	h	1194	B8N	O4-C4-N3	-2.71	115.39	119.98
3	h	1283	4AC	CM7-C7-N4	2.70	119.97	115.29
3	h	1274	OMG	C5-C6-N1	2.70	120.04	113.19
3	h	603	UY1	C6-C5-C4	2.70	120.08	118.20
3	h	598	OMG	C5-C6-N1	2.68	120.01	113.19
3	h	763	PSU	C6-C5-C4	2.66	120.06	118.20
3	h	246	OMG	C5-C6-N1	2.66	119.94	113.19
3	h	622	A2M	C3'-C2'-C1'	2.66	107.89	102.89
3	h	1106	PSU	O2-C2-N1	-2.65	119.87	122.79
3	h	392	OMG	C5-C6-N1	2.65	119.92	113.19
3	h	103	PSU	O2-C2-N1	-2.65	119.88	122.79
3	h	753	PSU	O2-C2-N1	-2.60	119.93	122.79
3	h	121	PSU	C6-C5-C4	2.59	120.01	118.20
3	h	362	PSU	O2-C2-N1	-2.59	119.94	122.79
3	h	1190	PSU	O2-C2-N1	-2.59	119.94	122.79
3	h	607	PSU	O2-C2-N1	-2.58	119.94	122.79
3	h	1217	PSU	C6-C5-C4	2.58	120.00	118.20
3	h	1293	PSU	O2-C2-N1	-2.58	119.95	122.79
3	h	606	PSU	C6-C5-C4	2.57	120.00	118.20
3	h	1433	OMG	C5-C6-N1	2.57	119.70	113.19
3	h	961	PSU	O2-C2-N1	-2.56	119.97	122.79
3	h	544	A2M	C6-C5-C4	2.56	120.62	117.18
3	h	1787	PSU	O2-C2-N1	-2.55	119.98	122.79
3	h	418	OMC	CM2-O2'-C2'	2.55	121.21	114.52
3	h	1178	PSU	O2-C2-N1	-2.54	120.00	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1184	PSU	O2-C2-N1	-2.54	120.00	122.79
3	h	1790	MA6	C4-C5-N7	-2.53	107.54	110.62
3	h	1308	PSU	O2-C2-N1	-2.53	120.01	122.79
3	h	584	PSU	O2-C2-N1	-2.53	120.01	122.79
3	h	809	PSU	O2-C2-N1	-2.53	120.01	122.79
3	h	1304	PSU	O2-C2-N1	-2.52	120.02	122.79
3	h	1485	PSU	O2-C2-N1	-2.52	120.02	122.79
3	h	635	PSU	O2-C2-N1	-2.51	120.02	122.79
3	h	1433	OMG	C2-N1-C6	-2.51	120.53	125.10
3	h	762	PSU	C6-C5-C4	2.50	119.95	118.20
3	h	950	PSU	O2-C2-N1	-2.50	120.04	122.79
3	h	1027	PSU	O2-C2-N1	-2.49	120.05	122.79
3	h	246	OMG	O6-C6-C5	-2.49	120.00	126.60
3	h	339	PSU	O2-C2-N1	-2.48	120.06	122.79
3	h	763	PSU	O2-C2-N1	-2.48	120.06	122.79
3	h	603	UY1	O2-C2-N1	-2.48	120.06	122.79
3	h	598	OMG	O6-C6-C5	-2.47	120.04	126.60
3	h	121	PSU	O2-C2-N1	-2.47	120.07	122.79
3	h	1567	PSU	O2-C2-N1	-2.47	120.07	122.79
3	h	1433	OMG	N9-C4-N3	2.47	130.89	125.94
3	h	1789	MA6	C4-N9-C8	2.46	108.40	105.73
3	h	1524	PSU	C6-C5-C4	2.46	119.92	118.20
3	h	605	PSU	O2-C2-N1	-2.46	120.09	122.79
3	h	598	OMG	N9-C4-N3	2.45	130.85	125.94
3	h	392	OMG	O6-C6-C5	-2.45	120.11	126.60
3	h	392	OMG	C8-N7-C5	2.44	108.65	104.24
3	h	1790	MA6	N3-C4-N9	2.44	131.10	127.08
3	h	1790	MA6	C4-N9-C8	2.43	108.36	105.73
3	h	1524	PSU	O2-C2-N1	-2.43	120.12	122.79
3	h	1274	OMG	N9-C4-N3	2.42	130.79	125.94
3	h	1217	PSU	O2-C2-N1	-2.41	120.13	122.79
3	h	1274	OMG	C8-N7-C5	2.41	108.60	104.24
3	h	598	OMG	C8-N7-C5	2.41	108.60	104.24
3	h	1274	OMG	O6-C6-C5	-2.41	120.21	126.60
3	h	417	PSU	O2-C2-N1	-2.40	120.15	122.79
3	h	1433	OMG	O6-C6-C5	-2.39	120.26	126.60
3	h	1535	PSU	O2-C2-N1	-2.38	120.17	122.79
3	h	1790	MA6	C4-N9-C1'	2.38	132.25	126.59
3	h	310	PSU	O2-C2-N1	-2.37	120.18	122.79
3	h	1634	PSU	O2-C2-N1	-2.37	120.19	122.79
3	h	451	PSU	O2-C2-N1	-2.35	120.20	122.79
3	h	1615	PSU	O2-C2-N1	-2.35	120.21	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	258	PSU	O2-C2-N1	-2.34	120.22	122.79
3	h	470	PSU	O2-C2-N1	-2.34	120.22	122.79
3	h	1781	4AC	C6-C5-C4	2.33	119.82	116.96
3	h	246	OMG	C8-N7-C5	2.33	108.45	104.24
3	h	762	PSU	O2-C2-N1	-2.32	120.23	122.79
3	h	95	PSU	O2-C2-N1	-2.32	120.23	122.79
3	h	392	OMG	N9-C4-N3	2.28	130.53	125.94
3	h	440	A2M	C6-C5-C4	2.28	120.25	117.18
3	h	622	A2M	C4-C5-N7	-2.27	107.85	110.62
3	h	607	PSU	O4'-C1'-C2'	2.27	108.34	105.14
3	h	306	PSU	O2-C2-N1	-2.26	120.30	122.79
3	h	606	PSU	O2-C2-N1	-2.26	120.31	122.79
3	h	28	A2M	C6-C5-C4	2.23	120.18	117.18
3	h	1758	A2M	C4'-O4'-C1'	-2.23	104.55	109.47
3	h	1433	OMG	C8-N7-C5	2.21	108.25	104.24
3	h	1758	A2M	C6-C5-C4	2.21	120.16	117.18
3	h	392	OMG	N2-C2-N1	2.19	121.38	116.71
3	h	598	OMG	N2-C2-N1	2.19	121.37	116.71
3	h	1579	A2M	C6-C5-C4	2.18	120.12	117.18
3	h	977	A2M	C6-C5-C4	2.17	120.11	117.18
3	h	451	PSU	O4'-C1'-C2'	2.17	108.21	105.14
3	h	1771	6MZ	C4-N9-C8	2.17	108.08	105.73
3	h	1329	A2M	C4-C5-N7	-2.16	107.99	110.62
3	h	1790	MA6	C5-C4-N9	2.16	108.29	105.78
3	h	1283	4AC	C6-C5-C4	2.15	119.59	116.96
3	h	1194	B8N	C31-N3-C4	2.15	120.47	117.31
3	h	162	A2M	C4'-O4'-C1'	-2.15	104.74	109.47
3	h	1329	A2M	C6-C5-C4	2.14	120.06	117.18
3	h	800	A2M	C6-C5-C4	2.13	120.04	117.18
3	h	622	A2M	C4'-O4'-C1'	-2.12	104.79	109.47
3	h	440	A2M	C4-C5-N7	-2.12	108.03	110.62
3	h	622	A2M	C4-N9-C8	2.12	108.02	105.73
3	h	1579	A2M	C4-C5-N7	-2.11	108.05	110.62
3	h	162	A2M	C6-C5-C4	2.11	120.02	117.18
3	h	424	A2M	C4'-O4'-C1'	-2.11	104.83	109.47
3	h	339	PSU	O4'-C1'-C2'	2.10	108.11	105.14
3	h	1274	OMG	N2-C2-N1	2.10	121.19	116.71
3	h	800	A2M	C4-C5-N7	-2.10	108.06	110.62
3	h	977	A2M	C4-C5-N7	-2.10	108.07	110.62
3	h	809	PSU	O4'-C1'-C2'	2.08	108.08	105.14
3	h	544	A2M	O4'-C4'-C3'	-2.08	101.01	105.11
3	h	1194	B8N	O4'-C1'-C2'	2.07	108.06	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	1194	B8N	O36-C34-C33	2.06	120.40	113.38
3	h	424	A2M	C4-N9-C8	2.06	107.96	105.73
3	h	1789	MA6	C4-C5-N7	-2.05	108.12	110.62
3	h	468	A2M	C6-C5-C4	2.05	119.94	117.18
3	h	468	A2M	C4-C5-N7	-2.04	108.13	110.62
3	h	392	OMG	C4-C5-N7	-2.04	107.50	110.72
3	h	468	A2M	C4'-O4'-C1'	-2.04	104.98	109.47
3	h	1433	OMG	N1-C2-N3	-2.03	119.53	123.32
3	h	424	A2M	C6-C5-C4	2.03	119.91	117.18
3	h	1002	PSU	O2-C2-N1	-2.02	120.57	122.79
3	h	28	A2M	C4-C5-N7	-2.02	108.16	110.62
3	h	392	OMG	C2'-C1'-N9	-2.02	110.31	114.22
3	h	544	A2M	C4-C5-N7	-2.01	108.17	110.62
3	h	1329	A2M	C4-N9-C8	2.01	107.91	105.73
3	h	1758	A2M	O4'-C1'-C2'	-2.00	103.05	106.57

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	h	123	OMU	O4'-C4'-C5'-O5'
3	h	140	OMC	C3'-C4'-C5'-O5'
3	h	140	OMC	O4'-C4'-C5'-O5'
3	h	392	OMG	O4'-C4'-C5'-O5'
3	h	418	OMC	C1'-C2'-O2'-CM2
3	h	418	OMC	C3'-C2'-O2'-CM2
3	h	584	PSU	C2'-C1'-C5-C4
3	h	584	PSU	O4'-C1'-C5-C6
3	h	584	PSU	C3'-C4'-C5'-O5'
3	h	584	PSU	O4'-C4'-C5'-O5'
3	h	598	OMG	O4'-C4'-C5'-O5'
3	h	622	A2M	C3'-C4'-C5'-O5'
3	h	886	OMU	C1'-C2'-O2'-CM2
3	h	1234	OMU	C3'-C4'-C5'-O5'
3	h	1234	OMU	O4'-C4'-C5'-O5'
3	h	1274	OMG	O4'-C4'-C5'-O5'
3	h	1274	OMG	C3'-C4'-C5'-O5'
3	h	1308	PSU	C2'-C1'-C5-C4
3	h	1579	A2M	O4'-C4'-C5'-O5'
3	h	1194	B8N	N34-C33-C34-O35
3	h	1787	PSU	C3'-C4'-C5'-O5'
3	h	1787	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	h	1790	MA6	O4'-C4'-C5'-O5'
3	h	1790	MA6	C3'-C4'-C5'-O5'
3	h	123	OMU	C3'-C4'-C5'-O5'
3	h	392	OMG	C3'-C4'-C5'-O5'
3	h	581	OMU	O4'-C4'-C5'-O5'
3	h	598	OMG	C3'-C4'-C5'-O5'
3	h	622	A2M	O4'-C4'-C5'-O5'
3	h	1272	OMU	O4'-C4'-C5'-O5'
3	h	1579	A2M	C3'-C4'-C5'-O5'
3	h	258	PSU	O4'-C4'-C5'-O5'
3	h	1194	B8N	N34-C33-C34-O36
3	h	258	PSU	C3'-C4'-C5'-O5'
3	h	544	A2M	C3'-C4'-C5'-O5'
3	h	886	OMU	C3'-C4'-C5'-O5'
3	h	581	OMU	C3'-C4'-C5'-O5'
3	h	598	OMG	C4'-C5'-O5'-P
3	h	886	OMU	O4'-C4'-C5'-O5'
3	h	622	A2M	C2'-C1'-N9-C8
3	h	1433	OMG	C4'-C5'-O5'-P
3	h	1790	MA6	C4'-C5'-O5'-P
3	h	584	PSU	O4'-C1'-C5-C4
3	h	961	PSU	O4'-C1'-C5-C4
3	h	1308	PSU	O4'-C1'-C5-C4
3	h	614	OMU	O4'-C4'-C5'-O5'
3	h	544	A2M	O4'-C1'-N9-C8
3	h	622	A2M	O4'-C1'-N9-C8
3	h	961	PSU	O4'-C1'-C5-C6
3	h	1524	PSU	O4'-C1'-C5-C6
3	h	1304	PSU	C4'-C5'-O5'-P
3	h	1524	PSU	O4'-C4'-C5'-O5'
3	h	622	A2M	C2'-C1'-N9-C4

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	h	95	PSU	1	0
3	h	1790	MA6	3	0
3	h	598	OMG	1	0
3	h	392	OMG	2	0
3	h	1447	OMU	1	0
3	h	1645	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	h	1781	4AC	1	0
3	h	1234	OMU	1	0
3	h	603	UY1	1	0
3	h	762	PSU	2	0
3	h	605	PSU	1	0
3	h	1789	MA6	2	0
3	h	763	PSU	1	0
3	h	1383	OMU	1	0
3	h	140	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 126 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	SPM	h	2017	-	13,13,13	0.34	0	12,12,12	0.85	0
39	SPM	h	2016	-	13,13,13	0.34	0	12,12,12	0.78	0
39	SPM	h	2018	-	13,13,13	0.35	0	12,12,12	0.90	0
38	SPD	h	2015	-	9,9,9	0.30	0	8,8,8	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SPM	h	2017	-	-	4/11/11/11	-
39	SPM	h	2016	-	-	5/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SPM	h	2018	-	-	2/11/11/11	-
38	SPD	h	2015	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	h	2016	SPM	C7-C8-C9-N10
38	h	2015	SPD	N6-C7-C8-C9
38	h	2015	SPD	C8-C7-N6-C5
39	h	2016	SPM	C8-C9-N10-C11
39	h	2018	SPM	N5-C6-C7-C8
39	h	2016	SPM	N10-C11-C12-C13
38	h	2015	SPD	C4-C5-N6-C7
39	h	2016	SPM	C7-C6-N5-C4
39	h	2017	SPM	C6-C7-C8-C9
39	h	2018	SPM	C11-C12-C13-N14
39	h	2017	SPM	C8-C9-N10-C11
39	h	2017	SPM	C7-C6-N5-C4
39	h	2016	SPM	N5-C6-C7-C8
39	h	2017	SPM	N10-C11-C12-C13

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	h	2016	SPM	1	0
39	h	2018	SPM	1	0
38	h	2015	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

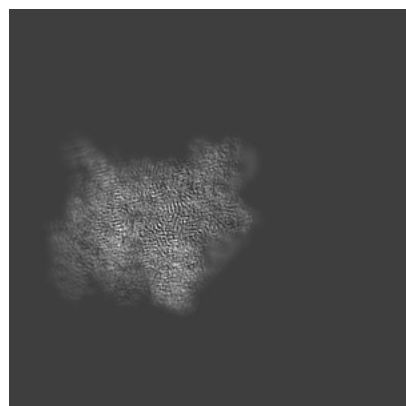
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15674. These allow visual inspection of the internal detail of the map and identification of artifacts.

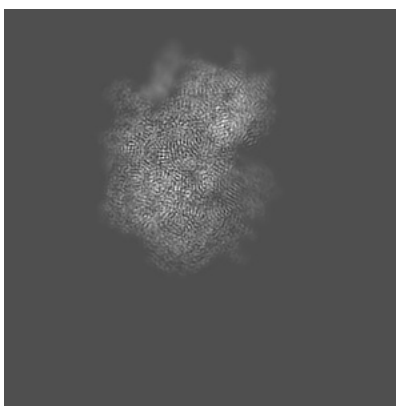
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

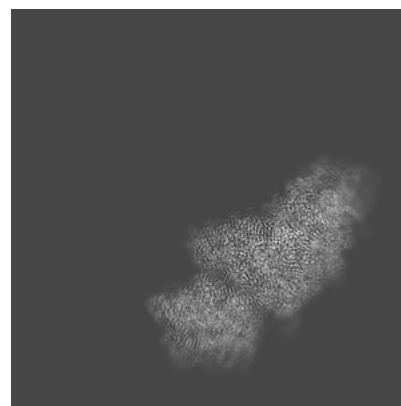
6.1.1 Primary map



X

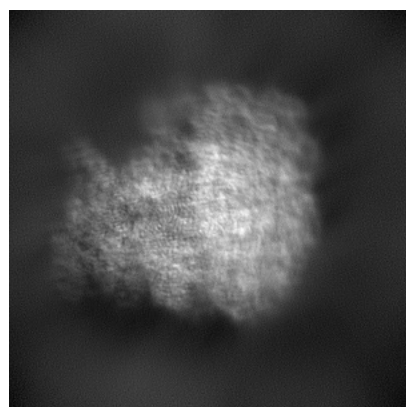


Y

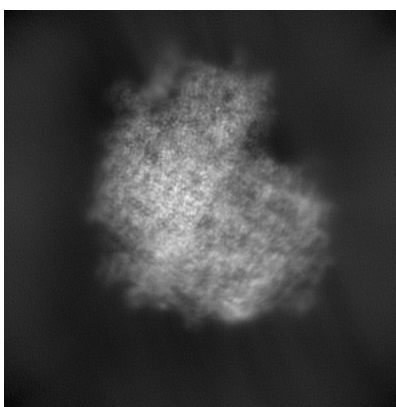


Z

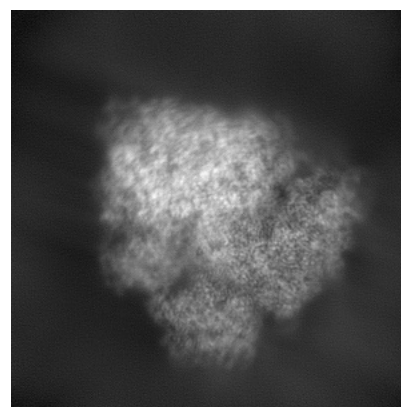
6.1.2 Raw map



X



Y

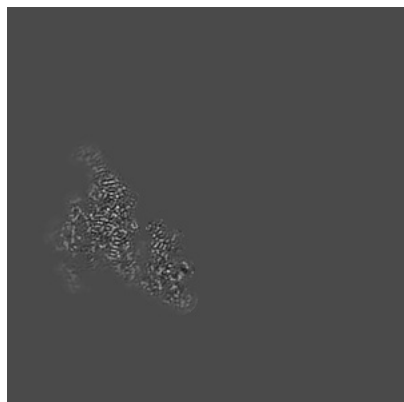


Z

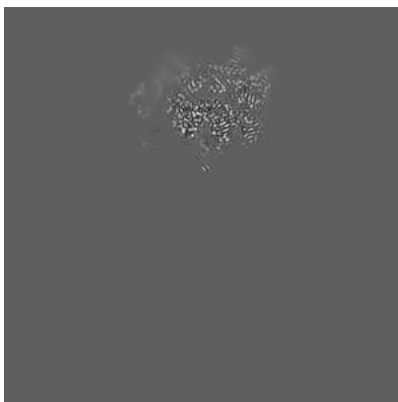
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

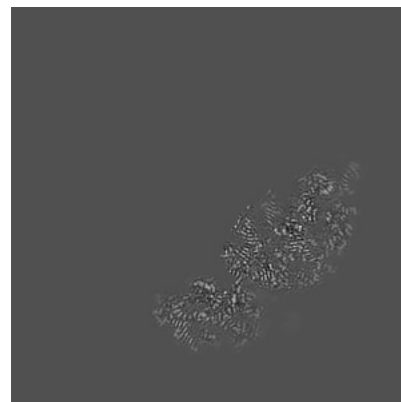
6.2.1 Primary map



X Index: 225

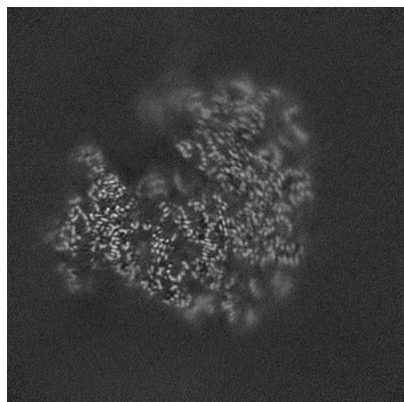


Y Index: 225

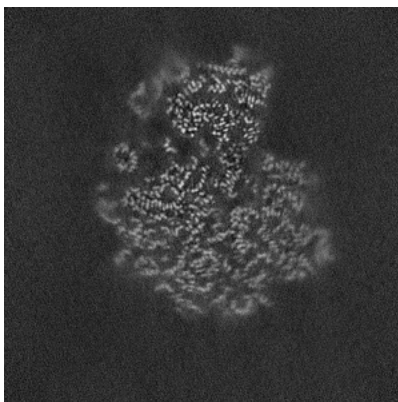


Z Index: 225

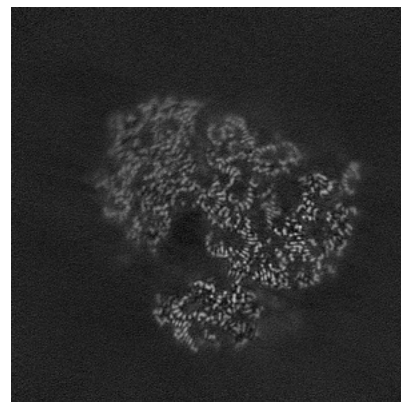
6.2.2 Raw map



X Index: 225



Y Index: 225

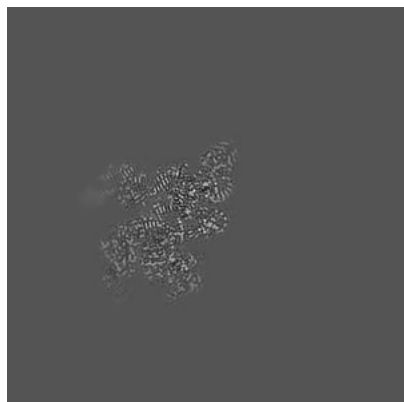


Z Index: 225

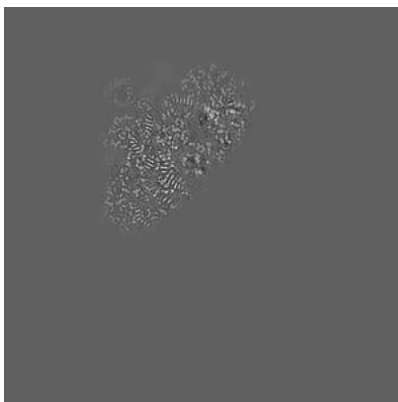
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

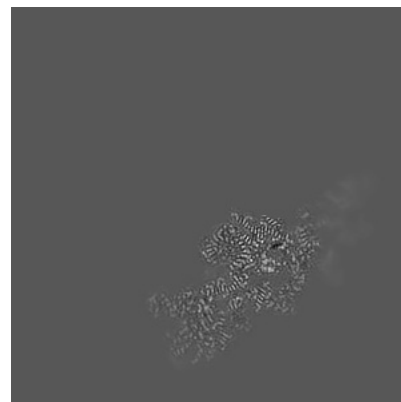
6.3.1 Primary map



X Index: 316

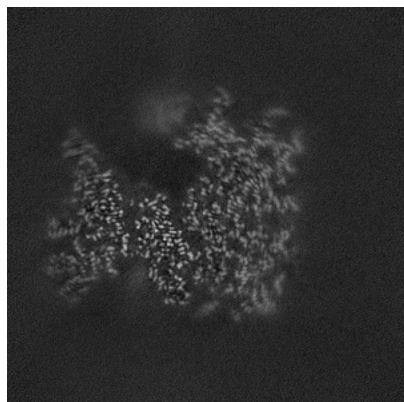


Y Index: 187

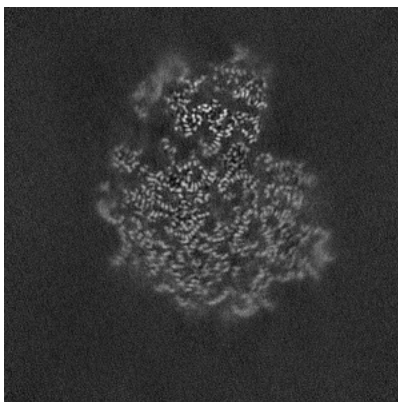


Z Index: 179

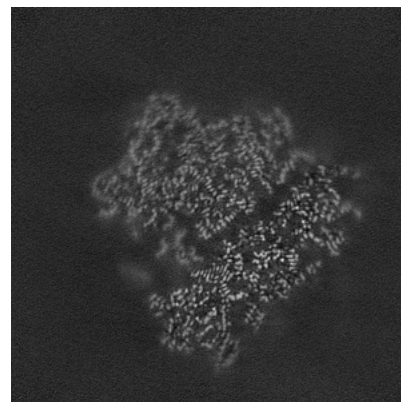
6.3.2 Raw map



X Index: 246



Y Index: 228

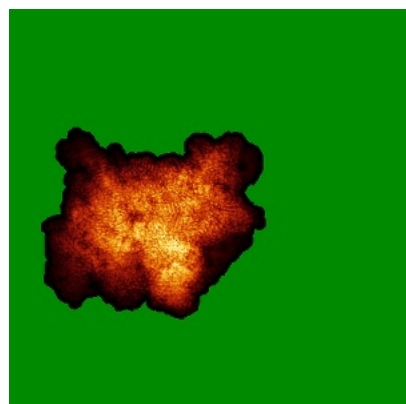


Z Index: 206

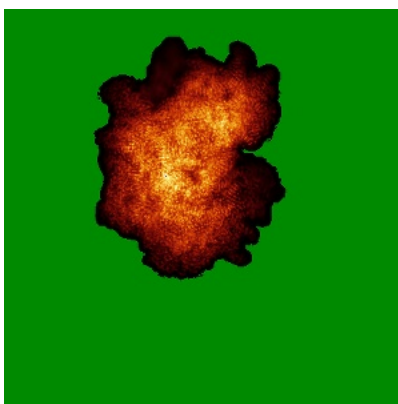
The images above show the largest variance slices of the map in three orthogonal directions.

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

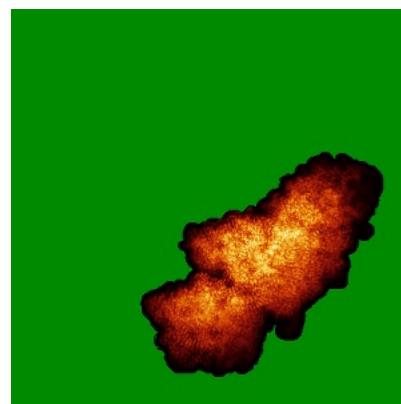
6.4.1 Primary map



X

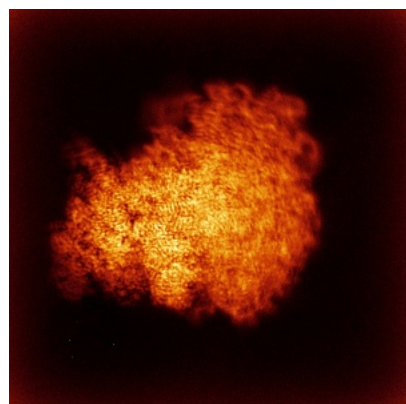


Y

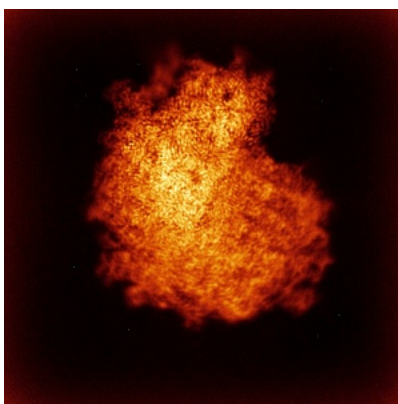


Z

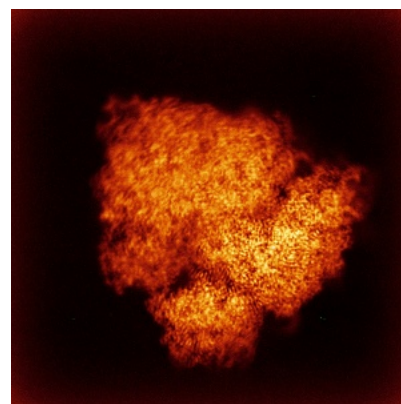
6.4.2 Raw map



X



Y

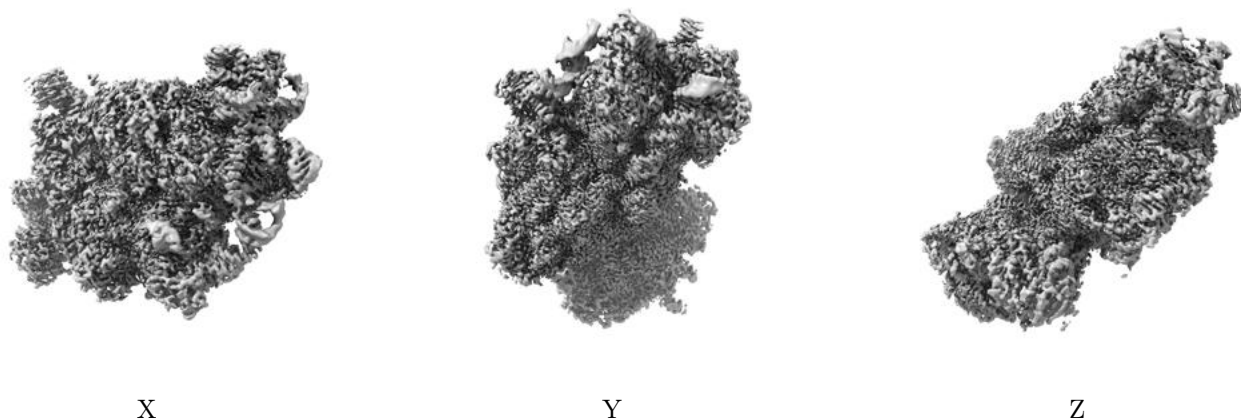


Z

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 0.426. 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.

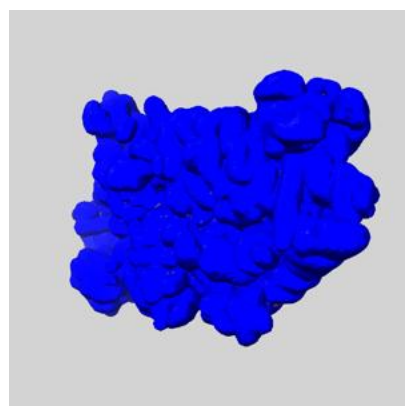
6.6 Mask visualisation [i](#)

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

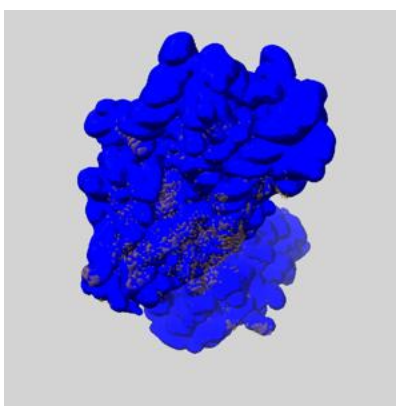
A mask typically either:

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

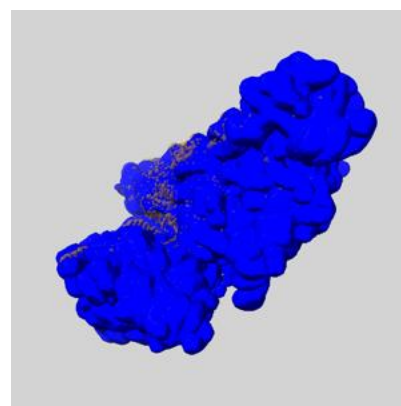
6.6.1 emd_15674_msk_1.map [i](#)



X



Y

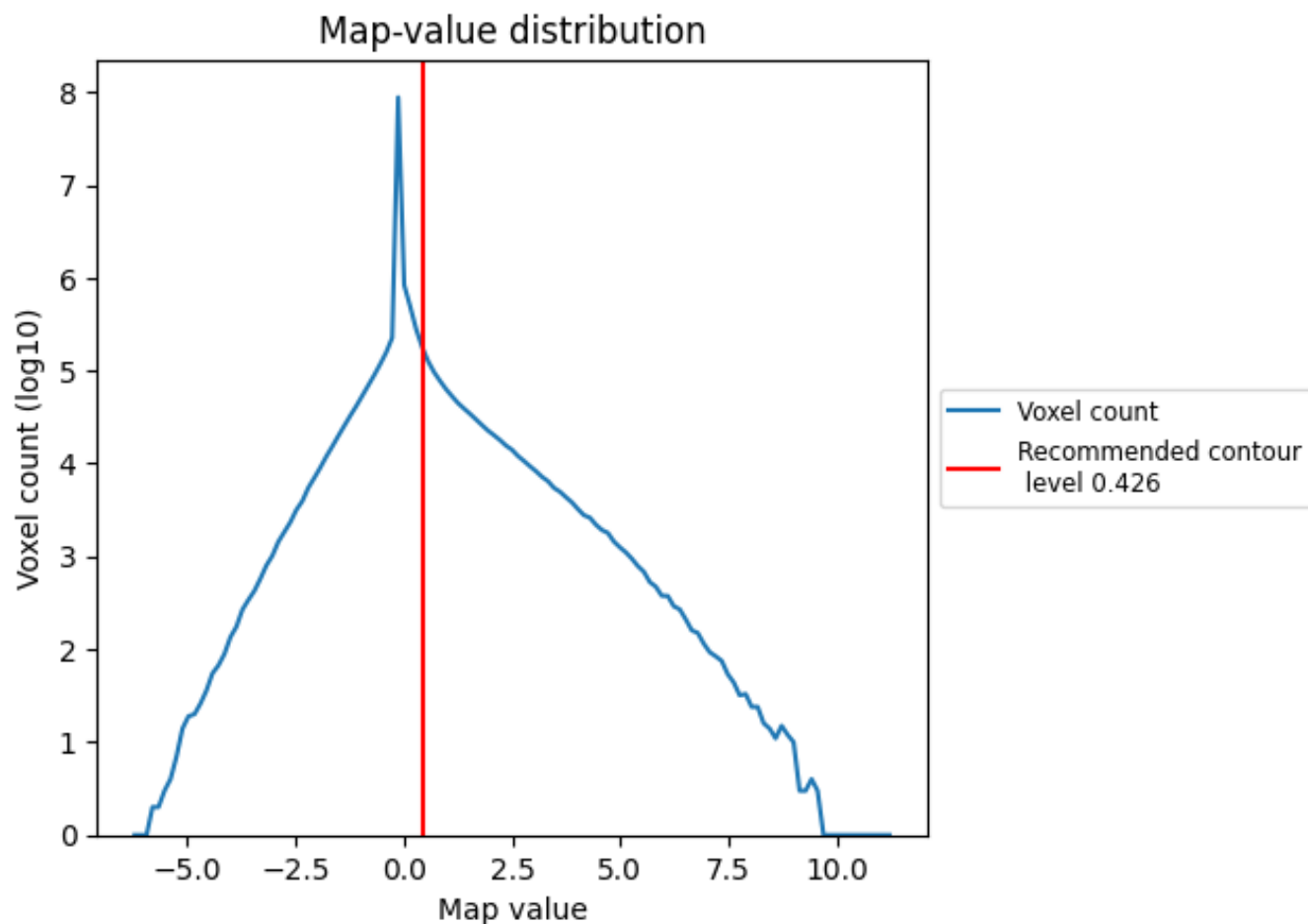


Z

7 Map analysis [i](#)

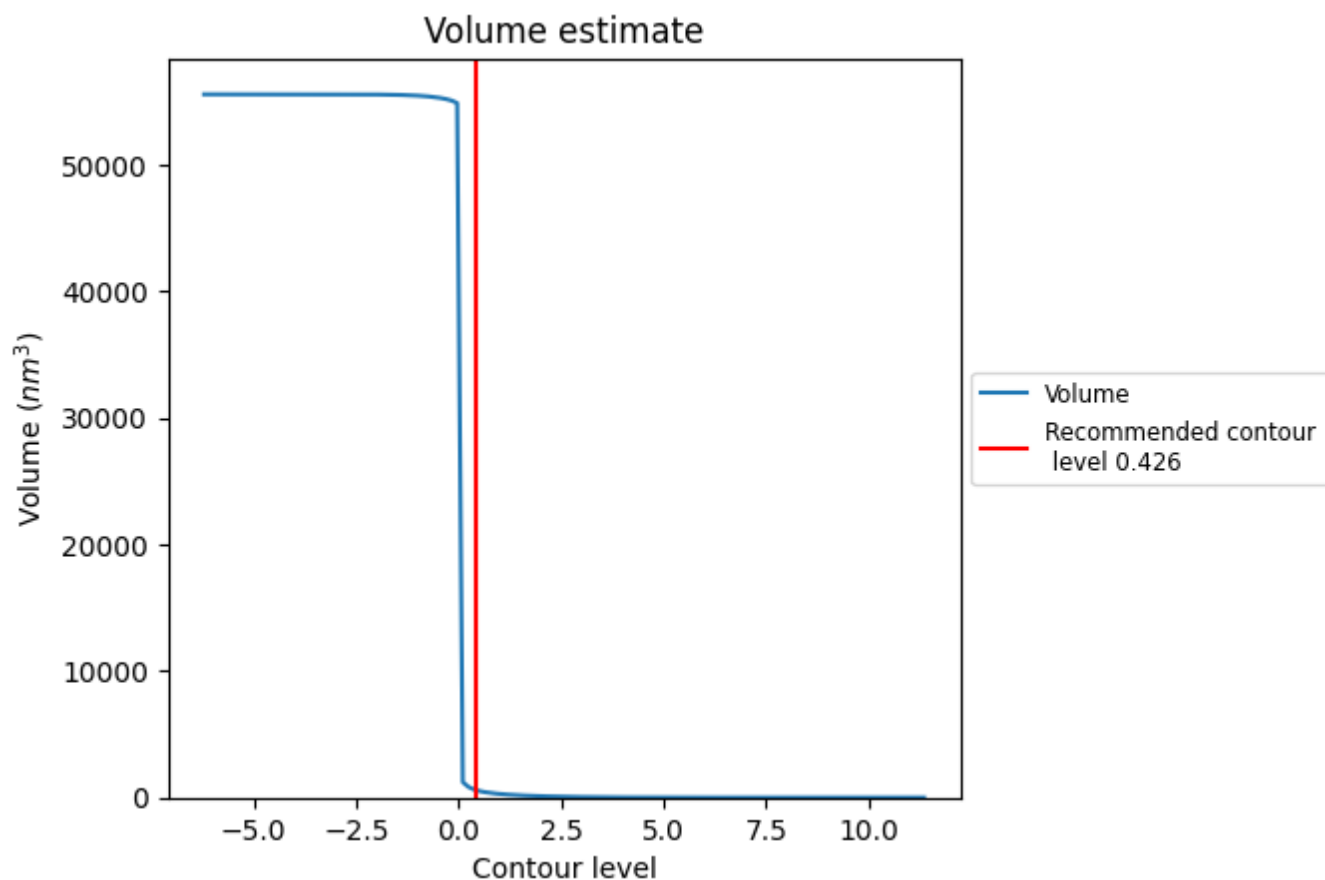
This section contains the results of statistical analysis of the map.

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.

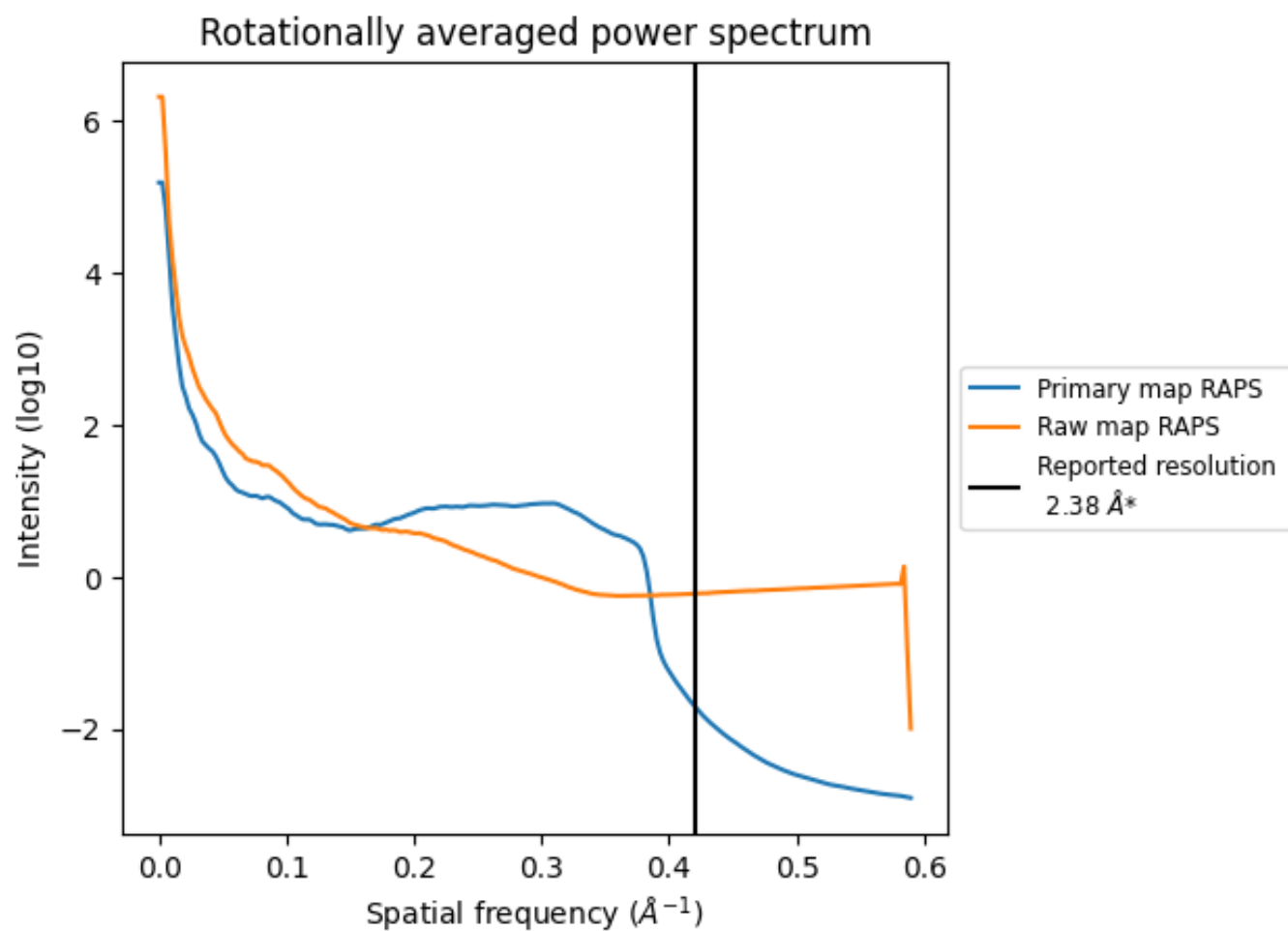
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 588 nm³; this corresponds to an approximate mass of 531 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 ⓘ

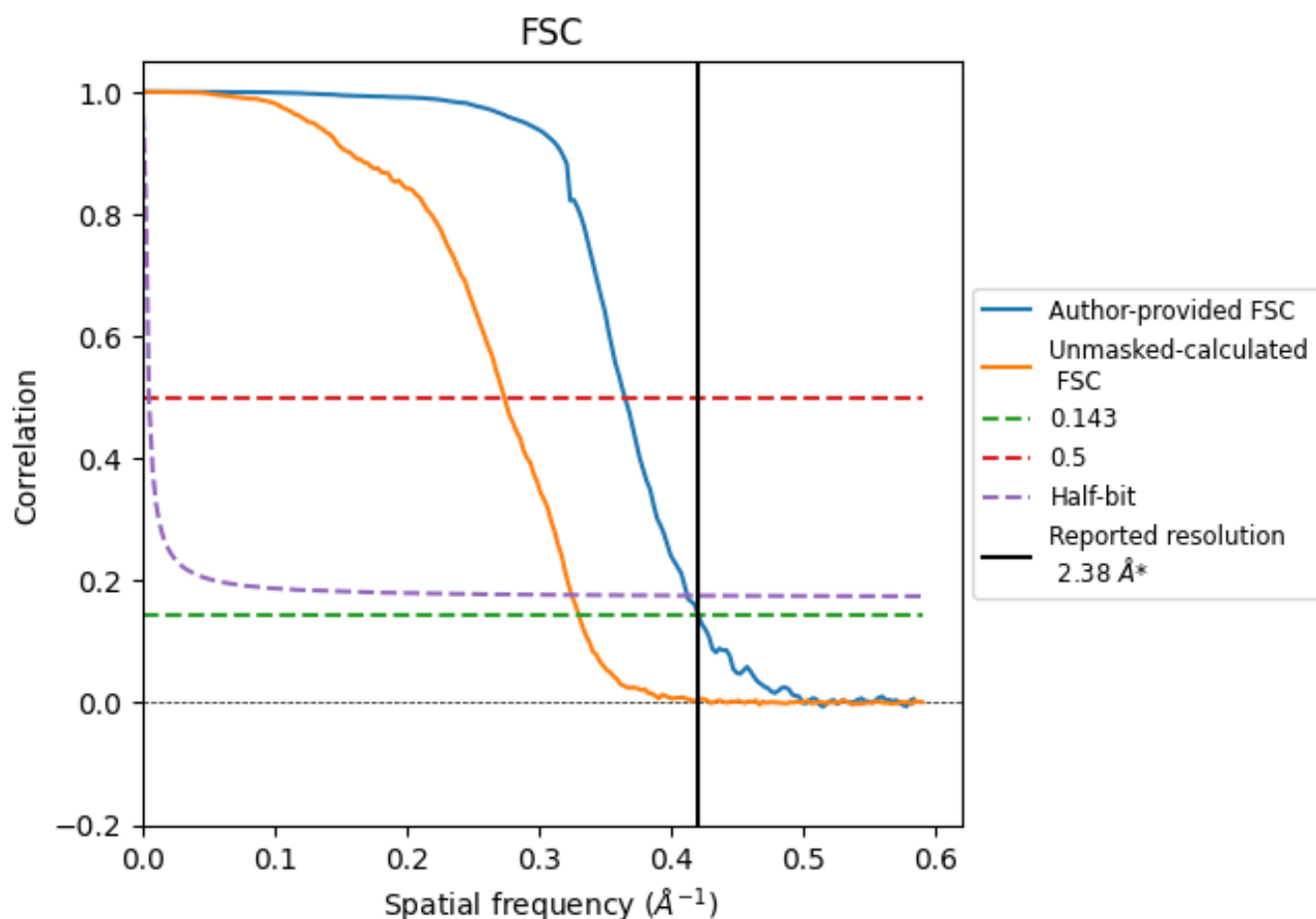


*Reported resolution corresponds to spatial frequency of $0.420 \text{ \AA}^{-1}$

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 0.420 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

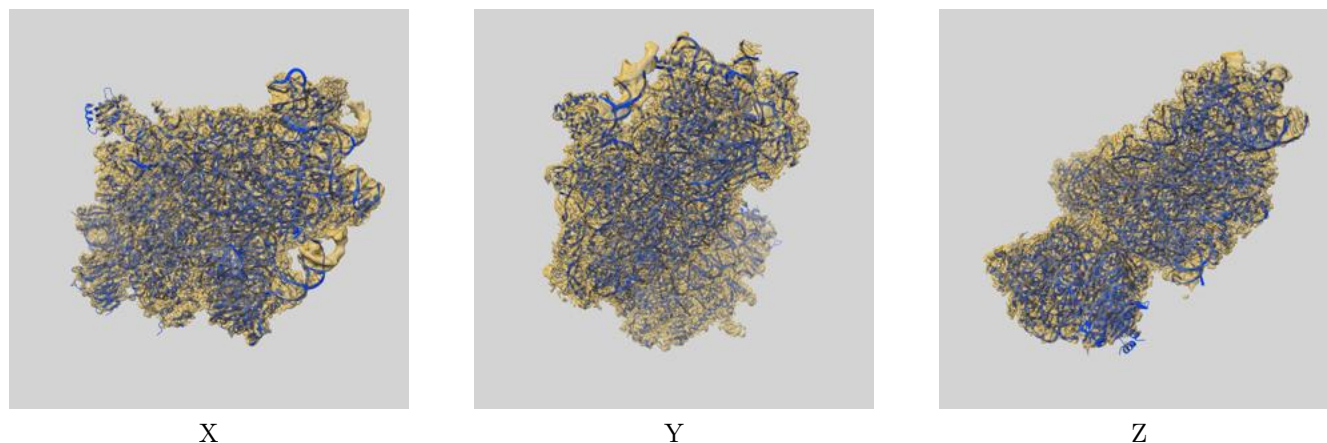
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	2.38	2.74	2.43
Unmasked-calculated*	3.03	3.65	3.08

*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 2.38 by more than 10 %

9 Map-model fit [i](#)

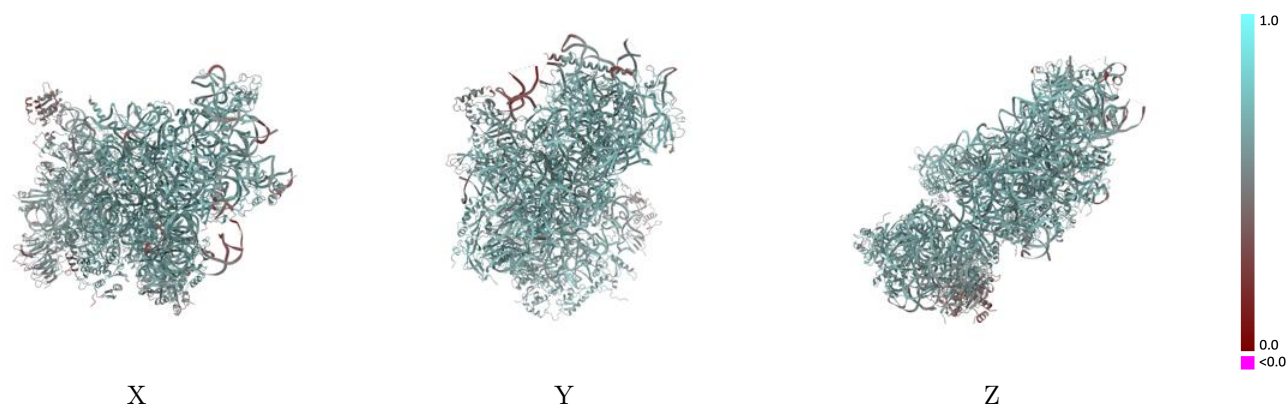
This section contains information regarding the fit between EMDB map EMD-15674 and PDB model 8AUV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



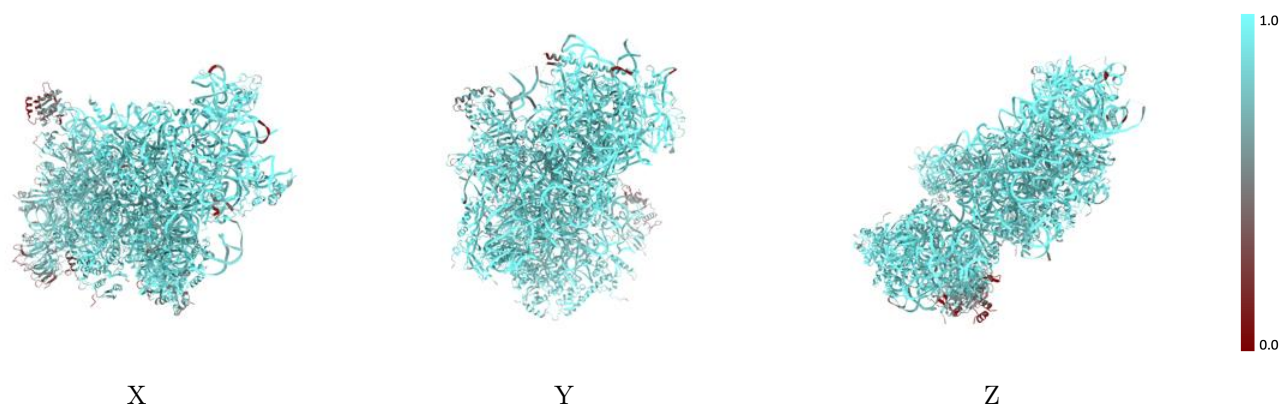
The images above show the 3D surface view of the map at the recommended contour level 0.426 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



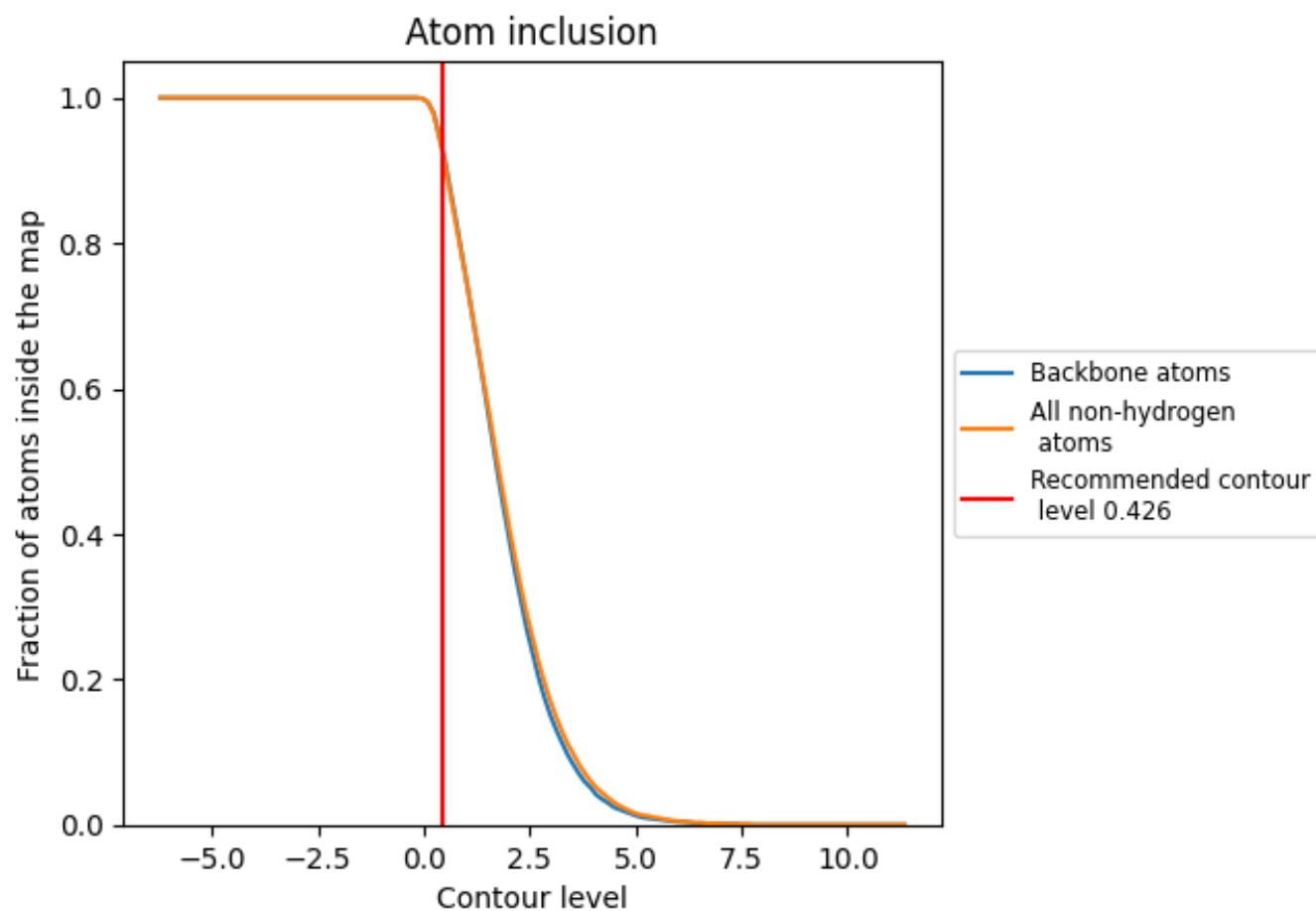
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.426).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.426) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.6220
A	 0.9670	 0.6530
B	 0.8800	 0.5470
C	 0.3740	 0.3990
D	 0.8060	 0.5530
E	 0.9670	 0.6350
F	 0.9620	 0.6480
G	 0.9250	 0.6170
H	 0.9320	 0.6210
I	 0.8940	 0.5860
J	 0.9630	 0.6630
K	 0.9120	 0.6070
L	 0.8940	 0.5850
M	 0.9290	 0.6230
N	 0.5330	 0.4480
O	 0.8090	 0.5630
P	 0.9480	 0.6440
Q	 0.6600	 0.4980
R	 0.8200	 0.5820
S	 0.9580	 0.6480
T	 0.9800	 0.6820
U	 0.9430	 0.6210
V	 0.9860	 0.6620
W	 0.9660	 0.6520
X	 0.9820	 0.6710
Y	 0.9160	 0.6000
Z	 0.9480	 0.6370
a	 0.8840	 0.5890
b	 0.9520	 0.6360
c	 0.9690	 0.6640
d	 0.9330	 0.6190
e	 0.9890	 0.6840
f	 0.9470	 0.6290
h	 0.9720	 0.6340
k	 0.8970	 0.6000
l	 0.8790	 0.5760

