



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 06:22 am BST

PDB ID : 8PPK / pdb_00008ppk
EMDB ID : EMD-17804
Title : Bat-Hp-CoV Nsp1 and eIF1 bound to the human 40S small ribosomal subunit
Authors : Schubert, K.; Karousis, E.D.; Ban, I.; Lapointe, C.P.; Leibundgut, M.; Baeumlin, E.; Kummerant, E.; Scaiola, A.; Schoenhut, T.; Ziegelmueller, J.; Puglisi, J.D.; Muehlemann, O.; Ban, N.
Deposited on : 2023-07-07
Resolution : 2.98 Å(reported)
Based on initial models : 6ZOL, 6ZOK

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:

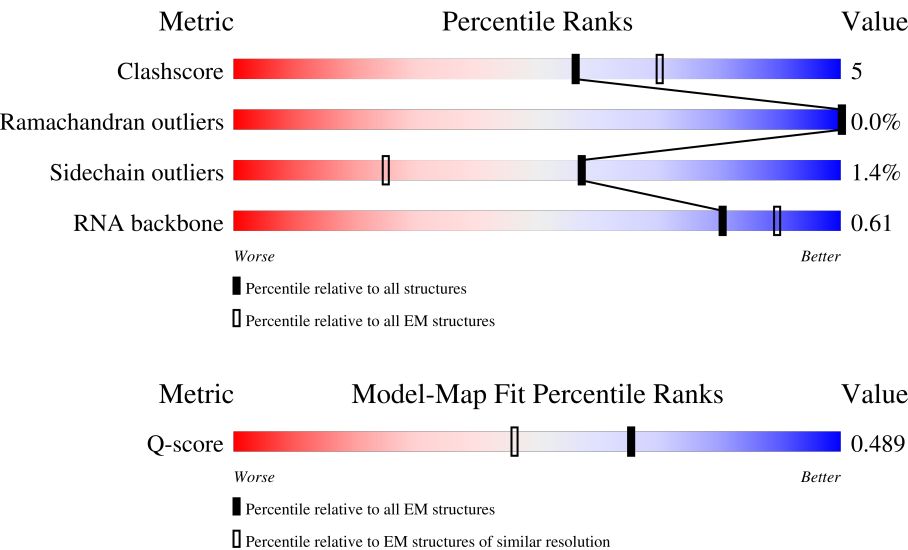
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

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

The reported resolution of this entry is 2.98 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.



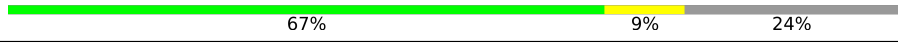
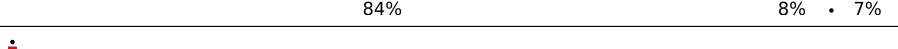
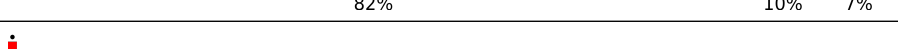
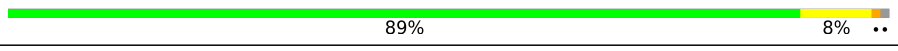
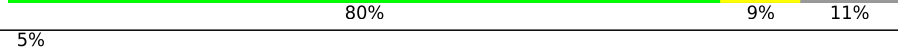
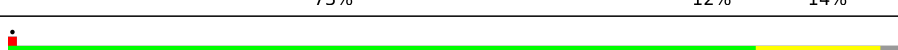
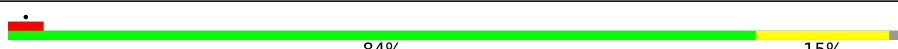
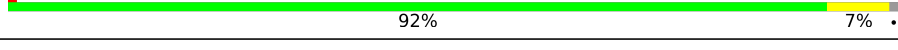
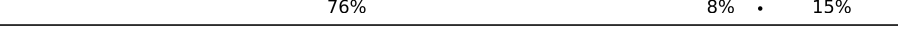
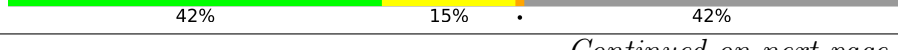
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	p	113	
2	2	1869	
3	A	295	

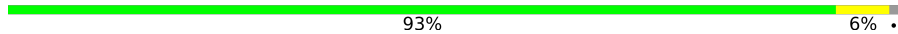
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Mol	Chain	Length	Quality of chain
4	B	264	
5	C	293	
6	D	243	
7	E	263	
8	F	204	
9	G	249	
10	H	194	
11	I	208	
12	J	194	
13	K	165	
14	L	158	
15	M	132	
16	N	151	
17	O	151	
18	P	145	
19	Q	146	
20	R	135	
21	S	152	
22	T	145	
23	U	119	
24	V	83	
25	W	130	
26	X	143	
27	Y	133	
28	Z	125	

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Mol	Chain	Length	Quality of chain
29	a	115	
30	b	84	
31	c	69	
32	d	56	
33	e	133	
34	f	156	
35	g	317	
36	h	25	
37	j	188	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 79548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	85	Total	C	N	O	S	0	0
			691	438	125	126	2		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1771	Total	C	N	O	P	0	0
			37855	16922	6786	12376	1771		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	223	Total	C	N	O	S	1	0
			1741	1124	300	307	10		

- Molecule 6 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 7 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 9 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	189	Total	C	N	O	S	0	0
			1523	972	280	270	1		

- Molecule 11 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 12 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 13 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 14 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	155	Total	C	N	O	S	0	0
			1267	807	237	217	6		

- Molecule 15 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 16 is a protein called 40S ribosomal protein S13.

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

- Molecule 17 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	modified residue	UNP P62263

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	124	Total	C	N	O	S	0	0
			1016	644	192	173	7		

- Molecule 19 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 20 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	145	Total	C	N	O	S	0	0
			1200	753	242	204	1		

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	144	Total	C	N	O	S	0	0
			1123	704	217	199	3		

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 24 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 25 is a protein called 40S ribosomal protein S15a.

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

- Molecule 26 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 29 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 30 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 31 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 32 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 33 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 36 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 37 is a protein called Nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	174	Total	C	N	O	S	0	0
			1363	867	239	253	4		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-13	MET	-	initiating methionine	UNP A0A088DIE1
j	-12	HIS	-	expression tag	UNP A0A088DIE1
j	-11	HIS	-	expression tag	UNP A0A088DIE1
j	-10	HIS	-	expression tag	UNP A0A088DIE1
j	-9	HIS	-	expression tag	UNP A0A088DIE1
j	-8	HIS	-	expression tag	UNP A0A088DIE1
j	-7	HIS	-	expression tag	UNP A0A088DIE1
j	-6	GLU	-	expression tag	UNP A0A088DIE1
j	-5	ASN	-	expression tag	UNP A0A088DIE1
j	-4	LEU	-	expression tag	UNP A0A088DIE1
j	-3	TYR	-	expression tag	UNP A0A088DIE1
j	-2	PHE	-	expression tag	UNP A0A088DIE1
j	-1	GLN	-	expression tag	UNP A0A088DIE1
j	0	SER	-	expression tag	UNP A0A088DIE1

- Molecule 38 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
38	2	108	Total 108	X 108	0
38	G	1	Total 1	X 1	0
38	H	1	Total 1	X 1	0
38	I	1	Total 1	X 1	0
38	J	1	Total 1	X 1	0
38	L	1	Total 1	X 1	0
38	N	1	Total 1	X 1	0
38	O	2	Total 2	X 2	0
38	X	1	Total 1	X 1	0

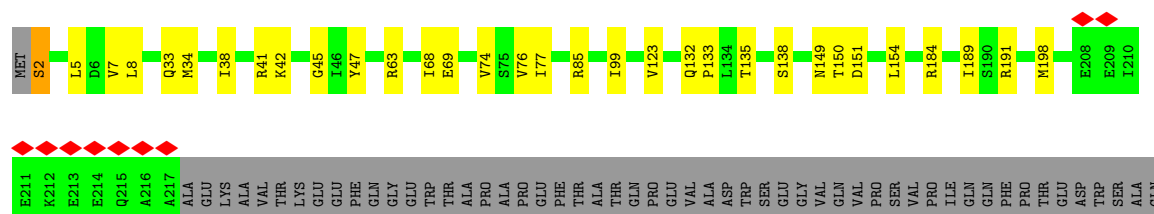
- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	2	110	Total 110	Mg 110	0
39	X	1	Total 1	Mg 1	0

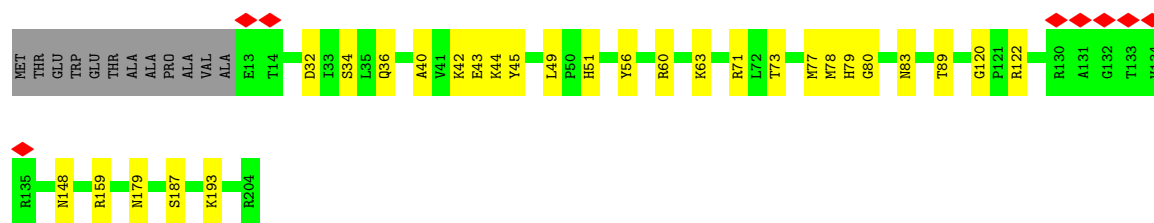
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	a	1	Total 1	Zn 1	0
40	d	1	Total 1	Zn 1	0
40	f	1	Total 1	Zn 1	0

- Molecule 3: 40S ribosomal protein SA

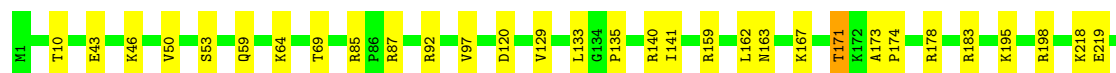


Chain F:  80% 14% 6%



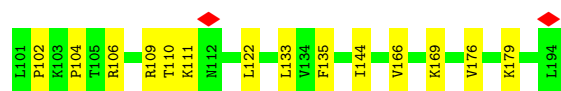
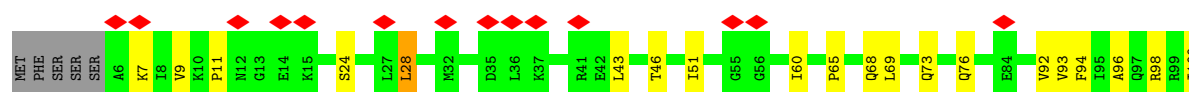
- Molecule 9: 40S ribosomal protein S6

Chain G: 82% 14%



- Molecule 10: 40S ribosomal protein S7

Chain H: 8% 80% 17%



- Molecule 11: 40S ribosomal protein S8

Chain I: 88% 11%



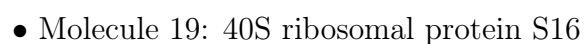
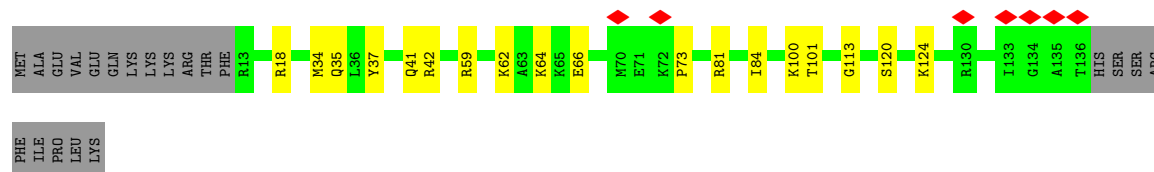
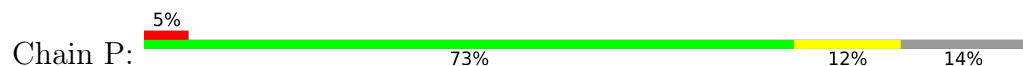
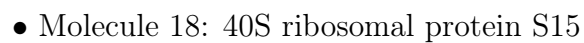
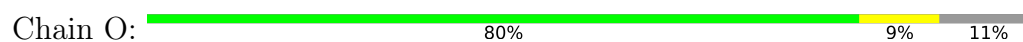
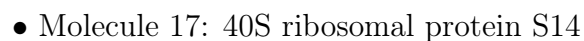
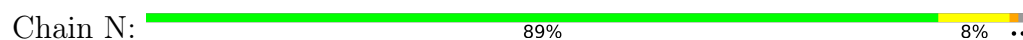
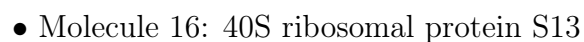
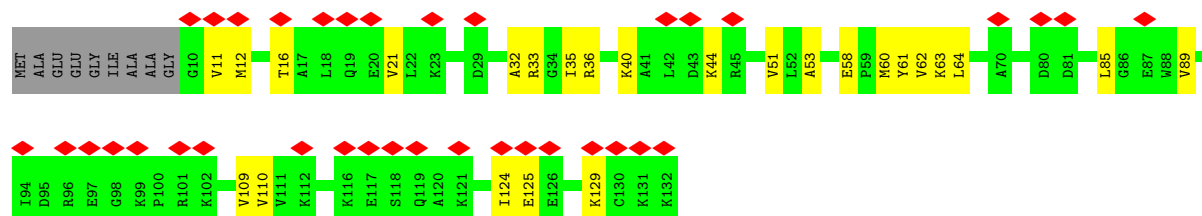
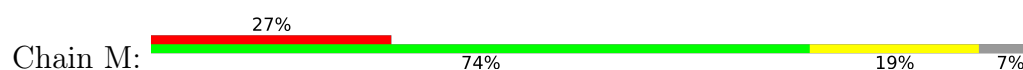
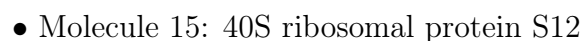
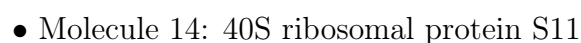
- Molecule 12: 40S ribosomal protein S9

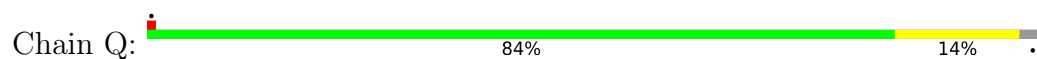
Chain J: 82% 10% 7%



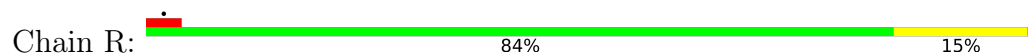
- Molecule 13: 40S ribosomal protein S10

Chain K: 48% 10% 41%

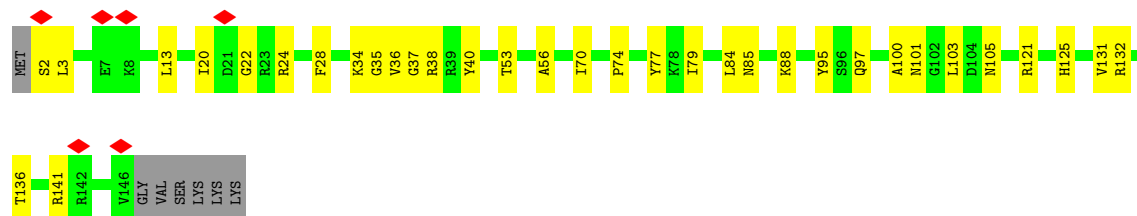




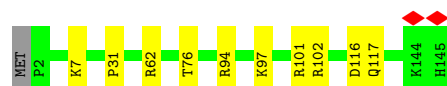
- Molecule 20: 40S ribosomal protein S17



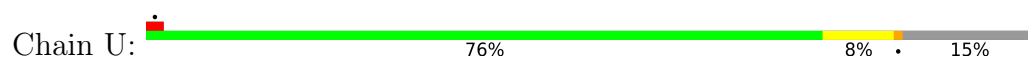
- Molecule 21: Small ribosomal subunit protein uS13



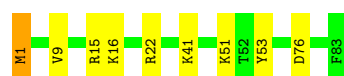
- Molecule 22: Small ribosomal subunit protein eS19



- Molecule 23: 40S ribosomal protein S20



- Molecule 24: 40S ribosomal protein S21



- Molecule 25: 40S ribosomal protein S15a

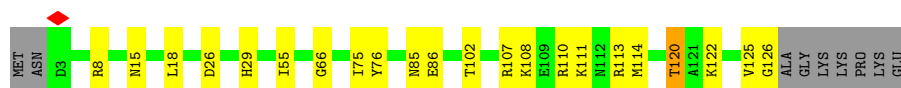
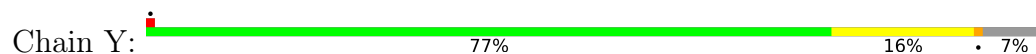




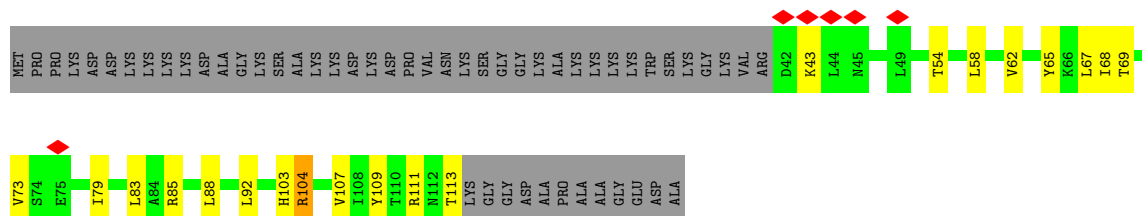
- Molecule 26: 40S ribosomal protein S23



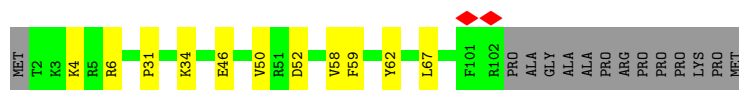
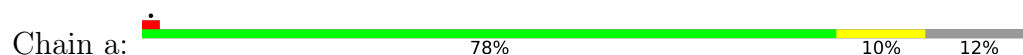
- Molecule 27: 40S ribosomal protein S24



- Molecule 28: 40S ribosomal protein S25



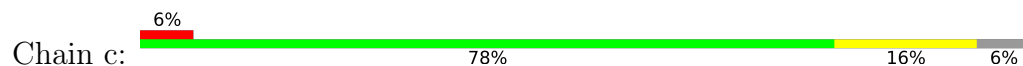
- Molecule 29: 40S ribosomal protein S26



- Molecule 30: 40S ribosomal protein S27



- Molecule 31: 40S ribosomal protein S28





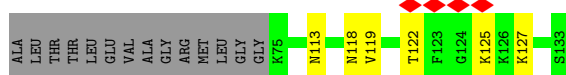
- Molecule 32: 40S ribosomal protein S29

Chain d: 89% 9% .



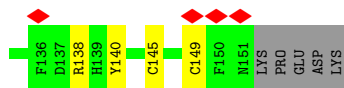
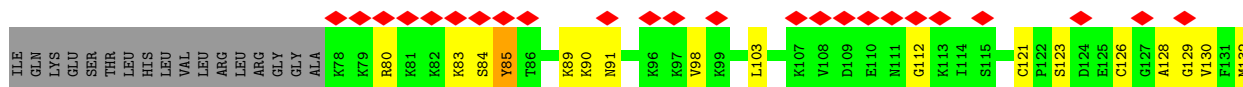
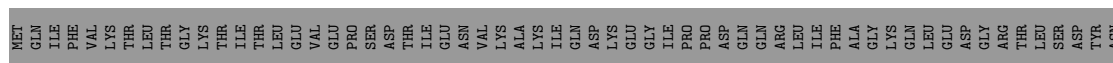
- Molecule 33: Small ribosomal subunit protein eS30

Chain e: 40% 5% 56%



- Molecule 34: Ubiquitin-40S ribosomal protein S27a

Chain f: 18% 34% 13% 53%



- Molecule 35: Receptor of activated protein C kinase 1

Chain g: 83% 15% ..

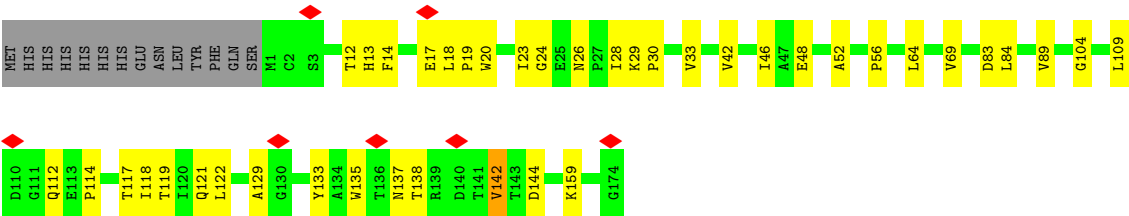


- Molecule 36: 60S ribosomal protein L41

Chain h: 12% 84% 16%



• Molecule 37: Nsp1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.378	Depositor
Minimum map value	-0.548	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IAS, A2M, AME, MG, MA6, OMG, B8N, OMU, G7M, 4AC, SAC, HY3, PSU, UNX, OMC, 6MZ, NMM

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	p	0.07	0/701	0.16	0/936
2	2	0.16	2/40280 (0.0%)	0.17	0/62782
3	A	0.10	0/1736	0.20	0/2359
4	B	0.10	0/1841	0.20	0/2459
5	C	0.11	0/1781	0.21	0/2405
6	D	0.09	0/1780	0.20	0/2397
7	E	0.12	0/2118	0.22	0/2849
8	F	0.08	0/1539	0.24	0/2071
9	G	0.09	0/1968	0.19	0/2619
10	H	0.09	0/1546	0.23	0/2071
11	I	0.10	0/1711	0.20	0/2282
12	J	0.11	0/1524	0.19	0/2035
13	K	0.08	0/840	0.22	0/1133
14	L	0.11	0/1289	0.19	0/1724
15	M	0.07	0/963	0.24	0/1291
16	N	0.10	0/1226	0.21	0/1649
17	O	0.10	0/1014	0.21	0/1358
18	P	0.06	0/1035	0.17	0/1383
19	Q	0.09	0/1146	0.21	0/1534
20	R	0.08	0/1097	0.20	0/1474
21	S	0.07	0/1209	0.20	0/1620
22	T	0.07	0/1130	0.17	0/1513
23	U	0.08	0/813	0.21	0/1092
24	V	0.10	0/635	0.19	0/850
25	W	0.13	0/1051	0.23	0/1406
26	X	0.11	0/1107	0.22	0/1475
27	Y	0.10	0/1031	0.19	0/1370
28	Z	0.09	0/580	0.24	0/780
29	a	0.11	0/828	0.21	0/1109
30	b	0.10	0/664	0.21	0/891
31	c	0.09	0/514	0.21	0/688

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.09	0/469	0.20	0/623
33	e	0.12	0/473	0.26	0/623
34	f	0.34	0/622	0.40	0/822
35	g	0.09	0/2497	0.24	0/3399
36	h	0.08	0/240	0.15	0/305
37	j	0.11	0/1399	0.27	0/1903
All	All	0.14	2/82397 (0.0%)	0.19	0/119280

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	627	OMU	O3'-P	5.17	1.61	1.56
2	2	1639	G7M	O3'-P	5.02	1.61	1.56

There are no bond angle outliers.

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	p	691	0	706	5	0
2	2	37855	0	19186	304	0
3	A	1708	0	1710	20	0
4	B	1815	0	1908	11	0
5	C	1741	0	1827	20	0
6	D	1752	0	1848	15	0
7	E	2076	0	2177	21	0
8	F	1517	0	1569	20	0
9	G	1945	0	2112	26	0
10	H	1523	0	1622	27	0
11	I	1682	0	1769	17	0
12	J	1499	0	1618	12	0
13	K	816	0	841	9	0
14	L	1267	0	1340	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	953	0	990	18	0
16	N	1202	0	1289	9	0
17	O	1010	0	1033	8	0
18	P	1016	0	1066	13	0
19	Q	1128	0	1195	11	0
20	R	1082	0	1137	15	0
21	S	1200	0	1262	22	0
22	T	1123	0	1152	7	0
23	U	803	0	873	5	0
24	V	639	0	638	9	0
25	W	1034	0	1080	12	0
26	X	1099	0	1162	7	0
27	Y	1014	0	1082	15	0
28	Z	574	0	627	12	0
29	a	814	0	863	7	0
30	b	650	0	672	3	0
31	c	512	0	541	7	0
32	d	458	0	448	3	0
33	e	467	0	516	2	0
34	f	610	0	634	19	0
35	g	2440	0	2396	32	0
36	h	239	0	289	3	0
37	j	1363	0	1342	20	0
38	2	108	0	0	0	0
38	G	1	0	0	0	0
38	H	1	0	0	0	0
38	I	1	0	0	0	0
38	J	1	0	0	0	0
38	L	1	0	0	0	0
38	N	1	0	0	0	0
38	O	2	0	0	0	0
38	X	1	0	0	0	0
39	2	110	0	0	0	0
39	X	1	0	0	0	0
40	a	1	0	0	0	0
40	d	1	0	0	0	0
40	f	1	0	0	0	0
All	All	79548	0	62520	641	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 5.

All (641) 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)
2:2:1091:C:HO2'	25:W:2:VAL:N	1.71	0.88
2:2:229:A:H62	2:2:887:U:H3	1.29	0.77
35:g:191:HIS:HE2	35:g:209:SER:HG	1.33	0.74
9:G:64:LYS:HB2	9:G:97:VAL:HG11	1.68	0.73
31:c:7:GLN:HE22	31:c:61:SER:H	1.37	0.72
2:2:512:A2M:HM'2	2:2:513:G:H5'	1.73	0.71
2:2:1842:4AC:O7	36:h:4:LYS:NZ	2.23	0.69
10:H:93:VAL:HG11	10:H:133:LEU:HD12	1.75	0.69
2:2:462:OMC:HM22	2:2:463:C:H5'	1.75	0.69
2:2:496:C:OP1	7:E:49:ARG:NH2	2.26	0.68
22:T:76:THR:HG22	22:T:94:ARG:HB3	1.76	0.68
2:2:1490:OMG:HM22	2:2:1491:G:H5'	1.75	0.67
2:2:798:G:H4'	10:H:110:THR:HG21	1.77	0.67
2:2:170:A:OP2	9:G:140:ARG:NH1	2.28	0.66
2:2:576:A2M:HM'2	2:2:577:U:H5'	1.77	0.66
35:g:87:LEU:HB2	35:g:101:PHE:HB2	1.77	0.66
35:g:11:LEU:HB2	35:g:307:VAL:HB	1.77	0.66
5:C:259:THR:HG21	24:V:16:LYS:H	1.60	0.66
2:2:436:OMG:HM22	2:2:437:G:H5'	1.78	0.66
35:g:40:ILE:HB	35:g:59:LEU:HB2	1.77	0.66
37:j:12:THR:HG23	37:j:135:TRP:HZ3	1.60	0.66
11:I:141:ARG:HB2	11:I:146:GLN:HG2	1.78	0.66
15:M:51:VAL:HB	15:M:109:VAL:HB	1.78	0.66
2:2:1677:U:H2'	2:2:1678:A2M:H8	1.76	0.66
2:2:1703:OMC:HM22	2:2:1704:C:H5'	1.78	0.66
9:G:230:LYS:O	9:G:234:LEU:N	2.26	0.66
2:2:126:G:OP2	9:G:195:LYS:NZ	2.28	0.65
4:B:63:LYS:HE3	4:B:90:ASP:HA	1.77	0.65
9:G:135:PRO:HG2	9:G:141:ILE:HD13	1.79	0.65
2:2:928:G:H1	2:2:1013:U:H3	1.42	0.64
2:2:1147:C:OP1	29:a:6:ARG:NH1	2.30	0.64
20:R:17:ILE:HG13	20:R:57:LEU:HD23	1.77	0.64
2:2:752:G:N2	2:2:792:C:O2	2.30	0.64
2:2:1017:U:OP1	16:N:62:GLN:NE2	2.31	0.64
21:S:101:ASN:O	21:S:105:ASN:ND2	2.30	0.64
2:2:547:G:H1'	2:2:548:C:H5''	1.78	0.64
2:2:1030:A:H2'	2:2:1031:A2M:H8	1.80	0.64
2:2:1239:U:H5''	18:P:124:LYS:HD3	1.79	0.63
16:N:99:ARG:NH2	16:N:119:GLU:OE2	2.30	0.63
2:2:1348:G:OP2	2:2:1348:G:N2	2.28	0.63
2:2:1565:C:OP2	22:T:101:ARG:NH1	2.31	0.63
2:2:282:G:H2'	2:2:283:G:O4'	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:165:G:OP2	2:2:165:G:N2	2.31	0.63
18:P:62:LYS:NZ	18:P:66:GLU:OE2	2.32	0.63
3:A:184:ARG:HD2	3:A:191:ARG:HG2	1.81	0.63
7:E:100:ARG:NH2	7:E:121:TYR:O	2.32	0.63
2:2:1570:G:N7	22:T:97:LYS:NZ	2.43	0.62
10:H:69:LEU:HD22	10:H:96:ALA:HB2	1.81	0.62
35:g:256:ILE:HB	35:g:270:LEU:HB2	1.81	0.62
18:P:41:GLN:NE2	18:P:113:GLY:O	2.33	0.62
2:2:1597:C:OP2	28:Z:85:ARG:NH2	2.32	0.62
31:c:44:ARG:NH2	31:c:60:GLU:O	2.33	0.61
2:2:1327:G:O2'	34:f:80:ARG:NH2	2.32	0.61
2:2:1507:G:N2	34:f:85:TYR:HB2	2.16	0.61
23:U:33:GLU:OE2	23:U:87:ARG:NH1	2.33	0.61
2:2:799:OMU:HM22	2:2:800:U:H5'	1.82	0.61
2:2:1383:A2M:HM'2	2:2:1384:C:H5'	1.82	0.61
2:2:1445:PSU:O2	2:2:1446:A:N6	2.33	0.61
12:J:136:ARG:HD3	12:J:160:SER:HA	1.83	0.61
2:2:1314:U:O2'	13:K:8:ARG:NH1	2.32	0.61
2:2:1528:G:O2'	2:2:1666:C:OP1	2.17	0.61
16:N:55:ARG:NH1	16:N:56:ASP:OD1	2.34	0.61
18:P:41:GLN:HG3	18:P:84:ILE:HD13	1.81	0.61
2:2:1153:C:OP2	25:W:71:LYS:NZ	2.31	0.60
3:A:85:ARG:NH2	20:R:82:ASP:O	2.34	0.60
6:D:179:GLN:HE22	37:j:142:VAL:HB	1.66	0.60
19:Q:5:GLY:O	19:Q:27:ARG:NH1	2.33	0.60
35:g:120:ILE:HB	35:g:132:TRP:HB2	1.82	0.60
11:I:101:ILE:HD12	11:I:190:LEU:HD11	1.83	0.60
21:S:13:LEU:HB2	21:S:20:ILE:HB	1.83	0.60
2:2:736:C:H2'	2:2:737:G:C8	2.36	0.60
2:2:1617:G:N1	2:2:1620:A:OP2	2.34	0.60
2:2:1060:A:O2'	2:2:1062:A:N7	2.30	0.60
10:H:104:PRO:O	10:H:109:ARG:NH1	2.35	0.60
37:j:13:HIS:HB3	37:j:121:GLN:HB3	1.83	0.60
2:2:70:G:OP2	9:G:167:LYS:NZ	2.35	0.59
2:2:145:G:O6	9:G:178:ARG:NH2	2.35	0.59
2:2:166:A2M:HM'2	2:2:167:G:H5'	1.84	0.59
6:D:175:VAL:HG13	6:D:182:LEU:HB3	1.84	0.59
2:2:1550:G:H3'	2:2:1579:A:H61	1.67	0.59
12:J:107:GLU:O	12:J:113:GLN:NE2	2.33	0.59
15:M:44:LYS:HD3	34:f:128:ALA:HB3	1.83	0.59
2:2:799:OMU:H5	10:H:109:ARG:HE	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:693:A:H2'	2:2:694:G:C8	2.37	0.58
2:2:370:G:O2'	11:I:10:LYS:NZ	2.31	0.58
34:f:121:CYS:HA	34:f:132:MET:HE3	1.84	0.58
7:E:174:LYS:O	7:E:179:ASN:ND2	2.37	0.58
35:g:215:GLN:HG3	35:g:231:ASP:HA	1.85	0.58
2:2:792:C:H2'	2:2:793:G:H8	1.69	0.58
3:A:42:LYS:NZ	20:R:99:ASP:OD2	2.30	0.58
33:e:125:LYS:HZ1	33:e:127:LYS:HG2	1.68	0.58
2:2:1118:C:O2'	30:b:75:GLU:OE1	2.19	0.58
2:2:206:G:O6	11:I:144:LYS:NZ	2.35	0.58
2:2:538:U:H2'	2:2:539:C:C6	2.39	0.58
2:2:1354:G:N2	2:2:1357:A:OP2	2.35	0.58
9:G:10:THR:HA	9:G:129:VAL:HG12	1.84	0.58
18:P:35:GLN:O	21:S:88:LYS:NZ	2.35	0.58
2:2:468:A2M:HM'2	2:2:469:A:H5'	1.86	0.58
2:2:1391:OMC:HM22	2:2:1392:U:H5'	1.86	0.58
2:2:1601:A:OP1	28:Z:43:LYS:NZ	2.34	0.57
25:W:6:VAL:HG12	25:W:34:ILE:HD11	1.87	0.57
27:Y:55:ILE:HG13	27:Y:75:ILE:HG12	1.86	0.57
2:2:509:OMG:HM22	2:2:510:G:H5'	1.86	0.57
4:B:108:ASP:OD1	4:B:108:ASP:N	2.36	0.57
24:V:22:ARG:NH2	25:W:19:LYS:O	2.38	0.57
2:2:1241:A:HO2'	2:2:1266:C:HO2'	1.51	0.57
2:2:835:C:H4'	2:2:836:G:N7	2.20	0.56
2:2:1447:OMG:HM22	2:2:1448:A:H5'	1.86	0.56
35:g:165:ILE:HG13	35:g:177:TRP:HB2	1.87	0.56
2:2:387:C:OP2	11:I:10:LYS:NZ	2.39	0.56
2:2:1863:A:OP2	29:a:4:LYS:NZ	2.35	0.56
21:S:36:VAL:HG13	21:S:40:TYR:HD2	1.69	0.56
6:D:42:THR:OG1	6:D:45:ARG:O	2.22	0.56
35:g:107:ASP:OD2	35:g:125:ARG:NH1	2.39	0.56
2:2:1241:A:O2'	2:2:1266:C:O2'	2.21	0.56
8:F:78:MET:HB3	8:F:79:HIS:HD2	1.70	0.56
35:g:88:ARG:HE	35:g:100:ARG:HH11	1.53	0.56
4:B:33:VAL:HA	4:B:96:CYS:HB2	1.88	0.56
17:O:28:PHE:HZ	29:a:58:VAL:HG21	1.71	0.56
2:2:1606:G:H22	2:2:1632:G:H1'	1.71	0.56
35:g:266:ILE:HD11	35:g:269:GLU:HB2	1.88	0.56
21:S:34:LYS:HG2	21:S:103:LEU:HD23	1.88	0.55
16:N:63:VAL:HG21	16:N:71:ILE:HD11	1.87	0.55
2:2:601:OMG:HM22	2:2:602:G:H5'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1098:C:H2'	2:2:1099:G:C8	2.40	0.55
2:2:792:C:H2'	2:2:793:G:C8	2.42	0.55
19:Q:53:GLU:OE1	19:Q:85:ARG:NH2	2.39	0.55
15:M:12:MET:HG3	15:M:16:THR:HB	1.89	0.55
2:2:925:G:H1	2:2:1017:U:H3	1.53	0.55
7:E:124:CYS:HB3	7:E:141:THR:HB	1.89	0.55
35:g:215:GLN:NE2	35:g:231:ASP:OD1	2.36	0.55
2:2:453:C:O2'	9:G:92:ARG:O	2.20	0.55
2:2:74:G:N2	2:2:74:G:OP2	2.39	0.55
2:2:234:C:H42	2:2:894:G:H1	1.55	0.55
34:f:83:LYS:C	34:f:85:TYR:H	2.14	0.55
2:2:677:G:N1	2:2:1027:A:OP2	2.26	0.54
2:2:834:C:O2	2:2:838:G:N2	2.38	0.54
2:2:377:G:H5'	11:I:98:LYS:HB3	1.88	0.54
21:S:24:ARG:HH21	21:S:28:PHE:HB3	1.72	0.54
23:U:78:ASP:OD2	32:d:44:ARG:NH1	2.40	0.54
2:2:1400:U:O4	2:2:1401:A:N6	2.40	0.54
9:G:228:ILE:HG12	9:G:231:ARG:HH21	1.71	0.54
35:g:220:ASP:HB2	35:g:227:LEU:HD21	1.90	0.54
2:2:690:G:N2	2:2:741:C:O2	2.41	0.54
2:2:1285:G:H5'	15:M:35:ILE:HG22	1.88	0.54
2:2:1344:A:N1	2:2:1385:G:O2'	2.37	0.54
4:B:123:ALA:HB2	4:B:165:ARG:HG3	1.90	0.53
6:D:40:ARG:NH2	6:D:47:GLU:OE1	2.42	0.53
2:2:551:U:H2'	2:2:552:G:H8	1.73	0.53
6:D:32:ASP:OD2	6:D:65:ARG:NH1	2.41	0.53
6:D:38:GLU:HB3	6:D:49:ILE:HB	1.90	0.53
8:F:40:ALA:HB1	8:F:45:TYR:CG	2.43	0.53
2:2:1005:G:OP2	4:B:162:ARG:NH1	2.41	0.53
9:G:234:LEU:HA	9:G:237:LEU:HB2	1.90	0.53
26:X:68:LYS:HB3	26:X:91:LEU:HD22	1.90	0.53
35:g:122:SER:OG	35:g:132:TRP:NE1	2.37	0.53
2:2:847:A:O2'	7:E:106:LYS:NZ	2.41	0.53
9:G:85:ARG:O	9:G:87:ARG:NH1	2.42	0.53
28:Z:73:VAL:HG21	28:Z:88:LEU:HD11	1.89	0.53
30:b:65:GLN:HE21	30:b:72:ARG:HD2	1.73	0.53
2:2:893:U:H2'	2:2:894:G:C8	2.44	0.53
35:g:304:ASP:O	35:g:305:ASN:ND2	2.42	0.53
11:I:81:VAL:HG22	11:I:102:VAL:HG12	1.90	0.53
15:M:40:LYS:HG3	34:f:129:GLY:HA3	1.90	0.53
15:M:64:LEU:HD22	34:f:103:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:34:PHE:HB3	17:O:41:PHE:HB2	1.91	0.52
2:2:1763:G:H2'	2:2:1764:G:C8	2.44	0.52
2:2:664:A:O2'	2:2:670:A:N1	2.38	0.52
2:2:887:U:H2'	2:2:888:U:C6	2.44	0.52
13:K:31:LYS:HA	13:K:41:PRO:HA	1.90	0.52
17:O:53:ILE:HG23	17:O:88:LEU:HD12	1.91	0.52
2:2:1310:U:H5''	34:f:130:VAL:HG13	1.90	0.52
9:G:159:ARG:HG2	9:G:173:ALA:HB2	1.91	0.52
2:2:126:G:OP1	9:G:198:ARG:NH1	2.43	0.52
2:2:186:C:H2'	2:2:187:G:C8	2.45	0.52
2:2:1751:C:O2	2:2:1782:G:N2	2.42	0.52
37:j:52:ALA:HB2	37:j:109:LEU:HD13	1.90	0.52
2:2:1033:G:N1	2:2:1080:A:O2'	2.34	0.52
2:2:1524:G:OP2	21:S:141:ARG:NH1	2.42	0.52
4:B:77:ASP:OD1	4:B:77:ASP:N	2.43	0.52
8:F:49:LEU:HD12	19:Q:50:LYS:HG2	1.91	0.52
2:2:1261:C:O2	32:d:10:HIS:NE2	2.40	0.52
2:2:1313:A:OP2	15:M:33:ARG:NH2	2.43	0.52
2:2:745:C:H4'	10:H:111:LYS:HE3	1.92	0.52
2:2:1762:C:H2'	2:2:1763:G:C8	2.45	0.52
2:2:1841:C:H2'	2:2:1842:4AC:H6	1.91	0.52
5:C:254:ASP:HB2	24:V:1:AME:HT22	1.92	0.52
3:A:77:ILE:HG12	3:A:99:ILE:HB	1.92	0.51
35:g:31:ILE:HB	35:g:43:TRP:HB2	1.92	0.51
1:p:105:ASP:OD1	1:p:105:ASP:N	2.42	0.51
2:2:1274:G:O4'	13:K:47:LYS:NZ	2.42	0.51
2:2:1315:U:H4'	13:K:2:LEU:HD12	1.93	0.51
2:2:1427:C:OP1	22:T:7:LYS:NZ	2.42	0.51
2:2:1648:G:O2'	2:2:1674:G:O6	2.27	0.51
17:O:95:ILE:HG21	17:O:116:LEU:HD12	1.93	0.51
2:2:17:C:O2'	2:2:1194:A:N1	2.41	0.51
2:2:641:A:OP1	12:J:40:LYS:NZ	2.43	0.51
2:2:1606:G:N2	2:2:1632:G:H1'	2.24	0.51
2:2:1779:G:H2'	2:2:1780:G:C8	2.45	0.51
9:G:218:LYS:NZ	9:G:219:GLU:OE2	2.44	0.51
21:S:22:GLY:HA2	21:S:56:ALA:HB3	1.92	0.51
35:g:68:ASP:HB3	35:g:111:VAL:HG12	1.92	0.51
37:j:69:VAL:HG22	37:j:89:VAL:HG22	1.90	0.51
2:2:227:U:N3	2:2:886:A:O2'	2.43	0.51
2:2:860:G:N2	25:W:107:SER:OG	2.43	0.51
2:2:1351:G:O2'	2:2:1378:A:N1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1521:C:OP2	21:S:136:THR:OG1	2.27	0.51
2:2:799:OMU:H5	10:H:109:ARG:NE	2.26	0.50
7:E:246:LEU:HB3	7:E:250:GLU:HG3	1.93	0.50
2:2:1662:U:O4	2:2:1663:A:N6	2.43	0.50
37:j:28:ILE:HD13	37:j:64:LEU:HD23	1.93	0.50
3:A:38:ILE:HD11	3:A:47:TYR:HB3	1.93	0.50
3:A:184:ARG:HG2	3:A:189:ILE:HG13	1.93	0.50
7:E:100:ARG:HG2	7:E:102:ILE:HG12	1.92	0.50
2:2:1430:C:H3'	2:2:1431:G:H21	1.77	0.50
4:B:2:ALA:N	17:O:62:VAL:O	2.45	0.50
5:C:187[A]:ARG:HD3	5:C:192:LEU:HD12	1.93	0.50
18:P:81:ARG:NH1	18:P:120:SER:OG	2.43	0.50
2:2:873:G:H4'	2:2:874:G:OP2	2.11	0.50
3:A:149:ASN:OD1	3:A:150:THR:N	2.39	0.50
2:2:121:OMU:HM22	2:2:122:G:H5'	1.94	0.50
2:2:1124:C:H5''	4:B:150:ILE:HG12	1.93	0.50
9:G:43:GLU:HA	9:G:46:LYS:HE3	1.93	0.50
37:j:18:LEU:HD21	37:j:46:ILE:HG23	1.92	0.50
4:B:105:LEU:HD13	4:B:213:ARG:HA	1.94	0.50
37:j:109:LEU:HD21	37:j:114:PRO:HG3	1.94	0.50
37:j:29:LYS:HD2	37:j:30:PRO:HD2	1.93	0.49
1:p:76:HIS:N	1:p:80:GLY:O	2.42	0.49
2:2:520:A:O2'	2:2:825:A:N3	2.42	0.49
2:2:689:U:C4	2:2:690:G:H1'	2.47	0.49
2:2:517:OMC:HM22	2:2:518:G:H5'	1.93	0.49
28:Z:68:ILE:HB	28:Z:109:TYR:HB2	1.94	0.49
2:2:1154:U:OP2	5:C:187[B]:ARG:NH2	2.45	0.49
2:2:551:U:H2'	2:2:552:G:C8	2.47	0.49
14:L:111:VAL:HG12	14:L:140:PHE:HB2	1.95	0.49
27:Y:113:ARG:NH2	27:Y:126:GLY:O	2.45	0.49
2:2:206:G:H2'	2:2:207:G:H8	1.77	0.49
5:C:209:VAL:HB	5:C:210:PRO:HD3	1.95	0.49
12:J:114:VAL:HG13	12:J:119:LEU:HB2	1.94	0.49
2:2:799:OMU:H5''	10:H:109:ARG:HB3	1.93	0.49
17:O:45:THR:HG22	17:O:52:THR:HA	1.95	0.49
27:Y:110:ARG:NH1	27:Y:125:VAL:O	2.41	0.49
37:j:17:GLU:HA	37:j:119:THR:HA	1.95	0.49
2:2:559:G:O2'	2:2:560:A:H5''	2.12	0.49
2:2:581:U:H4'	27:Y:66:GLY:HA2	1.95	0.49
2:2:867:G:H1	10:H:109:ARG:HH21	1.60	0.49
2:2:1763:G:H2'	2:2:1764:G:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:199:PRO:HG2	12:J:58:ARG:HE	1.78	0.49
10:H:166:VAL:HG12	10:H:169:LYS:HD3	1.94	0.49
2:2:122:G:H21	7:E:146:THR:HG21	1.78	0.49
2:2:868:G:OP2	2:2:868:G:N2	2.31	0.49
2:2:1726:G:H1	2:2:1808:U:H3	1.60	0.49
2:2:1630:A:H5''	21:S:37:GLY:H	1.77	0.48
19:Q:19:ALA:HB2	19:Q:75:GLY:HA3	1.94	0.48
2:2:1804:OMU:HM22	2:2:1805:G:H5'	1.95	0.48
35:g:233:GLY:HA3	35:g:252:THR:HG21	1.95	0.48
2:2:191:A:H3'	2:2:192:C:H5''	1.95	0.48
2:2:736:C:H2'	2:2:737:G:H8	1.76	0.48
4:B:104:ASP:OD1	4:B:105:LEU:N	2.46	0.48
5:C:169:TYR:OH	5:C:175:GLY:O	2.31	0.48
21:S:34:LYS:HB3	21:S:100:ALA:HA	1.95	0.48
27:Y:18:LEU:O	27:Y:85:ASN:ND2	2.47	0.48
2:2:436:OMG:OP2	2:2:471:G:O2'	2.30	0.48
2:2:1232:PSU:H2'	2:2:1233:G:C8	2.49	0.48
2:2:1272:OMC:HM22	2:2:1273:C:H5'	1.95	0.48
7:E:11:ARG:HA	7:E:28:ALA:HB2	1.95	0.48
10:H:106:ARG:HA	10:H:109:ARG:HB2	1.95	0.48
2:2:282:G:OP2	2:2:890:U:H5''	2.13	0.48
3:A:2:SAC:OAC	3:A:63:ARG:NH2	2.45	0.48
2:2:1271:C:H2'	2:2:1272:OMC:H6	1.79	0.48
2:2:1395:C:H1'	2:2:1474:A:C4	2.49	0.48
10:H:51:ILE:HD11	10:H:176:VAL:HG22	1.95	0.48
15:M:58:GLU:HG3	15:M:61:TYR:H	1.79	0.48
19:Q:98:LYS:O	35:g:57:ARG:NH1	2.40	0.48
25:W:80:ASP:OD1	25:W:124:LYS:NZ	2.46	0.48
37:j:14:PHE:CZ	37:j:122:LEU:HB2	2.49	0.48
2:2:751:G:H2'	2:2:752:G:C8	2.49	0.48
2:2:1386:A:OP2	6:D:160:SER:OG	2.31	0.48
23:U:49:LYS:HE3	23:U:92:HIS:HB2	1.95	0.48
2:2:280:G:H2'	2:2:281:C:C5	2.49	0.47
2:2:690:G:H2'	2:2:691:G:C8	2.49	0.47
10:H:60:ILE:HB	10:H:92:VAL:HG22	1.95	0.47
14:L:22:ARG:HH22	14:L:31:GLU:HA	1.78	0.47
20:R:31:ASN:ND2	20:R:55:THR:OG1	2.40	0.47
2:2:1679:A:OP1	31:c:20:ARG:NH2	2.46	0.47
35:g:163:PRO:HB2	35:g:179:LEU:HB3	1.95	0.47
2:2:96:C:H1'	2:2:474:G:H5'	1.95	0.47
2:2:546:G:O2'	2:2:548:C:OP1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:11:ARG:O	14:L:136:LYS:NZ	2.32	0.47
24:V:51:LYS:NZ	24:V:76:ASP:HB3	2.30	0.47
2:2:466:G:H1'	9:G:59:GLN:HE21	1.78	0.47
2:2:1337:4AC:H2'	2:2:1338:G:H8	1.80	0.47
8:F:77:MET:O	8:F:83:ASN:ND2	2.47	0.47
23:U:56:MET:HB2	23:U:86:LYS:HB3	1.95	0.47
35:g:86:THR:HG21	35:g:100:ARG:HH22	1.79	0.47
19:Q:34:VAL:HG22	19:Q:70:VAL:HB	1.97	0.47
37:j:20:TRP:CD1	37:j:118:ILE:HG13	2.49	0.47
2:2:874:G:H1	2:2:912:C:H42	1.62	0.47
2:2:1084:A:OP1	2:2:1858:G:O2'	2.29	0.47
2:2:1455:A:OP1	20:R:5:ARG:NH2	2.47	0.47
12:J:53:ILE:HD13	12:J:81:LEU:HD21	1.96	0.47
15:M:60:MET:HG3	34:f:103:LEU:HD22	1.96	0.47
27:Y:8:ARG:HB3	27:Y:26:ASP:HB2	1.95	0.47
27:Y:102:THR:HG23	27:Y:107:ARG:HH11	1.79	0.47
2:2:206:G:H2'	2:2:207:G:C8	2.50	0.47
2:2:699:C:H2'	2:2:700:G:H8	1.80	0.47
8:F:120:GLY:O	8:F:193:LYS:NZ	2.48	0.47
31:c:17:VAL:HA	31:c:30:VAL:HG12	1.97	0.47
2:2:233:C:H2'	2:2:234:C:C6	2.50	0.47
2:2:1221:G:H2'	2:2:1222:G:H8	1.80	0.47
15:M:125:GLU:HG3	15:M:129:LYS:HE3	1.97	0.47
2:2:359:U:OP2	26:X:18:ARG:HD3	2.14	0.47
2:2:1610:G:N2	21:S:85:ASN:O	2.48	0.47
2:2:1623:A:N6	21:S:132:ARG:HD3	2.30	0.47
9:G:231:ARG:HA	9:G:234:LEU:HB2	1.97	0.47
10:H:144:ILE:HB	25:W:52:ILE:HB	1.97	0.47
35:g:107:ASP:HB2	35:g:125:ARG:HD2	1.95	0.47
2:2:472:C:H4'	2:2:474:G:OP1	2.15	0.46
2:2:484:A2M:H8	2:2:484:A2M:O5'	2.15	0.46
3:A:5:LEU:HD13	24:V:41:LYS:HA	1.97	0.46
8:F:78:MET:HB2	8:F:159:ARG:CZ	2.45	0.46
35:g:122:SER:HG	35:g:132:TRP:HE1	1.60	0.46
2:2:165:G:H2'	2:2:166:A2M:H8	1.97	0.46
7:E:21:ASP:OD2	7:E:24:THR:OG1	2.29	0.46
8:F:71:ARG:NH2	8:F:148:ASN:OD1	2.49	0.46
10:H:9:VAL:HG12	10:H:11:PRO:HD3	1.98	0.46
18:P:18:ARG:NH1	21:S:88:LYS:O	2.49	0.46
2:2:629:A:O2'	2:2:631:U:OP1	2.33	0.46
5:C:83:LEU:O	24:V:15:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:122:ARG:HD2	31:c:57:THR:HG21	1.98	0.46
10:H:46:THR:HG23	10:H:65:PRO:HD3	1.98	0.46
11:I:57:ALA:HB2	11:I:183:GLY:HA2	1.97	0.46
6:D:163:PRO:O	6:D:167:TYR:HB2	2.15	0.46
10:H:69:LEU:O	10:H:73:GLN:HG2	2.15	0.46
21:S:74:PRO:HB3	21:S:79:ILE:HD12	1.97	0.46
2:2:836:G:N2	2:2:838:G:OP2	2.48	0.46
2:2:1112:U:H2'	2:2:1113:A:C8	2.50	0.46
8:F:78:MET:O	8:F:159:ARG:NH1	2.49	0.46
10:H:7:LYS:HB2	10:H:28:LEU:HD21	1.98	0.46
21:S:84:LEU:HD12	21:S:95:TYR:HB3	1.96	0.46
2:2:65:C:C2	9:G:133:LEU:HD22	2.51	0.46
2:2:380:G:P	11:I:56:ARG:HH22	2.37	0.46
2:2:540:U:H3'	2:2:541:U:H5''	1.97	0.46
8:F:42:LYS:HA	8:F:42:LYS:HD3	1.75	0.46
15:M:44:LYS:HE2	34:f:129:GLY:H	1.81	0.46
35:g:190:GLY:HA3	35:g:217:MET:HE1	1.96	0.46
2:2:1786:U:H2'	2:2:1787:G:H8	1.81	0.46
3:A:33:GLN:HB3	3:A:154:LEU:HD12	1.98	0.46
25:W:55:ASP:OD1	25:W:55:ASP:N	2.48	0.46
2:2:354:OMU:HM22	2:2:355:G:H5'	1.97	0.46
2:2:692:G:H3'	2:2:693:A:H8	1.80	0.46
7:E:45:ILE:HG13	7:E:61:VAL:HG21	1.98	0.46
8:F:179:ASN:HB2	8:F:187:SER:HB3	1.98	0.46
14:L:31:GLU:N	14:L:31:GLU:OE1	2.49	0.46
17:O:63:LYS:H	17:O:63:LYS:HD3	1.80	0.46
2:2:116:OMU:HM22	2:2:117:C:H5'	1.98	0.46
2:2:506:G:OP1	27:Y:108:LYS:NZ	2.36	0.46
2:2:919:A:OP2	16:N:64:ARG:NH1	2.45	0.46
8:F:80:GLY:HA2	8:F:83:ASN:OD1	2.15	0.46
15:M:63:LYS:HZ1	34:f:112:GLY:HA2	1.81	0.46
2:2:448:A:H5''	11:I:25:ARG:HA	1.98	0.45
2:2:1836:G:OP1	2:2:1839:U:H4'	2.16	0.45
5:C:252:THR:OG1	5:C:254:ASP:OD1	2.24	0.45
8:F:51:HIS:ND1	19:Q:82:TYR:OH	2.43	0.45
19:Q:89:SER:HB3	19:Q:112:LEU:HD13	1.99	0.45
24:V:53:TYR:OH	24:V:76:ASP:OD2	2.22	0.45
2:2:906:U:H2'	2:2:907:G:H8	1.81	0.45
2:2:1498:A:OP2	6:D:27:ARG:NH2	2.49	0.45
2:2:884:C:H2'	2:2:885:U:C6	2.52	0.45
2:2:1228:A:H2'	2:2:1229:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:9:VAL:HG23	10:H:24:SER:HB3	1.98	0.45
28:Z:111:ARG:HG3	28:Z:113:THR:HG23	1.99	0.45
2:2:1031:A2M:HM'2	2:2:1032:C:H5'	1.98	0.45
14:L:76:VAL:HG12	14:L:125:ILE:HD13	1.97	0.45
31:c:23:SER:OG	31:c:24:GLN:OE1	2.25	0.45
2:2:1231:C:O2'	2:2:1253:A:N6	2.49	0.45
3:A:68:ILE:HD12	3:A:74:VAL:HG22	1.97	0.45
2:2:317:C:OP2	9:G:183:ARG:NH1	2.36	0.45
10:H:51:ILE:HG21	10:H:179:LYS:HG2	1.97	0.45
2:2:192:C:H4'	2:2:192:C:OP1	2.16	0.45
2:2:1299:A:OP1	18:P:59:ARG:NH1	2.50	0.45
2:2:1412:C:H2'	2:2:1413:G:H8	1.80	0.45
3:A:76:VAL:HG12	3:A:123:VAL:HB	1.98	0.45
2:2:543:C:H3'	2:2:544:G:H8	1.80	0.45
2:2:1819:A:H2'	2:2:1820:G:C8	2.51	0.45
18:P:64:LYS:HA	18:P:73:PRO:HB3	1.98	0.45
34:f:138:ARG:HA	34:f:149:CYS:HA	1.98	0.45
2:2:668:A2M:HM'2	2:2:668:A2M:H1'	1.61	0.45
13:K:14:LEU:HD23	13:K:21:MET:HE1	1.99	0.45
35:g:3:GLU:HG3	35:g:314:ILE:HA	1.99	0.45
12:J:110:LEU:HB2	12:J:147:PHE:HB3	1.98	0.44
33:e:113:ASN:O	33:e:118:ASN:ND2	2.50	0.44
2:2:746:C:H4'	2:2:747:U:H5'	1.99	0.44
2:2:1221:G:H2'	2:2:1222:G:C8	2.52	0.44
3:A:135:THR:O	3:A:138:SER:OG	2.30	0.44
13:K:90:VAL:O	13:K:95:ARG:NH2	2.49	0.44
20:R:127:ASN:OD1	20:R:127:ASN:N	2.50	0.44
2:2:4:C:H4'	5:C:207:ALA:HB2	2.00	0.44
2:2:1016:U:OP1	30:b:30:SER:OG	2.29	0.44
2:2:1653:U:H3	2:2:1671:G:H1	1.64	0.44
2:2:1667:U:H2'	2:2:1668:U:C6	2.53	0.44
5:C:168:GLY:N	5:C:179:THR:O	2.38	0.44
7:E:71:LYS:HG2	7:E:76:VAL:HG22	1.99	0.44
14:L:120:VAL:HG22	14:L:145:VAL:HG11	2.00	0.44
18:P:37:TYR:O	18:P:42:ARG:NH2	2.51	0.44
21:S:70:ILE:HG12	21:S:77:TYR:CZ	2.52	0.44
27:Y:114:MET:O	27:Y:122:LYS:NZ	2.49	0.44
2:2:1442:OMU:HM22	2:2:1443:C:H5'	1.99	0.44
2:2:1452:A:OP2	20:R:32:LYS:NZ	2.51	0.44
2:2:1507:G:C2	34:f:85:TYR:CD2	3.05	0.44
11:I:21:TYR:CZ	11:I:22:HIS:HD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:25:ARG:HA	11:I:25:ARG:HD3	1.89	0.44
2:2:699:C:H2'	2:2:700:G:C8	2.53	0.44
4:B:68:GLU:OE2	4:B:85:LYS:NZ	2.50	0.44
5:C:236:PHE:O	5:C:240:THR:HG22	2.18	0.44
6:D:67:ARG:NH1	13:K:96:ARG:O	2.51	0.44
29:a:59:PHE:HB2	29:a:62:TYR:HB2	2.00	0.44
2:2:543:C:H3'	2:2:544:G:C8	2.53	0.44
2:2:1461:G:H3'	2:2:1463:U:H3	1.83	0.44
6:D:32:ASP:OD1	6:D:32:ASP:N	2.49	0.44
10:H:76:GLN:HE22	10:H:94:PHE:HB2	1.81	0.44
21:S:3:LEU:HB3	28:Z:83:LEU:HD11	1.99	0.44
21:S:125:HIS:CE1	21:S:131:VAL:HG21	2.53	0.44
37:j:83:ASP:OD1	37:j:84:LEU:N	2.51	0.44
2:2:753:C:H2'	2:2:754:G:C8	2.53	0.44
2:2:1288:OMU:HM22	2:2:1289:U:H5'	2.00	0.44
2:2:1531:A:H4'	2:2:1605:G:H4'	2.00	0.44
2:2:1808:U:H2'	2:2:1809:A:H8	1.83	0.44
35:g:20:GLN:HB3	35:g:69:VAL:HG12	2.00	0.44
1:p:38:ARG:HB2	1:p:44:LEU:HD13	2.00	0.44
2:2:587:A:H5'	2:2:592:C:H41	1.83	0.44
2:2:1452:A:H5''	20:R:48:ASN:HD22	1.83	0.44
16:N:20:ARG:HH21	25:W:56:HIS:HB3	1.82	0.44
17:O:117:ARG:NE	29:a:52:ASP:OD2	2.48	0.44
2:2:67:C:H41	9:G:163:ASN:HA	1.83	0.43
2:2:234:C:N4	2:2:894:G:H1	2.16	0.43
2:2:1376:A:OP2	20:R:67:ARG:NH2	2.51	0.43
10:H:100:ILE:HD13	10:H:122:LEU:HD12	1.99	0.43
28:Z:58:LEU:HD12	28:Z:62:VAL:HG21	2.00	0.43
2:2:641:A:O2'	2:2:645:C:OP1	2.33	0.43
2:2:753:C:H2'	2:2:754:G:H8	1.83	0.43
2:2:907:G:H2'	2:2:908:A:C8	2.53	0.43
2:2:1783:C:OP1	2:2:1784:G:H5'	2.18	0.43
15:M:32:ALA:HB3	15:M:110:VAL:HB	2.00	0.43
37:j:23:ILE:HG12	37:j:24:GLY:H	1.83	0.43
2:2:1013:U:OP1	2:2:1129:G:O2'	2.33	0.43
2:2:1752:C:H2'	2:2:1753:C:C6	2.54	0.43
6:D:202:LYS:HZ1	6:D:202:LYS:H	1.65	0.43
7:E:151:ASP:HB3	7:E:154:ILE:HG13	2.00	0.43
35:g:275:ILE:HD12	35:g:275:ILE:HA	1.87	0.43
2:2:379:C:H5'	11:I:33:ALA:HA	2.01	0.43
2:2:740:C:H2'	2:2:741:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1255:G:OP1	2:2:1256:G:O2'	2.26	0.43
2:2:1431:G:H2'	2:2:1432:U:C6	2.53	0.43
7:E:54:TYR:O	27:Y:15:ASN:ND2	2.52	0.43
7:E:183:VAL:HG11	7:E:220:THR:HG21	2.00	0.43
13:K:83:LEU:HB2	13:K:85:LEU:HG	2.01	0.43
19:Q:21:ALA:HB2	19:Q:72:VAL:HG13	1.99	0.43
28:Z:92:LEU:HD22	28:Z:109:TYR:HE1	1.83	0.43
34:f:90:LYS:HG3	34:f:91:ASN:N	2.34	0.43
2:2:546:G:H2'	2:2:548:C:C5	2.54	0.43
6:D:106:ARG:HH21	6:D:173:ARG:HB3	1.83	0.43
20:R:21:TYR:HA	20:R:24:LEU:HD12	2.00	0.43
2:2:1083:A:N7	2:2:1841:C:O2'	2.41	0.43
8:F:32:ASP:O	8:F:36:GLN:HG3	2.19	0.43
15:M:21:VAL:HG21	15:M:124:ILE:HD12	2.00	0.43
23:U:23:THR:HB	23:U:113:GLU:HB2	2.00	0.43
26:X:93:PHE:O	26:X:140:ARG:NH1	2.51	0.43
7:E:117:GLU:N	7:E:117:GLU:OE1	2.52	0.43
16:N:22:VAL:HG23	16:N:26:LEU:HD23	2.01	0.43
18:P:34:MET:HB3	18:P:42:ARG:HG3	2.00	0.43
21:S:35:GLY:O	21:S:97:GLN:NE2	2.52	0.43
26:X:84:PHE:HB2	26:X:118:VAL:HG11	2.01	0.43
2:2:27:A2M:HM'2	2:2:28:U:O4'	2.19	0.43
2:2:205:G:H2'	2:2:206:G:C8	2.54	0.43
2:2:584:A:OP1	12:J:169:ARG:NH2	2.51	0.43
2:2:834:C:H2'	2:2:835:C:O4'	2.19	0.43
2:2:1320:G:H2'	2:2:1321:G:O4'	2.18	0.43
6:D:166:TYR:O	6:D:200:PRO:HG3	2.18	0.43
19:Q:50:LYS:HB3	19:Q:85:ARG:HD2	2.01	0.43
2:2:1091:C:O2'	25:W:2:VAL:N	2.42	0.43
2:2:1543:U:OP2	22:T:62:ARG:NH2	2.38	0.43
2:2:1762:C:H2'	2:2:1763:G:H8	1.83	0.43
24:V:1:AME:HT23	24:V:1:AME:HA	1.61	0.43
25:W:30:CYS:SG	25:W:31:SER:N	2.91	0.43
35:g:238:ALA:H	35:g:251:ALA:HB3	1.84	0.43
36:h:2:ARG:HD3	36:h:5:TRP:NE1	2.34	0.43
2:2:1037:G:H4'	2:2:1845:A:H4'	2.01	0.42
2:2:1452:A:H5''	20:R:48:ASN:ND2	2.33	0.42
10:H:43:LEU:HD22	10:H:68:GLN:HB3	2.01	0.42
2:2:239:C:H2'	2:2:240:G:C8	2.54	0.42
12:J:63:LEU:O	12:J:70:ARG:NH1	2.52	0.42
15:M:85:LEU:O	15:M:89:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:101:PHE:CE2	35:g:136:GLY:HA2	2.54	0.42
35:g:272:GLN:H	35:g:272:GLN:HG2	1.63	0.42
2:2:495:U:OP1	7:E:49:ARG:NH1	2.52	0.42
3:A:41:ARG:HE	3:A:45:GLY:HA2	1.84	0.42
14:L:23:VAL:HG23	14:L:26:GLY:H	1.84	0.42
16:N:5:HIS:CD2	16:N:117:LEU:HD22	2.55	0.42
28:Z:103:HIS:CE1	28:Z:104:ARG:HG3	2.54	0.42
35:g:171:ASP:OD1	35:g:171:ASP:N	2.49	0.42
2:2:894:G:C6	2:2:895:G:C6	3.07	0.42
15:M:53:ALA:HB2	15:M:85:LEU:HD13	2.00	0.42
20:R:78:ARG:O	20:R:82:ASP:N	2.52	0.42
2:2:588:G:OP2	2:2:588:G:N2	2.52	0.42
2:2:1337:4AC:H2'	2:2:1338:G:C8	2.54	0.42
2:2:1816:G:H2'	2:2:1817:G:H8	1.84	0.42
34:f:89:LYS:HG2	34:f:90:LYS:H	1.85	0.42
2:2:1412:C:H2'	2:2:1413:G:C8	2.55	0.42
35:g:298:LEU:HD23	35:g:298:LEU:HA	1.91	0.42
2:2:146:G:H1	2:2:173:A:H61	1.68	0.42
2:2:420:G:O2'	2:2:660:C:N3	2.52	0.42
2:2:1374:C:H2'	2:2:1375:G:O4'	2.19	0.42
2:2:1575:G:H2'	2:2:1576:G:H8	1.85	0.42
7:E:36:HIS:CG	7:E:85:GLY:HA3	2.55	0.42
7:E:141:THR:OG1	7:E:143:ASP:OD1	2.32	0.42
8:F:73:THR:O	8:F:89:THR:HG21	2.20	0.42
9:G:159:ARG:HB3	9:G:171:THR:HG22	2.00	0.42
12:J:131:ARG:HD2	12:J:131:ARG:HA	1.88	0.42
26:X:40:PRO:HB2	26:X:81:ILE:HD11	2.01	0.42
29:a:46:GLU:O	29:a:50:VAL:HG23	2.20	0.42
37:j:56:PRO:HB3	37:j:104:GLY:N	2.35	0.42
2:2:151:C:OP1	27:Y:120:THR:OG1	2.31	0.42
2:2:681:PSU:H4'	26:X:9:THR:HG22	2.02	0.42
2:2:877:C:H2'	2:2:878:G:C8	2.54	0.42
2:2:1179:G:N2	2:2:1182:A:OP2	2.51	0.42
2:2:1511:U:H2'	2:2:1512:C:C6	2.55	0.42
8:F:34:SER:HA	31:c:55:VAL:HB	2.02	0.42
2:2:145:G:H2'	2:2:146:G:C8	2.55	0.42
3:A:198:MET:H	3:A:198:MET:HG2	1.71	0.42
14:L:84:ARG:HD3	14:L:115:PRO:HG3	2.00	0.42
28:Z:65:TYR:C	28:Z:67:LEU:H	2.28	0.42
3:A:151:ASP:OD1	3:A:151:ASP:N	2.48	0.42
5:C:271:ASP:O	5:C:274:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:17:ILE:HD11	20:R:54:VAL:HG13	2.00	0.42
2:2:384:U:O4	11:I:5:ARG:NH2	2.39	0.41
2:2:1415:C:H2'	2:2:1416:C:C6	2.55	0.41
2:2:1720:U:H3'	2:2:1721:U:H5''	2.01	0.41
2:2:1786:U:H2'	2:2:1787:G:C8	2.55	0.41
2:2:1808:U:H2'	2:2:1809:A:C8	2.54	0.41
14:L:135:SER:O	14:L:139:ARG:NH1	2.53	0.41
32:d:33:LYS:HE2	32:d:34:TYR:CZ	2.55	0.41
2:2:1156:U:O4	5:C:194:ARG:NH1	2.53	0.41
2:2:1770:G:H2'	2:2:1771:G:C8	2.55	0.41
3:A:69:GLU:HB2	5:C:270:THR:HG21	2.01	0.41
28:Z:88:LEU:HD23	28:Z:109:TYR:CD2	2.55	0.41
34:f:140:TYR:HE1	34:f:145:CYS:HA	1.85	0.41
2:2:894:G:H2'	2:2:895:G:C8	2.55	0.41
2:2:897:U:H2'	2:2:898:U:C6	2.55	0.41
2:2:913:A:N6	10:H:98:ARG:HB3	2.36	0.41
5:C:60:TRP:O	5:C:71:LYS:NZ	2.36	0.41
8:F:44:LYS:HE3	8:F:45:TYR:CE2	2.55	0.41
22:T:116:ASP:OD1	22:T:117:GLN:N	2.53	0.41
37:j:137:ASN:H	37:j:137:ASN:ND2	2.18	0.41
1:p:50:ILE:HB	1:p:56:LYS:HE2	2.03	0.41
2:2:115:U:O2'	2:2:381:C:O2	2.29	0.41
2:2:165:G:H4'	9:G:53:SER:HB3	2.02	0.41
2:2:835:C:C5	27:Y:8:ARG:HD2	2.54	0.41
2:2:1007:C:H2'	2:2:1008:A:C8	2.55	0.41
2:2:1819:A:H2'	2:2:1820:G:H8	1.84	0.41
9:G:120:ASP:OD1	9:G:120:ASP:N	2.50	0.41
11:I:6:ASP:OD1	11:I:9:HIS:ND1	2.38	0.41
16:N:5:HIS:HD2	16:N:117:LEU:HD22	1.84	0.41
37:j:42:VAL:HG21	37:j:69:VAL:HG21	2.02	0.41
2:2:494:C:N4	2:2:509:OMG:HN22	2.18	0.41
2:2:1778:C:H2'	2:2:1779:G:C8	2.55	0.41
8:F:56:TYR:HB3	8:F:63:LYS:HA	2.01	0.41
29:a:31:PRO:HG2	29:a:34:LYS:HB3	2.03	0.41
2:2:434:G:OP2	11:I:25:ARG:NH2	2.53	0.41
2:2:801:PSU:H2'	2:2:802:A:C8	2.55	0.41
2:2:991:G:C6	2:2:1134:G:H4'	2.56	0.41
2:2:1275:G:N2	2:2:1506:A:OP2	2.53	0.41
2:2:1446:A:O2'	2:2:1447:OMG:H8	2.04	0.41
5:C:259:THR:HG21	24:V:15:ARG:HA	2.02	0.41
2:2:1473:G:N2	2:2:1476:A:OP2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:171:ASP:OD1	7:E:171:ASP:N	2.52	0.41
37:j:26:ASN:HD22	37:j:112:GLN:HA	1.86	0.41
2:2:54:A:OP1	27:Y:111:LYS:NZ	2.41	0.41
2:2:300:U:H2'	2:2:301:A:C8	2.56	0.41
2:2:527:C:H4'	12:J:121:LYS:HD2	2.03	0.41
2:2:874:G:H2'	2:2:875:A:H8	1.84	0.41
2:2:906:U:H2'	2:2:907:G:C8	2.55	0.41
2:2:1772:C:H2'	2:2:1773:C:C6	2.55	0.41
28:Z:54:THR:HG21	28:Z:79:ILE:HD11	2.02	0.41
2:2:65:C:C6	9:G:174:PRO:HB3	2.56	0.41
2:2:741:C:O3'	10:H:102:PRO:HG3	2.21	0.41
2:2:1036:A:N3	2:2:1844:U:O2'	2.54	0.41
2:2:1453:C:O2'	20:R:52:GLY:HA3	2.21	0.41
2:2:1520:G:N3	2:2:1520:G:H2'	2.36	0.41
2:2:1679:A:H2'	8:F:60:ARG:HD2	2.02	0.41
2:2:1778:C:N4	2:2:1779:G:O6	2.54	0.41
2:2:1848:U:H2'	2:2:1850:MA6:OP2	2.21	0.41
3:A:38:ILE:HD12	3:A:38:ILE:HA	1.92	0.41
5:C:196:ILE:HB	5:C:223:TYR:HB2	2.03	0.41
12:J:48:PHE:CZ	12:J:52:LYS:HE3	2.55	0.41
18:P:100:LYS:HG2	18:P:101:THR:HG23	2.03	0.41
27:Y:76:TYR:OH	27:Y:86:GLU:OE1	2.33	0.41
34:f:83:LYS:C	34:f:85:TYR:N	2.79	0.41
2:2:540:U:H2'	2:2:542:U:OP2	2.21	0.41
2:2:795:A:H2'	2:2:796:G:H8	1.85	0.41
2:2:889:U:H2'	2:2:890:U:C6	2.56	0.41
2:2:1240:A:C2	18:P:100:LYS:HB2	2.56	0.41
2:2:1757:G:H2'	2:2:1758:G:C8	2.56	0.41
1:p:67:PHE:CE1	1:p:92:ASN:HB3	2.56	0.40
2:2:1733:U:H2'	2:2:1734:G:O4'	2.21	0.40
2:2:1846:G:N7	36:h:8:LYS:NZ	2.63	0.40
15:M:36:ARG:HH12	15:M:40:LYS:HB2	1.86	0.40
15:M:63:LYS:NZ	34:f:112:GLY:HA2	2.36	0.40
34:f:123:SER:HB2	34:f:126:CYS:SG	2.61	0.40
37:j:19:PRO:HA	37:j:117:THR:HA	2.02	0.40
2:2:186:C:H2'	2:2:187:G:H8	1.86	0.40
2:2:228:C:C2	2:2:901:G:H1'	2.56	0.40
2:2:689:U:C2	10:H:122:LEU:HD21	2.57	0.40
2:2:1432:U:H2'	2:2:1438:A:C8	2.56	0.40
2:2:1736:G:H2'	2:2:1737:G:C8	2.57	0.40
5:C:113:GLN:HE22	37:j:159:LYS:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:159:LYS:HA	5:C:162:ILE:HG13	2.04	0.40
8:F:43:GLU:H	8:F:43:GLU:CD	2.28	0.40
10:H:73:GLN:HB3	10:H:135:PHE:CE1	2.56	0.40
22:T:31:PRO:HB3	22:T:102:ARG:HH11	1.86	0.40
2:2:220:U:H2'	2:2:221:A:H8	1.87	0.40
7:E:62:LYS:HE3	7:E:62:LYS:HB3	1.93	0.40
13:K:4:PRO:HG2	13:K:7:ASN:CG	2.46	0.40
20:R:57:LEU:HD12	20:R:57:LEU:HA	1.95	0.40
2:2:428:OMU:H2'	2:2:428:OMU:H6	1.83	0.40
3:A:132:GLN:HB3	3:A:133:PRO:HD3	2.04	0.40
19:Q:44:PRO:HD2	19:Q:81:ILE:HD11	2.04	0.40
25:W:77:PRO:HD3	26:X:5:ARG:O	2.21	0.40
27:Y:29:HIS:ND1	27:Y:29:HIS:O	2.54	0.40
2:2:35:C:H2'	2:2:36:PSU:H6	1.87	0.40
2:2:280:G:H2'	2:2:281:C:C6	2.56	0.40
2:2:554:A:H5''	2:2:555:A:OP1	2.21	0.40
2:2:634:A:H2'	2:2:635:G:C8	2.57	0.40
2:2:1114:U:H3'	2:2:1115:U:H5'	2.04	0.40
2:2:1308:U:H2'	2:2:1309:C:C6	2.57	0.40
2:2:1486:A:OP2	6:D:151:LYS:NZ	2.38	0.40
2:2:1603:G:H4'	21:S:38:ARG:CZ	2.51	0.40
2:2:1767:C:O2	2:2:1768:A:N6	2.54	0.40
3:A:7:VAL:HG13	3:A:8:LEU:HG	2.04	0.40
9:G:162:LEU:HD12	9:G:162:LEU:HA	1.96	0.40
21:S:121:ARG:HG3	21:S:131:VAL:HG13	2.04	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	p	83/113 (74%)	82 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	214/295 (72%)	211 (99%)	3 (1%)	0	100	100
4	B	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
5	C	222/293 (76%)	218 (98%)	4 (2%)	0	100	100
6	D	223/243 (92%)	221 (99%)	2 (1%)	0	100	100
7	E	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
8	F	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
9	G	238/249 (96%)	236 (99%)	2 (1%)	0	100	100
10	H	187/194 (96%)	183 (98%)	4 (2%)	0	100	100
11	I	203/208 (98%)	201 (99%)	2 (1%)	0	100	100
12	J	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
13	K	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
14	L	153/158 (97%)	149 (97%)	4 (3%)	0	100	100
15	M	121/132 (92%)	117 (97%)	4 (3%)	0	100	100
16	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
17	O	131/151 (87%)	128 (98%)	3 (2%)	0	100	100
18	P	122/145 (84%)	122 (100%)	0	0	100	100
19	Q	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
20	R	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
21	S	143/152 (94%)	141 (99%)	2 (1%)	0	100	100
22	T	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
23	U	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
24	V	81/83 (98%)	81 (100%)	0	0	100	100
25	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
26	X	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
27	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
28	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
29	a	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
30	b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
31	c	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
32	d	53/56 (95%)	53 (100%)	0	0	100	100
33	e	57/133 (43%)	54 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	f	72/156 (46%)	63 (88%)	8 (11%)	1 (1%)	9	34
35	g	312/317 (98%)	297 (95%)	15 (5%)	0	100	100
36	h	23/25 (92%)	23 (100%)	0	0	100	100
37	j	172/188 (92%)	165 (96%)	6 (4%)	1 (1%)	21	53
All	All	5112/5876 (87%)	4994 (98%)	116 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	j	129	ALA
34	f	84	SER

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	p	74/96 (77%)	72 (97%)	2 (3%)	39	70
3	A	179/242 (74%)	178 (99%)	1 (1%)	78	88
4	B	203/231 (88%)	200 (98%)	3 (2%)	57	79
5	C	190/225 (84%)	190 (100%)	0	100	100
6	D	189/202 (94%)	186 (98%)	3 (2%)	55	78
7	E	224/225 (100%)	224 (100%)	0	100	100
8	F	162/170 (95%)	162 (100%)	0	100	100
9	G	209/218 (96%)	206 (99%)	3 (1%)	59	80
10	H	169/174 (97%)	168 (99%)	1 (1%)	78	88
11	I	178/180 (99%)	175 (98%)	3 (2%)	53	77
12	J	160/168 (95%)	159 (99%)	1 (1%)	78	88
13	K	88/136 (65%)	85 (97%)	3 (3%)	32	64
14	L	139/142 (98%)	138 (99%)	1 (1%)	76	87
15	M	104/108 (96%)	102 (98%)	2 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	130/131 (99%)	127 (98%)	3 (2%)	44	72
17	O	104/118 (88%)	103 (99%)	1 (1%)	68	83
18	P	110/130 (85%)	110 (100%)	0	100	100
19	Q	117/121 (97%)	114 (97%)	3 (3%)	40	70
20	R	121/122 (99%)	117 (97%)	4 (3%)	33	65
21	S	125/131 (95%)	124 (99%)	1 (1%)	73	86
22	T	113/114 (99%)	113 (100%)	0	100	100
23	U	93/107 (87%)	90 (97%)	3 (3%)	34	65
24	V	66/66 (100%)	65 (98%)	1 (2%)	57	79
25	W	112/113 (99%)	111 (99%)	1 (1%)	70	85
26	X	112/114 (98%)	111 (99%)	1 (1%)	70	85
27	Y	108/115 (94%)	107 (99%)	1 (1%)	70	85
28	Z	64/103 (62%)	61 (95%)	3 (5%)	23	56
29	a	88/98 (90%)	87 (99%)	1 (1%)	65	82
30	b	75/76 (99%)	74 (99%)	1 (1%)	61	81
31	c	58/62 (94%)	58 (100%)	0	100	100
32	d	48/49 (98%)	47 (98%)	1 (2%)	47	74
33	e	48/104 (46%)	46 (96%)	2 (4%)	26	59
34	f	67/140 (48%)	65 (97%)	2 (3%)	36	67
35	g	272/275 (99%)	267 (98%)	5 (2%)	51	76
36	h	24/24 (100%)	24 (100%)	0	100	100
37	j	144/158 (91%)	138 (96%)	6 (4%)	26	59
All	All	4467/4988 (90%)	4404 (99%)	63 (1%)	57	80

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	105	ASP
1	p	110	VAL
3	A	34	MET
4	B	33	VAL
4	B	108	ASP
4	B	228	LEU
6	D	32	ASP

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Mol	Chain	Res	Type
6	D	175	VAL
6	D	202	LYS
9	G	50	VAL
9	G	69	THR
9	G	171	THR
10	H	28	LEU
11	I	29	LEU
11	I	76	THR
11	I	107	THR
12	J	29	LEU
13	K	72	THR
13	K	93	THR
13	K	94	LEU
14	L	155	PHE
15	M	11	VAL
15	M	62	VAL
16	N	22	VAL
16	N	55	ARG
16	N	145	THR
17	O	119	LEU
19	Q	18	THR
19	Q	51	LEU
19	Q	100	VAL
20	R	6	THR
20	R	19	LYS
20	R	23	ARG
20	R	124	VAL
21	S	53	THR
23	U	25	THR
23	U	68	THR
23	U	78	ASP
24	V	9	VAL
25	W	105	THR
26	X	105	PHE
27	Y	120	THR
28	Z	69	THR
28	Z	104	ARG
28	Z	107	VAL
29	a	67	LEU
30	b	53	VAL
32	d	30	LEU
33	e	119	VAL

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Mol	Chain	Res	Type
33	e	122	THR
34	f	85	TYR
34	f	98	VAL
35	g	113	PHE
35	g	252	THR
35	g	266	ILE
35	g	294	ASP
35	g	298	LEU
37	j	33	VAL
37	j	48	GLU
37	j	133	TYR
37	j	138	THR
37	j	142	VAL
37	j	144	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	113	GLN
3	A	164	ASN
5	C	172	ASN
6	D	4	GLN
6	D	159	HIS
6	D	179	GLN
7	E	112	HIS
7	E	161	GLN
7	E	179	ASN
7	E	201	HIS
8	F	79	HIS
8	F	83	ASN
8	F	95	HIS
8	F	110	GLN
8	F	203	ASN
9	G	65	GLN
9	G	225	GLN
10	H	112	ASN
10	H	157	HIS
11	I	52	ASN
11	I	146	GLN
11	I	165	GLN
13	K	39	ASN
14	L	11	GLN

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Mol	Chain	Res	Type
14	L	18	GLN
14	L	19	ASN
14	L	112	HIS
15	M	19	GLN
16	N	5	HIS
16	N	49	GLN
17	O	103	ASN
19	Q	11	GLN
19	Q	77	HIS
20	R	29	HIS
21	S	105	ASN
23	U	18	HIS
23	U	81	GLN
24	V	2	GLN
24	V	49	GLN
25	W	15	ASN
25	W	44	HIS
25	W	90	GLN
26	X	16	HIS
26	X	61	GLN
29	a	25	ASN
29	a	80	HIS
30	b	9	HIS
30	b	65	GLN
30	b	83	GLN
31	c	7	GLN
33	e	118	ASN
33	e	132	ASN
34	f	111	ASN
35	g	20	GLN
35	g	62	HIS
35	g	181	ASN
35	g	226	HIS
35	g	305	ASN
35	g	311	GLN
37	j	10	GLN
37	j	22	GLN
37	j	26	ASN
37	j	74	ASN
37	j	85	GLN
37	j	121	GLN
37	j	137	ASN

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Mol	Chain	Res	Type
37	j	148	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1765/1869 (94%)	213 (12%)	1 (0%)

All (213) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	4	C
2	2	17	C
2	2	33	G
2	2	41	G
2	2	46	A
2	2	56	G
2	2	64	A
2	2	67	C
2	2	68	A
2	2	76	U
2	2	77	A
2	2	79	A
2	2	103	A
2	2	113	G
2	2	115	U
2	2	126	G
2	2	130	G
2	2	143	U
2	2	155	G
2	2	163	U
2	2	168	C
2	2	178	C
2	2	182	C
2	2	184	G
2	2	190	G
2	2	192	C
2	2	205	G
2	2	226	A
2	2	228	C
2	2	281	C
2	2	287	U

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Mol	Chain	Res	Type
2	2	295	C
2	2	309	G
2	2	312	G
2	2	319	C
2	2	325	C
2	2	326	C
2	2	328	U
2	2	330	G
2	2	335	G
2	2	347	G
2	2	362	C
2	2	364	A
2	2	369	C
2	2	385	G
2	2	386	C
2	2	400	C
2	2	409	C
2	2	421	G
2	2	448	A
2	2	450	C
2	2	470	G
2	2	471	G
2	2	472	C
2	2	474	G
2	2	482	G
2	2	487	U
2	2	492	C
2	2	508	A
2	2	512	A2M
2	2	525	A
2	2	542	U
2	2	547	G
2	2	548	C
2	2	555	A
2	2	559	G
2	2	560	A
2	2	563	G
2	2	564	A
2	2	588	G
2	2	591	U
2	2	607	U
2	2	608	C

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Mol	Chain	Res	Type
2	2	614	C
2	2	628	A
2	2	631	U
2	2	643	A
2	2	644	OMG
2	2	655	A
2	2	660	C
2	2	668	A2M
2	2	669	A
2	2	671	A
2	2	672	A
2	2	673	G
2	2	690	G
2	2	746	C
2	2	748	C
2	2	749	U
2	2	790	C
2	2	798	G
2	2	799	OMU
2	2	811	A
2	2	821	G
2	2	822	PSU
2	2	830	A
2	2	831	G
2	2	835	C
2	2	836	G
2	2	837	A
2	2	838	G
2	2	839	C
2	2	841	G
2	2	847	A
2	2	870	A
2	2	871	U
2	2	874	G
2	2	891	G
2	2	913	A
2	2	920	A
2	2	922	A
2	2	933	G
2	2	943	U
2	2	971	G
2	2	990	A

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Mol	Chain	Res	Type
2	2	992	A
2	2	1017	U
2	2	1023	A
2	2	1061	U
2	2	1062	A
2	2	1083	A
2	2	1085	C
2	2	1115	U
2	2	1144	A
2	2	1148	A
2	2	1153	C
2	2	1154	U
2	2	1157	G
2	2	1166	G
2	2	1171	G
2	2	1195	A
2	2	1215	C
2	2	1224	G
2	2	1227	G
2	2	1242	U
2	2	1251	A
2	2	1253	A
2	2	1256	G
2	2	1257	G
2	2	1259	A
2	2	1274	G
2	2	1275	G
2	2	1293	A
2	2	1300	U
2	2	1302	G
2	2	1303	C
2	2	1309	C
2	2	1342	U
2	2	1358	U
2	2	1371	U
2	2	1372	U
2	2	1378	A
2	2	1397	U
2	2	1405	A
2	2	1419	C
2	2	1420	G
2	2	1421	A

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Mol	Chain	Res	Type
2	2	1424	G
2	2	1435	C
2	2	1438	A
2	2	1439	A
2	2	1454	A
2	2	1463	U
2	2	1464	C
2	2	1466	G
2	2	1489	A
2	2	1490	OMG
2	2	1497	G
2	2	1507	G
2	2	1508	A
2	2	1521	C
2	2	1533	A
2	2	1553	C
2	2	1570	G
2	2	1579	A
2	2	1580	A
2	2	1585	U
2	2	1588	A
2	2	1594	A
2	2	1596	U
2	2	1599	U
2	2	1601	A
2	2	1618	C
2	2	1621	U
2	2	1623	A
2	2	1624	U
2	2	1637	A
2	2	1641	A
2	2	1665	G
2	2	1680	G
2	2	1695	A
2	2	1698	C
2	2	1699	A
2	2	1721	U
2	2	1722	G
2	2	1742	C
2	2	1757	G
2	2	1783	C
2	2	1784	G

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Mol	Chain	Res	Type
2	2	1824	A
2	2	1825	A
2	2	1831	A
2	2	1835	A
2	2	1836	G
2	2	1838	U
2	2	1849	G
2	2	1851	MA6
2	2	1861	G
2	2	1862	G
2	2	1863	A
2	2	1864	U
2	2	1865	C
2	2	1869	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	873	G

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

92 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	$\# Z > 2$
2	OMC	2	1703	2	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
2	PSU	2	109	2	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
2	MA6	2	1850	2	23,26,27	2.26	5 (21%)	34,38,41	3.70	13 (38%)
2	PSU	2	119	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	PSU	2	1238	2	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
2	A2M	2	512	2	22,25,26	1.45	4 (18%)	31,36,39	2.15	9 (29%)
2	PSU	2	651	2	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	2	1031	2	22,25,26	1.44	4 (18%)	31,36,39	2.12	10 (32%)
2	OMU	2	354	2	19,22,23	1.22	3 (15%)	26,31,34	1.72	5 (19%)
2	A2M	2	27	39,2	22,25,26	1.50	4 (18%)	31,36,39	2.14	10 (32%)
2	OMG	2	601	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	PSU	2	814	2	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
2	OMU	2	116	2	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
2	A2M	2	99	39,2	22,25,26	1.51	4 (18%)	31,36,39	2.14	10 (32%)
2	PSU	2	1174	2	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	6MZ	2	1832	39,2	22,25,26	1.42	4 (18%)	30,36,39	2.16	8 (26%)
2	PSU	2	1244	2	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
2	PSU	2	609	2	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	2	1367	2	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
2	A2M	2	1678	2	22,25,26	1.45	4 (18%)	31,36,39	2.16	9 (29%)
2	OMG	2	644	2	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
2	OMC	2	462	2	19,22,23	0.81	0	26,31,34	0.81	0
2	PSU	2	1643	39,2	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	2	1347	2	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	A2M	2	668	39,2	22,25,26	1.44	4 (18%)	31,36,39	2.11	9 (29%)
2	OMU	2	1326	39,2	19,22,23	1.19	2 (10%)	26,31,34	1.72	5 (19%)
2	PSU	2	1177	2	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
2	G7M	2	1639	2	23,26,27	3.11	8 (34%)	35,39,42	3.31	13 (37%)
2	OMU	2	1804	2	19,22,23	1.21	3 (15%)	26,31,34	1.71	4 (15%)
2	PSU	2	686	2	18,21,22	1.33	2 (11%)	22,30,33	1.93	4 (18%)
2	PSU	2	1081	2	18,21,22	1.38	3 (16%)	22,30,33	1.88	3 (13%)
2	OMU	2	121	2	19,22,23	1.21	3 (15%)	26,31,34	1.69	5 (19%)
2	PSU	2	966	2	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
2	OMU	2	1442	39,2	19,22,23	1.23	2 (10%)	26,31,34	1.70	4 (15%)
2	PSU	2	1232	2	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
2	OMG	2	1447	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	OMU	2	428	2	19,22,23	1.19	3 (15%)	26,31,34	1.71	5 (19%)
2	PSU	2	34	2	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
2	A2M	2	159	2	22,25,26	1.51	4 (18%)	31,36,39	2.13	10 (32%)
2	A2M	2	166	2	22,25,26	1.45	4 (18%)	31,36,39	2.16	10 (32%)
2	OMU	2	172	2	19,22,23	1.21	2 (10%)	26,31,34	1.73	5 (19%)
2	PSU	2	681	2	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	2	509	39,2	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
2	PSU	2	801	2	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
2	OMC	2	1272	2	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
2	PSU	2	1136	2	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
2	PSU	2	1004	2	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	OMG	2	1490	39,2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	OMC	2	517	2	19,22,23	0.82	0	26,31,34	0.82	0
2	OMC	2	1391	2	19,22,23	0.81	0	26,31,34	0.83	0
2	PSU	2	1692	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	A2M	2	1383	2	22,25,26	1.46	4 (18%)	31,36,39	2.16	10 (32%)
2	PSU	2	1625	2	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
2	PSU	2	1046	2	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
26	HY3	X	62	26	6,8,9	2.16	1 (16%)	5,10,12	1.16	1 (20%)
2	PSU	2	210	2	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	2	218	2	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
2	PSU	2	296	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	PSU	2	863	2	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
2	OMG	2	683	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	OMC	2	174	39,2	19,22,23	0.82	0	26,31,34	0.79	0
2	OMC	2	797	2	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
2	PSU	2	1445	2	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
2	PSU	2	105	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	PSU	2	406	2	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	IAS	O	138	17	6,7,8	0.97	0	6,8,10	1.32	1 (16%)
2	4AC	2	1337	2	21,24,25	1.10	2 (9%)	29,34,37	1.02	2 (6%)
2	PSU	2	866	2	18,21,22	1.34	2 (11%)	22,30,33	1.93	4 (18%)
22	NMM	T	67	22	9,11,12	0.59	0	6,12,14	0.55	0
2	B8N	2	1248	2	24,29,30	1.29	3 (12%)	29,42,45	1.26	3 (10%)
2	PSU	2	822	2	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
2	PSU	2	1056	2	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
2	PSU	2	93	2	18,21,22	1.38	2 (11%)	22,30,33	1.95	3 (13%)
2	OMG	2	436	2	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
2	OMU	2	799	2	19,22,23	1.21	3 (15%)	26,31,34	1.72	5 (19%)
2	MA6	2	1851	2	23,26,27	2.27	5 (21%)	34,38,41	3.64	12 (35%)
3	SAC	A	2	3	7,8,9	0.52	0	8,9,11	0.86	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	2	572	2	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
2	PSU	2	815	2	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
2	OMU	2	627	2	19,22,23	1.20	2 (10%)	26,31,34	1.67	5 (19%)
2	A2M	2	468	2	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
2	A2M	2	590	2	22,25,26	1.46	4 (18%)	31,36,39	2.19	7 (22%)
2	OMU	2	1288	2	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
2	4AC	2	1842	2	21,24,25	1.11	2 (9%)	29,34,37	1.23	3 (10%)
2	PSU	2	36	2	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
2	A2M	2	484	2	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
21	SAC	S	2	21	7,8,9	0.53	0	8,9,11	0.91	1 (12%)
2	A2M	2	576	2	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
24	AME	V	1	24	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
2	PSU	2	649	2	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
2	OMG	2	1328	2	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
2	PSU	2	1045	2	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)

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
2	OMC	2	1703	2	-	1/9/27/28	0/2/2/2
2	PSU	2	109	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1850	2	-	0/11/29/30	0/3/3/3
2	PSU	2	119	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1238	2	-	0/7/25/26	0/2/2/2
2	A2M	2	512	2	-	3/9/27/28	0/3/3/3
2	PSU	2	651	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1031	2	-	0/9/27/28	0/3/3/3
2	OMU	2	354	2	-	1/9/27/28	0/2/2/2
2	A2M	2	27	39,2	-	0/9/27/28	0/3/3/3
2	OMG	2	601	2	-	0/9/27/28	0/3/3/3
2	PSU	2	814	2	-	0/7/25/26	0/2/2/2
2	OMU	2	116	2	-	1/9/27/28	0/2/2/2
2	A2M	2	99	39,2	-	2/9/27/28	0/3/3/3
2	PSU	2	1174	2	-	0/7/25/26	0/2/2/2
2	6MZ	2	1832	39,2	-	0/9/27/28	0/3/3/3
2	PSU	2	1244	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	609	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1367	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1678	2	-	0/9/27/28	0/3/3/3
2	OMG	2	644	2	-	3/9/27/28	0/3/3/3
2	OMC	2	462	2	-	0/9/27/28	0/2/2/2
2	PSU	2	1643	39,2	-	0/7/25/26	0/2/2/2
2	PSU	2	1347	2	-	0/7/25/26	0/2/2/2
2	A2M	2	668	39,2	-	4/9/27/28	0/3/3/3
2	OMU	2	1326	39,2	-	0/9/27/28	0/2/2/2
2	PSU	2	1177	2	-	0/7/25/26	0/2/2/2
2	G7M	2	1639	2	-	0/7/25/26	0/3/3/3
2	OMU	2	1804	2	-	0/9/27/28	0/2/2/2
2	PSU	2	686	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1081	2	-	1/7/25/26	0/2/2/2
2	OMU	2	121	2	-	0/9/27/28	0/2/2/2
2	PSU	2	966	2	-	0/7/25/26	0/2/2/2
2	OMU	2	1442	39,2	-	0/9/27/28	0/2/2/2
2	PSU	2	1232	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1447	2	-	2/9/27/28	0/3/3/3
2	OMU	2	428	2	-	4/9/27/28	0/2/2/2
2	PSU	2	34	2	-	0/7/25/26	0/2/2/2
2	A2M	2	159	2	-	0/9/27/28	0/3/3/3
2	A2M	2	166	2	-	0/9/27/28	0/3/3/3
2	OMU	2	172	2	-	0/9/27/28	0/2/2/2
2	PSU	2	681	2	-	0/7/25/26	0/2/2/2
2	OMG	2	509	39,2	-	3/9/27/28	0/3/3/3
2	PSU	2	801	2	-	1/7/25/26	0/2/2/2
2	OMC	2	1272	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1136	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1004	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1490	39,2	-	0/9/27/28	0/3/3/3
2	OMC	2	517	2	-	0/9/27/28	0/2/2/2
2	OMC	2	1391	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1692	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1383	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1625	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1046	2	-	0/7/25/26	0/2/2/2
26	HY3	X	62	26	-	1/1/12/14	0/1/1/1
2	PSU	2	210	2	-	0/7/25/26	0/2/2/2
2	PSU	2	218	2	-	0/7/25/26	0/2/2/2
2	PSU	2	296	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	863	2	-	0/7/25/26	0/2/2/2
2	OMG	2	683	2	-	1/9/27/28	0/3/3/3
2	OMC	2	174	39,2	-	0/9/27/28	0/2/2/2
2	OMC	2	797	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1445	2	-	0/7/25/26	0/2/2/2
2	PSU	2	105	2	-	0/7/25/26	0/2/2/2
2	PSU	2	406	2	-	0/7/25/26	0/2/2/2
17	IAS	O	138	17	-	1/7/7/8	-
2	4AC	2	1337	2	-	2/11/29/30	0/2/2/2
2	PSU	2	866	2	-	0/7/25/26	0/2/2/2
22	NMM	T	67	22	-	0/9/11/13	-
2	B8N	2	1248	2	-	4/16/34/35	0/2/2/2
2	PSU	2	822	2	-	2/7/25/26	0/2/2/2
2	PSU	2	1056	2	-	0/7/25/26	0/2/2/2
2	PSU	2	93	2	-	0/7/25/26	0/2/2/2
2	OMG	2	436	2	-	0/9/27/28	0/3/3/3
2	OMU	2	799	2	-	2/9/27/28	0/2/2/2
2	MA6	2	1851	2	-	1/11/29/30	0/3/3/3
3	SAC	A	2	3	-	1/7/8/10	-
2	PSU	2	572	2	-	0/7/25/26	0/2/2/2
2	PSU	2	815	2	-	0/7/25/26	0/2/2/2
2	OMU	2	627	2	-	1/9/27/28	0/2/2/2
2	A2M	2	468	2	-	0/9/27/28	0/3/3/3
2	A2M	2	590	2	-	3/9/27/28	0/3/3/3
2	OMU	2	1288	2	-	0/9/27/28	0/2/2/2
2	4AC	2	1842	2	-	2/11/29/30	0/2/2/2
2	PSU	2	36	2	-	0/7/25/26	0/2/2/2
2	A2M	2	484	2	-	2/9/27/28	0/3/3/3
21	SAC	S	2	21	-	0/7/8/10	-
2	A2M	2	576	2	-	3/9/27/28	0/3/3/3
24	AME	V	1	24	-	2/9/10/12	-
2	PSU	2	649	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1328	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1045	2	-	0/7/25/26	0/2/2/2

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1639	G7M	C4-N9	7.91	1.58	1.38
2	2	1639	G7M	O6-C6	7.52	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1850	MA6	C5-N7	6.82	1.51	1.39
2	2	1851	MA6	C5-N7	6.81	1.51	1.39
2	2	1639	G7M	C5-C4	6.17	1.53	1.38
2	2	1850	MA6	C8-N9	-5.45	1.27	1.37
2	2	1851	MA6	C8-N9	-5.42	1.27	1.37
26	X	62	HY3	C3-CA	-4.94	1.50	1.55
2	2	159	A2M	C5-C4	4.61	1.47	1.39
2	2	99	A2M	C5-C4	4.54	1.47	1.39
2	2	27	A2M	C5-C4	4.52	1.47	1.39
2	2	590	A2M	C5-C4	4.52	1.47	1.39
2	2	1639	G7M	C2-N2	4.43	1.44	1.34
2	2	484	A2M	C5-C4	4.41	1.47	1.39
2	2	1678	A2M	C5-C4	4.40	1.47	1.39
2	2	1383	A2M	C5-C4	4.39	1.47	1.39
2	2	1832	6MZ	C5-C4	4.39	1.47	1.39
2	2	166	A2M	C5-C4	4.37	1.47	1.39
2	2	468	A2M	C5-C4	4.36	1.47	1.39
2	2	576	A2M	C5-C4	4.35	1.47	1.39
2	2	512	A2M	C5-C4	4.35	1.47	1.39
2	2	1031	A2M	C5-C4	4.31	1.47	1.39
2	2	668	A2M	C5-C4	4.31	1.47	1.39
2	2	1639	G7M	C2-N1	3.80	1.47	1.37
2	2	1851	MA6	C4-N9	-3.77	1.29	1.37
2	2	1850	MA6	C4-N9	-3.45	1.30	1.37
2	2	1851	MA6	C5-C4	3.35	1.45	1.39
2	2	1850	MA6	C5-C4	3.34	1.45	1.39
2	2	1639	G7M	C2-N3	3.32	1.41	1.33
2	2	1248	B8N	C4-N3	-3.18	1.34	1.40
2	2	1625	PSU	C6-C5	3.16	1.39	1.35
2	2	210	PSU	C6-C5	3.16	1.39	1.35
2	2	801	PSU	C6-C5	3.15	1.39	1.35
2	2	1238	PSU	C6-C5	3.15	1.39	1.35
2	2	1643	PSU	C6-C5	3.11	1.38	1.35
2	2	1445	PSU	C6-C5	3.11	1.38	1.35
2	2	609	PSU	C6-C5	3.10	1.38	1.35
2	2	218	PSU	C6-C5	3.09	1.38	1.35
2	2	296	PSU	C6-C5	3.09	1.38	1.35
2	2	651	PSU	C6-C5	3.08	1.38	1.35
2	2	1447	OMG	C5-C4	3.08	1.47	1.38
2	2	1328	OMG	C5-C4	3.07	1.47	1.38
2	2	866	PSU	C6-C5	3.07	1.38	1.35
2	2	1490	OMG	C5-C4	3.07	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1232	PSU	C6-C5	3.06	1.38	1.35
2	2	1174	PSU	C6-C5	3.06	1.38	1.35
2	2	1692	PSU	C6-C5	3.06	1.38	1.35
2	2	966	PSU	C6-C5	3.05	1.38	1.35
2	2	105	PSU	C6-C5	3.03	1.38	1.35
2	2	814	PSU	C6-C5	3.02	1.38	1.35
2	2	109	PSU	C6-C5	3.02	1.38	1.35
2	2	1248	B8N	C6-C5	3.02	1.39	1.34
2	2	863	PSU	C6-C5	3.02	1.38	1.35
2	2	1056	PSU	C6-C5	3.01	1.38	1.35
2	2	683	OMG	C5-C4	3.01	1.47	1.38
2	2	93	PSU	C6-C5	3.00	1.38	1.35
2	2	1244	PSU	C6-C5	3.00	1.38	1.35
2	2	644	OMG	C5-C4	3.00	1.47	1.38
2	2	1177	PSU	C6-C5	3.00	1.38	1.35
2	2	509	OMG	C5-C4	2.99	1.47	1.38
2	2	815	PSU	C6-C5	2.99	1.38	1.35
2	2	1367	PSU	C6-C5	2.99	1.38	1.35
2	2	1046	PSU	C6-C5	2.98	1.38	1.35
2	2	1004	PSU	C6-C5	2.98	1.38	1.35
2	2	601	OMG	C5-C4	2.98	1.47	1.38
2	2	1842	4AC	C4-N4	-2.97	1.35	1.39
2	2	1081	PSU	C6-C5	2.97	1.38	1.35
2	2	572	PSU	C6-C5	2.97	1.38	1.35
2	2	436	OMG	C5-C4	2.96	1.47	1.38
2	2	1347	PSU	C6-C5	2.96	1.38	1.35
2	2	681	PSU	C6-C5	2.95	1.38	1.35
2	2	1337	4AC	C4-N4	-2.95	1.35	1.39
2	2	1850	MA6	C6-N6	2.95	1.45	1.36
2	2	119	PSU	C6-C5	2.95	1.38	1.35
2	2	36	PSU	C6-C5	2.94	1.38	1.35
2	2	406	PSU	C6-C5	2.93	1.38	1.35
2	2	686	PSU	C6-C5	2.93	1.38	1.35
2	2	34	PSU	C6-C5	2.91	1.38	1.35
2	2	1851	MA6	C6-N6	2.91	1.45	1.36
2	2	822	PSU	C6-C5	2.89	1.38	1.35
2	2	36	PSU	C4-N3	-2.87	1.33	1.38
2	2	649	PSU	C6-C5	2.87	1.38	1.35
2	2	1045	PSU	C6-C5	2.86	1.38	1.35
2	2	1136	PSU	C6-C5	2.84	1.38	1.35
2	2	34	PSU	C4-N3	-2.84	1.33	1.38
2	2	93	PSU	C4-N3	-2.80	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1136	PSU	C4-N3	-2.79	1.33	1.38
2	2	1347	PSU	C4-N3	-2.79	1.33	1.38
2	2	1081	PSU	C4-N3	-2.79	1.33	1.38
2	2	649	PSU	C4-N3	-2.79	1.33	1.38
2	2	406	PSU	C4-N3	-2.78	1.33	1.38
2	2	572	PSU	C4-N3	-2.78	1.33	1.38
2	2	1045	PSU	C4-N3	-2.77	1.33	1.38
2	2	119	PSU	C4-N3	-2.77	1.33	1.38
2	2	681	PSU	C4-N3	-2.77	1.33	1.38
2	2	1367	PSU	C4-N3	-2.76	1.33	1.38
2	2	815	PSU	C4-N3	-2.76	1.33	1.38
2	2	651	PSU	C4-N3	-2.75	1.33	1.38
2	2	609	PSU	C4-N3	-2.75	1.33	1.38
2	2	814	PSU	C4-N3	-2.75	1.33	1.38
2	2	1177	PSU	C4-N3	-2.74	1.33	1.38
2	2	966	PSU	C4-N3	-2.74	1.33	1.38
2	2	1004	PSU	C4-N3	-2.74	1.33	1.38
2	2	296	PSU	C4-N3	-2.74	1.33	1.38
2	2	863	PSU	C4-N3	-2.73	1.33	1.38
2	2	105	PSU	C4-N3	-2.73	1.33	1.38
2	2	822	PSU	C4-N3	-2.73	1.33	1.38
2	2	1692	PSU	C4-N3	-2.72	1.33	1.38
2	2	159	A2M	C5-C6	2.72	1.48	1.41
2	2	1174	PSU	C4-N3	-2.72	1.33	1.38
2	2	1445	PSU	C4-N3	-2.71	1.33	1.38
2	2	801	PSU	C4-N3	-2.71	1.33	1.38
2	2	1643	PSU	C4-N3	-2.70	1.33	1.38
2	2	1056	PSU	C4-N3	-2.70	1.33	1.38
2	2	109	PSU	C4-N3	-2.69	1.33	1.38
2	2	99	A2M	C5-C6	2.69	1.48	1.41
2	2	1625	PSU	C4-N3	-2.69	1.33	1.38
2	2	27	A2M	C5-C6	2.69	1.48	1.41
2	2	166	A2M	C5-C6	2.68	1.48	1.41
2	2	866	PSU	C4-N3	-2.68	1.33	1.38
2	2	686	PSU	C4-N3	-2.68	1.33	1.38
2	2	1046	PSU	C4-N3	-2.67	1.33	1.38
2	2	1232	PSU	C4-N3	-2.67	1.33	1.38
2	2	218	PSU	C4-N3	-2.66	1.33	1.38
2	2	1244	PSU	C4-N3	-2.66	1.33	1.38
2	2	1238	PSU	C4-N3	-2.66	1.33	1.38
2	2	210	PSU	C4-N3	-2.65	1.33	1.38
2	2	644	OMG	C6-N1	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1383	A2M	C5-C6	2.64	1.48	1.41
2	2	590	A2M	C5-C6	2.64	1.48	1.41
2	2	468	A2M	C5-C6	2.63	1.48	1.41
2	2	172	OMU	C4-N3	-2.63	1.33	1.38
2	2	1678	A2M	C5-C6	2.63	1.48	1.41
2	2	509	OMG	C6-N1	-2.63	1.34	1.38
2	2	668	A2M	C5-C6	2.62	1.48	1.41
2	2	1031	A2M	C5-C6	2.61	1.48	1.41
2	2	1442	OMU	C4-N3	-2.59	1.33	1.38
2	2	116	OMU	C4-N3	-2.58	1.33	1.38
2	2	484	A2M	C5-C6	2.58	1.48	1.41
2	2	121	OMU	C4-N3	-2.58	1.33	1.38
2	2	354	OMU	C4-N3	-2.57	1.34	1.38
2	2	576	A2M	C5-C6	2.56	1.48	1.41
2	2	436	OMG	C6-N1	-2.56	1.34	1.38
2	2	428	OMU	C4-N3	-2.55	1.34	1.38
2	2	683	OMG	C6-N1	-2.55	1.34	1.38
2	2	1490	OMG	C6-N1	-2.54	1.34	1.38
2	2	512	A2M	C5-C6	2.53	1.48	1.41
2	2	1328	OMG	C6-N1	-2.53	1.34	1.38
2	2	1288	OMU	C4-N3	-2.51	1.34	1.38
2	2	1447	OMG	C6-N1	-2.49	1.34	1.38
2	2	601	OMG	C6-N1	-2.49	1.34	1.38
2	2	627	OMU	C4-N3	-2.49	1.34	1.38
2	2	799	OMU	C4-N3	-2.48	1.34	1.38
2	2	1326	OMU	C4-N3	-2.47	1.34	1.38
2	2	1804	OMU	C4-N3	-2.45	1.34	1.38
2	2	1248	B8N	C2-N3	-2.44	1.34	1.38
2	2	159	A2M	C8-N7	2.42	1.36	1.31
2	2	1832	6MZ	C5-N7	-2.42	1.34	1.39
2	2	1383	A2M	C8-N7	2.41	1.36	1.31
2	2	99	A2M	C8-N7	2.41	1.36	1.31
2	2	668	A2M	C8-N7	2.40	1.36	1.31
2	2	468	A2M	C8-N7	2.39	1.36	1.31
2	2	27	A2M	C5-N7	-2.37	1.34	1.39
2	2	27	A2M	C8-N7	2.36	1.36	1.31
2	2	166	A2M	C8-N7	2.35	1.36	1.31
2	2	1031	A2M	C8-N7	2.35	1.36	1.31
2	2	590	A2M	C5-N7	-2.34	1.34	1.39
2	2	1639	G7M	C5-N7	2.34	1.41	1.39
2	2	576	A2M	C8-N7	2.34	1.36	1.31
2	2	576	A2M	C5-N7	-2.32	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	512	A2M	C5-N7	-2.31	1.34	1.39
2	2	1678	A2M	C8-N7	2.31	1.36	1.31
2	2	1842	4AC	C7-N4	-2.30	1.32	1.37
2	2	1832	6MZ	C5-C6	2.30	1.47	1.41
2	2	354	OMU	C2-N3	-2.28	1.33	1.38
2	2	512	A2M	C8-N7	2.28	1.35	1.31
2	2	484	A2M	C8-N7	2.27	1.35	1.31
2	2	484	A2M	C5-N7	-2.26	1.34	1.39
2	2	159	A2M	C5-N7	-2.26	1.34	1.39
2	2	99	A2M	C5-N7	-2.25	1.34	1.39
2	2	644	OMG	C5-N7	-2.25	1.34	1.39
2	2	601	OMG	C5-N7	-2.25	1.34	1.39
2	2	668	A2M	C5-N7	-2.25	1.34	1.39
2	2	509	OMG	C5-N7	-2.25	1.34	1.39
2	2	1490	OMG	C5-N7	-2.25	1.34	1.39
2	2	428	OMU	C2-N3	-2.24	1.34	1.38
2	2	1678	A2M	C5-N7	-2.23	1.34	1.39
2	2	121	OMU	C2-N3	-2.23	1.34	1.38
2	2	590	A2M	C8-N7	2.23	1.35	1.31
2	2	116	OMU	C2-N3	-2.23	1.34	1.38
2	2	1442	OMU	C2-N3	-2.22	1.34	1.38
2	2	1639	G7M	C4-N3	2.22	1.39	1.34
2	2	172	OMU	C2-N3	-2.22	1.34	1.38
2	2	1031	A2M	C5-N7	-2.21	1.34	1.39
2	2	436	OMG	C5-N7	-2.21	1.34	1.39
2	2	683	OMG	C5-N7	-2.20	1.34	1.39
2	2	1447	OMG	C5-N7	-2.20	1.34	1.39
2	2	1383	A2M	C5-N7	-2.19	1.34	1.39
2	2	166	A2M	C5-N7	-2.19	1.34	1.39
2	2	468	A2M	C5-N7	-2.18	1.34	1.39
2	2	1328	OMG	C5-N7	-2.18	1.34	1.39
2	2	1326	OMU	C2-N3	-2.17	1.34	1.38
2	2	1832	6MZ	C8-N7	2.16	1.35	1.31
2	2	1337	4AC	C7-N4	-2.14	1.33	1.37
2	2	1804	OMU	C2-N3	-2.14	1.34	1.38
2	2	799	OMU	C2-N3	-2.13	1.34	1.38
2	2	1288	OMU	C2-N3	-2.10	1.34	1.38
2	2	121	OMU	C5-C4	-2.08	1.39	1.43
2	2	627	OMU	C2-N3	-2.07	1.34	1.38
2	2	1288	OMU	C2-N1	2.07	1.41	1.38
2	2	1081	PSU	C2-N3	-2.07	1.34	1.37
2	2	354	OMU	C5-C4	-2.06	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	428	OMU	C5-C4	-2.06	1.39	1.43
2	2	116	OMU	C5-C4	-2.04	1.39	1.43
2	2	1804	OMU	C2-N1	2.02	1.41	1.38
2	2	799	OMU	C5-C4	-2.02	1.39	1.43

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1850	MA6	C4-N9-C8	14.46	121.39	105.73
2	2	1851	MA6	C4-N9-C8	14.39	121.32	105.73
2	2	1639	G7M	C8-N7-C5	11.31	121.92	107.78
2	2	1850	MA6	N3-C4-N9	6.98	138.59	127.08
2	2	590	A2M	C5-C4-N3	-6.97	117.66	126.75
2	2	1639	G7M	N9-C4-N3	6.74	139.47	125.94
2	2	1832	6MZ	C5-C4-N3	-6.58	118.17	126.75
2	2	1851	MA6	N3-C4-N9	6.58	137.92	127.08
2	2	27	A2M	C5-C4-N3	-6.32	118.51	126.75
2	2	484	A2M	C5-C4-N3	-6.29	118.54	126.75
2	2	159	A2M	C5-C4-N3	-6.28	118.56	126.75
2	2	512	A2M	C5-C4-N3	-6.25	118.60	126.75
2	2	166	A2M	C5-C4-N3	-6.24	118.61	126.75
2	2	1639	G7M	C6-C5-N7	6.22	139.77	132.25
2	2	509	OMG	C5-C4-N3	-6.22	118.37	128.46
2	2	1328	OMG	C5-C4-N3	-6.21	118.38	128.46
2	2	822	PSU	N1-C2-N3	6.21	122.16	115.13
2	2	99	A2M	C5-C4-N3	-6.21	118.65	126.75
2	2	1383	A2M	C5-C4-N3	-6.19	118.68	126.75
2	2	468	A2M	C5-C4-N3	-6.17	118.70	126.75
2	2	1678	A2M	C5-C4-N3	-6.16	118.71	126.75
2	2	1447	OMG	C5-C4-N3	-6.15	118.49	128.46
2	2	668	A2M	C5-C4-N3	-6.14	118.73	126.75
2	2	644	OMG	C5-C4-N3	-6.13	118.51	128.46
2	2	36	PSU	N1-C2-N3	6.13	122.07	115.13
2	2	1490	OMG	C5-C4-N3	-6.13	118.52	128.46
2	2	34	PSU	N1-C2-N3	6.13	122.07	115.13
2	2	93	PSU	N1-C2-N3	6.11	122.05	115.13
2	2	572	PSU	N1-C2-N3	6.11	122.05	115.13
2	2	681	PSU	N1-C2-N3	6.09	122.03	115.13
2	2	436	OMG	C5-C4-N3	-6.09	118.59	128.46
2	2	1232	PSU	N1-C2-N3	6.08	122.02	115.13
2	2	683	OMG	C5-C4-N3	-6.07	118.61	128.46
2	2	651	PSU	N1-C2-N3	6.07	122.01	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	406	PSU	N1-C2-N3	6.06	122.00	115.13
2	2	601	OMG	C5-C4-N3	-6.06	118.63	128.46
2	2	105	PSU	N1-C2-N3	6.06	121.99	115.13
2	2	1445	PSU	N1-C2-N3	6.05	121.99	115.13
2	2	1639	G7M	CN7-N7-C5	-6.05	119.25	126.77
2	2	866	PSU	N1-C2-N3	6.05	121.98	115.13
2	2	1031	A2M	C5-C4-N3	-6.03	118.88	126.75
2	2	1136	PSU	N1-C2-N3	6.03	121.96	115.13
2	2	1692	PSU	N1-C2-N3	6.03	121.96	115.13
2	2	296	PSU	N1-C2-N3	6.02	121.96	115.13
2	2	815	PSU	N1-C2-N3	6.02	121.95	115.13
2	2	686	PSU	N1-C2-N3	6.01	121.94	115.13
2	2	119	PSU	N1-C2-N3	6.01	121.94	115.13
2	2	1625	PSU	N1-C2-N3	6.00	121.93	115.13
2	2	109	PSU	N1-C2-N3	6.00	121.93	115.13
2	2	1367	PSU	N1-C2-N3	6.00	121.92	115.13
2	2	649	PSU	N1-C2-N3	5.99	121.92	115.13
2	2	801	PSU	N1-C2-N3	5.98	121.91	115.13
2	2	1238	PSU	N1-C2-N3	5.98	121.91	115.13
2	2	1643	PSU	N1-C2-N3	5.98	121.91	115.13
2	2	1850	MA6	C5-C4-N3	-5.98	118.95	126.75
2	2	218	PSU	N1-C2-N3	5.98	121.90	115.13
2	2	1004	PSU	N1-C2-N3	5.98	121.90	115.13
2	2	966	PSU	N1-C2-N3	5.96	121.88	115.13
2	2	1045	PSU	N1-C2-N3	5.96	121.88	115.13
2	2	1056	PSU	N1-C2-N3	5.95	121.88	115.13
2	2	1347	PSU	N1-C2-N3	5.95	121.88	115.13
2	2	609	PSU	N1-C2-N3	5.95	121.87	115.13
2	2	814	PSU	N1-C2-N3	5.95	121.87	115.13
2	2	210	PSU	N1-C2-N3	5.95	121.87	115.13
2	2	863	PSU	N1-C2-N3	5.95	121.87	115.13
2	2	1174	PSU	N1-C2-N3	5.95	121.87	115.13
2	2	1046	PSU	N1-C2-N3	5.94	121.86	115.13
2	2	1177	PSU	N1-C2-N3	5.94	121.86	115.13
2	2	576	A2M	C5-C4-N3	-5.94	119.00	126.75
2	2	1244	PSU	N1-C2-N3	5.88	121.80	115.13
2	2	1081	PSU	N1-C2-N3	5.87	121.78	115.13
2	2	1850	MA6	C4-C5-N7	-5.85	103.49	110.62
2	2	1850	MA6	N9-C8-N7	-5.77	106.02	113.91
2	2	1851	MA6	C4-C5-N7	-5.71	103.66	110.62
2	2	1851	MA6	N9-C8-N7	-5.56	106.30	113.91
2	2	1851	MA6	C5-C4-N3	-5.52	119.54	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	590	A2M	N3-C4-N9	5.48	136.10	127.08
2	2	1832	6MZ	N3-C4-N9	5.42	136.01	127.08
2	2	436	OMG	C2-N3-C4	4.93	121.09	112.30
2	2	509	OMG	C2-N3-C4	4.91	121.05	112.30
2	2	1328	OMG	C2-N3-C4	4.90	121.03	112.30
2	2	27	A2M	N3-C4-N9	4.88	135.12	127.08
2	2	1447	OMG	C2-N3-C4	4.87	120.98	112.30
2	2	644	OMG	C2-N3-C4	4.87	120.98	112.30
2	2	484	A2M	N3-C4-N9	4.86	135.09	127.08
2	2	1490	OMG	C2-N3-C4	4.86	120.95	112.30
2	2	601	OMG	C2-N3-C4	4.85	120.95	112.30
2	2	512	A2M	N3-C4-N9	4.85	135.07	127.08
2	2	1678	A2M	N3-C4-N9	4.84	135.06	127.08
2	2	166	A2M	N3-C4-N9	4.83	135.05	127.08
2	2	683	OMG	C2-N3-C4	4.83	120.90	112.30
2	2	159	A2M	N3-C4-N9	4.82	135.03	127.08
2	2	1383	A2M	N3-C4-N9	4.75	134.91	127.08
2	2	468	A2M	N3-C4-N9	4.74	134.90	127.08
2	2	99	A2M	N3-C4-N9	4.71	134.85	127.08
2	2	668	A2M	N3-C4-N9	4.70	134.82	127.08
2	2	1639	G7M	C2-N3-C4	4.69	120.65	112.30
2	2	576	A2M	N3-C4-N9	4.67	134.77	127.08
2	2	509	OMG	N9-C4-N3	4.66	135.29	125.94
2	2	1031	A2M	N3-C4-N9	4.64	134.73	127.08
2	2	1328	OMG	N9-C4-N3	4.62	135.22	125.94
2	2	1490	OMG	N9-C4-N3	4.60	135.18	125.94
2	2	644	OMG	N9-C4-N3	4.60	135.17	125.94
2	2	1447	OMG	N9-C4-N3	4.58	135.14	125.94
2	2	1326	OMU	C4-N3-C2	-4.57	120.56	126.58
2	2	799	OMU	C4-N3-C2	-4.56	120.56	126.58
2	2	436	OMG	N9-C4-N3	4.56	135.09	125.94
2	2	683	OMG	N9-C4-N3	4.56	135.09	125.94
2	2	601	OMG	N9-C4-N3	4.54	135.05	125.94
2	2	172	OMU	C4-N3-C2	-4.51	120.62	126.58
2	2	428	OMU	C4-N3-C2	-4.51	120.63	126.58
2	2	1442	OMU	C4-N3-C2	-4.50	120.64	126.58
2	2	627	OMU	C4-N3-C2	-4.49	120.66	126.58
2	2	121	OMU	C4-N3-C2	-4.43	120.73	126.58
2	2	1851	MA6	N1-C2-N3	-4.41	121.70	128.60
2	2	1804	OMU	C4-N3-C2	-4.41	120.76	126.58
2	2	1842	4AC	N4-C4-N3	4.40	121.24	113.85
2	2	1639	G7M	C5-C4-N3	-4.40	119.71	128.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	116	OMU	C4-N3-C2	-4.39	120.78	126.58
2	2	1288	OMU	C4-N3-C2	-4.39	120.79	126.58
2	2	354	OMU	C4-N3-C2	-4.38	120.80	126.58
2	2	1850	MA6	N1-C2-N3	-4.27	121.93	128.60
2	2	1851	MA6	C2-N1-C6	4.25	121.78	111.75
2	2	799	OMU	N3-C2-N1	4.19	120.46	114.89
2	2	590	A2M	C2-N3-C4	4.18	121.63	111.75
2	2	116	OMU	N3-C2-N1	4.16	120.41	114.89
2	2	627	OMU	N3-C2-N1	4.15	120.40	114.89
2	2	93	PSU	C4-N3-C2	-4.15	120.36	126.34
2	2	172	OMU	N3-C2-N1	4.15	120.39	114.89
2	2	1442	OMU	N3-C2-N1	4.14	120.38	114.89
2	2	1850	MA6	C2-N1-C6	4.12	121.49	111.75
2	2	1326	OMU	N3-C2-N1	4.12	120.36	114.89
2	2	34	PSU	C4-N3-C2	-4.12	120.41	126.34
2	2	121	OMU	N3-C2-N1	4.10	120.33	114.89
2	2	1804	OMU	N3-C2-N1	4.10	120.33	114.89
2	2	354	OMU	N3-C2-N1	4.09	120.32	114.89
2	2	686	PSU	C4-N3-C2	-4.09	120.44	126.34
2	2	36	PSU	C4-N3-C2	-4.07	120.47	126.34
2	2	866	PSU	C4-N3-C2	-4.07	120.48	126.34
2	2	428	OMU	N3-C2-N1	4.06	120.29	114.89
2	2	1232	PSU	C4-N3-C2	-4.02	120.54	126.34
2	2	681	PSU	C4-N3-C2	-4.02	120.55	126.34
2	2	801	PSU	C4-N3-C2	-4.02	120.55	126.34
2	2	651	PSU	C4-N3-C2	-4.01	120.56	126.34
2	2	649	PSU	C4-N3-C2	-4.00	120.57	126.34
2	2	576	A2M	C2'-C1'-N9	-4.00	106.80	113.53
2	2	1288	OMU	N3-C2-N1	3.99	120.19	114.89
2	2	572	PSU	C4-N3-C2	-3.99	120.58	126.34
2	2	1136	PSU	C4-N3-C2	-3.99	120.58	126.34
2	2	109	PSU	C4-N3-C2	-3.99	120.59	126.34
2	2	1367	PSU	C4-N3-C2	-3.98	120.60	126.34
2	2	815	PSU	C4-N3-C2	-3.98	120.60	126.34
2	2	1347	PSU	C4-N3-C2	-3.98	120.60	126.34
2	2	1045	PSU	C4-N3-C2	-3.97	120.61	126.34
2	2	1445	PSU	C4-N3-C2	-3.96	120.63	126.34
2	2	406	PSU	C4-N3-C2	-3.95	120.65	126.34
2	2	105	PSU	C4-N3-C2	-3.95	120.65	126.34
2	2	1692	PSU	C4-N3-C2	-3.94	120.66	126.34
2	2	119	PSU	C4-N3-C2	-3.93	120.67	126.34
2	2	1174	PSU	C4-N3-C2	-3.93	120.68	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	296	PSU	C4-N3-C2	-3.92	120.69	126.34
2	2	814	PSU	C4-N3-C2	-3.91	120.70	126.34
2	2	166	A2M	C2-N3-C4	3.90	120.97	111.75
2	2	1056	PSU	C4-N3-C2	-3.90	120.72	126.34
2	2	1625	PSU	C4-N3-C2	-3.90	120.72	126.34
2	2	1081	PSU	C4-N3-C2	-3.90	120.72	126.34
2	2	1639	G7M	CN7-N7-C8	-3.90	118.83	124.84
2	2	609	PSU	C4-N3-C2	-3.89	120.73	126.34
2	2	1177	PSU	C4-N3-C2	-3.89	120.73	126.34
2	2	966	PSU	C4-N3-C2	-3.89	120.74	126.34
2	2	863	PSU	C4-N3-C2	-3.87	120.76	126.34
2	2	1639	G7M	C5-C6-N1	3.86	119.86	111.79
2	2	210	PSU	C4-N3-C2	-3.86	120.77	126.34
2	2	1004	PSU	C4-N3-C2	-3.86	120.78	126.34
2	2	1678	A2M	C2-N3-C4	3.86	120.86	111.75
2	2	1383	A2M	C2-N3-C4	3.85	120.85	111.75
2	2	512	A2M	C2-N3-C4	3.85	120.84	111.75
2	2	484	A2M	C2-N3-C4	3.85	120.84	111.75
2	2	1643	PSU	C4-N3-C2	-3.85	120.79	126.34
2	2	822	PSU	C4-N3-C2	-3.85	120.80	126.34
2	2	668	A2M	C2-N3-C4	3.84	120.81	111.75
2	2	468	A2M	C2-N3-C4	3.84	120.81	111.75
2	2	1832	6MZ	C2-N3-C4	3.83	120.80	111.75
2	2	1238	PSU	C4-N3-C2	-3.82	120.83	126.34
2	2	27	A2M	C2-N3-C4	3.82	120.77	111.75
2	2	1031	A2M	C2-N3-C4	3.81	120.76	111.75
2	2	99	A2M	C2-N3-C4	3.81	120.75	111.75
2	2	218	PSU	C4-N3-C2	-3.79	120.87	126.34
2	2	822	PSU	O2-C2-N1	-3.79	118.62	122.79
2	2	159	A2M	C2-N3-C4	3.78	120.68	111.75
2	2	576	A2M	C2-N3-C4	3.77	120.66	111.75
2	2	1046	PSU	C4-N3-C2	-3.76	120.92	126.34
2	2	1639	G7M	N9-C8-N7	-3.71	103.04	112.21
2	2	1244	PSU	C4-N3-C2	-3.70	121.01	126.34
2	2	1850	MA6	C1'-N9-C8	-3.66	118.88	127.14
2	2	34	PSU	O2-C2-N1	-3.65	118.77	122.79
2	2	512	A2M	C2'-C1'-N9	-3.64	107.41	113.53
2	2	428	OMU	C5-C4-N3	3.63	120.27	114.84
2	2	1326	OMU	C5-C4-N3	3.62	120.25	114.84
2	2	1288	OMU	C5-C4-N3	3.60	120.23	114.84
2	2	1442	OMU	C5-C4-N3	3.60	120.22	114.84
2	2	172	OMU	C5-C4-N3	3.59	120.22	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	93	PSU	O2-C2-N1	-3.59	118.83	122.79
2	2	1851	MA6	C6-C5-N7	3.56	139.25	133.28
2	2	121	OMU	C5-C4-N3	3.56	120.16	114.84
2	2	354	OMU	C5-C4-N3	3.55	120.16	114.84
2	2	1804	OMU	C5-C4-N3	3.54	120.13	114.84
2	2	218	PSU	O2-C2-N1	-3.53	118.90	122.79
2	2	1850	MA6	C2-N3-C4	3.53	120.09	111.75
2	2	686	PSU	O2-C2-N1	-3.52	118.92	122.79
2	2	99	A2M	C2'-C1'-N9	-3.52	107.61	113.53
2	2	36	PSU	O2-C2-N1	-3.51	118.93	122.79
2	2	1046	PSU	O2-C2-N1	-3.50	118.94	122.79
2	2	116	OMU	C5-C4-N3	3.50	120.07	114.84
2	2	1639	G7M	O6-C6-C5	-3.49	120.18	128.06
2	2	27	A2M	C2'-C1'-N9	-3.49	107.66	113.53
2	2	627	OMU	C5-C4-N3	3.48	120.05	114.84
2	2	1851	MA6	C2-N3-C4	3.48	119.98	111.75
2	2	1004	PSU	O2-C2-N1	-3.48	118.96	122.79
2	2	1445	PSU	O2-C2-N1	-3.47	118.97	122.79
2	2	1056	PSU	O2-C2-N1	-3.46	118.98	122.79
2	2	99	A2M	C4-C5-N7	-3.46	106.40	110.62
2	2	109	PSU	O2-C2-N1	-3.46	118.98	122.79
2	2	799	OMU	C5-C4-N3	3.46	120.01	114.84
2	2	572	PSU	O2-C2-N1	-3.45	118.99	122.79
2	2	210	PSU	O2-C2-N1	-3.44	119.01	122.79
2	2	1367	PSU	O2-C2-N1	-3.44	119.01	122.79
2	2	296	PSU	O2-C2-N1	-3.43	119.01	122.79
2	2	159	A2M	C4-C5-N7	-3.43	106.44	110.62
2	2	863	PSU	O2-C2-N1	-3.43	119.01	122.79
2	2	1232	PSU	O2-C2-N1	-3.43	119.02	122.79
2	2	866	PSU	O2-C2-N1	-3.42	119.02	122.79
2	2	1136	PSU	O2-C2-N1	-3.42	119.03	122.79
2	2	27	A2M	C4-C5-N7	-3.42	106.45	110.62
2	2	1639	G7M	C4-C5-N7	-3.42	102.08	107.67
2	2	1174	PSU	O2-C2-N1	-3.41	119.03	122.79
2	2	1678	A2M	C2'-C1'-N9	-3.40	107.80	113.53
2	2	406	PSU	O2-C2-N1	-3.40	119.04	122.79
2	2	1692	PSU	O2-C2-N1	-3.40	119.05	122.79
2	2	651	PSU	O2-C2-N1	-3.39	119.05	122.79
2	2	105	PSU	O2-C2-N1	-3.38	119.07	122.79
2	2	681	PSU	O2-C2-N1	-3.38	119.07	122.79
2	2	966	PSU	O2-C2-N1	-3.38	119.07	122.79
2	2	814	PSU	O2-C2-N1	-3.38	119.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	119	PSU	O2-C2-N1	-3.37	119.08	122.79
2	2	1851	MA6	C1'-N9-C8	-3.37	119.53	127.14
2	2	1031	A2M	C2'-C1'-N9	-3.36	107.87	113.53
2	2	1625	PSU	O2-C2-N1	-3.36	119.09	122.79
2	2	484	A2M	C4-C5-N7	-3.36	106.53	110.62
2	2	1238	PSU	O2-C2-N1	-3.35	119.10	122.79
2	2	801	PSU	O2-C2-N1	-3.35	119.10	122.79
2	2	159	A2M	C2'-C1'-N9	-3.35	107.89	113.53
2	2	815	PSU	O2-C2-N1	-3.34	119.11	122.79
2	2	1383	A2M	C4-C5-N7	-3.34	106.55	110.62
2	2	1643	PSU	O2-C2-N1	-3.34	119.11	122.79
2	2	1850	MA6	C6-C5-N7	3.34	138.88	133.28
2	2	649	PSU	O2-C2-N1	-3.33	119.12	122.79
2	2	1383	A2M	C2'-C1'-N9	-3.33	107.92	113.53
2	2	668	A2M	C4-C5-N7	-3.32	106.58	110.62
2	2	1244	PSU	O2-C2-N1	-3.32	119.14	122.79
2	2	609	PSU	O2-C2-N1	-3.31	119.14	122.79
2	2	166	A2M	C4-C5-N7	-3.31	106.59	110.62
2	2	1031	A2M	C4-C5-N7	-3.31	106.59	110.62
2	2	1177	PSU	O2-C2-N1	-3.31	119.15	122.79
2	2	1045	PSU	O2-C2-N1	-3.30	119.16	122.79
2	2	1248	B8N	C4-N3-C2	-3.28	121.31	125.46
2	2	468	A2M	C4-C5-N7	-3.28	106.62	110.62
2	2	1347	PSU	O2-C2-N1	-3.28	119.18	122.79
2	2	166	A2M	C2'-C1'-N9	-3.27	108.03	113.53
2	2	1337	4AC	N4-C4-N3	3.26	119.32	113.85
2	2	512	A2M	C4-C5-N7	-3.24	106.67	110.62
2	2	1678	A2M	C4-C5-N7	-3.22	106.69	110.62
2	2	436	OMG	C6-C5-N7	3.18	136.16	130.25
2	2	576	A2M	C4-C5-N7	-3.17	106.75	110.62
2	2	576	A2M	N3-C2-N1	-3.17	123.64	128.60
2	2	1678	A2M	N3-C2-N1	-3.17	123.65	128.60
2	2	1081	PSU	O2-C2-N1	-3.17	119.31	122.79
2	2	1031	A2M	N3-C2-N1	-3.16	123.66	128.60
2	2	590	A2M	N3-C2-N1	-3.16	123.66	128.60
2	2	644	OMG	C6-C5-N7	3.16	136.12	130.25
2	2	590	A2M	C4-C5-N7	-3.15	106.78	110.62
2	2	166	A2M	N3-C2-N1	-3.14	123.69	128.60
2	2	1851	MA6	C4-N9-C1'	-3.13	119.14	126.59
2	2	601	OMG	C6-C5-N7	3.11	136.03	130.25
2	2	683	OMG	C6-C5-N7	3.11	136.02	130.25
2	2	428	OMU	O4-C4-C5	-3.10	119.71	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1383	A2M	N3-C2-N1	-3.10	123.75	128.60
2	2	1328	OMG	C6-C5-N7	3.10	136.01	130.25
2	2	512	A2M	N3-C2-N1	-3.10	123.75	128.60
2	2	668	A2M	N3-C2-N1	-3.07	123.80	128.60
2	2	1326	OMU	O4-C4-C5	-3.07	119.76	125.16
2	2	468	A2M	N3-C2-N1	-3.06	123.81	128.60
2	2	468	A2M	C2'-C1'-N9	-3.06	108.38	113.53
2	2	799	OMU	O4-C4-C5	-3.06	119.78	125.16
2	2	1490	OMG	C6-C5-N7	3.05	135.92	130.25
2	2	354	OMU	O4-C4-C5	-3.05	119.80	125.16
2	2	1639	G7M	C2-N1-C6	-3.04	119.55	125.10
2	2	484	A2M	N3-C2-N1	-3.04	123.85	128.60
2	2	509	OMG	C6-C5-N7	3.04	135.90	130.25
2	2	1447	OMG	C6-C5-N7	3.04	135.89	130.25
2	2	1288	OMU	O4-C4-C5	-2.99	119.91	125.16
2	2	1248	B8N	N3-C2-N1	2.98	120.97	116.76
2	2	121	OMU	O4-C4-C5	-2.98	119.91	125.16
2	2	1804	OMU	O4-C4-C5	-2.98	119.92	125.16
2	2	116	OMU	O4-C4-C5	-2.98	119.92	125.16
2	2	172	OMU	O4-C4-C5	-2.96	119.95	125.16
2	2	1832	6MZ	N1-C2-N3	-2.94	124.01	128.60
2	2	627	OMU	O4-C4-C5	-2.92	120.02	125.16
2	2	1850	MA6	C4-N9-C1'	-2.88	119.72	126.59
2	2	27	A2M	C5-N7-C8	2.86	107.58	103.51
2	2	27	A2M	N3-C2-N1	-2.86	124.13	128.60
2	2	1442	OMU	O4-C4-C5	-2.86	120.14	125.16
2	2	1850	MA6	C5-C4-N9	-2.85	102.47	105.78
2	2	99	A2M	N3-C2-N1	-2.83	124.17	128.60
2	2	1832	6MZ	C4-C5-N7	-2.83	107.17	110.62
2	2	159	A2M	C5-N7-C8	2.81	107.50	103.51
2	2	99	A2M	C5-N7-C8	2.80	107.49	103.51
2	2	166	A2M	C5-N7-C8	2.80	107.48	103.51
2	2	1383	A2M	C5-N7-C8	2.80	107.48	103.51
2	2	1851	MA6	C5-C4-N9	-2.79	102.54	105.78
2	2	159	A2M	N3-C2-N1	-2.77	124.27	128.60
2	2	484	A2M	C5-N7-C8	2.77	107.44	103.51
2	2	668	A2M	C5-N7-C8	2.74	107.40	103.51
2	2	1678	A2M	C5-N7-C8	2.72	107.37	103.51
2	2	1031	A2M	C5-N7-C8	2.72	107.37	103.51
2	2	468	A2M	C5-N7-C8	2.71	107.36	103.51
2	2	512	A2M	C5-N7-C8	2.70	107.35	103.51
2	2	576	A2M	C5-N7-C8	2.69	107.33	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	576	A2M	C4-N9-C8	2.69	108.64	105.73
2	2	590	A2M	C5-N7-C8	2.67	107.31	103.51
2	2	1031	A2M	C4-N9-C8	2.63	108.58	105.73
2	2	1328	OMG	C4-C5-N7	-2.62	106.57	110.72
2	2	27	A2M	C4-N9-C8	2.61	108.56	105.73
2	2	644	OMG	C4-C5-N7	-2.58	106.63	110.72
2	2	683	OMG	C4-C5-N7	-2.57	106.65	110.72
2	2	159	A2M	C4-N9-C8	2.57	108.51	105.73
2	2	436	OMG	C4-C5-N7	-2.57	106.66	110.72
2	2	99	A2M	C4-N9-C8	2.56	108.50	105.73
2	2	668	A2M	C4-N9-C8	2.56	108.50	105.73
2	2	1678	A2M	C4-N9-C8	2.56	108.50	105.73
2	2	509	OMG	C4-C5-N7	-2.55	106.68	110.72
17	O	138	IAS	OD1-CG-CB	-2.55	118.01	125.43
2	2	1447	OMG	C4-C5-N7	-2.53	106.71	110.72
24	V	1	AME	O-C-CA	-2.53	118.14	124.78
2	2	1383	A2M	C4-N9-C8	2.53	108.47	105.73
2	2	601	OMG	C4-C5-N7	-2.53	106.72	110.72
2	2	1832	6MZ	C4-N9-C8	2.52	108.46	105.73
2	2	468	A2M	C4-N9-C8	2.52	108.46	105.73
2	2	166	A2M	C4-N9-C8	2.52	108.45	105.73
2	2	1832	6MZ	C5-N7-C8	2.51	107.07	103.51
2	2	1490	OMG	C4-C5-N7	-2.50	106.76	110.72
2	2	484	A2M	C4-N9-C8	2.49	108.43	105.73
2	2	512	A2M	C4-N9-C8	2.48	108.42	105.73
21	S	2	SAC	O-C-CA	-2.45	118.35	124.78
2	2	1842	4AC	C6-C5-C4	2.43	119.94	116.96
2	2	1337	4AC	C6-C5-C4	2.38	119.88	116.96
2	2	1639	G7M	C5-C4-N9	-2.32	100.81	105.89
3	A	2	SAC	O-C-CA	-2.32	118.70	124.78
2	2	1326	OMU	O2-C2-N1	-2.29	119.74	122.79
2	2	99	A2M	C6-C5-N7	2.28	136.27	132.02
2	2	428	OMU	O2-C2-N1	-2.27	119.77	122.79
2	2	1842	4AC	C5-C4-N4	-2.27	118.98	122.92
2	2	1832	6MZ	C6-C5-N7	2.26	134.83	132.39
2	2	1031	A2M	C6-C5-N7	2.26	136.23	132.02
26	X	62	HY3	O-C-CA	-2.26	118.54	124.83
2	2	484	A2M	C2'-C1'-N9	-2.25	109.75	113.53
2	2	166	A2M	C6-C5-N7	2.22	136.16	132.02
2	2	668	A2M	C6-C5-N7	2.22	136.16	132.02
2	2	1850	MA6	C5-N7-C8	2.20	106.64	103.51
2	2	1383	A2M	C6-C5-N7	2.20	136.12	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	159	A2M	C6-C5-N7	2.20	136.11	132.02
2	2	121	OMU	O2-C2-N1	-2.18	119.88	122.79
2	2	27	A2M	C6-C5-N7	2.18	136.08	132.02
2	2	1272	OMC	O2-C2-N3	-2.18	118.79	122.33
2	2	576	A2M	C6-C5-N7	2.18	136.08	132.02
2	2	172	OMU	O2-C2-N1	-2.18	119.89	122.79
2	2	601	OMG	O6-C6-C5	-2.18	120.83	126.60
2	2	1490	OMG	O6-C6-C5	-2.17	120.85	126.60
2	2	468	A2M	C6-C5-N7	2.16	136.05	132.02
2	2	1248	B8N	C5-C4-N3	2.16	120.18	116.17
2	2	1328	OMG	O6-C6-C5	-2.16	120.87	126.60
2	2	484	A2M	C6-C5-N7	2.16	136.04	132.02
2	2	644	OMG	O6-C6-C5	-2.15	120.90	126.60
2	2	509	OMG	O6-C6-C5	-2.14	120.92	126.60
2	2	683	OMG	O6-C6-C5	-2.13	120.94	126.60
2	2	436	OMG	O6-C6-C5	-2.12	120.97	126.60
2	2	354	OMU	O2-C2-N1	-2.12	119.97	122.79
2	2	1447	OMG	O6-C6-C5	-2.12	120.99	126.60
2	2	1703	OMC	O2-C2-N3	-2.11	118.89	122.33
2	2	822	PSU	O4'-C1'-C2'	2.11	108.12	105.14
2	2	1678	A2M	C6-C5-N7	2.11	135.94	132.02
2	2	27	A2M	N9-C8-N7	-2.10	111.05	113.91
2	2	576	A2M	N9-C8-N7	-2.10	111.05	113.91
2	2	797	OMC	O2-C2-N3	-2.09	118.93	122.33
2	2	590	A2M	C4-N9-C8	2.09	107.99	105.73
2	2	1031	A2M	N9-C8-N7	-2.08	111.07	113.91
2	2	866	PSU	C5-C6-N1	-2.07	119.00	122.11
2	2	668	A2M	N9-C8-N7	-2.07	111.08	113.91
2	2	512	A2M	C6-C5-N7	2.07	135.88	132.02
2	2	1383	A2M	N9-C8-N7	-2.07	111.08	113.91
2	2	799	OMU	O2-C2-N1	-2.06	120.05	122.79
2	2	99	A2M	N9-C8-N7	-2.05	111.10	113.91
2	2	627	OMU	O2-C2-N1	-2.05	120.06	122.79
2	2	649	PSU	C5-C6-N1	-2.04	119.04	122.11
2	2	166	A2M	N9-C8-N7	-2.03	111.13	113.91
2	2	159	A2M	N9-C8-N7	-2.03	111.14	113.91
2	2	651	PSU	C5-C6-N1	-2.03	119.06	122.11
2	2	468	A2M	N9-C8-N7	-2.02	111.16	113.91
2	2	1232	PSU	C5-C6-N1	-2.01	119.09	122.11
2	2	686	PSU	C5-C6-N1	-2.01	119.09	122.11

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	428	OMU	C2'-C1'-N1-C2
2	2	428	OMU	C2'-C1'-N1-C6
2	2	644	OMG	O4'-C4'-C5'-O5'
2	2	644	OMG	C3'-C4'-C5'-O5'
2	2	668	A2M	C1'-C2'-O2'-CM'
2	2	1248	B8N	N34-C33-C34-O35
2	2	1337	4AC	O7-C7-N4-C4
2	2	1337	4AC	CM7-C7-N4-C4
2	2	1842	4AC	N3-C4-N4-C7
2	2	1842	4AC	C5-C4-N4-C7
2	2	512	A2M	O4'-C4'-C5'-O5'
2	2	668	A2M	O4'-C4'-C5'-O5'
2	2	668	A2M	C3'-C4'-C5'-O5'
24	V	1	AME	CT2-CT1-N-CA
24	V	1	AME	OT-CT1-N-CA
2	2	1248	B8N	N34-C33-C34-O36
2	2	512	A2M	C3'-C4'-C5'-O5'
2	2	576	A2M	C3'-C4'-C5'-O5'
2	2	1447	OMG	C3'-C4'-C5'-O5'
2	2	509	OMG	C3'-C4'-C5'-O5'
2	2	799	OMU	C4'-C5'-O5'-P
2	2	99	A2M	O4'-C4'-C5'-O5'
2	2	576	A2M	O4'-C4'-C5'-O5'
2	2	509	OMG	O4'-C4'-C5'-O5'
2	2	1447	OMG	O4'-C4'-C5'-O5'
2	2	627	OMU	C4'-C5'-O5'-P
2	2	1851	MA6	C4'-C5'-O5'-P
2	2	822	PSU	C3'-C4'-C5'-O5'
2	2	590	A2M	C2'-C1'-N9-C4
3	A	2	SAC	C-CA-N-C1A
2	2	354	OMU	C3'-C2'-O2'-CM2
2	2	484	A2M	C3'-C2'-O2'-CM'
2	2	1248	B8N	C32-C33-C34-O36
2	2	1248	B8N	C32-C33-C34-O35
2	2	644	OMG	C4'-C5'-O5'-P
2	2	1703	OMC	C3'-C4'-C5'-O5'
2	2	590	A2M	C2'-C1'-N9-C8
2	2	576	A2M	C3'-C2'-O2'-CM'
2	2	428	OMU	O4'-C1'-N1-C6
2	2	668	A2M	C2'-C1'-N9-C8
2	2	801	PSU	O4'-C1'-C5-C4
2	2	509	OMG	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
2	2	512	A2M	C3'-C2'-O2'-CM'
2	2	797	OMC	C3'-C2'-O2'-CM2
2	2	1272	OMC	C3'-C2'-O2'-CM2
2	2	1391	OMC	C3'-C2'-O2'-CM2
2	2	590	A2M	O4'-C1'-N9-C8
2	2	822	PSU	O4'-C4'-C5'-O5'
2	2	484	A2M	C1'-C2'-O2'-CM'
2	2	428	OMU	O4'-C1'-N1-C2
26	X	62	HY3	O-C-CA-C3
2	2	116	OMU	O4'-C4'-C5'-O5'
2	2	799	OMU	O4'-C4'-C5'-O5'
17	O	138	IAS	CA-CB-CG-OD1
2	2	683	OMG	C3'-C2'-O2'-CM2
2	2	99	A2M	C3'-C4'-C5'-O5'
2	2	1081	PSU	C4'-C5'-O5'-P

There are no ring outliers.

38 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1703	OMC	1	0
2	2	1850	MA6	1	0
2	2	512	A2M	1	0
2	2	1031	A2M	2	0
2	2	354	OMU	1	0
2	2	27	A2M	1	0
2	2	601	OMG	1	0
2	2	116	OMU	1	0
2	2	1678	A2M	1	0
2	2	462	OMC	1	0
2	2	668	A2M	1	0
2	2	1804	OMU	1	0
2	2	121	OMU	1	0
2	2	1442	OMU	1	0
2	2	1232	PSU	1	0
2	2	1447	OMG	2	0
2	2	428	OMU	1	0
2	2	166	A2M	2	0
2	2	681	PSU	1	0
2	2	509	OMG	2	0
2	2	801	PSU	1	0
2	2	1272	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1490	OMG	1	0
2	2	517	OMC	1	0
2	2	1391	OMC	1	0
2	2	1383	A2M	1	0
2	2	1445	PSU	1	0
2	2	1337	4AC	2	0
2	2	436	OMG	2	0
2	2	799	OMU	4	0
3	A	2	SAC	1	0
2	2	468	A2M	1	0
2	2	1288	OMU	1	0
2	2	1842	4AC	2	0
2	2	36	PSU	1	0
2	2	484	A2M	1	0
2	2	576	A2M	1	0
24	V	1	AME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 117 are unknown and 114 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

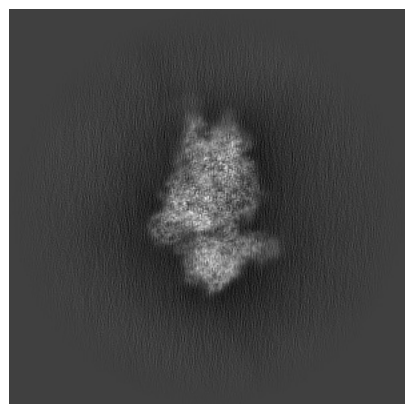
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17804. These allow visual inspection of the internal detail of the map and identification of artifacts.

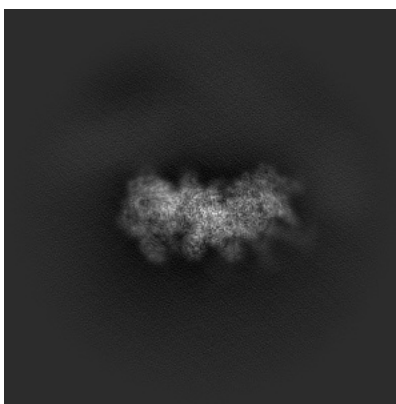
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

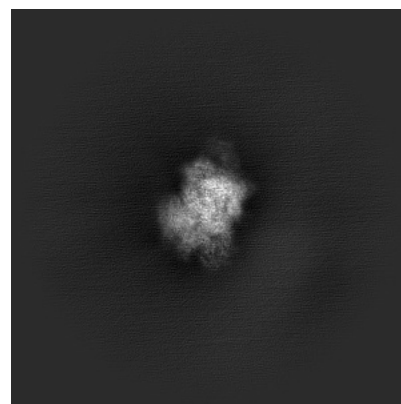
6.1.1 Primary map



X

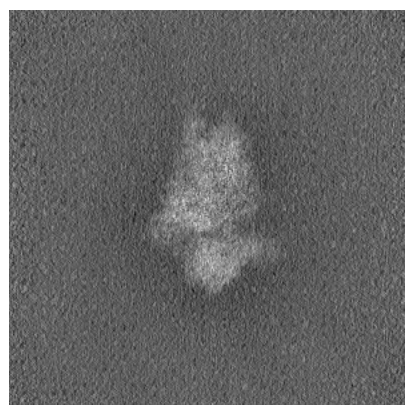


Y

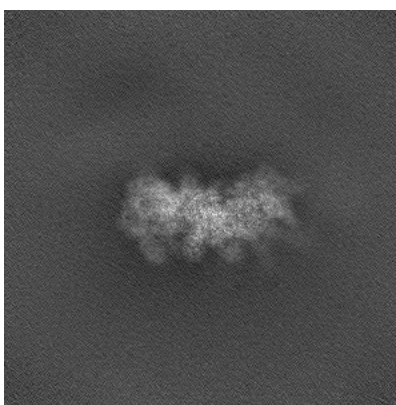


Z

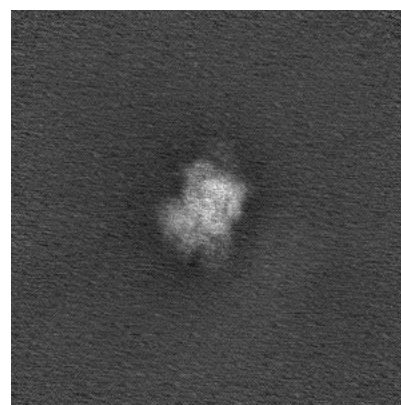
6.1.2 Raw map



X



Y

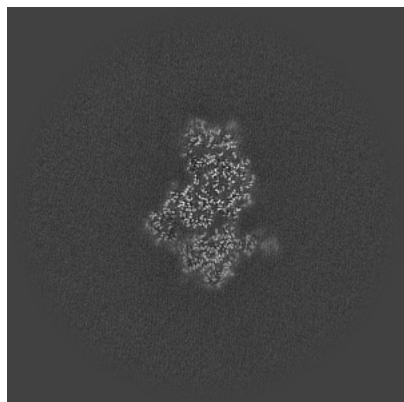


Z

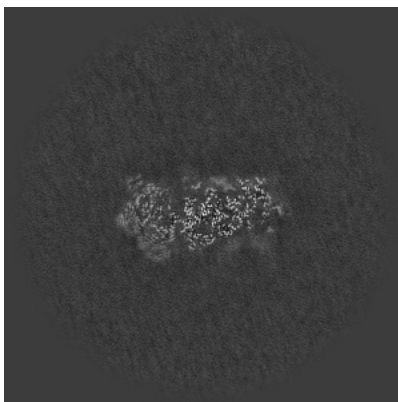
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

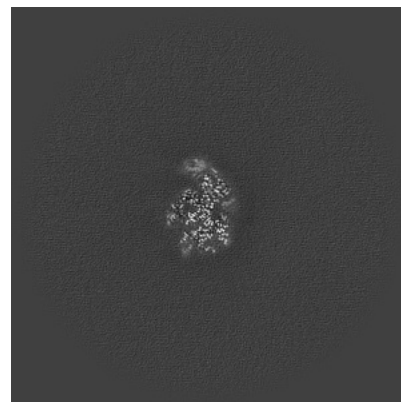
6.2.1 Primary map



X Index: 280

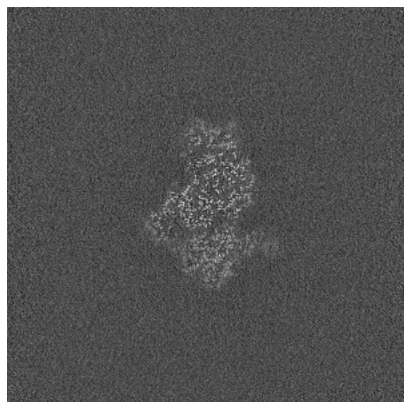


Y Index: 280

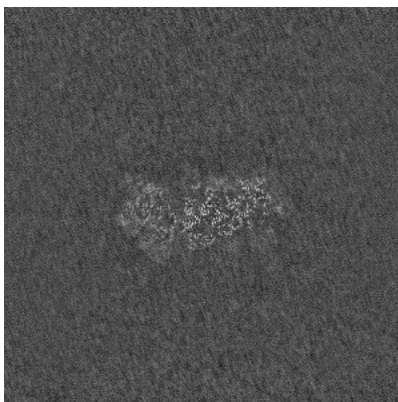


Z Index: 280

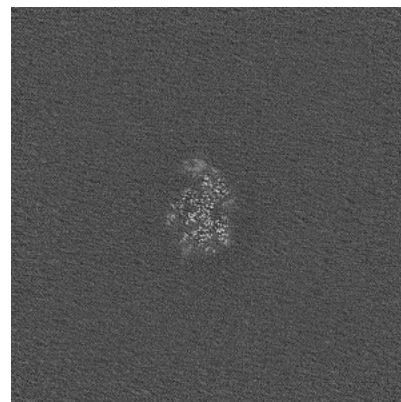
6.2.2 Raw map



X Index: 280



Y Index: 280

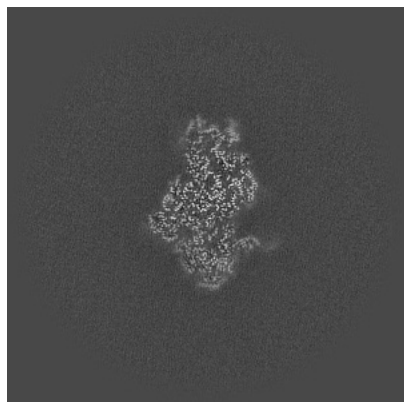


Z Index: 280

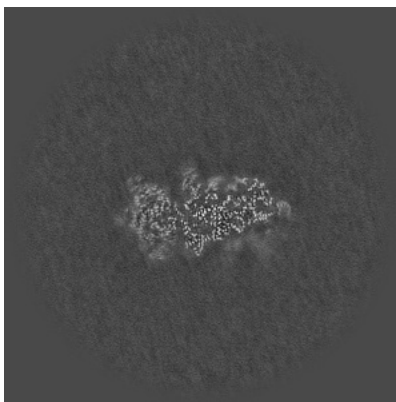
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

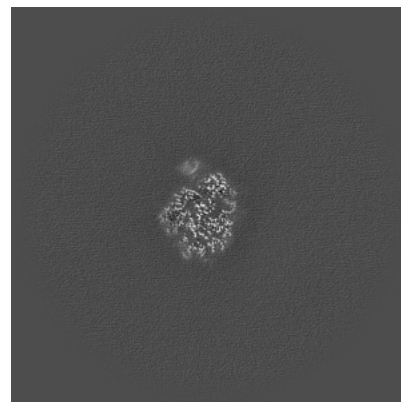
6.3.1 Primary map



X Index: 274

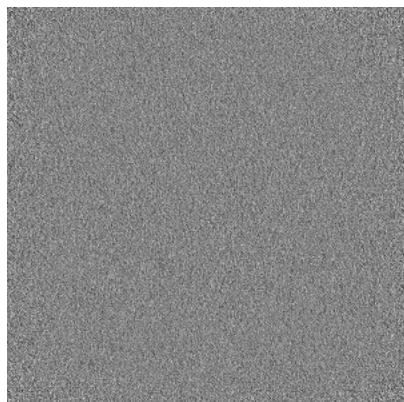


Y Index: 275

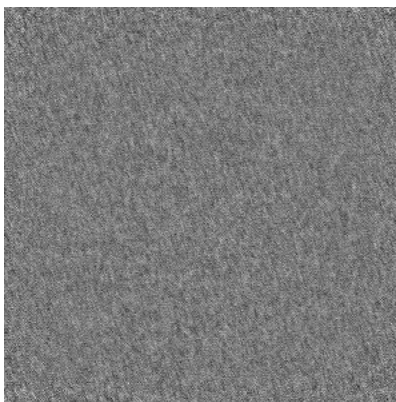


Z Index: 274

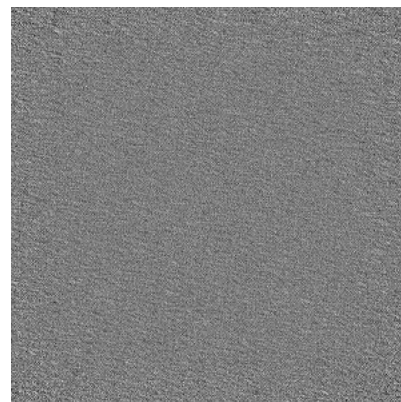
6.3.2 Raw map



X Index: 0



Y Index: 0

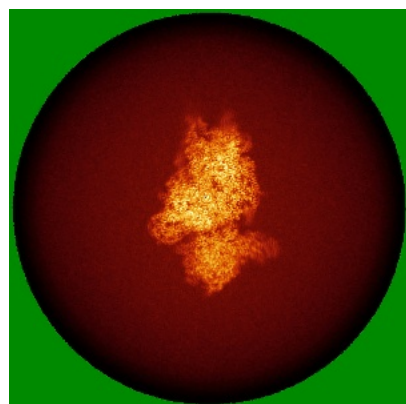


Z Index: 0

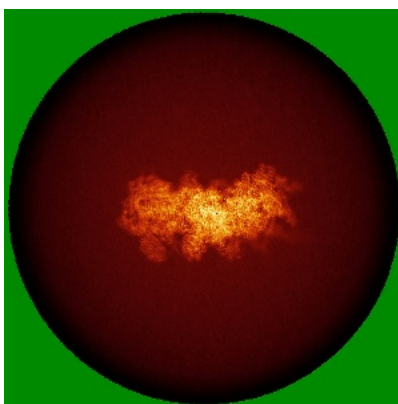
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

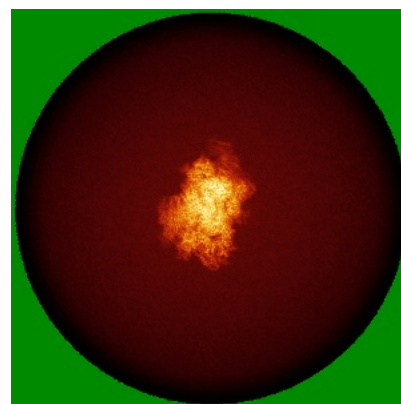
6.4.1 Primary map



X

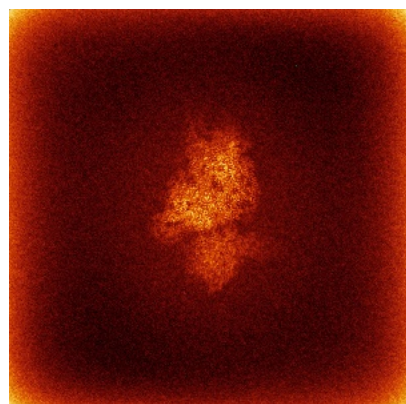


Y

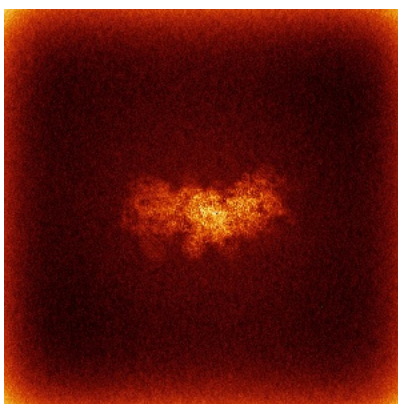


Z

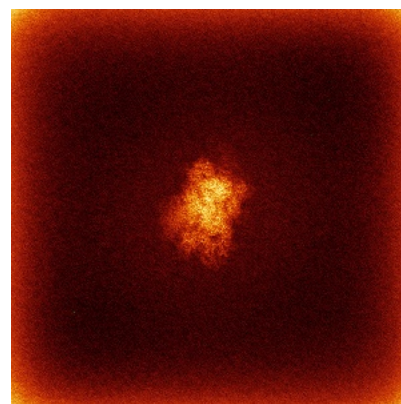
6.4.2 Raw map



X



Y

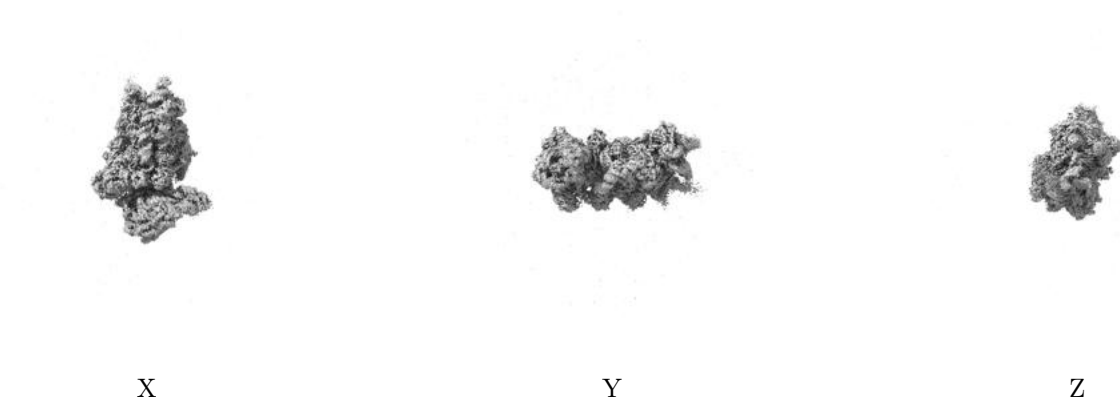


Z

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.

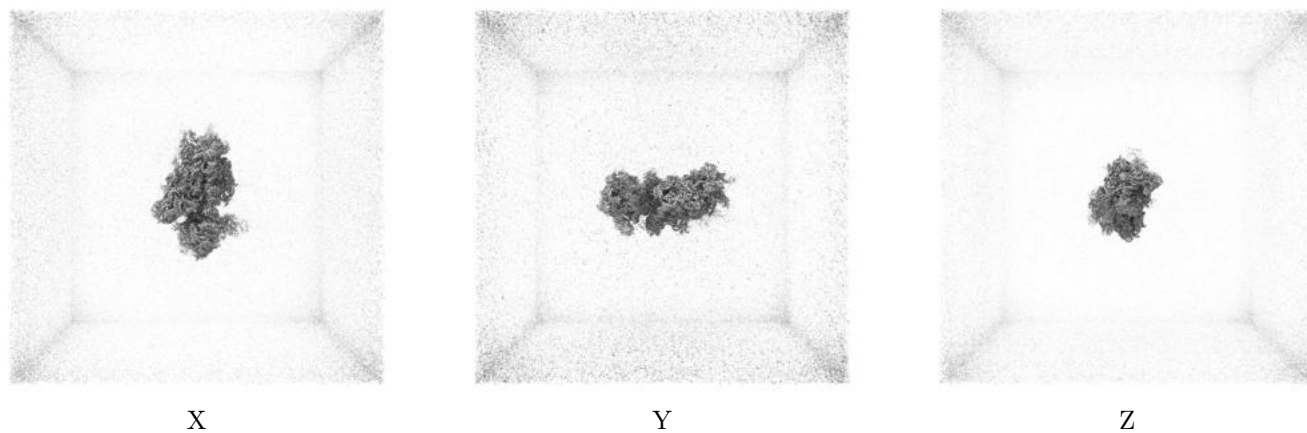
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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

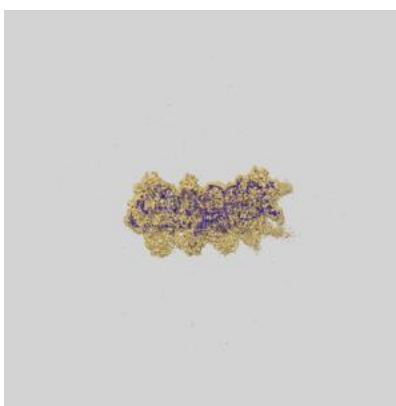
A mask typically either:

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

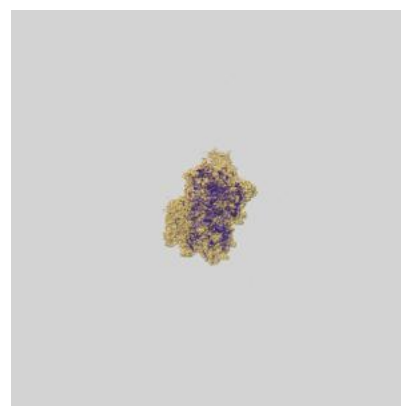
6.6.1 emd_17804_msk_1.map [i](#)



X

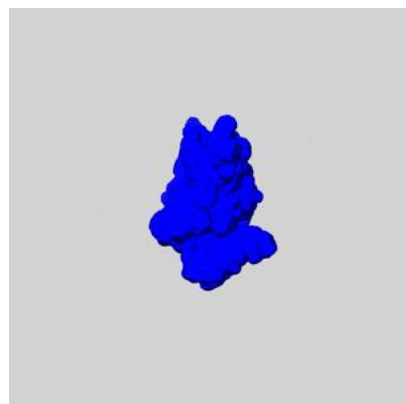


Y

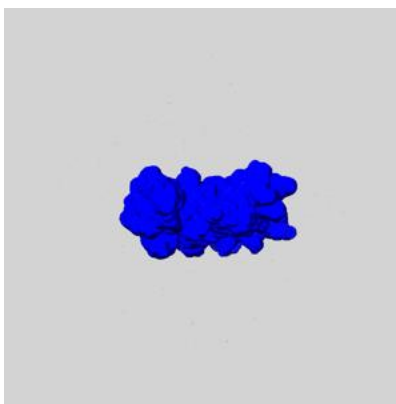


Z

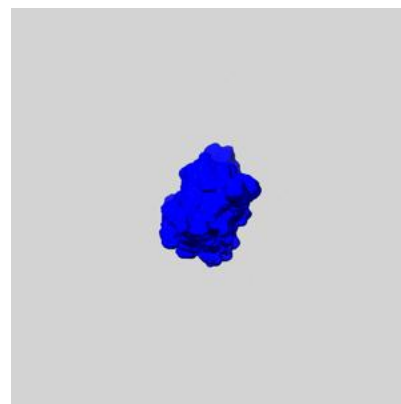
6.6.2 emd_17804_msk_2.map [i](#)



X



Y

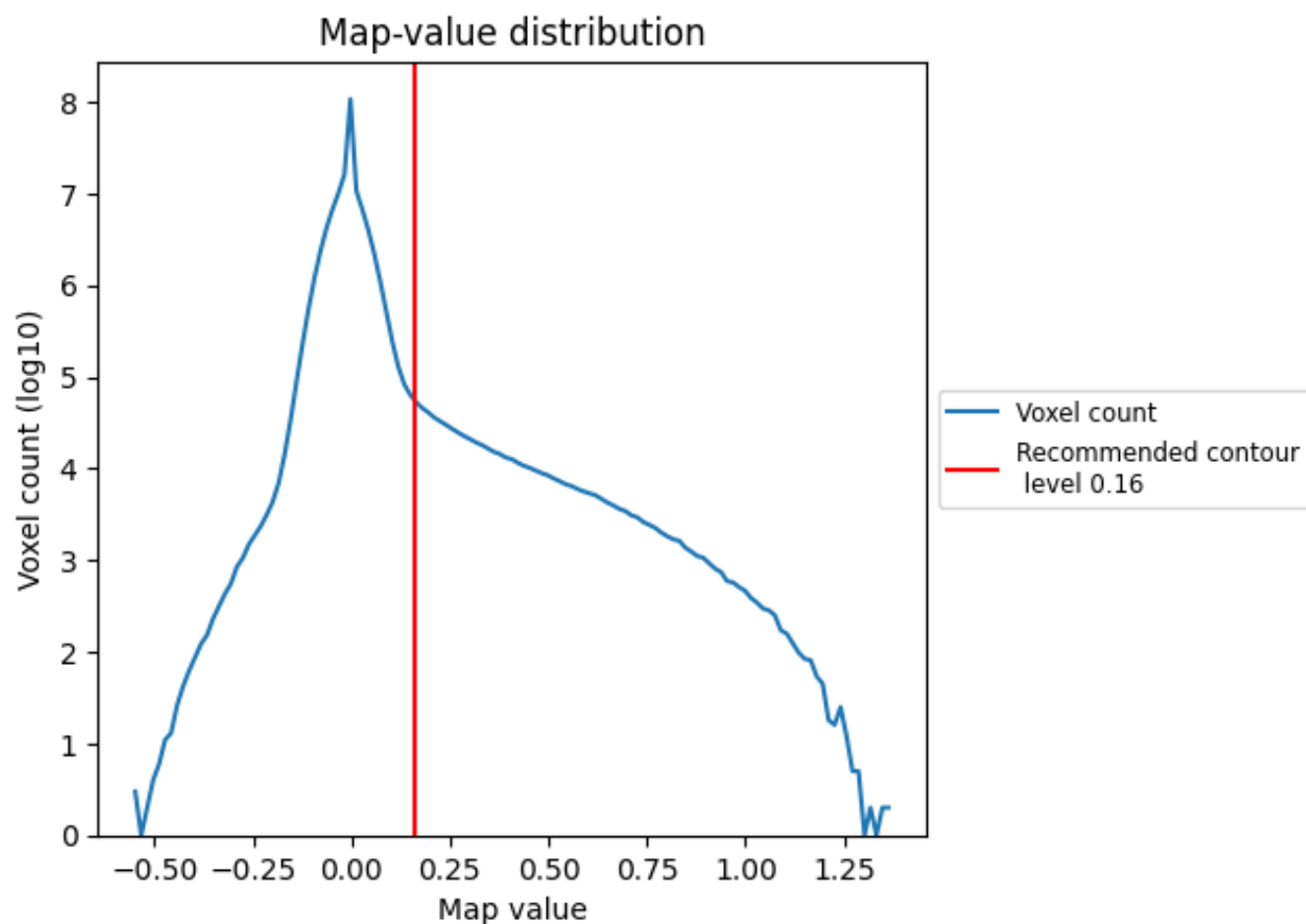


Z

7 Map analysis [i](#)

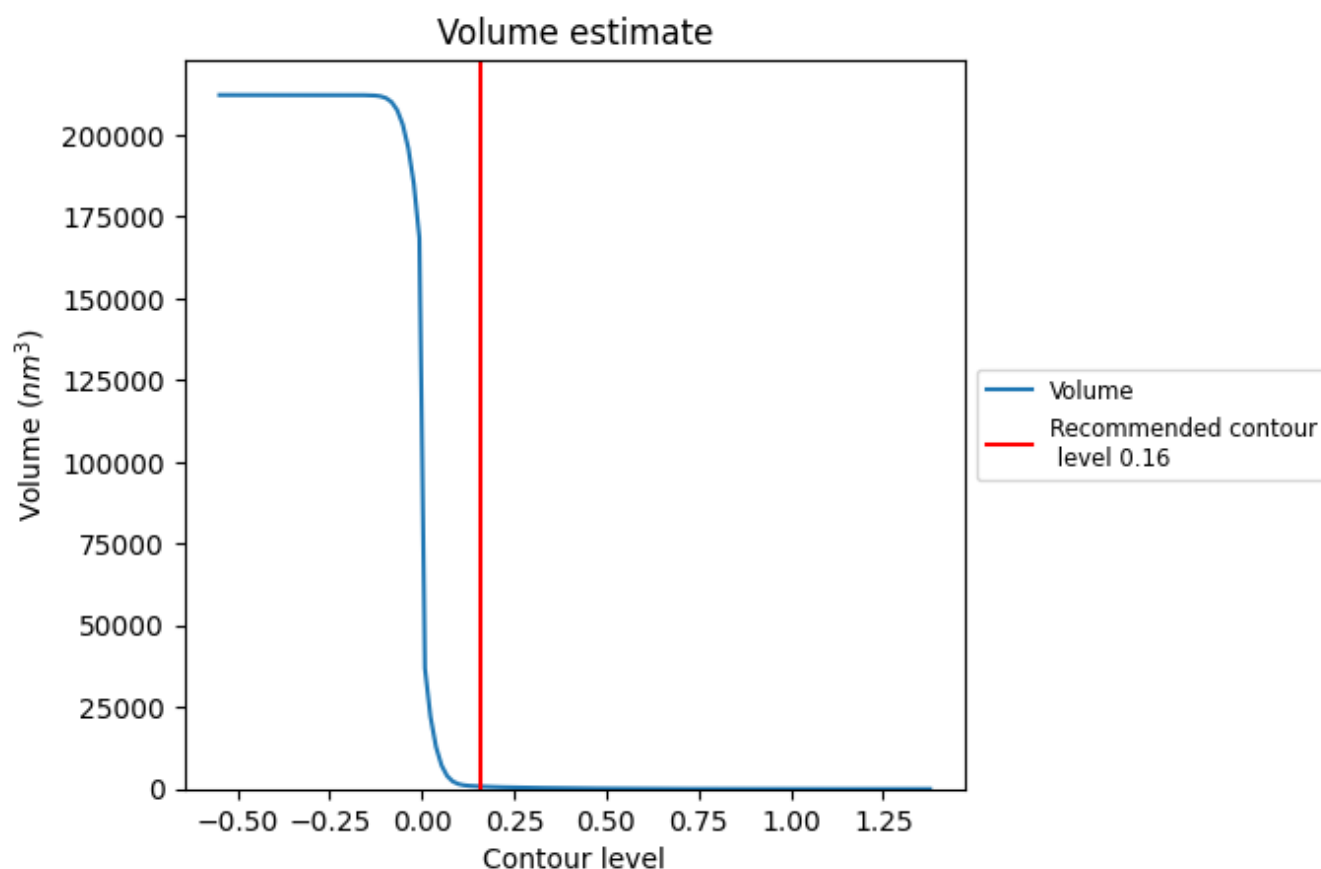
This section contains the results of statistical analysis of the map.

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.

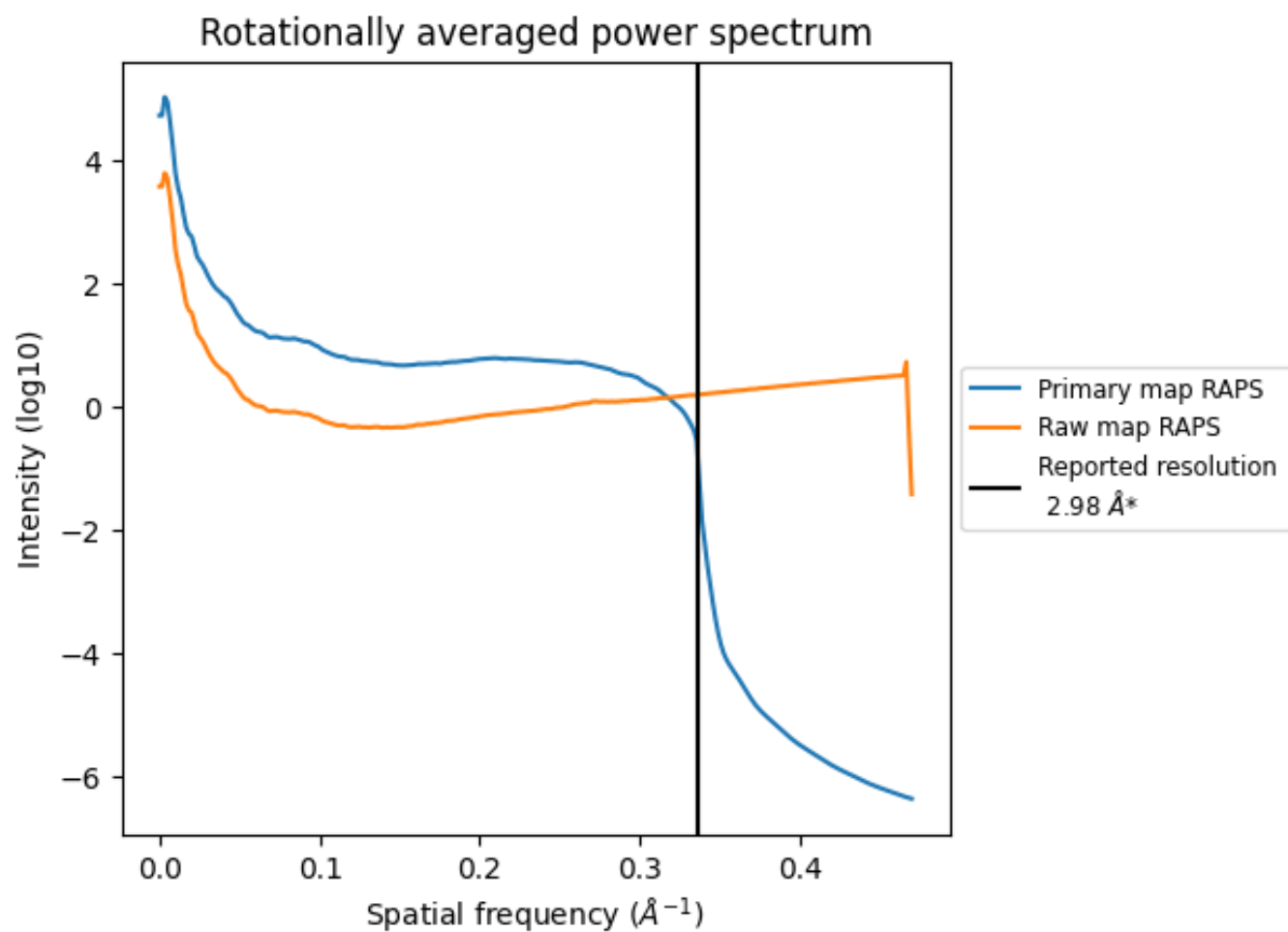
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm^3 ; this corresponds to an approximate mass of 680 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 ⓘ

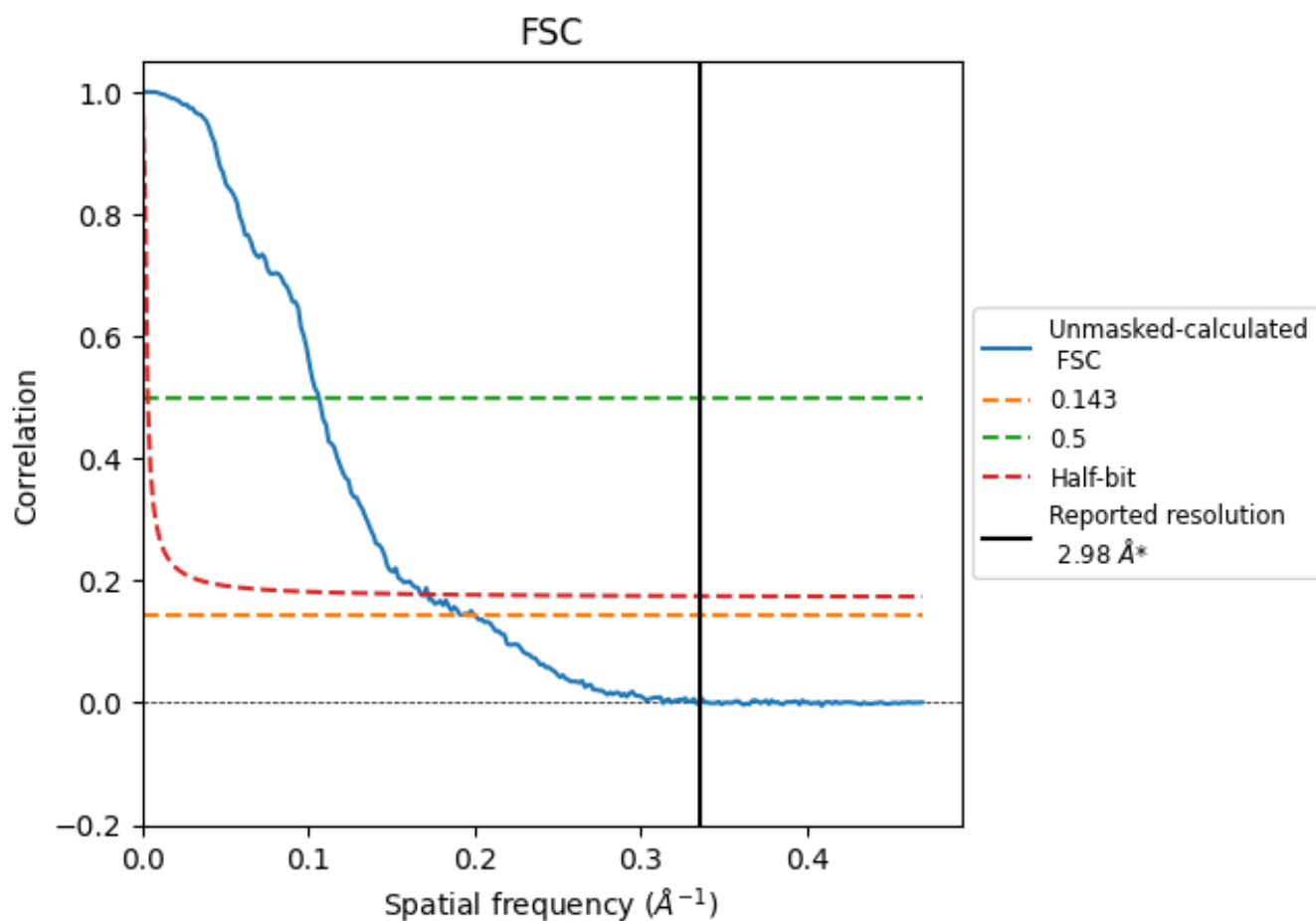


*Reported resolution corresponds to spatial frequency of 0.336 $\text{\AA}^{-1}$

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 0.336 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

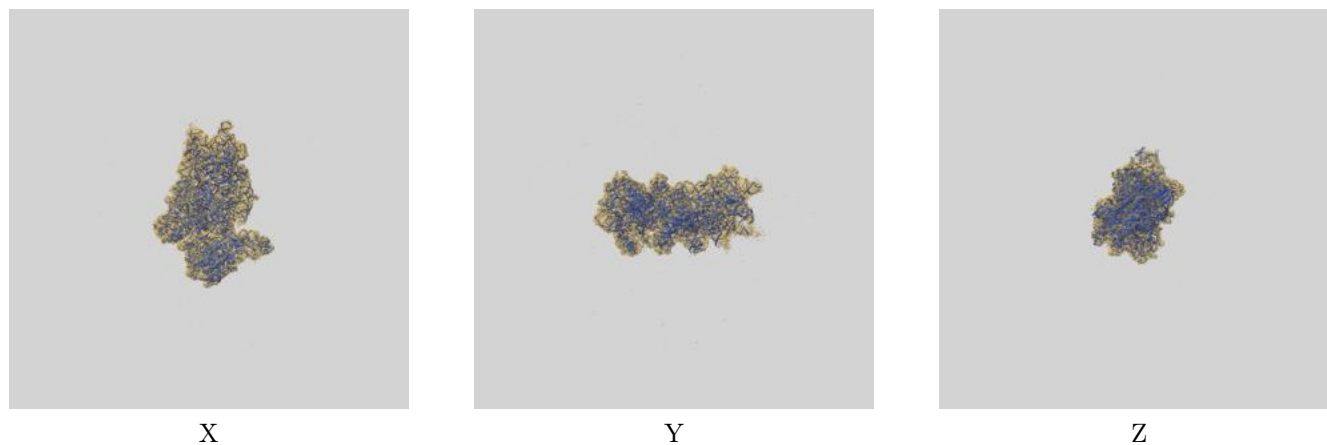
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.00	9.42	5.97

*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 5.00 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

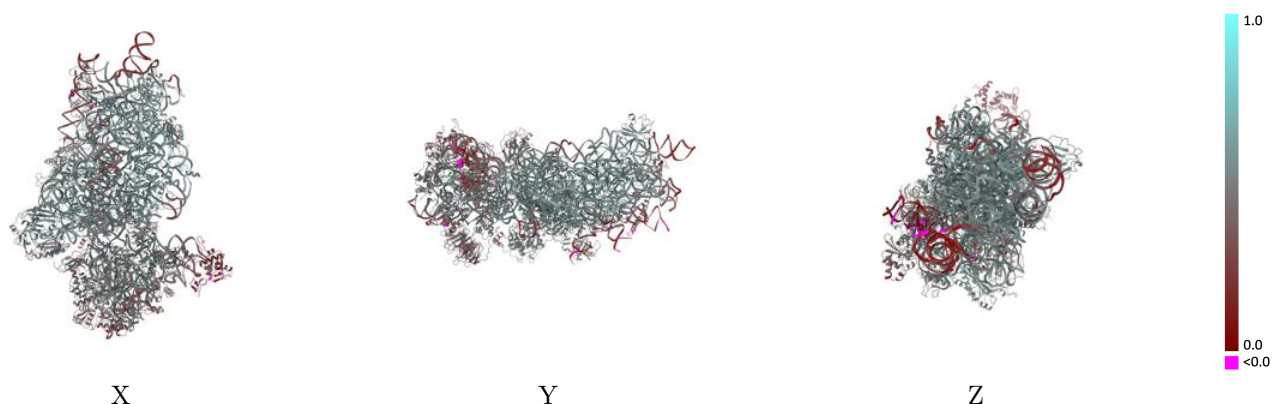
This section contains information regarding the fit between EMDB map EMD-17804 and PDB model 8PPK. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



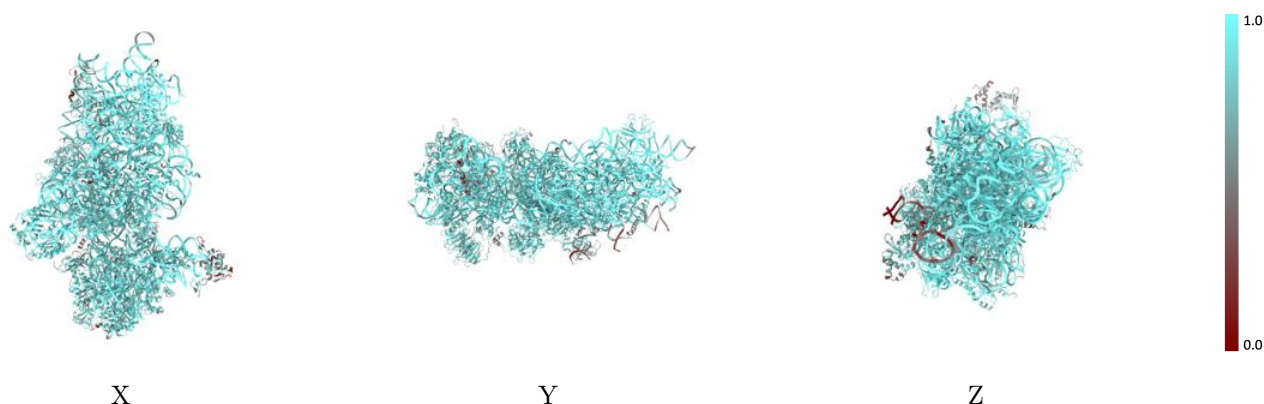
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



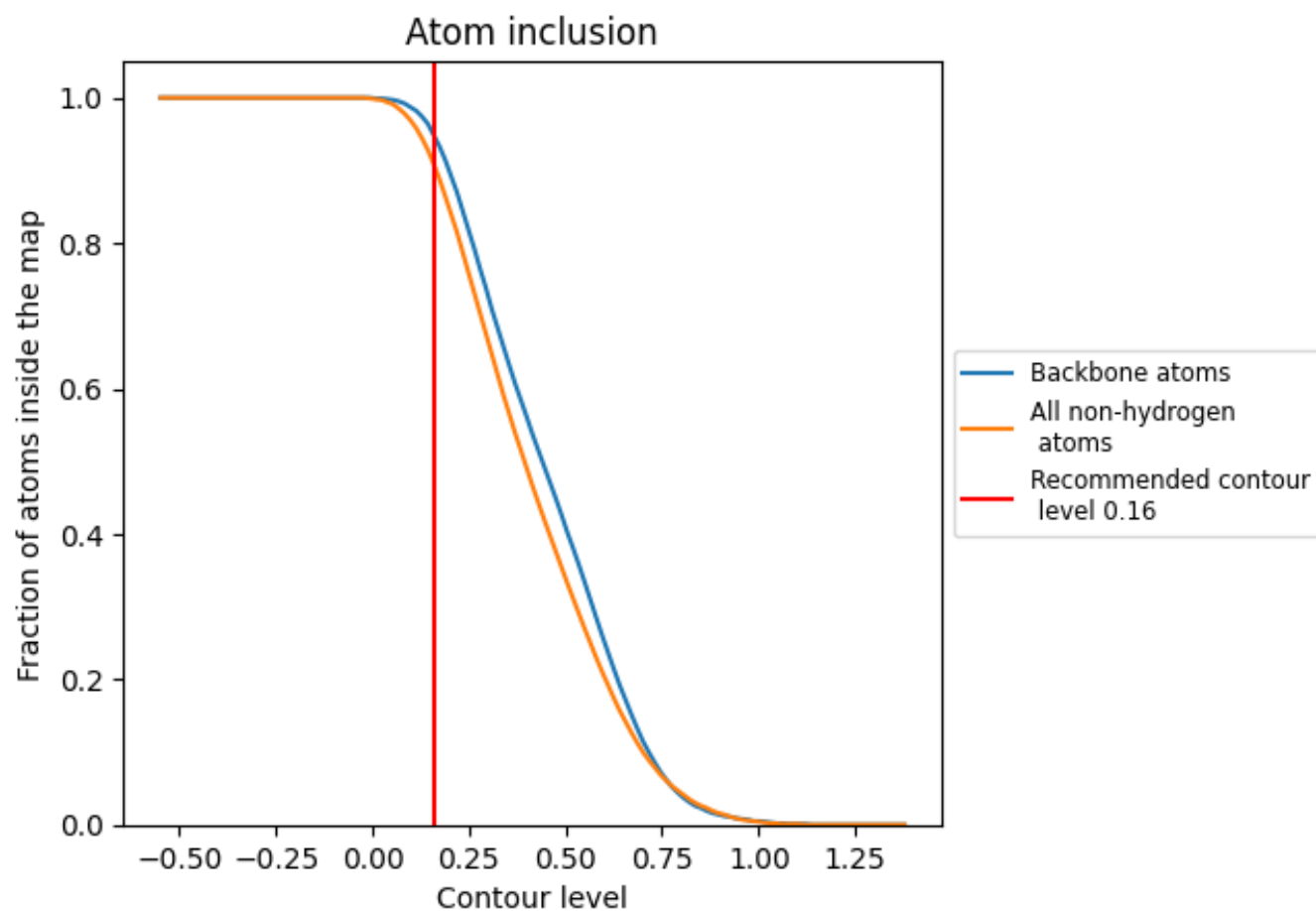
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4890
2	 0.9540	 0.4970
A	 0.9080	 0.5210
B	 0.9050	 0.5110
C	 0.9470	 0.5610
D	 0.8700	 0.4880
E	 0.9470	 0.5620
F	 0.8420	 0.4650
G	 0.8870	 0.4820
H	 0.7610	 0.4380
I	 0.9050	 0.5210
J	 0.9490	 0.5590
K	 0.8740	 0.4470
L	 0.8670	 0.5160
M	 0.5190	 0.2090
N	 0.9400	 0.5330
O	 0.9210	 0.5210
P	 0.8050	 0.4120
Q	 0.9010	 0.5030
R	 0.8180	 0.4470
S	 0.7800	 0.3990
T	 0.8730	 0.4730
U	 0.8440	 0.4530
V	 0.9390	 0.5570
W	 0.9590	 0.5730
X	 0.9510	 0.5700
Y	 0.9540	 0.5550
Z	 0.7380	 0.3720
a	 0.9250	 0.5380
b	 0.9070	 0.5000
c	 0.7700	 0.4200
d	 0.9500	 0.5380
e	 0.8500	 0.5220
f	 0.5080	 0.2000
g	 0.8130	 0.3880



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Chain	Atom inclusion	Q-score
h	 0.7710	 0.4760
j	 0.7960	 0.4640
p	 0.7730	 0.4460