



Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 07:47 PM EDT

PDB ID : 9NPX / pdb_00009npx
EMDB ID : EMD-49635
Title : SARS-CoV-2 nsp1 bound to the Rhinolophus lepidus 40S ribosomal subunit (local refinement of the 40S body)
Authors : Gen, R.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Veesler, D.
Deposited on : 2025-03-11
Resolution : 2.10 Å (reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

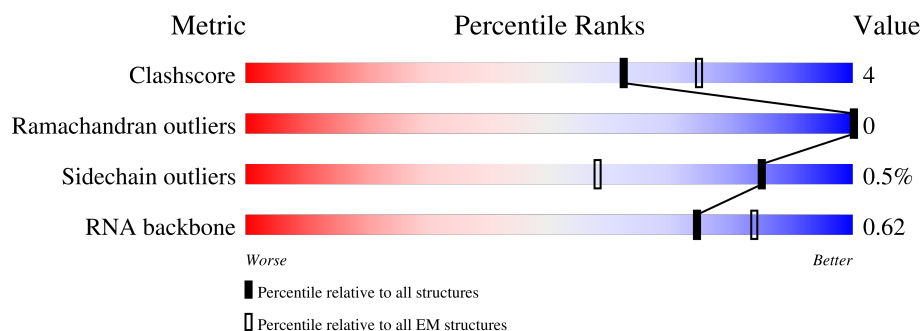
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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.





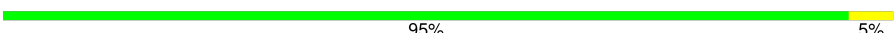









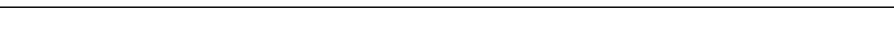



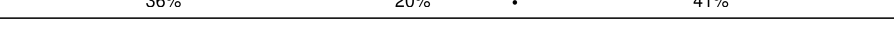
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	293	
2	D	263	
3	F	249	
4	H	208	
5	I	194	
6	M	151	
7	N	151	

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Mol	Chain	Length	Quality of chain
8	P	130	
9	R	135	
10	V	84	
11	W	143	
12	X	130	
13	Z	115	
14	a	84	
15	f	25	
16	h	295	
17	j	180	
18	k	113	
19	G	194	
20	K	158	
21	e	61	
22	C	264	
23	i	1869	
24	B	243	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 48314 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 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1679	1089	288	293	9		

- Molecule 2 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	260	Total	C	N	O	S	0	0
			2024	1297	378	341	8		

- Molecule 3 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	231	Total	C	N	O	S	0	0
			1724	1086	346	287	5		

- Molecule 4 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	205	Total	C	N	O	S	0	0
			1574	991	314	265	4		

- Molecule 5 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	179	Total	C	N	O	S	0	0
			1460	935	294	229	2		

- Molecule 6 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	149	Total	C	N	O	S	0	0
			1161	750	220	190	1		

- Molecule 7 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	133	Total	C	N	O	S	0	0
			971	596	194	175	6		

- Molecule 8 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	129	Total	C	N	O	S	0	0
			1029	657	193	173	6		

- Molecule 9 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	52	Total	C	N	O	S	0	0
			362	234	61	65	2		

- Molecule 10 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	84	Total	C	N	O	S	0	0
			627	388	115	119	5		

- Molecule 11 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	140	Total	C	N	O	S	0	0
			1079	682	214	180	3		

- Molecule 12 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	125	Total	C	N	O	S	0	0
			970	613	191	161	5		

- Molecule 13 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	98	Total	C	N	O	S	0	0
			740	467	151	117	5		

- Molecule 14 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	82	Total	C	N	O	S	0	0
			592	373	111	105	3		

- Molecule 15 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	22	Total	C	N	O	S	0	0
			186	114	48	22	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	208	Total	C	N	O	S	0	0
			1595	1019	285	283	8		

- Molecule 17 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	32	Total	C	N	O	S	0	0
			253	155	46	51	1		

- Molecule 18 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	52	Total	C	N	O	S	0	0
			309	186	64	58	1		

- Molecule 19 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	183	Total	C	N	O	S	0	0
			1304	846	249	209			

- Molecule 20 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	140	Total	C	N	O	S	0	0
			1131	721	212	192	6		

- Molecule 21 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	48	Total	C	N	O	S	0	0
			368	225	84	58	1		

- Molecule 22 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	217	Total	C	N	O	S	0	0
			1693	1078	310	291	14		

- Molecule 23 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	1095	Total	C	N	O	P	0	0
			23450	10491	4246	7618	1095		

- Molecule 24 is a protein called 40S ribosomal protein uS3, RPS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	44	Total	C	N	O	S	0	0
			322	204	61	53	4		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	F	1	Total	Mg	0
			1	1	
25	i	56	Total	Mg	0
			56	56	

- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
26	N	1	Total	K	0
			1	1	
26	Z	1	Total	K	0
			1	1	
26	i	11	Total	K	0
			11	11	

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	Z	1	Total	Zn	0
			1	1	

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	A	21	Total	O	0
			21	21	
28	D	37	Total	O	0
			37	37	
28	F	8	Total	O	0
			8	8	
28	H	22	Total	O	0
			22	22	
28	I	40	Total	O	0
			40	40	
28	M	18	Total	O	0
			18	18	
28	N	16	Total	O	0
			16	16	
28	P	27	Total	O	0
			27	27	
28	V	7	Total	O	0
			7	7	
28	W	28	Total	O	0
			28	28	
28	X	13	Total	O	0
			13	13	
28	Z	22	Total	O	0
			22	22	
28	a	6	Total	O	0
			6	6	
28	f	5	Total	O	0
			5	5	
28	h	4	Total	O	0
			4	4	
28	j	3	Total	O	0
			3	3	
28	G	2	Total	O	0
			2	2	
28	K	32	Total	O	0
			32	32	
28	e	6	Total	O	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
28	C	14	Total 14	O 14	0
28	i	1309	Total 1309	O 1309	0

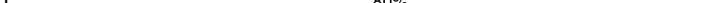
MET	ASN	ASP	T4	V5	T6	F12	R16	K21	L28	F60	G128	LYS	LYS
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- Chain Z:  75% 10% 15%

MET	T2	K3	N8	R28	K37	I44	V45	E46	V50	P65	K70	S88	R92	P99	ARG	PHE	ARG	ARG	PRO	ALA	ALA	GLY	ALA	ALA	ALA	ARG	ARG	PRO	PRO	PRO	LYS	PRO	MET
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- Chain a:  92% 6%

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: MET, P2, D34, T67, K70, F79, K82, Q83, HIS. The P2 position has the highest information content, with 'P' being the most frequent residue.

- Chain f:  80% 8% 12%

A schematic diagram of a protein structure. The protein is represented as a horizontal bar. The bar is divided into segments. The segments for residues M1, R11, R17, and Q22 are highlighted in green. The segments for residues ARG, SER, and LYS are highlighted in grey. The residues are labeled vertically below their respective segments.

- Chain h:  64% 6% 29%

[illegible][illegible]

GLU
TRP
SER

- Chain j:  16% 82%

MET	GLU	SER	LEU	VAL	PRO	GLY	PHE	ASN	GLU	LYS	THR	HIS	VAL	GLN	LEU	SER	LEU	PRO	VAL	VAL	LEU	VAL	VAL	ARG	ASP	VAL	LEU	VAL	VAL	ARG	GLY	GLY	PHE	ASP	ASP	VAL	VAL	GLU	GLU	ALA	ALA	ARG	GLN	HIS	LEU	LEU	LYS	ASP	VAL	VAL	GLU	GLU	GLY	THR	CYS	GLY	GLY	LEU	VAL	VAL	GLU	GLU	LYS	GLY	VAL
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LEU	PRO	GLN	LEU	GLN	PRO	TYR	PHE	ILE	LYS	ARG	SER	ASP	ALA	ARG	THR	ALA	HIS	GLY	HIS	VAL	MET	GLU	LEU	VAL	VAL	ALA	GLU	GLY	ILE	GLN	TYR	GLY	ARG	SER	GLY	GLU	THR	LEU	VAL	VAL	GLY	VAL	VAL	GLY	GLY	ILE	PRO	ALA	TYR	ARG
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VAL	LEU	LEU	ARG	LYS	ASN	GLY	ASN	LYS	GLY	ALA	GLY	GLY	HIS	SER	TYR	GLY	ASP	LEU	LYS	SER	PHE	ASP	LEU	GLY	ASP	E148	D152	L173	M174	R175	G179	GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120566	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.70	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/1716	0.30	0/2325
2	D	0.18	0/2066	0.30	0/2788
3	F	0.15	0/1747	0.26	0/2347
4	H	0.16	0/1602	0.28	0/2154
5	I	0.16	0/1485	0.27	0/1988
6	M	0.15	0/1185	0.27	0/1599
7	N	0.15	0/975	0.28	0/1309
8	P	0.19	0/1046	0.28	0/1401
9	R	0.09	0/368	0.22	0/503
10	V	0.15	0/632	0.27	0/849
11	W	0.16	0/1097	0.28	0/1467
12	X	0.16	0/987	0.27	0/1320
13	Z	0.16	0/753	0.28	0/1015
14	a	0.14	0/603	0.25	0/816
15	f	0.15	0/187	0.29	0/242
16	h	0.14	0/1627	0.25	0/2216
17	j	0.15	0/258	0.34	0/348
18	k	0.10	0/308	0.22	0/415
19	G	0.13	0/1323	0.25	0/1791
20	K	0.18	0/1151	0.27	0/1543
21	e	0.17	0/370	0.31	0/485
22	C	0.15	0/1719	0.27	0/2306
23	i	0.23	0/24757	0.28	0/38563
24	B	0.10	0/324	0.17	0/429
All	All	0.20	0/48286	0.27	0/70219

There are no bond length outliers.

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	A	1679	0	1743	13	0
2	D	2024	0	2102	13	0
3	F	1724	0	1750	10	0
4	H	1574	0	1556	12	0
5	I	1460	0	1564	11	0
6	M	1161	0	1216	12	0
7	N	971	0	979	3	0
8	P	1029	0	1076	10	0
9	R	362	0	331	2	0
10	V	627	0	611	3	0
11	W	1079	0	1139	6	0
12	X	970	0	982	3	0
13	Z	740	0	770	8	0
14	a	592	0	560	3	0
15	f	186	0	201	2	0
16	h	1595	0	1591	9	0
17	j	253	0	222	2	0
18	k	309	0	200	3	0
19	G	1304	0	1270	14	0
20	K	1131	0	1174	5	0
21	e	368	0	394	5	0
22	C	1693	0	1713	13	0
23	i	23450	0	11891	214	0
24	B	322	0	342	2	0
25	F	1	0	0	0	0
25	i	56	0	0	0	0
26	N	1	0	0	0	0
26	Z	1	0	0	0	0
26	i	11	0	0	0	0
27	Z	1	0	0	0	0
28	A	21	0	0	0	0
28	C	14	0	0	0	0
28	D	37	0	0	0	0
28	F	8	0	0	0	0
28	G	2	0	0	0	0
28	H	22	0	0	0	0
28	I	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	K	32	0	0	0	0
28	M	18	0	0	0	0
28	N	16	0	0	0	0
28	P	27	0	0	1	0
28	V	7	0	0	0	0
28	W	28	0	0	0	0
28	X	13	0	0	0	0
28	Z	22	0	0	1	0
28	a	6	0	0	0	0
28	e	6	0	0	0	0
28	f	5	0	0	0	0
28	h	4	0	0	0	0
28	i	1309	0	0	0	0
28	j	3	0	0	0	0
All	All	48314	0	35377	332	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (332) 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)
23:i:925:G:H1	23:i:1017:U:H3	1.27	0.82
8:P:2:VAL:N	23:i:1091:C:HO2'	1.79	0.81
23:i:928:G:H1	23:i:1013:U:H3	1.31	0.75
23:i:874:G:H2'	23:i:875:A:H8	1.54	0.72
13:Z:3:LYS:NZ	13:Z:8:ASN:OD1	2.24	0.70
23:i:981:A:H2'	23:i:982:G:C8	2.26	0.70
23:i:857:U:H2'	23:i:858:A:C8	2.28	0.67
8:P:80:ASP:OD1	8:P:124:LYS:NZ	2.26	0.67
23:i:1714:U:H2'	23:i:1715:A:C8	2.30	0.66
20:K:91:ASP:HB3	20:K:104:LYS:HE2	1.79	0.64
3:F:140:ARG:NH1	23:i:170:A:OP2	2.32	0.63
23:i:928:G:H2'	23:i:929:G:C8	2.34	0.62
19:G:19:PHE:HZ	19:G:60:ILE:HD12	1.63	0.62
23:i:640:A:H2'	23:i:641:A:C8	2.36	0.61
16:h:108:PHE:HB2	16:h:136:GLU:HG2	1.83	0.61
19:G:7:LYS:NZ	19:G:40:LEU:O	2.33	0.61
23:i:1030:A:H2'	23:i:1031:A2M:H8	1.83	0.61
1:A:65:LYS:HE3	1:A:273:LEU:HD13	1.83	0.61
4:H:22:HIS:HB3	23:i:433:A:H5''	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:36:GLN:O	16:h:53:ARG:NH1	2.33	0.59
23:i:797:OMC:H2'	23:i:798:G:C8	2.37	0.58
23:i:1705:C:H2'	23:i:1706:G:C8	2.37	0.58
23:i:1856:C:H2'	23:i:1857:G:C8	2.39	0.58
23:i:554:A:O2'	23:i:556:U:OP2	2.21	0.58
23:i:145:G:H2'	23:i:146:G:C8	2.38	0.58
23:i:942:G:H2'	23:i:943:U:C6	2.40	0.57
7:N:34:PHE:HB3	7:N:41:PHE:HB2	1.87	0.57
23:i:107:A:H2'	23:i:108:G:C8	2.39	0.57
8:P:3:ARG:HD3	8:P:6:VAL:HG12	1.86	0.56
22:C:124:HIS:HA	22:C:137:LEU:O	2.05	0.56
3:F:2:LYS:NZ	23:i:156:G:OP1	2.31	0.56
23:i:191:A:H3'	23:i:192:C:H5''	1.88	0.56
23:i:1797:U:H2'	23:i:1798:C:C6	2.41	0.56
23:i:16:G:H2'	23:i:17:C:C6	2.41	0.55
1:A:252:THR:OG1	1:A:254:ASP:OD1	2.22	0.55
23:i:1713:C:H2'	23:i:1714:U:C6	2.41	0.55
23:i:528:A:H2'	23:i:529:A:H8	1.71	0.55
23:i:190:G:O2'	23:i:209:A:N6	2.40	0.55
23:i:996:A:H2'	23:i:997:A:C8	2.42	0.55
22:C:136:ARG:HB2	22:C:218:LEU:HD11	1.88	0.55
8:P:91:ASN:ND2	28:P:201:HOH:O	2.39	0.55
21:e:110:MET:HE3	21:e:114:ARG:HH12	1.72	0.55
23:i:118:C:H1'	23:i:445:A:C5	2.43	0.54
23:i:1798:C:H2'	23:i:1799:G:O4'	2.07	0.54
6:M:64:ARG:NH1	23:i:919:A:OP2	2.38	0.54
23:i:528:A:H2'	23:i:529:A:C8	2.41	0.54
23:i:1845:A:H2'	23:i:1846:G:C8	2.43	0.54
5:I:40:LYS:NZ	23:i:641:A:OP1	2.36	0.54
23:i:1712:A:H2'	23:i:1713:C:C6	2.42	0.53
11:W:54:LYS:HE2	11:W:91:LEU:HG	1.90	0.53
23:i:1007:C:H2'	23:i:1008:A:C8	2.43	0.53
22:C:47:THR:OG1	22:C:65:ARG:NH1	2.42	0.53
23:i:1113:A:H2'	23:i:1114:U:C6	2.43	0.53
3:F:1:MET:HE2	3:F:106:LEU:HB2	1.90	0.53
5:I:136:ARG:HD3	5:I:160:SER:HA	1.91	0.53
23:i:12:U:H2'	23:i:13:C:C6	2.43	0.53
23:i:809:A:H2'	23:i:810:A:O4'	2.09	0.53
23:i:1088:U:H4'	23:i:1089:G:OP2	2.09	0.53
2:D:106:LYS:NZ	23:i:847:A:O2'	2.42	0.52
23:i:1819:A:H2'	23:i:1820:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:1201:U:H2'	23:i:1202:U:C6	2.44	0.52
23:i:29:G:H2'	23:i:30:C:C6	2.44	0.52
1:A:191:VAL:HG11	1:A:236:PHE:HA	1.92	0.52
20:K:128:VAL:HG12	20:K:142:VAL:HA	1.91	0.52
16:h:37:TYR:OH	16:h:57:LYS:NZ	2.40	0.52
23:i:1856:C:H2'	23:i:1857:G:H8	1.75	0.52
12:X:12:PHE:HZ	12:X:21:LYS:HD3	1.75	0.52
2:D:11:ARG:HA	2:D:28:ALA:HB2	1.92	0.51
4:H:5:ARG:NE	23:i:379:C:O2	2.40	0.51
22:C:134:LEU:HB3	22:C:219:LYS:HB2	1.92	0.51
23:i:1203:G:H2'	23:i:1204:A:C8	2.45	0.51
5:I:103:GLU:O	5:I:107:GLU:HG2	2.09	0.51
23:i:495:U:H2'	23:i:496:C:O4'	2.10	0.51
19:G:19:PHE:CZ	19:G:60:ILE:HD12	2.45	0.51
22:C:33:VAL:HG12	22:C:44:ILE:HD12	1.92	0.51
1:A:257:LYS:O	10:V:16:LYS:NZ	2.36	0.51
7:N:113:GLN:HE21	13:Z:46:GLU:H	1.59	0.51
23:i:15:U:H2'	23:i:16:G:O4'	2.11	0.51
4:H:98:LYS:HB3	23:i:377:G:H5'	1.92	0.51
16:h:77:ILE:HG12	16:h:99:ILE:HB	1.93	0.51
23:i:1736:G:H2'	23:i:1737:G:C8	2.45	0.51
19:G:114:GLN:HE22	23:i:874:G:H21	1.58	0.51
23:i:1098:C:H2'	23:i:1099:G:C8	2.46	0.50
20:K:18:GLN:HG2	20:K:33:LEU:HD11	1.93	0.50
23:i:115:U:H2'	23:i:116:OMU:C6	2.42	0.50
23:i:367:U:H4'	23:i:371:A:C8	2.46	0.50
23:i:1706:G:H2'	23:i:1707:U:H6	1.76	0.50
23:i:57:U:OP1	23:i:504:G:O2'	2.26	0.50
23:i:656:G:H5'	23:i:662:G:N2	2.26	0.50
4:H:57:ALA:HB2	4:H:183:GLY:HA2	1.94	0.50
8:P:91:ASN:HD21	23:i:2:A:H61	1.60	0.50
23:i:563:G:O2'	23:i:564:A:H8	1.95	0.50
23:i:952:G:H2'	23:i:953:C:C6	2.47	0.50
14:a:67:THR:OG1	14:a:70:LYS:O	2.28	0.49
23:i:629:A:O2'	23:i:631:U:OP1	2.30	0.49
23:i:1010:G:H2'	23:i:1011:A:C8	2.47	0.49
4:H:184:ARG:NH2	23:i:218:PSU:O4	2.45	0.49
21:e:117:VAL:HG11	23:i:552:G:H5'	1.94	0.49
23:i:573:U:O2	23:i:576:A2M:H8	2.12	0.49
23:i:1101:U:H2'	23:i:1102:G:C8	2.48	0.49
4:H:113:TYR:OH	4:H:156:ALA:O	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:1736:G:H2'	23:i:1737:G:H8	1.77	0.49
23:i:17:C:H2'	23:i:18:C:C6	2.47	0.49
23:i:51:U:H2'	23:i:52:G:C8	2.48	0.49
23:i:106:C:H2'	23:i:107:A:H8	1.78	0.49
9:R:116:ASN:OD1	9:R:116:ASN:N	2.46	0.49
23:i:1712:A:H2'	23:i:1713:C:H6	1.78	0.49
3:F:162:LEU:HB3	23:i:67:C:C5	2.48	0.49
23:i:674:C:H2'	23:i:675:U:C6	2.48	0.49
23:i:1836:G:OP1	23:i:1839:U:H4'	2.13	0.49
6:M:55:ARG:HD3	23:i:1017:U:H5'	1.94	0.48
23:i:99:A2M:O5'	23:i:99:A2M:H8	2.14	0.48
23:i:563:G:O2'	23:i:564:A:H5''	2.14	0.48
2:D:97:GLU:OE1	2:D:113:ARG:NH1	2.37	0.48
14:a:34:ASP:O	14:a:79:PHE:HA	2.13	0.48
16:h:137:ALA:HB1	16:h:142:LEU:HB3	1.94	0.48
2:D:124:CYS:HB3	2:D:141:THR:HB	1.94	0.48
2:D:175:PHE:HE2	2:D:198:ARG:HD2	1.79	0.48
8:P:30:CYS:SG	8:P:31:SER:N	2.85	0.48
19:G:69:LEU:HD22	19:G:96:ALA:HB2	1.94	0.48
2:D:107:GLY:HA2	2:D:189:LEU:HG	1.95	0.48
3:F:183:ARG:NH1	23:i:317:C:OP2	2.34	0.48
13:Z:2:THR:N	23:i:1199:A:OP1	2.46	0.48
23:i:614:C:H2'	23:i:626:G:C8	2.48	0.48
23:i:575:A:H2'	23:i:576:A2M:O4'	2.14	0.48
1:A:165:VAL:HG21	1:A:217:ALA:HB1	1.96	0.48
6:M:33:VAL:HG21	6:M:66:VAL:HG11	1.96	0.48
13:Z:28:ARG:NH2	28:Z:301:HOH:O	2.41	0.47
20:K:136:LYS:HB2	23:i:385:G:H3'	1.96	0.47
6:M:25:TRP:CD2	14:a:82:LYS:HD3	2.49	0.47
23:i:96:C:H2'	23:i:97:U:C6	2.50	0.47
23:i:874:G:H2'	23:i:875:A:C8	2.41	0.47
5:I:53:ILE:HD13	5:I:81:LEU:HD21	1.96	0.47
11:W:66:ILE:HD12	21:e:78:GLY:HA2	1.96	0.47
22:C:123:ALA:HB2	22:C:165:ARG:HG3	1.96	0.47
18:k:67:PHE:CE1	18:k:92:ASN:HB3	2.50	0.47
2:D:11:ARG:HD3	2:D:21:ASP:O	2.14	0.47
5:I:127:ARG:HD3	21:e:105:ARG:HD3	1.96	0.47
19:G:44:ASN:H	19:G:68:GLN:HE22	1.61	0.47
23:i:121:OMU:HM23	23:i:121:OMU:H1'	1.60	0.47
23:i:963:A:H2'	23:i:964:A:C8	2.50	0.47
6:M:31:ASP:O	6:M:35:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:28:U:H2'	23:i:29:G:H8	1.79	0.47
23:i:527:C:H2'	23:i:528:A:H8	1.80	0.47
23:i:443:U:H2'	23:i:444:G:O4'	2.15	0.47
23:i:1189:A:H2'	23:i:1190:A:C8	2.50	0.47
23:i:1845:A:H2'	23:i:1846:G:H8	1.79	0.47
4:H:101:ILE:HD12	4:H:190:LEU:HD11	1.96	0.46
23:i:320:G:H2'	23:i:321:C:C6	2.50	0.46
1:A:116:THR:OG1	1:A:119:GLY:O	2.17	0.46
22:C:168:MET:HG2	22:C:197:ILE:HG21	1.97	0.46
23:i:420:G:O2'	23:i:660:C:N3	2.46	0.46
23:i:352:U:H2'	23:i:353:C:C6	2.51	0.46
3:F:162:LEU:HD11	3:F:172:LYS:HD2	1.97	0.46
23:i:562:U:H2'	23:i:563:G:C8	2.51	0.46
23:i:1010:G:H2'	23:i:1011:A:H8	1.79	0.46
23:i:1164:G:O2'	23:i:1165:G:H5'	2.15	0.46
3:F:2:LYS:HD3	3:F:15:LEU:HD21	1.97	0.46
23:i:416:U:H2'	23:i:417:C:O4'	2.16	0.46
1:A:183:LYS:HA	1:A:195:LEU:O	2.15	0.46
4:H:106:SER:HB3	4:H:171:LEU:HG	1.98	0.46
5:I:134:HIS:ND1	5:I:163:SER:OG	2.40	0.46
23:i:559:G:O2'	23:i:560:A:H5''	2.16	0.46
23:i:1119:A:H2'	23:i:1120:U:C6	2.51	0.46
23:i:1139:C:H2'	23:i:1140:G:O4'	2.16	0.46
23:i:441:C:H2'	23:i:442:C:C6	2.51	0.46
23:i:533:A:H2'	23:i:534:G:H8	1.81	0.46
7:N:135:ILE:O	23:i:943:U:O2'	2.34	0.46
23:i:17:C:O2'	23:i:1194:A:N1	2.43	0.46
23:i:801:U:H2'	23:i:802:A:H8	1.81	0.46
23:i:964:A:H2'	23:i:965:U:C6	2.50	0.46
23:i:1148:A:H4'	23:i:1149:A:O4'	2.17	0.46
23:i:980:A:H2'	23:i:981:A:C8	2.51	0.45
23:i:1025:U:H2'	23:i:1026:C:O4'	2.16	0.45
23:i:1084:A:OP1	23:i:1858:G:O2'	2.28	0.45
23:i:1821:U:H2'	23:i:1822:A:C8	2.51	0.45
23:i:5:U:H2'	23:i:6:G:H8	1.82	0.45
23:i:1854:U:H2'	23:i:1855:G:H8	1.82	0.45
10:V:30:ALA:O	10:V:60:ARG:HD3	2.16	0.45
23:i:159:A2M:HM'3	23:i:159:A2M:H1'	1.63	0.45
23:i:878:G:H1	23:i:908:A:H61	1.63	0.45
23:i:1817:G:H2'	23:i:1818:A:C8	2.51	0.45
6:M:110:ASP:O	6:M:114:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:44:ILE:HD12	13:Z:65:PRO:HG2	1.99	0.45
23:i:530:U:H2'	23:i:531:A:H8	1.81	0.45
5:I:33:GLY:HA3	21:e:112:TYR:CG	2.52	0.45
6:M:9:LYS:HE3	23:i:1092:G:OP2	2.17	0.45
19:G:40:LEU:HD11	19:G:79:LEU:HD11	1.99	0.45
20:K:111:VAL:HG12	20:K:140:PHE:HB2	1.97	0.45
23:i:568:C:H2'	23:i:569:A:O4'	2.17	0.45
23:i:858:A:H2'	23:i:859:G:H8	1.82	0.45
23:i:940:U:H2'	23:i:941:C:C6	2.51	0.45
23:i:1199:A:H2'	23:i:1200:A:C8	2.52	0.45
8:P:42:MET:HE1	19:G:146:VAL:HG12	1.98	0.45
23:i:520:A:O2'	23:i:825:A:N3	2.42	0.45
23:i:634:A:H2'	23:i:635:G:C8	2.52	0.45
23:i:1714:U:H2'	23:i:1715:A:H8	1.80	0.45
13:Z:88:SER:O	13:Z:92:ARG:HG3	2.17	0.44
23:i:116:OMU:HM23	23:i:116:OMU:H1'	1.72	0.44
23:i:639:C:H2'	23:i:640:A:C8	2.52	0.44
23:i:1713:C:H2'	23:i:1714:U:H6	1.79	0.44
16:h:184:ARG:HD3	16:h:191:ARG:HG2	1.99	0.44
23:i:30:C:O2'	23:i:596:U:OP1	2.34	0.44
23:i:664:A:O2'	23:i:670:A:N1	2.45	0.44
23:i:1715:A:H2'	23:i:1716:C:H6	1.83	0.44
1:A:185:THR:OG1	23:i:1155:U:OP1	2.34	0.44
23:i:1101:U:H2'	23:i:1102:G:H8	1.83	0.44
11:W:68:LYS:HB3	11:W:91:LEU:HD22	1.99	0.44
17:j:152:ASP:HA	24:B:117:ARG:HH21	1.83	0.44
23:i:1036:A:H4'	23:i:1855:G:N2	2.33	0.44
13:Z:37:LYS:HG2	13:Z:70:LYS:HE2	2.00	0.44
17:j:173:LEU:C	17:j:175:ARG:H	2.25	0.44
23:i:99:A2M:HM'3	23:i:99:A2M:H1'	1.86	0.44
23:i:626:G:N3	23:i:626:G:H2'	2.33	0.44
23:i:329:G:H3'	23:i:330:G:H8	1.82	0.44
23:i:530:U:H2'	23:i:531:A:C8	2.53	0.44
8:P:77:PRO:HB2	11:W:7:LEU:HG	2.00	0.43
19:G:45:ILE:HG22	19:G:64:VAL:HG12	1.99	0.43
23:i:517:OMC:H2'	23:i:518:G:O4'	2.18	0.43
23:i:533:A:H2'	23:i:534:G:C8	2.53	0.43
23:i:804:U:H2'	23:i:805:U:C6	2.53	0.43
23:i:1692:PSU:H2'	23:i:1693:G:C8	2.53	0.43
1:A:72:ASP:OD2	1:A:272:HIS:NE2	2.43	0.43
16:h:80:ARG:O	16:h:84:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:551:U:H2'	23:i:552:G:C8	2.53	0.43
23:i:1711:U:H2'	23:i:1712:A:H8	1.83	0.43
2:D:20:LEU:HD21	2:D:46:ILE:HD12	2.00	0.43
22:C:104:ASP:OD1	22:C:105:LEU:N	2.51	0.43
4:H:4:SER:OG	4:H:6:ASP:OD2	2.28	0.43
23:i:958:G:H2'	23:i:959:G:C8	2.53	0.43
19:G:135:PHE:CG	19:G:136:PRO:HA	2.54	0.43
23:i:382:C:H2'	23:i:383:G:H8	1.84	0.43
23:i:433:A:H2'	23:i:434:G:C8	2.54	0.43
23:i:1711:U:H2'	23:i:1712:A:C8	2.54	0.43
23:i:1786:U:H2'	23:i:1787:G:H8	1.82	0.43
23:i:223:C:H2'	23:i:224:A:C8	2.54	0.43
23:i:634:A:H2'	23:i:635:G:H8	1.84	0.43
2:D:27:PHE:O	23:i:495:U:O2'	2.35	0.43
3:F:164:LYS:NZ	23:i:68:A:OP2	2.50	0.43
6:M:87:ASP:OD1	6:M:87:ASP:N	2.52	0.43
19:G:99:ARG:HH12	23:i:913:A:P	2.41	0.43
23:i:84:A:N3	23:i:150:A:O2'	2.47	0.43
23:i:332:G:O2'	23:i:333:G:H5'	2.19	0.43
16:h:69:GLU:OE1	16:h:69:GLU:N	2.51	0.43
23:i:943:U:C2	23:i:944:A:C8	3.07	0.43
23:i:1748:G:H2'	23:i:1749:G:H8	1.84	0.43
6:M:4:MET:HG2	6:M:5:HIS:CD2	2.54	0.43
2:D:45:ILE:HG13	2:D:61:VAL:HG21	2.01	0.42
5:I:111:GLN:HE21	5:I:123:ILE:HG13	1.84	0.42
18:k:68:ALA:HB1	23:i:1707:U:O2	2.18	0.42
23:i:116:OMU:O5'	23:i:116:OMU:H6	2.19	0.42
23:i:206:G:H2'	23:i:207:G:C8	2.53	0.42
24:B:138:VAL:HG12	24:B:142:LEU:HD21	2.00	0.42
8:P:86:LEU:HD21	8:P:113:HIS:HB2	2.01	0.42
23:i:160:U:O2'	23:i:162:C:OP2	2.33	0.42
23:i:472:C:H4'	23:i:474:G:OP1	2.18	0.42
23:i:1705:C:H2'	23:i:1706:G:H8	1.84	0.42
23:i:1801:A:H2'	23:i:1802:C:H6	1.84	0.42
3:F:98:ARG:NH2	3:F:103:ASP:OD1	2.52	0.42
3:F:133:LEU:HD22	23:i:65:C:C2	2.53	0.42
6:M:94:LYS:HG2	6:M:118:ILE:HD13	2.01	0.42
22:C:94:LYS:HD2	22:C:94:LYS:HA	1.81	0.42
23:i:1740:C:H2'	23:i:1741:U:C6	2.53	0.42
15:f:17:ARG:NH2	23:i:1173:A:OP1	2.52	0.42
23:i:106:C:H2'	23:i:107:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:67:ASP:HB3	5:I:70:ARG:HB3	2.00	0.42
23:i:344:U:H2'	23:i:345:U:C6	2.54	0.42
23:i:945:U:H2'	23:i:946:U:C6	2.54	0.42
23:i:1037:G:H4'	23:i:1845:A:H4'	2.00	0.42
18:k:70:ASN:OD1	18:k:71:GLY:N	2.51	0.42
19:G:100:ILE:HG12	19:G:125:VAL:HG21	2.02	0.42
23:i:1708:C:C2	23:i:1709:G:C8	3.08	0.42
2:D:182:MET:HE3	2:D:192:ILE:HD11	2.01	0.42
23:i:1118:C:H2'	23:i:1119:A:O4'	2.20	0.42
1:A:267:GLN:HE22	10:V:35:ASN:HD21	1.67	0.42
4:H:170:LYS:HE2	4:H:170:LYS:HB3	1.91	0.42
8:P:83:LEU:HD23	8:P:83:LEU:HA	1.90	0.42
1:A:271:ASP:O	1:A:274:VAL:HG12	2.20	0.41
6:M:93:LYS:HB3	6:M:93:LYS:HE2	1.78	0.41
22:C:231:LEU:HD12	22:C:231:LEU:HA	1.82	0.41
23:i:320:G:H2'	23:i:321:C:H6	1.85	0.41
23:i:418:A:H2'	23:i:419:G:C8	2.55	0.41
23:i:851:C:H5''	23:i:852:G:H5'	2.02	0.41
23:i:158:A:H2'	23:i:159:A2M:O4'	2.20	0.41
11:W:64:SER:OG	23:i:615:C:OP2	2.33	0.41
4:H:33:ALA:HA	23:i:379:C:H5'	2.02	0.41
23:i:186:C:H2'	23:i:187:G:H8	1.86	0.41
5:I:80:ARG:NH1	23:i:818:A:OP1	2.38	0.41
16:h:126:ASP:HB3	16:h:129:ALA:HB3	2.02	0.41
23:i:1819:A:H2'	23:i:1820:G:H8	1.82	0.41
19:G:46:THR:N	19:G:63:PHE:O	2.53	0.41
23:i:99:A2M:H2'	23:i:100:U:O4'	2.20	0.41
23:i:948:C:H2'	23:i:949:G:H8	1.86	0.41
23:i:1189:A:H2'	23:i:1190:A:H8	1.85	0.41
23:i:1831:A:H2'	23:i:1832:6MZ:H8	2.02	0.41
23:i:321:C:H2'	23:i:322:C:C6	2.55	0.41
23:i:1181:A:H2'	23:i:1182:A:C8	2.56	0.41
2:D:66:MET:HG3	23:i:502:C:O4'	2.20	0.41
23:i:5:U:H2'	23:i:6:G:C8	2.56	0.41
23:i:301:A:H2'	23:i:302:A:O4'	2.20	0.41
13:Z:46:GLU:O	13:Z:50:VAL:HG23	2.21	0.41
22:C:99:ASN:OD1	22:C:100:PHE:N	2.51	0.41
23:i:349:A:H2'	23:i:350:C:C6	2.56	0.41
23:i:398:A:OP1	23:i:399:C:O2'	2.32	0.41
23:i:462:OMC:H1'	23:i:462:OMC:HM23	1.86	0.41
23:i:601:OMG:HM23	23:i:601:OMG:H1'	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:848:U:H2'	23:i:849:A:H8	1.86	0.41
23:i:1043:G:H2'	23:i:1044:G:O4'	2.21	0.41
23:i:1706:G:H2'	23:i:1707:U:C6	2.55	0.41
22:C:146:ARG:HB2	22:C:149:GLN:HB2	2.03	0.41
23:i:51:U:H2'	23:i:52:G:H8	1.85	0.41
23:i:929:G:H2'	23:i:930:C:O4'	2.21	0.41
1:A:125:LYS:HG3	1:A:143:CYS:HB2	2.02	0.40
2:D:21:ASP:HB2	23:i:829:C:OP1	2.20	0.40
12:X:6:THR:OG1	12:X:28:LEU:HB2	2.20	0.40
15:f:11:ARG:HH12	23:i:1844:U:P	2.44	0.40
22:C:103:MET:HE1	22:C:212:VAL:O	2.21	0.40
23:i:28:U:H2'	23:i:29:G:C8	2.55	0.40
6:M:99:ARG:NH2	6:M:119:GLU:OE2	2.42	0.40
9:R:129:LYS:NZ	23:i:1126:G:OP2	2.49	0.40
23:i:468:A2M:H2'	23:i:469:A:O4'	2.21	0.40
1:A:207:ALA:HB2	23:i:4:C:H4'	2.03	0.40
5:I:170:PRO:HB3	5:I:174:LYS:HG2	2.02	0.40
11:W:124:LYS:HG2	11:W:129:SER:HA	2.03	0.40
12:X:60:PHE:O	23:i:571:U:O2'	2.39	0.40
19:G:63:PHE:HA	19:G:95:ILE:O	2.21	0.40
4:H:197:PHE:CZ	4:H:201:LYS:HE3	2.57	0.40
23:i:115:U:O2'	23:i:381:C:O2	2.33	0.40
23:i:204:G:H2'	23:i:205:G:H8	1.86	0.40
23:i:509:OMG:H1'	23:i:509:OMG:HM23	1.89	0.40
23:i:293:C:H2'	23:i:293:C:O2	2.22	0.40
23:i:639:C:H2'	23:i:640:A:H8	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
2	D	258/263 (98%)	254 (98%)	4 (2%)	0	100	100
3	F	229/249 (92%)	227 (99%)	2 (1%)	0	100	100
4	H	203/208 (98%)	203 (100%)	0	0	100	100
5	I	177/194 (91%)	174 (98%)	3 (2%)	0	100	100
6	M	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
7	N	129/151 (85%)	126 (98%)	3 (2%)	0	100	100
8	P	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	R	50/135 (37%)	50 (100%)	0	0	100	100
10	V	82/84 (98%)	82 (100%)	0	0	100	100
11	W	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
12	X	123/130 (95%)	123 (100%)	0	0	100	100
13	Z	96/115 (84%)	96 (100%)	0	0	100	100
14	a	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
15	f	20/25 (80%)	20 (100%)	0	0	100	100
16	h	206/295 (70%)	204 (99%)	2 (1%)	0	100	100
17	j	30/180 (17%)	27 (90%)	3 (10%)	0	100	100
18	k	46/113 (41%)	45 (98%)	1 (2%)	0	100	100
19	G	177/194 (91%)	176 (99%)	1 (1%)	0	100	100
20	K	136/158 (86%)	134 (98%)	2 (2%)	0	100	100
21	e	44/61 (72%)	44 (100%)	0	0	100	100
22	C	213/264 (81%)	213 (100%)	0	0	100	100
24	B	42/243 (17%)	42 (100%)	0	0	100	100
All	All	2971/3863 (77%)	2940 (99%)	31 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/223 (80%)	178 (99%)	1 (1%)	84	89
2	D	212/225 (94%)	212 (100%)	0	100	100
3	F	160/218 (73%)	160 (100%)	0	100	100
4	H	147/180 (82%)	147 (100%)	0	100	100
5	I	151/168 (90%)	151 (100%)	0	100	100
6	M	117/131 (89%)	117 (100%)	0	100	100
7	N	95/118 (80%)	94 (99%)	1 (1%)	70	77
8	P	111/113 (98%)	111 (100%)	0	100	100
9	R	33/121 (27%)	32 (97%)	1 (3%)	36	40
10	V	63/67 (94%)	63 (100%)	0	100	100
11	W	110/115 (96%)	108 (98%)	2 (2%)	54	61
12	X	94/112 (84%)	93 (99%)	1 (1%)	70	77
13	Z	75/98 (76%)	75 (100%)	0	100	100
14	a	57/76 (75%)	57 (100%)	0	100	100
15	f	15/24 (62%)	15 (100%)	0	100	100
16	h	161/240 (67%)	160 (99%)	1 (1%)	84	89
17	j	26/151 (17%)	26 (100%)	0	100	100
18	k	13/96 (14%)	13 (100%)	0	100	100
19	G	113/174 (65%)	113 (100%)	0	100	100
20	K	122/142 (86%)	120 (98%)	2 (2%)	58	65
21	e	34/49 (69%)	34 (100%)	0	100	100
22	C	176/231 (76%)	174 (99%)	2 (1%)	70	77
24	B	32/202 (16%)	32 (100%)	0	100	100
All	All	2296/3274 (70%)	2285 (100%)	11 (0%)	85	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	TYR
7	N	113	GLN
9	R	116	ASN
11	W	17	ARG
11	W	105	PHE
12	X	16	ARG
16	h	38	ILE

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Mol	Chain	Res	Type
20	K	8	ARG
20	K	141	ASN
22	C	43	ASN
22	C	225	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
2	D	214	ASN
3	F	70	HIS
3	F	163	ASN
4	H	111	GLN
4	H	116	HIS
4	H	146	GLN
6	M	58	HIS
6	M	69	ASN
6	M	90	HIS
7	N	113	GLN
8	P	91	ASN
8	P	120	HIS
9	R	127	ASN
10	V	2	GLN
10	V	21	ASN
11	W	87	ASN
12	X	89	HIS
13	Z	86	ASN
14	a	65	GLN
16	h	36	GLN
16	h	84	GLN
16	h	113	GLN
19	G	68	GLN
19	G	76	GLN
19	G	114	GLN
19	G	162	GLN
20	K	19	ASN
22	C	76	ASN
22	C	92	GLN
22	C	159	GLN
22	C	163	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	i	1076/1869 (57%)	129 (11%)	0

All (129) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
23	i	17	C
23	i	23	G
23	i	33	G
23	i	41	G
23	i	46	A
23	i	56	G
23	i	64	A
23	i	65	C
23	i	67	C
23	i	68	A
23	i	79	A
23	i	99	A2M
23	i	103	A
23	i	113	G
23	i	114	G
23	i	115	U
23	i	126	G
23	i	130	G
23	i	131	C
23	i	143	U
23	i	155	G
23	i	168	C
23	i	178	C
23	i	182	C
23	i	184	G
23	i	192	C
23	i	224	A
23	i	309	G
23	i	312	G
23	i	319	C
23	i	330	G
23	i	333	G
23	i	335	G
23	i	351	G
23	i	362	C
23	i	364	A

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Mol	Chain	Res	Type
23	i	369	C
23	i	385	G
23	i	386	C
23	i	400	C
23	i	409	C
23	i	421	G
23	i	448	A
23	i	449	A
23	i	450	C
23	i	467	G
23	i	471	G
23	i	472	C
23	i	474	G
23	i	482	G
23	i	487	U
23	i	492	C
23	i	516	A
23	i	559	G
23	i	560	A
23	i	563	G
23	i	576	A2M
23	i	588	G
23	i	591	U
23	i	604	A
23	i	607	U
23	i	608	C
23	i	614	C
23	i	628	A
23	i	629	A
23	i	631	U
23	i	643	A
23	i	644	OMG
23	i	655	A
23	i	660	C
23	i	668	A2M
23	i	669	A
23	i	671	A
23	i	672	A
23	i	673	G
23	i	683	OMG
23	i	799	OMU
23	i	811	A

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Mol	Chain	Res	Type
23	i	821	G
23	i	822	PSU
23	i	830	A
23	i	834	C
23	i	847	A
23	i	870	A
23	i	873	G
23	i	874	G
23	i	878	G
23	i	913	A
23	i	920	A
23	i	922	A
23	i	933	G
23	i	943	U
23	i	978	G
23	i	990	A
23	i	992	A
23	i	1017	U
23	i	1023	A
23	i	1061	U
23	i	1062	A
23	i	1083	A
23	i	1085	C
23	i	1126	G
23	i	1130	G
23	i	1133	A
23	i	1144	A
23	i	1153	C
23	i	1154	U
23	i	1157	G
23	i	1171	G
23	i	1195	A
23	i	1203	G
23	i	1207	G
23	i	1698	C
23	i	1699	A
23	i	1744	G
23	i	1805	G
23	i	1829	G
23	i	1831	A
23	i	1835	A
23	i	1836	G

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Mol	Chain	Res	Type
23	i	1838	U
23	i	1849	G
23	i	1851	MA6
23	i	1861	G
23	i	1862	G
23	i	1863	A
23	i	1864	U
23	i	1865	C
23	i	1869	A

There are no RNA pucker outliers to report.

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

63 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
23	PSU	i	686	23	18,21,22	4.73	8 (44%)	21,30,33	2.04	5 (23%)
23	PSU	i	572	23	18,21,22	4.72	8 (44%)	21,30,33	2.05	6 (28%)
23	PSU	i	1045	23	18,21,22	4.71	8 (44%)	21,30,33	1.98	5 (23%)
23	OMU	i	799	23	19,22,23	0.79	1 (5%)	25,31,34	1.25	4 (16%)
23	PSU	i	649	23	18,21,22	4.72	8 (44%)	21,30,33	2.02	5 (23%)
23	PSU	i	105	23	18,21,22	4.72	8 (44%)	21,30,33	2.01	5 (23%)
23	A2M	i	512	23	18,25,26	1.30	2 (11%)	20,36,39	1.98	5 (25%)
23	A2M	i	99	23,25	18,25,26	1.29	2 (11%)	20,36,39	1.91	5 (25%)
23	PSU	i	866	23	18,21,22	4.75	8 (44%)	21,30,33	2.05	5 (23%)
23	OMG	i	601	23	19,26,27	1.17	2 (10%)	21,38,41	0.83	1 (4%)
23	A2M	i	159	23	18,25,26	1.24	2 (11%)	20,36,39	1.80	6 (30%)
23	OMC	i	1703	23	19,22,23	0.80	1 (5%)	25,31,34	1.15	4 (16%)
23	PSU	i	1136	23	18,21,22	4.71	8 (44%)	21,30,33	2.06	6 (28%)
23	A2M	i	27	23,25	18,25,26	1.30	2 (11%)	20,36,39	1.89	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	i	218	23	18,21,22	4.71	8 (44%)	21,30,33	1.92	6 (28%)
23	6MZ	i	1832	23,25,26	17,25,26	1.60	4 (23%)	15,36,39	2.73	5 (33%)
23	PSU	i	609	23	18,21,22	4.72	8 (44%)	21,30,33	2.04	5 (23%)
23	A2M	i	484	23	18,25,26	1.21	1 (5%)	20,36,39	1.75	6 (30%)
23	OMC	i	517	23	19,22,23	0.78	1 (5%)	25,31,34	1.14	4 (16%)
23	PSU	i	1174	23	18,21,22	4.70	8 (44%)	21,30,33	2.01	5 (23%)
23	PSU	i	1177	23	18,21,22	4.72	8 (44%)	21,30,33	1.98	5 (23%)
23	A2M	i	166	23	18,25,26	1.30	2 (11%)	20,36,39	2.02	6 (30%)
23	4AC	i	1842	23	21,24,25	3.38	10 (47%)	28,34,37	1.03	4 (14%)
23	PSU	i	814	23	18,21,22	4.70	8 (44%)	21,30,33	1.93	5 (23%)
23	PSU	i	863	23	18,21,22	4.70	8 (44%)	21,30,33	2.02	5 (23%)
23	PSU	i	406	23	18,21,22	4.70	8 (44%)	21,30,33	2.04	5 (23%)
23	A2M	i	668	23,25	18,25,26	1.37	3 (16%)	20,36,39	1.96	6 (30%)
23	PSU	i	681	23	18,21,22	4.67	8 (44%)	21,30,33	1.98	5 (23%)
23	OMU	i	428	23	19,22,23	0.66	0	25,31,34	1.26	4 (16%)
23	OMG	i	509	23,25	19,26,27	1.19	2 (10%)	21,38,41	0.85	1 (4%)
23	OMU	i	172	23	19,22,23	0.59	0	25,31,34	1.36	4 (16%)
23	PSU	i	119	23	18,21,22	4.67	8 (44%)	21,30,33	1.92	5 (23%)
23	OMC	i	797	23	19,22,23	0.99	2 (10%)	25,31,34	1.09	2 (8%)
7	IAS	N	138	7	6,7,8	1.13	0	3,8,10	2.08	1 (33%)
23	A2M	i	576	23	18,25,26	1.25	2 (11%)	20,36,39	1.87	5 (25%)
23	OMU	i	627	23	19,22,23	0.68	1 (5%)	25,31,34	1.31	4 (16%)
23	OMG	i	683	23	19,26,27	1.20	2 (10%)	21,38,41	0.82	1 (4%)
23	MA6	i	1850	23	19,26,27	1.70	3 (15%)	18,38,41	3.27	4 (22%)
23	PSU	i	1692	23	18,21,22	4.71	8 (44%)	21,30,33	2.03	5 (23%)
23	PSU	i	822	23	18,21,22	4.72	9 (50%)	21,30,33	2.09	6 (28%)
23	PSU	i	36	23	18,21,22	4.70	8 (44%)	21,30,33	2.03	6 (28%)
23	PSU	i	651	23	18,21,22	4.69	8 (44%)	21,30,33	2.05	5 (23%)
23	OMU	i	1804	23	19,22,23	0.76	0	25,31,34	1.32	4 (16%)
23	PSU	i	34	23	18,21,22	4.70	8 (44%)	21,30,33	2.00	5 (23%)
23	A2M	i	590	23	18,25,26	1.30	2 (11%)	20,36,39	2.20	6 (30%)
23	OMC	i	462	23	19,22,23	0.81	1 (5%)	25,31,34	1.11	4 (16%)
23	OMG	i	644	23	19,26,27	1.19	3 (15%)	21,38,41	0.85	1 (4%)
23	PSU	i	815	23	18,21,22	4.70	8 (44%)	21,30,33	2.03	5 (23%)
23	A2M	i	1031	23	18,25,26	1.27	2 (11%)	20,36,39	1.93	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	i	966	23	18,21,22	4.75	8 (44%)	21,30,33	1.98	5 (23%)
23	PSU	i	109	23	18,21,22	4.71	8 (44%)	21,30,33	2.02	6 (28%)
23	OMC	i	174	23	19,22,23	0.78	1 (5%)	25,31,34	1.17	4 (16%)
23	PSU	i	1046	23	18,21,22	4.72	8 (44%)	21,30,33	1.98	6 (28%)
23	PSU	i	1056	23	18,21,22	4.73	8 (44%)	21,30,33	2.01	6 (28%)
23	PSU	i	1081	23	18,21,22	4.73	9 (50%)	21,30,33	1.99	6 (28%)
23	OMU	i	354	23	19,22,23	0.65	0	25,31,34	1.32	5 (20%)
23	OMU	i	116	23	19,22,23	0.68	0	25,31,34	1.17	3 (12%)
23	PSU	i	1004	23	18,21,22	4.72	8 (44%)	21,30,33	2.01	5 (23%)
23	OMG	i	436	23	19,26,27	1.21	3 (15%)	21,38,41	0.82	1 (4%)
23	MA6	i	1851	23	19,26,27	1.65	3 (15%)	18,38,41	3.44	4 (22%)
23	OMU	i	121	23	19,22,23	0.56	0	25,31,34	1.21	3 (12%)
23	A2M	i	468	23	18,25,26	1.33	2 (11%)	20,36,39	2.05	6 (30%)
23	PSU	i	93	23	18,21,22	4.70	8 (44%)	21,30,33	1.94	5 (23%)

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
23	PSU	i	686	23	-	0/7/25/26	0/2/2/2
23	PSU	i	572	23	-	0/7/25/26	0/2/2/2
23	PSU	i	1045	23	-	0/7/25/26	0/2/2/2
23	OMU	i	799	23	-	0/9/27/28	0/2/2/2
23	PSU	i	649	23	-	0/7/25/26	0/2/2/2
23	PSU	i	105	23	-	0/7/25/26	0/2/2/2
23	A2M	i	512	23	-	0/5/27/28	0/3/3/3
23	A2M	i	99	23,25	-	2/5/27/28	0/3/3/3
23	PSU	i	866	23	-	0/7/25/26	0/2/2/2
23	OMG	i	601	23	-	1/5/27/28	0/3/3/3
23	A2M	i	159	23	-	1/5/27/28	0/3/3/3
23	OMC	i	1703	23	-	0/9/27/28	0/2/2/2
23	PSU	i	1136	23	-	0/7/25/26	0/2/2/2
23	A2M	i	27	23,25	-	0/5/27/28	0/3/3/3
23	PSU	i	218	23	-	0/7/25/26	0/2/2/2
23	6MZ	i	1832	23,25,26	-	0/5/27/28	0/3/3/3
23	PSU	i	609	23	-	0/7/25/26	0/2/2/2
23	A2M	i	484	23	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	i	517	23	-	0/9/27/28	0/2/2/2
23	PSU	i	1174	23	-	0/7/25/26	0/2/2/2
23	PSU	i	1177	23	-	0/7/25/26	0/2/2/2
23	A2M	i	166	23	-	0/5/27/28	0/3/3/3
23	4AC	i	1842	23	-	0/11/29/30	0/2/2/2
23	PSU	i	814	23	-	0/7/25/26	0/2/2/2
23	PSU	i	863	23	-	0/7/25/26	0/2/2/2
23	PSU	i	406	23	-	0/7/25/26	0/2/2/2
23	A2M	i	668	23,25	-	2/5/27/28	0/3/3/3
23	PSU	i	681	23	-	0/7/25/26	0/2/2/2
23	OMU	i	428	23	-	4/9/27/28	0/2/2/2
23	OMG	i	509	23,25	-	0/5/27/28	0/3/3/3
23	OMU	i	172	23	-	0/9/27/28	0/2/2/2
23	PSU	i	119	23	-	0/7/25/26	0/2/2/2
23	OMC	i	797	23	-	1/9/27/28	0/2/2/2
7	IAS	N	138	7	-	0/7/7/8	-
23	A2M	i	576	23	-	2/5/27/28	0/3/3/3
23	OMU	i	627	23	-	0/9/27/28	0/2/2/2
23	OMG	i	683	23	-	2/5/27/28	0/3/3/3
23	MA6	i	1850	23	-	0/7/29/30	0/3/3/3
23	PSU	i	1692	23	-	0/7/25/26	0/2/2/2
23	PSU	i	822	23	-	0/7/25/26	0/2/2/2
23	PSU	i	36	23	-	0/7/25/26	0/2/2/2
23	PSU	i	651	23	-	0/7/25/26	0/2/2/2
23	OMU	i	1804	23	-	0/9/27/28	0/2/2/2
23	PSU	i	34	23	-	0/7/25/26	0/2/2/2
23	A2M	i	590	23	-	0/5/27/28	0/3/3/3
23	OMC	i	462	23	-	0/9/27/28	0/2/2/2
23	OMG	i	644	23	-	4/5/27/28	0/3/3/3
23	PSU	i	815	23	-	0/7/25/26	0/2/2/2
23	A2M	i	1031	23	-	0/5/27/28	0/3/3/3
23	PSU	i	966	23	-	0/7/25/26	0/2/2/2
23	PSU	i	109	23	-	0/7/25/26	0/2/2/2
23	OMC	i	174	23	-	0/9/27/28	0/2/2/2
23	PSU	i	1046	23	-	0/7/25/26	0/2/2/2
23	PSU	i	1056	23	-	0/7/25/26	0/2/2/2
23	PSU	i	1081	23	-	1/7/25/26	0/2/2/2
23	OMU	i	354	23	-	0/9/27/28	0/2/2/2
23	OMU	i	116	23	-	0/9/27/28	0/2/2/2
23	PSU	i	1004	23	-	0/7/25/26	0/2/2/2
23	OMG	i	436	23	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	MA6	i	1851	23	-	1/7/29/30	0/3/3/3
23	OMU	i	121	23	-	1/9/27/28	0/2/2/2
23	A2M	i	468	23	-	0/5/27/28	0/3/3/3
23	PSU	i	93	23	-	0/7/25/26	0/2/2/2

All (296) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	866	PSU	C6-C5	12.62	1.49	1.35
23	i	966	PSU	C6-C5	12.60	1.49	1.35
23	i	609	PSU	C6-C5	12.58	1.49	1.35
23	i	649	PSU	C6-C5	12.56	1.49	1.35
23	i	572	PSU	C6-C5	12.55	1.49	1.35
23	i	1177	PSU	C6-C5	12.54	1.49	1.35
23	i	686	PSU	C6-C5	12.53	1.49	1.35
23	i	822	PSU	C6-C5	12.51	1.49	1.35
23	i	105	PSU	C6-C5	12.51	1.49	1.35
23	i	1004	PSU	C6-C5	12.51	1.49	1.35
23	i	1081	PSU	C6-C5	12.49	1.49	1.35
23	i	109	PSU	C6-C5	12.49	1.49	1.35
23	i	1046	PSU	C6-C5	12.49	1.49	1.35
23	i	406	PSU	C6-C5	12.48	1.49	1.35
23	i	1692	PSU	C6-C5	12.48	1.49	1.35
23	i	814	PSU	C6-C5	12.47	1.49	1.35
23	i	651	PSU	C6-C5	12.47	1.49	1.35
23	i	36	PSU	C6-C5	12.47	1.49	1.35
23	i	1056	PSU	C6-C5	12.47	1.49	1.35
23	i	815	PSU	C6-C5	12.45	1.49	1.35
23	i	34	PSU	C6-C5	12.44	1.49	1.35
23	i	1174	PSU	C6-C5	12.44	1.49	1.35
23	i	863	PSU	C6-C5	12.43	1.49	1.35
23	i	218	PSU	C6-C5	12.42	1.49	1.35
23	i	93	PSU	C6-C5	12.41	1.49	1.35
23	i	1136	PSU	C6-C5	12.40	1.49	1.35
23	i	1045	PSU	C6-C5	12.40	1.49	1.35
23	i	681	PSU	C6-C5	12.37	1.49	1.35
23	i	119	PSU	C6-C5	12.34	1.49	1.35
23	i	1045	PSU	C2-N1	9.83	1.49	1.36
23	i	866	PSU	C2-N1	9.80	1.49	1.36
23	i	1056	PSU	C2-N1	9.80	1.49	1.36
23	i	1136	PSU	C2-N1	9.78	1.49	1.36
23	i	1046	PSU	C2-N1	9.75	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	34	PSU	C2-N1	9.75	1.49	1.36
23	i	1177	PSU	C2-N1	9.75	1.49	1.36
23	i	686	PSU	C2-N1	9.74	1.49	1.36
23	i	93	PSU	C2-N1	9.74	1.49	1.36
23	i	814	PSU	C2-N1	9.74	1.49	1.36
23	i	649	PSU	C2-N1	9.73	1.49	1.36
23	i	105	PSU	C2-N1	9.72	1.49	1.36
23	i	966	PSU	C2-N1	9.72	1.49	1.36
23	i	863	PSU	C2-N1	9.71	1.49	1.36
23	i	1081	PSU	C2-N1	9.70	1.49	1.36
23	i	572	PSU	C2-N1	9.68	1.49	1.36
23	i	1692	PSU	C2-N1	9.67	1.49	1.36
23	i	36	PSU	C2-N1	9.66	1.49	1.36
23	i	1174	PSU	C2-N1	9.66	1.49	1.36
23	i	651	PSU	C2-N1	9.66	1.49	1.36
23	i	609	PSU	C2-N1	9.66	1.49	1.36
23	i	1004	PSU	C2-N1	9.65	1.49	1.36
23	i	815	PSU	C2-N1	9.64	1.49	1.36
23	i	218	PSU	C2-N1	9.61	1.49	1.36
23	i	406	PSU	C2-N1	9.60	1.49	1.36
23	i	109	PSU	C2-N1	9.59	1.49	1.36
23	i	681	PSU	C2-N1	9.58	1.49	1.36
23	i	822	PSU	C2-N1	9.58	1.49	1.36
23	i	119	PSU	C2-N1	9.51	1.49	1.36
23	i	866	PSU	C2-N3	8.47	1.51	1.37
23	i	686	PSU	C2-N3	8.43	1.51	1.37
23	i	609	PSU	C2-N3	8.40	1.51	1.37
23	i	1004	PSU	C2-N3	8.40	1.51	1.37
23	i	966	PSU	C2-N3	8.39	1.51	1.37
23	i	1056	PSU	C2-N3	8.37	1.51	1.37
23	i	822	PSU	C2-N3	8.37	1.51	1.37
23	i	1692	PSU	C2-N3	8.36	1.51	1.37
23	i	406	PSU	C2-N3	8.36	1.51	1.37
23	i	815	PSU	C2-N3	8.35	1.51	1.37
23	i	1174	PSU	C2-N3	8.35	1.51	1.37
23	i	572	PSU	C2-N3	8.34	1.51	1.37
23	i	1046	PSU	C2-N3	8.34	1.51	1.37
23	i	218	PSU	C2-N3	8.32	1.51	1.37
23	i	105	PSU	C2-N3	8.30	1.51	1.37
23	i	36	PSU	C2-N3	8.30	1.51	1.37
23	i	119	PSU	C2-N3	8.30	1.51	1.37
23	i	109	PSU	C2-N3	8.30	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	863	PSU	C2-N3	8.29	1.51	1.37
23	i	651	PSU	C2-N3	8.29	1.51	1.37
23	i	34	PSU	C2-N3	8.29	1.51	1.37
23	i	1136	PSU	C2-N3	8.29	1.51	1.37
23	i	649	PSU	C2-N3	8.28	1.51	1.37
23	i	1177	PSU	C2-N3	8.27	1.51	1.37
23	i	93	PSU	C2-N3	8.26	1.51	1.37
23	i	1045	PSU	C2-N3	8.26	1.51	1.37
23	i	1081	PSU	C2-N3	8.23	1.51	1.37
23	i	681	PSU	C2-N3	8.23	1.51	1.37
23	i	814	PSU	C2-N3	8.20	1.51	1.37
23	i	1842	4AC	C4-N3	7.30	1.45	1.32
23	i	1842	4AC	C2-N3	6.22	1.48	1.36
23	i	1842	4AC	C6-C5	6.21	1.49	1.35
23	i	218	PSU	C6-N1	5.74	1.45	1.36
23	i	105	PSU	C6-N1	5.73	1.45	1.36
23	i	866	PSU	C6-N1	5.72	1.45	1.36
23	i	572	PSU	C6-N1	5.71	1.45	1.36
23	i	93	PSU	C6-N1	5.70	1.45	1.36
23	i	609	PSU	C6-N1	5.70	1.45	1.36
23	i	1045	PSU	C6-N1	5.70	1.45	1.36
23	i	1056	PSU	C6-N1	5.69	1.45	1.36
23	i	966	PSU	C6-N1	5.67	1.45	1.36
23	i	109	PSU	C6-N1	5.67	1.45	1.36
23	i	406	PSU	C6-N1	5.66	1.45	1.36
23	i	1004	PSU	C6-N1	5.66	1.45	1.36
23	i	1136	PSU	C6-N1	5.66	1.45	1.36
23	i	119	PSU	C6-N1	5.65	1.45	1.36
23	i	1174	PSU	C6-N1	5.65	1.45	1.36
23	i	1046	PSU	C6-N1	5.63	1.45	1.36
23	i	863	PSU	C6-N1	5.63	1.45	1.36
23	i	1177	PSU	C6-N1	5.63	1.45	1.36
23	i	34	PSU	C6-N1	5.63	1.45	1.36
23	i	686	PSU	C6-N1	5.63	1.45	1.36
23	i	814	PSU	C6-N1	5.61	1.45	1.36
23	i	1081	PSU	C6-N1	5.61	1.45	1.36
23	i	815	PSU	C6-N1	5.61	1.45	1.36
23	i	36	PSU	C6-N1	5.60	1.45	1.36
23	i	1692	PSU	C6-N1	5.58	1.45	1.36
23	i	651	PSU	C6-N1	5.58	1.45	1.36
23	i	681	PSU	C6-N1	5.58	1.45	1.36
23	i	649	PSU	C6-N1	5.56	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	822	PSU	C6-N1	5.55	1.45	1.36
23	i	1842	4AC	C7-N4	5.06	1.47	1.37
23	i	1842	4AC	C4-N4	5.03	1.47	1.39
23	i	1832	6MZ	C6-C5	-4.61	1.37	1.44
23	i	1851	MA6	C6-N6	4.59	1.48	1.37
23	i	1850	MA6	C6-N6	4.45	1.47	1.37
23	i	966	PSU	C4-N3	4.26	1.46	1.38
23	i	109	PSU	C4-N3	4.18	1.46	1.38
23	i	866	PSU	C4-N3	4.15	1.46	1.38
23	i	218	PSU	C4-N3	4.15	1.46	1.38
23	i	1004	PSU	C4-N3	4.14	1.46	1.38
23	i	815	PSU	C4-N3	4.13	1.46	1.38
23	i	814	PSU	C4-N3	4.12	1.46	1.38
23	i	649	PSU	C4-N3	4.11	1.46	1.38
23	i	1174	PSU	C4-N3	4.10	1.46	1.38
23	i	1046	PSU	C4-N3	4.10	1.46	1.38
23	i	119	PSU	C4-N3	4.10	1.46	1.38
23	i	1177	PSU	C4-N3	4.09	1.46	1.38
23	i	572	PSU	C4-N3	4.09	1.46	1.38
23	i	1136	PSU	C4-N3	4.09	1.46	1.38
23	i	822	PSU	C4-N3	4.08	1.46	1.38
23	i	1056	PSU	C4-N3	4.08	1.46	1.38
23	i	686	PSU	C4-N3	4.08	1.46	1.38
23	i	36	PSU	C4-N3	4.08	1.46	1.38
23	i	1692	PSU	C4-N3	4.07	1.46	1.38
23	i	93	PSU	C4-N3	4.06	1.46	1.38
23	i	651	PSU	C4-N3	4.06	1.46	1.38
23	i	681	PSU	C4-N3	4.06	1.46	1.38
23	i	34	PSU	C4-N3	4.05	1.46	1.38
23	i	1045	PSU	C4-N3	4.05	1.46	1.38
23	i	863	PSU	C4-N3	4.05	1.46	1.38
23	i	406	PSU	C4-N3	4.05	1.46	1.38
23	i	1081	PSU	C4-N3	4.04	1.46	1.38
23	i	609	PSU	C4-N3	4.03	1.46	1.38
23	i	105	PSU	C4-N3	4.03	1.46	1.38
23	i	1850	MA6	C6-C5	-3.97	1.38	1.44
23	i	1842	4AC	C2-N1	3.89	1.48	1.40
23	i	1842	4AC	C5-C4	3.87	1.49	1.41
23	i	1851	MA6	C6-C5	-3.64	1.39	1.44
23	i	512	A2M	O5'-C5'	-3.46	1.34	1.44
23	i	668	A2M	O5'-C5'	-3.45	1.34	1.44
23	i	27	A2M	O5'-C5'	-3.44	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	218	PSU	O4-C4	-3.40	1.17	1.23
23	i	468	A2M	O5'-C5'	-3.39	1.34	1.44
23	i	36	PSU	O4-C4	-3.39	1.17	1.23
23	i	863	PSU	O4-C4	-3.38	1.17	1.23
23	i	1692	PSU	O4-C4	-3.38	1.17	1.23
23	i	681	PSU	O4-C4	-3.37	1.17	1.23
23	i	1081	PSU	O4-C4	-3.37	1.17	1.23
23	i	166	A2M	O5'-C5'	-3.37	1.34	1.44
23	i	99	A2M	O5'-C5'	-3.37	1.34	1.44
23	i	484	A2M	O5'-C5'	-3.36	1.34	1.44
23	i	1031	A2M	O5'-C5'	-3.36	1.34	1.44
23	i	109	PSU	O4-C4	-3.35	1.17	1.23
23	i	686	PSU	O4-C4	-3.34	1.17	1.23
23	i	93	PSU	O4-C4	-3.33	1.17	1.23
23	i	649	PSU	O4-C4	-3.33	1.17	1.23
23	i	406	PSU	O4-C4	-3.33	1.17	1.23
23	i	1046	PSU	O4-C4	-3.33	1.17	1.23
23	i	1136	PSU	O4-C4	-3.33	1.17	1.23
23	i	105	PSU	O4-C4	-3.32	1.17	1.23
23	i	814	PSU	O4-C4	-3.32	1.17	1.23
23	i	1045	PSU	O4-C4	-3.32	1.17	1.23
23	i	119	PSU	O4-C4	-3.31	1.17	1.23
23	i	572	PSU	O4-C4	-3.31	1.17	1.23
23	i	822	PSU	O4-C4	-3.31	1.17	1.23
23	i	815	PSU	O4-C4	-3.30	1.17	1.23
23	i	651	PSU	O4-C4	-3.29	1.17	1.23
23	i	1056	PSU	O4-C4	-3.29	1.17	1.23
23	i	1004	PSU	O4-C4	-3.28	1.17	1.23
23	i	34	PSU	O4-C4	-3.28	1.17	1.23
23	i	1174	PSU	O4-C4	-3.28	1.17	1.23
23	i	609	PSU	O4-C4	-3.28	1.17	1.23
23	i	590	A2M	O5'-C5'	-3.25	1.34	1.44
23	i	1177	PSU	O4-C4	-3.25	1.17	1.23
23	i	966	PSU	O4-C4	-3.24	1.17	1.23
23	i	866	PSU	O4-C4	-3.22	1.17	1.23
23	i	576	A2M	O5'-C5'	-3.21	1.34	1.44
23	i	159	A2M	O5'-C5'	-3.17	1.34	1.44
23	i	1842	4AC	C6-N1	3.13	1.45	1.38
23	i	683	OMG	C8-N7	-3.12	1.29	1.34
23	i	509	OMG	C8-N7	-3.06	1.30	1.34
23	i	436	OMG	C8-N7	-3.06	1.30	1.34
23	i	644	OMG	C8-N7	-3.05	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	601	OMG	C8-N7	-3.04	1.30	1.34
23	i	1842	4AC	O2-C2	-2.94	1.18	1.23
23	i	218	PSU	C1'-C5	2.89	1.56	1.50
23	i	1081	PSU	C1'-C5	2.88	1.56	1.50
23	i	1850	MA6	C2-N3	2.83	1.36	1.32
23	i	1046	PSU	C1'-C5	2.78	1.56	1.50
23	i	109	PSU	C1'-C5	2.77	1.56	1.50
23	i	822	PSU	C1'-C5	2.76	1.56	1.50
23	i	966	PSU	C1'-C5	2.75	1.56	1.50
23	i	105	PSU	C1'-C5	2.74	1.56	1.50
23	i	406	PSU	O2-C2	-2.74	1.17	1.23
23	i	1056	PSU	C1'-C5	2.73	1.56	1.50
23	i	93	PSU	C1'-C5	2.73	1.56	1.50
23	i	863	PSU	O2-C2	-2.73	1.17	1.23
23	i	105	PSU	O2-C2	-2.72	1.17	1.23
23	i	681	PSU	O2-C2	-2.72	1.17	1.23
23	i	1081	PSU	O2-C2	-2.72	1.17	1.23
23	i	649	PSU	O2-C2	-2.72	1.17	1.23
23	i	1177	PSU	C1'-C5	2.71	1.56	1.50
23	i	814	PSU	C1'-C5	2.71	1.56	1.50
23	i	1692	PSU	C1'-C5	2.71	1.56	1.50
23	i	609	PSU	O2-C2	-2.70	1.17	1.23
23	i	36	PSU	O2-C2	-2.70	1.17	1.23
23	i	1136	PSU	C1'-C5	2.70	1.56	1.50
23	i	686	PSU	O2-C2	-2.70	1.17	1.23
23	i	119	PSU	C1'-C5	2.69	1.56	1.50
23	i	109	PSU	O2-C2	-2.69	1.17	1.23
23	i	822	PSU	O2-C2	-2.69	1.17	1.23
23	i	34	PSU	C1'-C5	2.69	1.56	1.50
23	i	1004	PSU	O2-C2	-2.69	1.17	1.23
23	i	1045	PSU	C1'-C5	2.69	1.56	1.50
23	i	34	PSU	O2-C2	-2.69	1.17	1.23
23	i	572	PSU	O2-C2	-2.69	1.17	1.23
23	i	1046	PSU	O2-C2	-2.68	1.17	1.23
23	i	814	PSU	O2-C2	-2.67	1.17	1.23
23	i	1004	PSU	C1'-C5	2.67	1.56	1.50
23	i	863	PSU	C1'-C5	2.67	1.56	1.50
23	i	815	PSU	O2-C2	-2.67	1.17	1.23
23	i	668	A2M	O4'-C4'	-2.67	1.39	1.45
23	i	119	PSU	O2-C2	-2.67	1.17	1.23
23	i	1136	PSU	O2-C2	-2.67	1.17	1.23
23	i	93	PSU	O2-C2	-2.66	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	1177	PSU	O2-C2	-2.66	1.17	1.23
23	i	649	PSU	C1'-C5	2.66	1.56	1.50
23	i	1045	PSU	O2-C2	-2.66	1.17	1.23
23	i	1692	PSU	O2-C2	-2.66	1.17	1.23
23	i	681	PSU	C1'-C5	2.66	1.56	1.50
23	i	1174	PSU	C1'-C5	2.65	1.56	1.50
23	i	966	PSU	O2-C2	-2.65	1.17	1.23
23	i	651	PSU	O2-C2	-2.65	1.17	1.23
23	i	1174	PSU	O2-C2	-2.64	1.17	1.23
23	i	406	PSU	C1'-C5	2.64	1.56	1.50
23	i	609	PSU	C1'-C5	2.64	1.56	1.50
23	i	36	PSU	C1'-C5	2.63	1.56	1.50
23	i	572	PSU	C1'-C5	2.63	1.56	1.50
23	i	686	PSU	C1'-C5	2.61	1.56	1.50
23	i	866	PSU	C1'-C5	2.61	1.56	1.50
23	i	1056	PSU	O2-C2	-2.61	1.17	1.23
23	i	815	PSU	C1'-C5	2.61	1.56	1.50
23	i	436	OMG	C5-C6	-2.60	1.42	1.47
23	i	576	A2M	C1'-N9	-2.59	1.43	1.49
23	i	218	PSU	O2-C2	-2.58	1.17	1.23
23	i	866	PSU	O2-C2	-2.58	1.17	1.23
23	i	683	OMG	C5-C6	-2.58	1.42	1.47
23	i	651	PSU	C1'-C5	2.57	1.56	1.50
23	i	797	OMC	C2-N1	2.56	1.45	1.40
23	i	644	OMG	C5-C6	-2.54	1.42	1.47
23	i	797	OMC	C4-N4	2.54	1.40	1.33
23	i	468	A2M	C1'-N9	-2.53	1.43	1.49
23	i	509	OMG	C5-C6	-2.52	1.42	1.47
23	i	1832	6MZ	C2-N3	2.48	1.35	1.32
23	i	601	OMG	C5-C6	-2.48	1.42	1.47
23	i	668	A2M	C1'-N9	-2.47	1.43	1.49
23	i	512	A2M	C1'-N9	-2.38	1.44	1.49
23	i	99	A2M	C1'-N9	-2.34	1.44	1.49
23	i	1842	4AC	O7-C7	-2.33	1.18	1.23
23	i	1081	PSU	O4'-C1'	-2.32	1.40	1.43
23	i	1851	MA6	C2-N3	2.31	1.35	1.32
23	i	822	PSU	O4'-C1'	-2.30	1.40	1.43
23	i	1031	A2M	C1'-N9	-2.29	1.44	1.49
23	i	166	A2M	C1'-N9	-2.27	1.44	1.49
23	i	27	A2M	C1'-N9	-2.25	1.44	1.49
23	i	462	OMC	C4-N4	2.21	1.39	1.33
23	i	174	OMC	C4-N4	2.18	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	590	A2M	O4'-C4'	-2.15	1.40	1.45
23	i	627	OMU	C4-N3	2.13	1.42	1.38
23	i	1703	OMC	C4-N4	2.11	1.39	1.33
23	i	1832	6MZ	C6-N1	-2.11	1.31	1.34
23	i	159	A2M	C1'-N9	-2.10	1.44	1.49
23	i	517	OMC	C4-N4	2.06	1.38	1.33
23	i	799	OMU	C2-N1	2.05	1.41	1.38
23	i	1832	6MZ	C2-N1	2.03	1.37	1.33
23	i	644	OMG	C5-C4	-2.02	1.38	1.43
23	i	436	OMG	C5-C4	-2.01	1.38	1.43

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	1851	MA6	N1-C6-N6	-11.78	103.22	116.83
23	i	1850	MA6	N1-C6-N6	-10.55	104.64	116.83
23	i	590	A2M	C4'-O4'-C1'	-6.53	103.94	109.92
23	i	1832	6MZ	N3-C2-N1	-6.33	120.08	128.67
23	i	1850	MA6	N3-C2-N1	-6.28	120.14	128.67
23	i	1851	MA6	N3-C2-N1	-6.10	120.39	128.67
23	i	1832	6MZ	C9-N6-C6	-5.46	117.79	122.85
23	i	1850	MA6	C1'-N9-C4	5.16	135.71	126.64
23	i	609	PSU	C4-N3-C2	-4.96	119.54	126.37
23	i	468	A2M	C4'-O4'-C1'	-4.95	105.39	109.92
23	i	1692	PSU	C4-N3-C2	-4.94	119.56	126.37
23	i	651	PSU	C4-N3-C2	-4.94	119.57	126.37
23	i	815	PSU	C4-N3-C2	-4.94	119.57	126.37
23	i	572	PSU	C4-N3-C2	-4.93	119.58	126.37
23	i	105	PSU	C4-N3-C2	-4.93	119.58	126.37
23	i	93	PSU	C4-N3-C2	-4.93	119.59	126.37
23	i	863	PSU	C4-N3-C2	-4.92	119.59	126.37
23	i	686	PSU	C4-N3-C2	-4.92	119.60	126.37
23	i	866	PSU	C4-N3-C2	-4.92	119.60	126.37
23	i	1136	PSU	C4-N3-C2	-4.91	119.61	126.37
23	i	649	PSU	C4-N3-C2	-4.91	119.61	126.37
23	i	406	PSU	C4-N3-C2	-4.90	119.62	126.37
23	i	1174	PSU	C4-N3-C2	-4.90	119.62	126.37
23	i	1081	PSU	C4-N3-C2	-4.88	119.65	126.37
23	i	109	PSU	C4-N3-C2	-4.87	119.66	126.37
23	i	36	PSU	C4-N3-C2	-4.86	119.67	126.37
23	i	1056	PSU	C4-N3-C2	-4.86	119.68	126.37
23	i	34	PSU	C4-N3-C2	-4.86	119.68	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	681	PSU	C4-N3-C2	-4.86	119.68	126.37
23	i	1046	PSU	C4-N3-C2	-4.85	119.69	126.37
23	i	1045	PSU	C4-N3-C2	-4.85	119.69	126.37
23	i	1004	PSU	C4-N3-C2	-4.82	119.73	126.37
23	i	1177	PSU	C4-N3-C2	-4.82	119.73	126.37
23	i	822	PSU	C4-N3-C2	-4.79	119.78	126.37
23	i	966	PSU	C4-N3-C2	-4.77	119.81	126.37
23	i	166	A2M	C4'-O4'-C1'	-4.77	105.56	109.92
23	i	814	PSU	C4-N3-C2	-4.75	119.82	126.37
23	i	218	PSU	C4-N3-C2	-4.75	119.83	126.37
23	i	119	PSU	C4-N3-C2	-4.72	119.87	126.37
23	i	1851	MA6	C1'-N9-C4	4.64	134.80	126.64
23	i	651	PSU	N1-C2-N3	4.63	120.05	115.17
23	i	822	PSU	N1-C2-N3	4.61	120.03	115.17
23	i	866	PSU	N1-C2-N3	4.57	119.99	115.17
23	i	609	PSU	N1-C2-N3	4.56	119.98	115.17
23	i	815	PSU	N1-C2-N3	4.56	119.97	115.17
23	i	105	PSU	N1-C2-N3	4.55	119.96	115.17
23	i	1174	PSU	N1-C2-N3	4.55	119.96	115.17
23	i	1692	PSU	N1-C2-N3	4.54	119.96	115.17
23	i	572	PSU	N1-C2-N3	4.54	119.95	115.17
23	i	686	PSU	N1-C2-N3	4.54	119.95	115.17
23	i	1136	PSU	N1-C2-N3	4.54	119.95	115.17
23	i	109	PSU	N1-C2-N3	4.53	119.95	115.17
23	i	406	PSU	N1-C2-N3	4.53	119.94	115.17
23	i	649	PSU	N1-C2-N3	4.52	119.94	115.17
23	i	36	PSU	N1-C2-N3	4.52	119.93	115.17
23	i	34	PSU	N1-C2-N3	4.49	119.90	115.17
23	i	512	A2M	C4'-O4'-C1'	-4.48	105.82	109.92
23	i	863	PSU	N1-C2-N3	4.47	119.88	115.17
23	i	1004	PSU	N1-C2-N3	4.47	119.88	115.17
23	i	966	PSU	N1-C2-N3	4.46	119.87	115.17
23	i	681	PSU	N1-C2-N3	4.46	119.87	115.17
23	i	1046	PSU	N1-C2-N3	4.45	119.86	115.17
23	i	1081	PSU	N1-C2-N3	4.42	119.83	115.17
23	i	1177	PSU	N1-C2-N3	4.41	119.82	115.17
23	i	119	PSU	N1-C2-N3	4.39	119.80	115.17
23	i	1056	PSU	N1-C2-N3	4.39	119.80	115.17
23	i	1045	PSU	N1-C2-N3	4.37	119.78	115.17
23	i	99	A2M	C4'-O4'-C1'	-4.37	105.92	109.92
23	i	93	PSU	N1-C2-N3	4.37	119.77	115.17
23	i	814	PSU	N1-C2-N3	4.34	119.75	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	1031	A2M	C4'-O4'-C1'	-4.33	105.96	109.92
23	i	218	PSU	N1-C2-N3	4.24	119.64	115.17
23	i	27	A2M	C4'-O4'-C1'	-4.15	106.12	109.92
23	i	1832	6MZ	C1'-N9-C4	-4.01	119.59	126.64
23	i	1832	6MZ	C2-N1-C6	3.95	119.66	116.60
23	i	512	A2M	C1'-N9-C4	-3.88	119.83	126.64
23	i	668	A2M	C1'-N9-C4	-3.85	119.88	126.64
23	i	468	A2M	C1'-N9-C4	-3.79	119.98	126.64
23	i	668	A2M	C4'-O4'-C1'	-3.79	106.46	109.92
23	i	576	A2M	C1'-N9-C4	-3.78	119.99	126.64
23	i	166	A2M	C1'-N9-C4	-3.61	120.30	126.64
23	i	1136	PSU	C6-C5-C4	3.59	120.59	118.17
23	i	576	A2M	C4'-O4'-C1'	-3.57	106.65	109.92
23	i	1031	A2M	C1'-N9-C4	-3.55	120.40	126.64
23	i	27	A2M	C1'-N9-C4	-3.53	120.44	126.64
23	i	484	A2M	C1'-N9-C4	-3.51	120.47	126.64
23	i	822	PSU	C6-N1-C2	-3.46	119.48	122.69
7	N	138	IAS	OD1-CG-CB	-3.46	115.32	125.38
23	i	166	A2M	C3'-C2'-C1'	-3.43	96.24	102.81
23	i	572	PSU	C6-C5-C4	3.42	120.48	118.17
23	i	159	A2M	C1'-N9-C4	-3.40	120.66	126.64
23	i	468	A2M	C3'-C2'-C1'	-3.40	96.29	102.81
23	i	866	PSU	C6-C5-C4	3.40	120.47	118.17
23	i	512	A2M	C3'-C2'-C1'	-3.40	96.30	102.81
23	i	651	PSU	C6-C5-C4	3.40	120.47	118.17
23	i	406	PSU	C6-C5-C4	3.38	120.45	118.17
23	i	1056	PSU	C6-C5-C4	3.38	120.45	118.17
23	i	99	A2M	C3'-C2'-C1'	-3.36	96.38	102.81
23	i	1850	MA6	C2-N1-C6	3.36	120.13	116.84
23	i	576	A2M	O3'-C3'-C2'	3.34	120.53	111.19
23	i	686	PSU	C6-C5-C4	3.32	120.42	118.17
23	i	468	A2M	O3'-C3'-C2'	3.32	120.49	111.19
23	i	822	PSU	C6-C5-C4	3.32	120.42	118.17
23	i	166	A2M	O3'-C3'-C2'	3.32	120.48	111.19
23	i	1703	OMC	C5-C4-N3	3.32	126.91	121.32
23	i	1174	PSU	C6-N1-C2	-3.32	119.61	122.69
23	i	36	PSU	C6-C5-C4	3.31	120.41	118.17
23	i	109	PSU	C6-N1-C2	-3.31	119.62	122.69
23	i	1031	A2M	C3'-C2'-C1'	-3.30	96.48	102.81
23	i	966	PSU	C6-N1-C2	-3.29	119.63	122.69
23	i	815	PSU	C6-C5-C4	3.29	120.40	118.17
23	i	1046	PSU	C6-N1-C2	-3.28	119.65	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	36	PSU	C6-N1-C2	-3.28	119.65	122.69
23	i	609	PSU	C6-C5-C4	3.27	120.38	118.17
23	i	649	PSU	C6-N1-C2	-3.26	119.67	122.69
23	i	866	PSU	C6-N1-C2	-3.26	119.67	122.69
23	i	119	PSU	C6-N1-C2	-3.25	119.67	122.69
23	i	99	A2M	C1'-N9-C4	-3.25	120.93	126.64
23	i	1004	PSU	C6-N1-C2	-3.25	119.67	122.69
23	i	609	PSU	C6-N1-C2	-3.25	119.68	122.69
23	i	863	PSU	C6-N1-C2	-3.24	119.69	122.69
23	i	686	PSU	C6-N1-C2	-3.23	119.69	122.69
23	i	651	PSU	C6-N1-C2	-3.23	119.69	122.69
23	i	1692	PSU	C6-C5-C4	3.23	120.35	118.17
23	i	105	PSU	C6-N1-C2	-3.21	119.71	122.69
23	i	590	A2M	O3'-C3'-C2'	3.21	120.17	111.19
23	i	815	PSU	C6-N1-C2	-3.21	119.71	122.69
23	i	681	PSU	C6-N1-C2	-3.20	119.72	122.69
23	i	34	PSU	C6-N1-C2	-3.19	119.73	122.69
23	i	1851	MA6	C2-N1-C6	3.19	119.97	116.84
23	i	1692	PSU	C6-N1-C2	-3.16	119.75	122.69
23	i	484	A2M	O3'-C3'-C2'	3.16	120.03	111.19
23	i	512	A2M	O3'-C3'-C2'	3.16	120.02	111.19
23	i	863	PSU	C6-C5-C4	3.15	120.30	118.17
23	i	34	PSU	C6-C5-C4	3.15	120.30	118.17
23	i	1136	PSU	C6-N1-C2	-3.14	119.77	122.69
23	i	517	OMC	C5-C4-N3	3.14	126.61	121.32
23	i	174	OMC	C5-C4-N3	3.14	126.61	121.32
23	i	1004	PSU	C6-C5-C4	3.14	120.29	118.17
23	i	99	A2M	O3'-C3'-C2'	3.14	119.96	111.19
23	i	572	PSU	C6-N1-C2	-3.12	119.79	122.69
23	i	1177	PSU	C6-N1-C2	-3.11	119.80	122.69
23	i	159	A2M	O3'-C3'-C2'	3.11	119.89	111.19
23	i	590	A2M	C1'-N9-C4	-3.11	121.18	126.64
23	i	406	PSU	C6-N1-C2	-3.11	119.81	122.69
23	i	1045	PSU	C6-C5-C4	3.10	120.27	118.17
23	i	1056	PSU	C6-N1-C2	-3.10	119.81	122.69
23	i	159	A2M	C4'-O4'-C1'	-3.09	107.09	109.92
23	i	462	OMC	C5-C4-N3	3.09	126.52	121.32
23	i	814	PSU	C6-N1-C2	-3.07	119.84	122.69
23	i	797	OMC	C5-C4-N3	3.07	126.50	121.32
23	i	1174	PSU	C6-C5-C4	3.07	120.25	118.17
23	i	218	PSU	C6-N1-C2	-3.07	119.84	122.69
23	i	966	PSU	C6-C5-C4	3.06	120.24	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	1177	PSU	C6-C5-C4	3.06	120.24	118.17
23	i	105	PSU	C6-C5-C4	3.03	120.22	118.17
23	i	1045	PSU	C6-N1-C2	-3.03	119.88	122.69
23	i	109	PSU	C6-C5-C4	3.01	120.20	118.17
23	i	1081	PSU	C6-N1-C2	-2.99	119.91	122.69
23	i	27	A2M	C3'-C2'-C1'	-2.99	97.08	102.81
23	i	668	A2M	O3'-C3'-C2'	2.99	119.54	111.19
23	i	93	PSU	C6-N1-C2	-2.98	119.93	122.69
23	i	649	PSU	C6-C5-C4	2.98	120.18	118.17
23	i	1031	A2M	O3'-C3'-C2'	2.98	119.52	111.19
23	i	681	PSU	C6-C5-C4	2.96	120.17	118.17
23	i	627	OMU	C4-N3-C2	-2.94	122.96	126.61
23	i	172	OMU	C4-N3-C2	-2.93	122.97	126.61
23	i	576	A2M	C3'-C2'-C1'	-2.92	97.22	102.81
23	i	814	PSU	C6-C5-C4	2.91	120.14	118.17
23	i	428	OMU	C4-N3-C2	-2.90	123.02	126.61
23	i	1832	6MZ	C6-C5-C4	2.90	120.75	117.68
23	i	1046	PSU	C6-C5-C4	2.90	120.13	118.17
23	i	27	A2M	O3'-C3'-C2'	2.86	119.19	111.19
23	i	1004	PSU	O2-C2-N1	-2.85	119.85	122.79
23	i	1804	OMU	C4-N3-C2	-2.82	123.11	126.61
23	i	1081	PSU	C6-C5-C4	2.82	120.08	118.17
23	i	822	PSU	O2-C2-N1	-2.79	119.91	122.79
23	i	116	OMU	C4-N3-C2	-2.79	123.16	126.61
23	i	93	PSU	C6-C5-C4	2.75	120.03	118.17
23	i	109	PSU	O2-C2-N1	-2.75	119.95	122.79
23	i	406	PSU	O2-C2-N1	-2.73	119.97	122.79
23	i	174	OMC	C4-N3-C2	-2.73	115.97	120.26
23	i	354	OMU	C4-N3-C2	-2.72	123.23	126.61
23	i	590	A2M	O4'-C1'-C2'	2.71	111.23	106.61
23	i	1692	PSU	O2-C2-N1	-2.71	119.99	122.79
23	i	121	OMU	C4-N3-C2	-2.71	123.25	126.61
23	i	668	A2M	O4'-C1'-C2'	2.70	111.20	106.61
23	i	1703	OMC	C4-N3-C2	-2.68	116.04	120.26
23	i	218	PSU	C6-C5-C4	2.68	119.98	118.17
23	i	517	OMC	C4-N3-C2	-2.65	116.08	120.26
23	i	799	OMU	C4-N3-C2	-2.65	123.33	126.61
23	i	462	OMC	C4-N3-C2	-2.64	116.11	120.26
23	i	649	PSU	O2-C2-N1	-2.63	120.07	122.79
23	i	866	PSU	O2-C2-N1	-2.63	120.08	122.79
23	i	686	PSU	O2-C2-N1	-2.62	120.08	122.79
23	i	36	PSU	O2-C2-N1	-2.62	120.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	119	PSU	C6-C5-C4	2.62	119.94	118.17
23	i	966	PSU	O2-C2-N1	-2.62	120.09	122.79
23	i	572	PSU	O2-C2-N1	-2.61	120.09	122.79
23	i	609	PSU	O2-C2-N1	-2.61	120.10	122.79
23	i	797	OMC	C4-N3-C2	-2.58	116.20	120.26
23	i	119	PSU	O2-C2-N1	-2.56	120.14	122.79
23	i	34	PSU	O2-C2-N1	-2.56	120.14	122.79
23	i	1174	PSU	O2-C2-N1	-2.56	120.14	122.79
23	i	1136	PSU	O2-C2-N1	-2.55	120.15	122.79
23	i	815	PSU	O2-C2-N1	-2.55	120.16	122.79
23	i	1177	PSU	O2-C2-N1	-2.55	120.16	122.79
23	i	1056	PSU	O2-C2-N1	-2.55	120.16	122.79
23	i	651	PSU	O2-C2-N1	-2.52	120.19	122.79
23	i	1045	PSU	O2-C2-N1	-2.52	120.19	122.79
23	i	681	PSU	O2-C2-N1	-2.51	120.20	122.79
23	i	863	PSU	O2-C2-N1	-2.50	120.21	122.79
23	i	172	OMU	CM2-O2'-C2'	-2.49	108.08	114.47
23	i	590	A2M	C4-C5-N7	2.48	111.96	109.34
23	i	509	OMG	O6-C6-C5	2.48	129.24	124.32
23	i	822	PSU	O4'-C1'-C2'	2.47	108.57	105.15
23	i	1081	PSU	O2-C2-N1	-2.47	120.24	122.79
23	i	1046	PSU	O2-C2-N1	-2.46	120.25	122.79
23	i	105	PSU	O2-C2-N1	-2.45	120.26	122.79
23	i	601	OMG	O6-C6-C5	2.43	129.13	124.32
23	i	484	A2M	O4'-C1'-C2'	2.42	110.73	106.61
23	i	512	A2M	C4-C5-N7	2.41	111.89	109.34
23	i	799	OMU	C6-C5-C4	2.40	122.60	119.53
23	i	644	OMG	O6-C6-C5	2.40	129.08	124.32
23	i	121	OMU	O4-C4-N3	-2.40	115.80	119.27
23	i	814	PSU	O2-C2-N1	-2.39	120.32	122.79
23	i	799	OMU	O4-C4-N3	-2.39	115.80	119.27
23	i	99	A2M	C4-C5-N7	2.39	111.86	109.34
23	i	627	OMU	CM2-O2'-C2'	-2.38	108.36	114.47
23	i	218	PSU	O2-C2-N1	-2.38	120.34	122.79
23	i	668	A2M	C4-C5-N7	2.37	111.84	109.34
23	i	1804	OMU	O4-C4-N3	-2.37	115.83	119.27
23	i	1804	OMU	C6-C5-C4	2.37	122.56	119.53
23	i	166	A2M	C4-C5-N7	2.37	111.84	109.34
23	i	1842	4AC	N4-C4-N3	2.35	117.69	113.87
23	i	1842	4AC	C6-C5-C4	2.35	119.83	117.00
23	i	428	OMU	CM2-O2'-C2'	-2.35	108.45	114.47
23	i	172	OMU	O4-C4-N3	-2.34	115.88	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	159	A2M	O4'-C1'-C2'	2.34	110.59	106.61
23	i	27	A2M	C4-C5-N7	2.34	111.81	109.34
23	i	484	A2M	C4'-O4'-C1'	-2.33	107.79	109.92
23	i	93	PSU	O2-C2-N1	-2.33	120.39	122.79
23	i	683	OMG	O6-C6-C5	2.33	128.94	124.32
23	i	1804	OMU	CM2-O2'-C2'	-2.32	108.51	114.47
23	i	576	A2M	C4-C5-N7	2.32	111.79	109.34
23	i	627	OMU	O4-C4-N3	-2.31	115.92	119.27
23	i	159	A2M	C4-C5-N7	2.31	111.78	109.34
23	i	354	OMU	O4-C4-N3	-2.31	115.93	119.27
23	i	1031	A2M	C4-C5-N7	2.30	111.77	109.34
23	i	484	A2M	C4-C5-N7	2.29	111.76	109.34
23	i	159	A2M	C3'-C2'-C1'	-2.28	98.44	102.81
23	i	468	A2M	C4-C5-N7	2.27	111.74	109.34
23	i	174	OMC	C5-C6-N1	-2.27	118.15	121.84
23	i	428	OMU	O4-C4-N3	-2.26	116.00	119.27
23	i	354	OMU	C6-C5-C4	2.23	122.38	119.53
23	i	436	OMG	O6-C6-C5	2.20	128.68	124.32
23	i	172	OMU	C6-C5-C4	2.18	122.33	119.53
23	i	627	OMU	C6-C5-C4	2.18	122.33	119.53
23	i	668	A2M	C2'-C1'-N9	2.17	117.39	112.56
23	i	517	OMC	C5-C6-N1	-2.16	118.33	121.84
23	i	468	A2M	O4'-C1'-C2'	2.16	110.28	106.61
23	i	428	OMU	C6-C5-C4	2.16	122.29	119.53
23	i	116	OMU	C6-C5-C4	2.15	122.29	119.53
23	i	218	PSU	O4'-C1'-C2'	2.15	108.13	105.15
23	i	1842	4AC	CM7-C7-N4	2.14	118.72	115.27
23	i	1031	A2M	O4'-C1'-C2'	2.14	110.25	106.61
23	i	121	OMU	C6-C5-C4	2.14	122.26	119.53
23	i	354	OMU	CM2-O2'-C2'	-2.13	109.02	114.47
23	i	590	A2M	C3'-C2'-C1'	-2.12	98.75	102.81
23	i	1136	PSU	O4'-C1'-C2'	2.12	108.08	105.15
23	i	166	A2M	O4'-C1'-C2'	2.11	110.21	106.61
23	i	1703	OMC	N4-C4-N3	-2.10	114.14	117.91
23	i	1081	PSU	O4'-C1'-C2'	2.10	108.06	105.15
23	i	116	OMU	O4-C4-N3	-2.10	116.23	119.27
23	i	109	PSU	O4'-C1'-C2'	2.10	108.05	105.15
23	i	27	A2M	O4'-C1'-C2'	2.09	110.17	106.61
23	i	462	OMC	C5-C6-N1	-2.08	118.45	121.84
23	i	572	PSU	O4'-C1'-C2'	2.08	108.03	105.15
23	i	517	OMC	N4-C4-N3	-2.05	114.24	117.91
23	i	174	OMC	N4-C4-N3	-2.04	114.25	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	i	1703	OMC	C5-C6-N1	-2.04	118.52	121.84
23	i	354	OMU	N3-C2-N1	2.04	117.55	114.89
23	i	36	PSU	O4'-C1'-C2'	2.04	107.97	105.15
23	i	484	A2M	O4'-C4'-C3'	2.03	109.18	105.15
23	i	1046	PSU	O4'-C1'-C2'	2.03	107.95	105.15
23	i	799	OMU	O4-C4-C5	2.01	128.64	125.16
23	i	1056	PSU	O4'-C1'-C2'	2.01	107.94	105.15
23	i	462	OMC	N4-C4-N3	-2.01	114.31	117.91
23	i	1842	4AC	C5-C4-N3	-2.00	119.47	122.60

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	i	121	OMU	C1'-C2'-O2'-CM2
23	i	159	A2M	C1'-C2'-O2'-CM'
23	i	601	OMG	C1'-C2'-O2'-CM2
23	i	644	OMG	O4'-C4'-C5'-O5'
23	i	644	OMG	C1'-C2'-O2'-CM2
23	i	797	OMC	C1'-C2'-O2'-CM2
23	i	576	A2M	C3'-C4'-C5'-O5'
23	i	683	OMG	C3'-C4'-C5'-O5'
23	i	576	A2M	O4'-C4'-C5'-O5'
23	i	644	OMG	C3'-C4'-C5'-O5'
23	i	428	OMU	C2'-C1'-N1-C6
23	i	668	A2M	O4'-C4'-C5'-O5'
23	i	668	A2M	C3'-C4'-C5'-O5'
23	i	683	OMG	O4'-C4'-C5'-O5'
23	i	428	OMU	C2'-C1'-N1-C2
23	i	428	OMU	O4'-C1'-N1-C6
23	i	99	A2M	O4'-C4'-C5'-O5'
23	i	428	OMU	O4'-C1'-N1-C2
23	i	1851	MA6	C4'-C5'-O5'-P
23	i	644	OMG	C4'-C5'-O5'-P
23	i	1081	PSU	C4'-C5'-O5'-P
23	i	99	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	i	99	A2M	3	0
23	i	601	OMG	1	0
23	i	159	A2M	2	0
23	i	218	PSU	1	0
23	i	1832	6MZ	1	0
23	i	517	OMC	1	0
23	i	509	OMG	1	0
23	i	797	OMC	1	0
23	i	576	A2M	2	0
23	i	1692	PSU	1	0
23	i	462	OMC	1	0
23	i	1031	A2M	1	0
23	i	116	OMU	3	0
23	i	121	OMU	1	0
23	i	468	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 71 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 [i](#)

There are no chain breaks in this entry.

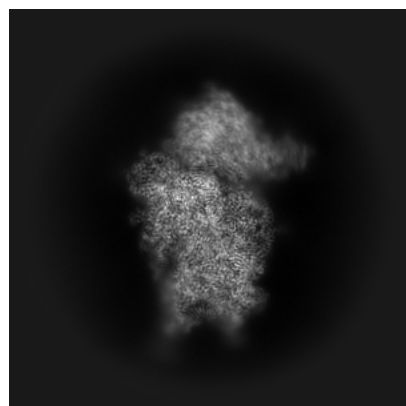
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49635. These allow visual inspection of the internal detail of the map and identification of artifacts.

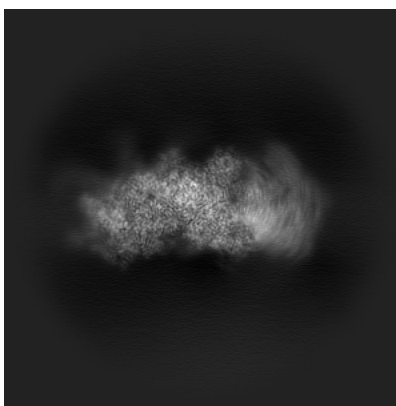
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

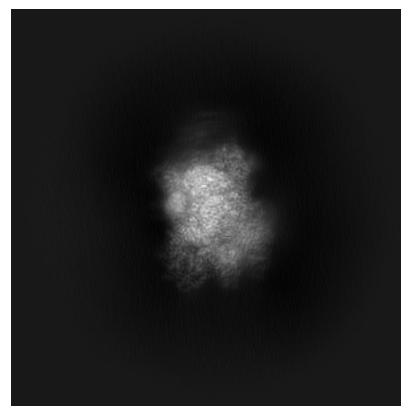
6.1.1 Primary map



X

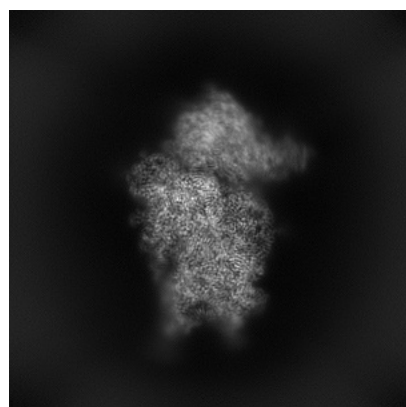


Y

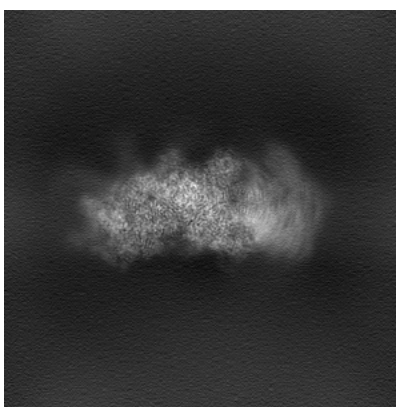


Z

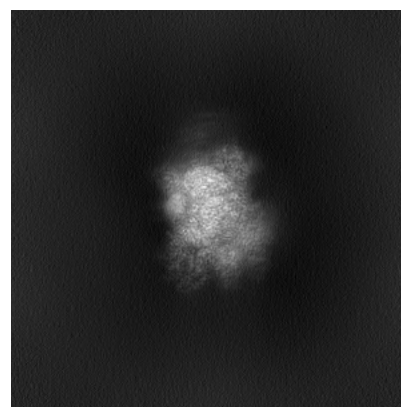
6.1.2 Raw map



X



Y

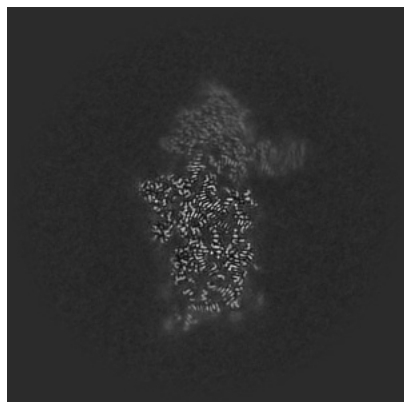


Z

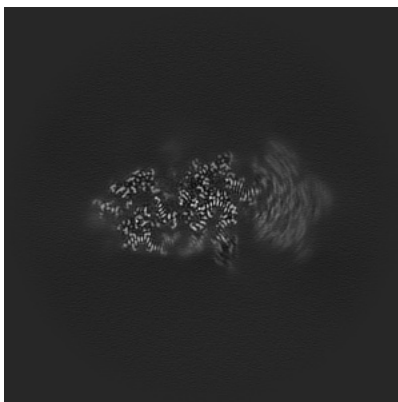
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

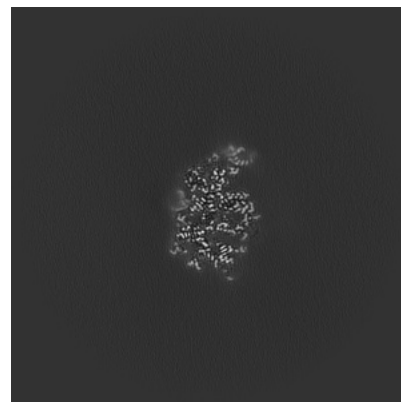
6.2.1 Primary map



X Index: 256

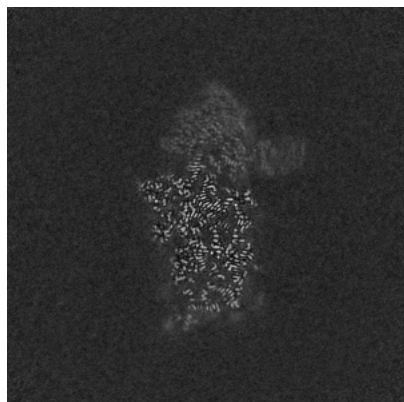


Y Index: 256

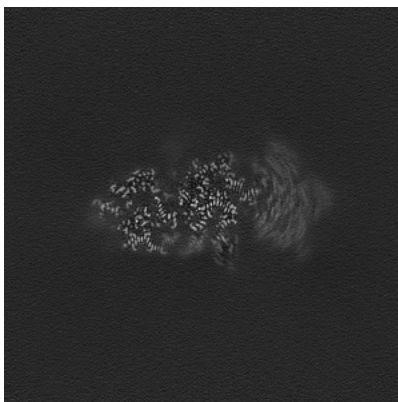


Z Index: 256

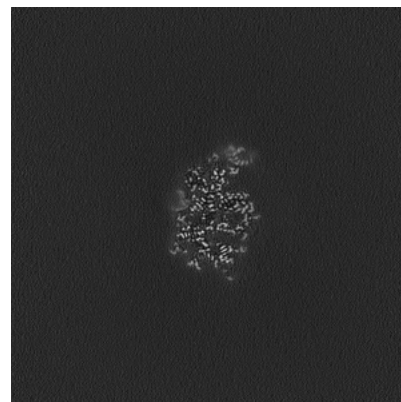
6.2.2 Raw map



X Index: 256



Y Index: 256

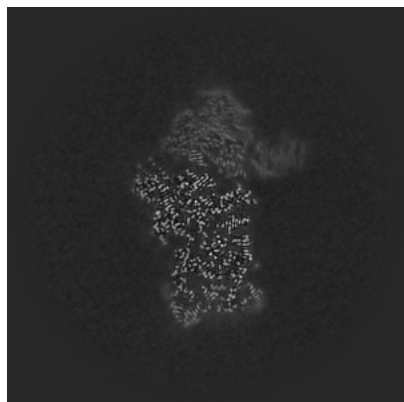


Z Index: 256

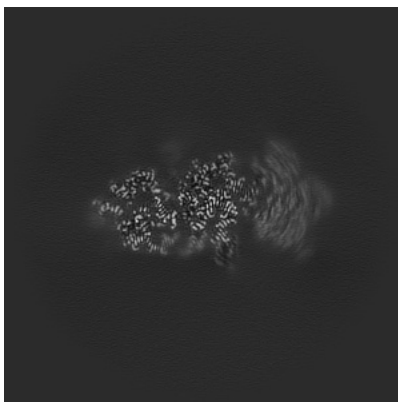
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

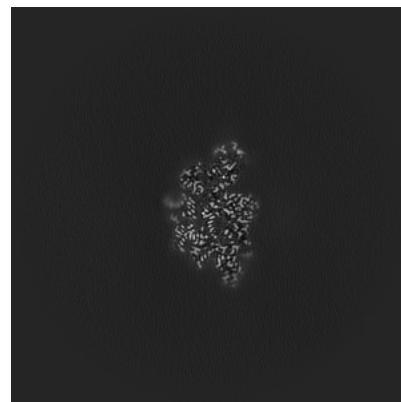
6.3.1 Primary map



X Index: 249

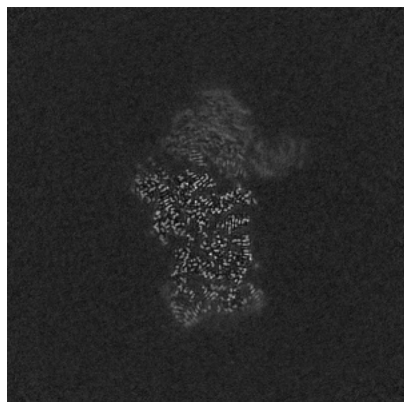


Y Index: 255

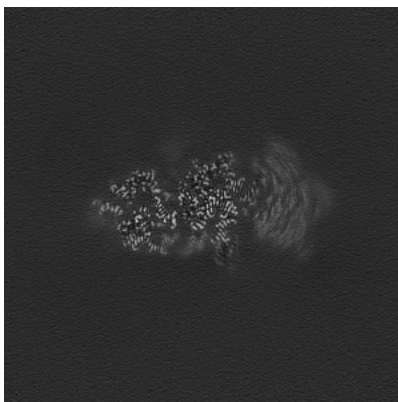


Z Index: 246

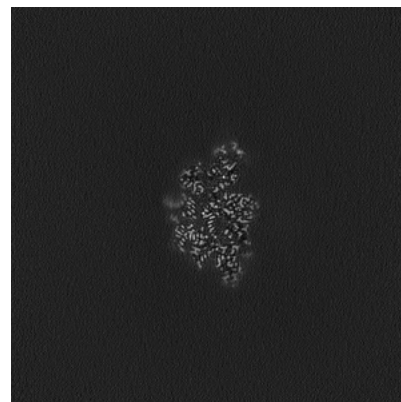
6.3.2 Raw map



X Index: 249



Y Index: 255

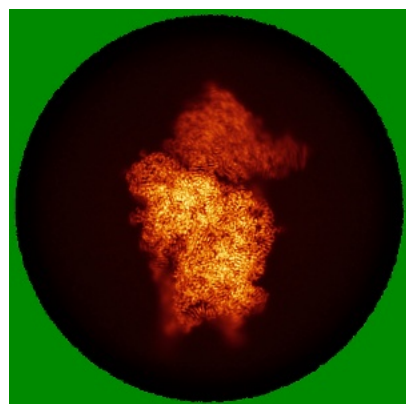


Z Index: 246

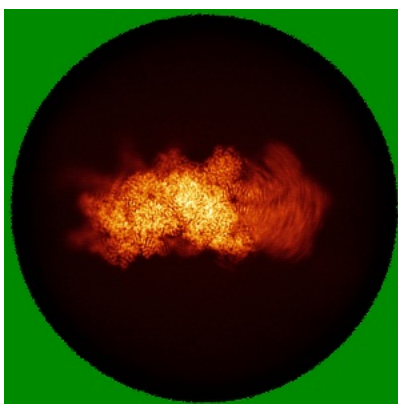
The images above show the largest variance slices of the map in three orthogonal directions.

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

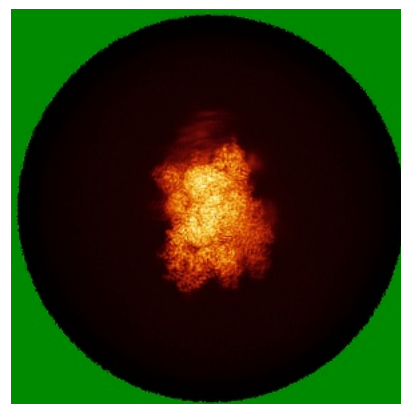
6.4.1 Primary map



X

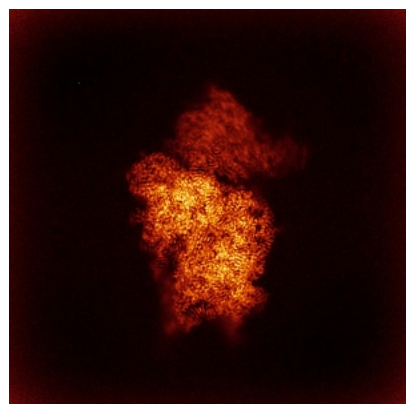


Y

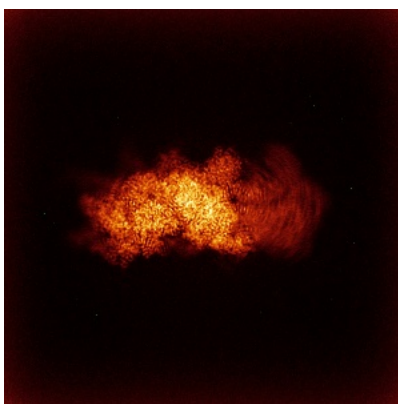


Z

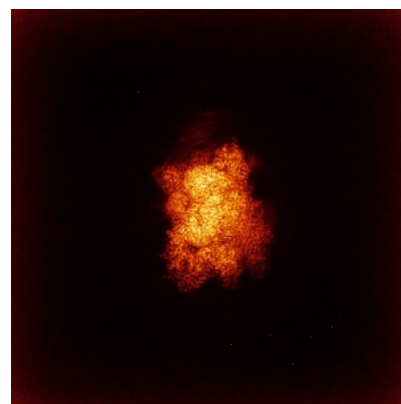
6.4.2 Raw map



X



Y

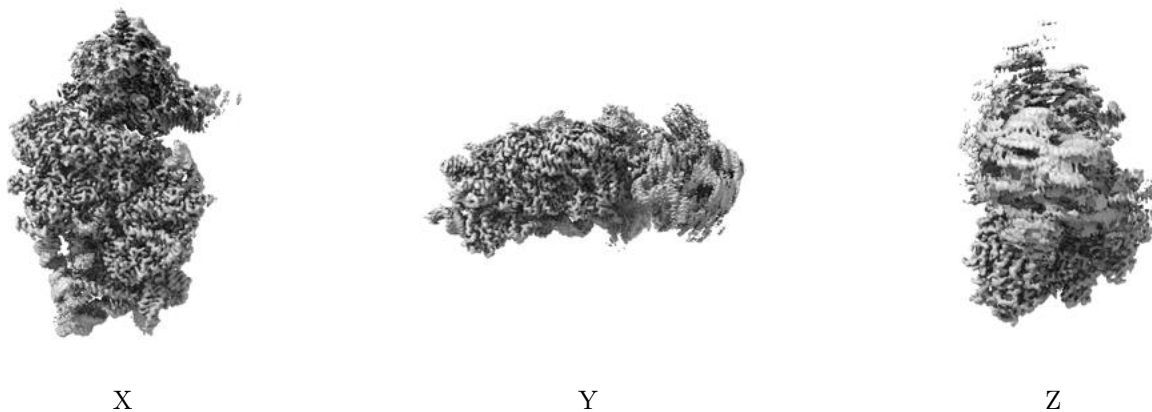


Z

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 0.035. 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.

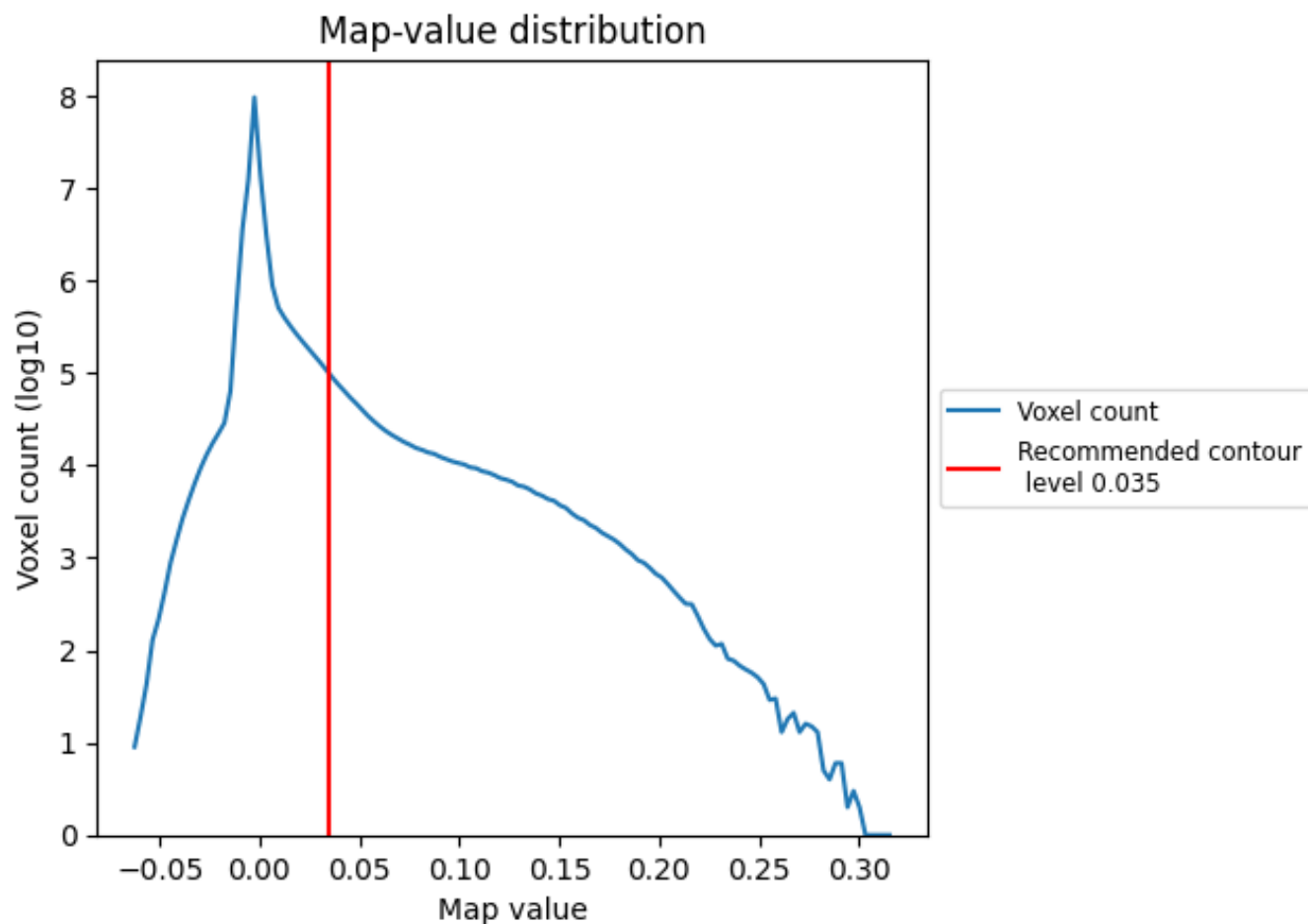
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

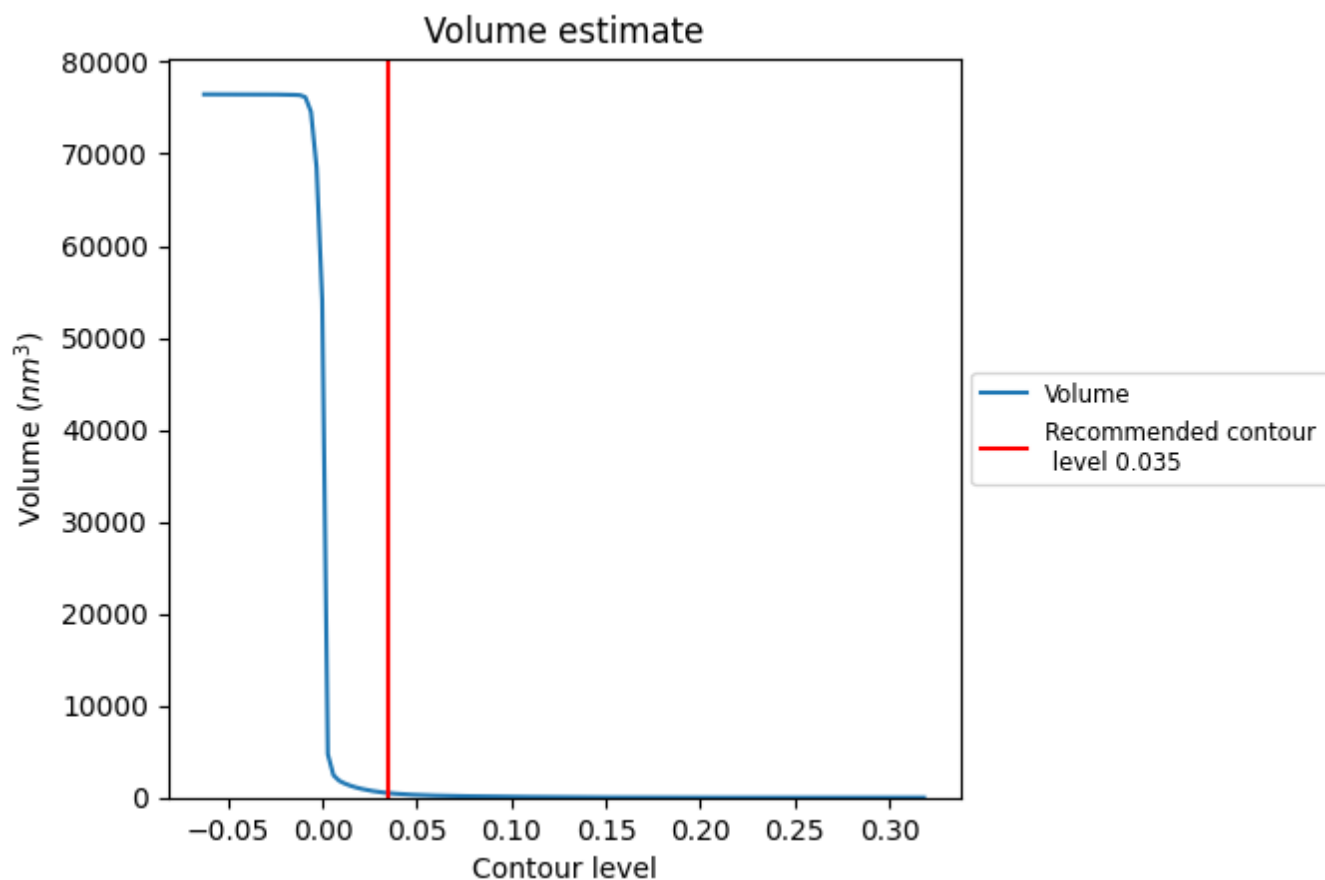
This section contains the results of statistical analysis of the map.

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.

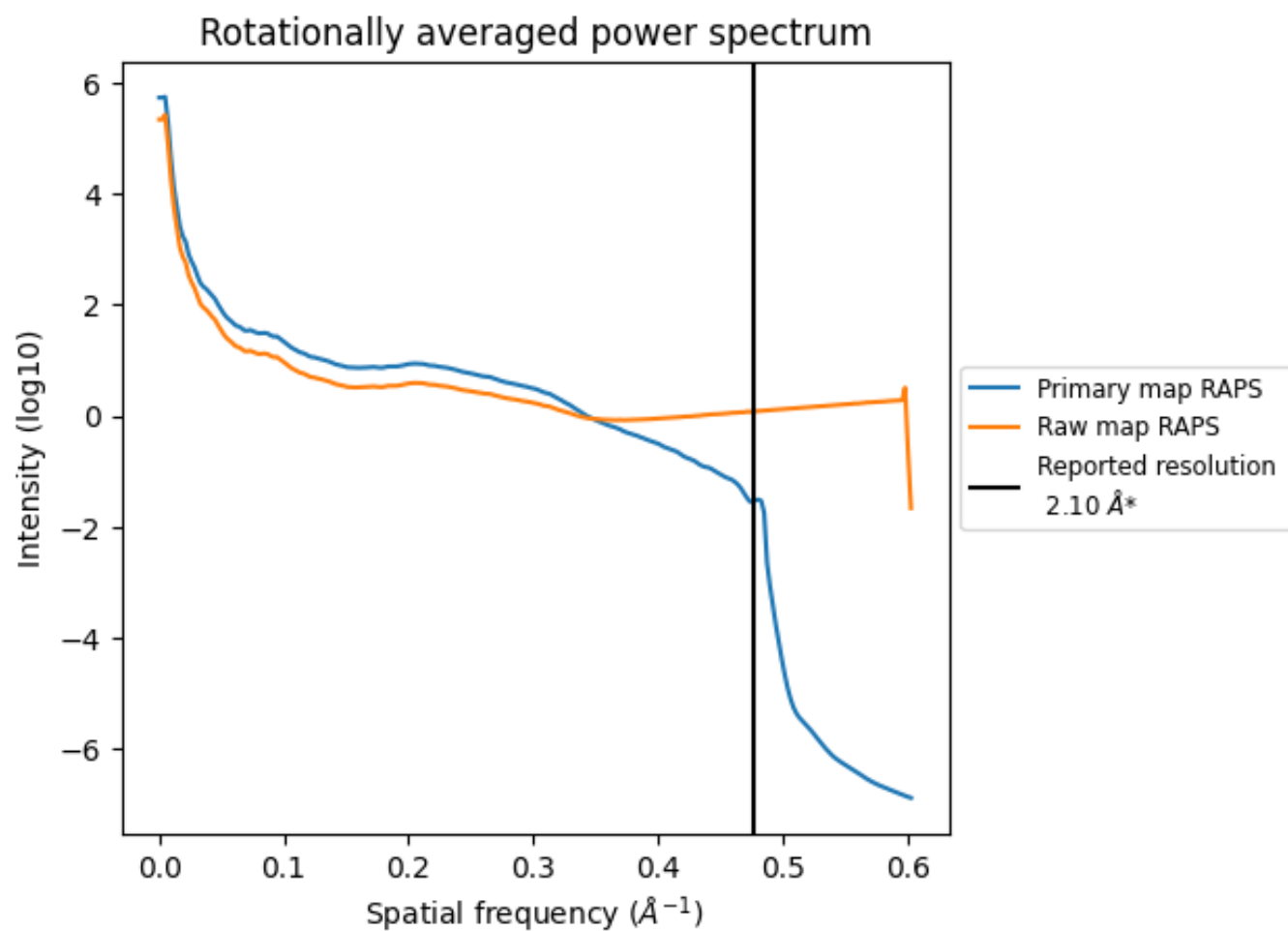
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm³; this corresponds to an approximate mass of 442 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 ⓘ

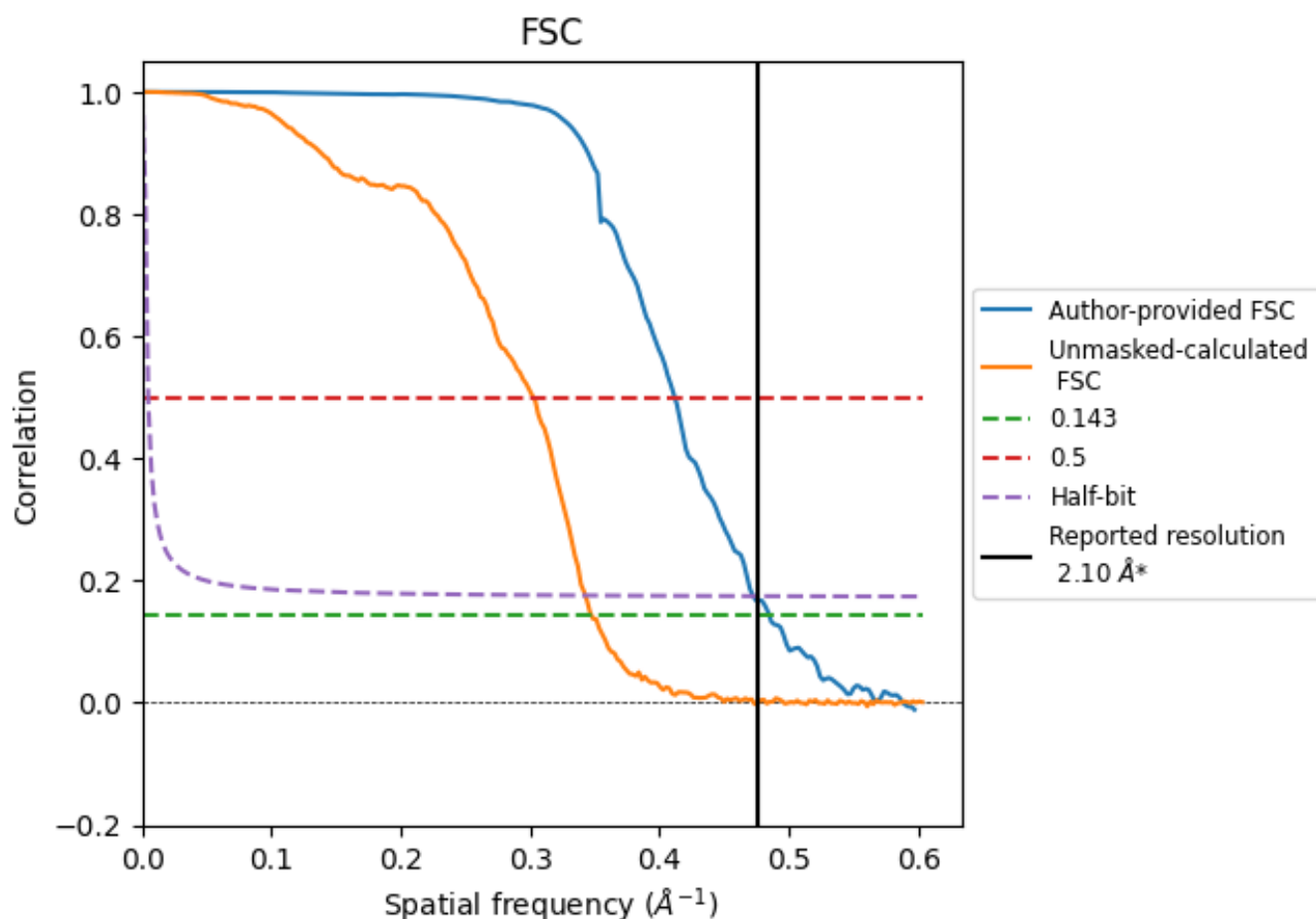


*Reported resolution corresponds to spatial frequency of 0.476 \AA^{-1}

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 0.476 \AA^{-1}

8.2 Resolution estimates

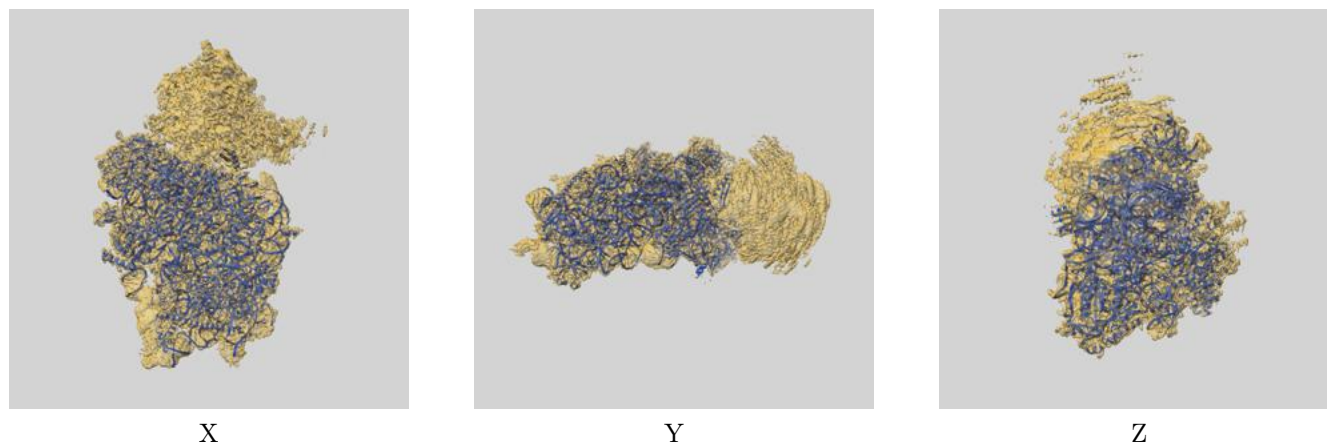
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.06	2.43	2.12
Unmasked-calculated*	2.88	3.31	2.92

*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 2.88 differs from the reported value 2.1 by more than 10 %

9 Map-model fit [i](#)

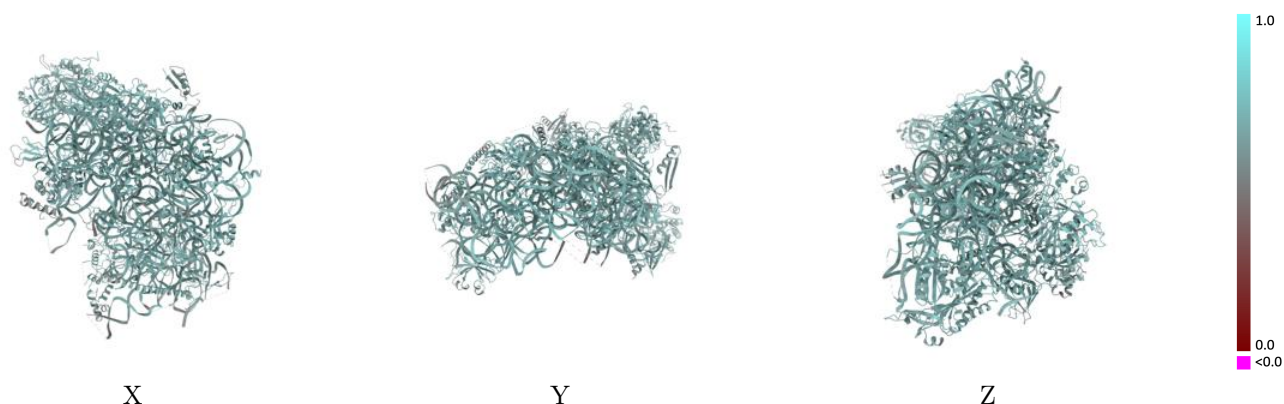
This section contains information regarding the fit between EMDB map EMD-49635 and PDB model 9NPX. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



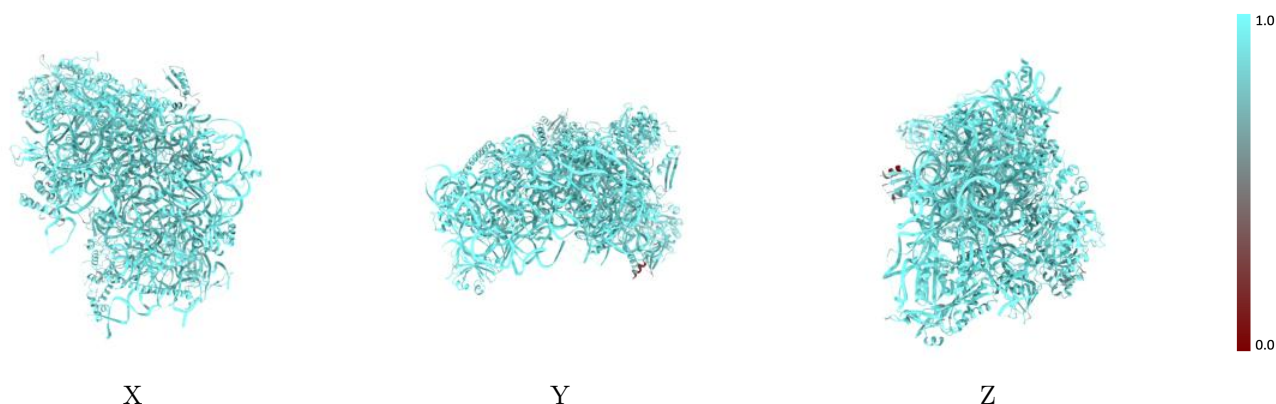
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



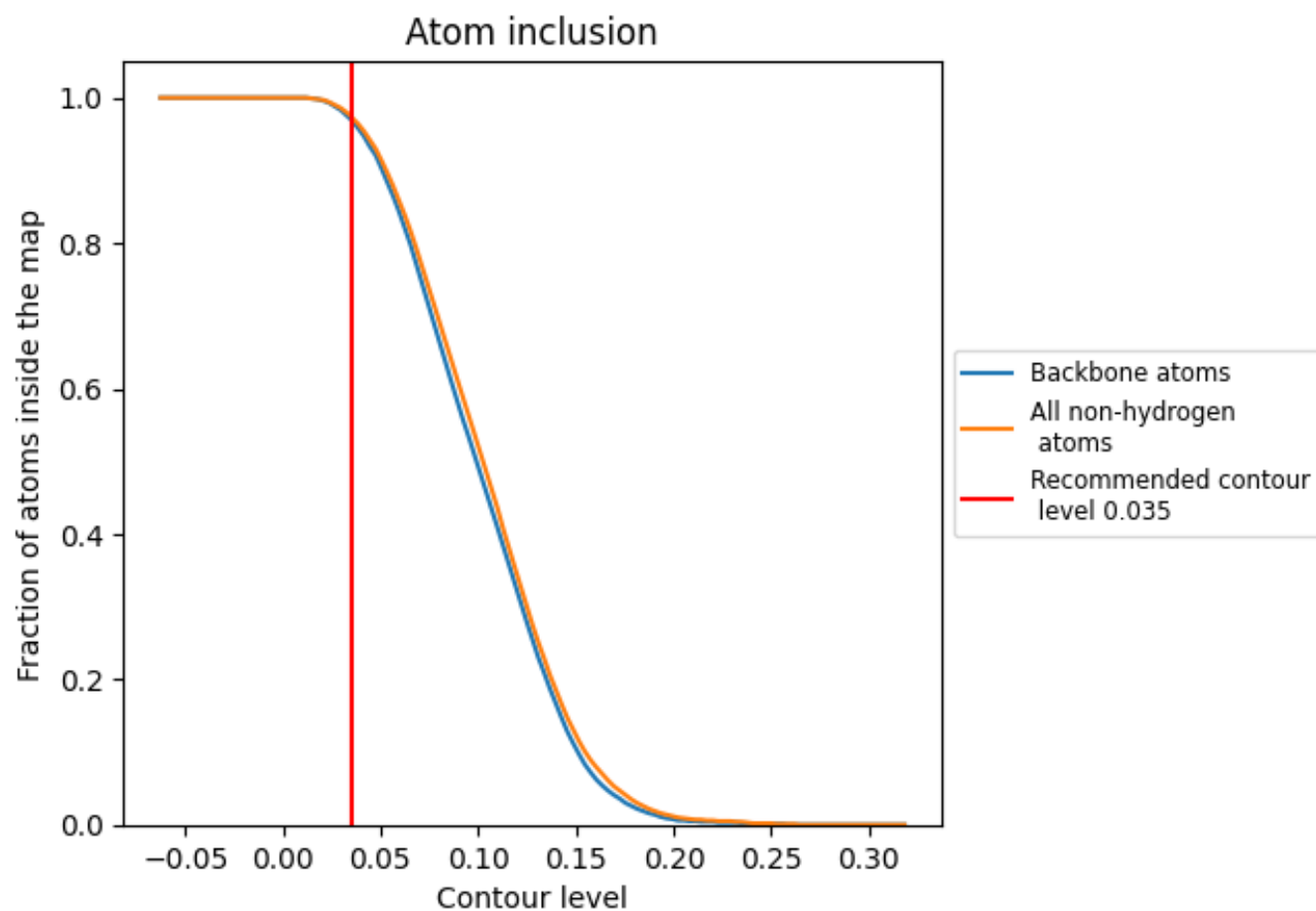
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6540
A	 0.9700	 0.6710
B	 0.8110	 0.5620
C	 0.9520	 0.6460
D	 0.9820	 0.6710
F	 0.9590	 0.6290
G	 0.8880	 0.6080
H	 0.9810	 0.6540
I	 0.9710	 0.6700
K	 0.9790	 0.6760
M	 0.9680	 0.6570
N	 0.9630	 0.6520
P	 0.9770	 0.6830
R	 0.8440	 0.6130
V	 0.9610	 0.6630
W	 0.9780	 0.6780
X	 0.9780	 0.6640
Z	 0.9850	 0.6700
a	 0.9670	 0.6550
e	 0.9720	 0.6650
f	 0.9650	 0.6500
h	 0.9760	 0.6600
i	 0.9920	 0.6530
j	 0.9270	 0.6630
k	 0.6750	 0.5900

