



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:04 AM EDT

PDB ID : 9BKD / pdb_00009bkd
EMDB ID : EMD-44641
Title : The structure of human Pdcd4 bound to the 40S small ribosomal subunit
Authors : Brito Querido, J.; Sokabe, M.; Diaz-Lopez, I.; Gordiyenko, Y.; Zuber, P.; Albacete-Albacete, L.; Ramakrishnan, V.; S.Fraser, C.
Deposited on : 2024-04-27
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

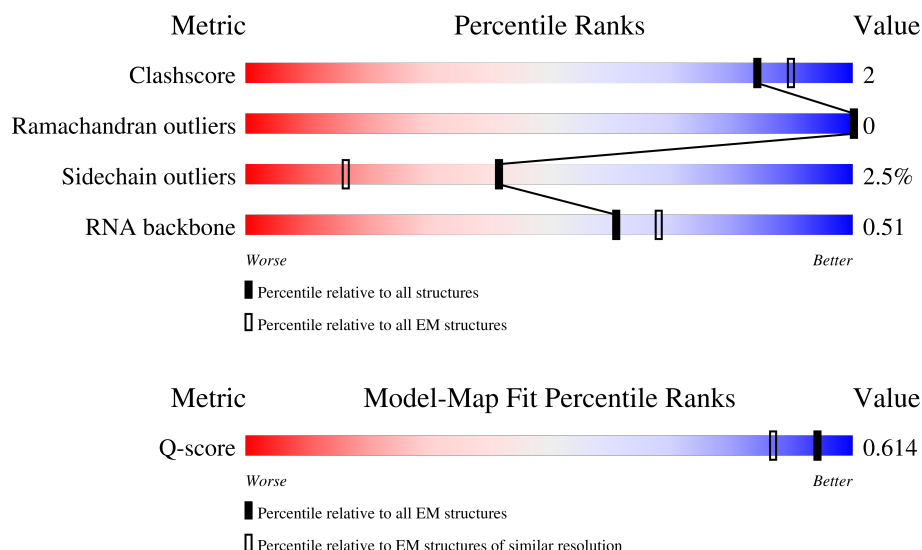
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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.



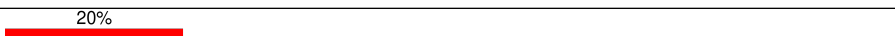
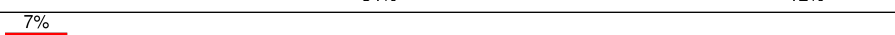
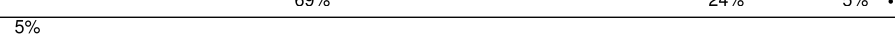
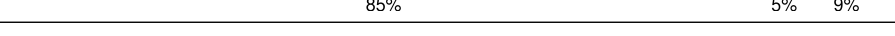
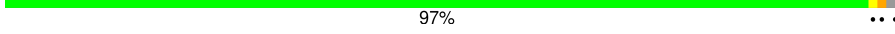
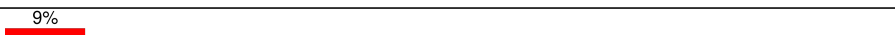
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	S	249	
2	G	194	
3	H	84	

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Mol	Chain	Length	Quality of chain
4	K	83	
5	L	293	
6	O	264	
7	N	295	
8	Q	115	
9	P	151	
10	I	151	
11	9	25	
12	A	1719	
13	B	158	
14	C	263	
15	D	194	
16	E	143	
17	F	59	
18	J	130	
19	R	208	
20	T	133	
21	V	204	
22	Y	146	
23	Z	243	
24	a	165	
25	b	145	
26	c	317	
27	d	145	
28	e	125	

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Mol	Chain	Length	Quality of chain
29	f	152	37%81%12%7%
30	i	56	86%12%
31	k	156	30%31%67%
32	m	132	91%72%20%8%
33	n	69	28%83%9%9%
34	M	135	10%83%13%
35	h	119	23%81%5%13%
36	U	469	9%90%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 74436 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 Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 2 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	173	Total	C	N	O	S	0	0
			1399	895	255	248	1		

- Molecule 3 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 4 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 6 is a protein called 40S ribosomal protein S3a.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 8 is a protein called 40S ribosomal protein S26.

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

- Molecule 9 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	131	Total	C	N	O	S	0	0
			981	600	193	182	6		

- Molecule 10 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 11 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 12 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1672	Total	C	N	O	P	0	0
			35720	15962	6403	11683	1672		

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	143	Total	C	N	O	S	0	0
			1177	749	222	200	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 15 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	47	Total	C	N	O	S	0	0
			378	231	85	61	1		

- Molecule 18 is a protein called 40S ribosomal protein S15a.

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

- Molecule 19 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 20 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 21 is a protein called 40S ribosomal protein S5.

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

- Molecule 22 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 24 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 25 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	118	Total	C	N	O	S	0	0
			972	617	182	166	7		

- Molecule 26 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 27 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 28 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	69	Total	C	N	O	S	0	0
			551	356	100	94	1		

- Molecule 29 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 31 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	52	Total	C	N	O	S	0	0
			429	271	82	69	7		

- Molecule 32 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 34 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 35 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 36 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	U	47	Total	C	N	O	0	0
			354	217	67	70		

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	Q	1	Total	Zn	0
			1	1	
37	i	1	Total	Zn	0
			1	1	
37	k	1	Total	Zn	0
			1	1	

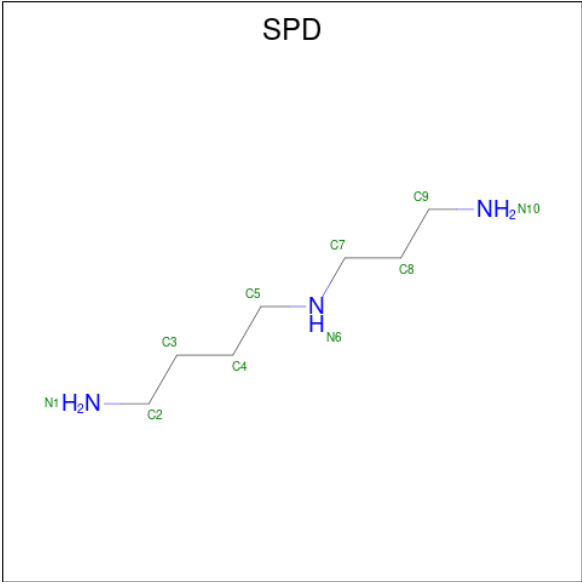
- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	P	1	Total	K	0
			1	1	
38	A	17	Total	K	0
			17	17	
38	i	1	Total	K	0
			1	1	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
39	A	87	Total	Mg	0
			87	87	
39	f	1	Total	Mg	0
			1	1	

- Molecule 40 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).

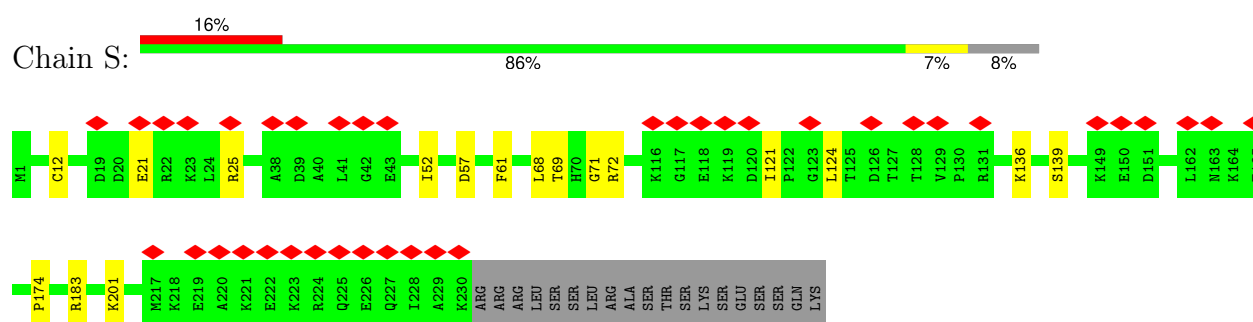


Mol	Chain	Residues	Atoms			AltConf
40	A	1	Total	C	N	0
			10	7	3	

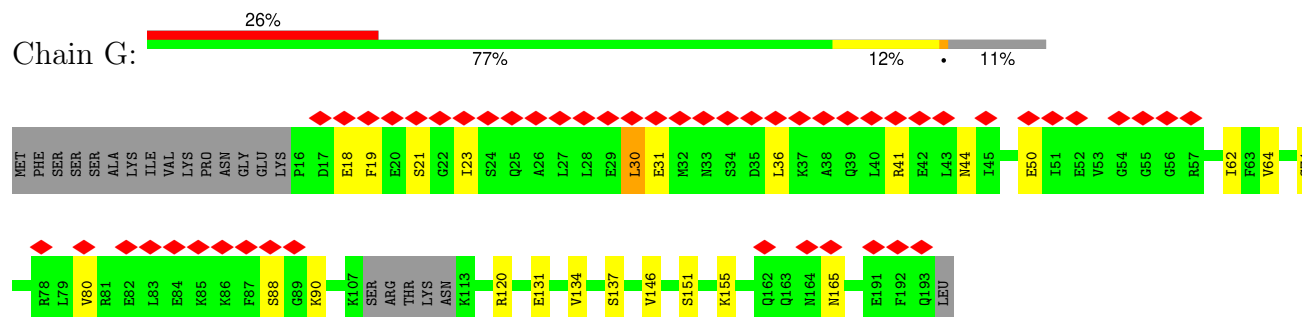
3 Residue-property plots [i](#)

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

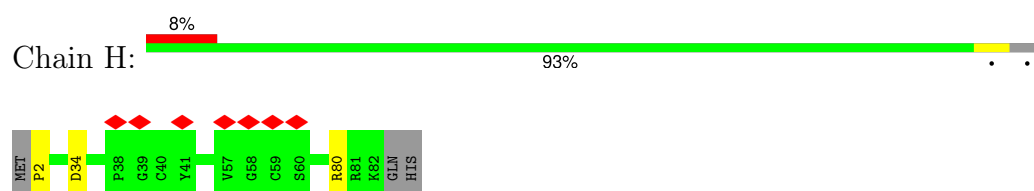
- Molecule 1: Small ribosomal subunit protein eS6



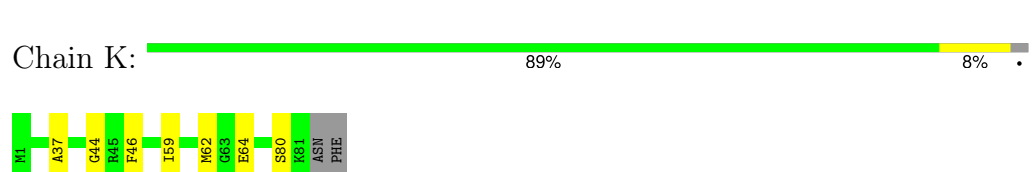
- Molecule 2: Small ribosomal subunit protein eS7



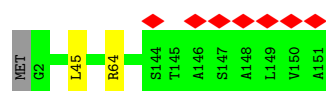
- Molecule 3: 40S ribosomal protein S27

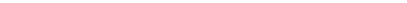


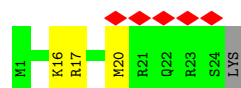
- Molecule 4: 40S ribosomal protein S21

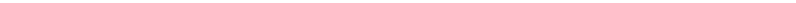


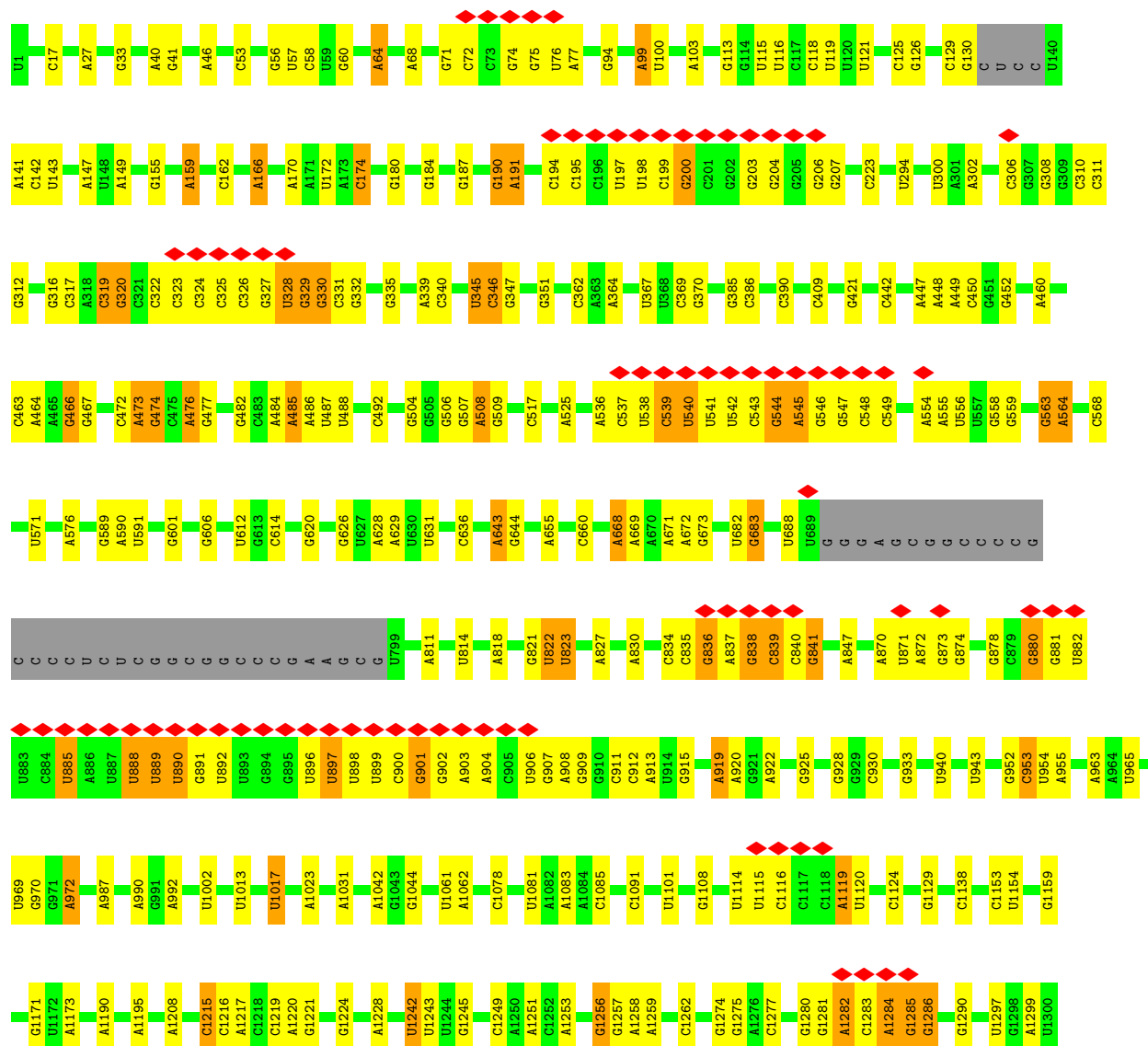
- Molecule 10: 40S ribosomal protein S13

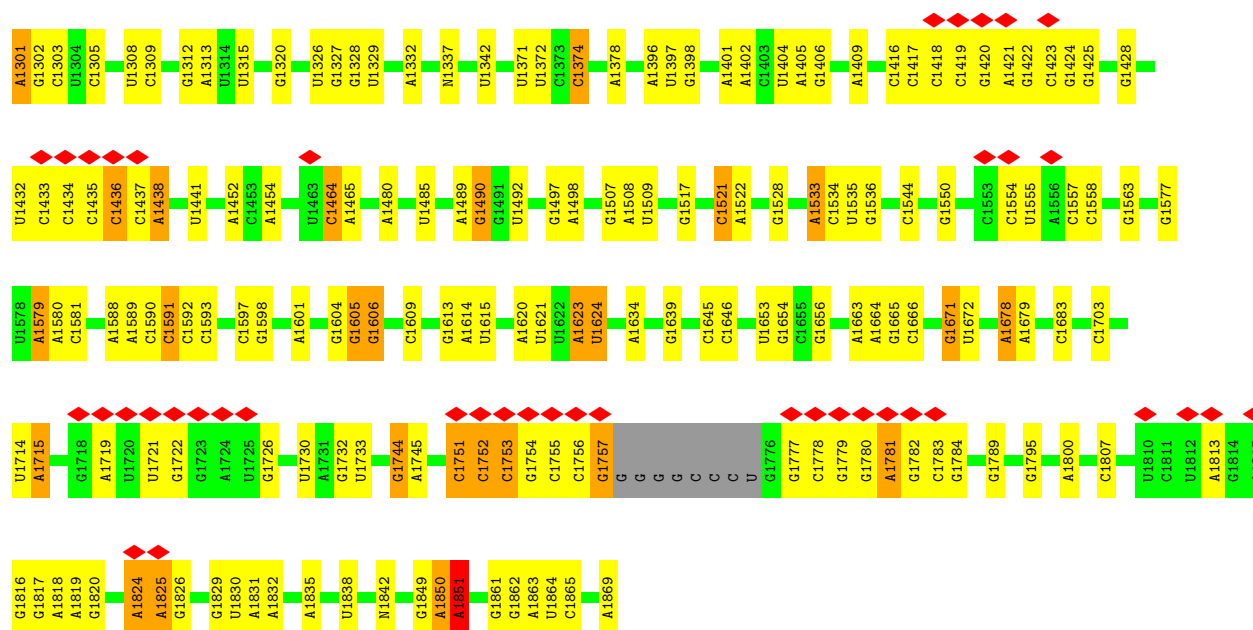


- Chain 9:  20% 84% 12%

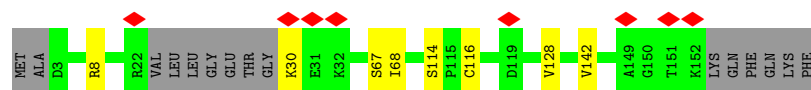
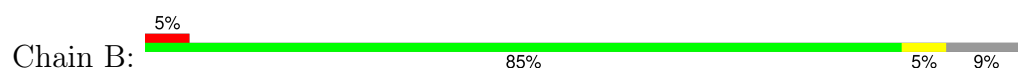


- Chain A:  7% 69% 24% 5%

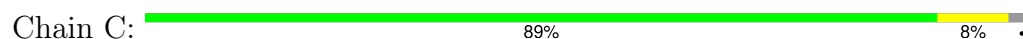




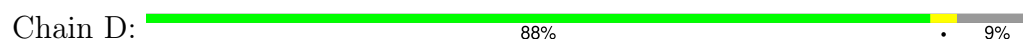
- Molecule 13: Small ribosomal subunit protein uS17



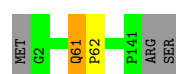
- Molecule 14: Small ribosomal subunit protein eS4, X isoform



- Molecule 15: Small ribosomal subunit protein uS4



- Molecule 16: Small ribosomal subunit protein uS12



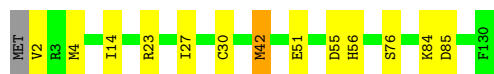
- Molecule 17: Small ribosomal subunit protein eS30

Chain F:  78% 20%



- Molecule 18: 40S ribosomal protein S15a

Chain J:  89% 9% ..



- Molecule 19: Small ribosomal subunit protein eS8

Chain R:  7% 87% 8% 5%



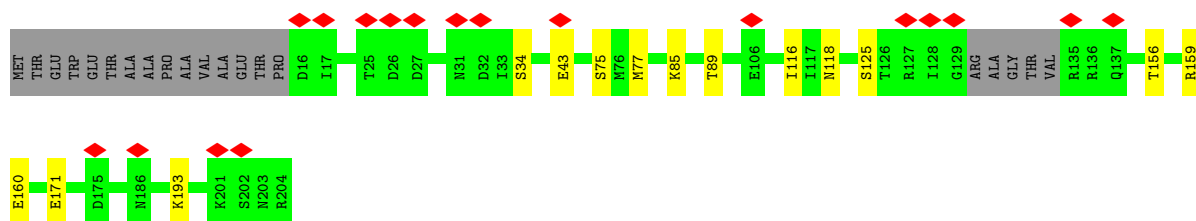
- Molecule 20: Small ribosomal subunit protein eS24

Chain T:  86% 6% 7%



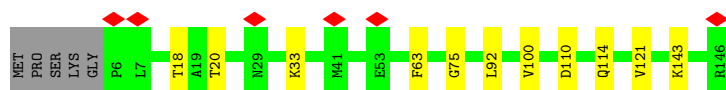
- Molecule 21: 40S ribosomal protein S5

Chain V:  9% 83% 7% 10%



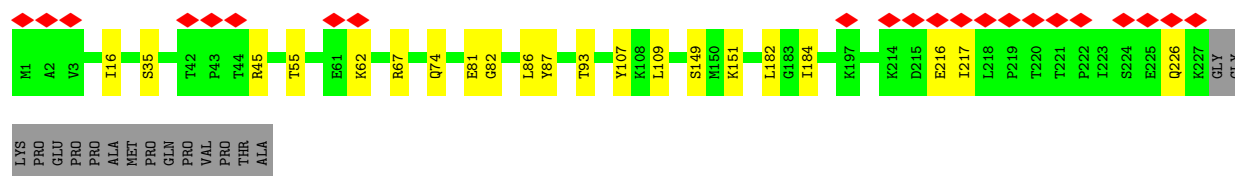
- Molecule 22: 40S ribosomal protein S16

Chain Y:  89% 8%

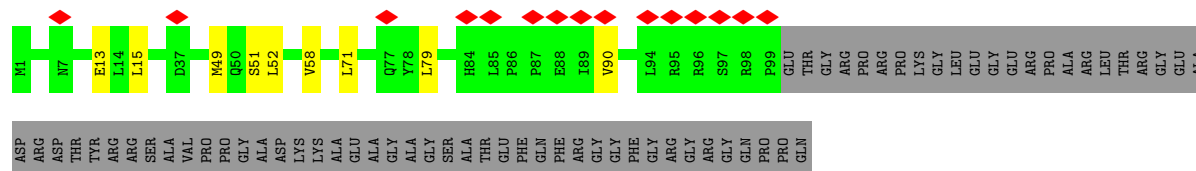


- Molecule 23: Small ribosomal subunit protein uS3

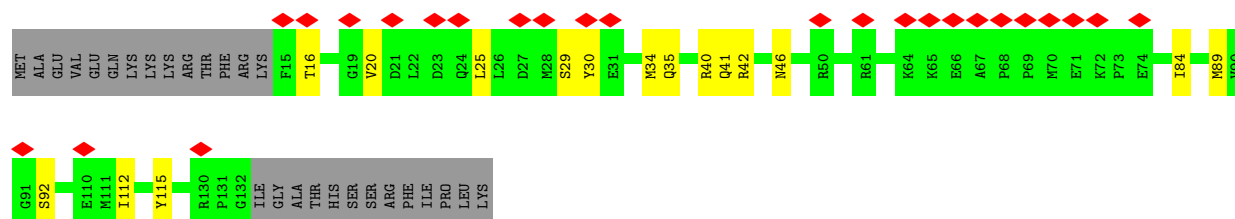
Chain Z:  9% 85% 9% 7%



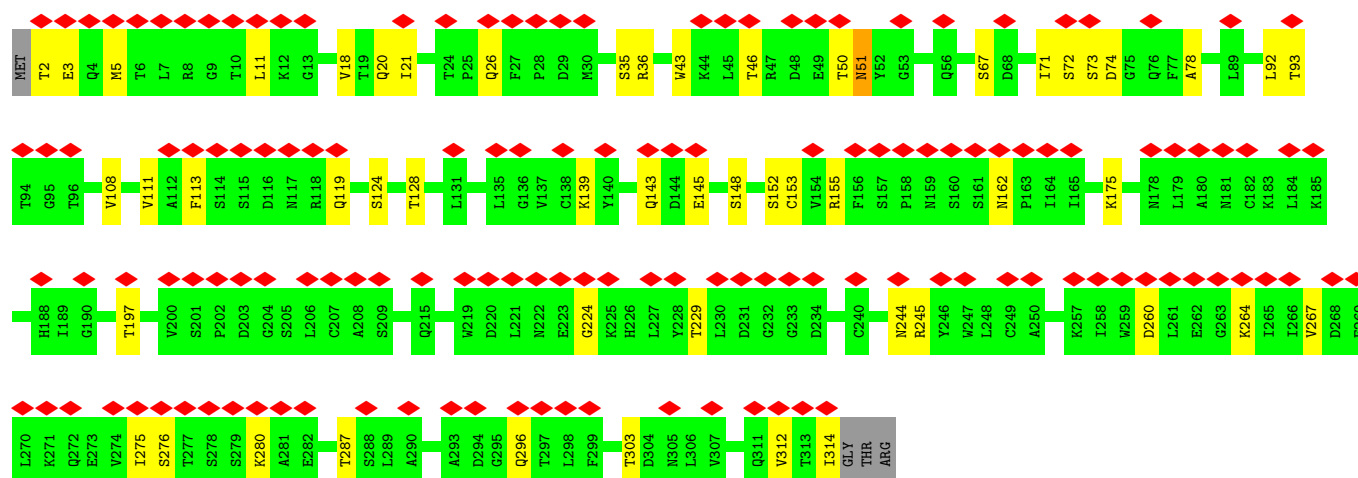
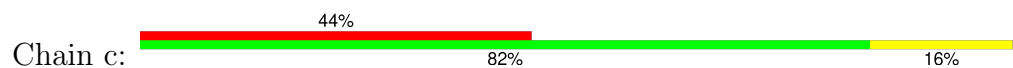
• Molecule 24: Small ribosomal subunit protein eS10



• Molecule 25: 40S ribosomal protein S15

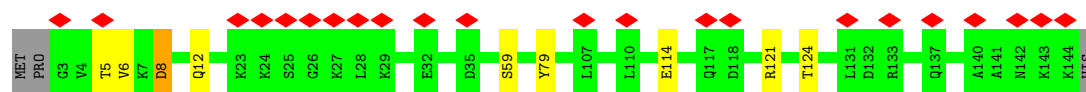


• Molecule 26: Receptor of activated protein C kinase 1

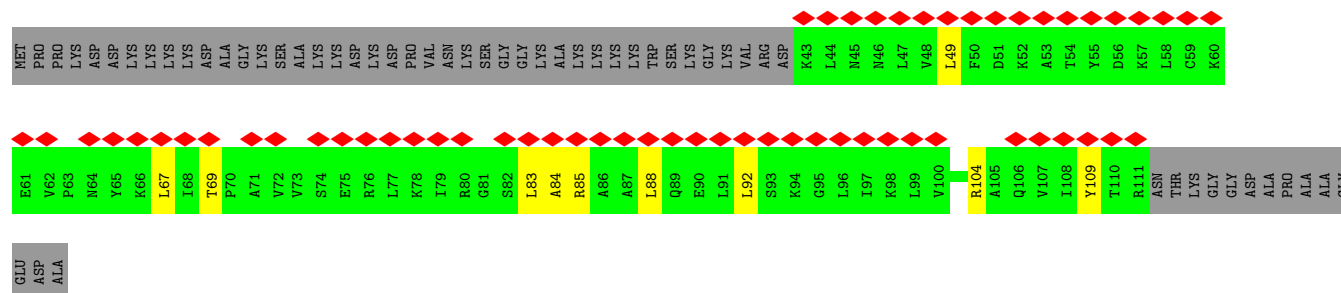


• Molecule 27: 40S ribosomal protein S19

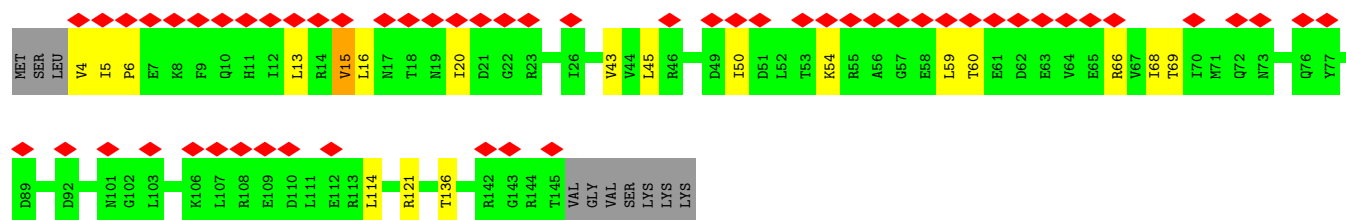
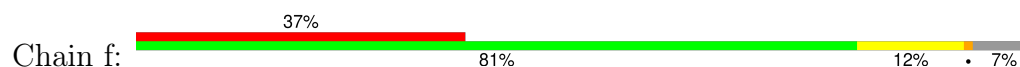




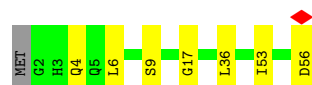
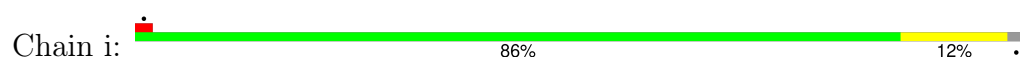
- Molecule 28: Small ribosomal subunit protein eS25



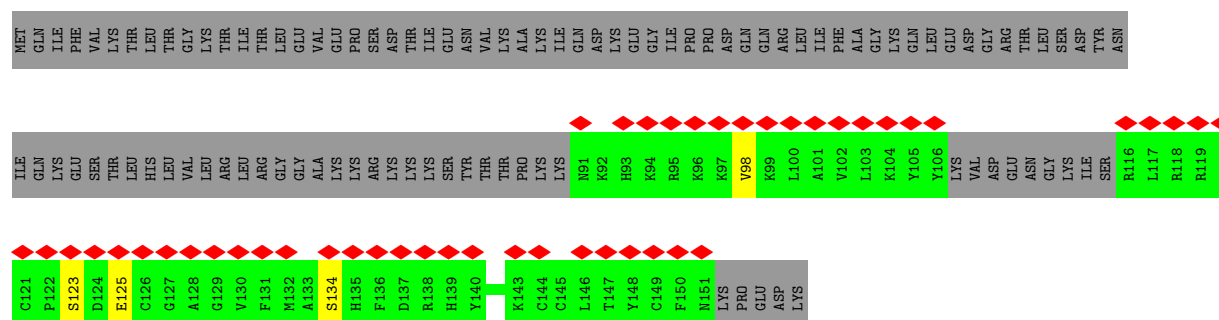
- Molecule 29: Small ribosomal subunit protein uS13



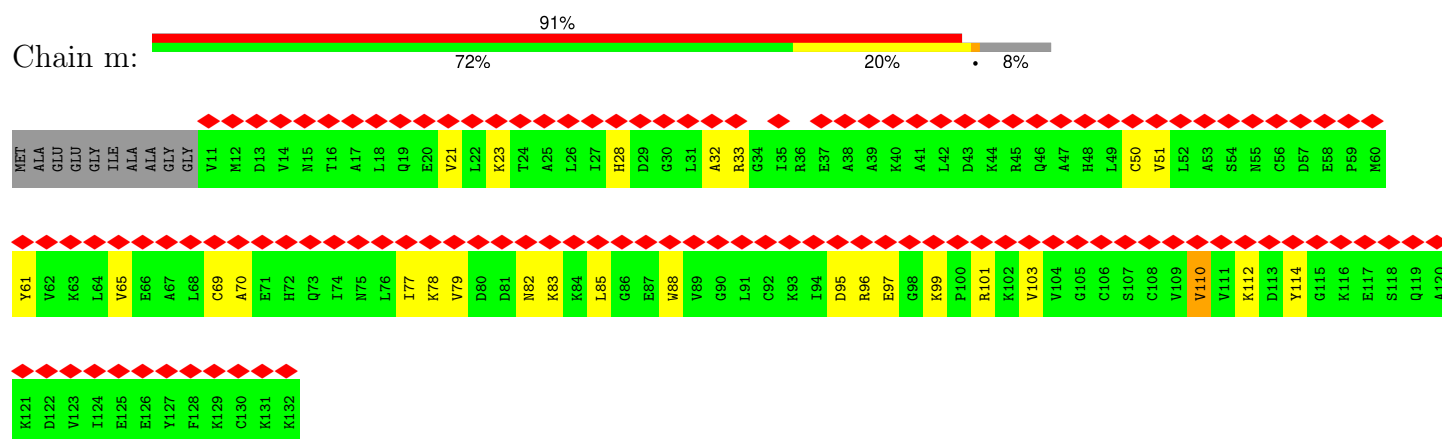
- Molecule 30: 40S ribosomal protein S29



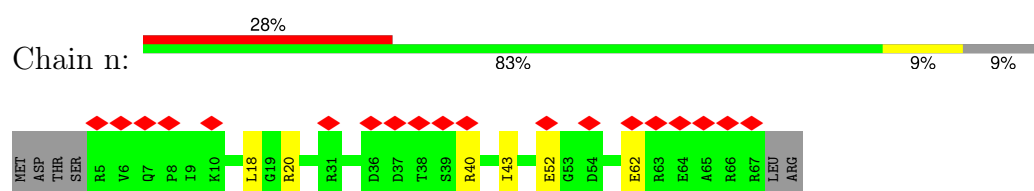
- Molecule 31: Ubiquitin-40S ribosomal protein S27a



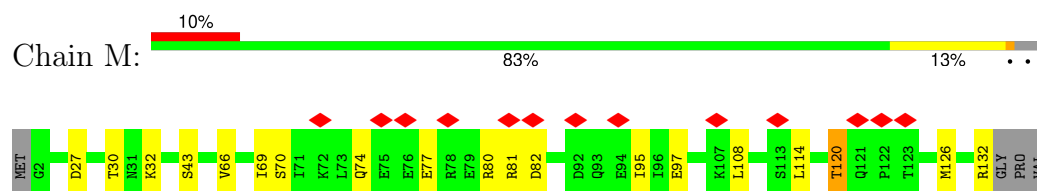
- Molecule 32: 40S ribosomal protein S12



- Molecule 33: 40S ribosomal protein S28



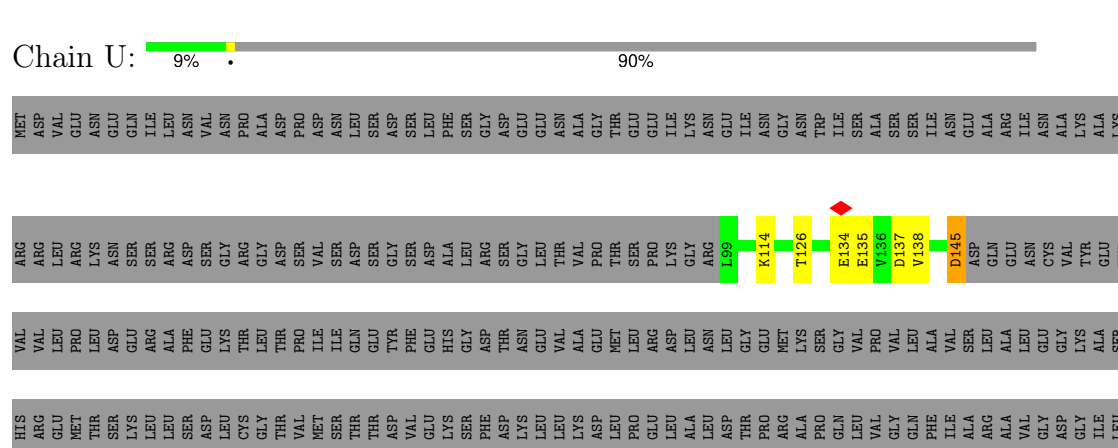
- Molecule 34: 40S ribosomal protein S17



- Molecule 35: 40S ribosomal protein S20



- Molecule 36: Programmed cell death protein 4



CYS	LEU	THR	PHE
ASN	LYS	ILE	VAL
THR	GLU	THR	SER
TYR	TYR	VAL	GLU
ILE	LEU	ASP	GLY
ASP	LEU	GLN	ASP
SER	SER	MET	GLY
TYR	GLY	LYS	GLY
LYS	ASP	ARG	ARG
THR	ILE	GLY	LEU
THR	SER	TYR	LYS
VAL	GLU	GLU	PRO
ASP	ALA	ARG	GLU
CYS	GLU	ILE	SER
VAL	HIS	TYR	TYR
GLN	CYS	ASN	ASN
ALA	LEU	GLU	ILE
ARG	LYS	ILE	PRO
ALA	GLU	ASP	ASP
ALA	LEU	ILE	ASP
LEU	GLU	ASN	ILE
ASP	VAL	ASN	ASN
LYS	PRO	LEU	LEU
ALA	HIS	ASP	VAL
THR	PHE	VAL	PRO
VAL	HIS	PRO	HIS
LEU	HIS	HIS	SER
LEU	GLU	SER	THR
SER	LEU	TYR	SER
MET	VAL	SER	VAL
SER	TYR	VAL	LEU
LYS	GLU	LEU	GLU
GLY	ALA	ARG	ARG
LYS	ILE	ILE	ARG
ARG	ILE	ILE	ASP
ASP	VAL	ASP	LEU
VAL	GLU	LEU	LEU
ASP	SER	ASP	CYS
THR	VAL	SER	PRO
TRP	THR	GLN	SER
GLY	GLY	ALA	ARG
SER	GLU	GLY	GLY
GLY	SER	ILE	ARG
GLY	THR	ILE	GLY
GLN	PHE	SER	ARG
GLN	LYS	LYS	ARG
GLN	MET	GLN	LYS
SER	ILE	LEU	LYS
VAL	LEU	ARG	SER
ASN	ASP	ASP	TYR
HIS	LEU	LEU	
LEU	LEU	LEU	
VAL	LYS	PRO	
LYS	SER	LEU	
TRP	LEU	GLY	
ILE	TRP	GLY	
ASP	LYS	ARG	
MET	SER	LYS	
LEU	SER	ARG	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85656	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	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, MG, UR3, A2M, 6MZ, MA6, 5MC, K, PSU, JMH, OMC, OMU, 4AC, 5MU, OMG, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	S	0.22	0/1885	0.44	0/2510
2	G	0.22	0/1420	0.45	0/1901
3	H	0.21	0/644	0.39	0/864
4	K	0.24	0/623	0.42	0/833
5	L	0.29	0/1743	0.43	0/2354
6	O	0.27	0/1742	0.46	0/2330
7	N	0.24	0/1670	0.40	0/2271
8	Q	0.27	0/805	0.40	0/1079
9	P	0.23	0/993	0.42	0/1330
10	I	0.24	0/1232	0.39	0/1656
11	9	0.26	0/231	0.46	0/294
12	A	0.33	0/39097	0.39	1/60929 (0.0%)
13	B	0.26	0/1197	0.39	0/1599
14	C	0.24	0/2077	0.40	0/2796
15	D	0.24	0/1502	0.43	0/2008
16	E	0.29	0/1105	0.45	0/1476
17	F	0.23	0/380	0.41	0/496
18	J	0.31	0/1051	0.55	2/1406 (0.1%)
19	R	0.24	0/1654	0.42	0/2203
20	T	0.25	0/1028	0.45	0/1366
21	V	0.21	0/1481	0.41	0/1988
22	Y	0.23	0/1142	0.46	0/1528
23	Z	0.23	0/1793	0.40	0/2414
24	a	0.28	0/859	0.52	0/1159
25	b	0.24	0/991	0.49	0/1325
26	c	0.21	0/2493	0.46	0/3394
27	d	0.22	0/1123	0.43	0/1504
28	e	0.21	0/557	0.42	0/748
29	f	0.22	0/1194	0.46	0/1599
30	i	0.27	0/470	0.46	0/623
31	k	0.20	0/438	0.44	0/580
32	m	0.24	0/960	0.53	0/1286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	n	0.26	0/500	0.53	0/669
34	M	0.23	0/1078	0.46	0/1447
35	h	0.25	0/827	0.45	0/1110
36	U	0.24	0/360	0.38	0/482
All	All	0.29	0/78345	0.41	3/113557 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	O	0	1
9	P	0	1
18	J	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	55	ASP	N-CA-C	-7.40	99.86	110.59
12	A	953	C	P-O3'-C3'	-6.27	110.80	120.20
18	J	56	HIS	N-CA-C	-5.33	107.32	112.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	J	23	ARG	Sidechain
6	O	151	ARG	Sidechain
9	P	137	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	1862	0	2018	9	0
2	G	1399	0	1481	14	0
3	H	631	0	657	2	0
4	K	617	0	622	4	0
5	L	1707	0	1794	5	0
6	O	1715	0	1785	12	0
7	N	1633	0	1640	7	0
8	Q	792	0	841	2	0
9	P	981	0	1005	2	0
10	I	1208	0	1293	1	0
11	9	230	0	276	2	0
12	A	35720	0	18065	129	0
13	B	1177	0	1246	4	0
14	C	2035	0	2138	12	0
15	D	1477	0	1589	5	0
16	E	1087	0	1154	1	0
17	F	378	0	417	1	0
18	J	1034	0	1080	7	0
19	R	1627	0	1706	7	0
20	T	1011	0	1083	6	0
21	V	1461	0	1511	6	0
22	Y	1124	0	1193	6	0
23	Z	1765	0	1865	10	0
24	a	834	0	861	6	0
25	b	972	0	1014	13	0
26	c	2436	0	2393	21	0
27	d	1105	0	1138	6	0
28	e	551	0	610	8	0
29	f	1176	0	1233	8	0
30	i	459	0	448	5	0
31	k	429	0	424	0	0
32	m	950	0	987	14	0
33	n	498	0	525	4	0
34	M	1064	0	1118	9	0
35	h	817	0	882	4	0
36	U	354	0	345	4	0
37	Q	1	0	0	0	0
37	i	1	0	0	0	0
37	k	1	0	0	0	0
38	A	17	0	0	0	0
38	P	1	0	0	0	0
38	i	1	0	0	0	0
39	A	87	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	f	1	0	0	0	0
40	A	10	0	19	0	0
All	All	74436	0	58456	296	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 2.

All (296) 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)
24:a:15:LEU:HD22	24:a:49:MET:HE1	1.44	0.99
12:A:928:G:H1	12:A:1013:U:H3	1.20	0.89
12:A:925:G:H1	12:A:1017:U:H3	1.22	0.87
27:d:59:SER:HG	27:d:79:TYR:HH	1.23	0.81
25:b:89:MET:O	25:b:92:SER:OG	2.04	0.76
12:A:1604:G:O2'	12:A:1605:G:O5'	2.03	0.75
12:A:543:C:O2'	12:A:545:A:OP1	2.06	0.74
12:A:1114:U:H3	12:A:1119:A:H61	1.35	0.73
1:S:121:ILE:HG21	1:S:124:LEU:HD13	1.71	0.72
5:L:200:ARG:O	15:D:54:ARG:NH2	2.22	0.72
12:A:1554:C:OP2	12:A:1555:U:O2'	2.05	0.72
12:A:1091:C:HO2'	18:J:2:VAL:N	1.88	0.71
27:d:8:ASP:OD1	27:d:8:ASP:N	2.23	0.71
32:m:95:ASP:O	32:m:96:ARG:NH1	2.24	0.71
12:A:1593:C:OP2	28:e:104:ARG:NH1	2.23	0.71
26:c:153:CYS:SG	26:c:155:ARG:NH1	2.64	0.70
12:A:1521:C:OP2	29:f:136:THR:OG1	2.08	0.70
14:C:117:GLU:N	14:C:117:GLU:OE2	2.24	0.70
12:A:878:G:O6	12:A:908:A:N1	2.24	0.69
12:A:1299:A:O2'	12:A:1301:A:OP1	2.11	0.69
25:b:35:GLN:N	25:b:35:GLN:OE1	2.25	0.69
12:A:319:C:O2'	12:A:320:G:O5'	2.08	0.69
12:A:1744:G:O2'	12:A:1789:G:N2	2.26	0.69
36:U:145:ASP:OD1	36:U:145:ASP:N	2.24	0.68
12:A:1396:A:O2'	12:A:1398:G:N7	2.27	0.68
12:A:1544:C:O2'	22:Y:75:GLY:O	2.08	0.68
12:A:839:C:O2'	12:A:841:G:O4'	2.12	0.67
12:A:1605:G:O2'	12:A:1606:G:O5'	2.10	0.67
26:c:78:ALA:HB2	26:c:92:LEU:HD21	1.77	0.67
12:A:1620:A:OP1	25:b:115:TYR:OH	2.09	0.67
6:O:130:THR:OG1	6:O:180:ASP:OD1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1528:G:O2'	12:A:1666:C:OP1	2.12	0.66
33:n:18:LEU:HD11	33:n:43:ILE:HD12	1.76	0.66
7:N:42:LYS:HD2	7:N:48:ILE:HD11	1.78	0.66
26:c:67:SER:OG	26:c:108:VAL:O	2.06	0.65
1:S:21:GLU:OE1	1:S:25:ARG:NH1	2.30	0.65
12:A:1286:G:N2	12:A:1312:G:O2'	2.28	0.65
21:V:118:ASN:O	21:V:193:LYS:NZ	2.28	0.65
8:Q:32:LYS:NZ	12:A:987:A:OP1	2.29	0.65
1:S:183:ARG:NH1	12:A:317:C:OP2	2.29	0.65
33:n:40:ARG:NH2	33:n:62:GLU:OE2	2.30	0.65
2:G:134:VAL:O	2:G:137:SER:OG	2.13	0.64
12:A:1589:A:N3	12:A:1653:U:O2'	2.28	0.64
32:m:23:LYS:NZ	32:m:88:TRP:O	2.28	0.64
2:G:31:GLU:OE2	2:G:41:ARG:NH1	2.31	0.64
12:A:538:U:H3	12:A:544:G:H1	1.45	0.64
5:L:72:ASP:OD2	5:L:272:HIS:NE2	2.24	0.64
12:A:1242:U:O2	12:A:1517:G:O2'	2.13	0.64
11:9:17:ARG:NH1	12:A:1173:A:OP1	2.30	0.64
6:O:69:VAL:HG21	6:O:74:LEU:HD13	1.80	0.63
7:N:38:ILE:HD11	7:N:150:THR:HG22	1.81	0.62
12:A:190:G:O2'	12:A:191:A:OP1	2.12	0.62
12:A:1591:C:OP1	21:V:85:LYS:NZ	2.27	0.62
18:J:84:LYS:NZ	18:J:85:ASP:OD2	2.32	0.62
19:R:69:SER:OG	19:R:191:GLU:OE2	2.07	0.62
12:A:1598:G:O6	28:e:85:ARG:NH1	2.33	0.61
26:c:260:ASP:O	26:c:264:LYS:N	2.34	0.61
12:A:880:G:H1	12:A:906:U:H3	1.48	0.61
4:K:59:ILE:HD13	4:K:62:MET:HE3	1.83	0.61
26:c:72:SER:OG	26:c:74:ASP:OD1	2.17	0.61
18:J:14:ILE:HD11	18:J:27:ILE:HD11	1.82	0.61
12:A:329:G:O2'	12:A:330:G:OP1	2.16	0.60
26:c:5:MET:SD	26:c:312:VAL:HG12	2.41	0.60
12:A:636:C:OP1	17:F:98:LYS:NZ	2.34	0.60
34:M:66:VAL:HG11	34:M:69:ILE:HD12	1.82	0.60
12:A:1329:U:O2'	12:A:1332:A:OP2	2.18	0.60
21:V:171:GLU:OE2	28:e:69:THR:OG1	2.08	0.60
12:A:1751:C:O2'	12:A:1752:C:O5'	2.17	0.60
12:A:1277:C:OP1	24:a:51:SER:OG	2.15	0.60
12:A:1535:U:O4	21:V:159:ARG:NH1	2.35	0.60
12:A:880:G:O6	12:A:906:U:O4	2.20	0.59
1:S:136:LYS:NZ	12:A:64:A:OP1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:200:G:OP2	12:A:200:G:N2	2.20	0.59
12:A:940:U:H3	12:A:1002:U:H3	1.47	0.59
23:Z:216:GLU:OE2	23:Z:217:ILE:N	2.35	0.59
8:Q:60:ASP:OD2	8:Q:60:ASP:N	2.36	0.59
14:C:87:MET:HE1	14:C:236:ILE:HD13	1.84	0.59
12:A:1436:C:O2'	12:A:1438:A:O5'	2.19	0.59
12:A:1672:U:OP1	22:Y:18:THR:OG1	2.17	0.58
23:Z:109:LEU:HD12	23:Z:184:ILE:HD11	1.86	0.58
2:G:50:GLU:OE2	2:G:90:LYS:NZ	2.36	0.58
12:A:1604:G:HO2'	12:A:1605:G:P	2.25	0.58
26:c:119:GLN:OE1	26:c:139:LYS:NZ	2.25	0.58
2:G:41:ARG:NH2	2:G:44:ASN:OD1	2.36	0.58
12:A:506:G:OP1	20:T:108:LYS:NZ	2.36	0.57
26:c:244:ASN:OD1	26:c:245:ARG:N	2.36	0.57
12:A:818:A:OP1	15:D:80:ARG:NH2	2.37	0.57
34:M:77:GLU:OE1	34:M:81:ARG:NH2	2.37	0.57
12:A:1124:C:O2'	34:M:126:MET:O	2.22	0.57
12:A:1285:G:N2	32:m:82:ASN:OD1	2.36	0.57
32:m:99:LYS:O	32:m:101:ARG:NH1	2.37	0.57
12:A:1480:A:O2'	30:i:56:ASP:O	2.21	0.57
23:Z:16:ILE:HD11	30:i:36:LEU:HD23	1.87	0.57
11:9:16:LYS:O	11:9:20:MET:HE2	2.04	0.57
34:M:97:GLU:OE2	34:M:120:THR:OG1	2.22	0.56
12:A:823:PSU:N1	15:D:143:ASN:OD1	2.32	0.56
19:R:88:ASN:OD1	19:R:205:ARG:NH1	2.38	0.56
12:A:539:C:O2'	12:A:540:U:O5'	2.17	0.56
12:A:1597:C:OP2	28:e:85:ARG:NH2	2.39	0.56
22:Y:110:ASP:OD1	22:Y:114:GLN:NE2	2.39	0.56
12:A:1613:G:OP1	25:b:42:ARG:NH2	2.39	0.55
29:f:15:VAL:HG12	29:f:68:ILE:HD11	1.89	0.55
12:A:643:A:OP1	15:D:41:ARG:NH2	2.38	0.55
27:d:114:GLU:OE1	27:d:124:THR:HG22	2.07	0.54
12:A:1256:G:O6	35:h:65:THR:HG22	2.07	0.54
12:A:888:U:O2'	12:A:889:U:O5'	2.11	0.54
12:A:57:U:OP1	12:A:504:G:O2'	2.23	0.53
29:f:66:ARG:O	29:f:69:THR:OG1	2.22	0.53
12:A:538:U:O4	12:A:544:G:O6	2.26	0.53
12:A:1824:A:O2'	12:A:1825:A:OP2	2.20	0.53
32:m:77:ILE:HG22	32:m:78:LYS:H	1.73	0.53
19:R:142:SER:OG	19:R:143:LYS:N	2.42	0.53
5:L:271:ASP:OD1	5:L:272:HIS:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:24:LEU:HD11	35:h:89:ILE:HD12	1.90	0.53
12:A:1593:C:O2	27:d:12:GLN:NE2	2.42	0.53
12:A:1757:G:OP2	12:A:1757:G:N2	2.36	0.52
29:f:45:LEU:HD22	29:f:50:ILE:HD11	1.91	0.52
4:K:37:ALA:HB1	4:K:46:PHE:CD1	2.45	0.52
25:b:29:SER:OG	25:b:30:TYR:N	2.39	0.52
32:m:51:VAL:HG21	32:m:79:VAL:HG23	1.90	0.52
4:K:44:GLY:O	7:N:191:ARG:NH2	2.42	0.52
12:A:563:G:HO2'	12:A:564:A:H8	1.57	0.52
3:H:34:ASP:OD2	3:H:80:ARG:NH1	2.42	0.52
24:a:15:LEU:CD2	24:a:49:MET:HE1	2.29	0.52
26:c:18:VAL:O	26:c:287:THR:OG1	2.27	0.52
16:E:61:GLN:HG3	16:E:62:PRO:HA	1.92	0.52
22:Y:63:PHE:CZ	22:Y:92:LEU:HD22	2.45	0.52
13:B:114:SER:OG	13:B:116:CYS:SG	2.60	0.51
12:A:1425:G:O3'	22:Y:33:LYS:NZ	2.43	0.51
12:A:1850:MA6:H92	12:A:1851:MA6:H93	1.91	0.51
2:G:19:PHE:CZ	2:G:23:ILE:HD11	2.46	0.51
20:T:50:THR:OG1	20:T:51:THR:N	2.43	0.51
26:c:145:GLU:O	26:c:175:LYS:NZ	2.44	0.51
12:A:53:C:O2'	12:A:507:G:N7	2.35	0.51
12:A:885:U:N3	12:A:901:G:N1	2.51	0.50
12:A:890:U:O4	12:A:897:U:O2'	2.29	0.50
12:A:1563:G:OP1	27:d:121:ARG:NH1	2.43	0.50
20:T:7:ILE:HD13	20:T:44:LEU:HD22	1.93	0.50
32:m:32:ALA:HB3	32:m:110:VAL:HG22	1.94	0.50
6:O:44:ILE:HD11	6:O:86:LEU:HD12	1.93	0.50
7:N:12:GLU:OE1	7:N:12:GLU:N	2.45	0.50
12:A:345:U:O2'	12:A:346:C:OP1	2.27	0.50
12:A:447:A:OP1	19:R:49:ARG:NH2	2.44	0.50
12:A:1533:A:N3	12:A:1536:G:O2'	2.37	0.50
12:A:1577:G:O2'	12:A:1579:A:N3	2.39	0.50
12:A:60:G:H22	12:A:316:G:H21	1.60	0.49
6:O:138:PHE:O	6:O:213:ARG:N	2.45	0.49
12:A:1678:A2M:HM'2	12:A:1679:A:O4'	2.12	0.49
24:a:49:MET:HE2	24:a:52:LEU:HD12	1.94	0.49
7:N:89:LYS:NZ	34:M:82:ASP:O	2.41	0.49
32:m:51:VAL:CG2	32:m:79:VAL:HG23	2.41	0.49
7:N:13:GLU:OE1	7:N:13:GLU:N	2.43	0.49
26:c:11:LEU:HD12	26:c:43:TRP:CE3	2.47	0.49
34:M:77:GLU:OE2	34:M:80:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:473:A:O2'	12:A:474:G:OP2	2.31	0.49
12:A:969:U:OP1	12:A:970:G:O2'	2.15	0.49
13:B:128:VAL:HG12	13:B:142:VAL:HA	1.95	0.49
26:c:35:SER:OG	26:c:36:ARG:N	2.45	0.48
34:M:95:ILE:O	34:M:95:ILE:HD12	2.13	0.48
35:h:33:GLU:OE2	35:h:55:ARG:NH1	2.46	0.48
5:L:174:ILE:O	5:L:200:ARG:NH2	2.46	0.48
12:A:836:G:O2'	12:A:838:G:O6	2.31	0.48
1:S:72:ARG:NH2	12:A:466:G:O2'	2.44	0.48
14:C:176:ASP:OD1	14:C:177:THR:N	2.47	0.48
21:V:77:MET:HB3	21:V:89:THR:HG21	1.96	0.48
3:H:2:PRO:HA	4:K:64:GLU:OE1	2.13	0.48
12:A:1623:A:O2'	12:A:1624:U:OP1	2.29	0.48
12:A:1614:A:OP2	25:b:42:ARG:NH1	2.47	0.48
26:c:162:ASN:O	26:c:162:ASN:ND2	2.47	0.48
12:A:1550:G:O2'	12:A:1558:C:O2	2.26	0.47
14:C:54:TYR:O	20:T:15:ASN:ND2	2.47	0.47
12:A:1245:G:O2'	12:A:1492:U:OP1	2.32	0.47
12:A:1534:C:O2	12:A:1598:G:N2	2.48	0.47
13:B:68:ILE:O	13:B:68:ILE:HG22	2.14	0.47
12:A:329:G:HO2'	12:A:330:G:P	2.37	0.47
36:U:137:ASP:OD1	36:U:138:VAL:N	2.48	0.47
6:O:39:PHE:CE1	6:O:74:LEU:HD23	2.50	0.47
6:O:229:MET:N	6:O:229:MET:HE2	2.30	0.47
12:A:1850:MA6:C9	12:A:1851:MA6:H93	2.44	0.47
34:M:27:ASP:OD2	34:M:30:THR:OG1	2.27	0.47
12:A:1432:U:O2'	12:A:1436:C:O2	2.19	0.47
14:C:44:LEU:HD13	14:C:72:ILE:HD11	1.95	0.47
2:G:146:VAL:HG12	18:J:42:MET:HE1	1.97	0.47
26:c:78:ALA:CB	26:c:92:LEU:HD21	2.44	0.47
29:f:4:VAL:HG23	29:f:5:ILE:HG23	1.97	0.47
6:O:133:TYR:CE2	6:O:181:LEU:HD22	2.50	0.46
14:C:102:ILE:HG23	14:C:182:MET:HE1	1.98	0.46
23:Z:81:GLU:OE1	23:Z:82:GLY:N	2.49	0.46
12:A:1679:A:OP1	33:n:20:ARG:NH2	2.47	0.46
12:A:1485:U:OP1	23:Z:151:LYS:NZ	2.48	0.46
26:c:26:GLN:NE2	26:c:73:SER:O	2.49	0.46
32:m:83:LYS:HZ1	32:m:103:VAL:HG21	1.81	0.46
1:S:174:PRO:O	12:A:77:A:O2'	2.24	0.46
12:A:1013:U:OP1	12:A:1129:G:O2'	2.33	0.46
12:A:1753:C:N3	12:A:1781:A:N6	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:885:U:O4	12:A:901:G:O6	2.34	0.46
12:A:955:A:N1	12:A:972:A:C5	2.83	0.46
2:G:19:PHE:CE1	2:G:23:ILE:HD11	2.50	0.45
12:A:94:G:HO2'	12:A:508:A:HO2'	1.57	0.45
12:A:885:U:O2	12:A:901:G:N2	2.49	0.45
24:a:49:MET:HE2	24:a:49:MET:HA	1.99	0.45
27:d:5:THR:HG22	27:d:6:VAL:H	1.81	0.45
14:C:174:LYS:O	14:C:179:ASN:ND2	2.50	0.45
25:b:41:GLN:HG3	25:b:84:ILE:HD13	1.98	0.45
2:G:23:ILE:HD13	2:G:62:ILE:CD1	2.46	0.45
25:b:20:VAL:HG13	25:b:25:LEU:CD1	2.46	0.45
23:Z:109:LEU:HD13	23:Z:182:LEU:CD2	2.47	0.45
32:m:50:CYS:SG	32:m:51:VAL:N	2.88	0.45
12:A:1620:A:O2'	25:b:40:ARG:NH1	2.50	0.45
23:Z:226:GLN:NE2	26:c:224:GLY:O	2.50	0.45
9:P:27:VAL:H	9:P:91:THR:CG2	2.30	0.45
12:A:1249:C:O2'	22:Y:143:LYS:NZ	2.46	0.45
23:Z:62:LYS:O	23:Z:67:ARG:NH2	2.47	0.45
15:D:21:GLU:OE2	15:D:23:SER:OG	2.34	0.45
30:i:4:GLN:OE1	30:i:4:GLN:N	2.50	0.44
9:P:44:VAL:HG11	9:P:85:CYS:SG	2.57	0.44
10:I:64:ARG:NH2	12:A:919:A:OP2	2.45	0.44
12:A:953:C:H2'	12:A:954:U:O4'	2.17	0.44
12:A:1228:A:O2'	12:A:1634:A:N3	2.48	0.44
12:A:1374:5MC:O2'	12:A:1464:C:O2	2.33	0.44
12:A:94:G:O2'	12:A:508:A:O2'	2.28	0.44
2:G:23:ILE:HD13	2:G:62:ILE:HD12	1.99	0.44
12:A:1190:A:N3	12:A:1714:U:O2'	2.46	0.44
6:O:57:ILE:HD12	6:O:60:ASP:H	1.83	0.43
26:c:50:THR:OG1	26:c:51:ASN:N	2.51	0.43
1:S:57:ASP:OD1	1:S:61:PHE:N	2.49	0.43
26:c:296:GLN:O	26:c:312:VAL:HG13	2.18	0.43
12:A:1282:A:O2'	12:A:1283:C:O5'	2.32	0.43
30:i:6:LEU:C	30:i:9:SER:HG	2.25	0.43
19:R:115:SER:OG	19:R:136:ILE:HD11	2.18	0.43
20:T:7:ILE:CD1	20:T:44:LEU:HD22	2.48	0.43
29:f:54:LYS:NZ	29:f:59:LEU:HD12	2.32	0.43
14:C:184:THR:C	14:C:189:LEU:HD13	2.44	0.43
12:A:1284:A:N7	32:m:33:ARG:NH1	2.67	0.43
12:A:40:A:O2'	12:A:485:A:O2'	2.22	0.43
12:A:328:U:O2	12:A:328:U:O2'	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:LYS:NZ	18:J:51:GLU:OE1	2.36	0.43
6:O:29:ASP:OD1	6:O:29:ASP:N	2.50	0.43
32:m:69:CYS:SG	32:m:70:ALA:N	2.92	0.43
2:G:30:LEU:HD22	2:G:36:LEU:HD12	2.01	0.43
6:O:120:MET:HE1	12:A:987:A:C6	2.54	0.43
28:e:49:LEU:HD13	29:f:6:PRO:HA	2.01	0.43
14:C:88:ASP:OD1	14:C:122:LYS:NZ	2.50	0.42
12:A:545:A:O2'	12:A:547:G:O6	2.33	0.42
12:A:1615:U:O4	25:b:40:ARG:NH2	2.52	0.42
1:S:69:THR:HG22	1:S:71:GLY:H	1.84	0.42
12:A:1101:U:OP1	34:M:132:ARG:NH1	2.52	0.42
12:A:1262:C:O2	30:i:17:GLY:N	2.50	0.42
12:A:1579:A:O2'	12:A:1581:C:OP2	2.29	0.42
14:C:20:LEU:HD21	14:C:46:ILE:HD12	2.01	0.42
12:A:1159:G:OP1	18:J:76:SER:OG	2.33	0.42
12:A:1715:A:H61	12:A:1818:A:H2	1.66	0.42
14:C:91:SER:OG	14:C:98:ASN:OD1	2.34	0.42
36:U:134:GLU:OE2	36:U:135:GLU:N	2.50	0.42
5:L:68:ARG:NH2	5:L:72:ASP:OD1	2.44	0.42
12:A:463:C:O2'	12:A:466:G:O6	2.29	0.42
12:A:476:A:N3	12:A:488:U:O2'	2.29	0.42
12:A:888:U:HO2'	12:A:889:U:P	2.36	0.42
12:A:1215:C:O2'	12:A:1645:C:OP2	2.35	0.42
25:b:20:VAL:HG13	25:b:25:LEU:HD11	2.01	0.42
12:A:955:A:C2	12:A:972:A:C5	3.08	0.41
33:n:52:GLU:N	33:n:52:GLU:OE1	2.52	0.41
26:c:20:GLN:OE1	26:c:21:ILE:N	2.49	0.41
26:c:276:SER:O	26:c:280:LYS:NZ	2.43	0.41
29:f:114:LEU:HD23	29:f:121:ARG:HB3	2.02	0.41
21:V:156:THR:OG1	21:V:160:GLU:OE1	2.38	0.41
2:G:18:GLU:O	2:G:21:SER:OG	2.21	0.41
12:A:952:G:H2'	12:A:953:C:C6	2.55	0.41
12:A:390:C:O2'	13:B:8:ARG:NH2	2.53	0.41
1:S:201:LYS:NZ	12:A:125:C:OP2	2.50	0.41
2:G:120:ARG:NH2	12:A:915:G:OP1	2.54	0.41
12:A:563:G:O2'	12:A:564:A:O4'	2.39	0.41
23:Z:107:TYR:OH	36:U:137:ASP:OD2	2.39	0.41
32:m:61:TYR:O	32:m:65:VAL:HG23	2.20	0.41
2:G:165:ASN:OD1	2:G:165:ASN:N	2.54	0.41
6:O:69:VAL:CG2	6:O:74:LEU:HD13	2.49	0.41
26:c:2:THR:OG1	26:c:3:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:92:LEU:HD22	28:e:109:TYR:HE1	1.86	0.41
7:N:206:ASP:N	7:N:206:ASP:OD1	2.54	0.41
14:C:189:LEU:HD12	14:C:190:GLY:N	2.36	0.41
28:e:88:LEU:HD23	28:e:109:TYR:CD2	2.56	0.41
6:O:25:PHE:HA	6:O:28:LYS:HD2	2.03	0.40
23:Z:45:ARG:NH2	23:Z:87:TYR:OH	2.54	0.40
24:a:71:LEU:HD11	24:a:79:LEU:HD12	2.04	0.40
32:m:79:VAL:HG11	32:m:85:LEU:HB2	2.01	0.40
12:A:328:U:O2'	12:A:329:G:N7	2.53	0.40
12:A:1653:U:H3	12:A:1671:G:H1	1.69	0.40
19:R:22:HIS:ND1	19:R:23:LYS:O	2.34	0.40
25:b:16:THR:OG1	25:b:20:VAL:N	2.54	0.40
28:e:84:ALA:O	28:e:88:LEU:HD13	2.20	0.40
35:h:20:ILE:HG21	35:h:98:VAL:HG11	2.01	0.40
12:A:539:C:O2'	12:A:545:A:N6	2.54	0.40
12:A:571:U:O2'	20:T:60:PHE:O	2.35	0.40
12:A:682:U:O2'	18:J:4:MET:SD	2.77	0.40
19:R:117:TYR:CD1	19:R:156:ALA:HB2	2.56	0.40
25:b:34:MET:HE1	25:b:46:ASN:HA	2.03	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	S	228/249 (92%)	220 (96%)	8 (4%)	0	100	100
2	G	169/194 (87%)	164 (97%)	5 (3%)	0	100	100
3	H	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
4	K	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
5	L	218/293 (74%)	212 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	O	209/264 (79%)	207 (99%)	2 (1%)	0	100	100
7	N	205/295 (70%)	204 (100%)	1 (0%)	0	100	100
8	Q	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
9	P	129/151 (85%)	126 (98%)	3 (2%)	0	100	100
10	I	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
11	9	22/25 (88%)	22 (100%)	0	0	100	100
13	B	139/158 (88%)	134 (96%)	5 (4%)	0	100	100
14	C	254/263 (97%)	252 (99%)	2 (1%)	0	100	100
15	D	175/194 (90%)	173 (99%)	2 (1%)	0	100	100
16	E	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
17	F	43/59 (73%)	43 (100%)	0	0	100	100
18	J	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
19	R	194/208 (93%)	189 (97%)	5 (3%)	0	100	100
20	T	122/133 (92%)	121 (99%)	1 (1%)	0	100	100
21	V	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
22	Y	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
23	Z	225/243 (93%)	218 (97%)	7 (3%)	0	100	100
24	a	97/165 (59%)	96 (99%)	1 (1%)	0	100	100
25	b	116/145 (80%)	111 (96%)	5 (4%)	0	100	100
26	c	311/317 (98%)	291 (94%)	20 (6%)	0	100	100
27	d	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
28	e	67/125 (54%)	62 (92%)	5 (8%)	0	100	100
29	f	140/152 (92%)	133 (95%)	7 (5%)	0	100	100
30	i	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
31	k	48/156 (31%)	42 (88%)	6 (12%)	0	100	100
32	m	120/132 (91%)	110 (92%)	10 (8%)	0	100	100
33	n	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
34	M	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
35	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
36	U	45/469 (10%)	45 (100%)	0	0	100	100
All	All	4747/5970 (80%)	4597 (97%)	150 (3%)	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	S	200/218 (92%)	196 (98%)	4 (2%)	48	74
2	G	155/174 (89%)	148 (96%)	7 (4%)	24	50
3	H	73/76 (96%)	73 (100%)	0	100	100
4	K	65/67 (97%)	64 (98%)	1 (2%)	57	80
5	L	186/225 (83%)	185 (100%)	1 (0%)	81	92
6	O	192/231 (83%)	191 (100%)	1 (0%)	81	92
7	N	173/243 (71%)	169 (98%)	4 (2%)	44	71
8	Q	86/98 (88%)	83 (96%)	3 (4%)	32	59
9	P	102/119 (86%)	100 (98%)	2 (2%)	48	74
10	I	130/131 (99%)	129 (99%)	1 (1%)	73	88
11	9	23/24 (96%)	23 (100%)	0	100	100
13	B	130/142 (92%)	128 (98%)	2 (2%)	57	80
14	C	220/225 (98%)	218 (99%)	2 (1%)	70	87
15	D	158/168 (94%)	158 (100%)	0	100	100
16	E	112/115 (97%)	111 (99%)	1 (1%)	70	87
17	F	38/48 (79%)	38 (100%)	0	100	100
18	J	112/113 (99%)	110 (98%)	2 (2%)	51	76
19	R	172/180 (96%)	168 (98%)	4 (2%)	44	71
20	T	107/115 (93%)	104 (97%)	3 (3%)	38	66
21	V	156/170 (92%)	151 (97%)	5 (3%)	34	62
22	Y	117/121 (97%)	114 (97%)	3 (3%)	40	68
23	Z	190/202 (94%)	184 (97%)	6 (3%)	34	62
24	a	90/136 (66%)	87 (97%)	3 (3%)	33	61
25	b	106/130 (82%)	105 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	272/275 (99%)	255 (94%)	17 (6%)	16	36
27	d	112/115 (97%)	111 (99%)	1 (1%)	70	87
28	e	61/103 (59%)	59 (97%)	2 (3%)	33	61
29	f	123/132 (93%)	117 (95%)	6 (5%)	22	47
30	i	48/49 (98%)	47 (98%)	1 (2%)	47	73
31	k	46/140 (33%)	42 (91%)	4 (9%)	9	21
32	m	104/108 (96%)	98 (94%)	6 (6%)	18	39
33	n	56/62 (90%)	56 (100%)	0	100	100
34	M	119/122 (98%)	112 (94%)	7 (6%)	18	38
35	h	94/107 (88%)	93 (99%)	1 (1%)	65	84
36	U	36/404 (9%)	33 (92%)	3 (8%)	10	23
All	All	4164/5088 (82%)	4060 (98%)	104 (2%)	42	69

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	12	CYS
1	S	52	ILE
1	S	68	LEU
1	S	139	SER
2	G	30	LEU
2	G	64	VAL
2	G	71	SER
2	G	80	VAL
2	G	88	SER
2	G	131	GLU
2	G	151	SER
4	K	80	SER
5	L	63	VAL
6	O	52	THR
7	N	2	SER
7	N	38	ILE
7	N	190	SER
7	N	191	ARG
8	Q	2	THR
8	Q	30	VAL
8	Q	42	ARG
9	P	47	LEU

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Mol	Chain	Res	Type
9	P	93	LEU
10	I	45	LEU
13	B	30	LYS
13	B	67	SER
14	C	91	SER
14	C	105	THR
16	E	61	GLN
18	J	30	CYS
18	J	42	MET
19	R	4	SER
19	R	62	VAL
19	R	100	CYS
19	R	167	GLN
20	T	4	THR
20	T	44	LEU
20	T	102	THR
21	V	34	SER
21	V	43	GLU
21	V	75	SER
21	V	116	ILE
21	V	125	SER
22	Y	20	THR
22	Y	100	VAL
22	Y	121	VAL
23	Z	35	SER
23	Z	55	THR
23	Z	74	GLN
23	Z	86	LEU
23	Z	93	THR
23	Z	149	SER
24	a	13	GLU
24	a	58	VAL
24	a	90	VAL
25	b	112	ILE
26	c	46	THR
26	c	51	ASN
26	c	71	ILE
26	c	93	THR
26	c	111	VAL
26	c	113	PHE
26	c	124	SER
26	c	128	THR

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Mol	Chain	Res	Type
26	c	143	GLN
26	c	148	SER
26	c	152	SER
26	c	197	THR
26	c	229	THR
26	c	267	VAL
26	c	275	ILE
26	c	303	THR
26	c	314	ILE
27	d	8	ASP
28	e	67	LEU
28	e	83	LEU
29	f	13	LEU
29	f	15	VAL
29	f	16	LEU
29	f	20	ILE
29	f	43	VAL
29	f	60	THR
30	i	53	ILE
31	k	98	VAL
31	k	123	SER
31	k	125	GLU
31	k	134	SER
32	m	21	VAL
32	m	28	HIS
32	m	97	GLU
32	m	110	VAL
32	m	112	LYS
32	m	114	TYR
34	M	32	LYS
34	M	43	SER
34	M	70	SER
34	M	74	GLN
34	M	108	LEU
34	M	114	LEU
34	M	120	THR
35	h	65	THR
36	U	114	LYS
36	U	126	THR
36	U	145	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	56	ASN
1	S	197	GLN
1	S	227	GLN
6	O	40	ASN
6	O	53	GLN
6	O	186	ASN
9	P	83	GLN
10	I	62	GLN
13	B	11	GLN
13	B	94	HIS
14	C	142	HIS
16	E	61	GLN
16	E	127	ASN
19	R	35	ASN
20	T	106	GLN
21	V	118	ASN
21	V	203	ASN
25	b	46	ASN
30	i	26	ASN
32	m	72	HIS
34	M	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	A	1667/1719 (96%)	362 (21%)	19 (1%)

All (362) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	A	17	C
12	A	33	G
12	A	41	G
12	A	46	A
12	A	56	G
12	A	58	C
12	A	64	A
12	A	68	A
12	A	71	G
12	A	72	C
12	A	74	G
12	A	75	G

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Mol	Chain	Res	Type
12	A	76	U
12	A	99	A2M
12	A	100	U
12	A	103	A
12	A	113	G
12	A	115	U
12	A	118	C
12	A	126	G
12	A	129	C
12	A	130	G
12	A	141	A
12	A	142	C
12	A	143	U
12	A	147	A
12	A	149	A
12	A	155	G
12	A	159	A2M
12	A	162	C
12	A	166	A2M
12	A	170	A
12	A	172	U
12	A	174	OMC
12	A	180	G
12	A	184	G
12	A	187	G
12	A	190	G
12	A	191	A
12	A	194	C
12	A	195	C
12	A	197	U
12	A	198	U
12	A	199	C
12	A	200	G
12	A	204	G
12	A	206	G
12	A	207	G
12	A	223	C
12	A	294	U
12	A	300	U
12	A	302	A
12	A	306	C
12	A	308	G

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Mol	Chain	Res	Type
12	A	311	C
12	A	312	G
12	A	319	C
12	A	320	G
12	A	322	C
12	A	323	C
12	A	324	C
12	A	325	C
12	A	326	C
12	A	327	G
12	A	328	U
12	A	330	G
12	A	331	C
12	A	332	G
12	A	335	G
12	A	339	A
12	A	340	C
12	A	346	C
12	A	347	G
12	A	351	G
12	A	362	C
12	A	364	A
12	A	367	U
12	A	369	C
12	A	370	G
12	A	385	G
12	A	386	C
12	A	409	C
12	A	421	G
12	A	442	C
12	A	448	A
12	A	449	A
12	A	450	C
12	A	452	G
12	A	460	A
12	A	464	A
12	A	466	G
12	A	467	G
12	A	472	C
12	A	473	A
12	A	474	G
12	A	476	A

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Mol	Chain	Res	Type
12	A	477	G
12	A	482	G
12	A	485	A
12	A	486	A
12	A	487	U
12	A	492	C
12	A	508	A
12	A	525	A
12	A	536	A
12	A	537	C
12	A	540	U
12	A	541	U
12	A	542	U
12	A	544	G
12	A	545	A
12	A	546	G
12	A	548	C
12	A	549	C
12	A	554	A
12	A	555	A
12	A	556	U
12	A	558	G
12	A	559	G
12	A	563	G
12	A	564	A
12	A	568	C
12	A	576	A
12	A	589	G
12	A	590	A
12	A	591	U
12	A	606	G
12	A	614	C
12	A	620	G
12	A	626	G
12	A	628	A
12	A	629	A
12	A	631	U
12	A	643	A
12	A	655	A
12	A	660	C
12	A	668	A2M
12	A	669	A

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Mol	Chain	Res	Type
12	A	671	A
12	A	672	A
12	A	673	G
12	A	683	OMG
12	A	688	U
12	A	811	A
12	A	821	G
12	A	822	PSU
12	A	827	A
12	A	830	A
12	A	834	C
12	A	835	C
12	A	836	G
12	A	837	A
12	A	838	G
12	A	839	C
12	A	840	C
12	A	841	G
12	A	847	A
12	A	870	A
12	A	871	U
12	A	872	A
12	A	873	G
12	A	874	G
12	A	880	G
12	A	881	G
12	A	882	U
12	A	885	U
12	A	888	U
12	A	889	U
12	A	890	U
12	A	891	G
12	A	892	U
12	A	896	U
12	A	897	U
12	A	898	U
12	A	899	U
12	A	900	C
12	A	901	G
12	A	902	G
12	A	903	A
12	A	904	A

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Mol	Chain	Res	Type
12	A	907	G
12	A	909	G
12	A	912	C
12	A	913	A
12	A	919	A
12	A	920	A
12	A	922	A
12	A	930	C
12	A	933	G
12	A	943	U
12	A	963	A
12	A	965	U
12	A	972	A
12	A	990	A
12	A	992	A
12	A	1017	U
12	A	1023	A
12	A	1042	A
12	A	1044	G
12	A	1061	U
12	A	1062	A
12	A	1078	C
12	A	1083	A
12	A	1085	C
12	A	1108	G
12	A	1115	U
12	A	1116	C
12	A	1119	A
12	A	1120	U
12	A	1138	C
12	A	1153	C
12	A	1154	U
12	A	1171	G
12	A	1195	A
12	A	1208	A
12	A	1215	C
12	A	1216	C
12	A	1217	A
12	A	1220	A
12	A	1221	G
12	A	1224	G
12	A	1242	U

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Mol	Chain	Res	Type
12	A	1251	A
12	A	1253	A
12	A	1256	G
12	A	1257	G
12	A	1258	A
12	A	1259	A
12	A	1274	G
12	A	1275	G
12	A	1280	G
12	A	1281	G
12	A	1282	A
12	A	1284	A
12	A	1285	G
12	A	1286	G
12	A	1290	G
12	A	1297	U
12	A	1301	A
12	A	1302	G
12	A	1303	C
12	A	1305	C
12	A	1308	U
12	A	1309	C
12	A	1313	A
12	A	1315	U
12	A	1320	G
12	A	1326	U
12	A	1327	G
12	A	1342	U
12	A	1371	U
12	A	1372	U
12	A	1378	A
12	A	1397	U
12	A	1401	A
12	A	1402	A
12	A	1404	U
12	A	1405	A
12	A	1406	G
12	A	1409	A
12	A	1416	C
12	A	1417	C
12	A	1418	C
12	A	1419	C

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Mol	Chain	Res	Type
12	A	1420	G
12	A	1421	A
12	A	1422	G
12	A	1423	C
12	A	1424	G
12	A	1428	G
12	A	1433	C
12	A	1434	C
12	A	1435	C
12	A	1436	C
12	A	1437	C
12	A	1438	A
12	A	1441	U
12	A	1452	A
12	A	1454	A
12	A	1464	C
12	A	1465	A
12	A	1489	A
12	A	1490	OMG
12	A	1497	G
12	A	1498	A
12	A	1507	G
12	A	1508	A
12	A	1509	U
12	A	1521	C
12	A	1522	A
12	A	1533	A
12	A	1557	C
12	A	1579	A
12	A	1580	A
12	A	1588	A
12	A	1590	C
12	A	1591	C
12	A	1592	C
12	A	1601	A
12	A	1605	G
12	A	1606	G
12	A	1609	C
12	A	1621	U
12	A	1623	A
12	A	1624	U
12	A	1639	G

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Mol	Chain	Res	Type
12	A	1646	C
12	A	1654	G
12	A	1656	G
12	A	1663	A
12	A	1664	A
12	A	1665	G
12	A	1671	G
12	A	1683	C
12	A	1715	A
12	A	1719	A
12	A	1721	U
12	A	1722	G
12	A	1726	G
12	A	1730	U
12	A	1732	G
12	A	1733	U
12	A	1744	G
12	A	1745	A
12	A	1751	C
12	A	1752	C
12	A	1753	C
12	A	1754	G
12	A	1755	C
12	A	1756	C
12	A	1757	G
12	A	1777	G
12	A	1778	C
12	A	1779	G
12	A	1780	G
12	A	1781	A
12	A	1782	G
12	A	1783	C
12	A	1784	G
12	A	1795	G
12	A	1800	A
12	A	1807	C
12	A	1813	A
12	A	1816	G
12	A	1817	G
12	A	1819	A
12	A	1820	G
12	A	1824	A

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Mol	Chain	Res	Type
12	A	1825	A
12	A	1826	G
12	A	1829	G
12	A	1831	A
12	A	1835	A
12	A	1838	U
12	A	1849	G
12	A	1851	MA6
12	A	1861	G
12	A	1862	G
12	A	1863	A
12	A	1864	U
12	A	1865	C
12	A	1869	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	A	74	G
12	A	190	G
12	A	198	U
12	A	203	G
12	A	310	C
12	A	324	C
12	A	326	C
12	A	329	G
12	A	339	A
12	A	345	U
12	A	476	A
12	A	539	C
12	A	544	G
12	A	548	C
12	A	871	U
12	A	911	C
12	A	1605	G
12	A	1751	C
12	A	1781	A

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

34 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$
12	OMG	A	1328	38,12	23,26,27	2.36	9 (39%)	32,38,41	2.20	12 (37%)
12	A2M	A	99	39,12	22,25,26	3.52	9 (40%)	30,36,39	2.56	13 (43%)
12	A2M	A	27	39,12	22,25,26	3.50	9 (40%)	30,36,39	2.49	13 (43%)
12	JMH	A	1219	39,12	18,22,23	2.64	6 (33%)	23,32,35	1.12	2 (8%)
12	PSU	A	612	39,12	18,21,22	4.35	8 (44%)	21,30,33	2.18	6 (28%)
12	MA6	A	1850	12	23,26,27	1.45	4 (17%)	33,38,41	3.65	13 (39%)
12	6MZ	A	1832	39,38,12	22,25,26	3.02	6 (27%)	29,36,39	2.46	12 (41%)
12	OMG	A	644	12	23,26,27	2.35	9 (39%)	32,38,41	2.18	13 (40%)
12	OMU	A	116	12	19,22,23	3.14	8 (42%)	25,31,34	1.88	6 (24%)
12	OMG	A	683	12	23,26,27	2.36	9 (39%)	32,38,41	2.24	15 (46%)
12	OMU	A	121	12	19,22,23	3.18	8 (42%)	25,31,34	1.80	5 (20%)
12	A2M	A	668	39,12	22,25,26	3.41	10 (45%)	30,36,39	2.43	15 (50%)
12	A2M	A	1031	12	22,25,26	3.50	10 (45%)	30,36,39	2.40	15 (50%)
12	PSU	A	1081	12	18,21,22	4.42	8 (44%)	21,30,33	1.98	5 (23%)
12	OMC	A	1703	12	19,22,23	2.97	8 (42%)	25,31,34	0.74	0
12	PSU	A	822	12	18,21,22	4.37	8 (44%)	21,30,33	2.05	6 (28%)
12	PSU	A	1243	12	18,21,22	4.42	7 (38%)	21,30,33	2.10	5 (23%)
12	5MU	A	814	12	19,22,23	0.61	0	27,32,35	0.80	1 (3%)
12	A2M	A	166	12	22,25,26	3.50	9 (40%)	30,36,39	2.62	16 (53%)
12	OMC	A	174	39,12	19,22,23	3.03	8 (42%)	25,31,34	0.84	0
12	OMG	A	1490	39,12	23,26,27	2.33	8 (34%)	32,38,41	2.11	12 (37%)
12	UR3	A	1830	12	19,22,23	3.10	7 (36%)	26,32,35	1.77	4 (15%)
12	PSU	A	119	12	18,21,22	4.41	7 (38%)	21,30,33	1.82	4 (19%)
12	OMG	A	509	39,12	23,26,27	2.30	8 (34%)	32,38,41	2.10	9 (28%)
12	A2M	A	159	12	22,25,26	3.52	10 (45%)	30,36,39	2.48	15 (50%)
12	OMG	A	601	12	23,26,27	2.33	9 (39%)	32,38,41	2.18	13 (40%)
12	MA6	A	1851	12	23,26,27	1.52	4 (17%)	33,38,41	3.64	13 (39%)
12	4AC	A	1337	12	21,24,25	3.01	10 (47%)	28,34,37	1.88	6 (21%)
12	OMC	A	517	12	19,22,23	2.93	8 (42%)	25,31,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	A2M	A	484	12	22,25,26	3.50	10 (45%)	30,36,39	2.47	15 (50%)
12	PSU	A	823	12	18,21,22	4.43	7 (38%)	21,30,33	1.92	4 (19%)
12	A2M	A	1678	12	22,25,26	3.53	9 (40%)	30,36,39	2.51	12 (40%)
12	5MC	A	1374	12	19,22,23	3.86	8 (42%)	26,32,35	1.04	2 (7%)
12	4AC	A	1842	12	21,24,25	2.97	10 (47%)	28,34,37	1.05	2 (7%)

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
12	OMG	A	1328	38,12	-	0/9/27/28	0/3/3/3
12	A2M	A	99	39,12	-	2/9/27/28	0/3/3/3
12	A2M	A	27	39,12	-	0/9/27/28	0/3/3/3
12	JMH	A	1219	39,12	-	0/7/25/26	0/2/2/2
12	PSU	A	612	39,12	-	0/7/25/26	0/2/2/2
12	MA6	A	1850	12	-	0/11/29/30	0/3/3/3
12	6MZ	A	1832	39,38,12	-	2/9/27/28	0/3/3/3
12	OMG	A	644	12	-	1/9/27/28	0/3/3/3
12	OMU	A	116	12	-	0/9/27/28	0/2/2/2
12	OMG	A	683	12	-	2/9/27/28	0/3/3/3
12	OMU	A	121	12	-	0/9/27/28	0/2/2/2
12	A2M	A	668	39,12	-	2/9/27/28	0/3/3/3
12	A2M	A	1031	12	-	0/9/27/28	0/3/3/3
12	PSU	A	1081	12	-	1/7/25/26	0/2/2/2
12	OMC	A	1703	12	-	1/9/27/28	0/2/2/2
12	PSU	A	822	12	-	2/7/25/26	0/2/2/2
12	PSU	A	1243	12	-	0/7/25/26	0/2/2/2
12	5MU	A	814	12	-	0/7/25/26	0/2/2/2
12	A2M	A	166	12	-	2/9/27/28	0/3/3/3
12	OMC	A	174	39,12	-	3/9/27/28	0/2/2/2
12	OMG	A	1490	39,12	-	1/9/27/28	0/3/3/3
12	UR3	A	1830	12	-	0/7/25/26	0/2/2/2
12	PSU	A	119	12	-	0/7/25/26	0/2/2/2
12	OMG	A	509	39,12	-	0/9/27/28	0/3/3/3
12	A2M	A	159	12	-	2/9/27/28	0/3/3/3
12	OMG	A	601	12	-	0/9/27/28	0/3/3/3
12	MA6	A	1851	12	-	4/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	4AC	A	1337	12	-	2/11/29/30	0/2/2/2
12	OMC	A	517	12	-	0/9/27/28	0/2/2/2
12	A2M	A	484	12	-	0/9/27/28	0/3/3/3
12	PSU	A	823	12	-	2/7/25/26	0/2/2/2
12	A2M	A	1678	12	-	0/9/27/28	0/3/3/3
12	5MC	A	1374	12	-	0/7/25/26	0/2/2/2
12	4AC	A	1842	12	-	0/11/29/30	0/2/2/2

All (268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1832	6MZ	C6-N6	12.51	1.48	1.34
12	A	1081	PSU	C6-C5	11.08	1.47	1.35
12	A	119	PSU	C6-C5	11.06	1.47	1.35
12	A	823	PSU	C6-C5	10.90	1.47	1.35
12	A	612	PSU	C6-C5	10.86	1.47	1.35
12	A	822	PSU	C6-C5	10.80	1.47	1.35
12	A	1243	PSU	C6-C5	10.73	1.47	1.35
12	A	823	PSU	C2-N1	9.87	1.49	1.36
12	A	1243	PSU	C2-N1	9.79	1.49	1.36
12	A	1081	PSU	C2-N1	9.45	1.49	1.36
12	A	119	PSU	C2-N1	9.44	1.49	1.36
12	A	612	PSU	C2-N1	9.34	1.48	1.36
12	A	822	PSU	C2-N1	9.32	1.48	1.36
12	A	1678	A2M	C2'-C1'	-9.15	1.30	1.53
12	A	99	A2M	C2'-C1'	-9.02	1.30	1.53
12	A	484	A2M	C2'-C1'	-8.94	1.31	1.53
12	A	1374	5MC	C6-C5	8.93	1.49	1.34
12	A	27	A2M	C2'-C1'	-8.90	1.31	1.53
12	A	159	A2M	C2'-C1'	-8.90	1.31	1.53
12	A	166	A2M	O4'-C1'	8.89	1.62	1.42
12	A	1031	A2M	C2'-C1'	-8.87	1.31	1.53
12	A	166	A2M	C2'-C1'	-8.80	1.31	1.53
12	A	159	A2M	O4'-C1'	8.72	1.62	1.42
12	A	99	A2M	O4'-C1'	8.71	1.62	1.42
12	A	1678	A2M	O4'-C1'	8.67	1.62	1.42
12	A	1031	A2M	O4'-C1'	8.65	1.62	1.42
12	A	27	A2M	O4'-C1'	8.58	1.61	1.42
12	A	1830	UR3	C2-N1	8.29	1.50	1.38
12	A	484	A2M	O4'-C1'	8.27	1.61	1.42
12	A	668	A2M	C2'-C1'	-8.17	1.33	1.53
12	A	668	A2M	O4'-C1'	8.13	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	121	OMU	C2-N3	7.80	1.51	1.38
12	A	116	OMU	C2-N3	7.73	1.51	1.38
12	A	121	OMU	C2-N1	7.22	1.49	1.38
12	A	174	OMC	C2-N3	7.19	1.50	1.36
12	A	668	A2M	O4'-C4'	-7.18	1.29	1.45
12	A	1243	PSU	C2-N3	7.08	1.49	1.37
12	A	1703	OMC	C2-N3	7.01	1.50	1.36
12	A	517	OMC	C2-N3	6.97	1.50	1.36
12	A	116	OMU	C2-N1	6.95	1.49	1.38
12	A	119	PSU	C2-N3	6.90	1.48	1.37
12	A	1374	5MC	C2-N3	6.86	1.50	1.36
12	A	822	PSU	C2-N3	6.79	1.48	1.37
12	A	1081	PSU	C2-N3	6.79	1.48	1.37
12	A	1830	UR3	C6-C5	6.76	1.50	1.35
12	A	1219	JMH	C2-N1	6.73	1.47	1.38
12	A	484	A2M	O4'-C4'	-6.72	1.30	1.45
12	A	612	PSU	C2-N3	6.71	1.48	1.37
12	A	27	A2M	O4'-C4'	-6.70	1.30	1.45
12	A	1842	4AC	C4-N3	6.70	1.44	1.32
12	A	1678	A2M	O4'-C4'	-6.65	1.30	1.45
12	A	159	A2M	O4'-C4'	-6.62	1.30	1.45
12	A	1031	A2M	O4'-C4'	-6.60	1.30	1.45
12	A	1374	5MC	C4-N4	6.57	1.50	1.34
12	A	1337	4AC	C4-N3	6.51	1.43	1.32
12	A	99	A2M	O4'-C4'	-6.49	1.30	1.45
12	A	174	OMC	C6-C5	6.48	1.50	1.35
12	A	166	A2M	O4'-C4'	-6.45	1.30	1.45
12	A	517	OMC	C6-C5	6.40	1.49	1.35
12	A	1703	OMC	C6-C5	6.34	1.49	1.35
12	A	823	PSU	C2-N3	6.32	1.47	1.37
12	A	823	PSU	O4-C4	-6.25	1.11	1.23
12	A	683	OMG	C4-N3	6.23	1.48	1.34
12	A	1490	OMG	C4-N3	6.09	1.48	1.34
12	A	1328	OMG	C4-N3	6.08	1.48	1.34
12	A	644	OMG	C4-N3	5.97	1.47	1.34
12	A	1374	5MC	C4-N3	5.96	1.43	1.34
12	A	509	OMG	C4-N3	5.94	1.47	1.34
12	A	1219	JMH	C6-C5	5.94	1.48	1.35
12	A	1374	5MC	C5-C4	5.90	1.48	1.44
12	A	116	OMU	C6-C5	5.89	1.48	1.35
12	A	601	OMG	C4-N3	5.89	1.47	1.34
12	A	121	OMU	C6-C5	5.89	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1337	4AC	C6-C5	5.86	1.48	1.35
12	A	822	PSU	O4-C4	-5.83	1.12	1.23
12	A	612	PSU	O4-C4	-5.77	1.12	1.23
12	A	119	PSU	O4-C4	-5.75	1.12	1.23
12	A	1842	4AC	C6-C5	5.74	1.48	1.35
12	A	1081	PSU	O4-C4	-5.71	1.12	1.23
12	A	1243	PSU	O4-C4	-5.70	1.12	1.23
12	A	1842	4AC	C2-N3	5.61	1.47	1.36
12	A	1830	UR3	C2-N3	5.56	1.50	1.39
12	A	1337	4AC	C2-N3	5.54	1.47	1.36
12	A	823	PSU	C6-N1	5.07	1.44	1.36
12	A	1219	JMH	C2-N3	4.99	1.48	1.39
12	A	1243	PSU	C6-N1	4.91	1.44	1.36
12	A	174	OMC	C4-N3	4.89	1.44	1.34
12	A	119	PSU	C6-N1	4.89	1.44	1.36
12	A	822	PSU	C6-N1	4.85	1.44	1.36
12	A	1328	OMG	C2-N3	4.83	1.44	1.33
12	A	1703	OMC	C4-N3	4.81	1.44	1.34
12	A	683	OMG	C2-N3	4.77	1.44	1.33
12	A	1081	PSU	C6-N1	4.74	1.44	1.36
12	A	644	OMG	C2-N3	4.70	1.44	1.33
12	A	612	PSU	C6-N1	4.70	1.44	1.36
12	A	509	OMG	C2-N3	4.68	1.44	1.33
12	A	1490	OMG	C2-N3	4.67	1.44	1.33
12	A	1328	OMG	C2-N2	4.60	1.45	1.34
12	A	601	OMG	C2-N3	4.60	1.44	1.33
12	A	517	OMC	C4-N3	4.53	1.43	1.34
12	A	1490	OMG	C2-N2	4.50	1.44	1.34
12	A	683	OMG	C2-N2	4.48	1.44	1.34
12	A	601	OMG	C2-N2	4.40	1.44	1.34
12	A	166	A2M	C6-N6	4.39	1.45	1.34
12	A	159	A2M	C6-N6	4.37	1.45	1.34
12	A	644	OMG	C2-N2	4.37	1.44	1.34
12	A	1678	A2M	C6-N6	4.28	1.45	1.34
12	A	1374	5MC	C6-N1	4.26	1.45	1.38
12	A	99	A2M	C6-N6	4.25	1.45	1.34
12	A	27	A2M	C6-N6	4.22	1.45	1.34
12	A	509	OMG	C2-N2	4.18	1.44	1.34
12	A	174	OMC	C2-N1	4.17	1.48	1.40
12	A	484	A2M	C6-N6	4.14	1.44	1.34
12	A	1031	A2M	C6-N6	4.09	1.44	1.34
12	A	116	OMU	C4-N3	4.06	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	668	A2M	C6-N6	4.05	1.44	1.34
12	A	517	OMC	C2-N1	4.03	1.48	1.40
12	A	1337	4AC	C7-N4	4.03	1.45	1.37
12	A	1703	OMC	C2-N1	3.98	1.48	1.40
12	A	1243	PSU	C4-N3	3.93	1.46	1.38
12	A	1337	4AC	C4-N4	3.91	1.45	1.39
12	A	121	OMU	C4-N3	3.86	1.45	1.38
12	A	1374	5MC	C2-N1	3.84	1.48	1.40
12	A	612	PSU	O2-C2	-3.80	1.15	1.23
12	A	119	PSU	C4-N3	3.76	1.45	1.38
12	A	1081	PSU	O2-C2	-3.75	1.15	1.23
12	A	1337	4AC	C5-C4	3.69	1.49	1.41
12	A	1851	MA6	C5-N7	-3.69	1.32	1.39
12	A	119	PSU	O2-C2	-3.68	1.15	1.23
12	A	822	PSU	C4-N3	3.67	1.45	1.38
12	A	1842	4AC	C2-N1	3.65	1.47	1.40
12	A	1842	4AC	C7-N4	3.63	1.44	1.37
12	A	612	PSU	C4-N3	3.63	1.45	1.38
12	A	822	PSU	O2-C2	-3.63	1.15	1.23
12	A	823	PSU	O2-C2	-3.62	1.15	1.23
12	A	1081	PSU	C4-N3	3.61	1.45	1.38
12	A	509	OMG	C5-N7	-3.59	1.31	1.39
12	A	174	OMC	C4-N4	3.58	1.42	1.33
12	A	1851	MA6	C5-C4	-3.58	1.32	1.39
12	A	1243	PSU	O2-C2	-3.57	1.15	1.23
12	A	1703	OMC	C4-N4	3.55	1.42	1.33
12	A	1830	UR3	O4-C4	-3.52	1.16	1.23
12	A	1850	MA6	C5-N7	-3.48	1.32	1.39
12	A	1842	4AC	C4-N4	3.47	1.45	1.39
12	A	1337	4AC	C2-N1	3.46	1.47	1.40
12	A	1490	OMG	C5-N7	-3.43	1.32	1.39
12	A	823	PSU	C4-N3	3.43	1.45	1.38
12	A	1031	A2M	C5-C4	-3.37	1.33	1.39
12	A	601	OMG	C5-N7	-3.36	1.32	1.39
12	A	1850	MA6	C5-C4	-3.33	1.33	1.39
12	A	1842	4AC	C5-C4	3.32	1.48	1.41
12	A	484	A2M	C5-C4	-3.30	1.33	1.39
12	A	99	A2M	C5-C4	-3.28	1.33	1.39
12	A	517	OMC	C4-N4	3.28	1.41	1.33
12	A	644	OMG	C5-N7	-3.27	1.32	1.39
12	A	1842	4AC	O2-C2	-3.23	1.17	1.23
12	A	27	A2M	C5-C4	-3.22	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1703	OMC	C6-N1	3.21	1.45	1.38
12	A	174	OMC	C6-N1	3.21	1.45	1.38
12	A	1678	A2M	C5-C4	-3.21	1.33	1.39
12	A	517	OMC	C6-N1	3.19	1.45	1.38
12	A	683	OMG	C5-N7	-3.18	1.32	1.39
12	A	668	A2M	C5-C4	-3.17	1.33	1.39
12	A	1337	4AC	O2-C2	-3.16	1.17	1.23
12	A	166	A2M	C5-C4	-3.14	1.33	1.39
12	A	1703	OMC	O2-C2	-3.13	1.17	1.23
12	A	644	OMG	O6-C6	-3.12	1.17	1.23
12	A	1328	OMG	C5-N7	-3.11	1.32	1.39
12	A	121	OMU	O4-C4	-3.11	1.18	1.24
12	A	517	OMC	O2-C2	-3.10	1.17	1.23
12	A	668	A2M	C5-N7	-3.10	1.33	1.39
12	A	1832	6MZ	C5-C4	-3.09	1.33	1.39
12	A	509	OMG	O6-C6	-3.09	1.17	1.23
12	A	27	A2M	O3'-C3'	-3.08	1.35	1.43
12	A	1678	A2M	O2'-C2'	3.07	1.50	1.42
12	A	99	A2M	C5-N7	-3.06	1.33	1.39
12	A	116	OMU	O4-C4	-3.06	1.18	1.24
12	A	484	A2M	O2'-C2'	3.04	1.50	1.42
12	A	166	A2M	O3'-C3'	-3.04	1.35	1.43
12	A	174	OMC	O2-C2	-3.03	1.18	1.23
12	A	484	A2M	C5-N7	-3.01	1.33	1.39
12	A	159	A2M	O3'-C3'	-2.98	1.35	1.43
12	A	601	OMG	O6-C6	-2.98	1.17	1.23
12	A	1031	A2M	O3'-C3'	-2.98	1.35	1.43
12	A	159	A2M	C5-C4	-2.98	1.33	1.39
12	A	1832	6MZ	C5-N7	-2.98	1.33	1.39
12	A	644	OMG	C4-N9	-2.93	1.30	1.38
12	A	99	A2M	O3'-C3'	-2.91	1.35	1.43
12	A	159	A2M	O2'-C2'	2.90	1.49	1.42
12	A	1678	A2M	O3'-C3'	-2.90	1.35	1.43
12	A	1842	4AC	C6-N1	2.90	1.45	1.38
12	A	484	A2M	O3'-C3'	-2.86	1.35	1.43
12	A	601	OMG	C4-N9	-2.86	1.30	1.38
12	A	99	A2M	O2'-C2'	2.85	1.49	1.42
12	A	1337	4AC	C6-N1	2.84	1.44	1.38
12	A	1490	OMG	O6-C6	-2.84	1.18	1.23
12	A	1490	OMG	C4-N9	-2.82	1.30	1.38
12	A	159	A2M	C5-N7	-2.81	1.34	1.39
12	A	683	OMG	O6-C6	-2.81	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1031	A2M	O2'-C2'	2.80	1.49	1.42
12	A	1328	OMG	O6-C6	-2.79	1.18	1.23
12	A	668	A2M	O2'-C2'	2.79	1.49	1.42
12	A	1850	MA6	C6-N6	2.78	1.44	1.36
12	A	509	OMG	C4-N9	-2.77	1.31	1.38
12	A	27	A2M	C5-N7	-2.77	1.34	1.39
12	A	27	A2M	O2'-C2'	2.75	1.49	1.42
12	A	166	A2M	O2'-C2'	2.75	1.49	1.42
12	A	1830	UR3	O2-C2	-2.75	1.17	1.22
12	A	1031	A2M	C5-N7	-2.73	1.34	1.39
12	A	1328	OMG	C4-N9	-2.70	1.31	1.38
12	A	116	OMU	C6-N1	2.68	1.44	1.38
12	A	166	A2M	C5-N7	-2.67	1.34	1.39
12	A	484	A2M	C8-N9	-2.62	1.33	1.37
12	A	683	OMG	C4-N9	-2.60	1.31	1.38
12	A	121	OMU	C6-N1	2.60	1.44	1.38
12	A	668	A2M	O3'-C3'	-2.59	1.36	1.43
12	A	1219	JMH	C6-N1	2.58	1.44	1.38
12	A	822	PSU	O4'-C1'	-2.58	1.40	1.43
12	A	1328	OMG	C2-N1	2.57	1.43	1.37
12	A	1842	4AC	O7-C7	-2.54	1.17	1.23
12	A	1832	6MZ	C6-N1	-2.53	1.31	1.35
12	A	1851	MA6	C6-N6	2.52	1.43	1.36
12	A	683	OMG	C2-N1	2.52	1.43	1.37
12	A	644	OMG	C2-N1	2.48	1.43	1.37
12	A	1830	UR3	C6-N1	2.48	1.44	1.38
12	A	1081	PSU	O4'-C1'	-2.47	1.40	1.43
12	A	1374	5MC	O2-C2	-2.47	1.19	1.23
12	A	1851	MA6	C4-N9	-2.47	1.32	1.37
12	A	601	OMG	C2-N1	2.45	1.43	1.37
12	A	27	A2M	C8-N9	-2.45	1.33	1.37
12	A	1830	UR3	C5-C4	2.45	1.50	1.43
12	A	1678	A2M	C5-N7	-2.44	1.34	1.39
12	A	174	OMC	C5-C4	2.42	1.48	1.42
12	A	683	OMG	C5-C6	2.39	1.53	1.44
12	A	668	A2M	C8-N9	-2.37	1.33	1.37
12	A	121	OMU	O2-C2	-2.36	1.18	1.23
12	A	1031	A2M	C8-N9	-2.35	1.33	1.37
12	A	159	A2M	C8-N9	-2.34	1.33	1.37
12	A	1490	OMG	C2-N1	2.34	1.43	1.37
12	A	121	OMU	C5-C4	2.33	1.48	1.43
12	A	1219	JMH	C5-C4	2.33	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	99	A2M	C8-N9	-2.32	1.33	1.37
12	A	517	OMC	C5-C4	2.32	1.48	1.42
12	A	644	OMG	C5-C6	2.31	1.53	1.44
12	A	1328	OMG	C6-N1	2.31	1.43	1.38
12	A	601	OMG	C5-C6	2.30	1.53	1.44
12	A	1031	A2M	C4-N9	-2.30	1.32	1.37
12	A	509	OMG	C2-N1	2.29	1.43	1.37
12	A	116	OMU	O2-C2	-2.28	1.19	1.23
12	A	1703	OMC	C5-C4	2.27	1.48	1.42
12	A	1337	4AC	O7-C7	-2.27	1.18	1.23
12	A	1328	OMG	C5-C6	2.26	1.52	1.44
12	A	116	OMU	C5-C4	2.24	1.48	1.43
12	A	601	OMG	C6-N1	2.22	1.43	1.38
12	A	668	A2M	C4-N9	-2.20	1.33	1.37
12	A	166	A2M	C8-N9	-2.19	1.33	1.37
12	A	1678	A2M	C8-N9	-2.19	1.33	1.37
12	A	683	OMG	C6-N1	2.18	1.42	1.38
12	A	1219	JMH	O2-C2	-2.18	1.18	1.22
12	A	509	OMG	C5-C6	2.18	1.52	1.44
12	A	644	OMG	C6-N1	2.16	1.42	1.38
12	A	1490	OMG	C5-C6	2.13	1.52	1.44
12	A	484	A2M	C4-N9	-2.12	1.33	1.37
12	A	1832	6MZ	C4-N9	-2.11	1.33	1.37
12	A	159	A2M	C4-N9	-2.10	1.33	1.37
12	A	1832	6MZ	C8-N9	-2.10	1.34	1.37
12	A	1850	MA6	C4-N9	-2.07	1.33	1.37
12	A	612	PSU	O4'-C1'	-2.07	1.41	1.43

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1851	MA6	N1-C6-N6	-11.49	102.86	116.86
12	A	1850	MA6	N1-C6-N6	-9.80	104.91	116.86
12	A	1850	MA6	C1'-N9-C8	-8.61	108.00	127.09
12	A	1850	MA6	C4-N9-C1'	7.90	145.12	126.63
12	A	1851	MA6	C5-C6-N6	7.87	137.78	125.33
12	A	1850	MA6	C5-C6-N6	7.24	136.79	125.33
12	A	1851	MA6	C1'-N9-C8	-7.22	111.06	127.09
12	A	1851	MA6	C4-N9-C1'	6.94	142.87	126.63
12	A	1337	4AC	CM7-C7-N4	6.62	125.95	115.27
12	A	1830	UR3	C4-N3-C2	-6.21	119.58	124.58
12	A	1832	6MZ	N1-C2-N3	-5.89	119.66	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	27	A2M	N3-C2-N1	-5.67	120.00	128.58
12	A	1850	MA6	N1-C2-N3	-5.67	120.00	128.58
12	A	99	A2M	N3-C2-N1	-5.64	120.04	128.58
12	A	1678	A2M	N3-C2-N1	-5.53	120.21	128.58
12	A	166	A2M	N3-C2-N1	-5.51	120.24	128.58
12	A	668	A2M	N3-C2-N1	-5.47	120.30	128.58
12	A	1851	MA6	N1-C2-N3	-5.42	120.38	128.58
12	A	484	A2M	N3-C2-N1	-5.37	120.46	128.58
12	A	121	OMU	C4-N3-C2	-5.35	119.97	126.61
12	A	823	PSU	C4-N3-C2	-5.34	119.01	126.37
12	A	1031	A2M	N3-C2-N1	-5.34	120.50	128.58
12	A	159	A2M	N3-C2-N1	-5.30	120.56	128.58
12	A	1243	PSU	C4-N3-C2	-5.26	119.13	126.37
12	A	116	OMU	C4-N3-C2	-5.26	120.08	126.61
12	A	99	A2M	C5-C4-N3	-5.08	119.72	126.72
12	A	612	PSU	N1-C2-N3	5.07	120.52	115.17
12	A	822	PSU	C4-N3-C2	-4.98	119.52	126.37
12	A	1328	OMG	C1'-N9-C8	-4.97	112.62	126.73
12	A	509	OMG	C1'-N9-C8	-4.97	112.62	126.73
12	A	612	PSU	C4-N3-C2	-4.96	119.54	126.37
12	A	1678	A2M	C1'-N9-C8	-4.91	116.19	127.09
12	A	166	A2M	C5-C4-N3	-4.91	119.96	126.72
12	A	1081	PSU	C4-N3-C2	-4.88	119.65	126.37
12	A	1832	6MZ	C1'-N9-C8	-4.88	116.28	127.09
12	A	1678	A2M	N9-C8-N7	-4.84	107.08	113.94
12	A	509	OMG	C1'-N9-C4	4.83	140.74	126.49
12	A	484	A2M	C5-C4-N3	-4.79	120.12	126.72
12	A	1490	OMG	C1'-N9-C8	-4.79	113.12	126.73
12	A	166	A2M	C1'-N9-C8	-4.78	116.49	127.09
12	A	99	A2M	C1'-N9-C8	-4.76	116.54	127.09
12	A	119	PSU	C4-N3-C2	-4.75	119.82	126.37
12	A	601	OMG	C1'-N9-C8	-4.74	113.27	126.73
12	A	644	OMG	C1'-N9-C8	-4.72	113.33	126.73
12	A	683	OMG	C1'-N9-C8	-4.71	113.35	126.73
12	A	159	A2M	C5-C4-N3	-4.68	120.28	126.72
12	A	668	A2M	C5-C4-N3	-4.64	120.32	126.72
12	A	1243	PSU	N1-C2-N3	4.63	120.06	115.17
12	A	1031	A2M	N9-C8-N7	-4.62	107.39	113.94
12	A	683	OMG	C2-N3-C4	4.61	120.23	112.30
12	A	1851	MA6	C5-C4-N3	-4.59	120.40	126.72
12	A	27	A2M	C5-C4-N3	-4.57	120.43	126.72
12	A	1081	PSU	N1-C2-N3	4.56	119.98	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1678	A2M	C5-C4-N3	-4.55	120.45	126.72
12	A	1850	MA6	C4-C5-C6	4.54	120.60	115.91
12	A	509	OMG	C5-C4-N3	-4.52	121.20	128.39
12	A	683	OMG	C5-C4-N3	-4.50	121.22	128.39
12	A	1328	OMG	C1'-N9-C4	4.50	139.77	126.49
12	A	822	PSU	N1-C2-N3	4.50	119.91	115.17
12	A	27	A2M	C1'-N9-C8	-4.49	117.13	127.09
12	A	601	OMG	C2-N3-C4	4.48	120.01	112.30
12	A	1328	OMG	C2-N3-C4	4.44	119.95	112.30
12	A	166	A2M	N9-C8-N7	-4.44	107.64	113.94
12	A	159	A2M	C1'-N9-C8	-4.43	117.26	127.09
12	A	1832	6MZ	N9-C8-N7	-4.43	107.65	113.94
12	A	27	A2M	N9-C8-N7	-4.43	107.65	113.94
12	A	1850	MA6	C5-C4-N3	-4.42	120.63	126.72
12	A	601	OMG	C1'-N9-C4	4.41	139.51	126.49
12	A	1832	6MZ	C5-C4-N3	-4.39	120.68	126.72
12	A	1490	OMG	C1'-N9-C4	4.38	139.43	126.49
12	A	644	OMG	C2-N3-C4	4.38	119.84	112.30
12	A	1328	OMG	C5-C4-N3	-4.36	121.45	128.39
12	A	823	PSU	N1-C2-N3	4.35	119.75	115.17
12	A	1490	OMG	C2-N3-C4	4.34	119.78	112.30
12	A	1031	A2M	C1'-N9-C8	-4.33	117.48	127.09
12	A	1031	A2M	C5-C4-N3	-4.31	120.78	126.72
12	A	644	OMG	C1'-N9-C4	4.28	139.13	126.49
12	A	99	A2M	N9-C8-N7	-4.25	107.90	113.94
12	A	644	OMG	C5-C4-N3	-4.23	121.66	128.39
12	A	159	A2M	N9-C8-N7	-4.22	107.94	113.94
12	A	601	OMG	C5-C4-N3	-4.18	121.74	128.39
12	A	484	A2M	N9-C8-N7	-4.15	108.05	113.94
12	A	1490	OMG	C5-C4-N3	-4.15	121.79	128.39
12	A	1850	MA6	N9-C8-N7	-4.13	108.07	113.94
12	A	119	PSU	N1-C2-N3	4.12	119.52	115.17
12	A	683	OMG	C1'-N9-C4	4.11	138.63	126.49
12	A	484	A2M	C1'-N9-C8	-4.06	118.09	127.09
12	A	116	OMU	N3-C2-N1	4.05	120.16	114.89
12	A	668	A2M	N9-C8-N7	-4.05	108.19	113.94
12	A	1851	MA6	C4-C5-C6	4.00	120.05	115.91
12	A	509	OMG	C2-N3-C4	3.97	119.13	112.30
12	A	612	PSU	C6-N1-C2	-3.92	119.05	122.69
12	A	1830	UR3	C5-C4-N3	3.90	120.18	115.04
12	A	1851	MA6	N9-C8-N7	-3.90	108.40	113.94
12	A	1850	MA6	C2-N1-C6	3.87	121.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1832	6MZ	C4-N9-C1'	3.87	135.68	126.63
12	A	668	A2M	C2'-C1'-N9	3.81	120.03	113.75
12	A	99	A2M	C4-N9-C1'	3.79	135.50	126.63
12	A	1851	MA6	C5-C4-N9	3.77	109.92	105.81
12	A	121	OMU	N3-C2-N1	3.76	119.79	114.89
12	A	166	A2M	C4-N9-C1'	3.70	135.28	126.63
12	A	99	A2M	C5-C6-N6	-3.60	114.38	123.29
12	A	1678	A2M	C5-C6-N6	-3.54	114.53	123.29
12	A	683	OMG	N9-C8-N7	-3.51	106.90	113.40
12	A	668	A2M	C1'-N9-C8	-3.48	119.36	127.09
12	A	159	A2M	C4-N9-C1'	3.47	134.75	126.63
12	A	121	OMU	C5-C4-N3	3.46	119.65	114.80
12	A	99	A2M	C2-N3-C4	3.41	120.17	111.83
12	A	1851	MA6	C2-N1-C6	3.39	120.12	111.83
12	A	166	A2M	C2-N3-C4	3.38	120.10	111.83
12	A	1678	A2M	C4-N9-C1'	3.38	134.53	126.63
12	A	116	OMU	C5-C4-N3	3.38	119.53	114.80
12	A	166	A2M	C5-C6-N6	-3.37	114.93	123.29
12	A	27	A2M	C4-N9-C1'	3.35	134.47	126.63
12	A	99	A2M	N6-C6-N1	3.33	125.79	118.38
12	A	1243	PSU	C6-N1-C2	-3.30	119.63	122.69
12	A	644	OMG	N9-C8-N7	-3.29	107.29	113.40
12	A	27	A2M	C2-N3-C4	3.29	119.86	111.83
12	A	1337	4AC	O7-C7-N4	-3.27	116.76	121.90
12	A	484	A2M	C2-N3-C4	3.26	119.80	111.83
12	A	1678	A2M	C4-N9-C8	3.26	109.16	105.74
12	A	1328	OMG	N9-C8-N7	-3.26	107.36	113.40
12	A	159	A2M	C5-C6-N6	-3.25	115.24	123.29
12	A	1678	A2M	C2-N3-C4	3.25	119.77	111.83
12	A	1490	OMG	N9-C8-N7	-3.24	107.38	113.40
12	A	159	A2M	C2-N3-C4	3.24	119.74	111.83
12	A	1832	6MZ	C2-N3-C4	3.24	119.73	111.83
12	A	1850	MA6	C5-N7-C8	3.23	108.53	103.45
12	A	601	OMG	N9-C8-N7	-3.23	107.41	113.40
12	A	1851	MA6	C2-N3-C4	3.22	119.70	111.83
12	A	119	PSU	C6-N1-C2	-3.22	119.71	122.69
12	A	484	A2M	C4-N9-C1'	3.20	134.13	126.63
12	A	668	A2M	C2-N3-C4	3.20	119.66	111.83
12	A	27	A2M	C5-C6-N6	-3.19	115.38	123.29
12	A	822	PSU	C6-N1-C2	-3.19	119.73	122.69
12	A	1832	6MZ	C4-C5-C6	3.19	119.43	116.78
12	A	116	OMU	O4-C4-C5	-3.17	119.69	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	612	PSU	C6-C5-C4	3.15	120.30	118.17
12	A	1031	A2M	C4-N9-C1'	3.14	133.99	126.63
12	A	1832	6MZ	C5-N7-C8	3.13	108.38	103.45
12	A	166	A2M	C5-N7-C8	3.12	108.35	103.45
12	A	1374	5MC	C5-C6-N1	-3.10	119.95	123.31
12	A	1031	A2M	C2-N3-C4	3.09	119.38	111.83
12	A	1337	4AC	C5-C4-N4	3.08	128.12	122.94
12	A	1678	A2M	N6-C6-N1	3.08	125.23	118.38
12	A	601	OMG	C2-N1-C6	-3.08	119.53	125.11
12	A	121	OMU	O4-C4-C5	-3.07	119.86	125.16
12	A	1243	PSU	O2-C2-N1	-3.07	119.62	122.79
12	A	509	OMG	C2-N1-C6	-3.06	119.56	125.11
12	A	1031	A2M	C5-N7-C8	3.05	108.25	103.45
12	A	644	OMG	C2-N1-C6	-3.05	119.58	125.11
12	A	99	A2M	N3-C4-N9	3.05	132.35	127.17
12	A	1337	4AC	C5-C4-N3	-3.05	117.83	122.60
12	A	1678	A2M	C5-N7-C8	3.05	108.24	103.45
12	A	27	A2M	C5-N7-C8	3.04	108.23	103.45
12	A	99	A2M	C5-N7-C8	3.04	108.23	103.45
12	A	1081	PSU	C6-N1-C2	-3.03	119.88	122.69
12	A	1850	MA6	C2-N3-C4	3.01	119.19	111.83
12	A	1219	JMH	C1'-N1-C2	3.01	121.97	117.04
12	A	612	PSU	O2-C2-N1	-3.01	119.69	122.79
12	A	484	A2M	C5-C6-N6	-3.00	115.85	123.29
12	A	484	A2M	C5-N7-C8	2.98	108.14	103.45
12	A	1328	OMG	C2-N1-C6	-2.98	119.70	125.11
12	A	683	OMG	C2-N1-C6	-2.96	119.73	125.11
12	A	1851	MA6	C5-N7-C8	2.96	108.10	103.45
12	A	668	A2M	C5-N7-C8	2.94	108.07	103.45
12	A	159	A2M	N6-C6-N1	2.94	124.92	118.38
12	A	166	A2M	N6-C6-N1	2.93	124.90	118.38
12	A	116	OMU	O2-C2-N1	-2.93	118.99	122.80
12	A	668	A2M	C5-C6-N6	-2.92	116.05	123.29
12	A	159	A2M	C5-N7-C8	2.92	108.04	103.45
12	A	1678	A2M	N3-C4-N9	2.92	132.14	127.17
12	A	1850	MA6	C5-C4-N9	2.90	108.97	105.81
12	A	1031	A2M	C5-C6-N6	-2.88	116.15	123.29
12	A	27	A2M	N6-C6-N1	2.88	124.79	118.38
12	A	166	A2M	N3-C4-N9	2.86	132.03	127.17
12	A	601	OMG	C5-C6-N1	2.76	120.28	113.25
12	A	601	OMG	N2-C2-N1	2.75	122.57	116.76
12	A	1243	PSU	C6-C5-C4	2.74	120.03	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	683	OMG	C5-C6-N1	2.74	120.22	113.25
12	A	484	A2M	O4'-C1'-N9	2.72	113.32	108.09
12	A	644	OMG	C5-C6-N1	2.71	120.16	113.25
12	A	484	A2M	C4-C5-N7	-2.70	107.50	110.58
12	A	1328	OMG	C5-C6-N1	2.70	120.12	113.25
12	A	668	A2M	N6-C6-N1	2.69	124.37	118.38
12	A	1081	PSU	C6-C5-C4	2.69	119.99	118.17
12	A	1337	4AC	O7-C7-CM7	-2.67	117.29	122.05
12	A	668	A2M	C4-N9-C1'	2.67	132.88	126.63
12	A	1031	A2M	C4-N9-C8	2.66	108.53	105.74
12	A	1850	MA6	C4-C5-N7	-2.65	107.55	110.58
12	A	1081	PSU	O2-C2-N1	-2.63	120.08	122.79
12	A	644	OMG	N2-C2-N1	2.62	122.30	116.76
12	A	1842	4AC	C5-C4-N3	-2.62	118.50	122.60
12	A	159	A2M	C4-C5-N7	-2.62	107.59	110.58
12	A	27	A2M	N3-C4-N9	2.62	131.62	127.17
12	A	484	A2M	N6-C6-N1	2.62	124.20	118.38
12	A	1374	5MC	CM5-C5-C6	-2.61	119.31	122.85
12	A	159	A2M	C2'-C1'-N9	-2.61	109.45	113.75
12	A	1830	UR3	C6-N1-C2	-2.61	119.67	121.80
12	A	1219	JMH	C6-N1-C2	-2.60	119.67	121.80
12	A	1337	4AC	C6-C5-C4	2.59	120.12	117.00
12	A	1851	MA6	C4-C5-N7	-2.59	107.62	110.58
12	A	509	OMG	N9-C8-N7	-2.56	108.66	113.40
12	A	668	A2M	C4-C5-N7	-2.56	107.66	110.58
12	A	1031	A2M	C4-C5-N7	-2.55	107.66	110.58
12	A	683	OMG	C8-N7-C5	2.55	108.81	104.26
12	A	509	OMG	C5-C6-N1	2.55	119.74	113.25
12	A	1832	6MZ	C4-C5-N7	-2.54	107.68	110.58
12	A	1031	A2M	N6-C6-N1	2.53	124.02	118.38
12	A	27	A2M	C4-N9-C8	2.53	108.39	105.74
12	A	1328	OMG	N2-C2-N1	2.52	122.08	116.76
12	A	644	OMG	O6-C6-C5	-2.51	119.91	126.53
12	A	484	A2M	C3'-C2'-C1'	2.51	107.61	102.81
12	A	484	A2M	C5-C4-N9	2.50	108.53	105.81
12	A	1328	OMG	O6-C6-C5	-2.49	119.95	126.53
12	A	822	PSU	O2-C2-N1	-2.49	120.22	122.79
12	A	1490	OMG	N2-C2-N1	2.47	121.98	116.76
12	A	27	A2M	C4-C5-N7	-2.46	107.77	110.58
12	A	484	A2M	N3-C4-N9	2.46	131.35	127.17
12	A	119	PSU	O2-C2-N1	-2.46	120.25	122.79
12	A	166	A2M	C4-C5-N7	-2.46	107.77	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	822	PSU	C6-C5-C4	2.45	119.83	118.17
12	A	159	A2M	N3-C4-N9	2.42	131.28	127.17
12	A	601	OMG	O6-C6-C5	-2.42	120.16	126.53
12	A	1490	OMG	C5-C6-N1	2.41	119.39	113.25
12	A	159	A2M	C5-C4-N9	2.41	108.44	105.81
12	A	668	A2M	N3-C4-N9	2.40	131.25	127.17
12	A	668	A2M	C5-C4-N9	2.39	108.42	105.81
12	A	166	A2M	C4-N9-C8	2.37	108.23	105.74
12	A	822	PSU	O4'-C1'-C2'	2.36	108.42	105.15
12	A	601	OMG	C5-C4-N9	2.36	109.88	105.66
12	A	814	5MU	C6-N1-C2	-2.36	118.95	121.30
12	A	823	PSU	C6-N1-C2	-2.35	120.51	122.69
12	A	683	OMG	O6-C6-C5	-2.35	120.32	126.53
12	A	166	A2M	O4'-C1'-N9	2.35	112.60	108.09
12	A	1490	OMG	N1-C2-N3	-2.35	119.02	123.32
12	A	27	A2M	C2'-C1'-N9	-2.32	109.94	113.75
12	A	683	OMG	C2'-C1'-N9	-2.31	109.85	114.24
12	A	644	OMG	C8-N7-C5	2.31	108.37	104.26
12	A	1832	6MZ	N3-C4-N9	2.29	131.07	127.17
12	A	1328	OMG	C8-N7-C5	2.29	108.33	104.26
12	A	1031	A2M	N3-C4-N9	2.28	131.05	127.17
12	A	1490	OMG	O6-C6-C5	-2.28	120.51	126.53
12	A	683	OMG	C4-C5-N7	-2.28	107.06	110.67
12	A	1490	OMG	C8-N7-C5	2.28	108.32	104.26
12	A	601	OMG	C8-N7-C5	2.27	108.31	104.26
12	A	99	A2M	C4-C5-N7	-2.27	107.98	110.58
12	A	668	A2M	O4'-C1'-N9	-2.27	103.73	108.09
12	A	612	PSU	O4'-C1'-C2'	2.27	108.29	105.15
12	A	1832	6MZ	C5-C4-N9	2.24	108.25	105.81
12	A	1490	OMG	C2-N1-C6	-2.24	121.05	125.11
12	A	116	OMU	C6-N1-C2	-2.23	118.28	121.00
12	A	1031	A2M	C2'-C1'-N9	-2.23	110.08	113.75
12	A	644	OMG	C5-C4-N9	2.23	109.64	105.66
12	A	509	OMG	O6-C6-C5	-2.22	120.67	126.53
12	A	644	OMG	C4-C5-N7	-2.20	107.18	110.67
12	A	1832	6MZ	C4-N9-C8	2.20	108.04	105.74
12	A	683	OMG	N2-C2-N1	2.19	121.39	116.76
12	A	823	PSU	C5-C4-N3	2.19	121.37	116.55
12	A	601	OMG	C4-C5-N7	-2.18	107.21	110.67
12	A	1678	A2M	C4-C5-N7	-2.17	108.11	110.58
12	A	1031	A2M	C5-C4-N9	2.16	108.17	105.81
12	A	509	OMG	C5-C4-N9	2.16	109.52	105.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1842	4AC	C6-C5-C4	2.16	119.60	117.00
12	A	601	OMG	C6-C5-N7	2.15	134.21	130.29
12	A	159	A2M	C4-N9-C8	2.14	107.99	105.74
12	A	1328	OMG	C4-C5-N7	-2.14	107.28	110.67
12	A	1830	UR3	C1'-N1-C2	2.14	120.54	117.04
12	A	668	A2M	C3'-C2'-C1'	2.12	106.87	102.81
12	A	166	A2M	C2'-C1'-N9	-2.12	110.27	113.75
12	A	99	A2M	C4-N9-C8	2.11	107.96	105.74
12	A	99	A2M	C6-C5-C4	2.10	120.05	117.18
12	A	1328	OMG	C5-C4-N9	2.10	109.42	105.66
12	A	484	A2M	O3'-C3'-C2'	-2.09	105.34	111.19
12	A	166	A2M	C5'-C4'-C3'	-2.06	107.79	115.21
12	A	1490	OMG	C5-C4-N9	2.06	109.34	105.66
12	A	159	A2M	O4'-C1'-N9	2.04	112.01	108.09
12	A	644	OMG	C6-C5-N7	2.04	134.00	130.29
12	A	683	OMG	C6-C5-N7	2.04	134.00	130.29
12	A	166	A2M	C5-C4-N9	2.02	108.01	105.81
12	A	683	OMG	C5-C4-N9	2.01	109.26	105.66
12	A	1031	A2M	O4'-C1'-N9	2.01	111.95	108.09
12	A	121	OMU	O2-C2-N1	-2.00	120.19	122.80
12	A	683	OMG	N1-C2-N3	-2.00	119.66	123.32

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	166	A2M	O4'-C4'-C5'-O5'
12	A	166	A2M	C3'-C4'-C5'-O5'
12	A	823	PSU	O4'-C1'-C5-C4
12	A	823	PSU	O4'-C1'-C5-C6
12	A	1832	6MZ	N1-C6-N6-C9
12	A	1851	MA6	C5-C6-N6-C10
12	A	99	A2M	O4'-C4'-C5'-O5'
12	A	159	A2M	O4'-C4'-C5'-O5'
12	A	159	A2M	C3'-C4'-C5'-O5'
12	A	683	OMG	O4'-C4'-C5'-O5'
12	A	668	A2M	O4'-C4'-C5'-O5'
12	A	822	PSU	O4'-C4'-C5'-O5'
12	A	1851	MA6	N1-C6-N6-C10
12	A	668	A2M	C3'-C4'-C5'-O5'
12	A	822	PSU	C3'-C4'-C5'-O5'
12	A	174	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
12	A	683	OMG	C3'-C4'-C5'-O5'
12	A	174	OMC	O4'-C4'-C5'-O5'
12	A	99	A2M	C3'-C4'-C5'-O5'
12	A	1337	4AC	O7-C7-N4-C4
12	A	1337	4AC	CM7-C7-N4-C4
12	A	1832	6MZ	C5-C6-N6-C9
12	A	644	OMG	C4'-C5'-O5'-P
12	A	1081	PSU	C4'-C5'-O5'-P
12	A	1490	OMG	C4'-C5'-O5'-P
12	A	174	OMC	C4'-C5'-O5'-P
12	A	1851	MA6	C4'-C5'-O5'-P
12	A	1703	OMC	O4'-C4'-C5'-O5'
12	A	1851	MA6	C5-C6-N6-C9

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1850	MA6	2	0
12	A	1851	MA6	2	0
12	A	823	PSU	1	0
12	A	1678	A2M	1	0
12	A	1374	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 110 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	SPD	A	2005	-	9,9,9	0.31	0	8,8,8	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SPD	A	2005	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

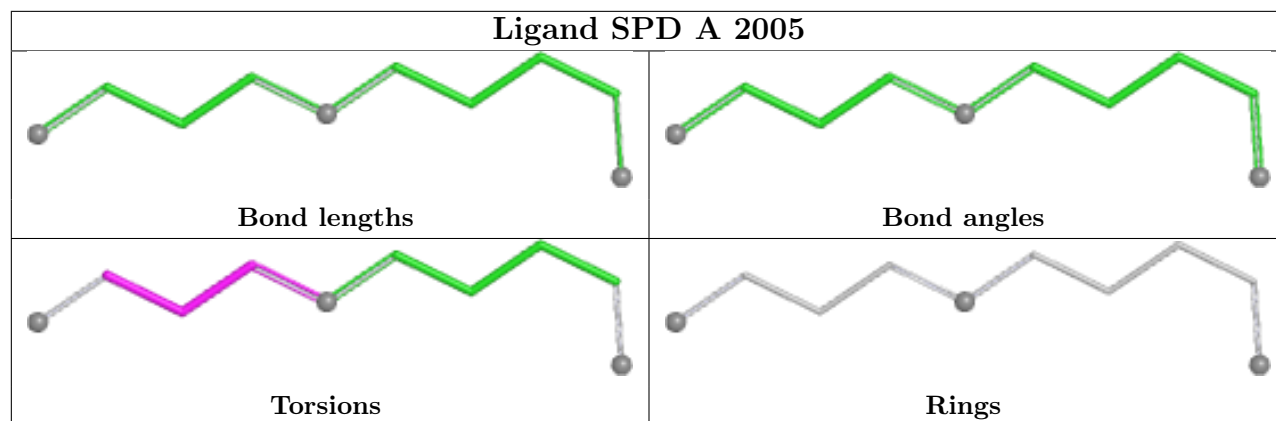
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	A	2005	SPD	C8-C7-N6-C5
40	A	2005	SPD	N6-C7-C8-C9
40	A	2005	SPD	C7-C8-C9-N10

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	225:G	O3'	287:U	P	7.96

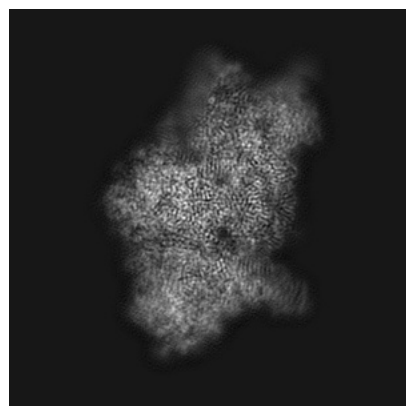
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44641. These allow visual inspection of the internal detail of the map and identification of artifacts.

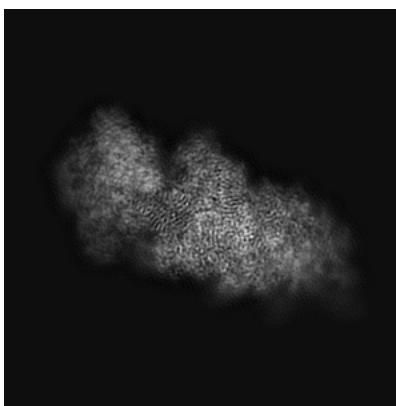
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

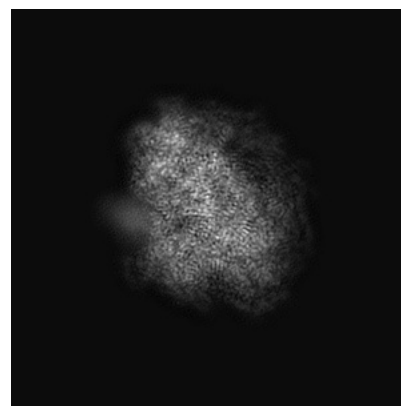
6.1.1 Primary map



X

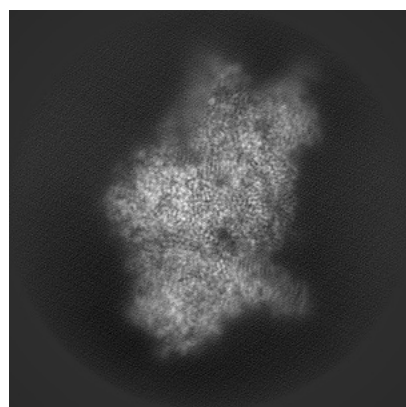


Y

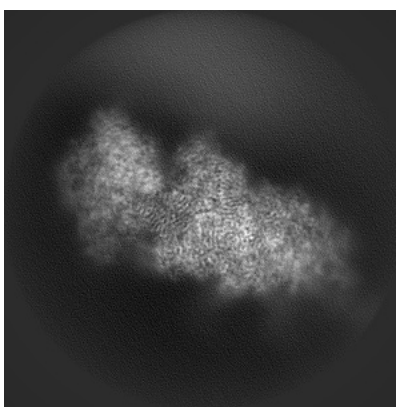


Z

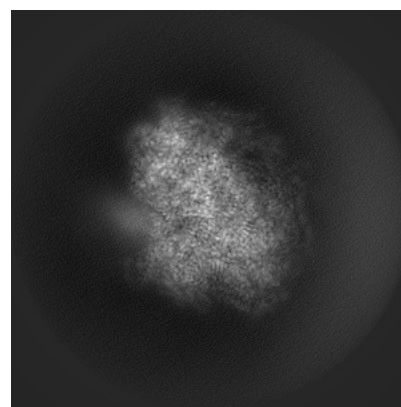
6.1.2 Raw map



X



Y

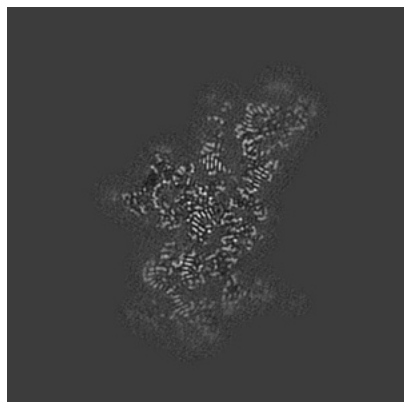


Z

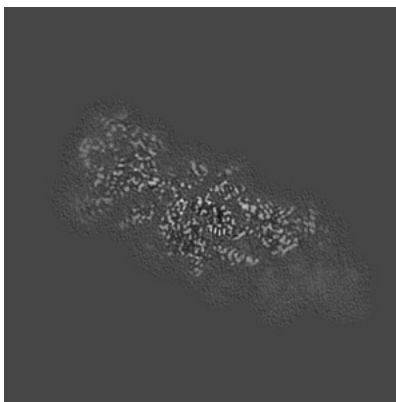
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

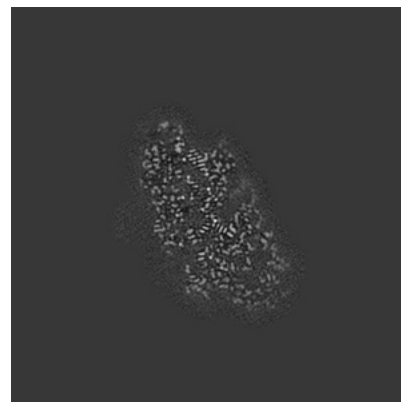
6.2.1 Primary map



X Index: 200

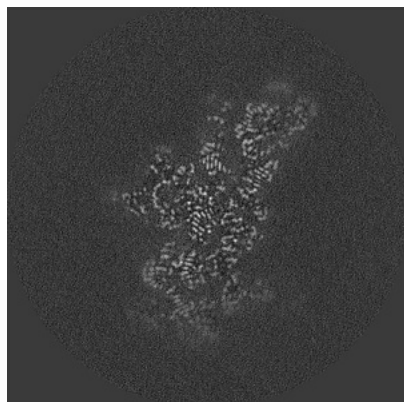


Y Index: 200

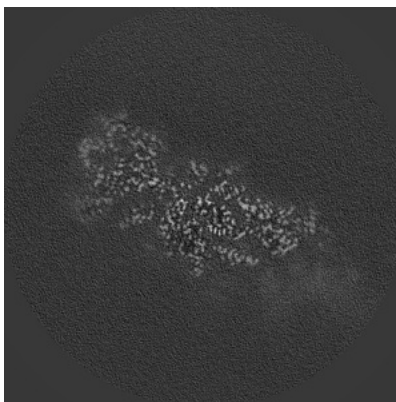


Z Index: 200

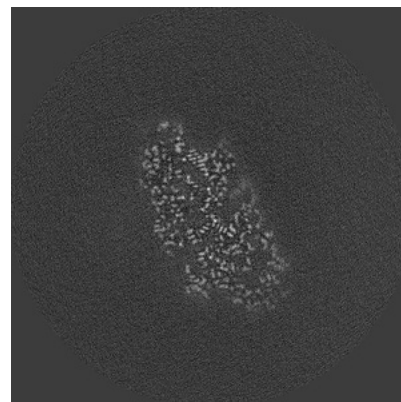
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

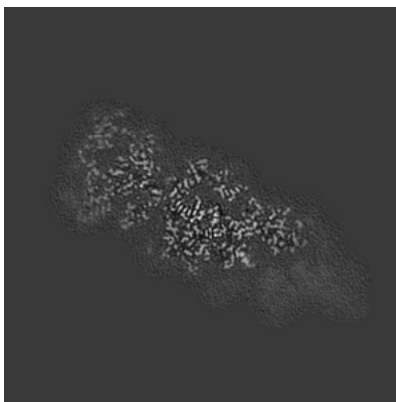
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

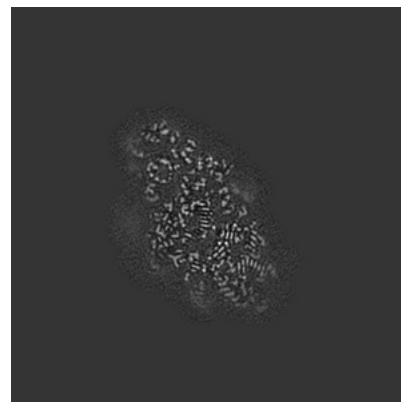
6.3.1 Primary map



X Index: 193

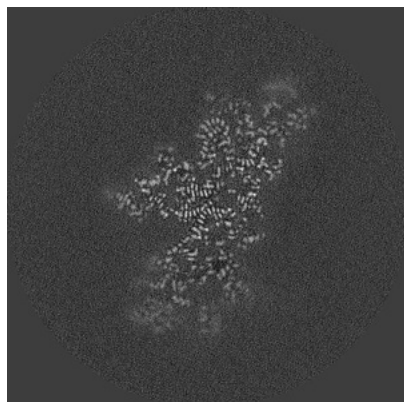


Y Index: 195

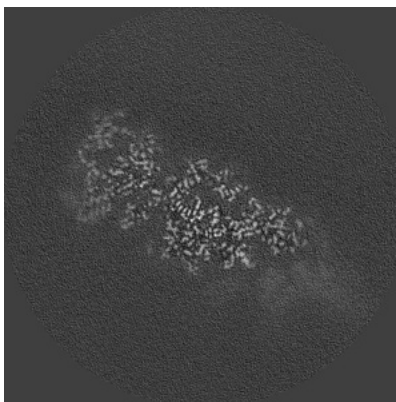


Z Index: 216

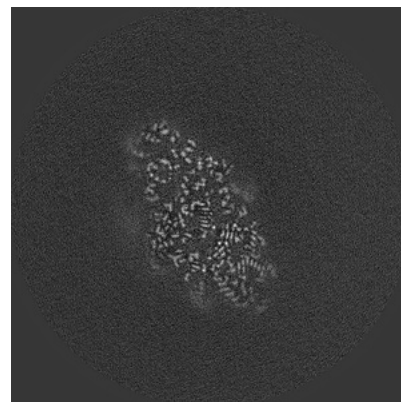
6.3.2 Raw map



X Index: 193



Y Index: 195

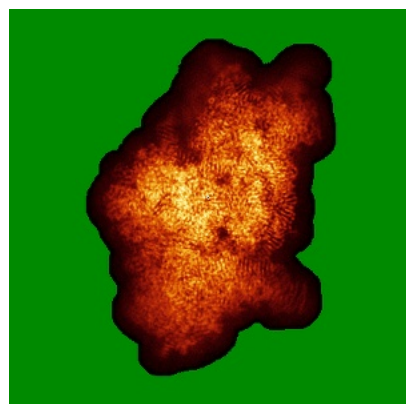


Z Index: 216

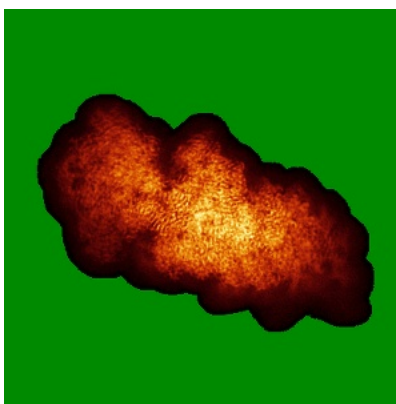
The images above show the largest variance slices of the map in three orthogonal directions.

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

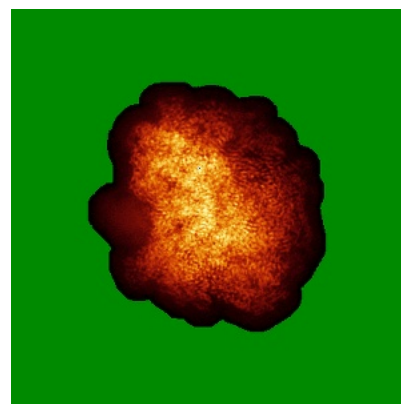
6.4.1 Primary map



X

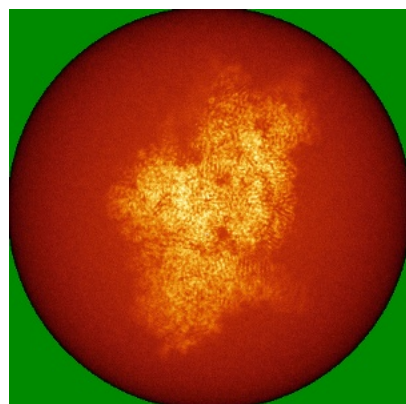


Y

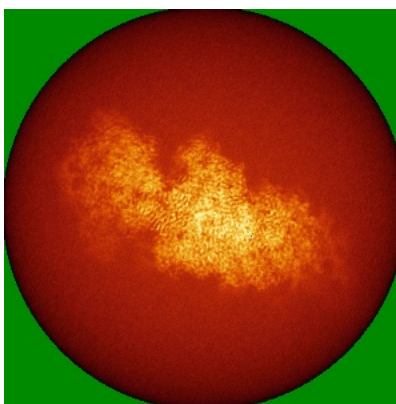


Z

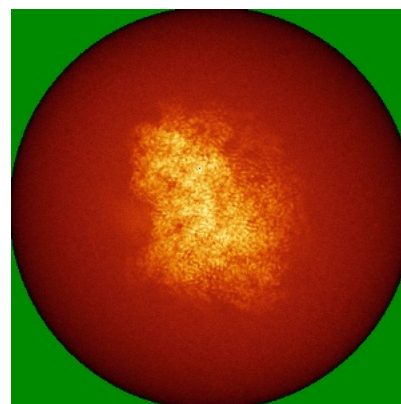
6.4.2 Raw map



X



Y

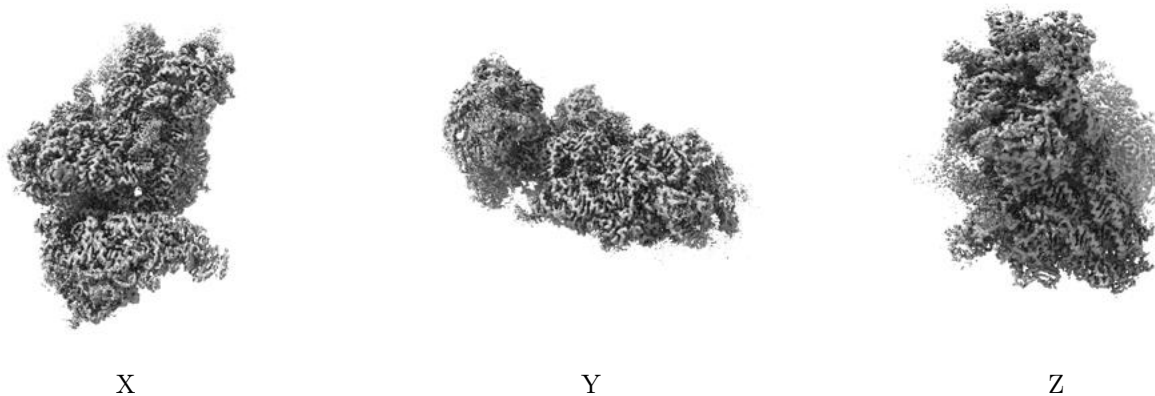


Z

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.

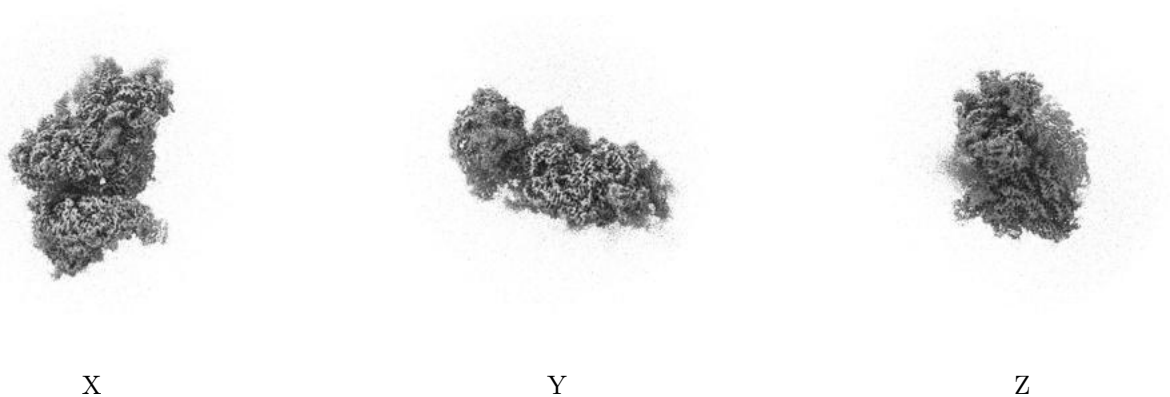
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

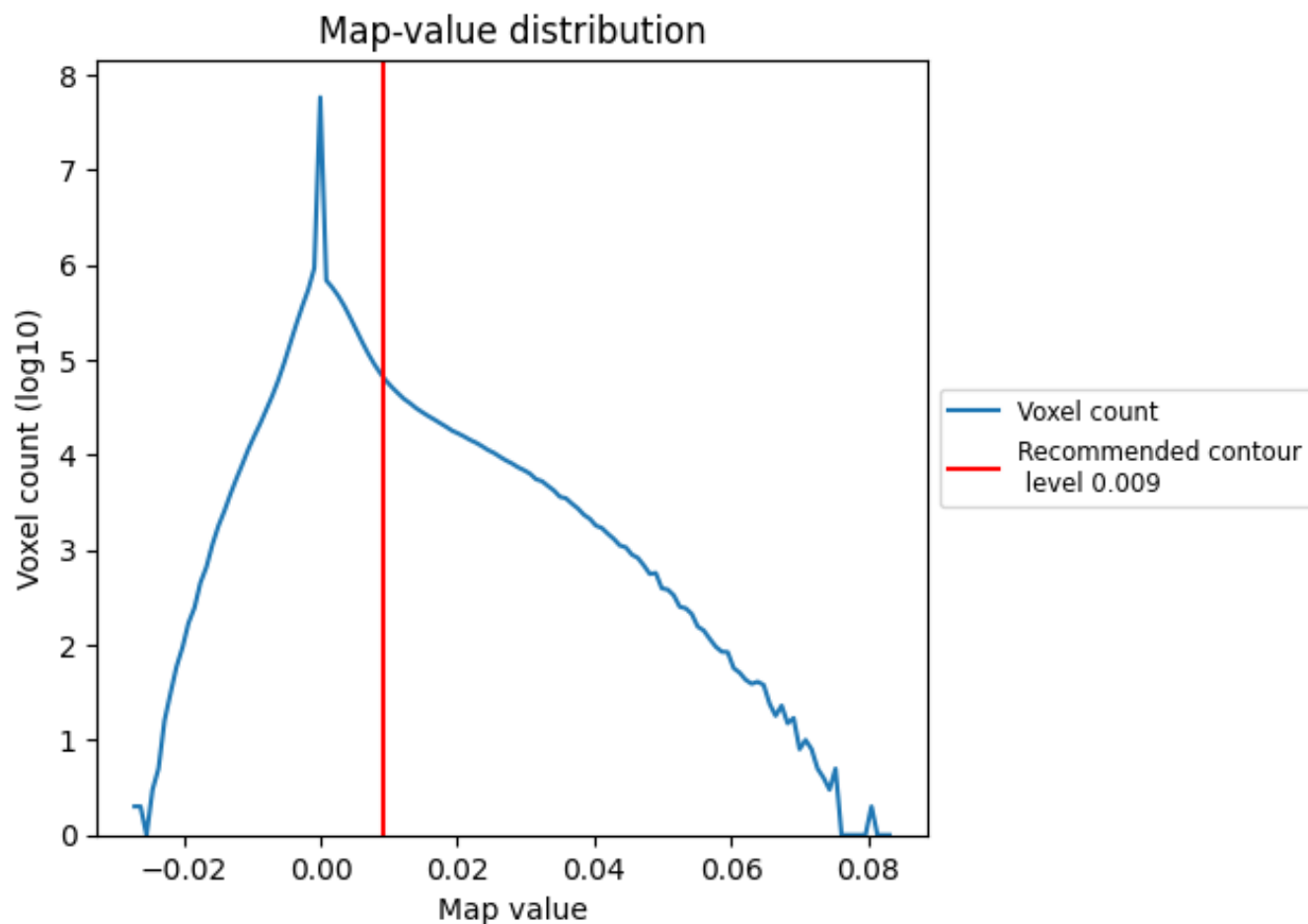
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

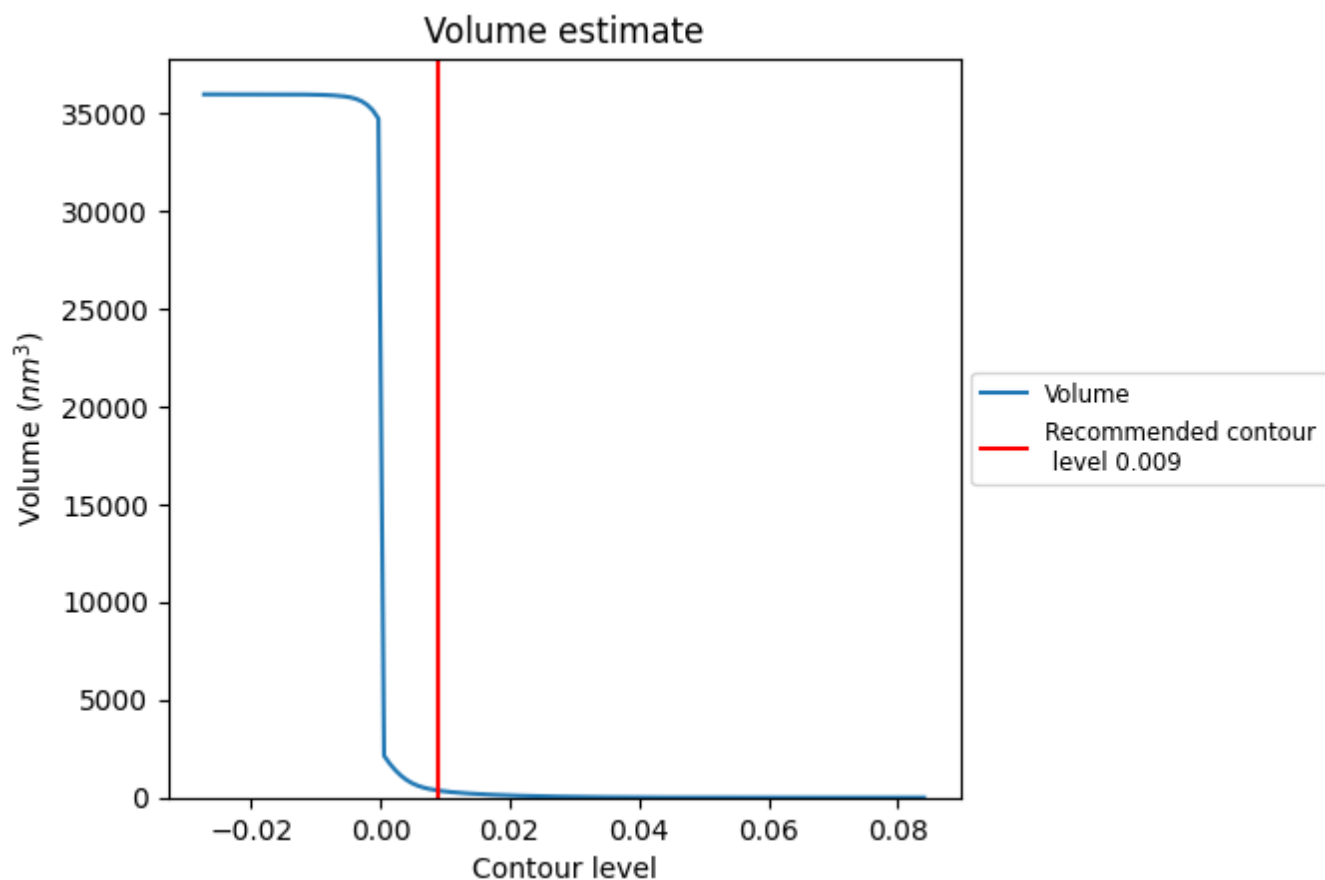
This section contains the results of statistical analysis of the map.

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.

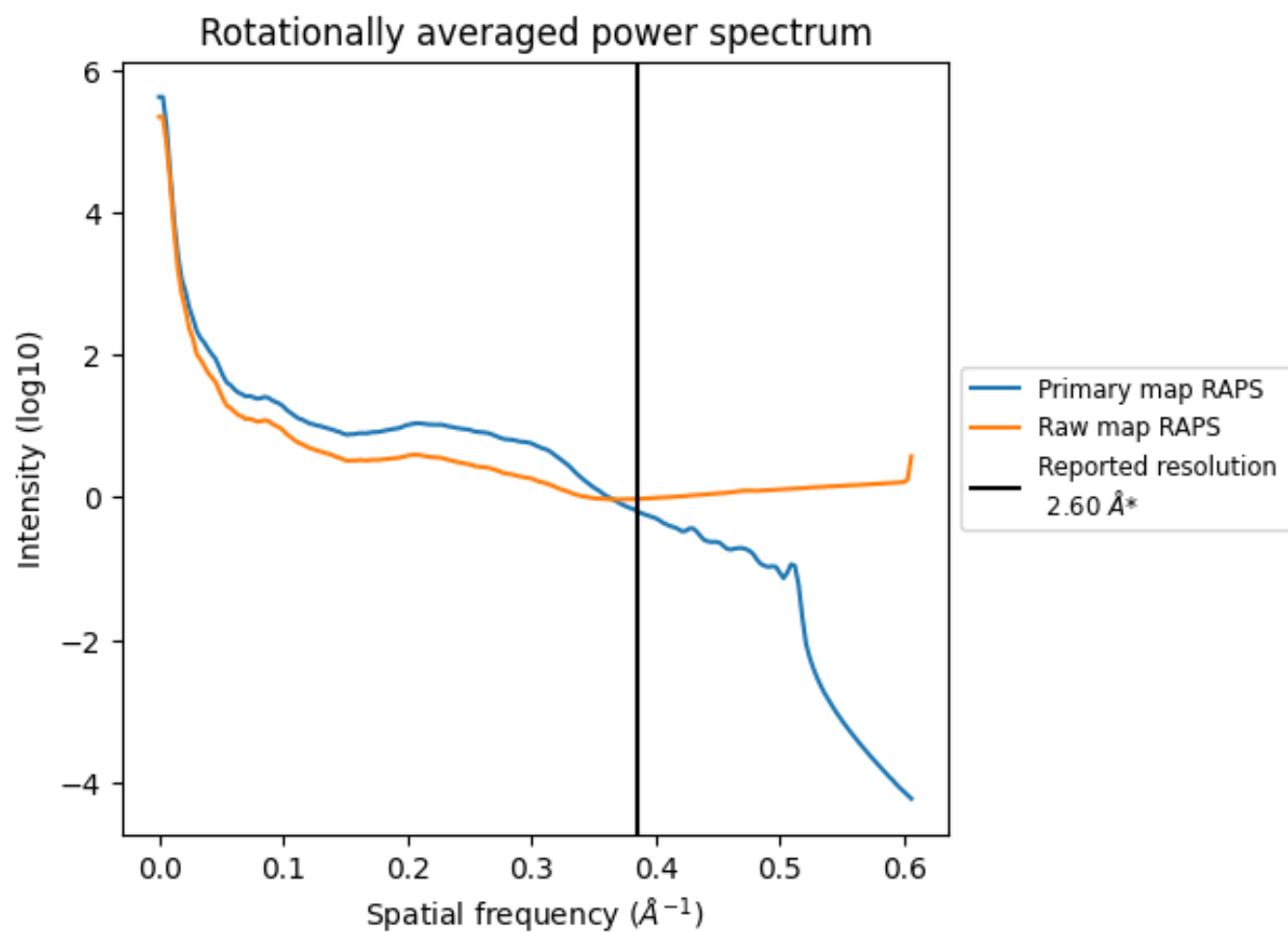
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 359 nm^3 ; this corresponds to an approximate mass of 324 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 ⓘ

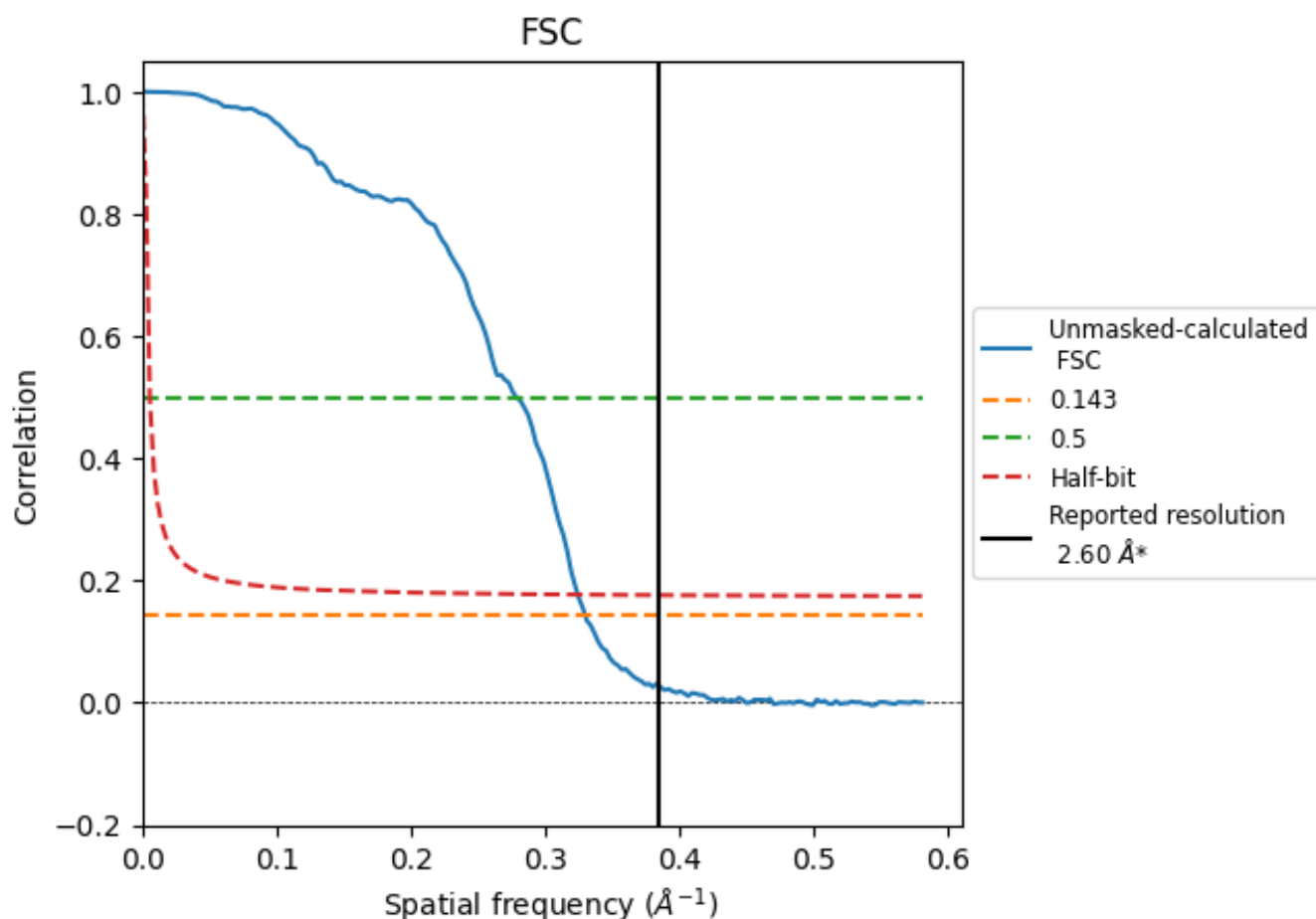


*Reported resolution corresponds to spatial frequency of $0.385 \text{ \AA}^{-1}$

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

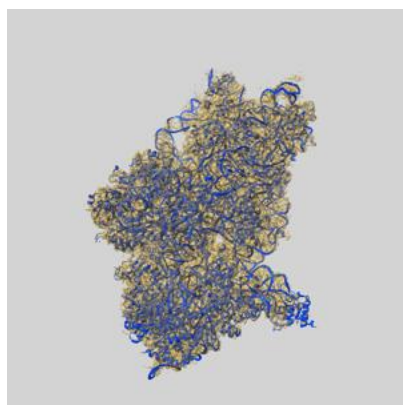
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.03	3.59	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.6 by more than 10 %

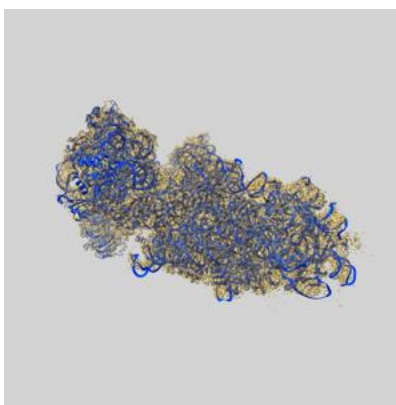
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44641 and PDB model 9BKD. Per-residue inclusion information can be found in section [3](#) on page [12](#).

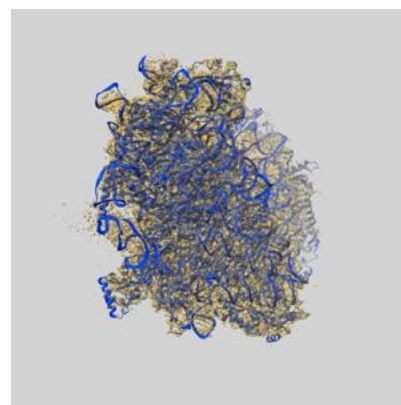
9.1 Map-model overlay [i](#)



X



Y



Z

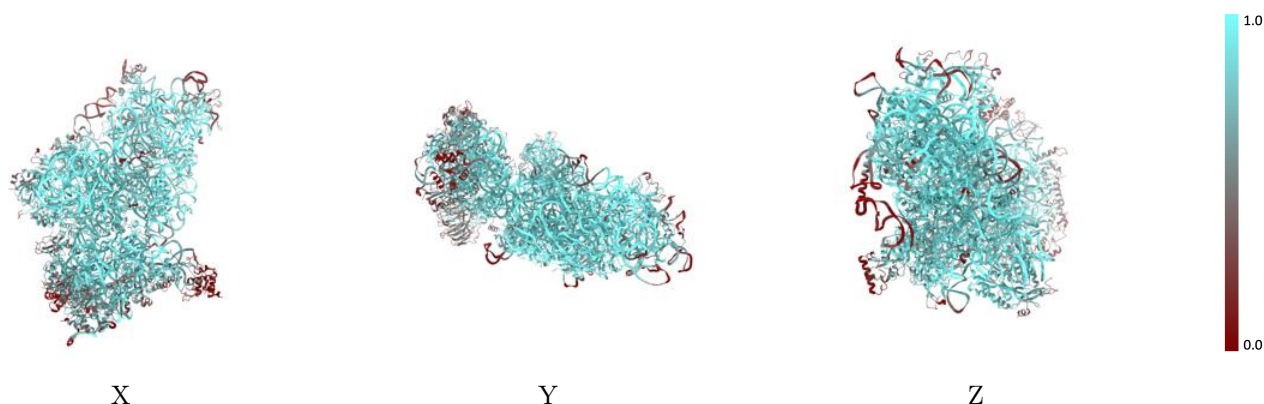
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



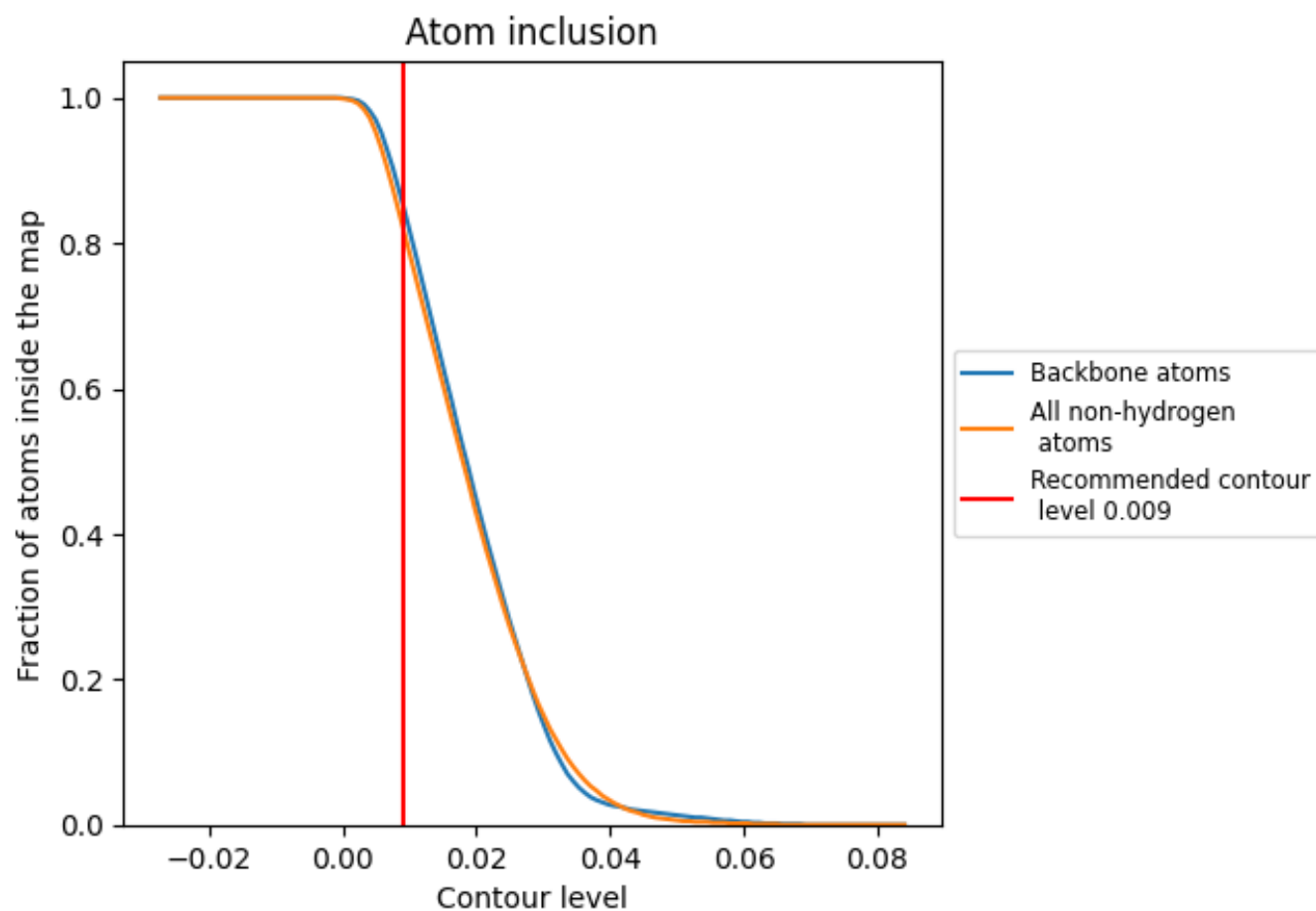
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8230	 0.6140
9	 0.7750	 0.6240
A	 0.8950	 0.6180
B	 0.9050	 0.6690
C	 0.9580	 0.6850
D	 0.9360	 0.6820
E	 0.9560	 0.6920
F	 0.9170	 0.6800
G	 0.5900	 0.5580
H	 0.8040	 0.6290
I	 0.8810	 0.6640
J	 0.9670	 0.6990
K	 0.9220	 0.6740
L	 0.9330	 0.6870
M	 0.7400	 0.6080
N	 0.9370	 0.6760
O	 0.7890	 0.6270
P	 0.8530	 0.6370
Q	 0.9170	 0.6750
R	 0.8320	 0.6290
S	 0.7090	 0.5810
T	 0.9110	 0.6650
U	 0.8690	 0.6330
V	 0.7120	 0.5820
Y	 0.7760	 0.6070
Z	 0.8090	 0.6300
a	 0.7190	 0.5790
b	 0.6080	 0.5600
c	 0.4520	 0.5040
d	 0.7030	 0.5830
e	 0.1780	 0.4490
f	 0.4910	 0.5240
h	 0.6490	 0.5680
i	 0.9280	 0.6720
k	 0.1470	 0.3940



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Chain	Atom inclusion	Q-score
m	 0.0630	 0.3490
n	 0.5560	 0.5180