



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:29 AM UTC

PDB ID : 3J5Y / pdb_00003j5y
EMDB ID : EMD-5801
Title : Structure of the mammalian ribosomal pre-termination complex associated with eRF1-eRF3-GDPNP
Authors : des Georges, A.; Hashem, Y.; Unbehaun, A.; Grassucci, R.A.; Taylor, D.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2013-11-21
Resolution : 9.70 Å (reported)
Based on initial models : 3VMF, 1R5O, 3E1Y, 1R5B, 2KTU

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:

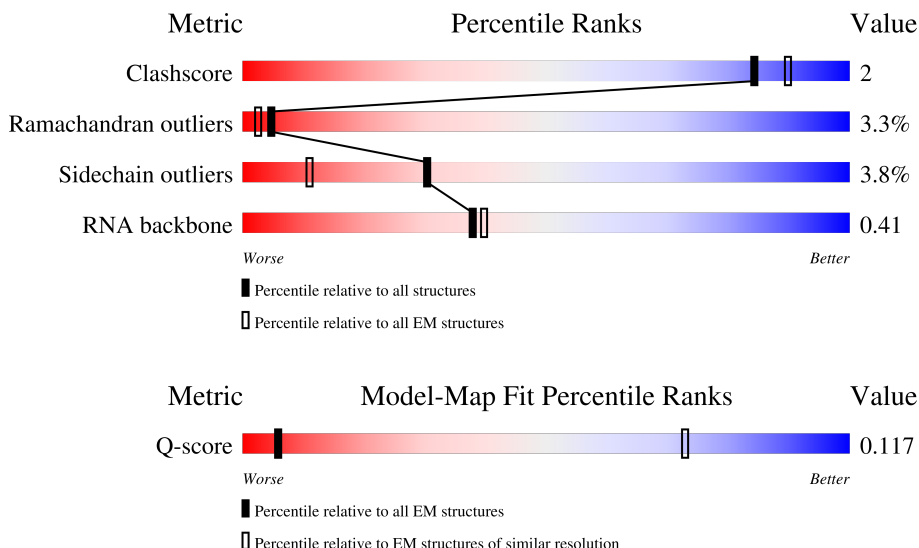
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	165 (9.20 - 10.20)

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

Mol	Chain	Length	Quality of chain
1	A	414	
2	B	428	
3	C	10	

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Mol	Chain	Length	Quality of chain
4	D	88	7% 9% 41% 25% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3269	2080	557	621	11		

- Molecule 2 is a protein called Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3367	2144	578	624	21		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	369	ILE	ASN	conflict	UNP P15170
B	389	SER	ASN	conflict	UNP P15170
B	407	ILE	LEU	conflict	UNP P15170
B	418	THR	ILE	conflict	UNP P15170
B	436	ILE	VAL	conflict	UNP P15170

- Molecule 3 is a RNA chain called 5'-R(*AP*UP*UP*GP*UP*AP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	10	Total	C	N	O	P	0	0
			212	97	41	65	9		

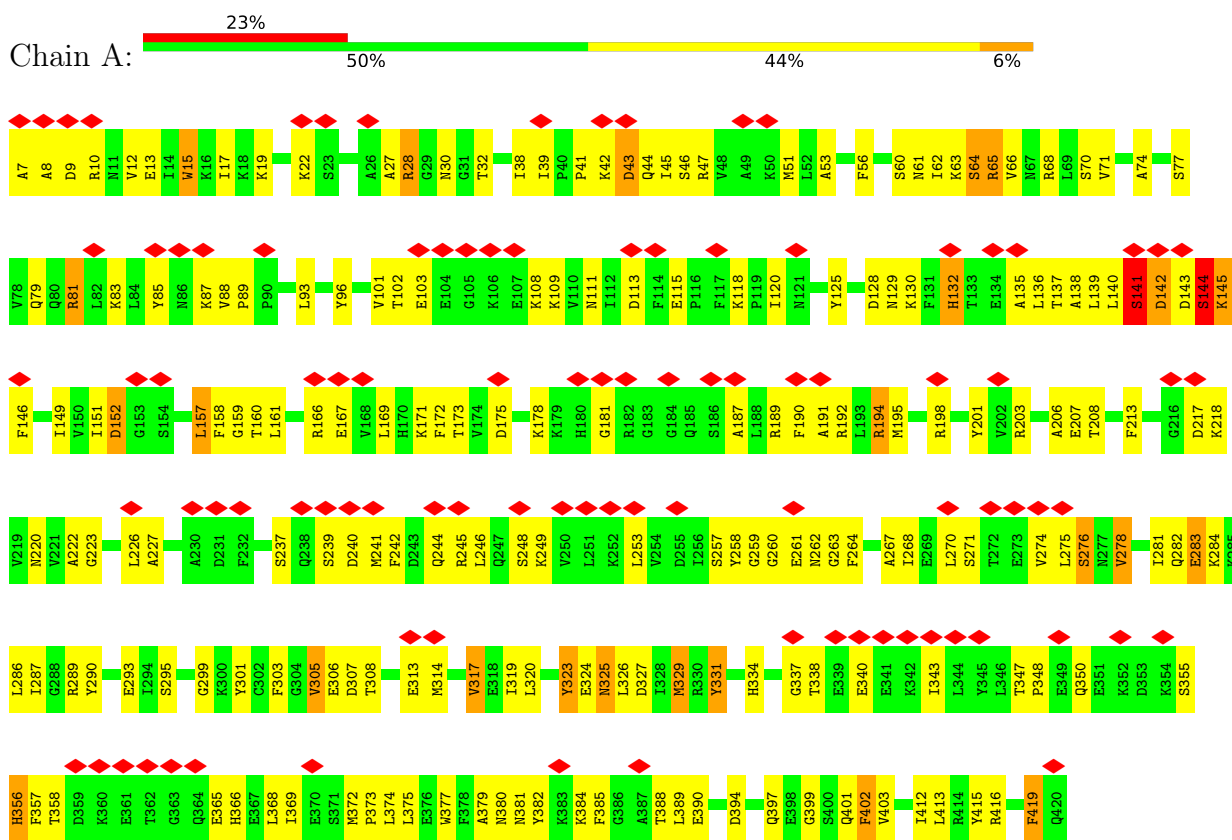
- Molecule 4 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	P	0	0
			1876	836	339	614	87		

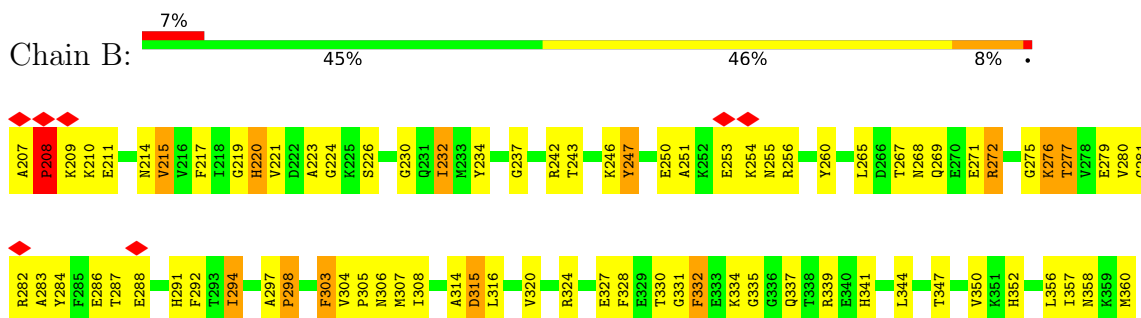
3 Residue-property plots

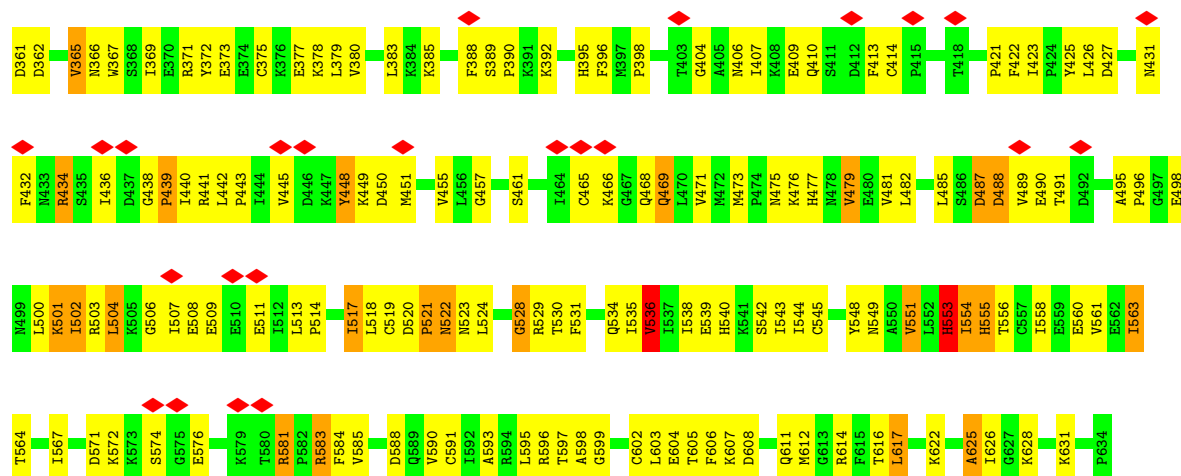
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



- Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

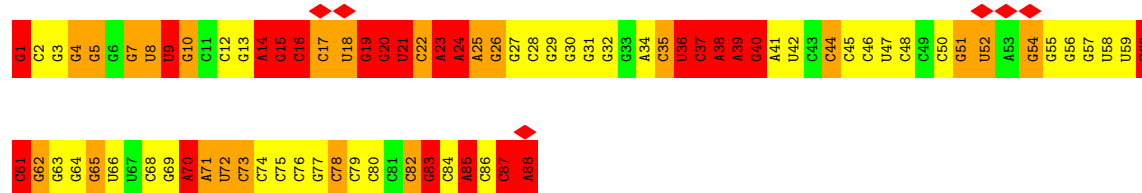




- Molecule 3: 5'-R(*AP*UP*UP*GP*UP*AP*AP*AP*AP*A)-3'



- Molecule 4: tRNA-Leu



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each Particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	456.0, 456.0, 456.0	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.13	88/3322 (2.6%)	2.38	194/4466 (4.3%)
2	B	2.11	105/3434 (3.1%)	2.44	219/4630 (4.7%)
3	C	2.17	6/238 (2.5%)	2.01	7/369 (1.9%)
4	D	2.04	50/2095 (2.4%)	1.86	69/3266 (2.1%)
All	All	2.10	249/9089 (2.7%)	2.27	489/12731 (3.8%)

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
1	A	0	17
2	B	0	23
3	C	0	7
4	D	0	42
All	All	0	89

All (249) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ASN	CA-C	13.36	1.60	1.52
2	B	558	ILE	CA-C	9.61	1.65	1.52
1	A	366	HIS	N-CA	9.00	1.57	1.45
4	D	14	A	P-O5'	-9.00	1.46	1.59
1	A	125	TYR	CA-CB	8.84	1.67	1.53
1	A	227	ALA	CA-C	8.73	1.63	1.52
2	B	528	GLY	CA-C	-8.59	1.42	1.51
4	D	22	C	O3'-P	-8.59	1.48	1.61
1	A	385	PHE	C-N	8.54	1.41	1.33
1	A	313	GLU	CA-CB	8.21	1.67	1.53
1	A	415	TYR	CA-C	8.14	1.62	1.52
3	C	99	A	C3'-C2'	8.13	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	485	LEU	CA-C	-7.98	1.42	1.53
1	A	207	GLU	N-CA	7.94	1.55	1.46
2	B	443	PRO	C-N	7.79	1.42	1.33
4	D	22	C	P-O5'	-7.77	1.48	1.59
1	A	87	LYS	CA-CB	7.77	1.66	1.53
1	A	88	VAL	CA-CB	-7.63	1.44	1.54
2	B	508	GLU	N-CA	-7.62	1.36	1.45
2	B	608	ASP	CA-C	7.60	1.62	1.52
2	B	536	VAL	CA-C	7.50	1.62	1.52
1	A	192	ARG	CD-NE	7.47	1.56	1.46
2	B	625	ALA	N-CA	-7.34	1.37	1.46
3	C	95	A	C2'-C1'	-7.32	1.42	1.53
1	A	89	PRO	CA-C	7.30	1.58	1.52
2	B	327	GLU	CA-C	7.25	1.62	1.52
2	B	468	GLN	CA-C	-7.25	1.44	1.52
1	A	381	ASN	C-N	7.13	1.43	1.34
2	B	347	THR	CA-C	7.13	1.62	1.52
1	A	167	GLU	C-O	-7.10	1.15	1.24
1	A	17	ILE	C-N	7.04	1.42	1.33
1	A	258	TYR	CA-C	-7.04	1.44	1.52
4	D	31	G	P-O5'	-7.02	1.49	1.59
1	A	263	GLY	CA-C	7.01	1.61	1.51
2	B	277	THR	C-N	6.99	1.43	1.33
2	B	339	ARG	CD-NE	6.99	1.56	1.46
1	A	9	ASP	CA-CB	6.98	1.65	1.53
1	A	324	GLU	CA-CB	6.92	1.64	1.53
2	B	406	ASN	N-CA	6.90	1.54	1.46
1	A	402	PHE	C-N	6.89	1.42	1.33
2	B	553	HIS	ND1-CE1	6.87	1.39	1.32
4	D	60	C	P-O5'	-6.87	1.49	1.59
2	B	625	ALA	C-N	6.85	1.42	1.33
2	B	450	ASP	CA-CB	6.84	1.65	1.53
2	B	427	ASP	N-CA	-6.83	1.38	1.46
2	B	390	PRO	N-CA	-6.80	1.40	1.46
1	A	317	VAL	N-CA	6.74	1.54	1.46
1	A	401	GLN	N-CA	-6.74	1.37	1.46
1	A	143	ASP	N-CA	-6.72	1.37	1.45
1	A	308	THR	N-CA	-6.72	1.38	1.46
2	B	631	LYS	CA-CB	6.71	1.63	1.53
2	B	404	GLY	N-CA	-6.69	1.35	1.45
2	B	626	ILE	CA-CB	-6.67	1.46	1.54
4	D	64	G	O5'-C5'	6.67	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLY	CA-C	-6.64	1.43	1.51
2	B	548	TYR	CA-C	6.64	1.61	1.52
1	A	64	SER	C-N	6.58	1.43	1.33
2	B	611	GLN	CA-C	6.55	1.61	1.52
1	A	307	ASP	N-CA	6.54	1.54	1.46
4	D	9	U	C5'-C4'	6.52	1.61	1.51
4	D	21	U	O5'-C5'	6.52	1.52	1.42
2	B	426	LEU	CA-C	6.52	1.61	1.52
2	B	442	LEU	CA-C	6.51	1.60	1.52
2	B	380	VAL	C-O	-6.51	1.19	1.24
1	A	248	SER	CA-CB	6.50	1.62	1.53
3	C	91	U	C4'-O4'	-6.49	1.36	1.45
1	A	372	MET	CA-C	6.44	1.60	1.52
4	D	82	C	C2'-C1'	-6.43	1.43	1.53
1	A	191	ALA	N-CA	-6.42	1.38	1.46
2	B	256	ARG	CA-CB	6.38	1.63	1.53
4	D	15	G	P-O5'	-6.36	1.50	1.59
2	B	614	ARG	CA-CB	6.34	1.62	1.53
2	B	284	TYR	CA-C	6.34	1.60	1.52
1	A	253	LEU	CA-CB	6.34	1.63	1.53
1	A	28	ARG	NE-CZ	6.33	1.40	1.33
1	A	416	ARG	CA-C	-6.33	1.44	1.52
2	B	251	ALA	CA-C	-6.33	1.44	1.52
1	A	257	SER	CA-C	-6.33	1.44	1.52
2	B	315	ASP	CA-CB	6.31	1.64	1.53
1	A	189	ARG	CD-NE	6.28	1.55	1.46
2	B	220	HIS	ND1-CE1	6.27	1.38	1.32
3	C	91	U	O3'-P	-6.27	1.51	1.61
4	D	18	U	C4'-C3'	6.26	1.62	1.53
1	A	189	ARG	CA-CB	6.23	1.63	1.53
4	D	27	G	C1'-N9	6.22	1.57	1.48
4	D	37	C	C3'-O3'	6.22	1.51	1.42
2	B	534	GLN	CA-CB	-6.22	1.44	1.53
2	B	330	THR	CA-C	6.21	1.60	1.52
2	B	426	LEU	N-CA	-6.20	1.38	1.46
2	B	520	ASP	N-CA	-6.18	1.37	1.45
4	D	45	C	P-O5'	-6.18	1.50	1.59
4	D	61	C	O3'-P	-6.17	1.51	1.61
4	D	41	A	O5'-C5'	6.15	1.51	1.42
1	A	140	LEU	C-N	6.12	1.42	1.33
1	A	158	PHE	CA-C	-6.12	1.45	1.52
1	A	198	ARG	CA-CB	6.11	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	7	G	C5'-C4'	6.10	1.60	1.51
2	B	352	HIS	CD2-NE2	6.08	1.44	1.37
4	D	75	C	C3'-O3'	6.08	1.51	1.42
3	C	90	A	O4'-C1'	-6.07	1.32	1.41
2	B	500	LEU	N-CA	-6.06	1.38	1.45
2	B	477	HIS	C-N	6.05	1.41	1.33
2	B	628	LYS	CA-CB	6.01	1.62	1.53
1	A	145	LYS	CA-CB	6.00	1.63	1.53
2	B	602	CYS	CA-C	-5.98	1.45	1.52
1	A	96	TYR	CA-C	5.98	1.59	1.52
1	A	101	VAL	CA-C	5.95	1.60	1.52
4	D	51	G	C4'-C3'	5.94	1.61	1.52
1	A	178	LYS	N-CA	-5.93	1.39	1.46
4	D	72	U	C1'-N1	5.93	1.56	1.47
4	D	22	C	C3'-O3'	5.92	1.52	1.43
4	D	56	G	C1'-N9	5.91	1.56	1.48
4	D	87	C	P-O5'	5.90	1.68	1.59
2	B	265	LEU	CA-CB	5.89	1.62	1.53
2	B	291	HIS	ND1-CE1	5.87	1.38	1.32
2	B	286	GLU	N-CA	-5.86	1.39	1.46
1	A	65	ARG	CA-CB	5.86	1.63	1.53
1	A	173	THR	N-CA	5.86	1.53	1.45
2	B	315	ASP	C-N	5.86	1.41	1.33
4	D	35	C	O5'-C5'	5.86	1.51	1.42
2	B	479	VAL	CA-CB	-5.84	1.48	1.55
4	D	66	U	O3'-P	-5.84	1.52	1.61
1	A	375	LEU	CA-C	5.83	1.60	1.52
2	B	581	ARG	CA-C	5.82	1.60	1.52
1	A	195	MET	N-CA	5.82	1.53	1.46
2	B	352	HIS	ND1-CE1	5.82	1.38	1.32
4	D	24	A	C1'-N9	-5.81	1.39	1.48
1	A	45	ILE	CA-CB	-5.81	1.46	1.54
2	B	389	SER	CA-C	-5.78	1.46	1.53
2	B	590	VAL	CA-C	5.77	1.59	1.52
2	B	407	ILE	CB-CG1	5.75	1.65	1.53
4	D	15	G	C5'-C4'	5.75	1.59	1.51
4	D	32	G	P-O5'	-5.75	1.51	1.59
4	D	17	C	C4'-C3'	5.74	1.61	1.52
1	A	278	VAL	C-N	5.74	1.41	1.33
2	B	396	PHE	N-CA	-5.71	1.39	1.46
2	B	477	HIS	CG-CD2	5.70	1.42	1.35
4	D	72	U	O4'-C1'	-5.68	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	ALA	C-N	5.68	1.41	1.33
4	D	56	G	O5'-C5'	5.67	1.50	1.42
2	B	286	GLU	C-O	-5.67	1.17	1.24
1	A	102	THR	CA-CB	5.66	1.61	1.53
2	B	441	ARG	CA-C	-5.66	1.45	1.52
1	A	306	GLU	CA-CB	5.64	1.62	1.53
2	B	498	GLU	CA-C	5.64	1.60	1.52
4	D	36	U	C3'-O3'	5.64	1.50	1.42
4	D	62	G	C2'-C1'	-5.63	1.45	1.53
2	B	279	GLU	CA-C	5.62	1.59	1.52
4	D	63	G	P-O5'	-5.62	1.51	1.59
4	D	79	C	C2'-C1'	-5.61	1.45	1.53
4	D	19	G	P-O5'	-5.60	1.51	1.59
4	D	16	C	C3'-O3'	-5.59	1.34	1.43
2	B	334	LYS	N-CA	-5.58	1.39	1.46
2	B	316	LEU	CA-C	5.57	1.59	1.52
2	B	471	VAL	CA-C	-5.57	1.45	1.52
2	B	395	HIS	C-N	5.56	1.41	1.33
1	A	397	GLN	CA-CB	5.54	1.63	1.53
2	B	612	MET	C-N	5.54	1.41	1.33
1	A	305	VAL	N-CA	5.51	1.53	1.46
2	B	469	GLN	CA-C	5.51	1.59	1.52
2	B	324	ARG	CA-C	-5.50	1.46	1.52
2	B	561	VAL	CA-C	-5.50	1.46	1.52
1	A	358	THR	CA-C	-5.50	1.46	1.52
4	D	13	G	C1'-N9	5.50	1.56	1.48
2	B	414	CYS	CA-CB	5.49	1.60	1.53
1	A	419	PHE	CA-CB	5.49	1.63	1.53
4	D	2	C	O4'-C1'	-5.46	1.33	1.41
4	D	77	G	C4'-C3'	5.46	1.60	1.52
2	B	369	ILE	CA-C	5.46	1.59	1.52
2	B	307	MET	CA-C	5.45	1.59	1.52
2	B	377	GLU	CA-C	-5.45	1.45	1.52
2	B	529	ARG	N-CA	-5.44	1.40	1.46
4	D	57	G	O3'-P	-5.44	1.52	1.61
4	D	50	C	C5'-C4'	5.43	1.59	1.51
2	B	254	LYS	N-CA	-5.42	1.39	1.46
2	B	518	LEU	N-CA	-5.42	1.39	1.45
1	A	329	MET	CA-CB	5.42	1.63	1.53
1	A	138	ALA	CA-C	-5.42	1.45	1.52
2	B	583	ARG	CD-NE	5.42	1.53	1.46
1	A	213	PHE	C-N	5.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	383	LEU	C-N	5.41	1.40	1.33
2	B	491	THR	CA-C	-5.40	1.46	1.52
2	B	287	THR	C-N	5.38	1.41	1.33
1	A	141	SER	C-N	5.37	1.40	1.33
1	A	390	GLU	CA-C	-5.36	1.46	1.52
2	B	520	ASP	CA-C	5.36	1.58	1.53
4	D	5	G	C4'-C3'	5.35	1.60	1.52
1	A	319	ILE	CA-CB	5.35	1.61	1.54
1	A	139	LEU	CA-C	5.34	1.59	1.52
2	B	611	GLN	CA-CB	5.33	1.62	1.53
2	B	280	VAL	C-N	5.33	1.40	1.32
2	B	513	LEU	CA-C	5.32	1.59	1.52
1	A	79	GLN	N-CA	5.31	1.52	1.46
4	D	85	A	C3'-O3'	5.31	1.50	1.42
2	B	612	MET	CA-CB	5.30	1.61	1.53
1	A	194	ARG	CD-NE	5.30	1.53	1.46
2	B	306	ASN	CA-CB	5.30	1.61	1.53
1	A	289	ARG	CD-NE	5.29	1.53	1.46
2	B	267	THR	CA-CB	-5.27	1.45	1.53
2	B	479	VAL	C-O	-5.27	1.17	1.23
1	A	9	ASP	N-CA	-5.24	1.39	1.46
1	A	103	GLU	CA-C	5.23	1.59	1.52
1	A	109	LYS	CA-CB	5.23	1.59	1.53
2	B	436	ILE	C-N	5.23	1.40	1.33
1	A	135	ALA	N-CA	-5.22	1.40	1.46
2	B	367	TRP	CA-C	-5.21	1.46	1.53
2	B	260	TYR	CA-CB	5.21	1.61	1.53
2	B	373	GLU	N-CA	-5.21	1.40	1.46
1	A	74	ALA	N-CA	-5.20	1.39	1.46
2	B	501	LYS	CA-CB	5.19	1.61	1.52
4	D	65	G	O4'-C1'	5.19	1.49	1.41
1	A	375	LEU	CA-CB	5.18	1.61	1.53
2	B	379	LEU	C-O	-5.18	1.18	1.24
2	B	607	LYS	CA-CB	5.17	1.61	1.53
4	D	78	C	C5'-C4'	5.17	1.59	1.51
1	A	222	ALA	CA-C	5.17	1.59	1.52
2	B	291	HIS	CA-CB	5.16	1.60	1.53
1	A	299	GLY	CA-C	-5.16	1.44	1.51
2	B	455	VAL	CA-C	5.15	1.58	1.52
2	B	294	ILE	N-CA	-5.14	1.39	1.46
2	B	584	PHE	CA-C	-5.12	1.46	1.52
1	A	323	TYR	N-CA	-5.12	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	SER	CA-CB	5.10	1.60	1.53
2	B	327	GLU	CA-CB	5.10	1.61	1.53
2	B	466	LYS	CA-CB	5.09	1.61	1.53
2	B	535	ILE	CA-C	-5.09	1.46	1.52
2	B	421	PRO	CA-CB	5.08	1.61	1.53
1	A	368	LEU	CA-C	-5.08	1.46	1.52
4	D	75	C	O5'-C5'	5.07	1.50	1.42
1	A	81	ARG	CA-C	-5.07	1.45	1.52
1	A	218	LYS	CA-CB	-5.05	1.44	1.53
4	D	26	G	C1'-N9	5.05	1.55	1.48
1	A	7	ALA	C-N	5.04	1.40	1.33
1	A	88	VAL	CA-C	-5.04	1.47	1.52
2	B	605	THR	N-CA	5.04	1.52	1.45
4	D	77	G	C5'-C4'	5.04	1.58	1.51
1	A	245	ARG	NE-CZ	5.04	1.38	1.33
1	A	357	PHE	CA-CB	5.03	1.60	1.53
2	B	219	GLY	CA-C	-5.03	1.46	1.51
3	C	93	G	O3'-P	-5.02	1.53	1.61
1	A	286	LEU	CA-C	5.02	1.59	1.52
2	B	395	HIS	CE1-NE2	-5.02	1.27	1.32
2	B	457	GLY	N-CA	-5.02	1.40	1.45
4	D	7	G	C3'-O3'	5.02	1.49	1.42
1	A	384	LYS	CA-CB	5.01	1.61	1.54
1	A	206	ALA	N-CA	-5.01	1.40	1.46
1	A	261	GLU	CA-CB	5.01	1.62	1.53
1	A	27	ALA	CA-C	5.01	1.59	1.53
2	B	221	VAL	C-N	-5.01	1.26	1.33

All (489) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	520	ASP	CA-CB-CG	15.77	128.37	112.60
3	C	91	U	P-O3'-C3'	15.70	143.75	120.20
4	D	23	A	P-O3'-C3'	15.15	142.93	120.20
2	B	380	VAL	CA-C-O	-11.98	110.66	118.69
1	A	158	PHE	CA-CB-CG	-10.89	102.91	113.80
2	B	303	PHE	CA-CB-CG	-10.85	102.95	113.80
1	A	325	ASN	CA-CB-CG	-10.64	101.96	112.60
2	B	481	VAL	O-C-N	-9.96	111.75	122.61
1	A	44	GLN	OE1-CD-NE2	9.61	132.21	122.60
4	D	60	C	C2'-C3'-O3'	9.48	123.72	109.50
2	B	413	PHE	CA-CB-CG	9.46	123.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	482	LEU	O-C-N	-9.37	111.14	122.48
1	A	166	ARG	NE-CZ-NH2	9.29	127.56	119.20
3	C	91	U	C2'-C3'-O3'	9.29	123.43	109.50
4	D	16	C	P-O3'-C3'	9.24	134.06	120.20
2	B	598	ALA	CA-C-N	9.14	133.90	122.85
2	B	598	ALA	C-N-CA	9.14	133.90	122.85
1	A	357	PHE	CA-CB-CG	-9.06	104.73	113.80
1	A	213	PHE	CA-CB-CG	-8.94	104.86	113.80
1	A	306	GLU	N-CA-C	8.72	121.66	111.02
1	A	115	GLU	CA-C-O	-8.65	112.46	119.99
2	B	373	GLU	CA-C-N	8.60	131.81	120.28
2	B	373	GLU	C-N-CA	8.60	131.81	120.28
2	B	395	HIS	CB-CG-CD2	-8.55	120.09	131.20
2	B	380	VAL	N-CA-CB	8.45	117.04	110.45
4	D	85	A	P-O3'-C3'	-8.42	107.56	120.20
2	B	555	HIS	CA-CB-CG	8.39	122.19	113.80
4	D	70	A	P-O3'-C3'	8.39	132.78	120.20
1	A	137	THR	N-CA-CB	8.34	122.39	110.12
2	B	536	VAL	N-CA-CB	8.30	123.13	112.34
1	A	203	ARG	NE-CZ-NH2	-8.23	111.80	119.20
1	A	412	ILE	CA-C-N	8.07	135.31	120.95
1	A	412	ILE	C-N-CA	8.07	135.31	120.95
1	A	152	ASP	O-C-N	-8.04	114.82	123.42
1	A	132	HIS	CA-CB-CG	-8.00	105.80	113.80
2	B	275	GLY	CA-C-O	-7.91	110.13	119.46
1	A	276	SER	O-C-N	-7.91	113.94	123.27
1	A	385	PHE	CA-CB-CG	-7.90	105.90	113.80
2	B	219	GLY	CA-C-O	-7.88	112.46	121.68
4	D	24	A	O3'-P-O5'	-7.86	92.21	104.00
4	D	52	U	P-O5'-C5'	7.82	132.63	120.90
2	B	208	PRO	N-CA-CB	7.78	111.42	103.25
4	D	14	A	P-O5'-C5'	7.77	132.56	120.90
2	B	520	ASP	CA-C-O	-7.74	112.12	120.17
1	A	381	ASN	CA-CB-CG	7.72	120.32	112.60
1	A	46	SER	N-CA-C	7.71	120.66	111.33
1	A	12	VAL	N-CA-C	7.71	118.48	110.62
1	A	118	LYS	N-CA-C	-7.66	98.76	110.32
1	A	355	SER	N-CA-C	7.61	121.83	112.54
2	B	297	ALA	CA-C-N	7.57	129.30	119.84
2	B	297	ALA	C-N-CA	7.57	129.30	119.84
1	A	15	TRP	CA-C-N	7.55	130.74	120.54
1	A	15	TRP	C-N-CA	7.55	130.74	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ILE	N-CA-C	7.50	117.62	110.42
1	A	239	SER	O-C-N	-7.48	114.00	122.75
2	B	223	ALA	N-CA-C	7.47	122.08	113.19
2	B	265	LEU	N-CA-CB	7.45	120.50	110.59
2	B	507	ILE	CA-C-O	7.45	126.36	119.20
1	A	192	ARG	N-CA-C	7.40	126.56	110.80
2	B	357	ILE	N-CA-CB	7.37	120.06	111.66
1	A	28	ARG	CA-C-N	7.34	135.80	121.41
1	A	28	ARG	C-N-CA	7.34	135.80	121.41
2	B	519	CYS	CA-C-N	7.32	130.57	120.39
2	B	519	CYS	C-N-CA	7.32	130.57	120.39
1	A	399	GLY	CA-C-N	7.31	131.78	120.82
1	A	399	GLY	C-N-CA	7.31	131.78	120.82
1	A	42	LYS	N-CA-C	7.30	121.54	111.90
2	B	529	ARG	CA-C-O	7.29	126.59	119.08
2	B	350	VAL	CA-C-O	-7.29	113.43	121.23
2	B	530	THR	OG1-CB-CG2	-7.29	94.72	109.30
2	B	395	HIS	CB-CG-ND1	7.26	133.59	122.70
1	A	38	ILE	CA-C-N	7.25	131.12	122.85
1	A	38	ILE	C-N-CA	7.25	131.12	122.85
2	B	438	GLY	O-C-N	-7.25	114.52	121.77
2	B	449	LYS	CB-CA-C	7.24	121.69	109.75
4	D	9	U	P-O3'-C3'	7.17	130.95	120.20
2	B	383	LEU	CA-C-N	7.16	129.75	120.44
2	B	383	LEU	C-N-CA	7.16	129.75	120.44
4	D	73	C	C4'-C3'-C2'	-7.15	95.45	102.60
1	A	287	ILE	CA-C-O	-7.14	112.54	120.25
2	B	271	GLU	CA-C-O	7.13	128.11	120.55
2	B	224	GLY	CA-C-N	7.13	130.55	120.28
2	B	224	GLY	C-N-CA	7.13	130.55	120.28
1	A	246	LEU	N-CA-C	7.11	119.03	111.28
4	D	50	C	O4'-C1'-N1	7.11	119.17	108.50
2	B	361	ASP	CA-C-N	7.08	132.35	121.03
2	B	361	ASP	C-N-CA	7.08	132.35	121.03
2	B	422	PHE	N-CA-C	7.07	118.64	111.07
1	A	257	SER	O-C-N	-7.06	112.38	122.41
2	B	581	ARG	CA-C-N	7.05	128.65	119.84
2	B	581	ARG	C-N-CA	7.05	128.65	119.84
2	B	465	CYS	CA-C-N	6.98	131.04	121.05
2	B	465	CYS	C-N-CA	6.98	131.04	121.05
1	A	32	THR	CA-C-O	6.98	129.24	120.65
2	B	304	VAL	O-C-N	-6.98	113.14	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	31	G	C4'-C3'-C2'	-6.97	95.62	102.60
1	A	343	ILE	O-C-N	-6.97	115.53	122.99
4	D	22	C	P-O3'-C3'	6.91	130.56	120.20
2	B	362	ASP	CA-C-N	6.90	128.46	119.84
2	B	362	ASP	C-N-CA	6.90	128.46	119.84
4	D	31	G	C1'-O4'-C4'	-6.88	103.02	109.90
1	A	70	SER	CA-C-N	6.88	129.47	120.60
1	A	70	SER	C-N-CA	6.88	129.47	120.60
1	A	377	TRP	CA-C-N	6.86	129.47	120.28
1	A	377	TRP	C-N-CA	6.86	129.47	120.28
1	A	135	ALA	N-CA-C	6.83	118.72	111.28
2	B	282	ARG	NE-CZ-NH2	-6.82	113.06	119.20
1	A	268	ILE	N-CA-C	-6.79	104.38	111.58
2	B	591	CYS	CA-C-N	6.76	131.57	123.19
2	B	591	CYS	C-N-CA	6.76	131.57	123.19
2	B	432	PHE	CA-C-O	6.74	127.51	120.30
1	A	287	ILE	O-C-N	6.71	131.02	121.82
2	B	563	ILE	CA-CB-CG2	-6.71	99.09	110.50
2	B	506	GLY	O-C-N	-6.71	113.98	122.70
2	B	603	LEU	O-C-N	-6.71	115.06	123.17
2	B	538	ILE	CA-CB-CG2	-6.70	99.12	110.50
1	A	379	ALA	CA-C-O	6.69	127.64	120.55
2	B	256	ARG	CA-C-N	6.69	129.57	120.54
2	B	256	ARG	C-N-CA	6.69	129.57	120.54
1	A	241	MET	CA-C-O	6.68	127.65	119.97
1	A	146	PHE	CA-C-O	-6.67	113.62	121.16
2	B	337	GLN	CA-C-N	6.67	129.21	120.28
2	B	337	GLN	C-N-CA	6.67	129.21	120.28
1	A	264	PHE	CA-CB-CG	6.65	120.45	113.80
4	D	73	C	P-O5'-C5'	-6.65	110.93	120.90
2	B	622	LYS	N-CA-CB	-6.64	100.12	111.21
4	D	1	G	O3'-P-O5'	-6.63	94.05	104.00
2	B	373	GLU	O-C-N	-6.62	115.10	122.12
2	B	522	ASN	O-C-N	-6.62	113.79	122.59
1	A	172	PHE	O-C-N	-6.61	115.11	123.24
2	B	255	ASN	N-CA-C	6.59	120.74	111.52
2	B	341	HIS	N-CA-C	6.58	118.53	111.36
1	A	365	GLU	CA-C-O	-6.58	113.79	121.16
2	B	588	ASP	CA-CB-CG	6.56	119.16	112.60
2	B	551	VAL	O-C-N	-6.55	115.22	122.69
1	A	203	ARG	NH1-CZ-NH2	6.54	127.81	119.30
4	D	22	C	C2'-C3'-O3'	6.53	119.30	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASP	CA-CB-CG	-6.51	106.09	112.60
2	B	434	ARG	N-CA-C	6.51	118.38	111.28
1	A	113	ASP	N-CA-CB	6.49	120.65	110.71
4	D	19	G	P-O3'-C3'	6.48	129.93	120.20
2	B	487	ASP	CA-CB-CG	-6.47	106.13	112.60
2	B	358	ASN	CA-C-N	6.45	131.31	122.34
2	B	358	ASN	C-N-CA	6.45	131.31	122.34
4	D	16	C	O4'-C1'-N1	6.45	117.87	108.20
2	B	495	ALA	O-C-N	-6.44	111.98	121.12
2	B	281	GLY	O-C-N	6.43	128.63	123.49
2	B	425	TYR	CA-C-N	6.43	129.76	120.38
2	B	425	TYR	C-N-CA	6.43	129.76	120.38
1	A	290	TYR	CB-CA-C	6.41	121.12	110.92
2	B	272	ARG	CD-NE-CZ	-6.39	115.46	124.40
2	B	232	ILE	CA-C-N	6.36	131.45	120.58
2	B	232	ILE	C-N-CA	6.36	131.45	120.58
2	B	320	VAL	CB-CA-C	-6.36	102.27	110.98
2	B	554	ILE	O-C-N	-6.34	116.21	123.00
4	D	19	G	O3'-P-O5'	-6.34	94.48	104.00
2	B	209	LYS	CA-C-N	6.33	129.86	120.87
2	B	209	LYS	C-N-CA	6.33	129.86	120.87
2	B	306	ASN	CA-C-N	6.33	128.76	120.28
2	B	306	ASN	C-N-CA	6.33	128.76	120.28
1	A	258	TYR	O-C-N	-6.33	115.83	123.10
2	B	356	LEU	O-C-N	-6.33	115.16	123.13
2	B	477	HIS	CA-CB-CG	6.33	120.13	113.80
1	A	375	LEU	CA-C-N	6.31	128.74	120.28
1	A	375	LEU	C-N-CA	6.31	128.74	120.28
4	D	20	G	C1'-O4'-C4'	-6.31	103.59	109.90
1	A	51	MET	N-CA-CB	6.31	121.04	110.32
1	A	101	VAL	CB-CA-C	6.30	121.07	111.68
4	D	64	G	O4'-C1'-C2'	-6.30	101.30	107.60
2	B	544	ILE	N-CA-C	-6.30	99.35	108.17
3	C	92	U	C4'-C3'-O3'	-6.30	103.55	113.00
2	B	542	SER	CA-C-N	6.29	133.30	121.97
2	B	542	SER	C-N-CA	6.29	133.30	121.97
4	D	22	C	C4'-C3'-O3'	6.29	118.84	109.40
1	A	81	ARG	CA-C-O	6.29	127.11	119.31
1	A	187	ALA	N-CA-C	6.29	120.55	113.01
2	B	531	PHE	N-CA-C	6.29	118.69	108.76
2	B	243	THR	N-CA-CB	6.28	119.46	110.16
1	A	324	GLU	O-C-N	-6.28	115.46	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	54	G	C3'-C2'-O2'	6.28	120.11	110.70
3	C	98	A	P-O5'-C5'	6.27	130.31	120.90
1	A	348	PRO	N-CA-CB	6.27	110.41	103.26
1	A	191	ALA	CA-C-O	-6.25	114.44	121.00
2	B	523	ASN	CA-CB-CG	-6.25	106.35	112.60
4	D	85	A	O4'-C4'-C3'	-6.24	97.76	104.00
1	A	271	SER	CA-C-N	6.24	133.45	121.54
1	A	271	SER	C-N-CA	6.24	133.45	121.54
2	B	563	ILE	O-C-N	-6.24	115.04	122.77
2	B	255	ASN	OD1-CG-ND2	-6.23	116.37	122.60
4	D	72	U	P-O5'-C5'	-6.22	111.57	120.90
1	A	237	SER	O-C-N	6.21	128.47	122.07
4	D	21	U	P-O5'-C5'	-6.21	111.58	120.90
1	A	293	GLU	N-CA-C	-6.21	103.10	112.04
2	B	455	VAL	CB-CA-C	-6.20	100.49	110.28
1	A	380	ASN	CA-CB-CG	6.17	118.77	112.60
2	B	423	ILE	O-C-N	-6.17	114.07	121.10
2	B	469	GLN	O-C-N	-6.16	115.72	123.12
4	D	19	G	C3'-C2'-C1'	6.16	107.46	101.30
2	B	226	SER	N-CA-CB	6.15	119.36	110.20
2	B	332	PHE	N-CA-CB	-6.14	101.57	110.47
2	B	485	LEU	CA-C-O	-6.13	113.57	121.11
1	A	295	SER	O-C-N	-6.13	113.32	122.39
4	D	62	G	P-O5'-C5'	6.13	130.09	120.90
2	B	521	PRO	CA-C-O	-6.12	109.45	120.60
1	A	340	GLU	CA-CB-CG	6.12	126.34	114.10
1	A	283	GLU	CA-C-N	6.12	128.97	120.29
1	A	283	GLU	C-N-CA	6.12	128.97	120.29
4	D	34	A	C4'-C3'-O3'	-6.11	103.83	113.00
1	A	17	ILE	N-CA-CB	6.11	117.70	110.55
1	A	403	VAL	CA-C-N	6.11	128.96	120.29
1	A	403	VAL	C-N-CA	6.11	128.96	120.29
2	B	365	VAL	N-CA-CB	-6.10	103.52	111.82
1	A	260	GLY	O-C-N	-6.09	116.08	122.60
2	B	242	ARG	NE-CZ-NH1	6.08	127.58	121.50
2	B	234	TYR	CA-C-O	6.08	126.97	120.70
3	C	92	U	O4'-C1'-N1	6.07	117.60	108.50
2	B	366	ASN	CB-CG-ND2	6.06	125.49	116.40
4	D	42	U	P-O5'-C5'	6.05	129.98	120.90
4	D	70	A	C2'-C3'-O3'	6.04	118.57	109.50
1	A	242	PHE	CA-CB-CG	6.04	119.84	113.80
2	B	617	LEU	CA-C-N	6.02	130.78	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	617	LEU	C-N-CA	6.02	130.78	122.77
1	A	366	HIS	CA-CB-CG	-6.02	107.78	113.80
2	B	606	PHE	CA-C-N	6.02	128.35	120.28
2	B	606	PHE	C-N-CA	6.02	128.35	120.28
4	D	51	G	C2'-C3'-O3'	6.01	122.72	113.70
2	B	495	ALA	N-CA-CB	-6.01	101.74	109.55
4	D	79	C	O4'-C1'-N1	6.00	117.50	108.50
1	A	307	ASP	CA-CB-CG	-5.98	106.62	112.60
2	B	622	LYS	O-C-N	-5.96	115.95	122.92
2	B	576	GLU	CB-CA-C	-5.95	100.28	110.22
1	A	79	GLN	CB-CG-CD	-5.95	102.49	112.60
2	B	599	GLY	N-CA-C	-5.94	105.66	112.79
4	D	74	C	C4'-C3'-C2'	-5.94	96.66	102.60
1	A	108	LYS	O-C-N	-5.94	116.32	123.27
1	A	149	ILE	N-CA-CB	5.94	118.94	111.46
2	B	561	VAL	CA-C-N	5.94	132.35	122.73
2	B	561	VAL	C-N-CA	5.94	132.35	122.73
4	D	40	G	C5'-C4'-C3'	-5.94	107.10	116.00
2	B	555	HIS	CE1-NE2-CD2	-5.93	103.06	109.00
1	A	270	LEU	N-CA-C	5.93	120.24	112.89
1	A	166	ARG	NH1-CZ-NH2	-5.92	111.60	119.30
2	B	398	PRO	CB-CA-C	5.91	119.19	110.85
2	B	536	VAL	O-C-N	-5.91	117.65	122.97
1	A	8	ALA	CA-C-N	5.91	132.06	121.66
1	A	8	ALA	C-N-CA	5.91	132.06	121.66
2	B	221	VAL	N-CA-C	5.91	117.36	110.62
1	A	151	ILE	N-CA-CB	-5.90	102.42	110.56
4	D	45	C	O4'-C1'-N1	5.89	117.33	108.50
4	D	60	C	P-O3'-C3'	5.88	129.03	120.20
4	D	48	C	C5'-C4'-C3'	5.87	124.80	116.00
1	A	89	PRO	CA-C-N	5.87	125.54	119.56
1	A	89	PRO	C-N-CA	5.87	125.54	119.56
2	B	276	LYS	O-C-N	-5.86	116.74	123.42
3	C	95	A	P-O5'-C5'	5.85	129.67	120.90
2	B	375	CYS	N-CA-C	5.84	117.65	111.28
4	D	87	C	O4'-C1'-C2'	-5.84	101.76	107.60
2	B	522	ASN	CB-CA-C	5.84	122.03	110.42
1	A	159	GLY	O-C-N	-5.83	117.01	123.66
2	B	253	GLU	CA-C-O	5.82	126.54	119.38
1	A	8	ALA	CA-C-O	5.80	126.60	119.05
1	A	152	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	81	ARG	NH1-CZ-NH2	-5.79	111.78	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	518	LEU	N-CA-C	5.78	118.65	110.50
1	A	10	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	A	278	VAL	CA-C-N	5.78	132.10	121.70
1	A	278	VAL	C-N-CA	5.78	132.10	121.70
2	B	476	LYS	CG-CD-CE	5.78	124.58	111.30
4	D	66	U	P-O5'-C5'	5.77	129.56	120.90
2	B	563	ILE	CB-CA-C	5.77	118.58	111.25
4	D	23	A	C4'-C3'-O3'	5.77	118.05	109.40
2	B	438	GLY	CA-C-N	5.76	125.78	119.90
2	B	438	GLY	C-N-CA	5.76	125.78	119.90
1	A	128	ASP	N-CA-CB	-5.76	100.75	110.49
2	B	369	ILE	CA-C-N	5.76	127.93	120.44
2	B	369	ILE	C-N-CA	5.76	127.93	120.44
2	B	488	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	347	THR	CA-C-N	5.75	125.87	119.32
1	A	347	THR	C-N-CA	5.75	125.87	119.32
2	B	554	ILE	CA-CB-CG2	-5.74	100.73	110.50
1	A	303	PHE	CB-CG-CD1	5.74	130.46	120.70
2	B	268	ASN	O-C-N	-5.74	116.31	122.85
1	A	152	ASP	CA-C-O	5.74	127.37	121.23
1	A	157	LEU	CA-C-N	5.74	131.25	122.93
1	A	157	LEU	C-N-CA	5.74	131.25	122.93
1	A	120	ILE	CA-C-O	5.72	127.91	121.11
4	D	44	C	O4'-C4'-C3'	-5.71	98.29	104.00
2	B	604	GLU	N-CA-C	-5.70	101.58	110.42
2	B	276	LYS	CA-C-N	5.70	132.42	121.54
2	B	276	LYS	C-N-CA	5.70	132.42	121.54
2	B	335	GLY	O-C-N	-5.70	116.23	122.84
2	B	585	VAL	O-C-N	-5.67	116.93	123.00
2	B	385	LYS	N-CA-C	5.67	117.26	111.14
1	A	103	GLU	CA-C-O	5.66	127.50	121.16
1	A	416	ARG	NE-CZ-NH1	5.66	127.16	121.50
4	D	57	G	C4'-C3'-C2'	-5.66	96.94	102.60
1	A	129	ASN	CA-C-N	5.65	131.37	122.21
1	A	129	ASN	C-N-CA	5.65	131.37	122.21
2	B	220	HIS	N-CA-CB	5.65	118.34	110.26
4	D	25	A	P-O3'-C3'	-5.65	111.72	120.20
1	A	337	GLY	CA-C-N	5.64	132.31	121.54
1	A	337	GLY	C-N-CA	5.64	132.31	121.54
4	D	3	G	C5'-C4'-C3'	5.64	124.46	116.00
1	A	138	ALA	N-CA-C	5.63	118.96	111.75
4	D	84	C	P-O5'-C5'	5.63	129.34	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	GLY	CA-C-O	-5.62	116.87	121.76
1	A	120	ILE	O-C-N	-5.62	116.09	122.72
2	B	491	THR	CA-C-O	5.61	127.74	121.40
2	B	330	THR	CA-C-O	5.61	126.36	120.42
2	B	491	THR	CA-CB-OG1	5.61	118.01	109.60
4	D	87	C	C4'-C3'-C2'	-5.61	96.99	102.60
4	D	16	C	C2'-C3'-O3'	5.60	117.91	109.50
1	A	158	PHE	N-CA-C	-5.60	100.58	109.59
4	D	58	U	C3'-C2'-O2'	5.59	119.09	110.70
1	A	83	LYS	N-CA-CB	-5.58	101.70	110.46
1	A	289	ARG	CA-C-O	-5.58	114.63	120.55
1	A	13	GLU	CA-C-N	5.57	128.33	120.42
1	A	13	GLU	C-N-CA	5.57	128.33	120.42
1	A	120	ILE	CA-C-N	5.57	131.88	122.79
1	A	120	ILE	C-N-CA	5.57	131.88	122.79
2	B	250	GLU	CA-CB-CG	5.57	125.24	114.10
2	B	341	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	A	66	VAL	CA-CB-CG2	-5.57	100.94	110.40
2	B	421	PRO	N-CA-C	5.56	119.00	111.22
2	B	523	ASN	CB-CA-C	-5.56	102.34	111.68
1	A	289	ARG	CA-C-N	5.53	128.48	120.79
1	A	289	ARG	C-N-CA	5.53	128.48	120.79
1	A	394	ASP	N-CA-CB	-5.53	102.25	110.61
1	A	397	GLN	O-C-N	-5.52	115.21	122.39
2	B	256	ARG	NE-CZ-NH1	5.52	127.02	121.50
2	B	540	HIS	CA-C-N	5.51	131.62	121.70
2	B	540	HIS	C-N-CA	5.51	131.62	121.70
2	B	572	LYS	CA-C-N	5.51	129.30	121.42
2	B	572	LYS	C-N-CA	5.51	129.30	121.42
2	B	439	PRO	N-CA-CB	5.50	108.09	103.25
2	B	502	ILE	CA-CB-CG2	-5.50	101.16	110.50
1	A	53	ALA	N-CA-C	-5.50	105.31	112.23
1	A	334	HIS	N-CA-CB	5.49	118.29	110.44
1	A	415	TYR	O-C-N	-5.48	116.80	123.10
2	B	555	HIS	ND1-CE1-NE2	5.48	113.88	108.40
2	B	215	VAL	CA-C-O	-5.47	114.54	120.67
2	B	514	PRO	O-C-N	-5.47	116.16	123.06
1	A	111	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	220	ASN	N-CA-C	-5.46	104.20	111.24
2	B	324	ARG	NE-CZ-NH1	5.46	126.96	121.50
2	B	596	ARG	O-C-N	-5.45	116.86	123.29
2	B	304	VAL	CA-C-N	5.43	125.25	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	304	VAL	C-N-CA	5.43	125.25	119.28
1	A	262	ASN	OD1-CG-ND2	-5.43	117.17	122.60
2	B	237	GLY	CA-C-N	5.43	129.78	120.72
2	B	237	GLY	C-N-CA	5.43	129.78	120.72
1	A	314	MET	CG-SD-CE	-5.40	89.02	100.90
2	B	365	VAL	O-C-N	-5.39	117.57	123.18
1	A	347	THR	CA-C-O	-5.39	115.11	120.66
1	A	161	LEU	CA-C-O	5.39	126.15	120.33
2	B	554	ILE	N-CA-C	-5.39	100.07	108.86
4	D	80	C	O3'-P-O5'	-5.39	95.92	104.00
1	A	85	TYR	N-CA-C	5.38	118.11	110.10
1	A	281	ILE	N-CA-CB	5.38	116.84	110.55
4	D	40	G	P-O5'-C5'	5.37	128.95	120.90
1	A	145	LYS	N-CA-CB	5.37	119.56	110.49
4	D	65	G	C5'-C4'-O4'	-5.36	101.76	109.80
2	B	603	LEU	CA-C-O	5.36	127.46	121.40
1	A	13	GLU	N-CA-CB	5.36	117.92	109.94
2	B	409	GLU	CA-C-O	5.35	127.16	121.11
4	D	39	A	P-O3'-C3'	5.35	128.23	120.20
2	B	361	ASP	N-CA-CB	5.35	119.02	110.73
1	A	39	ILE	CA-C-O	-5.34	115.19	119.25
1	A	71	VAL	N-CA-CB	5.34	116.44	110.51
3	C	95	A	C2'-C3'-O3'	5.34	117.50	109.50
1	A	369	ILE	CA-C-O	-5.33	115.49	120.34
4	D	35	C	C1'-O4'-C4'	-5.33	104.57	109.90
2	B	283	ALA	O-C-N	-5.33	117.09	123.27
2	B	208	PRO	CA-N-CD	-5.33	104.54	112.00
2	B	482	LEU	CA-C-O	5.33	124.67	118.97
2	B	410	GLN	N-CA-C	5.32	117.89	109.96
4	D	4	G	O4'-C1'-C2'	-5.31	102.29	107.60
4	D	44	C	O4'-C1'-N1	5.31	116.47	108.50
2	B	500	LEU	CA-C-O	-5.31	115.37	121.47
1	A	419	PHE	CA-C-O	5.30	127.12	121.45
2	B	556	THR	CA-CB-OG1	5.30	117.55	109.60
1	A	30	ASN	N-CA-C	-5.30	101.02	109.07
1	A	191	ALA	N-CA-C	5.30	116.74	110.97
1	A	377	TRP	CB-CG-CD2	-5.29	119.39	126.80
1	A	201	TYR	N-CA-C	-5.29	105.09	112.45
1	A	290	TYR	CA-C-O	-5.29	115.25	121.07
2	B	410	GLN	CG-CD-NE2	5.28	124.33	116.40
2	B	511	GLU	O-C-N	-5.28	116.00	122.34
4	D	61	C	O4'-C1'-N1	5.28	116.42	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	THR	N-CA-C	5.28	122.04	110.80
2	B	247	TYR	N-CA-C	5.27	117.03	111.28
1	A	77	SER	N-CA-C	5.27	117.70	111.33
2	B	560	GLU	CB-CG-CD	-5.27	103.65	112.60
2	B	584	PHE	N-CA-C	5.26	116.00	108.74
2	B	442	LEU	CA-C-N	5.26	125.56	119.93
2	B	442	LEU	C-N-CA	5.26	125.56	119.93
1	A	60	SER	CA-C-N	5.25	127.95	121.64
1	A	60	SER	C-N-CA	5.25	127.95	121.64
2	B	560	GLU	O-C-N	-5.25	116.80	122.79
1	A	118	LYS	CA-C-N	5.25	125.25	119.90
1	A	118	LYS	C-N-CA	5.25	125.25	119.90
2	B	210	LYS	CA-C-N	-5.25	113.42	120.87
2	B	210	LYS	C-N-CA	-5.25	113.42	120.87
2	B	489	VAL	CA-CB-CG2	5.24	119.31	110.40
2	B	367	TRP	CZ3-CH2-CZ2	-5.24	114.69	121.50
2	B	344	LEU	N-CA-C	5.23	116.79	111.14
2	B	360	MET	O-C-N	-5.23	115.80	122.34
1	A	83	LYS	CA-C-O	5.23	125.40	119.18
1	A	136	LEU	O-C-N	-5.23	115.24	122.46
2	B	448	TYR	N-CA-CB	5.23	119.33	110.49
1	A	343	ILE	CA-C-O	5.23	126.23	120.48
2	B	490	GLU	O-C-N	-5.22	116.47	122.95
1	A	350	GLN	CA-C-N	5.22	127.27	120.28
1	A	350	GLN	C-N-CA	5.22	127.27	120.28
1	A	141	SER	N-CA-C	5.20	121.87	110.80
2	B	496	PRO	O-C-N	-5.20	116.67	123.06
1	A	377	TRP	CE2-CD2-CE3	5.19	123.99	118.80
2	B	288	GLU	CA-C-O	5.19	125.91	119.79
4	D	88	A	C1'-O4'-C4'	-5.19	104.51	109.70
1	A	161	LEU	O-C-N	-5.19	116.28	123.12
1	A	81	ARG	N-CA-C	5.18	119.32	112.89
2	B	315	ASP	CA-CB-CG	-5.18	107.42	112.60
4	D	74	C	O4'-C1'-N1	5.18	116.27	108.50
1	A	144	SER	O-C-N	-5.18	115.70	122.59
2	B	597	THR	O-C-N	-5.18	116.95	122.85
1	A	198	ARG	NE-CZ-NH1	5.17	126.67	121.50
4	D	88	A	O4'-C4'-C3'	-5.17	100.93	106.10
2	B	268	ASN	CA-C-O	5.17	127.91	121.81
1	A	175	ASP	CA-C-O	5.17	125.94	120.36
2	B	593	ALA	O-C-N	5.17	129.42	123.17
1	A	203	ARG	CA-C-O	-5.17	115.40	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	SER	N-CA-C	5.17	116.60	111.07
1	A	388	THR	O-C-N	-5.16	117.08	123.33
2	B	217	PHE	CB-CA-C	-5.16	102.38	110.79
2	B	593	ALA	CA-C-O	-5.16	115.57	121.40
4	D	38	A	C1'-O4'-C4'	5.16	115.06	109.90
1	A	13	GLU	O-C-N	-5.15	116.73	122.09
4	D	51	G	C4'-C3'-O3'	-5.15	105.28	113.00
2	B	522	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	356	HIS	O-C-N	5.14	129.42	122.59
2	B	316	LEU	CA-C-O	5.14	126.03	120.43
1	A	356	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
2	B	269	GLN	N-CA-C	5.13	116.87	111.28
2	B	339	ARG	CB-CA-C	-5.13	102.83	110.88
2	B	479	VAL	CA-C-O	-5.13	116.14	120.96
1	A	132	HIS	CA-C-O	5.12	126.01	120.43
2	B	286	GLU	CA-C-N	5.11	131.11	122.12
2	B	286	GLU	C-N-CA	5.11	131.11	122.12
2	B	232	ILE	CA-CB-CG1	5.10	119.08	110.40
2	B	451	MET	CG-SD-CE	-5.10	89.67	100.90
2	B	271	GLU	O-C-N	-5.10	116.71	122.12
2	B	409	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	149	ILE	CA-CB-CG1	-5.09	101.75	110.40
1	A	226	LEU	N-CA-CB	-5.09	102.58	110.57
1	A	249	LYS	CA-C-O	5.07	124.31	119.08
1	A	173	THR	CA-C-N	5.07	131.19	122.67
1	A	173	THR	C-N-CA	5.07	131.19	122.67
4	D	34	A	O4'-C1'-C2'	5.06	112.66	107.60
2	B	504	LEU	CA-C-N	5.06	130.05	122.86
2	B	504	LEU	C-N-CA	5.06	130.05	122.86
4	D	82	C	C3'-C2'-C1'	5.06	106.36	101.30
1	A	194	ARG	NE-CZ-NH1	5.06	126.56	121.50
2	B	445	VAL	N-CA-C	5.06	116.16	111.81
1	A	93	LEU	O-C-N	-5.05	117.33	123.29
1	A	390	GLU	N-CA-C	5.05	116.64	108.41
2	B	477	HIS	ND1-CE1-NE2	5.05	113.45	108.40
1	A	282	GLN	OE1-CD-NE2	5.05	127.65	122.60
2	B	631	LYS	CA-C-O	-5.05	114.90	120.30
2	B	211	GLU	CA-C-O	-5.04	115.51	121.16
2	B	230	GLY	O-C-N	-5.04	116.14	122.70
4	D	46	C	P-O5'-C5'	5.04	128.46	120.90
1	A	142	ASP	O-C-N	-5.04	117.34	123.29
1	A	267	ALA	N-CA-C	5.04	119.06	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	LEU	O-C-N	-5.04	116.78	122.12
1	A	327	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	287	ILE	N-CA-C	-5.03	104.70	111.44
1	A	167	GLU	O-C-N	-5.02	117.43	123.31
1	A	337	GLY	O-C-N	5.02	129.76	122.68
1	A	22	LYS	N-CA-C	-5.01	105.28	111.40
2	B	545	CYS	CA-C-N	5.01	126.11	119.84
2	B	545	CYS	C-N-CA	5.01	126.11	119.84
2	B	555	HIS	CG-CD2-NE2	5.01	112.21	107.20
1	A	146	PHE	CA-CB-CG	-5.01	108.79	113.80
4	D	88	A	C1'-C2'-O2'	-5.01	104.28	111.80
4	D	7	G	C4'-C3'-C2'	5.01	107.61	102.60
1	A	217	ASP	CA-CB-CG	-5.00	107.59	112.60
1	A	93	LEU	N-CA-CB	5.00	118.42	110.57
4	D	2	C	C3'-C2'-C1'	-5.00	96.30	101.30
1	A	325	ASN	CA-C-O	5.00	125.76	120.36

There are no chirality outliers.

All (89) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	HIS	Sidechain
1	A	141	SER	Peptide
1	A	142	ASP	Peptide
1	A	144	SER	Peptide
1	A	194	ARG	Sidechain
1	A	275	LEU	Peptide
1	A	276	SER	Peptide
1	A	278	VAL	Peptide
1	A	28	ARG	Sidechain
1	A	301	TYR	Sidechain
1	A	323	TYR	Sidechain
1	A	325	ASN	Peptide
1	A	331	TYR	Sidechain
1	A	356	HIS	Sidechain
1	A	402	PHE	Sidechain
1	A	419	PHE	Sidechain
1	A	81	ARG	Sidechain
2	B	232	ILE	Mainchain
2	B	247	TYR	Sidechain
2	B	272	ARG	Sidechain
2	B	292	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	B	303	PHE	Sidechain
2	B	314	ALA	Peptide
2	B	328	PHE	Sidechain
2	B	371	ARG	Sidechain
2	B	372	TYR	Sidechain
2	B	439	PRO	Peptide
2	B	448	TYR	Sidechain
2	B	469	GLN	Peptide
2	B	473	MET	Peptide
2	B	503	ARG	Sidechain
2	B	517	ILE	Peptide
2	B	521	PRO	Peptide
2	B	524	LEU	Peptide
2	B	528	GLY	Peptide
2	B	536	VAL	Peptide
2	B	539	GLU	Peptide
2	B	553	HIS	Sidechain
2	B	581	ARG	Sidechain
2	B	583	ARG	Sidechain
3	C	90	A	Sidechain
3	C	91	U	Sidechain
3	C	92	U	Sidechain
3	C	93	G	Sidechain
3	C	95	A	Sidechain
3	C	97	A	Sidechain
3	C	98	A	Sidechain
4	D	1	G	Sidechain
4	D	10	G	Sidechain
4	D	12	C	Sidechain
4	D	14	A	Sidechain
4	D	15	G	Sidechain
4	D	18	U	Sidechain
4	D	19	G	Sidechain
4	D	20	G	Sidechain
4	D	21	U	Sidechain
4	D	23	A	Sidechain
4	D	24	A	Sidechain
4	D	26	G	Sidechain
4	D	28	C	Sidechain
4	D	29	G	Sidechain
4	D	30	G	Sidechain
4	D	36	U	Sidechain

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Mol	Chain	Res	Type	Group
4	D	37	C	Sidechain
4	D	38	A	Sidechain
4	D	39	A	Sidechain
4	D	4	G	Sidechain
4	D	40	G	Sidechain
4	D	44	C	Sidechain
4	D	47	U	Sidechain
4	D	5	G	Sidechain
4	D	51	G	Sidechain
4	D	54	G	Sidechain
4	D	55	G	Sidechain
4	D	59	U	Sidechain
4	D	61	C	Sidechain
4	D	62	G	Sidechain
4	D	65	G	Sidechain
4	D	69	G	Sidechain
4	D	70	A	Sidechain
4	D	71	A	Sidechain
4	D	76	C	Sidechain
4	D	78	C	Sidechain
4	D	8	U	Sidechain
4	D	83	G	Sidechain
4	D	85	A	Sidechain
4	D	87	C	Sidechain
4	D	88	A	Sidechain
4	D	9	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3269	0	3314	10	0
2	B	3367	0	3424	11	0
3	C	212	0	106	8	0
4	D	1876	0	938	15	0
All	All	8724	0	7782	37	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 (37) 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)
3:C:91:U:N3	4:D:39:A:N1	2.19	0.90
3:C:92:U:C2	4:D:38:A:C2	2.81	0.69
4:D:39:A:H3'	4:D:40:G:C8	2.30	0.67
2:B:308:ILE:HG21	2:B:553:HIS:CE1	2.34	0.63
2:B:617:LEU:HD23	2:B:625:ALA:HB3	1.84	0.57
1:A:15:TRP:CD1	1:A:19:LYS:HE2	2.39	0.57
3:C:91:U:C2	4:D:39:A:C2	2.93	0.57
3:C:92:U:O2	4:D:38:A:C2	2.62	0.52
3:C:91:U:C4	4:D:39:A:N1	2.76	0.52
1:A:274:VAL:HG12	1:A:274:VAL:O	2.13	0.48
4:D:15:G:H3'	4:D:16:C:H5''	1.96	0.47
4:D:1:G:C2	4:D:85:A:C2	3.02	0.47
2:B:215:VAL:HG13	2:B:294:ILE:HD13	1.97	0.47
2:B:563:ILE:HG22	2:B:595:LEU:CD2	2.44	0.47
1:A:329:MET:HB2	1:A:331:TYR:CE1	2.50	0.46
2:B:563:ILE:HG22	2:B:595:LEU:HD23	1.97	0.46
1:A:152:ASP:HB2	1:A:259:GLY:HA3	1.96	0.46
3:C:91:U:C2	4:D:39:A:N1	2.83	0.46
3:C:92:U:N3	4:D:38:A:C2	2.81	0.46
1:A:43:ASP:CG	1:A:47:ARG:HH21	2.25	0.45
2:B:220:HIS:CE1	2:B:331:GLY:HA3	2.52	0.44
2:B:332:PHE:CD1	2:B:378:LYS:HG2	2.52	0.44
4:D:14:A:H1'	4:D:25:A:C6	2.52	0.44
1:A:317:VAL:HA	1:A:413:LEU:HA	1.99	0.44
1:A:160:THR:HG23	1:A:169:LEU:HD11	2.00	0.44
2:B:536:VAL:O	2:B:625:ALA:HA	2.18	0.43
4:D:24:A:C2	4:D:60:C:C2	3.06	0.43
4:D:37:C:C2	4:D:38:A:C8	3.06	0.43
2:B:214:ASN:N	2:B:214:ASN:HD22	2.16	0.43
4:D:82:C:H2'	4:D:83:G:C8	2.54	0.43
2:B:479:VAL:HG21	2:B:504:LEU:HD23	2.02	0.42
1:A:382:TYR:CG	1:A:389:LEU:HB2	2.56	0.41
2:B:207:ALA:HB1	2:B:208:PRO:HD2	2.03	0.41
1:A:317:VAL:HG12	1:A:413:LEU:HD23	2.03	0.41
1:A:157:LEU:HD12	1:A:171:LYS:HD2	2.03	0.41
4:D:85:A:C2	4:D:86:C:C4	3.09	0.40
3:C:92:U:O2	3:C:93:G:C5	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/414 (100%)	365 (89%)	34 (8%)	13 (3%)	3	21
2	B	426/428 (100%)	374 (88%)	37 (9%)	15 (4%)	3	20
All	All	838/842 (100%)	739 (88%)	71 (8%)	28 (3%)	5	21

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	145	LYS
1	A	326	LEU
2	B	298	PRO
2	B	315	ASP
1	A	43	ASP
1	A	144	SER
1	A	338	THR
2	B	277	THR
2	B	461	SER
2	B	543	ILE
2	B	564	THR
2	B	567	ILE
1	A	62	ILE
1	A	244	GLN
2	B	208	PRO
2	B	487	ASP
2	B	574	SER
1	A	64	SER
2	B	431	ASN
2	B	509	GLU
2	B	522	ASN
2	B	555	HIS
1	A	68	ARG
1	A	373	PRO

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Mol	Chain	Res	Type
2	B	475	ASN
1	A	63	LYS
1	A	190	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/357 (100%)	348 (98%)	9 (2%)	42	63
2	B	372/372 (100%)	353 (95%)	19 (5%)	21	42
All	All	729/729 (100%)	701 (96%)	28 (4%)	30	50

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	56	PHE
1	A	130	LYS
1	A	141	SER
1	A	208	THR
1	A	283	GLU
1	A	284	LYS
1	A	305	VAL
1	A	320	LEU
2	B	246	LYS
2	B	276	LYS
2	B	298	PRO
2	B	305	PRO
2	B	365	VAL
2	B	388	PHE
2	B	392	LYS
2	B	434	ARG
2	B	440	ILE
2	B	488	ASP
2	B	501	LYS

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Mol	Chain	Res	Type
2	B	502	ILE
2	B	517	ILE
2	B	536	VAL
2	B	549	ASN
2	B	551	VAL
2	B	554	ILE
2	B	571	ASP
2	B	616	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	111	ASN
1	A	334	HIS
1	A	350	GLN
1	A	356	HIS
2	B	214	ASN
2	B	431	ASN
2	B	540	HIS
2	B	553	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	9/10 (90%)	6 (66%)	1 (11%)
4	D	87/88 (98%)	23 (26%)	6 (6%)
All	All	96/98 (97%)	29 (30%)	7 (7%)

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	91	U
3	C	92	U
3	C	94	U
3	C	96	A
3	C	97	A
3	C	99	A
4	D	7	G
4	D	8	U

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Mol	Chain	Res	Type
4	D	10	G
4	D	16	C
4	D	17	C
4	D	19	G
4	D	20	G
4	D	21	U
4	D	22	C
4	D	23	A
4	D	24	A
4	D	35	C
4	D	36	U
4	D	40	G
4	D	52	U
4	D	61	C
4	D	68	C
4	D	71	A
4	D	72	U
4	D	73	C
4	D	83	G
4	D	87	C
4	D	88	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	91	U
4	D	9	U
4	D	22	C
4	D	23	A
4	D	60	C
4	D	70	A
4	D	72	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

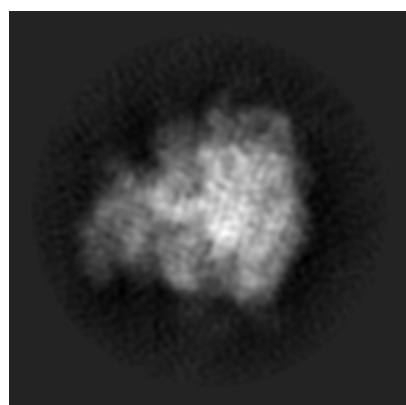
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5801. These allow visual inspection of the internal detail of the map and identification of artifacts.

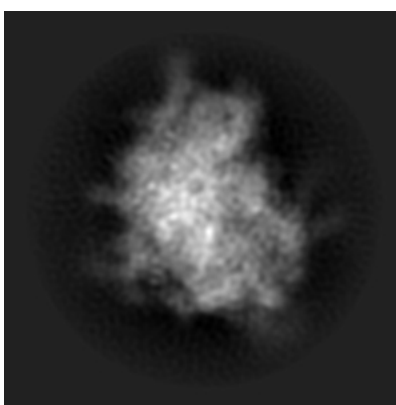
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

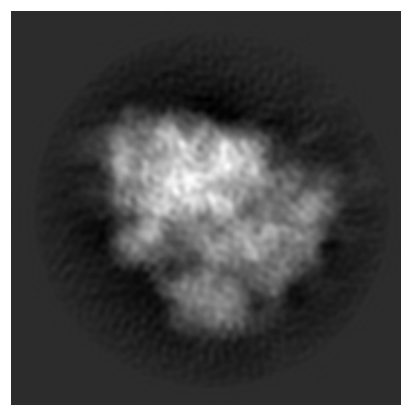
6.1.1 Primary map



X



Y

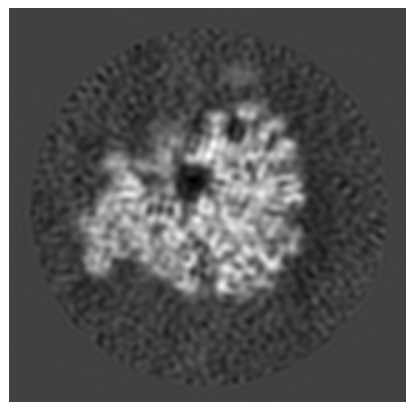


Z

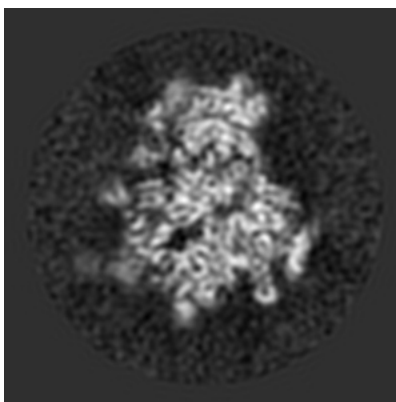
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

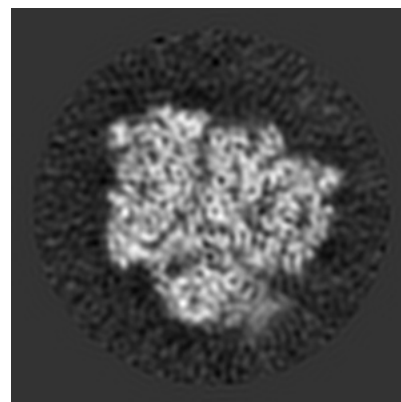
6.2.1 Primary map



X Index: 152



Y Index: 152

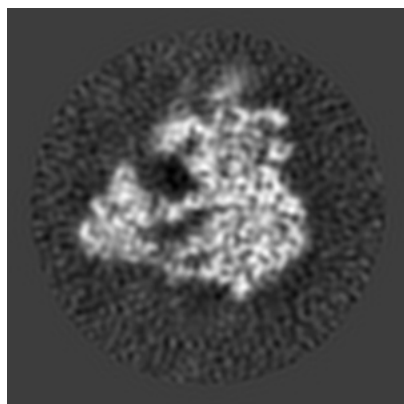


Z Index: 152

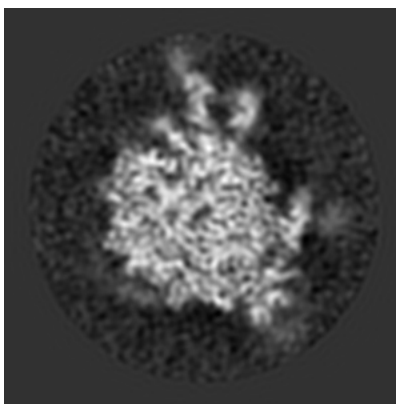
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

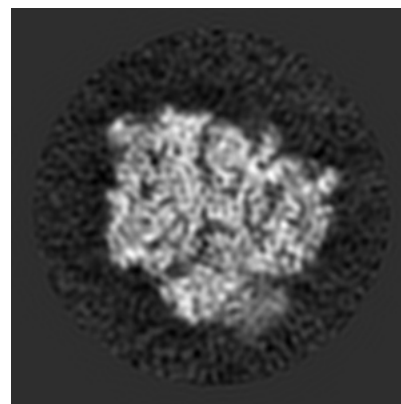
6.3.1 Primary map



X Index: 139



Y Index: 178

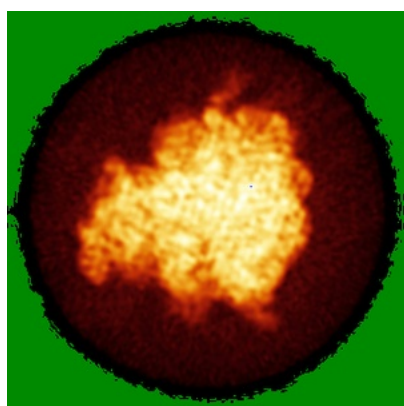


Z Index: 155

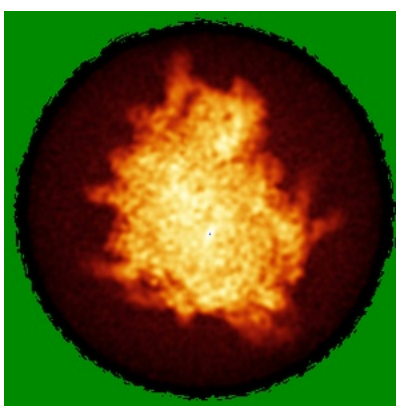
The images above show the largest variance slices of the map in three orthogonal directions.

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

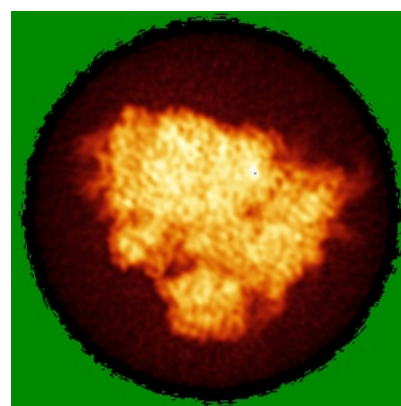
6.4.1 Primary map



X



Y



Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

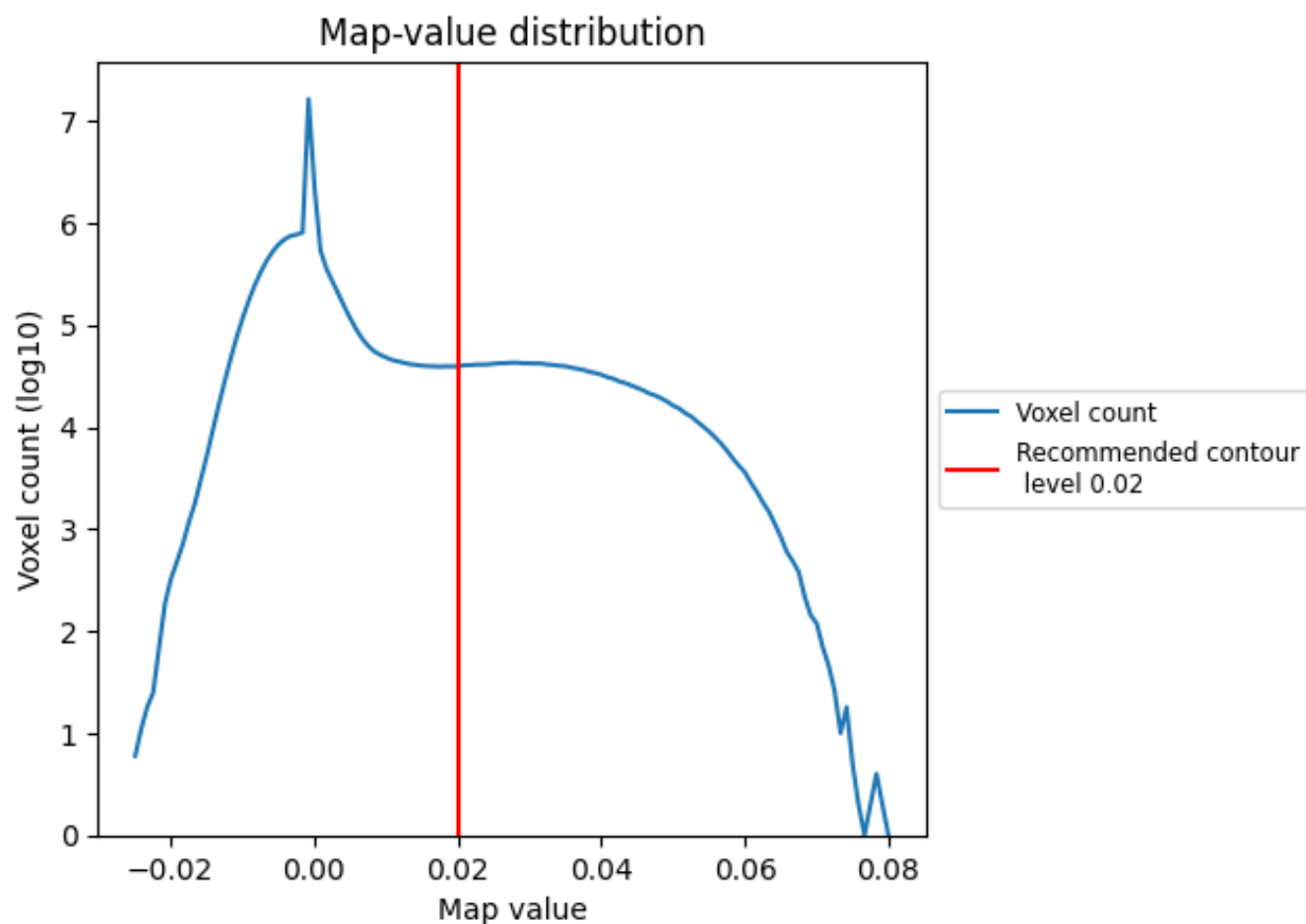
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

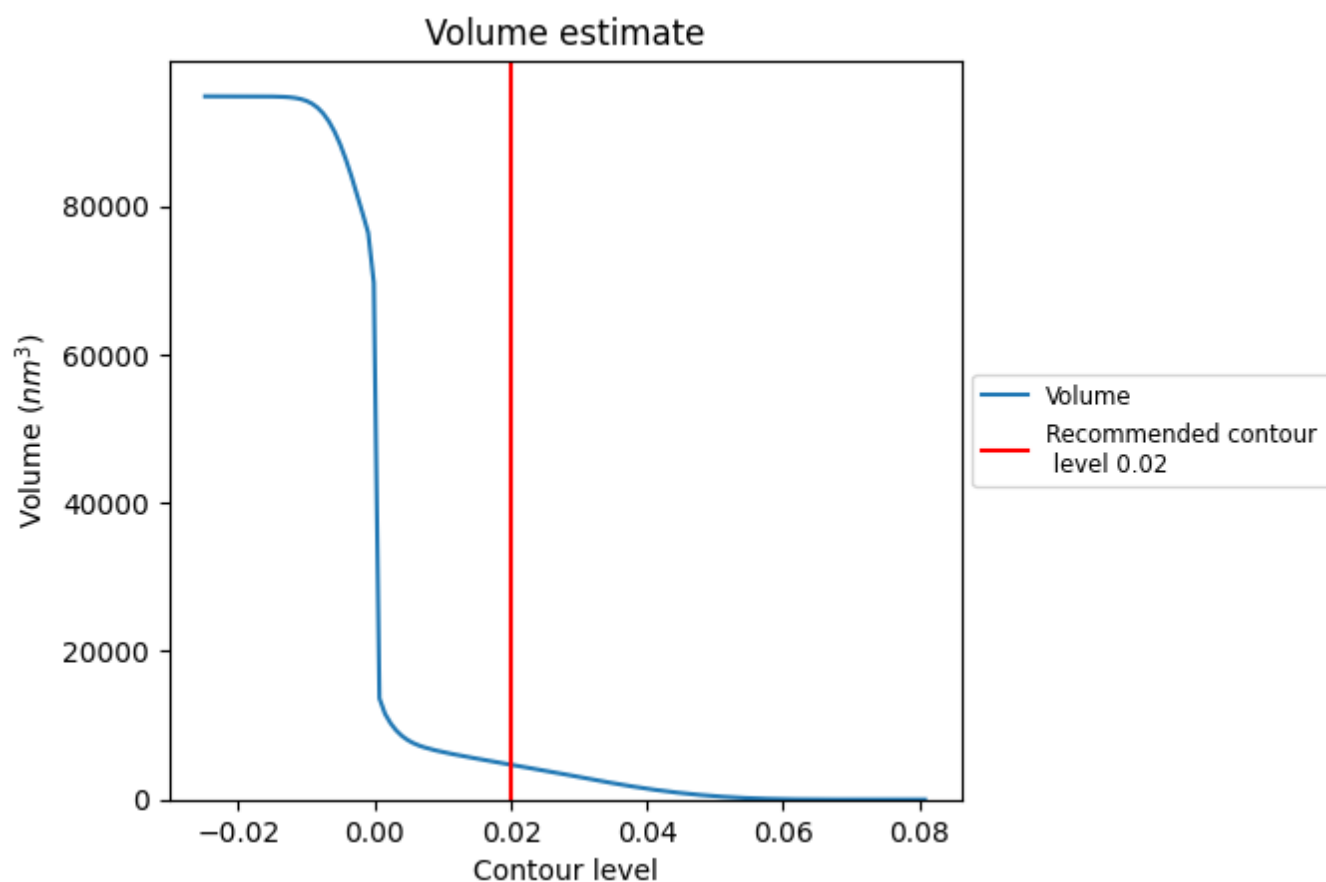
This section contains the results of statistical analysis of the map.

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.

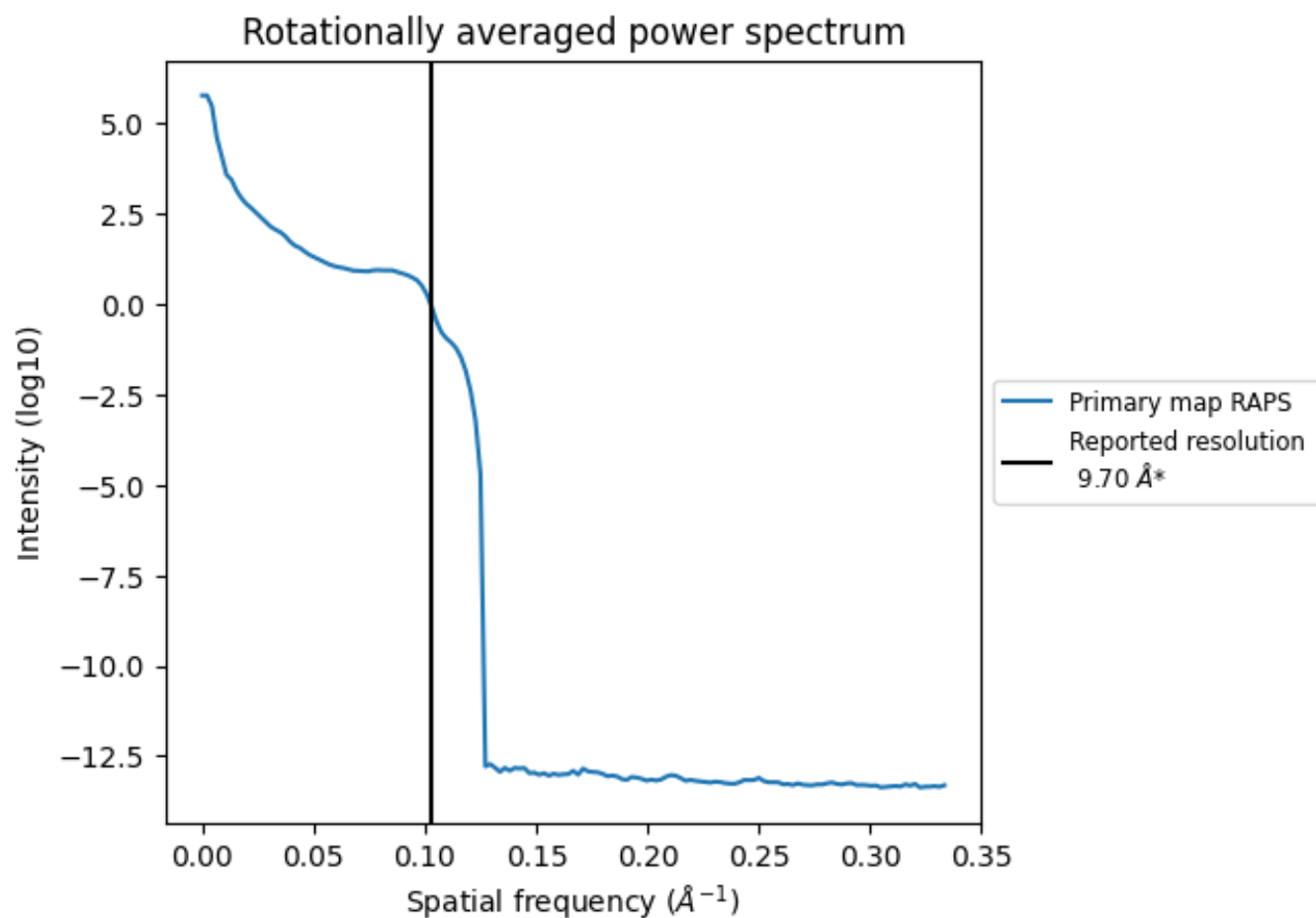
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4726 nm³; this corresponds to an approximate mass of 4270 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 ⓘ

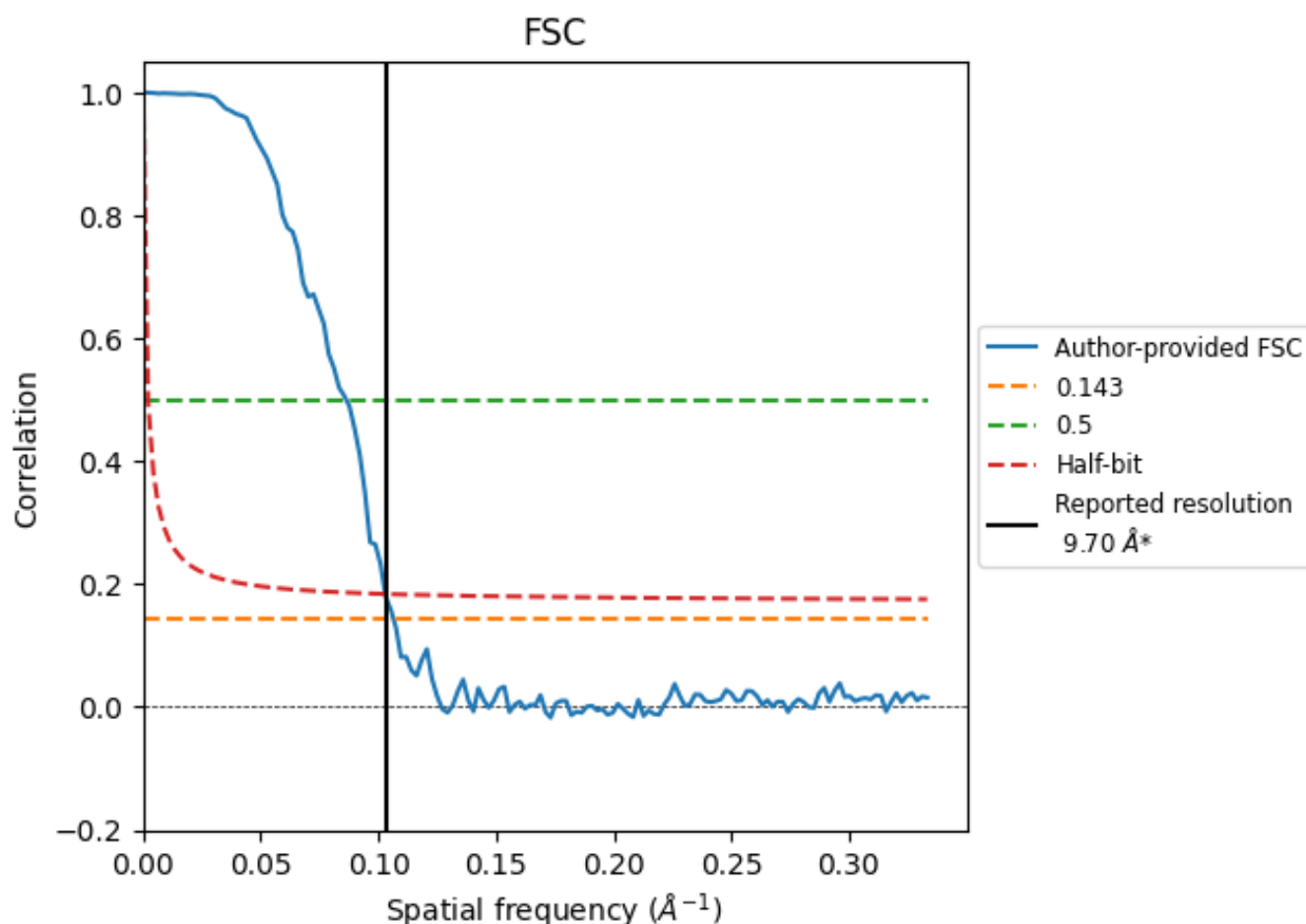


*Reported resolution corresponds to spatial frequency of 0.103 Å⁻¹

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 0.103 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

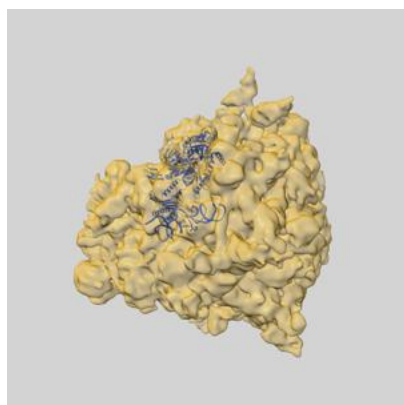
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.70	-	-
Author-provided FSC curve	9.40	11.59	9.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

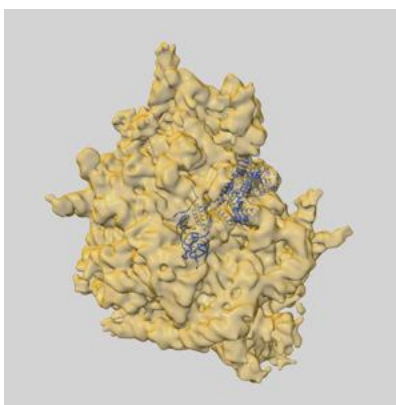
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5801 and PDB model 3J5Y. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

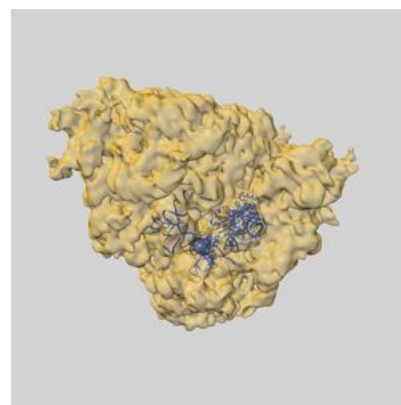
9.1 Map-model overlay [i](#)



X



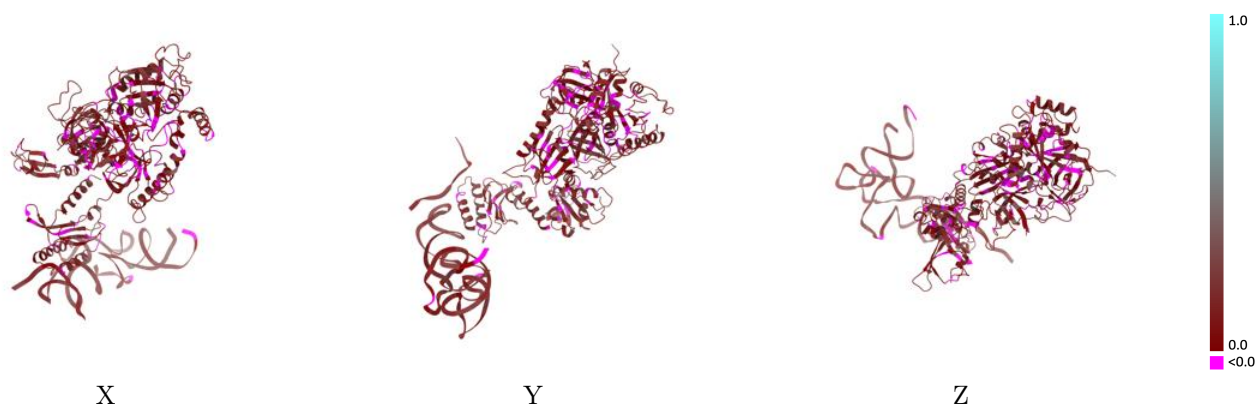
Y



Z

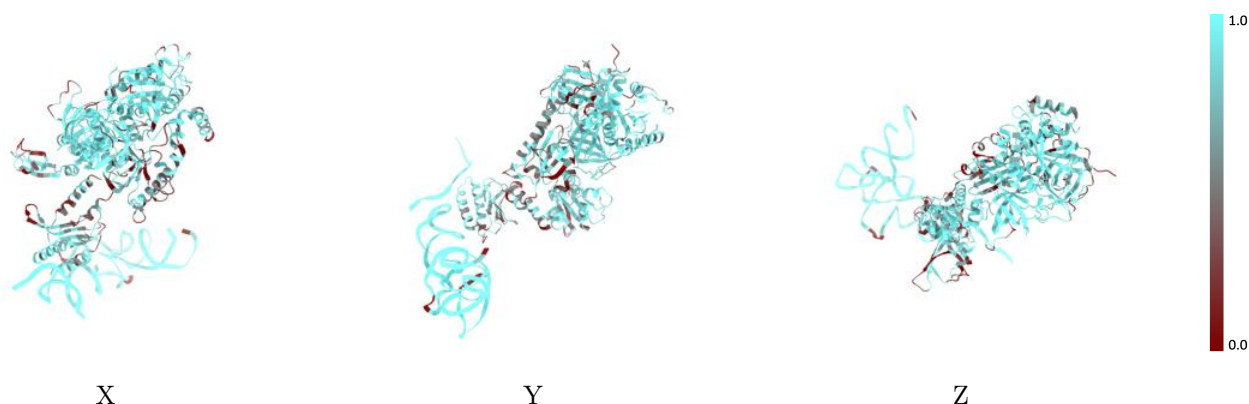
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



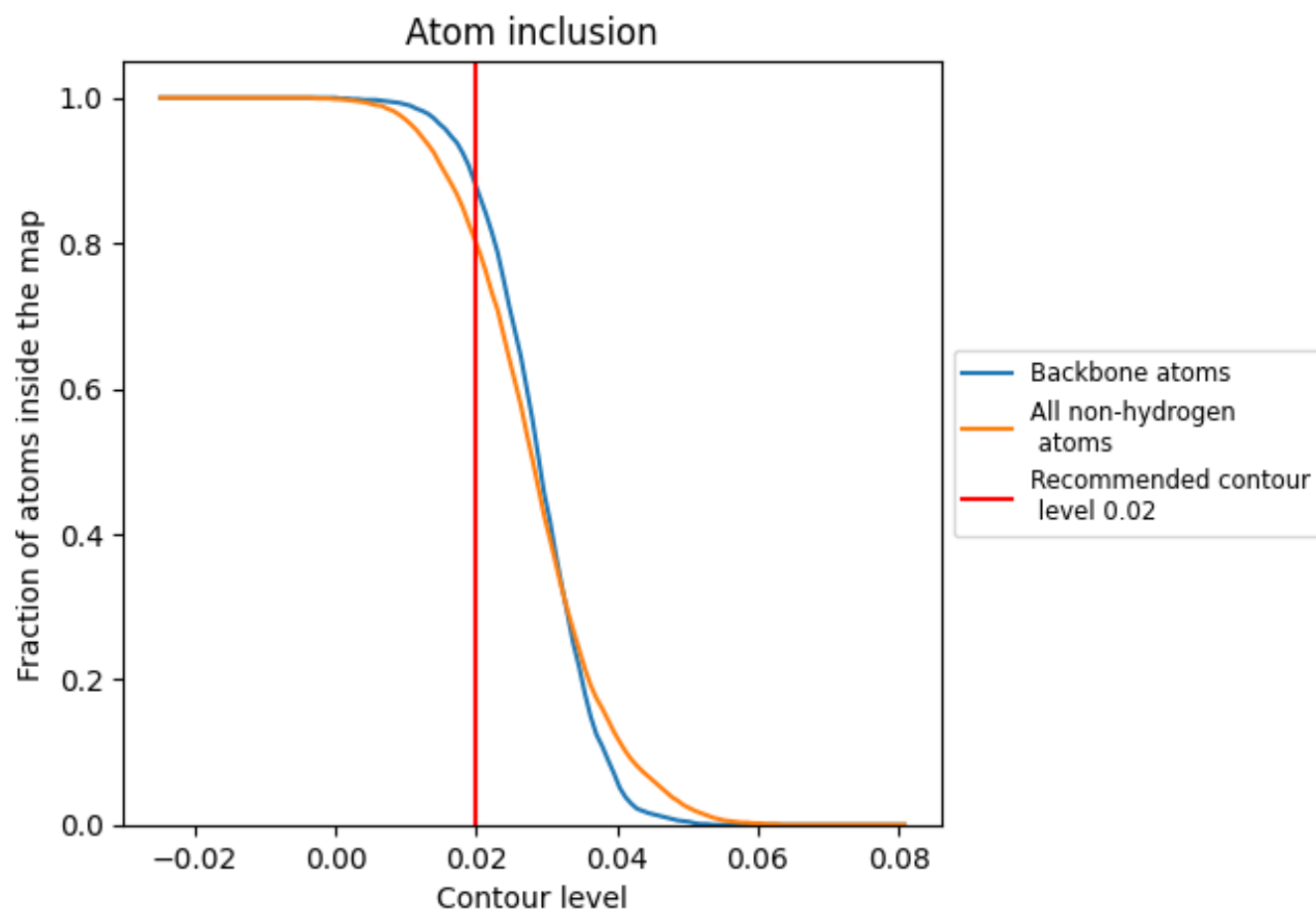
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.1170
A	0.6690	0.1050
B	0.8470	0.1060
C	1.0000	0.1560
D	0.9130	0.1540

