



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:27 PM UTC

PDB ID : 8TVX / pdb_00008tvx
EMDB ID : EMD-41654
Title : Cryo-EM structure of CPD-stalled Pol II (Conformation 2)
Authors : Sarsam, R.D.; Lahiri, I.; Leschziner, A.E.
Deposited on : 2023-08-18
Resolution : 3.70 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
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

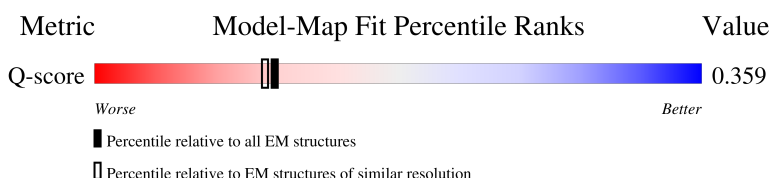
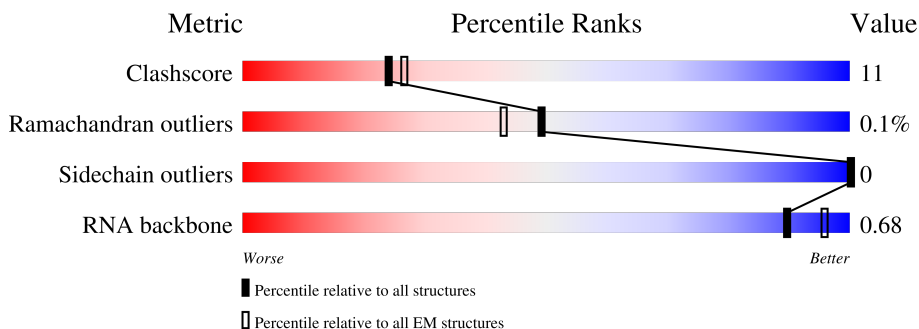
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1733	 63% 16% 21%
2	B	1224	 70% 15% 15%
3	C	318	 72% 12% 16%

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	47	
14	T	47	
15	R	10	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 59080 atoms, of which 28632 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1367	Total	C	H	N	O	S	0	0
			21595	6779	10846	1885	2024	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1041	Total	C	H	N	O	S	0	0
			16378	5223	8141	1435	1526	53		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	266	Total	C	H	N	O	S	0	0
			4146	1317	2051	348	417	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	142	Total	C	H	N	O	S	0	0
			2066	667	990	191	216	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	215	Total	C	H	N	O	S	0	0
			3548	1116	1788	310	322	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	81	Total	C	H	N	O	S	0	0
			1330	419	673	111	124	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			1806	701	696	198	207	4		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	133	Total	C	H	N	O	S	0	0
			2090	668	1030	174	213	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1303	479	515	151	153	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	65	Total	C	H	N	O	S	0	0
			1074	339	542	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	104	Total	C	H	N	O	S	0	0
			1673	534	839	142	157	1		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			751	224	387	72	64	4		

- Molecule 13 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	17	Total	C	N	O	P	0	0
			361	168	81	96	16		

- Molecule 14 is a DNA chain called DNA (TS).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	29	Total	C	H	N	O	P	0	0
			620	287	24	88	191	30		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	R	10	Total	C	H	N	O	P	0	0
			330	98	110	45	67	10		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	C	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

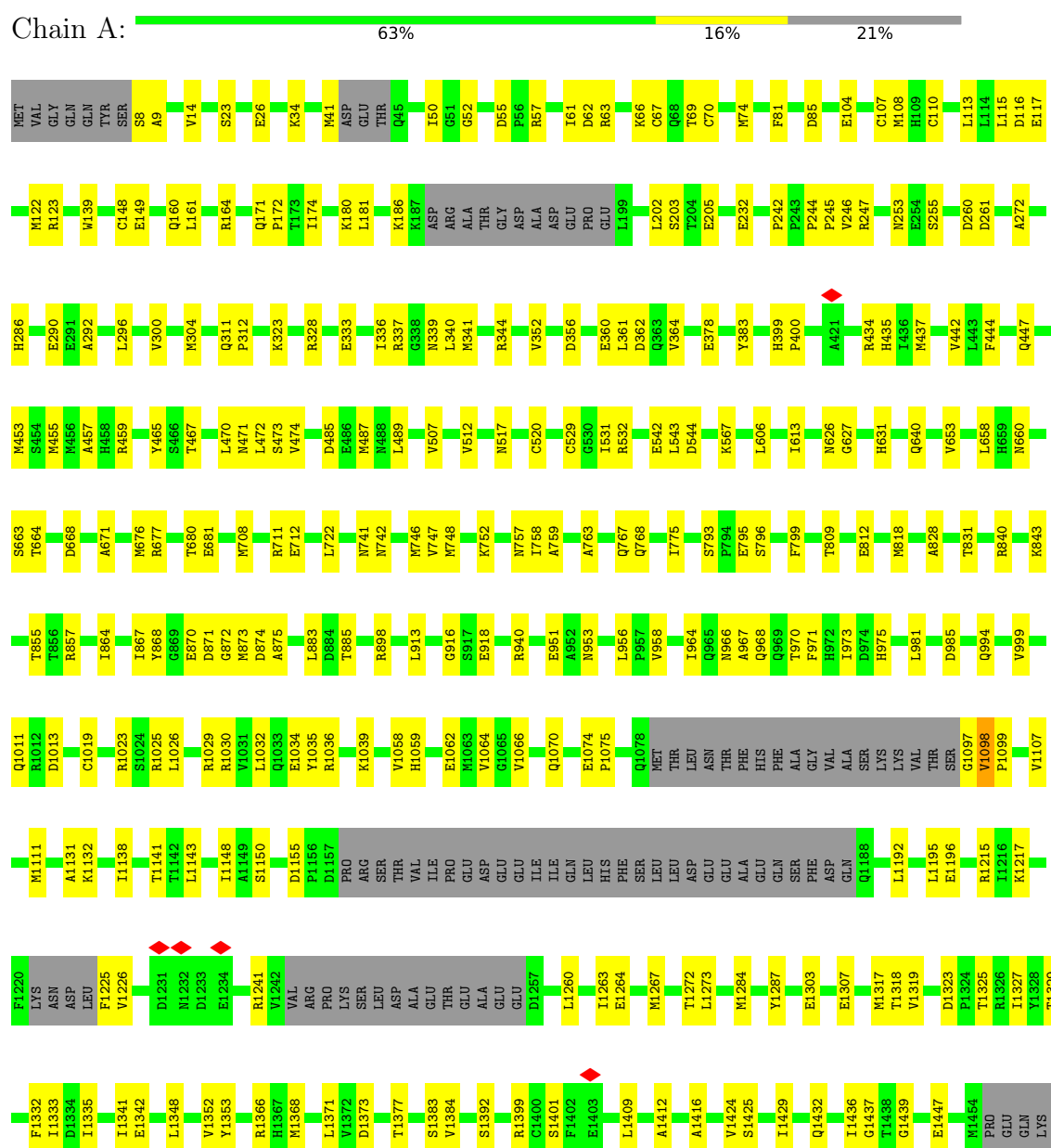
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	

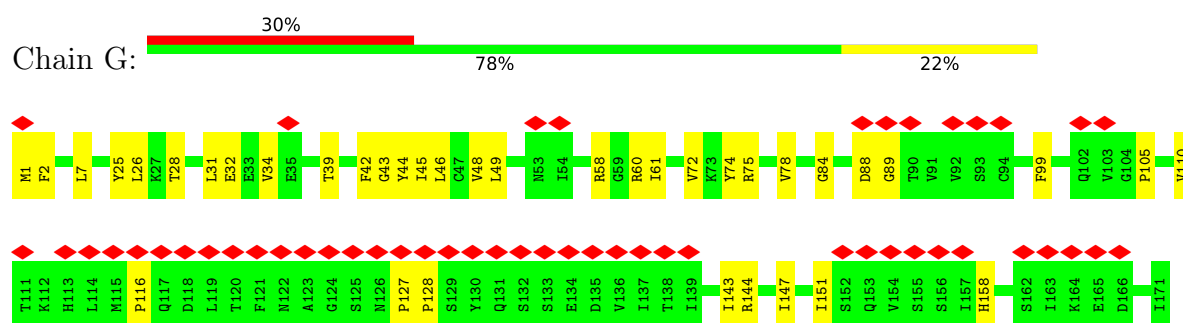
3 Residue-property plots

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.

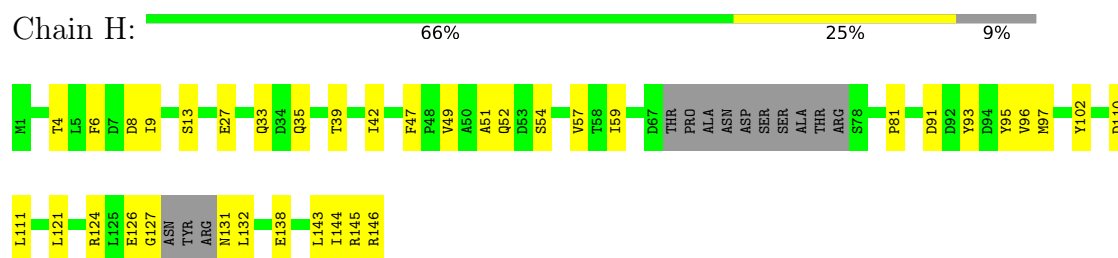
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



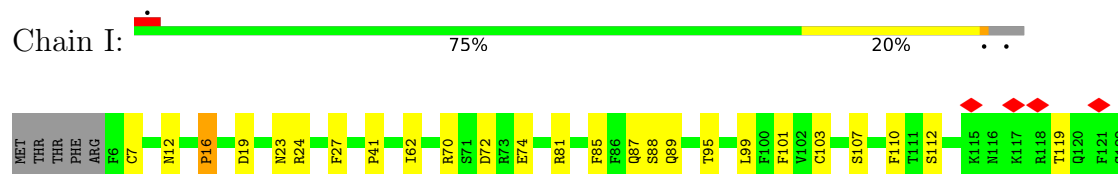




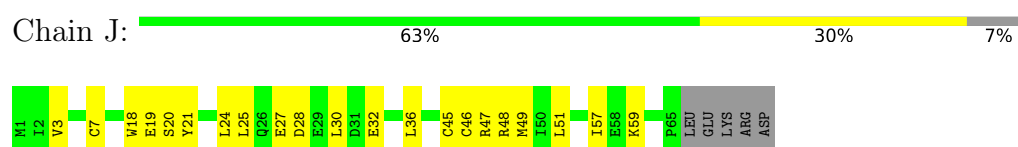
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



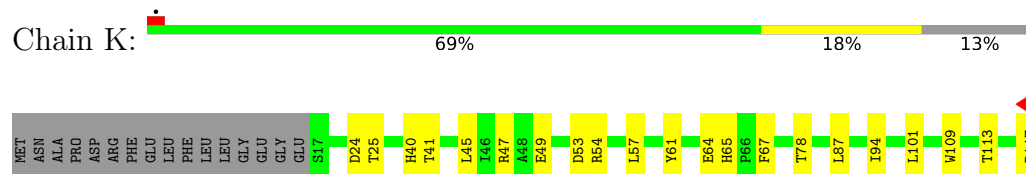
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



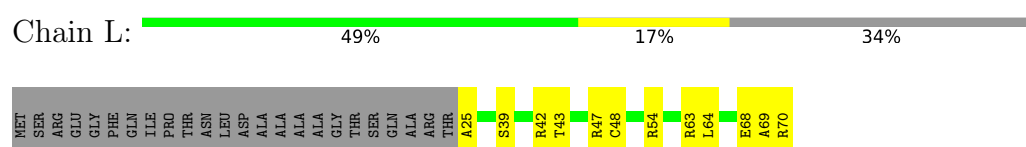
- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



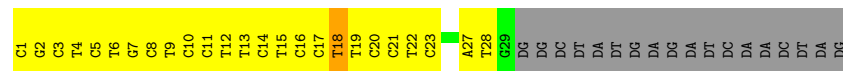
- Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



- Molecule 13: DNA (NTS)

[illegible]

Chain T: 9% 51% 0% 38%



Chain R: 80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.994	Depositor
Minimum map value	-0.720	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TTD, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/10939	0.32	0/14785
2	B	0.17	0/8396	0.33	1/11323 (0.0%)
3	C	0.18	0/2133	0.31	0/2891
4	D	0.14	0/1084	0.40	0/1460
5	E	0.14	0/1796	0.34	0/2416
6	F	0.19	0/669	0.40	0/903
7	G	0.22	0/1126	0.65	4/1531 (0.3%)
8	H	0.19	0/1076	0.36	0/1455
9	I	0.16	0/798	0.57	2/1082 (0.2%)
10	J	0.21	0/541	0.38	0/727
11	K	0.18	0/850	0.29	0/1148
12	L	0.14	0/366	0.34	0/485
13	N	0.19	0/407	0.29	0/629
14	T	0.19	0/615	0.35	0/941
15	R	0.12	0/247	0.18	0/384
All	All	0.17	0/31043	0.36	7/42160 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	116	PRO	N-CA-CB	8.81	111.12	103.19
2	B	877	PRO	N-CA-CB	8.76	111.11	103.31
7	G	127	PRO	N-CA-CB	7.71	111.08	102.60
9	I	41	PRO	N-CA-CB	7.61	111.09	103.48
9	I	16	PRO	N-CA-CB	7.49	111.11	103.25
7	G	128	PRO	N-CA-CB	7.47	111.09	103.25
7	G	105	PRO	N-CA-CB	7.25	111.08	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10749	10846	10846	213	0
2	B	8237	8141	8178	138	0
3	C	2095	2051	2053	23	0
4	D	1076	990	1032	26	0
5	E	1760	1788	1788	33	0
6	F	657	673	673	26	0
7	G	1110	696	882	23	0
8	H	1060	1030	1030	32	0
9	I	788	515	622	16	0
10	J	532	542	542	19	0
11	K	834	839	839	17	0
12	L	364	387	388	8	0
13	N	361	0	189	49	0
14	T	596	24	343	57	0
15	R	220	110	110	2	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	30448	28632	29515	614	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 11.

All (614) 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)
14:T:21:DC:H2''	14:T:22:DT:H5'	1.27	1.08
14:T:12:DT:H2'	14:T:13:DT:H71	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:LEU:HD23	6:F:122:MET:HE2	1.50	0.93
1:A:1062:GLU:OE1	6:F:88:TYR:OH	1.89	0.90
4:D:56:ARG:NH2	4:D:152:SER:OG	2.04	0.89
14:T:27:DA:H2''	14:T:28:DT:H5''	1.55	0.88
5:E:77:SER:OG	5:E:103:LYS:NZ	2.07	0.87
12:L:47:ARG:NH1	12:L:48:CYS:O	2.08	0.87
13:N:35:DA:H2''	13:N:36:DA:H5'	1.54	0.86
8:H:54:SER:O	8:H:146:ARG:NH1	2.08	0.86
1:A:485:ASP:OD1	15:R:10:A:O3'	1.97	0.82
14:T:21:DC:C2'	14:T:22:DT:H5'	2.08	0.82
6:F:85:MET:HE3	6:F:90:ARG:HB2	1.62	0.82
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.14	0.80
1:A:871:ASP:OD2	1:A:1366:ARG:NH2	2.15	0.78
1:A:567:LYS:NZ	8:H:91:ASP:O	2.17	0.78
1:A:328:ARG:NE	2:B:1206:GLU:OE2	2.17	0.77
13:N:37:DG:N2	14:T:11:DC:O2	2.15	0.77
1:A:1353:TYR:HA	1:A:1368:MET:HE1	1.68	0.76
1:A:870:GLU:OE1	5:E:202:SER:OG	2.01	0.75
5:E:66:GLU:N	5:E:66:GLU:OE1	2.20	0.75
5:E:157:SER:N	5:E:160:GLU:OE2	2.19	0.74
1:A:360:GLU:N	1:A:360:GLU:OE1	2.20	0.74
2:B:776:GLN:NE2	15:R:9:G:OP1	2.21	0.73
2:B:216:GLU:OE1	2:B:500:THR:OG1	2.04	0.73
1:A:855:THR:OG1	1:A:857:ARG:NH1	2.22	0.73
13:N:37:DG:N1	14:T:11:DC:N3	2.37	0.72
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.22	0.72
7:G:84:GLY:N	7:G:147:ILE:O	2.21	0.72
13:N:43:DG:H2''	13:N:44:DA:C8	2.25	0.72
2:B:233:PRO:O	2:B:260:GLY:N	2.23	0.71
12:L:25:ALA:N	12:L:39:SER:O	2.23	0.71
13:N:39:DA:OP2	13:N:39:DA:H2'	1.90	0.71
14:T:9:DT:H2''	14:T:10:DC:C5'	2.21	0.71
2:B:442:PHE:N	2:B:444:MET:SD	2.64	0.71
2:B:1122:ARG:N	14:T:22:DT:OP1	2.24	0.70
2:B:816:GLU:OE2	10:J:59:LYS:NZ	2.19	0.70
7:G:26:LEU:HD21	7:G:72:VAL:HG21	1.72	0.70
1:A:567:LYS:NZ	8:H:93:TYR:O	2.22	0.70
2:B:309:GLN:OE1	2:B:392:ARG:NH2	2.25	0.70
1:A:1447:GLU:OE1	1:A:1447:GLU:N	2.24	0.70
1:A:1260:LEU:O	1:A:1264:GLU:N	2.25	0.70
4:D:203:SER:OG	4:D:205:ASP:OD1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ASN:O	10:J:48:ARG:NH1	2.25	0.69
1:A:517:ASN:ND2	1:A:875:ALA:O	2.26	0.69
3:C:241:ASP:OD2	11:K:109:TRP:NE1	2.24	0.69
1:A:885:THR:O	1:A:940:ARG:NH1	2.25	0.69
1:A:1352:VAL:HG12	1:A:1368:MET:HE3	1.75	0.69
9:I:74:GLU:OE2	9:I:81:ARG:NE	2.25	0.69
14:T:6:DT:H2''	14:T:7:DG:C8	2.28	0.69
1:A:1263:ILE:CG2	1:A:1267:MET:HE1	2.22	0.69
1:A:1225:PHE:N	1:A:1241:ARG:O	2.26	0.68
3:C:75:MET:O	3:C:246:ARG:NH2	2.26	0.68
10:J:24:LEU:HD12	10:J:30:LEU:HD12	1.74	0.68
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.26	0.68
7:G:7:LEU:O	7:G:74:TYR:N	2.27	0.68
1:A:1329:THR:HG22	1:A:1335:ILE:HD11	1.75	0.67
13:N:32:DG:H2''	13:N:33:DA:OP2	1.94	0.67
2:B:523:CYS:SG	2:B:750:GLY:N	2.67	0.67
4:D:141:LEU:HD21	7:G:44:TYR:OH	1.94	0.67
1:A:117:GLU:O	1:A:123:ARG:NH1	2.28	0.67
1:A:149:GLU:N	1:A:149:GLU:OE1	2.28	0.66
1:A:532:ARG:NH2	1:A:748:MET:SD	2.68	0.66
13:N:32:DG:N2	14:T:17:DC:O2	2.28	0.66
14:T:8:DC:H2'	14:T:9:DT:H71	1.77	0.66
13:N:35:DA:N6	14:T:13:DT:O4	2.20	0.65
13:N:41:DC:H2''	13:N:42:DA:C8	2.32	0.65
2:B:614:SER:OG	2:B:632:ARG:NH1	2.29	0.65
13:N:46:DC:H6	13:N:46:DC:H5'	1.62	0.65
14:T:21:DC:H2''	14:T:22:DT:C5'	2.17	0.65
1:A:171:GLN:O	1:A:186:LYS:NZ	2.25	0.64
2:B:1053:GLU:OE1	2:B:1053:GLU:N	2.29	0.64
7:G:7:LEU:N	7:G:74:TYR:O	2.31	0.64
10:J:27:GLU:OE1	10:J:27:GLU:N	2.31	0.64
14:T:15:DT:H2''	14:T:16:DC:H5'	1.79	0.64
2:B:397:ASP:OD2	2:B:515:HIS:NE2	2.30	0.64
1:A:994:GLN:OE1	1:A:1023:ARG:NH1	2.31	0.63
13:N:38:DG:H2''	13:N:39:DA:H8	1.62	0.63
1:A:66:LYS:O	1:A:69:THR:N	2.31	0.63
1:A:148:CYS:SG	1:A:171:GLN:NE2	2.70	0.63
2:B:485:ARG:NH2	2:B:791:THR:O	2.32	0.63
14:T:9:DT:H2''	14:T:10:DC:H5'	1.80	0.63
1:A:69:THR:O	1:A:69:THR:HG22	1.97	0.63
2:B:841:MET:HE2	2:B:846:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:42:DA:H2''	13:N:43:DG:C8	2.33	0.63
8:H:138:GLU:OE1	8:H:138:GLU:N	2.28	0.62
14:T:6:DT:OP2	14:T:6:DT:H2'	1.99	0.62
2:B:186:GLU:N	2:B:186:GLU:OE1	2.32	0.62
1:A:640:GLN:OE1	1:A:640:GLN:N	2.30	0.62
14:T:19:DT:O2	14:T:19:DT:H2'	2.00	0.62
7:G:39:THR:O	7:G:43:GLY:N	2.33	0.61
1:A:50:ILE:HG22	1:A:52:GLY:H	1.65	0.61
2:B:199:MET:HE3	2:B:199:MET:HA	1.81	0.61
2:B:239:GLU:O	2:B:240:ILE:HD13	1.99	0.61
7:G:99:PHE:O	7:G:110:VAL:N	2.33	0.61
13:N:47:DG:H5'	13:N:47:DG:C8	2.35	0.61
1:A:795:GLU:OE1	1:A:795:GLU:N	2.28	0.61
2:B:221:ASN:N	2:B:241:ARG:O	2.33	0.61
1:A:1287:TYR:O	1:A:1303:GLU:N	2.34	0.61
3:C:5:GLY:O	3:C:24:ASN:ND2	2.32	0.61
8:H:143:LEU:O	8:H:144:ILE:HD13	2.00	0.61
1:A:471:ASN:O	1:A:474:VAL:HG12	2.01	0.61
13:N:31:DG:H1'	13:N:32:DG:C8	2.35	0.61
2:B:1100:ASP:O	2:B:1122:ARG:NH2	2.34	0.61
2:B:842:ASN:OD1	2:B:844:SER:N	2.34	0.61
14:T:7:DG:H2''	14:T:8:DC:H6	1.65	0.61
10:J:7:CYS:HA	10:J:49:MET:HE3	1.82	0.60
9:I:85:PHE:CD1	9:I:99:LEU:HD23	2.37	0.60
13:N:43:DG:H2''	13:N:44:DA:H8	1.67	0.60
2:B:327:ARG:NH2	2:B:371:GLU:OE2	2.33	0.60
2:B:999:MET:HE3	2:B:1011:ILE:HD11	1.84	0.60
1:A:1353:TYR:CA	1:A:1368:MET:HE1	2.32	0.60
1:A:344:ARG:NE	2:B:1120:GLU:OE2	2.28	0.59
14:T:11:DC:H2''	14:T:12:DT:C6	2.37	0.59
4:D:39:ASN:ND2	4:D:45:GLU:OE2	2.35	0.59
5:E:169:ARG:NE	6:F:140:ASP:OD2	2.34	0.59
1:A:383:TYR:CZ	6:F:111:LEU:HD21	2.38	0.59
14:T:27:DA:H2''	14:T:28:DT:H6	1.65	0.59
1:A:722:LEU:HD12	1:A:799:PHE:CE1	2.37	0.59
7:G:25:TYR:O	7:G:28:THR:OG1	2.17	0.59
9:I:103:CYS:O	9:I:107:SER:N	2.36	0.59
1:A:966:ASN:O	1:A:970:THR:HG23	2.03	0.58
13:N:36:DA:H2''	13:N:37:DG:C8	2.38	0.58
1:A:1263:ILE:HG23	1:A:1267:MET:HE1	1.85	0.58
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:THR:HG21	2:B:679:TYR:HD1	1.68	0.58
2:B:1210:MET:HA	2:B:1210:MET:HE2	1.86	0.58
1:A:531:ILE:HG12	1:A:653:VAL:HG21	1.85	0.58
1:A:1392:SER:O	1:A:1399:ARG:NH1	2.35	0.58
2:B:120:ARG:NE	2:B:956:THR:O	2.36	0.58
2:B:183:GLU:N	2:B:183:GLU:OE1	2.33	0.58
1:A:975:HIS:O	1:A:1036:ARG:NE	2.37	0.58
5:E:28:TYR:OH	5:E:76:GLY:O	2.12	0.58
1:A:1436:ILE:O	1:A:1439:GLY:N	2.35	0.58
2:B:842:ASN:CG	2:B:844:SER:HG	2.09	0.58
3:C:185:LYS:NZ	3:C:210:GLU:OE2	2.35	0.58
1:A:174:ILE:HG22	1:A:181:LEU:HD12	1.86	0.58
14:T:7:DG:H2''	14:T:8:DC:C6	2.39	0.58
14:T:21:DC:H2'	14:T:22:DT:H71	1.85	0.58
2:B:46:GLN:HB2	2:B:545:ILE:HG22	1.86	0.57
6:F:119:ARG:HA	6:F:122:MET:HE3	1.86	0.57
1:A:203:SER:OG	1:A:205:GLU:OE1	2.22	0.57
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.33	0.57
9:I:87:GLN:NE2	9:I:88:SER:O	2.36	0.57
2:B:620:ARG:NH1	9:I:89:GLN:OE1	2.37	0.57
2:B:298:LEU:O	2:B:302:CYS:N	2.37	0.57
3:C:55:THR:OG1	3:C:152:GLU:N	2.37	0.57
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.37	0.57
13:N:37:DG:H2''	13:N:38:DG:H8	1.69	0.57
5:E:82:PHE:CE1	5:E:111:VAL:HG21	2.40	0.57
6:F:131:PRO:C	6:F:132:LEU:HD22	2.30	0.57
6:F:133:VAL:HG23	6:F:146:TRP:C	2.28	0.57
14:T:16:DC:H1'	14:T:17:DC:C1'	2.35	0.57
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.85	0.57
2:B:326:ASP:OD1	2:B:328:GLU:N	2.37	0.56
4:D:163:VAL:HG23	4:D:214:LEU:HD11	1.86	0.56
7:G:49:LEU:N	7:G:75:ARG:O	2.38	0.56
14:T:5:DC:H2'	14:T:6:DT:H71	1.86	0.56
14:T:15:DT:H2''	14:T:16:DC:C5'	2.35	0.56
8:H:110:ASP:OD1	8:H:111:LEU:N	2.38	0.56
14:T:27:DA:C2'	14:T:28:DT:H5''	2.30	0.56
7:G:28:THR:O	7:G:32:GLU:OE1	2.22	0.56
1:A:711:ARG:NH2	9:I:95:THR:OG1	2.38	0.56
2:B:496:ARG:NH2	2:B:540:SER:O	2.36	0.56
6:F:86:THR:HB	6:F:89:GLU:OE1	2.06	0.56
13:N:39:DA:H2''	13:N:40:DG:OP2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:VAL:N	2:B:396:ASP:OD2	2.38	0.56
1:A:383:TYR:CE1	6:F:111:LEU:HD21	2.41	0.56
1:A:1263:ILE:HG22	1:A:1267:MET:HE1	1.87	0.56
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.87	0.56
2:B:106:ASP:OD2	12:L:54:ARG:NH2	2.39	0.55
5:E:160:GLU:OE1	5:E:160:GLU:N	2.35	0.55
13:N:31:DG:H1'	13:N:32:DG:H5'	1.87	0.55
1:A:447:GLN:NE2	2:B:1134:GLU:OE2	2.38	0.55
1:A:1143:LEU:HD12	1:A:1273:LEU:HD11	1.88	0.55
2:B:499:ASN:OD1	2:B:500:THR:N	2.40	0.55
2:B:135:ARG:NH1	2:B:136:THR:O	2.39	0.55
3:C:163:ILE:HG22	3:C:165:LYS:H	1.72	0.55
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.42	0.55
14:T:4:DT:H2''	14:T:5:DC:OP2	2.07	0.55
14:T:16:DC:H1'	14:T:17:DC:N1	2.21	0.55
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.89	0.55
8:H:127:GLY:O	8:H:132:LEU:N	2.39	0.55
13:N:39:DA:H2''	13:N:40:DG:H8	1.72	0.55
14:T:5:DC:H2''	14:T:6:DT:C6	2.40	0.55
13:N:38:DG:H2''	13:N:39:DA:C8	2.41	0.55
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.41	0.55
1:A:304:MET:HB3	2:B:1210:MET:HE1	1.89	0.55
11:K:24:ASP:OD1	11:K:25:THR:N	2.38	0.54
1:A:344:ARG:NH1	14:T:21:DC:OP1	2.41	0.54
1:A:1019:CYS:SG	1:A:1023:ARG:NH1	2.77	0.54
2:B:259:TYR:O	2:B:266:ALA:N	2.40	0.54
5:E:116:ILE:HD13	5:E:121:MET:CE	2.37	0.54
13:N:32:DG:O6	14:T:16:DC:N4	2.41	0.54
10:J:32:GLU:O	10:J:36:LEU:HD23	2.08	0.54
14:T:7:DG:H2''	14:T:8:DC:OP2	2.08	0.54
1:A:66:LYS:O	1:A:70:CYS:N	2.39	0.54
11:K:113:THR:O	11:K:117:ASP:N	2.40	0.54
1:A:174:ILE:CG2	1:A:181:LEU:HD12	2.37	0.54
1:A:1307:GLU:OE1	1:A:1307:GLU:N	2.41	0.54
8:H:4:THR:OG1	8:H:59:ILE:O	2.25	0.53
1:A:41:MET:HE2	1:A:41:MET:HA	1.91	0.53
14:T:12:DT:H4'	14:T:12:DT:OP1	2.07	0.53
2:B:287:ARG:HH12	2:B:292:ILE:HG23	1.73	0.53
4:D:154:PHE:CZ	4:D:214:LEU:HD12	2.42	0.53
2:B:102:VAL:HG22	2:B:112:LEU:HD13	1.90	0.53
4:D:67:ARG:NH1	4:D:132:GLN:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:HD2	1:A:437:MET:HE2	1.89	0.53
5:E:79:TRP:NE1	5:E:81:GLU:OE1	2.39	0.53
3:C:25:VAL:N	3:C:226:ASP:OD1	2.40	0.53
4:D:189:ASP:O	4:D:193:THR:HG23	2.09	0.53
8:H:57:VAL:HG22	8:H:144:ILE:HD12	1.90	0.53
13:N:47:DG:H5'	13:N:47:DG:H8	1.74	0.53
14:T:2:DG:H2''	14:T:3:DC:H5'	1.89	0.53
1:A:708:MET:HB3	1:A:712:GLU:OE2	2.09	0.52
1:A:970:THR:HG1	1:A:971:PHE:HD1	1.52	0.52
10:J:20:SER:O	10:J:24:LEU:HD23	2.09	0.52
1:A:362:ASP:O	1:A:459:ARG:N	2.41	0.52
1:A:529:CYS:SG	2:B:1015:HIS:NE2	2.81	0.52
13:N:34:DG:H2''	13:N:35:DA:H8	1.74	0.52
2:B:40:GLU:OE1	2:B:681:TRP:N	2.42	0.52
13:N:46:DC:H5'	13:N:46:DC:C6	2.42	0.52
14:T:22:DT:H2'	14:T:23:DC:C6	2.45	0.52
3:C:89:GLU:O	3:C:91:HIS:N	2.43	0.52
7:G:39:THR:N	7:G:43:GLY:O	2.35	0.52
7:G:60:ARG:NH1	7:G:61:ILE:O	2.42	0.52
1:A:626:ASN:O	1:A:631:HIS:ND1	2.40	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.90	0.52
2:B:579:ARG:NH2	2:B:623:GLU:OE2	2.42	0.52
5:E:1:MET:SD	5:E:7:ARG:NH2	2.82	0.52
1:A:14:VAL:N	1:A:1432:GLN:OE1	2.35	0.52
1:A:1138:ILE:CD1	1:A:1319:VAL:HG21	2.40	0.52
1:A:951:GLU:OE2	1:A:953:ASN:ND2	2.42	0.51
10:J:24:LEU:HD13	10:J:28:ASP:OD2	2.10	0.51
1:A:115:LEU:HB2	1:A:122:MET:HE3	1.92	0.51
6:F:96:THR:O	6:F:100:GLN:OE1	2.29	0.51
4:D:172:LEU:HD23	4:D:177:VAL:HG22	1.93	0.51
1:A:544:ASP:OD1	11:K:47:ARG:NH1	2.34	0.51
1:A:336:ILE:HG23	1:A:337:ARG:N	2.25	0.51
4:D:141:LEU:HD21	7:G:44:TYR:CZ	2.46	0.51
1:A:840:ARG:NH1	1:A:1384:VAL:HG23	2.25	0.51
14:T:5:DC:H2''	14:T:6:DT:OP2	2.11	0.51
1:A:292:ALA:O	1:A:296:LEU:HD23	2.10	0.51
13:N:45:DG:H2''	13:N:46:DC:H5'	1.91	0.51
1:A:1030:ARG:NE	1:A:1034:GLU:OE1	2.32	0.51
8:H:27:GLU:OE2	8:H:27:GLU:HA	2.11	0.51
6:F:110:ASP:OD2	6:F:123:LYS:NZ	2.44	0.51
7:G:2:PHE:CE2	7:G:46:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:4:DT:H2''	14:T:5:DC:C6	2.46	0.51
2:B:261:ARG:O	2:B:266:ALA:HB3	2.11	0.50
4:D:157:GLN:O	4:D:160:VAL:N	2.44	0.50
1:A:453:MET:HE2	1:A:520:CYS:SG	2.51	0.50
1:A:1074:GLU:CD	1:A:1075:PRO:HD3	2.37	0.50
1:A:1424:VAL:HG13	1:A:1425:SER:N	2.26	0.50
1:A:746:MET:HE1	2:B:1015:HIS:HA	1.92	0.50
5:E:3:GLN:NE2	5:E:51:GLY:O	2.43	0.50
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.92	0.50
13:N:37:DG:H2''	13:N:38:DG:C8	2.47	0.50
1:A:180:LYS:NZ	1:A:202:LEU:O	2.45	0.50
1:A:1226:VAL:HG23	1:A:1226:VAL:O	2.11	0.50
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.92	0.50
1:A:272:ALA:HB1	1:A:296:LEU:HD22	1.93	0.50
2:B:239:GLU:C	2:B:240:ILE:HD13	2.37	0.50
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.91	0.50
1:A:61:ILE:HG22	1:A:62:ASP:N	2.27	0.50
1:A:809:THR:OG1	1:A:812:GLU:OE1	2.20	0.50
13:N:41:DC:OP2	13:N:41:DC:H2'	2.12	0.50
1:A:361:LEU:HD21	1:A:473:SER:OG	2.12	0.50
1:A:874:ASP:OD1	1:A:875:ALA:N	2.44	0.50
5:E:116:ILE:HD11	5:E:120:ALA:HB1	1.94	0.50
2:B:101:MET:HE2	2:B:101:MET:HA	1.94	0.50
5:E:54:GLN:O	5:E:56:LYS:N	2.45	0.50
1:A:1215:ARG:NE	1:A:1272:THR:O	2.41	0.49
1:A:1317:MET:HE1	1:A:1327:ILE:HG21	1.94	0.49
2:B:370:PHE:O	2:B:374:LYS:N	2.43	0.49
2:B:859:TYR:OH	2:B:945:GLU:OE1	2.23	0.49
13:N:36:DA:H2''	13:N:37:DG:H8	1.77	0.49
1:A:606:LEU:CD2	8:H:102:TYR:OH	2.60	0.49
1:A:951:GLU:OE2	1:A:953:ASN:N	2.45	0.49
2:B:980:PHE:CD1	2:B:990:ILE:HD11	2.47	0.49
1:A:160:GLN:NE2	1:A:161:LEU:O	2.44	0.49
1:A:1148:ILE:N	1:A:1196:GLU:O	2.40	0.49
2:B:212:LEU:HD21	2:B:461:LEU:CD1	2.41	0.49
4:D:57:LEU:HD21	4:D:155:ARG:O	2.12	0.49
1:A:1059:HIS:HB3	6:F:86:THR:HG23	1.94	0.49
1:A:613:ILE:HG21	8:H:102:TYR:CD1	2.48	0.49
1:A:613:ILE:HG21	8:H:102:TYR:CE1	2.47	0.49
1:A:1059:HIS:ND1	6:F:86:THR:HG23	2.27	0.49
4:D:163:VAL:CG2	4:D:214:LEU:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:ILE:N	7:G:158:HIS:O	2.45	0.49
8:H:54:SER:OG	8:H:146:ARG:NH1	2.43	0.49
1:A:232:GLU:OE1	1:A:232:GLU:N	2.40	0.49
14:T:14:DC:H2''	14:T:15:DT:H71	1.93	0.49
6:F:125:LEU:C	6:F:125:LEU:HD23	2.38	0.49
8:H:13:SER:N	8:H:27:GLU:O	2.43	0.49
9:I:7:CYS:N	9:I:12:ASN:O	2.42	0.49
9:I:19:ASP:N	9:I:24:ARG:O	2.40	0.49
11:K:45:LEU:HD11	11:K:94:ILE:HD12	1.93	0.49
11:K:101:LEU:O	11:K:101:LEU:HD23	2.12	0.49
14:T:12:DT:C2'	14:T:13:DT:H71	2.32	0.49
1:A:399:HIS:O	1:A:435:HIS:ND1	2.43	0.48
1:A:362:ASP:HA	1:A:507:VAL:HG21	1.95	0.48
2:B:711:GLU:O	2:B:715:ALA:N	2.36	0.48
4:D:117:GLU:O	4:D:155:ARG:NE	2.38	0.48
11:K:101:LEU:HD23	11:K:101:LEU:C	2.38	0.48
1:A:828:ALA:O	1:A:831:THR:OG1	2.30	0.48
1:A:973:ILE:O	1:A:975:HIS:ND1	2.46	0.48
1:A:1131:ALA:CB	1:A:1284:MET:HE2	2.43	0.48
5:E:116:ILE:HD11	5:E:120:ALA:CB	2.42	0.48
9:I:101:PHE:N	9:I:110:PHE:O	2.44	0.48
1:A:107:CYS:HB2	1:A:110:CYS:HB3	1.94	0.48
1:A:985:ASP:OD2	1:A:1039:LYS:NZ	2.35	0.48
1:A:1013:ASP:O	5:E:205:SER:OG	2.30	0.48
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.14	0.48
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.95	0.48
12:L:42:ARG:HE	12:L:43:THR:H	1.61	0.48
13:N:40:DG:H2''	13:N:41:DC:OP2	2.14	0.48
1:A:341:MET:HE3	1:A:1401:SER:CB	2.42	0.48
2:B:1201:LYS:NZ	2:B:1205:GLN:OE1	2.45	0.48
1:A:1143:LEU:HD12	1:A:1273:LEU:CD1	2.43	0.48
2:B:101:MET:O	2:B:169:ARG:NH2	2.39	0.48
2:B:287:ARG:NH1	2:B:292:ILE:HG23	2.27	0.48
5:E:200:ARG:NH1	5:E:210:SER:OG	2.45	0.48
8:H:127:GLY:O	8:H:131:ASN:N	2.47	0.48
1:A:1097:GLY:O	1:A:1098:VAL:HB	2.14	0.48
1:A:916:GLY:N	1:A:918:GLU:OE1	2.46	0.48
1:A:1371:LEU:C	1:A:1371:LEU:HD23	2.38	0.48
10:J:24:LEU:HD12	10:J:30:LEU:CD1	2.42	0.48
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.95	0.47
2:B:212:LEU:HD21	2:B:461:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:130:ILE:HB	6:F:148:VAL:HG11	1.95	0.47
1:A:116:ASP:OD2	1:A:164:ARG:NE	2.46	0.47
1:A:286:HIS:NE2	1:A:290:GLU:OE2	2.47	0.47
1:A:457:ALA:O	1:A:507:VAL:HG23	2.14	0.47
7:G:89:GLY:N	7:G:143:ILE:O	2.47	0.47
2:B:651:LEU:HD22	2:B:710:LEU:CD2	2.45	0.47
2:B:1129:ARG:HE	14:T:20:DC:H5''	1.78	0.47
4:D:51:ASN:OD1	4:D:52:LEU:N	2.47	0.47
9:I:112:SER:O	9:I:119:THR:HG21	2.14	0.47
1:A:108:MET:HE3	1:A:172:PRO:HD2	1.97	0.47
1:A:336:ILE:HG23	1:A:337:ARG:H	1.79	0.47
8:H:81:PRO:HG2	11:K:57:LEU:HD23	1.96	0.47
10:J:51:LEU:HD23	10:J:51:LEU:O	2.15	0.47
1:A:74:MET:O	2:B:1116:ARG:NH2	2.41	0.47
1:A:531:ILE:CG1	1:A:653:VAL:HG21	2.43	0.47
1:A:767:GLN:NE2	1:A:768:GLN:O	2.34	0.47
1:A:775:ILE:HG23	1:A:818:MET:HE1	1.96	0.47
1:A:864:ILE:HD12	1:A:1377:THR:HG21	1.96	0.47
1:A:1155:ASP:CB	1:A:1192:LEU:HD11	2.45	0.47
2:B:382:ILE:HG22	2:B:386:LEU:HD23	1.97	0.47
3:C:58:LEU:HD11	10:J:57:ILE:HD13	1.97	0.47
4:D:178:ALA:HB1	7:G:1:MET:HE3	1.96	0.47
8:H:51:ALA:HB1	8:H:52:GLN:OE1	2.15	0.47
13:N:38:DG:H2''	13:N:39:DA:OP2	2.15	0.47
1:A:1155:ASP:HB2	1:A:1192:LEU:HD11	1.97	0.47
2:B:526:GLU:OE2	2:B:752:ALA:N	2.48	0.47
2:B:693:ILE:HG23	2:B:697:GLU:HB2	1.95	0.47
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.97	0.47
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.97	0.47
1:A:344:ARG:NH1	2:B:1127:GLY:O	2.48	0.47
1:A:444:PHE:CD1	1:A:487:MET:HE3	2.49	0.47
8:H:33:GLN:OE1	8:H:35:GLN:NE2	2.47	0.47
13:N:32:DG:H1'	13:N:33:DA:O4'	2.15	0.47
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.97	0.47
2:B:540:SER:OG	2:B:543:SER:OG	2.27	0.47
1:A:352:VAL:O	1:A:467:THR:OG1	2.28	0.46
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.97	0.46
3:C:241:ASP:OD1	3:C:242:GLN:N	2.48	0.46
1:A:999:VAL:N	1:A:1011:GLN:OE1	2.47	0.46
2:B:562:GLY:O	2:B:590:HIS:ND1	2.47	0.46
1:A:898:ARG:O	1:A:1029:ARG:NE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.46	0.46
13:N:44:DA:H2''	13:N:45:DG:H8	1.80	0.46
1:A:658:LEU:HD13	2:B:830:TYR:O	2.15	0.46
4:D:167:LEU:HD22	4:D:177:VAL:HG13	1.98	0.46
8:H:42:ILE:HG23	8:H:95:TYR:CE2	2.50	0.46
11:K:57:LEU:HD21	11:K:78:THR:HG22	1.97	0.46
1:A:663:SER:OG	2:B:827:ILE:O	2.22	0.46
1:A:775:ILE:HD12	1:A:818:MET:HE3	1.97	0.46
1:A:1141:THR:O	1:A:1273:LEU:N	2.47	0.46
13:N:40:DG:H2''	13:N:41:DC:C6	2.51	0.46
2:B:711:GLU:O	2:B:714:GLU:N	2.48	0.46
14:T:3:DC:H2'	14:T:4:DT:H71	1.98	0.46
1:A:62:ASP:OD1	1:A:63:ARG:N	2.48	0.46
1:A:542:GLU:OE1	1:A:543:LEU:N	2.40	0.46
1:A:759:ALA:O	1:A:763:ALA:N	2.48	0.46
1:A:1138:ILE:HD11	1:A:1319:VAL:HG21	1.98	0.46
1:A:455:MET:HE2	2:B:1138:MET:HE3	1.97	0.46
1:A:883:LEU:HD21	1:A:956:LEU:HD11	1.97	0.46
5:E:157:SER:OG	5:E:160:GLU:OE1	2.30	0.46
14:T:16:DC:H2''	14:T:17:DC:C6	2.51	0.46
1:A:677:ARG:O	1:A:680:THR:N	2.49	0.46
1:A:1143:LEU:HD22	1:A:1267:MET:HB3	1.98	0.46
6:F:119:ARG:HA	6:F:122:MET:CE	2.46	0.45
12:L:68:GLU:OE2	12:L:70:ARG:NE	2.49	0.45
1:A:512:VAL:O	1:A:512:VAL:HG13	2.16	0.45
1:A:626:ASN:OD1	1:A:627:GLY:N	2.50	0.45
1:A:1332:PHE:CE2	1:A:1348:LEU:HD12	2.51	0.45
5:E:93:MET:HE3	5:E:116:ILE:HD11	1.98	0.45
11:K:64:GLU:HA	11:K:64:GLU:OE2	2.16	0.45
1:A:1074:GLU:HG3	1:A:1075:PRO:HD2	1.99	0.45
2:B:1152:MET:HE3	2:B:1152:MET:HA	1.99	0.45
7:G:34:VAL:HG11	7:G:48:VAL:HG22	1.98	0.45
8:H:35:GLN:OE1	8:H:35:GLN:N	2.36	0.45
13:N:46:DC:H2''	13:N:47:DG:C8	2.50	0.45
1:A:668:ASP:O	1:A:741:ASN:ND2	2.39	0.45
7:G:89:GLY:O	7:G:143:ILE:O	2.35	0.45
14:T:11:DC:C2'	14:T:12:DT:H71	2.47	0.45
1:A:8:SER:OG	2:B:1193:GLN:OE1	2.34	0.45
1:A:472:LEU:HD22	2:B:835:GLN:CG	2.47	0.45
1:A:775:ILE:HD12	1:A:818:MET:CE	2.47	0.45
1:A:873:MET:HA	1:A:873:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PRO:O	2:B:716:ASN:N	2.48	0.45
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.50	0.45
6:F:125:LEU:HD23	6:F:125:LEU:O	2.17	0.45
1:A:356:ASP:OD2	11:K:65:HIS:NE2	2.37	0.45
1:A:339:ASN:ND2	2:B:1117:GLN:OE1	2.40	0.45
1:A:472:LEU:HD22	2:B:835:GLN:HG3	1.98	0.45
4:D:167:LEU:HD12	4:D:168:LYS:N	2.32	0.45
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.52	0.45
1:A:968:GLN:HA	1:A:973:ILE:HD12	1.98	0.44
2:B:664:THR:HG21	2:B:679:TYR:CD1	2.51	0.44
4:D:141:LEU:HB3	4:D:145:MET:HE1	1.99	0.44
1:A:668:ASP:OD1	1:A:742:ASN:N	2.46	0.44
1:A:913:LEU:HD21	1:A:1032:LEU:HD22	2.00	0.44
1:A:1412:ALA:O	1:A:1416:ALA:N	2.50	0.44
6:F:118:LEU:CD2	6:F:122:MET:HE2	2.34	0.44
2:B:613:VAL:HG22	2:B:628:THR:HG22	1.99	0.44
3:C:181:ASP:OD1	3:C:185:LYS:N	2.48	0.44
1:A:1317:MET:HE2	1:A:1317:MET:HA	2.00	0.44
5:E:103:LYS:HD2	5:E:103:LYS:O	2.17	0.44
12:L:63:ARG:NH1	12:L:64:LEU:O	2.51	0.44
1:A:8:SER:OG	1:A:9:ALA:N	2.48	0.44
1:A:898:ARG:O	1:A:1029:ARG:NH2	2.47	0.44
2:B:737:THR:HG21	9:I:70:ARG:NH1	2.32	0.44
9:I:112:SER:C	9:I:119:THR:HG21	2.43	0.44
13:N:42:DA:H8	13:N:42:DA:OP2	2.01	0.44
1:A:364:VAL:HG21	1:A:444:PHE:CZ	2.52	0.44
1:A:1409:LEU:HD13	2:B:1207:LEU:CD2	2.48	0.44
2:B:596:LEU:O	2:B:600:LEU:HD23	2.17	0.44
2:B:789:MET:HA	2:B:789:MET:HE2	1.99	0.44
5:E:50:MET:SD	5:E:52:ARG:HB2	2.58	0.44
14:T:1:DC:H2"	14:T:2:DG:OP2	2.18	0.44
2:B:1194:ILE:HG22	2:B:1196:ILE:HG23	2.00	0.44
1:A:113:LEU:O	1:A:164:ARG:NH1	2.45	0.44
1:A:242:PRO:O	1:A:247:ARG:NH2	2.47	0.44
5:E:28:TYR:CD2	5:E:62:ALA:HB1	2.53	0.43
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.47	0.43
1:A:296:LEU:O	1:A:300:VAL:HG12	2.17	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.61	0.43
1:A:671:ALA:HB3	1:A:676:MET:HE3	2.01	0.43
2:B:224:GLN:O	2:B:239:GLU:N	2.50	0.43
2:B:621:GLU:HB2	2:B:623:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:MET:HE3	2:B:850:LEU:HD23	2.01	0.43
2:B:619:ILE:HG21	9:I:62:ILE:HA	1.99	0.43
5:E:5:ASN:CG	5:E:7:ARG:NH1	2.77	0.43
8:H:96:VAL:HG13	8:H:143:LEU:CD2	2.47	0.43
13:N:44:DA:H2''	13:N:45:DG:C8	2.53	0.43
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.33	0.43
2:B:520:GLY:O	2:B:540:SER:OG	2.35	0.43
2:B:629:ASP:OD1	2:B:630:ALA:N	2.52	0.43
4:D:160:VAL:O	4:D:163:VAL:HG12	2.18	0.43
9:I:19:ASP:O	9:I:23:ASN:N	2.52	0.43
1:A:964:ILE:O	1:A:967:ALA:HB3	2.18	0.43
13:N:37:DG:H8	13:N:37:DG:OP2	2.01	0.43
14:T:9:DT:H2'	14:T:10:DC:C6	2.53	0.43
1:A:253:ASN:O	1:A:255:SER:N	2.52	0.43
3:C:11:ARG:NH1	3:C:206:ASN:OD1	2.43	0.43
1:A:752:LYS:O	1:A:752:LYS:HG3	2.19	0.43
1:A:1217:LYS:HA	1:A:1226:VAL:HG11	2.01	0.43
13:N:32:DG:H2''	13:N:33:DA:C8	2.54	0.43
14:T:11:DC:H2''	14:T:12:DT:H71	2.01	0.43
1:A:333:GLU:O	1:A:333:GLU:CD	2.62	0.43
1:A:1353:TYR:N	1:A:1368:MET:HE1	2.34	0.43
3:C:169:LYS:NZ	12:L:69:ALA:O	2.48	0.43
5:E:54:GLN:HB3	5:E:57:MET:HE2	2.01	0.43
6:F:83:PRO:O	6:F:151:LEU:HD23	2.19	0.43
6:F:128:LYS:HE3	6:F:153:VAL:HG23	2.01	0.43
13:N:42:DA:H2''	13:N:43:DG:H8	1.81	0.43
14:T:5:DC:C2'	14:T:6:DT:H71	2.48	0.43
2:B:1152:MET:HE3	2:B:1152:MET:CA	2.49	0.42
5:E:56:LYS:HG3	5:E:57:MET:SD	2.59	0.42
13:N:40:DG:H2''	13:N:41:DC:H6	1.82	0.42
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.42	0.42
1:A:246:VAL:O	1:A:328:ARG:NH2	2.52	0.42
1:A:470:LEU:HD21	1:A:487:MET:HE1	2.00	0.42
5:E:46:TYR:CD1	5:E:58:MET:HG2	2.54	0.42
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.99	0.42
2:B:175:ARG:NH2	2:B:198:ASP:O	2.46	0.42
2:B:546:SER:N	2:B:632:ARG:O	2.36	0.42
2:B:845:SER:HB3	2:B:850:LEU:HD22	2.01	0.42
3:C:105:GLY:HA3	3:C:148:ARG:O	2.19	0.42
5:E:171:LYS:N	5:E:174:GLN:OE1	2.43	0.42
9:I:72:ASP:OD1	9:I:72:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:45:CYS:SG	10:J:46:CYS:N	2.92	0.42
13:N:46:DC:H2''	13:N:47:DG:H8	1.83	0.42
13:N:46:DC:H2''	13:N:47:DG:OP2	2.19	0.42
14:T:12:DT:H2''	14:T:13:DT:H6	1.83	0.42
1:A:260:ASP:OD1	1:A:261:ASP:N	2.52	0.42
1:A:913:LEU:HD22	1:A:981:LEU:O	2.19	0.42
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.49	0.42
2:B:639:ILE:HD12	2:B:689:LEU:C	2.45	0.42
2:B:1174:LYS:O	2:B:1178:ASN:N	2.52	0.42
3:C:3:GLU:O	3:C:7:GLN:NE2	2.45	0.42
6:F:109:VAL:HG13	6:F:124:GLU:OE2	2.20	0.42
7:G:28:THR:O	7:G:31:LEU:N	2.52	0.42
13:N:43:DG:H8	13:N:43:DG:OP2	2.03	0.42
14:T:4:DT:H2''	14:T:5:DC:H6	1.85	0.42
14:T:5:DC:OP2	14:T:5:DC:H6	2.02	0.42
1:A:311:GLN:N	1:A:312:PRO:CD	2.82	0.42
1:A:1025:ARG:C	1:A:1026:LEU:HD22	2.45	0.42
2:B:102:VAL:N	2:B:110:HIS:O	2.37	0.42
8:H:97:MET:HE3	8:H:121:LEU:HD12	2.01	0.42
1:A:664:THR:HG22	2:B:1014:PRO:HB3	2.02	0.42
2:B:223:VAL:HG11	2:B:384:ARG:HD3	2.00	0.42
2:B:992:ILE:HD12	11:K:67:PHE:CE1	2.54	0.42
14:T:18:TTD:H2''	14:T:18:TTD:H6	1.89	0.42
1:A:244:PRO:N	1:A:245:PRO:CD	2.83	0.42
1:A:1111:MET:HE1	1:A:1333:ILE:HD12	2.01	0.42
2:B:997:GLU:OE1	2:B:997:GLU:N	2.38	0.42
1:A:383:TYR:OH	6:F:111:LEU:HD21	2.20	0.42
1:A:465:TYR:CD1	2:B:976:ILE:HD12	2.55	0.42
1:A:872:GLY:O	1:A:1058:VAL:HG12	2.19	0.42
1:A:1323:ASP:OD1	1:A:1325:THR:OG1	2.31	0.42
1:A:722:LEU:HD12	1:A:799:PHE:CD1	2.54	0.42
2:B:841:MET:HE2	2:B:846:ILE:CG1	2.46	0.42
4:D:154:PHE:CE2	4:D:214:LEU:HD12	2.55	0.42
14:T:22:DT:OP2	14:T:22:DT:H3'	2.19	0.42
2:B:230:ALA:HB3	2:B:231:PRO:HD3	2.03	0.41
2:B:604:ARG:NH2	2:B:692:TYR:O	2.53	0.41
2:B:763:GLN:HB2	2:B:1021:MET:HB2	2.02	0.41
8:H:4:THR:OG1	8:H:6:PHE:O	2.31	0.41
1:A:867:ILE:HG22	1:A:872:GLY:N	2.35	0.41
1:A:1436:ILE:O	1:A:1437:GLY:C	2.61	0.41
4:D:172:LEU:HD11	4:D:176:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:61:TYR:CD1	11:K:61:TYR:C	2.98	0.41
12:L:47:ARG:CZ	12:L:48:CYS:O	2.68	0.41
1:A:677:ARG:O	1:A:681:GLU:OE1	2.39	0.41
7:G:39:THR:HG21	7:G:42:PHE:HD2	1.84	0.41
8:H:8:ASP:OD1	8:H:9:ILE:N	2.46	0.41
8:H:96:VAL:HG13	8:H:143:LEU:HD23	2.01	0.41
8:H:96:VAL:HG22	8:H:143:LEU:HD22	2.02	0.41
11:K:53:ASP:OD1	11:K:54:ARG:N	2.53	0.41
2:B:44:VAL:HG11	2:B:495:LEU:HD23	2.02	0.41
2:B:444:MET:SD	2:B:444:MET:N	2.93	0.41
2:B:694:ASP:OD1	2:B:694:ASP:C	2.64	0.41
2:B:812:LEU:N	2:B:812:LEU:HD12	2.36	0.41
14:T:15:DT:H4'	14:T:15:DT:OP1	2.20	0.41
1:A:55:ASP:OD2	1:A:57:ARG:NE	2.48	0.41
8:H:27:GLU:OE2	8:H:39:THR:OG1	2.27	0.41
8:H:143:LEU:C	8:H:144:ILE:HD13	2.45	0.41
1:A:66:LYS:O	1:A:67:CYS:C	2.63	0.41
8:H:145:ARG:O	8:H:146:ARG:HB2	2.21	0.41
13:N:42:DA:OP2	13:N:42:DA:H2'	2.20	0.41
1:A:660:ASN:OD1	2:B:1082:MET:HB3	2.21	0.41
1:A:1318:THR:HG22	5:E:141:VAL:HG21	2.02	0.41
2:B:46:GLN:HG2	2:B:47:GLN:N	2.36	0.41
3:C:181:ASP:OD1	3:C:184:ASN:N	2.54	0.41
4:D:154:PHE:HZ	4:D:214:LEU:HD12	1.83	0.41
14:T:9:DT:H2''	14:T:10:DC:O5'	2.21	0.41
1:A:81:PHE:CZ	2:B:1208:MET:HB2	2.56	0.41
1:A:1097:GLY:O	1:A:1099:PRO:HD2	2.20	0.41
1:A:1132:LYS:CG	1:A:1284:MET:HE1	2.51	0.41
2:B:640:VAL:HG12	2:B:649:LYS:HG2	2.03	0.41
2:B:779:GLY:O	2:B:795:ILE:HA	2.20	0.41
2:B:950:ASP:OD2	2:B:967:ARG:NE	2.45	0.41
2:B:999:MET:HE2	2:B:999:MET:HB3	1.95	0.41
6:F:124:GLU:HG3	6:F:130:ILE:CD1	2.50	0.41
1:A:23:SER:O	1:A:26:GLU:N	2.53	0.41
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.03	0.41
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.56	0.41
1:A:964:ILE:CG2	1:A:1035:TYR:CD1	3.03	0.41
2:B:46:GLN:OE1	2:B:46:GLN:N	2.38	0.41
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.03	0.41
2:B:832:GLY:O	2:B:835:GLN:HG2	2.21	0.41
4:D:192:LYS:HD2	4:D:199:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:19:GLU:OE1	10:J:19:GLU:N	2.41	0.41
14:T:11:DC:H2''	14:T:12:DT:H6	1.81	0.41
5:E:5:ASN:HB3	5:E:7:ARG:NH1	2.35	0.41
5:E:100:ILE:O	5:E:104:ASN:N	2.54	0.41
7:G:45:ILE:HG12	7:G:78:VAL:HG12	2.03	0.41
14:T:13:DT:H2''	14:T:14:DC:H5'	2.02	0.41
1:A:793:SER:O	1:A:796:SER:OG	2.28	0.40
1:A:1066:VAL:HG12	1:A:1070:GLN:OE1	2.20	0.40
2:B:368:GLU:OE1	2:B:368:GLU:N	2.46	0.40
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.55	0.40
5:E:116:ILE:HG21	5:E:121:MET:HE3	2.02	0.40
7:G:88:ASP:HA	7:G:144:ARG:HA	2.03	0.40
8:H:47:PHE:O	8:H:49:VAL:N	2.54	0.40
1:A:757:ASN:HA	2:B:1021:MET:HE1	2.02	0.40
1:A:843:LYS:NZ	1:A:1401:SER:O	2.54	0.40
3:C:66:ARG:NH1	10:J:3:VAL:O	2.50	0.40
3:C:99:LEU:HD23	3:C:99:LEU:N	2.36	0.40
5:E:43:LYS:O	5:E:47:CYS:N	2.52	0.40
6:F:111:LEU:N	6:F:111:LEU:HD12	2.36	0.40
13:N:39:DA:H2''	13:N:40:DG:C8	2.52	0.40
1:A:1107:VAL:HG23	1:A:1383:SER:HB3	2.02	0.40
2:B:292:ILE:N	2:B:293:PRO:CD	2.85	0.40
2:B:597:MET:HE3	2:B:617:ARG:HB2	2.03	0.40
10:J:51:LEU:HD23	10:J:51:LEU:C	2.46	0.40
13:N:34:DG:H2''	13:N:35:DA:C8	2.56	0.40
1:A:323:LYS:HD2	1:A:323:LYS:O	2.22	0.40
1:A:1138:ILE:HD11	1:A:1319:VAL:HG11	2.04	0.40
1:A:1150:SER:HA	1:A:1195:LEU:HD13	2.03	0.40
1:A:1424:VAL:HG13	1:A:1425:SER:H	1.85	0.40
2:B:640:VAL:HG23	2:B:740:HIS:HA	2.04	0.40
6:F:138:LEU:HD12	6:F:142:SER:OG	2.21	0.40
14:T:2:DG:H1'	14:T:3:DC:H5''	2.02	0.40
1:A:757:ASN:ND2	2:B:1018:PRO:O	2.54	0.40
4:D:173:HIS:O	4:D:177:VAL:HG23	2.22	0.40
4:D:207:LEU:O	4:D:211:LEU:HD13	2.21	0.40
9:I:16:PRO:HA	9:I:27:PHE:HA	2.04	0.40
13:N:35:DA:C2'	13:N:36:DA:H5'	2.39	0.40
13:N:40:DG:OP2	13:N:40:DG:H8	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1353/1733 (78%)	1292 (96%)	59 (4%)	2 (0%)	48	78
2	B	1019/1224 (83%)	973 (96%)	46 (4%)	0	100	100
3	C	264/318 (83%)	259 (98%)	5 (2%)	0	100	100
4	D	138/221 (62%)	136 (99%)	2 (1%)	0	100	100
5	E	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
6	F	79/155 (51%)	76 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	21	52
8	H	127/146 (87%)	113 (89%)	14 (11%)	0	100	100
9	I	115/122 (94%)	111 (96%)	4 (4%)	0	100	100
10	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
11	K	102/120 (85%)	101 (99%)	1 (1%)	0	100	100
12	L	44/70 (63%)	40 (91%)	4 (9%)	0	100	100
All	All	3686/4565 (81%)	3531 (96%)	152 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1098	VAL
1	A	958	VAL
7	G	58	ARG

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	1192/1520 (78%)	1192 (100%)	0	100	100
2	B	885/1061 (83%)	885 (100%)	0	100	100
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	109/200 (54%)	109 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	75/152 (49%)	75 (100%)	0	100	100
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	64/116 (55%)	64 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	89/102 (87%)	89 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3134/4009 (78%)	3134 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	118	HIS
1	A	358	ASN
1	A	545	GLN
1	A	972	HIS
2	B	648	HIS
2	B	1040	ASN
2	B	1093	GLN
9	I	108	HIS
9	I	114	GLN
9	I	120	GLN
10	J	64	ASN
11	K	44	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	9/10 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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
14	TTD	T	18	14	42,45,46	1.26	8 (19%)	61,74,77	2.21	14 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	TTD	T	18	14	-	14/22/109/110	0/5/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	18	TTD	C2T-N1T	3.20	1.42	1.36
14	T	18	TTD	C5-C6	-2.60	1.52	1.55
14	T	18	TTD	C2T-N3T	-2.57	1.33	1.38
14	T	18	TTD	C4T-N3T	-2.54	1.33	1.37
14	T	18	TTD	C2-N3	-2.53	1.33	1.38
14	T	18	TTD	C5T-C6T	-2.41	1.52	1.55
14	T	18	TTD	C4-N3	-2.33	1.33	1.37
14	T	18	TTD	C1R-N1T	2.02	1.48	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	18	TTD	N3T-C2T-N1T	6.97	124.08	116.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	18	TTD	C5-C4-N3	5.36	120.58	116.09
14	T	18	TTD	O4'-C1'-N1	4.97	114.54	108.65
14	T	18	TTD	C2'-C1'-N1	-4.92	108.94	115.59
14	T	18	TTD	N3-C2-N1	4.89	121.90	116.78
14	T	18	TTD	C5T-C4T-N3T	4.71	120.04	116.09
14	T	18	TTD	O2T-C2T-N1T	-4.69	116.42	123.44
14	T	18	TTD	O4-C4-C5	-4.35	118.66	122.71
14	T	18	TTD	O4T-C4T-C5T	-4.34	118.67	122.71
14	T	18	TTD	O4R-C1R-N1T	3.13	112.36	108.65
14	T	18	TTD	O2-C2-N1	-2.57	119.59	123.44
14	T	18	TTD	C2R-C1R-N1T	-2.25	112.55	115.59
14	T	18	TTD	C6T-C6-N1	-2.22	110.20	118.51
14	T	18	TTD	C6-C6T-N1T	-2.22	110.22	118.51

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	18	TTD	O4'-C4R-C5'-O5'
14	T	18	TTD	O4'-C1'-N1-C2
14	T	18	TTD	C5R-O5R-PB-O3R
14	T	18	TTD	C5R-O5R-PB-O5P
14	T	18	TTD	C5R-O5R-PB-O4P
14	T	18	TTD	O4R-C4'-C5R-O5R
14	T	18	TTD	O4'-C1'-N1-C6
14	T	18	TTD	C3R-C4R-C5'-O5'
14	T	18	TTD	C3'-C4'-C5R-O5R
14	T	18	TTD	C4'-C5R-O5R-PB
14	T	18	TTD	C2R-C1R-N1T-C2T
14	T	18	TTD	C2'-C1'-N1-C6
14	T	18	TTD	C4R-C5'-O5'-P
14	T	18	TTD	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	18	TTD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

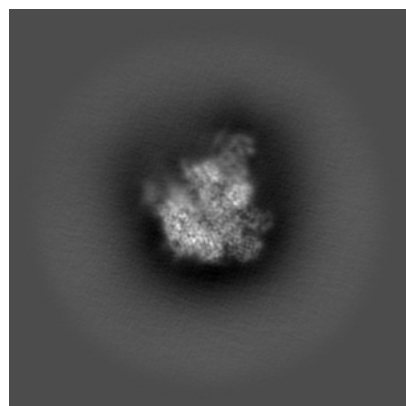
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41654. These allow visual inspection of the internal detail of the map and identification of artifacts.

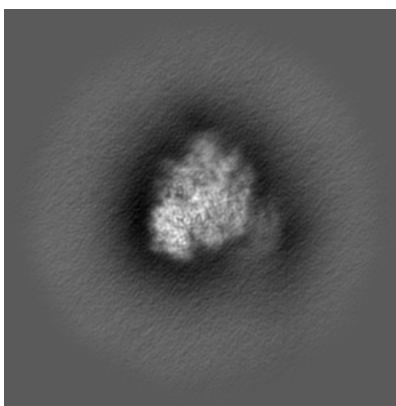
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

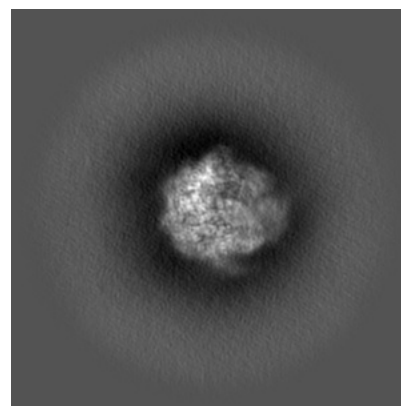
6.1.1 Primary map



X

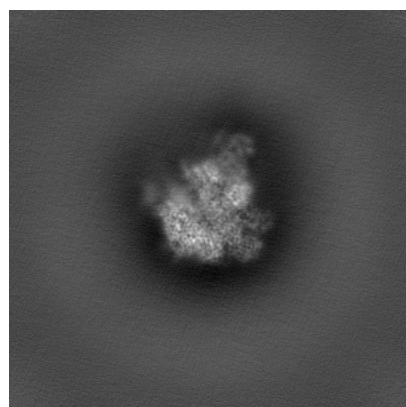


Y

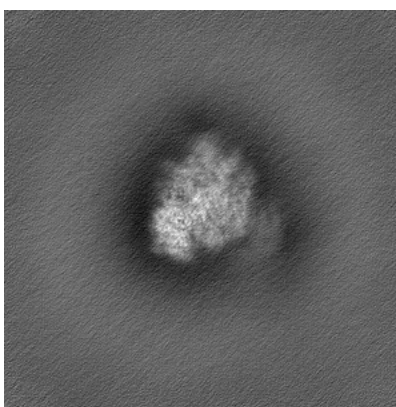


Z

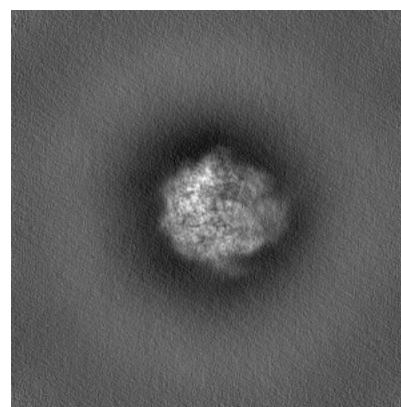
6.1.2 Raw map



X



Y

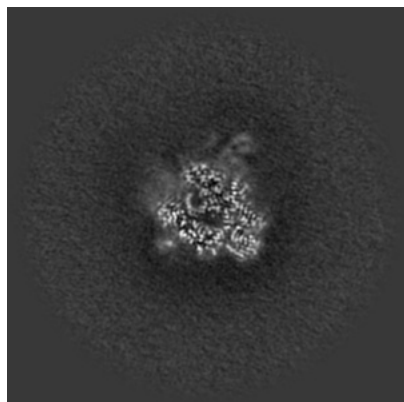


Z

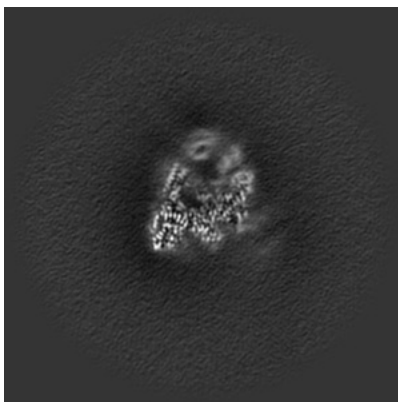
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

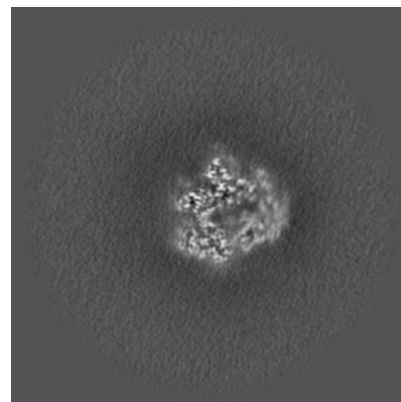
6.2.1 Primary map



X Index: 192

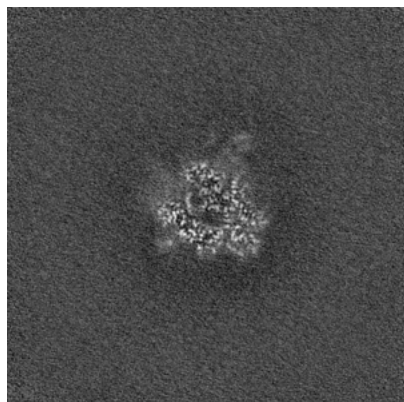


Y Index: 192

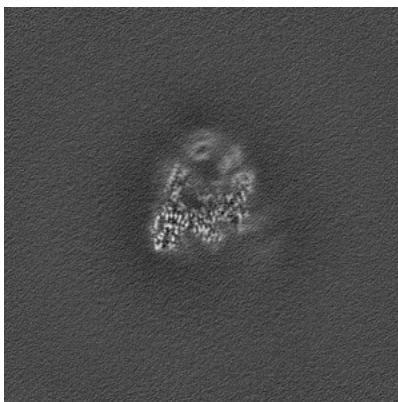


Z Index: 192

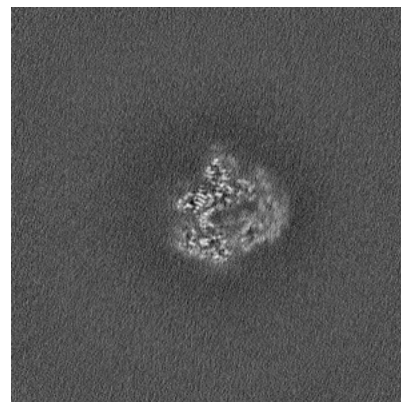
6.2.2 Raw map



X Index: 192



Y Index: 192

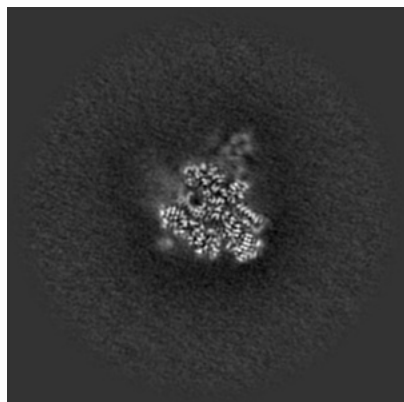


Z Index: 192

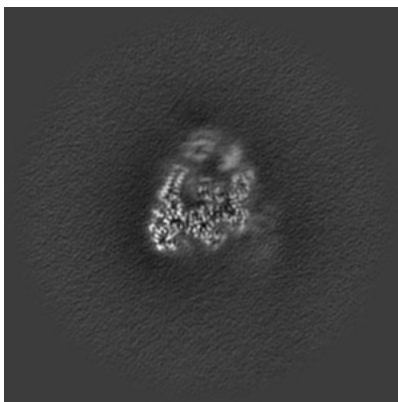
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

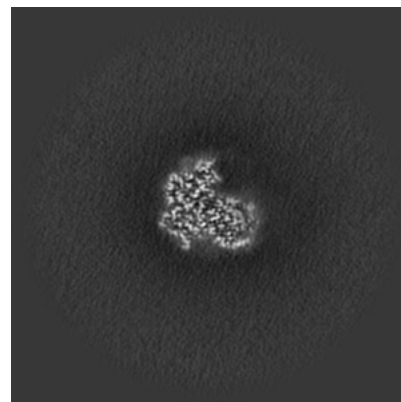
6.3.1 Primary map



X Index: 189

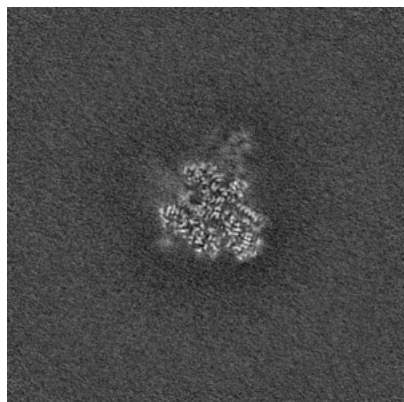


Y Index: 195

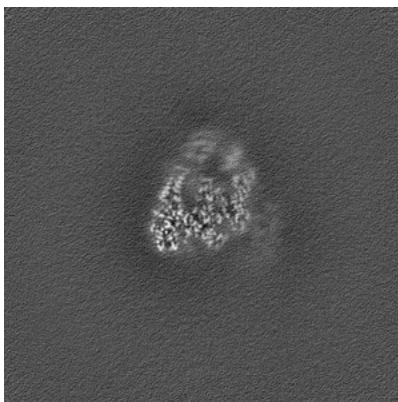


Z Index: 164

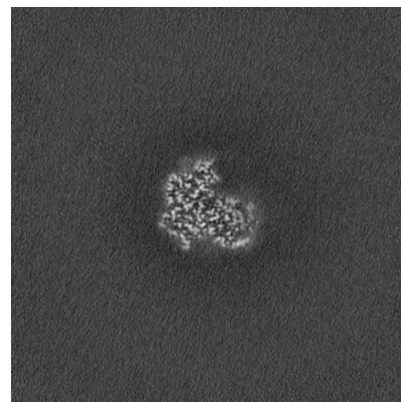
6.3.2 Raw map



X Index: 188



Y Index: 196

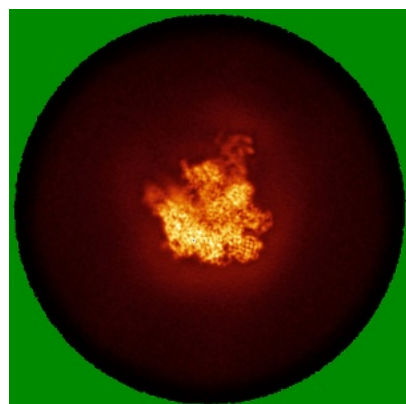


Z Index: 165

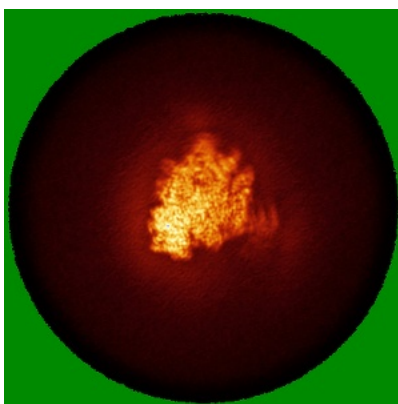
The images above show the largest variance slices of the map in three orthogonal directions.

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

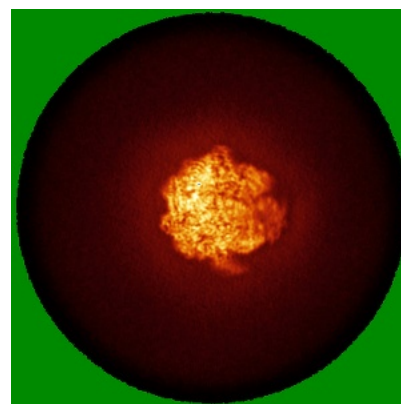
6.4.1 Primary map



X

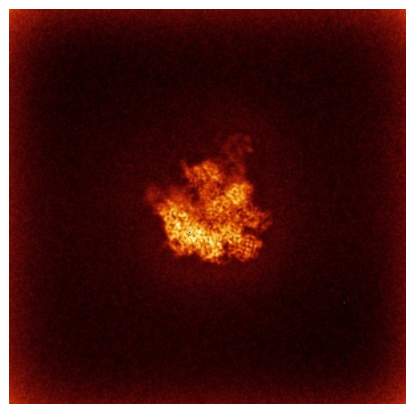


Y

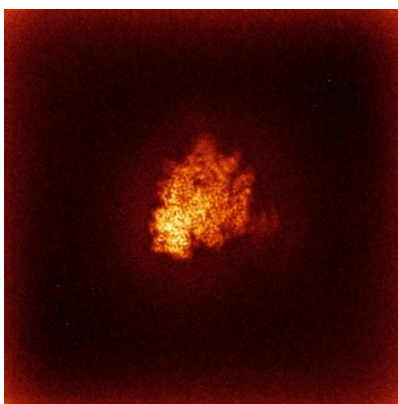


Z

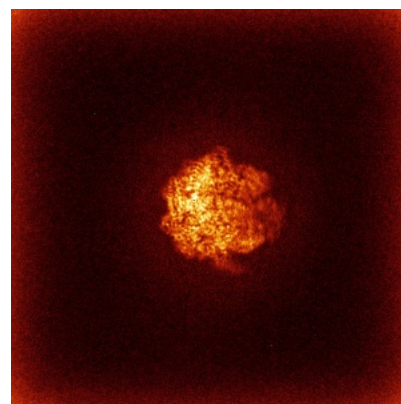
6.4.2 Raw map



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



X



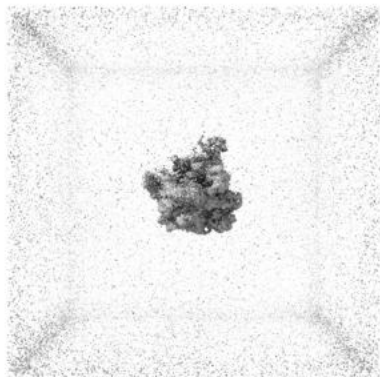
Y



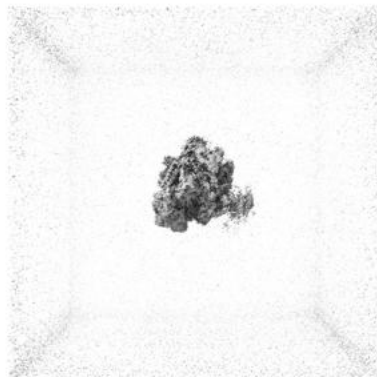
Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

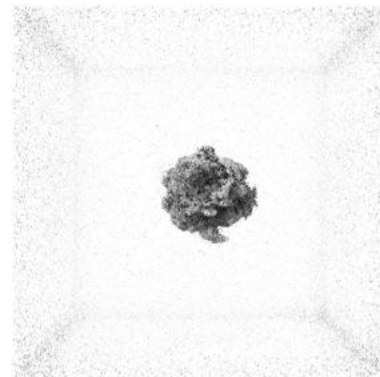
6.5.2 Raw map



X



Y



Z

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.

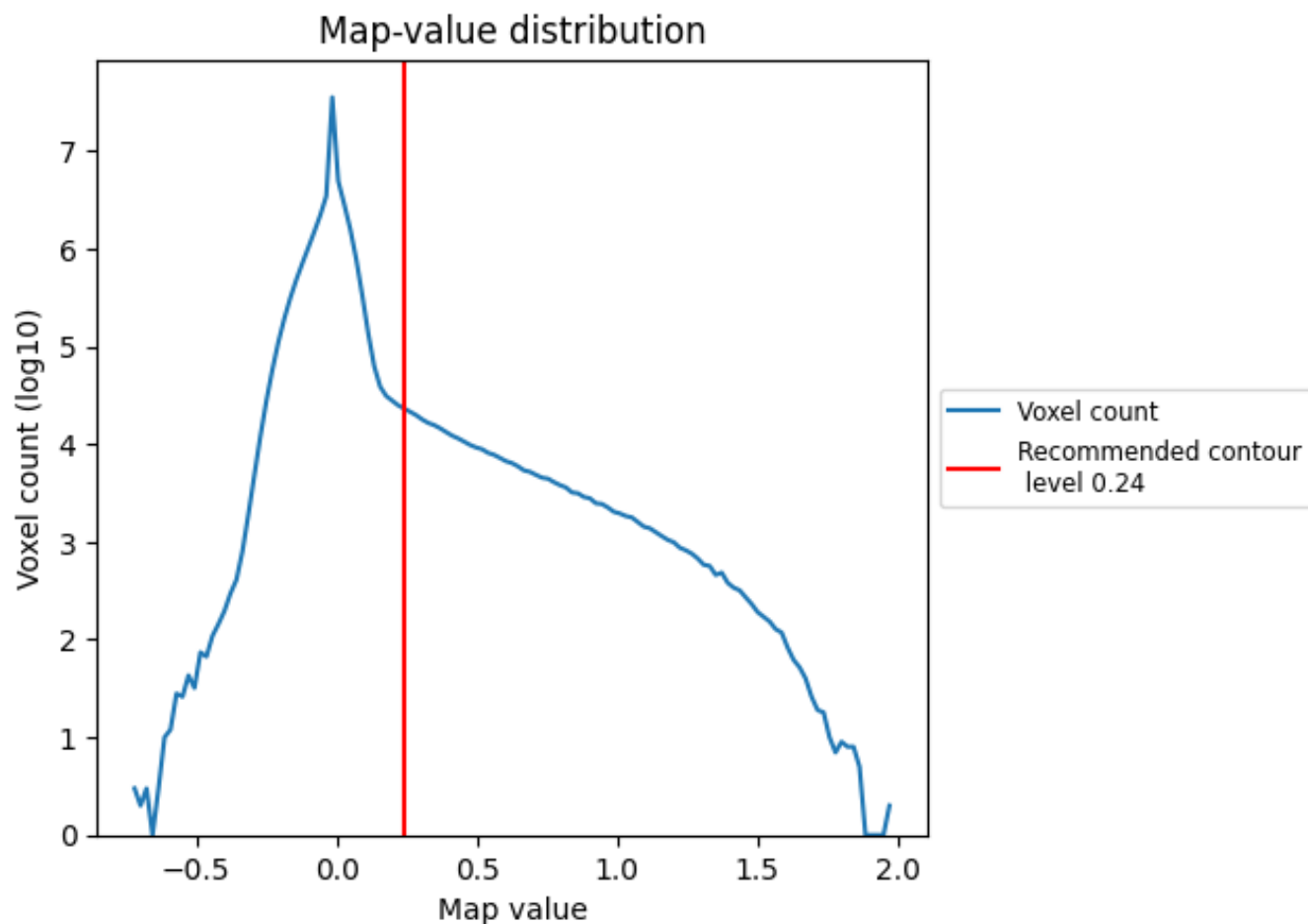
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

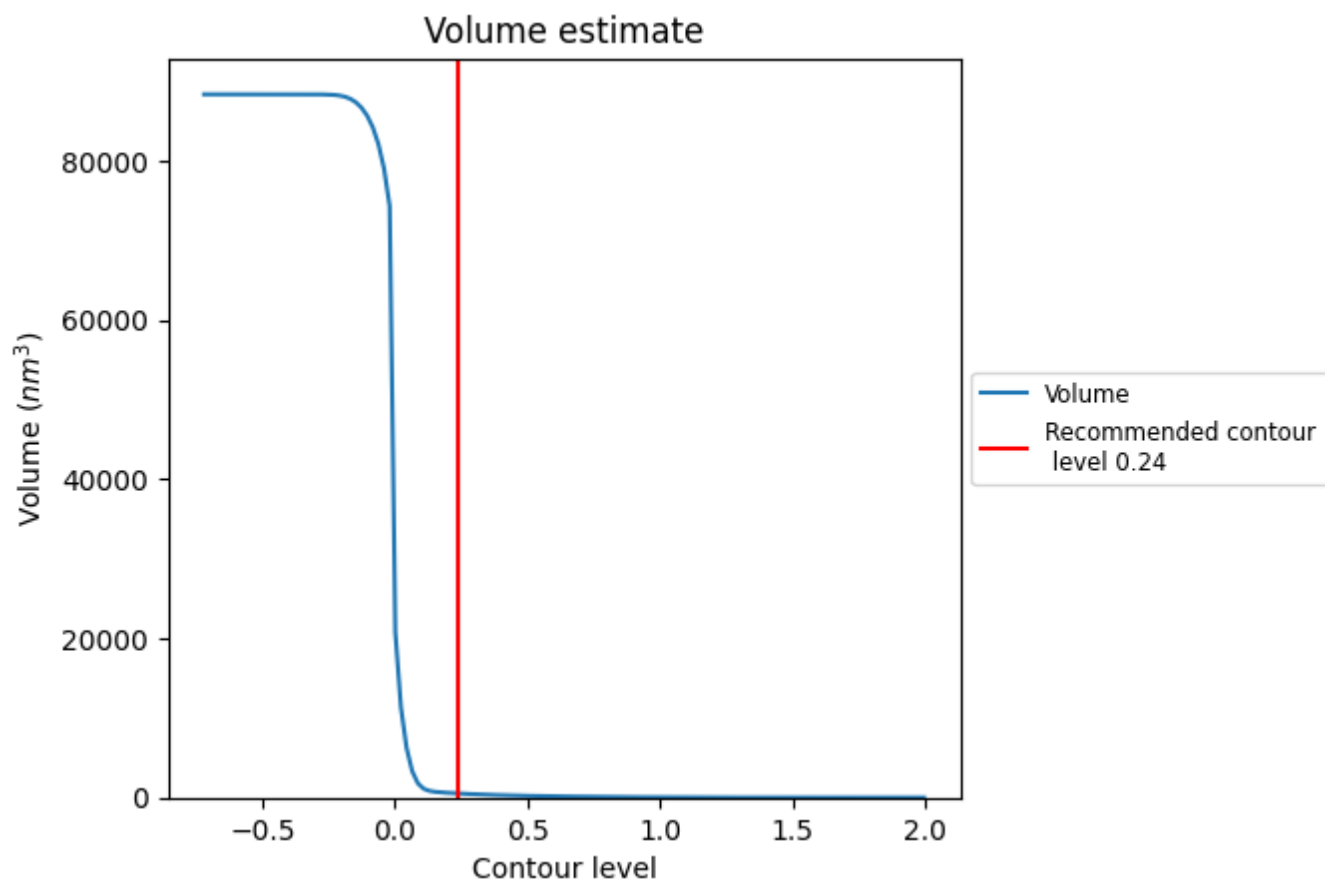
This section contains the results of statistical analysis of the map.

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.

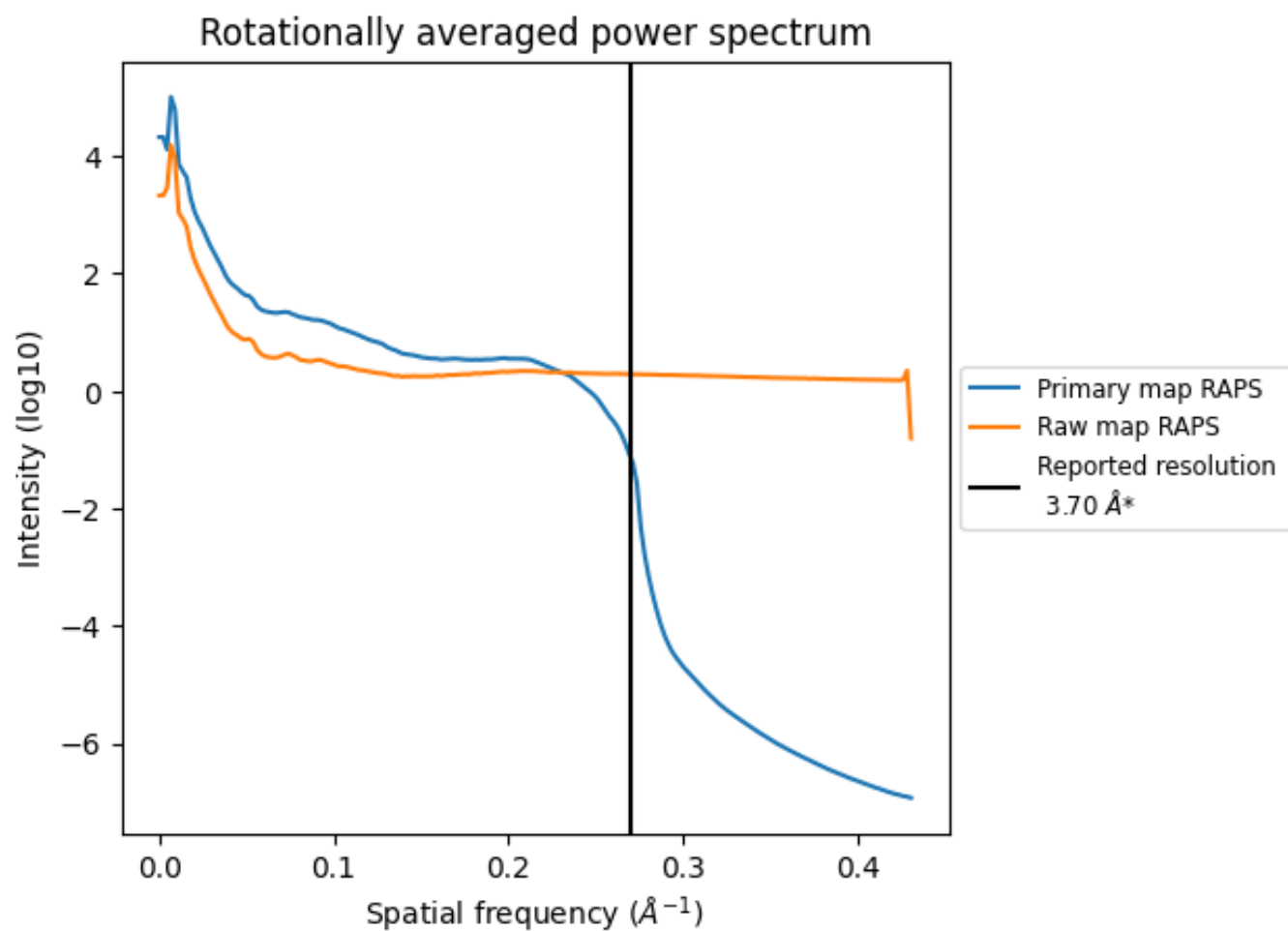
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 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 ⓘ

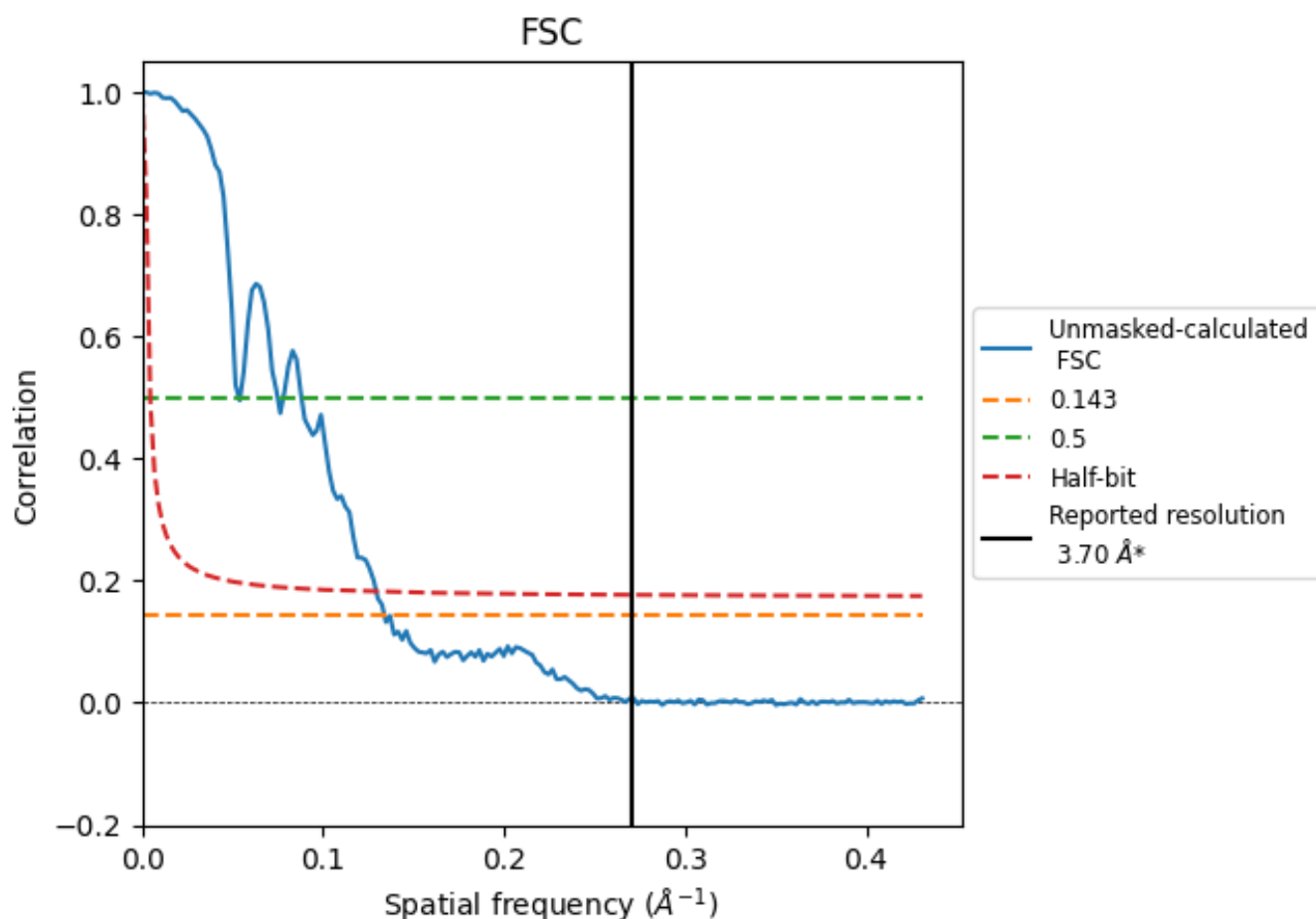


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

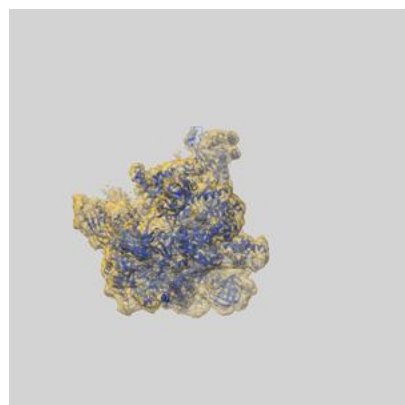
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.47	18.73	7.73

*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 7.47 differs from the reported value 3.7 by more than 10 %

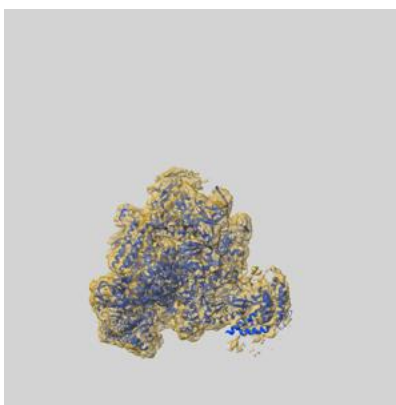
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41654 and PDB model 8TVX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

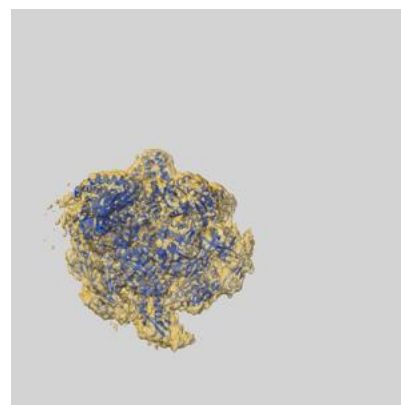
9.1 Map-model overlay [i](#)



X



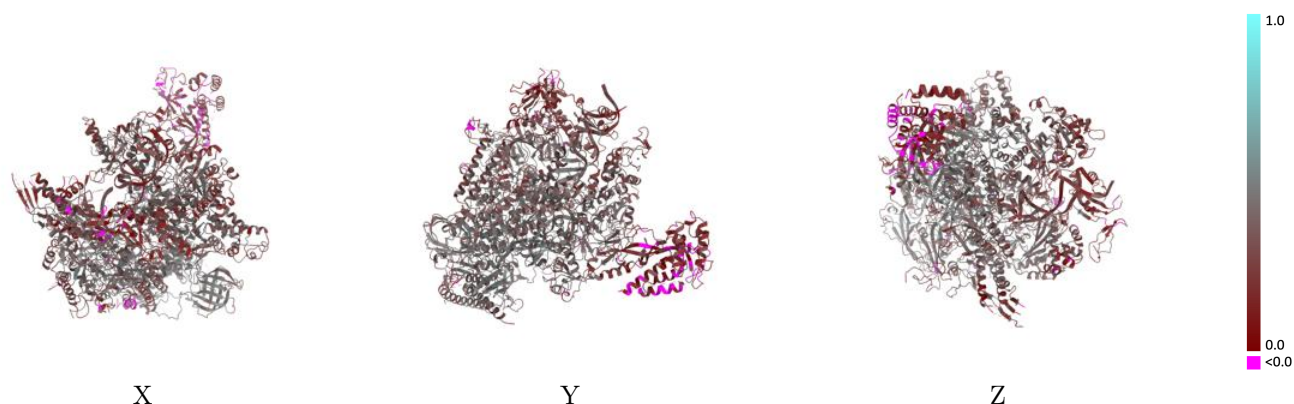
Y



Z

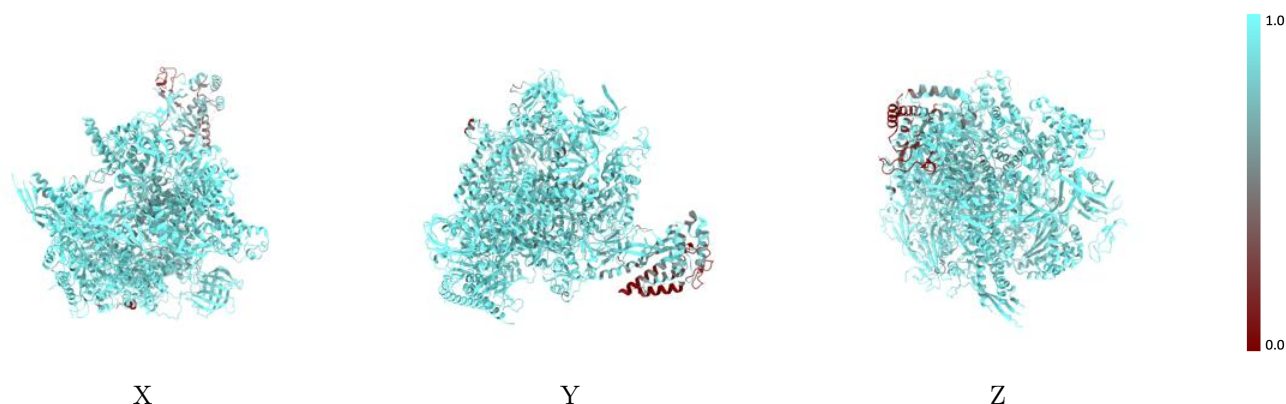
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



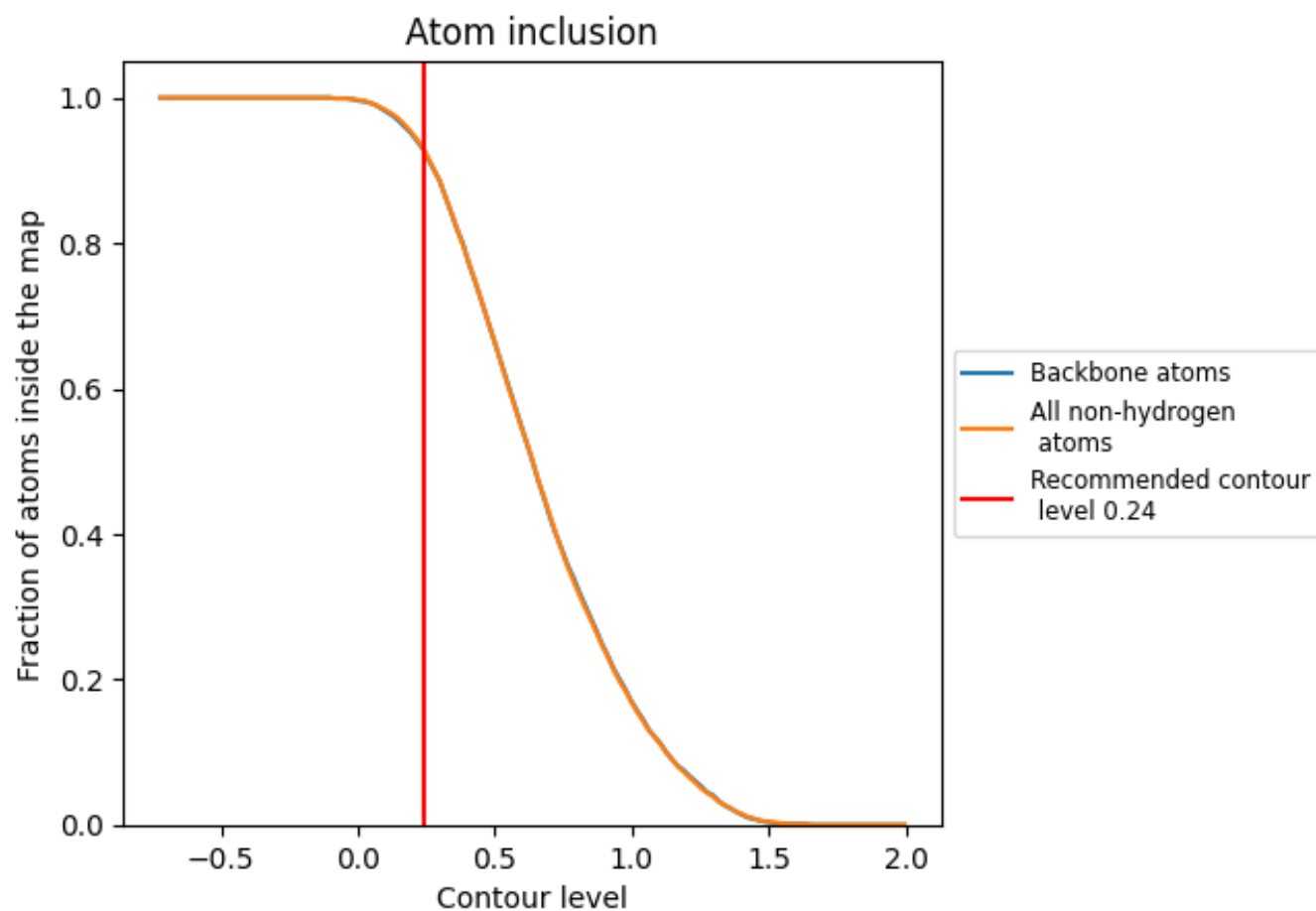
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.3590
A	 0.9390	 0.3710
B	 0.9610	 0.3830
C	 0.9830	 0.4330
D	 0.5930	 0.1340
E	 0.9740	 0.3330
F	 0.9610	 0.3950
G	 0.7070	 0.1950
H	 0.9780	 0.3890
I	 0.9130	 0.2690
J	 0.9920	 0.4260
K	 0.9670	 0.4110
L	 0.9830	 0.3320
N	 0.9360	 0.2310
R	 0.9180	 0.3460
T	 0.9660	 0.3270

