



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 04:47 AM UTC

PDB ID : 8PBL / pdb_00008pbl
EMDB ID : EMD-17586
Title : E. coli RNA polymerase elongation complex stalled at thymine dimer lesion
Authors : Woodgate, J.; Zenkin, N.
Deposited on : 2023-06-09
Resolution : 2.87 Å(reported)
Based on initial models : 8FVR, 1SL2

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:

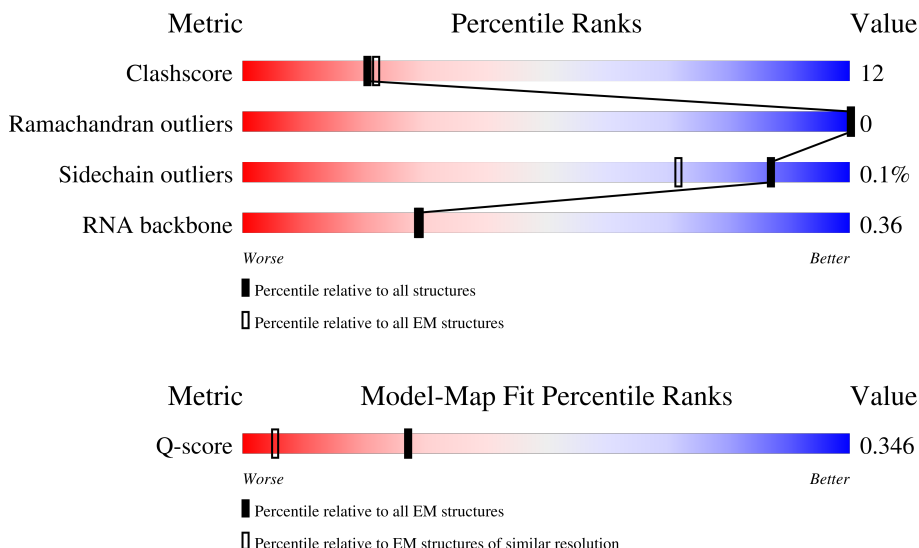
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.87 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	12062 (2.37 - 3.37)

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	49	
2	B	49	
3	D	239	

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Mol	Chain	Length	Quality of chain
3	E	239	
4	F	1342	
5	G	1407	
6	H	91	
7	R	19	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26261 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	27	Total	C	N	O	P	0	0
			557	264	111	156	26		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	27	Total	C	N	O	P	0	0
			563	270	96	170	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	229	Total	C	N	O	S	0	0
			1779	1108	316	349	6		
3	E	220	Total	C	N	O	S	0	0
			1695	1057	299	333	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	236	VAL	-	expression tag	UNP A0A5B9AW69
D	237	LEU	-	expression tag	UNP A0A5B9AW69
D	238	PHE	-	expression tag	UNP A0A5B9AW69
D	239	GLN	-	expression tag	UNP A0A5B9AW69
E	236	VAL	-	expression tag	UNP A0A5B9AW69
E	237	LEU	-	expression tag	UNP A0A5B9AW69
E	238	PHE	-	expression tag	UNP A0A5B9AW69
E	239	GLN	-	expression tag	UNP A0A5B9AW69

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	1319	Total	C	N	O	S	3	0
			10427	6544	1820	2019	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	1330	Total	C	N	O	S	0	0
			10352	6506	1846	1950	50		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	14	Total	C	N	O	P	0	0
			303	135	57	97	14		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	G	2	Total	Zn	0
			2	2	

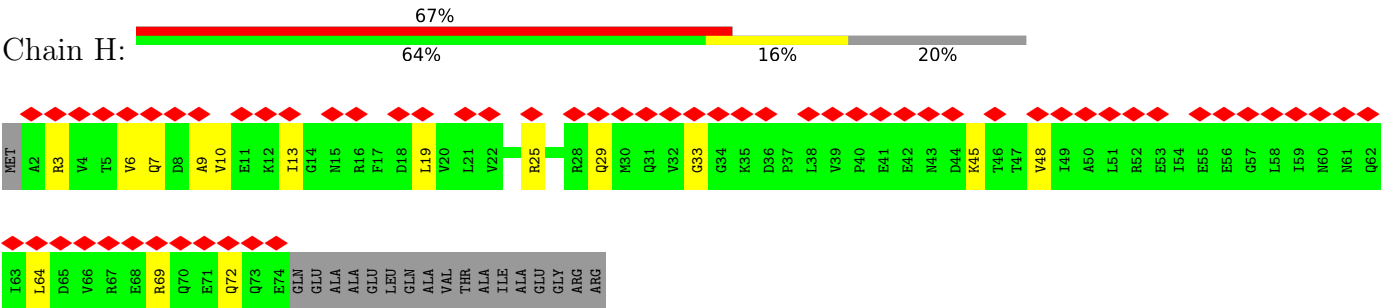
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	R	1	Total	Mg	0
			1	1	

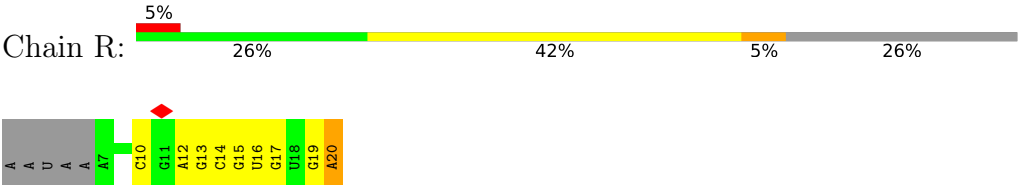


L1356	I1233	E1146	R978	S887	F773	T674	M485	R362	R259	R123	GLU	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
H1366	V1237	A1147	N979	G893	T776	A675	S486	L363	R260	R126	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
R1373	Q1238	P1150	E981	V894	K789	G677	T487	H364	A261	L126	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	Y1241	K1151	R990	G900	G794	V682	V574	K370	T262	D129	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1246	E1152	E993	R901	L800	E678	L579	K371	D264	L132	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	K1247	P1153	V1002	L903	L800	R678	L579	M372	L265	R133	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	D1250	Q1084	L1003	L903	L800	V682	L579	L374	N266	D134	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	K1251	G1085	L1003	L903	L800	V682	L579	L374	R275	V138	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1255	D1086	L1004	L903	L800	E678	L579	K378	R278	V146	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	I1256	R1173	A1004	L903	L800	E678	L579	P379	R281	I147	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1257	R1174	A1004	L903	L800	E678	L579	P379	L282	I147	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	R1258	R1175	A1004	L903	L800	E678	L579	P379	G149	I147	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	Q1259	P1091	G1014	L903	L800	E678	L579	P379	A286	G150	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	R1262	P1091	G1014	L903	L800	E678	L579	P379	R291	L154	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	K1263	P1091	G1014	L903	L800	E678	L579	P379	L291	L154	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	F1274	P1091	G1014	L903	L800	E678	L579	P379	E295	Q157	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	E1278	P1091	G1014	L903	L800	E678	L579	P379	M298	Q158	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	Q1279	P1091	G1014	L903	L800	E678	L579	P379	V303	Q158	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1280	P1091	G1014	L903	L800	E678	L579	P379	D308	Q158	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	E1281	P1091	G1014	L903	L800	E678	L579	P379	R311	E211	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	L1292	P1091	G1014	L903	L800	E678	L579	P379	R312	E211	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	K1297	P1091	G1014	L903	L800	E678	L579	P379	G313	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1298	P1091	G1014	L903	L800	E678	L579	P379	R314	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	G1299	P1091	G1014	L903	L800	E678	L579	P379	A315	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	D1305	P1091	G1014	L903	L800	E678	L579	P379	I316	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	Q1308	P1091	G1014	L903	L800	E678	L579	P379	T317	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	I1309	P1091	G1014	L903	L800	E678	L579	P379	G318	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	F1319	P1091	G1014	L903	L800	E678	L579	P379	S319	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	E1327	P1091	G1014	L903	L800	E678	L579	P379	P323	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	T1328	P1091	G1014	L903	L800	E678	L579	P379	L324	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	E1334	P1091	G1014	L903	L800	E678	L579	P379	I331	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	A1335	P1091	G1014	L903	L800	E678	L579	P379	K332	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	G1336	P1091	G1014	L903	L800	E678	L579	P379	Q335	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1337	P1091	G1014	L903	L800	E678	L579	P379	R339	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	D1342	P1091	G1014	L903	L800	E678	L579	P379	Q340	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	G1346	P1091	G1014	L903	L800	E678	L579	P379	G344	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	L1347	P1091	G1014	L903	L800	E678	L579	P379	K345	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	K1348	P1091	G1014	L903	L800	E678	L579	P379	R346	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	E1349	P1091	G1014	L903	L800	E678	L579	P379	G346	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	N1350	P1091	G1014	L903	L800	E678	L579	P379	Y349	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1351	P1091	G1014	L903	L800	E678	L579	P379	R353	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	I1352	P1091	G1014	L903	L800	E678	L579	P379	S353	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	V1353	P1091	G1014	L903	L800	E678	L579	P379	E554	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET
ALA	E1356	P1091	G1014	L903	L800	E678	L579	P379	V357	R214	THR	THR	THR	GLN	ALA	LYS	PHE	LEU	LEU	ASP	LYS	MET

● Molecule 6: DNA-directed RNA polymerase subunit omega



● Molecule 7: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	240000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00102	Depositor
Map size (Å)	287.0, 287.0, 287.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	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: ZN, MG, TTD

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	0.18	0/626	0.36	0/963
2	B	0.51	2/583 (0.3%)	1.02	4/894 (0.4%)
3	D	0.16	0/1801	0.35	0/2440
3	E	0.15	0/1714	0.39	0/2322
4	F	0.18	0/10602	0.39	1/14303 (0.0%)
5	G	0.17	0/10508	0.40	2/14185 (0.0%)
6	H	0.10	0/584	0.32	0/786
7	R	0.14	0/339	0.24	0/527
All	All	0.18	2/26757 (0.0%)	0.42	7/36420 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	DA	O4'-C1'	6.96	1.55	1.41
2	B	13	DA	C5'-C4'	5.88	1.64	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	DA	C5'-C4'-C3'	-21.72	82.32	114.90
2	B	13	DA	C4'-C3'-O3'	11.84	127.76	110.00
2	B	13	DA	C5'-C4'-O4'	-7.44	98.24	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	DA	C1'-O4'-C4'	-6.16	100.47	109.70
5	G	504	GLN	CB-CA-C	-5.53	109.71	117.23
5	G	1144	LEU	N-CA-C	-5.41	105.73	112.93
4	F	630	VAL	N-CA-C	-5.33	108.09	113.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	901	ARG	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	557	0	304	21	0
2	B	563	0	318	30	0
3	D	1779	0	1806	23	0
3	E	1695	0	1726	35	0
4	F	10427	0	10455	271	0
5	G	10352	0	10575	306	0
6	H	582	0	593	10	0
7	R	303	0	152	7	0
8	G	2	0	0	0	0
9	R	1	0	0	0	0
All	All	26261	0	25929	628	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 12.

All (628) 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:E:47:LEU:HD12	3:E:183:ILE:CD1	1.54	1.35
3:E:47:LEU:CD1	3:E:183:ILE:HD12	1.67	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1333:LEU:HD21	5:G:115:TRP:CH2	1.76	1.19
3:D:43:LEU:O	3:D:47:LEU:HD13	1.47	1.13
3:E:47:LEU:CD1	3:E:183:ILE:CD1	2.26	1.13
3:E:47:LEU:HD13	3:E:183:ILE:HD12	1.35	1.09
5:G:701:LEU:CD2	5:G:723:TYR:HB2	1.83	1.08
5:G:701:LEU:HD21	5:G:723:TYR:HB2	1.32	1.05
4:F:184:LEU:HD12	4:F:184:LEU:O	1.64	0.96
3:E:47:LEU:HD12	3:E:183:ILE:HD11	1.46	0.94
4:F:1333:LEU:CD2	5:G:115:TRP:CH2	2.57	0.86
2:B:14:TTD:H1'	2:B:14:TTD:H5R1	1.57	0.85
1:A:15:DG:H22	4:F:199:ASP:HB3	1.42	0.84
5:G:701:LEU:HD21	5:G:723:TYR:CB	2.11	0.80
3:D:43:LEU:O	3:D:47:LEU:CD1	2.27	0.80
4:F:1333:LEU:HD21	5:G:115:TRP:CZ2	2.17	0.79
3:D:70:THR:HG23	4:F:729:ALA:HB3	1.66	0.78
5:G:701:LEU:HD23	5:G:701:LEU:O	1.83	0.78
4:F:102:LEU:HB3	4:F:118:LYS:HB2	1.66	0.77
5:G:886:VAL:HG11	5:G:1230:THR:HG21	1.67	0.77
4:F:592:ARG:HG3	4:F:655:VAL:HG12	1.65	0.76
5:G:482:ALA:O	5:G:488:ASN:ND2	2.17	0.76
4:F:176:ILE:HG23	4:F:405:PHE:HZ	1.49	0.76
5:G:701:LEU:HD23	5:G:723:TYR:HB2	1.68	0.76
3:E:181:GLU:HA	5:G:535:ARG:HH21	1.52	0.75
2:B:16:DC:H5'	4:F:1269:ARG:HG2	1.69	0.75
4:F:528:ARG:NH2	4:F:576:SER:O	2.19	0.75
5:G:836:ARG:NH1	5:G:869:CYS:SG	2.60	0.74
5:G:1005:LYS:HB3	5:G:1009:GLU:HG3	1.69	0.74
4:F:1243:MET:HE3	5:G:372:MET:HG3	1.69	0.73
4:F:802:VAL:HG12	4:F:1096:ILE:HB	1.69	0.73
5:G:147:ILE:O	5:G:156:ARG:NH1	2.22	0.72
5:G:701:LEU:CD2	5:G:723:TYR:CB	2.64	0.72
5:G:926:PRO:HB3	5:G:1246:VAL:HG11	1.71	0.72
1:A:21:DC:H2'	1:A:22:DG:C8	2.25	0.72
4:F:1303:LYS:HG3	4:F:1315:MET:HG3	1.71	0.71
3:E:182:ARG:HB3	3:E:206:GLU:HB2	1.70	0.71
5:G:807:LEU:HD23	5:G:1255:VAL:HG13	1.71	0.71
5:G:430:HIS:CE1	5:G:432:LEU:HB2	2.26	0.70
5:G:510:LEU:HD11	5:G:624:ILE:HG23	1.72	0.70
3:D:207:THR:HG23	3:D:209:GLY:H	1.58	0.69
4:F:10:ARG:HE	4:F:791:LEU:HD12	1.55	0.69
3:E:91:ARG:HE	3:E:124:VAL:HG22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:417:ARG:O	6:H:45:LYS:NZ	2.26	0.69
5:G:123:ARG:NH2	5:G:1334:GLU:OE2	2.26	0.68
5:G:485:MET:O	5:G:489:ASN:ND2	2.27	0.68
4:F:980:VAL:HG13	4:F:984:VAL:HG23	1.75	0.68
3:D:28:LEU:HD21	3:E:231:PHE:HZ	1.58	0.68
1:A:9:DG:OP2	5:G:275:ARG:NH1	2.28	0.67
4:F:389:PHE:HB3	4:F:420:LEU:HD12	1.76	0.67
5:G:1025:MET:HB2	5:G:1124:ILE:HB	1.77	0.67
5:G:606:ASN:OD1	5:G:610:ARG:NH2	2.29	0.66
5:G:923:ILE:O	5:G:1241:TYR:OH	2.14	0.66
4:F:987:GLU:O	4:F:991:LYS:NZ	2.23	0.66
5:G:1173:ARG:NH2	5:G:1194:ARG:O	2.28	0.66
5:G:552:ILE:HD11	5:G:570:LYS:HD2	1.77	0.66
5:G:701:LEU:CD2	5:G:723:TYR:CD1	2.80	0.65
5:G:1238:GLN:NE2	5:G:1250:ASP:OD1	2.28	0.65
5:G:1346:GLY:O	5:G:1350:ASN:ND2	2.27	0.65
5:G:825:VAL:HG23	5:G:838:ARG:HH12	1.62	0.65
5:G:1022:PRO:O	5:G:1126:GLN:NE2	2.30	0.65
4:F:706:ARG:NH1	4:F:791:LEU:O	2.29	0.64
5:G:800:LEU:HD22	5:G:1256:ILE:HD13	1.79	0.64
3:E:52:PRO:HA	3:E:150:ARG:HG2	1.80	0.64
5:G:813:ASP:OD1	5:G:883:ARG:NH1	2.28	0.64
2:B:18:DC:H2'	2:B:19:DA:C8	2.33	0.64
3:D:11:PRO:HB2	3:D:28:LEU:HD22	1.80	0.64
5:G:362:ARG:HD2	5:G:364:HIS:CE1	2.34	0.63
4:F:180:ARG:HB3	4:F:396:ASP:HB3	1.80	0.63
5:G:362:ARG:HD2	5:G:364:HIS:HE1	1.63	0.63
3:D:83:LEU:HD13	4:F:694:ARG:HH11	1.63	0.63
4:F:890:LYS:HD3	4:F:914:LYS:HG3	1.80	0.63
5:G:1219:ASP:HA	5:G:1222:ARG:HG2	1.81	0.63
4:F:817:LEU:HB3	4:F:1097:VAL:HB	1.80	0.63
5:G:773:PHE:O	5:G:776:THR:OG1	2.15	0.63
3:E:47:LEU:HD12	3:E:183:ILE:HD13	1.72	0.63
4:F:145:ILE:HB	4:F:456:VAL:HG22	1.80	0.63
4:F:434:ASP:HB2	4:F:439:LYS:HB3	1.78	0.63
4:F:1243:MET:HE1	5:G:371:LYS:HB2	1.79	0.63
2:B:18:DC:OP1	4:F:1262:LYS:N	2.31	0.63
5:G:430:HIS:CD2	5:G:925:GLU:HG3	2.34	0.63
4:F:197:ARG:NH1	4:F:201:ARG:O	2.31	0.62
4:F:1129:ASN:HD22	4:F:1177:ARG:HG3	1.62	0.62
5:G:519:ASN:ND2	5:G:707:ILE:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1147:ALA:H	5:G:1308:GLY:HA2	1.63	0.62
5:G:353:SER:OG	5:G:372:MET:SD	2.57	0.62
4:F:59:ILE:HG12	4:F:472:GLU:HG3	1.80	0.62
4:F:178:PRO:HD3	4:F:183:TRP:HB3	1.81	0.62
4:F:979:LEU:HD23	4:F:989:LEU:HD11	1.82	0.62
4:F:843:THR:OG1	4:F:846:GLY:O	2.18	0.62
5:G:1274:PHE:HE1	5:G:1280:VAL:HG11	1.64	0.62
3:D:104:LYS:HG2	3:D:110:VAL:HG22	1.81	0.62
4:F:241:LEU:HD21	4:F:285:ILE:HD12	1.82	0.62
4:F:360:LEU:HD11	4:F:378:ARG:HE	1.64	0.62
4:F:4:SER:H	4:F:8:LYS:HE2	1.65	0.61
5:G:63:GLY:O	5:G:98:ARG:NH1	2.33	0.61
4:F:142:GLU:HB3	4:F:760:ASN:HD21	1.66	0.61
4:F:1119[A]:MET:HB2	4:F:1228:GLY:HA2	1.82	0.61
5:G:515:ARG:NH2	5:G:717:VAL:O	2.34	0.61
5:G:674:THR:OG1	5:G:677:GLU:OE1	2.17	0.61
5:G:803:VAL:HG21	5:G:1309:ILE:HG13	1.82	0.61
3:D:179:PRO:O	3:D:207:THR:OG1	2.17	0.61
4:F:563:THR:O	4:F:684:ASN:ND2	2.30	0.61
4:F:225:PHE:HZ	4:F:345:PRO:HA	1.66	0.61
5:G:1144:LEU:HD21	5:G:1233:ILE:HG23	1.81	0.61
5:G:1099:TYR:HE1	5:G:1199:PHE:HB3	1.65	0.61
2:B:11:DC:OP2	5:G:311:ARG:NH1	2.34	0.61
4:F:715:THR:HG22	4:F:786:GLY:H	1.65	0.61
5:G:517:CYS:HB3	5:G:520:ALA:HB2	1.83	0.61
5:G:848:VAL:HG12	5:G:857:LEU:HD12	1.82	0.61
4:F:1260:GLY:O	5:G:346:ARG:NH1	2.34	0.60
4:F:968:GLU:HG2	4:F:972:PHE:HD2	1.66	0.60
5:G:367:GLY:HA3	5:G:448:GLN:HB2	1.82	0.60
1:A:17:DA:H2	4:F:183:TRP:HE1	1.46	0.60
5:G:1348:LYS:HA	5:G:1351:VAL:HG22	1.83	0.60
4:F:1107:MET:HB3	5:G:763:PHE:HE2	1.65	0.60
5:G:644:MET:CE	5:G:740:LEU:HD13	2.31	0.60
4:F:18:ARG:NH2	4:F:622:ASN:OD1	2.34	0.60
5:G:878:ASP:O	5:G:990:ARG:NH1	2.35	0.60
4:F:1117:LEU:HD13	4:F:1195:ILE:HG12	1.83	0.60
4:F:839:VAL:HG22	4:F:1049:ILE:HG12	1.82	0.60
4:F:870:ILE:O	4:F:944:ARG:NH1	2.35	0.60
5:G:495:ASN:ND2	5:G:1247:LYS:O	2.34	0.60
2:B:18:DC:H2'	2:B:19:DA:H8	1.68	0.59
5:G:660:GLU:HG3	5:G:685:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:416:ILE:HG13	5:G:439:PRO:HG2	1.82	0.59
5:G:701:LEU:HD23	5:G:723:TYR:CD1	2.36	0.59
4:F:1004:ASP:OD1	4:F:1005:GLU:N	2.36	0.59
5:G:22:ILE:HG21	5:G:1335:ALA:HB1	1.84	0.59
5:G:644:MET:HB2	5:G:764:ARG:HD2	1.83	0.59
2:B:14:TTD:H2'	2:B:14:TTD:O4P	2.02	0.58
3:D:135:ASP:HB3	3:D:138:ALA:HB2	1.86	0.58
4:F:118:LYS:HD2	4:F:488:MET:HE1	1.85	0.58
4:F:697:LYS:O	4:F:799:ASN:ND2	2.36	0.58
3:D:192:VAL:HG12	3:D:194:GLN:H	1.69	0.58
4:F:808:ASN:H	5:G:633:ALA:HB2	1.68	0.58
4:F:1241:ASP:O	4:F:1262:LYS:HD2	2.03	0.58
5:G:1106:ILE:HB	5:G:1123:ARG:HB2	1.84	0.58
3:E:43:LEU:HD23	3:E:46:ILE:HD11	1.85	0.58
4:F:1308:ILE:HD11	5:G:472:LEU:HD21	1.85	0.58
3:D:48:LEU:HG	3:D:183:ILE:HD12	1.85	0.58
4:F:1073:LYS:NZ	5:G:462:ASP:O	2.27	0.58
5:G:54:ASP:OD1	5:G:60:ARG:NH2	2.36	0.58
4:F:257:ALA:N	4:F:260:LYS:O	2.37	0.57
4:F:339:ASN:H	4:F:343:HIS:HB2	1.69	0.57
4:F:472:GLU:HA	4:F:475:VAL:HG12	1.84	0.57
2:B:3:DC:H2''	2:B:4:DG:C8	2.39	0.57
5:G:724:MET:O	5:G:728:SER:HB3	2.04	0.57
5:G:211:GLU:HA	5:G:214:ARG:HB2	1.86	0.57
5:G:604:MET:HE2	5:G:620:PHE:HZ	1.68	0.57
5:G:1230:THR:HG22	5:G:1257:VAL:HG11	1.86	0.57
1:A:28:DG:H2''	1:A:29:DA:C8	2.40	0.57
4:F:257:ALA:HA	4:F:282:VAL:HG21	1.86	0.57
5:G:789:LYS:NZ	5:G:930:LEU:O	2.37	0.57
5:G:822:MET:HE1	5:G:838:ARG:HB2	1.87	0.57
4:F:89:GLY:HA2	4:F:140:GLY:HA3	1.87	0.57
5:G:146:VAL:HG21	5:G:154:LEU:HD13	1.87	0.57
4:F:562:GLU:OE1	4:F:662:SER:OG	2.15	0.57
5:G:1158:GLU:OE1	5:G:1222:ARG:NH1	2.37	0.57
2:B:21:DG:H2''	4:F:143:ARG:HH22	1.69	0.56
3:E:46:ILE:HG13	3:E:220:ALA:HB1	1.86	0.56
4:F:1066:MET:HG2	4:F:1232:MET:HE3	1.86	0.56
3:D:9:LEU:HB3	3:D:30:PRO:HG2	1.85	0.56
5:G:704:GLU:HG3	5:G:718:SER:HA	1.87	0.56
5:G:1319:PHE:CE1	5:G:1342:ASP:HB2	2.39	0.56
6:H:3:ARG:HD3	6:H:48:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:40:GLU:O	4:F:73:TYR:OH	2.23	0.56
4:F:252:SER:O	4:F:265:LYS:NZ	2.36	0.56
4:F:688:GLN:OE1	4:F:1237:HIS:NE2	2.38	0.56
5:G:332:LYS:HG2	5:G:1328:THR:HB	1.87	0.56
5:G:429:LEU:HB3	5:G:925:GLU:HG2	1.88	0.56
5:G:699:ASP:OD1	5:G:700:ASN:N	2.39	0.56
7:R:14:C:H2'	7:R:15:G:H8	1.70	0.56
5:G:129:ASP:OD2	5:G:220:ARG:NH1	2.38	0.56
4:F:151:ARG:HH21	4:F:156:PHE:HB2	1.71	0.56
5:G:553:THR:HG23	5:G:567:THR:HG22	1.88	0.56
5:G:597:GLY:O	5:G:601:ILE:HG13	2.06	0.56
5:G:1062:LEU:O	5:G:1067:ARG:NH1	2.38	0.56
7:R:14:C:H2'	7:R:15:G:C8	2.41	0.56
3:E:16:ILE:HG12	3:E:26:VAL:HG13	1.88	0.56
4:F:489:PRO:HA	4:F:492:MET:HG2	1.88	0.56
5:G:1144:LEU:CD2	5:G:1233:ILE:HG23	2.36	0.56
2:B:17:DA:OP2	5:G:346:ARG:NH2	2.39	0.55
4:F:32:LEU:HA	4:F:130:MET:HE1	1.87	0.55
5:G:974:VAL:HG23	5:G:1002:VAL:HG22	1.88	0.55
5:G:591:ILE:O	5:G:594:GLN:NE2	2.39	0.55
4:F:833:ILE:HA	4:F:1054:LEU:O	2.06	0.55
4:F:529[A]:ARG:NH1	4:F:574:SER:OG	2.39	0.55
4:F:812:PHE:HB3	5:G:357:VAL:HG21	1.89	0.55
4:F:889:PRO:HA	4:F:913:VAL:HG12	1.89	0.55
2:B:11:DC:H2'	2:B:12:DC:C6	2.42	0.55
4:F:463:GLN:HG2	4:F:505:PHE:HB2	1.89	0.55
4:F:10:ARG:HD3	4:F:697:LYS:HD3	1.88	0.55
2:B:11:DC:H4'	5:G:1327:GLU:HG2	1.89	0.54
5:G:44:ILE:HG22	5:G:51:PRO:HA	1.88	0.54
5:G:521:LYS:NZ	5:G:540:GLY:O	2.28	0.54
5:G:978:ARG:HE	5:G:979:ASN:H	1.55	0.54
4:F:199:ASP:O	4:F:201:ARG:HG3	2.08	0.54
5:G:245:LEU:HD23	5:G:250:ARG:HD2	1.90	0.54
4:F:272:ARG:HA	4:F:275:ARG:HG2	1.89	0.54
4:F:935:THR:OG1	4:F:1048:LYS:NZ	2.40	0.54
5:G:814:CYS:SG	5:G:883:ARG:NH2	2.81	0.54
2:B:26:DA:H2''	2:B:27:DT:H5'	1.88	0.54
5:G:533:ALA:HB1	5:G:574:VAL:HG13	1.88	0.54
4:F:590:PRO:HB3	4:F:605:TYR:CE1	2.43	0.54
5:G:166:LEU:HD23	5:G:169:LEU:HD21	1.90	0.54
4:F:214:ASN:HA	4:F:359:ARG:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:942:ASP:O	4:F:946:LEU:N	2.37	0.54
1:A:16:DA:H2'	4:F:183:TRP:CZ2	2.43	0.53
4:F:176:ILE:HD12	4:F:184:LEU:HD11	1.88	0.53
5:G:807:LEU:HD22	5:G:1259:GLN:HE21	1.73	0.53
1:A:16:DA:H2'	4:F:183:TRP:HZ2	1.72	0.53
4:F:408:SER:OG	4:F:431:LYS:NZ	2.42	0.53
4:F:1098:LEU:HD11	4:F:1230:MET:HE1	1.91	0.53
4:F:943:LYS:HA	4:F:946:LEU:HB2	1.91	0.53
5:G:250:ARG:O	5:G:266:ASN:ND2	2.42	0.53
5:G:370:LYS:HG2	5:G:441:LEU:HD22	1.91	0.53
5:G:1356:LEU:O	5:G:1366:HIS:NE2	2.34	0.53
3:D:158:ARG:NH2	3:D:173:VAL:O	2.41	0.53
5:G:430:HIS:HD2	5:G:925:GLU:HG3	1.71	0.53
4:F:968:GLU:HG2	4:F:972:PHE:CD2	2.43	0.53
5:G:1222:ARG:HG3	5:G:1223:LEU:HG	1.90	0.53
3:D:43:LEU:C	3:D:47:LEU:HD13	2.28	0.53
4:F:520:PRO:HG3	4:F:714:VAL:HG21	1.90	0.53
5:G:502:PRO:O	5:G:598:LYS:NZ	2.42	0.53
2:B:13:DA:OP1	5:G:339:ARG:NH1	2.35	0.53
3:E:43:LEU:O	3:E:47:LEU:HG	2.09	0.53
4:F:1304:MET:HG3	4:F:1305:TYR:N	2.24	0.53
4:F:1127:LYS:HD3	4:F:1144:PHE:CZ	2.43	0.52
4:F:1289:GLU:OE2	5:G:473:THR:OG1	2.22	0.52
5:G:423:LEU:HD22	5:G:468:VAL:HG22	1.91	0.52
4:F:1254:VAL:O	5:G:99:ARG:NH2	2.43	0.52
5:G:278:ARG:NH1	5:G:295:GLU:OE2	2.42	0.52
5:G:536:LEU:HB3	5:G:542:ALA:HB3	1.91	0.52
5:G:1094:ASP:OD1	5:G:1094:ASP:N	2.43	0.52
6:H:6:VAL:HG12	6:H:10:VAL:HG23	1.91	0.52
1:A:25:DG:H2''	1:A:26:DA:H5''	1.92	0.52
3:E:105:SER:HA	3:E:133:LEU:HD12	1.92	0.52
4:F:705:GLU:HB3	4:F:794:LEU:H	1.74	0.52
5:G:900:GLY:O	5:G:909:ILE:HD12	2.09	0.52
2:B:4:DG:C8	2:B:4:DG:H5'	2.45	0.52
4:F:563:THR:O	4:F:680:LEU:HD11	2.09	0.52
4:F:667:LEU:HD11	4:F:708:VAL:HG21	1.92	0.52
4:F:1274:GLU:CG	5:G:424:ASN:HD21	2.23	0.52
4:F:255:ILE:HD11	4:F:263:VAL:HB	1.92	0.52
4:F:1107:MET:HB3	5:G:763:PHE:CE2	2.45	0.52
3:E:4:SER:OG	3:E:5:VAL:N	2.42	0.51
4:F:461:GLU:HG2	4:F:465:ARG:HE	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:559:CYS:HB2	4:F:662:SER:HB3	1.91	0.51
5:G:701:LEU:CD2	5:G:723:TYR:HD1	2.23	0.51
5:G:899:TYR:CE1	5:G:1251:LYS:HB3	2.45	0.51
3:E:155:ALA:N	3:E:174:ASP:OD1	2.43	0.51
4:F:657:THR:HG22	4:F:1187:PHE:HB2	1.92	0.51
5:G:118:LYS:HD3	5:G:312:ARG:HG3	1.93	0.51
6:H:6:VAL:HG13	6:H:9:ALA:HB3	1.93	0.51
5:G:701:LEU:HD23	5:G:723:TYR:CG	2.46	0.51
5:G:872:LEU:HD22	5:G:877:VAL:HG21	1.93	0.51
4:F:254:ASP:OD1	4:F:265:LYS:N	2.44	0.51
5:G:614:LEU:HD23	6:H:7:GLN:NE2	2.26	0.51
5:G:1045:THR:HA	5:G:1067:ARG:HD2	1.93	0.51
4:F:10:ARG:NH1	4:F:1175:ASN:O	2.43	0.51
4:F:1274:GLU:HG3	5:G:424:ASN:HD21	1.75	0.51
5:G:247:PRO:HA	5:G:250:ARG:NH1	2.25	0.51
3:E:44:ARG:NH1	5:G:538:ARG:HB3	2.26	0.50
5:G:1178:THR:HG22	5:G:1185:PRO:HG3	1.92	0.50
4:F:74:ARG:HH22	4:F:121:GLU:CD	2.19	0.50
4:F:693:LEU:HD21	4:F:1057:LYS:HZ2	1.75	0.50
4:F:1003:THR:HA	4:F:1008:GLN:HB3	1.93	0.50
4:F:1293:VAL:HG13	4:F:1304:MET:SD	2.51	0.50
4:F:1300:GLY:HA2	4:F:1303:LYS:NZ	2.26	0.50
5:G:111:THR:O	5:G:239:LEU:N	2.39	0.50
5:G:724:MET:O	5:G:728:SER:CB	2.60	0.50
4:F:1072:ASN:HD22	4:F:1111:GLN:CD	2.19	0.50
5:G:1165:PHE:HA	5:G:1175:LEU:HD22	1.93	0.50
4:F:798:GLN:NE2	4:F:827:ARG:O	2.45	0.50
4:F:1100:PRO:HB2	5:G:639:VAL:HG23	1.93	0.50
5:G:647:PRO:HG3	5:G:697:MET:HA	1.94	0.50
1:A:18:DT:C4	4:F:542:ARG:HD2	2.46	0.50
2:B:14:TTD:O4P	2:B:14:TTD:H1	2.12	0.50
2:B:14:TTD:O2	5:G:794:GLY:HA3	2.12	0.50
4:F:557:ARG:NH2	4:F:611:GLU:OE1	2.37	0.50
4:F:1291:LEU:HA	5:G:345:LYS:HD2	1.94	0.50
5:G:829:GLY:HA2	5:G:993:GLU:HG2	1.93	0.50
5:G:682:VAL:HA	5:G:685:ILE:HG12	1.94	0.50
5:G:668:PHE:HB2	5:G:678:ARG:HD3	1.94	0.49
4:F:88:ARG:HA	4:F:934:PHE:CE1	2.47	0.49
4:F:188:PHE:HE1	4:F:436:ARG:HH11	1.58	0.49
5:G:425:ARG:HB2	5:G:466:MET:HE2	1.93	0.49
3:D:100:LEU:HD21	3:D:121:VAL:HG21	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:30:ILE:HD13	5:G:243:PRO:HD3	1.94	0.49
5:G:126:LEU:HD21	5:G:219:LYS:HG3	1.93	0.49
3:E:191:ARG:HG2	3:E:196:THR:HG22	1.95	0.49
4:F:1269:ARG:NH1	5:G:344:GLY:O	2.45	0.49
4:F:1313:HIS:HB3	5:G:473:THR:HG22	1.94	0.49
3:D:111:THR:HG22	3:D:129:VAL:HG22	1.94	0.49
4:F:194:LEU:HD11	4:F:436:ARG:HH22	1.76	0.49
5:G:442:ILE:HG22	5:G:444:GLY:H	1.76	0.49
3:D:153:VAL:O	3:D:158:ARG:NH1	2.45	0.49
4:F:598:VAL:HG22	4:F:628:HIS:NE2	2.28	0.49
3:E:185:TYR:HB2	3:E:201:LEU:HD11	1.95	0.49
4:F:1061:GLN:HE22	5:G:445:LYS:HE2	1.77	0.49
2:B:18:DC:H5''	4:F:1262:LYS:HB2	1.94	0.49
4:F:194:LEU:HG	4:F:436:ARG:HH12	1.77	0.49
4:F:821:ARG:HA	4:F:824:GLN:HE21	1.77	0.49
5:G:275:ARG:HH11	5:G:298:MET:HB3	1.78	0.48
1:A:15:DG:H2''	1:A:16:DA:O5'	2.13	0.48
3:E:47:LEU:HD21	3:E:217:ILE:HA	1.96	0.48
5:G:510:LEU:HD12	5:G:601:ILE:HD13	1.94	0.48
3:D:45:ARG:NH1	4:F:1215:GLY:O	2.40	0.48
5:G:370:LYS:HE2	5:G:443:GLU:HA	1.95	0.48
5:G:476:ALA:HA	5:G:479:GLU:HG2	1.95	0.48
6:H:13:ILE:HG21	6:H:19:LEU:HB2	1.95	0.48
2:B:19:DA:H2'	2:B:20:DC:C6	2.48	0.48
4:F:84:GLU:HA	4:F:87:ILE:HG22	1.96	0.48
4:F:1101:LEU:HD21	5:G:508:LEU:HD22	1.95	0.48
4:F:1246:ARG:NH2	4:F:1258:PRO:HB2	2.29	0.48
1:A:16:DA:N6	4:F:181:GLY:O	2.46	0.48
5:G:430:HIS:HE1	5:G:432:LEU:HB2	1.78	0.48
5:G:894:VAL:HG22	5:G:1258:ARG:NH1	2.28	0.48
5:G:1153:PRO:HB3	5:G:1216:ALA:HB2	1.96	0.48
2:B:9:DC:H2''	2:B:10:DG:C8	2.49	0.48
4:F:303:ASP:HB2	4:F:310:ILE:HD11	1.96	0.48
4:F:765:ILE:HA	4:F:787:PRO:HG3	1.96	0.48
4:F:819:SER:HB2	4:F:1085:MET:HE2	1.95	0.48
5:G:24:LEU:HD21	5:G:116:PHE:HZ	1.79	0.48
5:G:1143:ASP:HB2	5:G:1148:ARG:HG3	1.96	0.48
4:F:153:PRO:HA	4:F:177:ILE:HG23	1.95	0.48
5:G:489:ASN:O	5:G:499:ILE:HD11	2.14	0.48
5:G:743:MET:HE2	5:G:745:GLY:HA2	1.95	0.48
4:F:204:LEU:HB3	4:F:208:ILE:HD12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1226:VAL:O	5:G:1230:THR:HG23	2.14	0.47
4:F:147:SER:HB3	4:F:453:ILE:HG23	1.97	0.47
4:F:432:LEU:O	4:F:435:ILE:HG22	2.14	0.47
5:G:253:VAL:HG21	7:R:12:A:H1'	1.96	0.47
4:F:961:SER:O	4:F:964:LEU:HG	2.13	0.47
5:G:701:LEU:HD23	5:G:723:TYR:CB	2.38	0.47
4:F:431:LYS:HA	4:F:434:ASP:OD2	2.13	0.47
4:F:1270:PHE:CZ	4:F:1274:GLU:HB3	2.49	0.47
1:A:17:DA:H2	4:F:183:TRP:NE1	2.12	0.47
3:E:109:PRO:HA	3:E:132:HIS:CE1	2.50	0.47
4:F:1313:HIS:HB3	5:G:473:THR:HA	1.97	0.47
5:G:222:LYS:NZ	5:G:1278:GLU:HG2	2.29	0.47
3:D:75:GLN:NE2	4:F:771:VAL:O	2.40	0.47
4:F:548:ARG:NH1	4:F:567:PRO:O	2.36	0.47
4:F:697:LYS:HE2	4:F:1181:PRO:HG3	1.97	0.47
4:F:808:ASN:HD21	4:F:1216:ARG:HH22	1.62	0.47
4:F:953:LEU:HD21	4:F:1036:ILE:HG21	1.95	0.47
4:F:1340:GLU:OE1	4:F:1340:GLU:N	2.47	0.47
5:G:118:LYS:HG2	5:G:311:ARG:HB3	1.96	0.47
5:G:227:PHE:CZ	5:G:237:MET:HE1	2.50	0.47
5:G:250:ARG:O	5:G:250:ARG:HG2	2.15	0.47
5:G:734:ALA:O	5:G:738:ARG:HG3	2.15	0.47
5:G:746:LEU:HD23	5:G:758:PRO:HB3	1.97	0.47
2:B:19:DA:H2'	2:B:20:DC:H6	1.80	0.47
4:F:444:ASP:HB3	4:F:447:HIS:HB2	1.96	0.47
4:F:681:MET:O	4:F:685:MET:HB2	2.15	0.47
3:E:180:VAL:HG13	3:E:205:MET:HE1	1.96	0.47
4:F:1261:GLY:O	4:F:1266:GLY:N	2.31	0.47
5:G:118:LYS:HE2	5:G:311:ARG:HB3	1.96	0.47
7:R:12:A:H2'	7:R:13:G:H8	1.79	0.47
3:E:182:ARG:NH1	5:G:534:GLU:OE2	2.48	0.47
4:F:839:VAL:O	4:F:886:LYS:NZ	2.48	0.47
4:F:978:VAL:HG21	4:F:1014:LEU:HD13	1.96	0.46
4:F:979:LEU:HG	4:F:985:GLU:HB2	1.96	0.46
4:F:1192:GLU:HG3	5:G:641:ILE:HD13	1.97	0.46
5:G:807:LEU:HD22	5:G:1259:GLN:NE2	2.29	0.46
4:F:968:GLU:O	4:F:972:PHE:N	2.35	0.46
4:F:1205:PRO:HG2	4:F:1210:ILE:HG12	1.97	0.46
5:G:601:ILE:O	5:G:604:MET:HG2	2.16	0.46
5:G:1146:GLU:HA	5:G:1309:ILE:H	1.81	0.46
1:A:25:DG:H1	2:B:6:DC:H42	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:194:GLN:OE1	5:G:409:TRP:NE1	2.48	0.46
4:F:622:ASN:ND2	4:F:631:GLU:OE2	2.49	0.46
5:G:447:ILE:HD11	5:G:466:MET:HB3	1.97	0.46
5:G:644:MET:HE1	5:G:740:LEU:HD13	1.97	0.46
5:G:1144:LEU:HD22	5:G:1237:VAL:CG2	2.46	0.46
5:G:308:ASP:HB3	5:G:311:ARG:HD3	1.98	0.46
5:G:899:TYR:HD2	5:G:909:ILE:HD13	1.80	0.46
5:G:1079:LYS:HB3	5:G:1079:LYS:HE3	1.75	0.46
2:B:18:DC:O3'	4:F:1262:LYS:HE3	2.15	0.46
5:G:113:HIS:HB3	5:G:116:PHE:HD2	1.80	0.46
2:B:7:DG:H2''	2:B:8:DG:C8	2.50	0.46
3:E:110:VAL:H	3:E:132:HIS:CE1	2.34	0.46
4:F:1114:GLU:OE1	4:F:1230:MET:HG3	2.15	0.46
5:G:129:ASP:HB3	5:G:220:ARG:HD3	1.98	0.46
1:A:12:DT:H3'	1:A:13:DG:H2'	1.98	0.46
2:B:11:DC:P	5:G:311:ARG:HH12	2.39	0.46
4:F:724:VAL:HG11	4:F:727:VAL:HG23	1.98	0.46
4:F:1003:THR:HG22	4:F:1009:ASN:HB3	1.98	0.46
5:G:848:VAL:HB	5:G:858:VAL:HG22	1.97	0.46
5:G:976:THR:HG22	5:G:1028:ILE:HG22	1.98	0.46
3:E:79:LEU:HD11	5:G:526:VAL:HG21	1.98	0.46
4:F:150:HIS:CE1	4:F:454:ARG:HB2	2.50	0.46
4:F:471:VAL:HG22	4:F:497:PRO:HG2	1.97	0.46
5:G:425:ARG:NH1	7:R:20:A:O3'	2.49	0.46
5:G:867:GLN:O	5:G:871:LEU:HG	2.16	0.46
2:B:6:DC:H5'	4:F:191:LYS:HE2	1.97	0.46
3:D:97:GLU:HG3	3:D:145:LYS:HE3	1.97	0.46
4:F:14:ASP:HA	4:F:1183:ALA:HB3	1.98	0.46
4:F:56:VAL:HG12	4:F:59:ILE:HD11	1.98	0.46
4:F:142:GLU:HG2	4:F:515:MET:HE2	1.98	0.46
4:F:942:ASP:OD1	4:F:943:LYS:N	2.45	0.46
4:F:1289:GLU:HG2	4:F:1316:GLU:OE2	2.15	0.46
5:G:925:GLU:HB3	5:G:926:PRO:HD3	1.97	0.46
5:G:1136:GLY:C	5:G:1139:PRO:HD2	2.40	0.46
4:F:107:ARG:HG2	4:F:108:GLU:OE1	2.16	0.46
4:F:444:ASP:OD2	4:F:447:HIS:N	2.49	0.45
4:F:1246:ARG:HH21	4:F:1267:GLY:N	2.14	0.45
5:G:24:LEU:HD21	5:G:116:PHE:CZ	2.51	0.45
5:G:520:ALA:HB3	5:G:546:ALA:HA	1.98	0.45
5:G:549:LYS:HE2	5:G:569:LEU:HG	1.97	0.45
5:G:850:LYS:HB2	5:G:857:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:865:HIS:CD2	5:G:901:ARG:HH12	2.34	0.45
4:F:205:PRO:HG2	4:F:208:ILE:HD11	1.97	0.45
4:F:549:ASP:OD1	4:F:550:VAL:N	2.50	0.45
5:G:490:ILE:O	5:G:499:ILE:HG12	2.16	0.45
4:F:732:ILE:HD11	4:F:769:PRO:HB3	1.98	0.45
5:G:701:LEU:HD22	5:G:723:TYR:HD1	1.80	0.45
3:E:186:ASN:OD1	3:E:202:VAL:HB	2.16	0.45
5:G:18:ASP:OD1	5:G:18:ASP:N	2.46	0.45
5:G:349:TYR:CE1	5:G:379:PRO:HG3	2.51	0.45
5:G:749:LYS:CG	5:G:750:PRO:HD2	2.46	0.45
5:G:1212:ASP:N	5:G:1212:ASP:OD1	2.50	0.45
4:F:311:CYS:HB3	4:F:321:LEU:HD11	1.99	0.45
5:G:492:SER:OG	5:G:495:ASN:OD1	2.35	0.45
5:G:527:LEU:HB2	5:G:550:VAL:HG22	1.98	0.45
5:G:1146:GLU:HG2	5:G:1309:ILE:H	1.81	0.45
5:G:1177:ILE:O	5:G:1185:PRO:HB3	2.17	0.45
7:R:12:A:H2'	7:R:13:G:C8	2.51	0.45
1:A:21:DC:H4'	5:G:1148:ARG:NH1	2.32	0.45
2:B:3:DC:H2''	2:B:4:DG:N7	2.32	0.45
2:B:27:DT:H2''	2:B:28:DT:H5''	1.98	0.45
4:F:688:GLN:HB3	4:F:1235:LEU:HD12	1.99	0.45
4:F:1122:LYS:HG2	4:F:1229:TYR:CE1	2.52	0.45
4:F:1269:ARG:HB2	5:G:346:ARG:HE	1.81	0.45
5:G:227:PHE:CE1	5:G:1337:VAL:HG13	2.52	0.45
5:G:520:ALA:HB1	5:G:543:SER:OG	2.16	0.45
5:G:650:LYS:HE2	5:G:654:ILE:HD11	1.98	0.45
4:F:80:PHE:CE1	4:F:1038:GLN:HG2	2.52	0.45
4:F:804:PHE:O	5:G:638:SER:OG	2.23	0.45
4:F:1176:LEU:HD13	4:F:1180:MET:SD	2.57	0.45
5:G:706:VAL:HG21	5:G:716:GLN:HE21	1.82	0.45
4:F:607:SER:OG	4:F:610:GLU:OE1	2.34	0.45
5:G:43:THR:HG22	5:G:56:LEU:HD12	1.99	0.45
3:E:107:ILE:HG23	3:E:134:THR:HA	1.99	0.45
4:F:666:SER:HA	4:F:1186:VAL:HG11	1.99	0.45
5:G:740:LEU:C	5:G:740:LEU:HD12	2.42	0.45
4:F:485:ASP:H	4:F:487:LEU:HG	1.82	0.44
5:G:148:GLU:OE2	5:G:150:GLY:N	2.50	0.44
5:G:741:ALA:C	5:G:762:ASN:HD22	2.26	0.44
4:F:815:SER:HB3	4:F:1077:SER:OG	2.17	0.44
4:F:1063:GLY:HA3	4:F:1239:VAL:HG11	1.99	0.44
3:E:16:ILE:HG23	3:E:26:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:141:THR:HB	4:F:514:PHE:HE1	1.81	0.44
4:F:310:ILE:HD12	4:F:330:HIS:HE1	1.81	0.44
4:F:80:PHE:HE1	4:F:1038:GLN:HG2	1.82	0.44
4:F:807:TRP:HB2	4:F:1097:VAL:HG11	1.99	0.44
4:F:1278:LEU:HB2	4:F:1287:LEU:HD21	1.99	0.44
1:A:20:DG:H2'	1:A:21:DC:C6	2.53	0.44
5:G:932:MET:HB2	5:G:1136:GLY:HA3	1.99	0.44
5:G:527:LEU:HD21	5:G:536:LEU:HD12	1.98	0.44
5:G:805:GLN:HG2	5:G:1348:LYS:HE2	2.00	0.44
5:G:374:LEU:O	5:G:378:LYS:HG3	2.17	0.44
5:G:599:LYS:O	5:G:603:LYS:HG2	2.18	0.44
1:A:9:DG:H1'	1:A:10:DC:O4'	2.17	0.44
2:B:14:TTD:H72	2:B:14:TTD:H5A1	1.71	0.44
4:F:400:VAL:HA	4:F:403:MET:HG2	2.00	0.44
4:F:720:ARG:NH1	4:F:745:GLU:OE2	2.51	0.44
5:G:282:LEU:HD21	5:G:291:ILE:HG22	2.00	0.44
5:G:504:GLN:HG3	5:G:731:ARG:NH2	2.33	0.44
5:G:1146:GLU:HG2	5:G:1309:ILE:N	2.33	0.44
4:F:177:ILE:HD12	4:F:183:TRP:CD1	2.53	0.43
5:G:518:VAL:HG11	5:G:714:GLU:HB2	1.99	0.43
5:G:865:HIS:HD2	5:G:901:ARG:HH12	1.66	0.43
5:G:1150:PRO:O	5:G:1153:PRO:HD3	2.18	0.43
4:F:250:THR:OG1	4:F:251:ALA:N	2.51	0.43
4:F:845:LEU:HD23	4:F:889:PRO:HB2	1.99	0.43
5:G:26:SER:HB2	5:G:29:MET:H	1.83	0.43
1:A:3:DA:N3	1:A:3:DA:H2'	2.34	0.43
4:F:1035:LYS:HA	4:F:1038:GLN:HB2	2.00	0.43
4:F:1281:TYR:CE2	5:G:431:ARG:HG2	2.53	0.43
4:F:1286:THR:N	5:G:479:GLU:OE2	2.52	0.43
5:G:661:VAL:HG12	5:G:685:ILE:HD11	1.99	0.43
5:G:893:GLY:O	5:G:1258:ARG:NH2	2.52	0.43
5:G:1196:LEU:HG	5:G:1210:ILE:HG22	1.99	0.43
7:R:16:U:H2'	7:R:17:G:C8	2.53	0.43
5:G:868:TRP:O	5:G:872:LEU:HG	2.18	0.43
4:F:227:LYS:HE2	4:F:298:ALA:HB1	2.01	0.43
4:F:1128:ILE:HG13	4:F:1144:PHE:HE2	1.84	0.43
5:G:158:GLN:OE1	5:G:158:GLN:N	2.52	0.43
5:G:507:VAL:HG12	5:G:728:SER:OG	2.18	0.43
5:G:701:LEU:CD2	5:G:723:TYR:CG	3.02	0.43
5:G:847:ASP:HB3	5:G:856:ILE:HG23	2.00	0.43
5:G:865:HIS:H	5:G:868:TRP:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1158:GLU:OE1	5:G:1223:LEU:HD21	2.18	0.43
5:G:1292:LEU:HD22	5:G:1297:LYS:HE3	2.01	0.43
3:E:29:GLU:HA	3:E:30:PRO:HA	1.69	0.43
4:F:1061:GLN:HE21	4:F:1239:VAL:HG23	1.83	0.43
5:G:134:ASP:O	5:G:138:VAL:HG23	2.19	0.43
5:G:702:GLN:HB3	5:G:723:TYR:CE1	2.54	0.43
5:G:1292:LEU:HD12	5:G:1299:GLY:HA2	2.01	0.43
3:D:29:GLU:HA	3:D:30:PRO:HA	1.80	0.43
4:F:377:THR:HB	4:F:380:ALA:HB3	2.00	0.43
4:F:962:GLU:HA	4:F:965:GLN:HB2	2.01	0.43
5:G:335:GLN:HA	5:G:340:GLN:HG3	2.00	0.43
5:G:1119:ASP:N	5:G:1119:ASP:OD1	2.52	0.43
5:G:1305:ASP:OD1	5:G:1305:ASP:N	2.48	0.43
6:H:69:ARG:O	6:H:72:GLN:HG2	2.19	0.43
4:F:648:ASP:OD1	4:F:648:ASP:N	2.51	0.43
4:F:800:MET:O	4:F:1229:TYR:HA	2.18	0.43
5:G:818:GLU:HG3	5:G:887:SER:HB2	2.01	0.43
4:F:109:ALA:HB1	4:F:113:THR:HB	2.01	0.42
4:F:817:LEU:HD11	4:F:1080:ASN:HB2	2.01	0.42
4:F:1341:ASP:OD1	4:F:1342:GLU:N	2.52	0.42
5:G:132:LEU:HD11	5:G:312:ARG:HH22	1.84	0.42
5:G:522:GLY:HA2	5:G:525:MET:HE2	2.01	0.42
6:H:25:ARG:NH1	6:H:64:LEU:HB3	2.34	0.42
4:F:737:ASN:O	4:F:741:MET:HG3	2.18	0.42
4:F:1032:LYS:O	4:F:1036:ILE:HG12	2.18	0.42
5:G:317:THR:HG22	5:G:323:PRO:HA	2.01	0.42
5:G:432:LEU:HD13	5:G:499:ILE:HD13	2.01	0.42
5:G:706:VAL:HG21	5:G:716:GLN:NE2	2.34	0.42
5:G:807:LEU:HD11	5:G:894:VAL:HG23	2.00	0.42
5:G:836:ARG:HG3	5:G:869:CYS:SG	2.59	0.42
5:G:1036:ARG:NH1	5:G:1111:ASP:OD1	2.52	0.42
5:G:1350:ASN:HA	5:G:1353:VAL:HG22	2.00	0.42
1:A:18:DT:N3	4:F:542:ARG:HD2	2.35	0.42
5:G:759:ILE:H	5:G:759:ILE:HD12	1.84	0.42
5:G:255:LEU:HG	5:G:261:ALA:HB2	2.01	0.42
3:E:179:PRO:HG3	3:E:211:ILE:HD12	2.01	0.42
4:F:884:VAL:O	4:F:917:SER:HB2	2.20	0.42
5:G:549:LYS:HG2	5:G:569:LEU:HG	2.00	0.42
5:G:425:ARG:HD3	5:G:459:ALA:HB2	2.00	0.42
5:G:615:LYS:HB2	5:G:616:PRO:HD3	2.02	0.42
5:G:865:HIS:HA	5:G:901:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1152:GLU:HG3	5:G:1214:PRO:HD2	2.00	0.42
4:F:668:ILE:HD12	4:F:1069:ARG:O	2.20	0.42
4:F:805:MET:HE1	4:F:1221:PHE:CZ	2.55	0.42
4:F:813:GLU:OE2	5:G:731:ARG:NH2	2.46	0.42
4:F:1085:MET:HE1	4:F:1097:VAL:HG23	2.00	0.42
5:G:264:ASP:HB3	5:G:324:LEU:HB3	2.01	0.42
5:G:423:LEU:HB3	5:G:466:MET:SD	2.59	0.42
5:G:504:GLN:HE21	5:G:731:ARG:NH1	2.17	0.42
5:G:907:HIS:ND1	5:G:908:ILE:O	2.45	0.42
4:F:474:ALA:O	4:F:477:GLU:HG3	2.19	0.42
4:F:1301:ARG:HA	4:F:1304:MET:HG2	2.01	0.42
4:F:1329:GLU:HG3	5:G:331:ILE:HD11	2.02	0.42
5:G:513:MET:HE2	5:G:579:LEU:HG	2.02	0.42
5:G:865:HIS:H	5:G:868:TRP:CD1	2.38	0.42
4:F:1308:ILE:HG21	5:G:379:PRO:HB2	2.01	0.42
5:G:663:GLU:CD	5:G:667:GLN:HE21	2.28	0.42
6:H:45:LYS:HA	6:H:45:LYS:HD3	1.89	0.42
4:F:60:GLN:O	4:F:476:LYS:NZ	2.40	0.42
4:F:197:ARG:HD3	4:F:200:ARG:HA	2.02	0.42
4:F:750:ILE:HD13	4:F:963:GLU:HG2	2.02	0.42
4:F:976:ARG:O	4:F:980:VAL:HG23	2.20	0.42
4:F:997:TRP:HE3	4:F:1000:LEU:HD22	1.85	0.42
5:G:528:THR:N	5:G:532:GLU:OE1	2.45	0.42
5:G:864:LEU:HD11	5:G:869:CYS:HB3	2.02	0.42
6:H:29:GLN:O	6:H:33:GLY:N	2.42	0.42
5:G:111:THR:HG21	5:G:303:VAL:HB	2.02	0.41
3:E:197:ASP:OD1	3:E:197:ASP:N	2.44	0.41
4:F:151:ARG:HH12	4:F:175:ARG:HH21	1.67	0.41
4:F:338:THR:HG23	4:F:343:HIS:O	2.21	0.41
4:F:367:TYR:O	4:F:371:ARG:N	2.29	0.41
5:G:510:LEU:HA	5:G:513:MET:HG2	2.02	0.41
1:A:29:DA:H2"	1:A:30:DA:H5"	2.01	0.41
4:F:12:ARG:O	4:F:1157:GLN:NE2	2.43	0.41
4:F:590:PRO:HB3	4:F:605:TYR:HE1	1.84	0.41
5:G:1161:GLY:C	5:G:1203:ARG:HG3	2.45	0.41
5:G:1259:GLN:OE1	5:G:1262:ARG:NH1	2.53	0.41
4:F:452:ARG:HB3	4:F:586:PHE:CE1	2.55	0.41
4:F:560:PRO:HG3	5:G:773:PHE:CD1	2.55	0.41
4:F:724:VAL:CG1	4:F:727:VAL:HG23	2.50	0.41
4:F:1065:LYS:HD3	4:F:1073:LYS:NZ	2.35	0.41
5:G:367:GLY:CA	5:G:448:GLN:HB2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:370:LYS:HG2	5:G:441:LEU:HB3	2.02	0.41
5:G:1173:ARG:NH2	5:G:1192:LYS:O	2.53	0.41
4:F:176:ILE:HG23	4:F:405:PHE:CZ	2.40	0.41
4:F:1107:MET:HE2	5:G:763:PHE:CE2	2.55	0.41
5:G:364:HIS:HB3	5:G:487:THR:HG23	2.03	0.41
4:F:685:MET:SD	4:F:1073:LYS:HB2	2.60	0.41
4:F:753:LEU:HB3	4:F:767:GLN:HB2	2.03	0.41
5:G:554:GLU:CD	5:G:589:TYR:H	2.28	0.41
5:G:885:VAL:HG12	5:G:894:VAL:HG11	2.03	0.41
4:F:1230:MET:HE3	4:F:1232:MET:SD	2.60	0.41
5:G:416:ILE:HD13	5:G:441:LEU:HG	2.02	0.41
5:G:538:ARG:HD2	5:G:538:ARG:HA	1.84	0.41
2:B:2:DT:H6	2:B:2:DT:H2'	1.72	0.41
4:F:100:LEU:HD12	4:F:122:VAL:HG21	2.02	0.41
4:F:515:MET:HA	4:F:526:HIS:CE1	2.56	0.41
4:F:812:PHE:HE1	5:G:504:GLN:HB2	1.83	0.41
4:F:1072:ASN:HD22	4:F:1111:GLN:NE2	2.19	0.41
4:F:1073:LYS:NZ	5:G:463:GLY:HA3	2.36	0.41
5:G:250:ARG:HG2	5:G:266:ASN:ND2	2.36	0.41
1:A:10:DC:H41	5:G:316:ILE:HG12	1.85	0.41
3:D:79:LEU:HD11	4:F:1057:LYS:NZ	2.36	0.41
3:E:57:THR:HG22	3:E:175:ALA:HB2	2.03	0.41
4:F:722:GLY:HA2	4:F:737:ASN:CG	2.45	0.41
4:F:990:ASP:OD1	4:F:991:LYS:N	2.51	0.41
4:F:1118:GLY:C	4:F:1229:TYR:HB2	2.46	0.41
4:F:1134:GLN:OE1	4:F:1136:GLN:NE2	2.54	0.41
4:F:1171[B]:ARG:HE	4:F:1171[B]:ARG:HB3	1.53	0.41
5:G:102:MET:SD	5:G:246:PRO:HD3	2.60	0.41
5:G:1060:VAL:HG22	5:G:1106:ILE:HD12	2.03	0.41
4:F:14:ASP:HB3	4:F:1157:GLN:HB2	2.03	0.41
4:F:1288:GLN:O	4:F:1292:THR:OG1	2.29	0.41
5:G:707:ILE:HD13	5:G:713:GLU:HG3	2.02	0.41
4:F:742:TYR:O	4:F:745:GLU:HG2	2.20	0.40
4:F:878:THR:HA	4:F:925:SER:HA	2.02	0.40
4:F:1316:GLU:N	4:F:1317:PRO:HD2	2.36	0.40
5:G:1068:THR:HG23	5:G:1070:GLY:H	1.86	0.40
4:F:196:VAL:N	4:F:204:LEU:O	2.43	0.40
4:F:1105:SER:HA	5:G:736:GLN:OE1	2.20	0.40
4:F:1151:LEU:HD11	4:F:1197:GLU:HB3	2.03	0.40
4:F:12:ARG:HA	4:F:1181:PRO:HB2	2.02	0.40
4:F:317:LEU:HD23	4:F:317:LEU:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:395:TYR:CE2	4:F:420:LEU:HG	2.56	0.40
4:F:404:LYS:HD3	4:F:404:LYS:HA	1.94	0.40
4:F:1186:VAL:HG23	4:F:1187:PHE:HD1	1.87	0.40
4:F:1278:LEU:HD12	4:F:1287:LEU:HD23	2.04	0.40
5:G:496:GLY:HA2	5:G:903:LEU:O	2.22	0.40
5:G:732:GLY:HA2	5:G:736:GLN:OE1	2.22	0.40
4:F:802:VAL:HA	4:F:1096:ILE:O	2.21	0.40
4:F:1125:GLY:HA3	4:F:1179:GLY:HA2	2.03	0.40
5:G:234:PRO:HA	5:G:237:MET:HE3	2.02	0.40
5:G:1154:ALA:H	5:G:1215:GLU:HA	1.87	0.40
5:G:1263:LYS:NZ	5:G:1281:GLU:HG2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	227/239 (95%)	225 (99%)	2 (1%)	0	100	100
3	E	216/239 (90%)	209 (97%)	7 (3%)	0	100	100
4	F	1318/1342 (98%)	1278 (97%)	40 (3%)	0	100	100
5	G	1322/1407 (94%)	1281 (97%)	41 (3%)	0	100	100
6	H	71/91 (78%)	69 (97%)	2 (3%)	0	100	100
All	All	3154/3318 (95%)	3062 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	
3	D	197/206 (96%)	197 (100%)	0	100	100
3	E	188/206 (91%)	188 (100%)	0	100	100
4	F	1141/1157 (99%)	1140 (100%)	1 (0%)	88	97
5	G	1116/1168 (96%)	1114 (100%)	2 (0%)	87	96
6	H	63/75 (84%)	63 (100%)	0	100	100
All	All	2705/2812 (96%)	2702 (100%)	3 (0%)	87	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	327	GLN
5	G	901	ARG
5	G	951	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	93	GLN
3	D	147	GLN
3	D	227	GLN
3	E	18	GLN
3	E	23	HIS
3	E	41	ASN
3	E	132	HIS
4	F	83	GLN
4	F	150	HIS
4	F	752	ASN
4	F	824	GLN
4	F	952	GLN
4	F	1061	GLN
4	F	1116	HIS
4	F	1136	GLN
4	F	1257	GLN
5	G	153	ASN
5	G	186	GLN
5	G	266	ASN

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Mol	Chain	Res	Type
5	G	276	ASN
5	G	340	GLN
5	G	341	ASN
5	G	364	HIS
5	G	424	ASN
5	G	469	HIS
5	G	545	HIS
5	G	665	GLN
5	G	669	GLN
5	G	771	GLN
5	G	865	HIS
5	G	951	GLN
5	G	1244	GLN
5	G	1367	GLN
6	H	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	13/19 (68%)	3 (23%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	10	C
7	R	19	G
7	R	20	A

There are no RNA pucker outliers to report.

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

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
2	TTD	B	14	2	42,45,46	1.38	9 (21%)	61,74,77	2.64	22 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTD	B	14	2	-	12/22/109/110	0/5/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	TTD	C5-C6	3.63	1.59	1.55
2	B	14	TTD	C2T-N3T	-3.19	1.32	1.38
2	B	14	TTD	C2-N3	-2.79	1.33	1.38
2	B	14	TTD	C6T-C6	2.69	1.64	1.56
2	B	14	TTD	C1R-N1T	-2.61	1.42	1.45
2	B	14	TTD	C6-N1	2.35	1.50	1.46
2	B	14	TTD	C2T-N1T	-2.28	1.32	1.36
2	B	14	TTD	C2'-C3R	-2.22	1.48	1.52
2	B	14	TTD	C5T-C6T	2.02	1.57	1.55

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	TTD	C2R-C1R-N1T	-7.63	105.28	115.59
2	B	14	TTD	O3'-C3'-C2R	-7.58	84.52	110.88
2	B	14	TTD	C6T-C6-N1	4.87	136.70	118.51
2	B	14	TTD	C5T-C5-C4	4.63	127.88	112.84
2	B	14	TTD	O4R-C1R-N1T	4.59	114.09	108.65
2	B	14	TTD	C5-C4-N3	4.51	119.88	116.09
2	B	14	TTD	C5T-C4T-N3T	4.45	119.82	116.09
2	B	14	TTD	C2'-C1'-N1	-4.36	109.70	115.59
2	B	14	TTD	C5-C5T-C4T	4.03	125.94	112.84
2	B	14	TTD	N3-C2-N1	-3.98	112.61	116.78
2	B	14	TTD	C5-C6-N1	-3.94	110.42	115.65
2	B	14	TTD	O4'-C1'-N1	3.94	113.32	108.65
2	B	14	TTD	O4-C4-C5	-3.63	119.33	122.71
2	B	14	TTD	O4T-C4T-C5T	-3.15	119.78	122.71
2	B	14	TTD	O4'-C1'-C2'	-3.11	100.43	106.25
2	B	14	TTD	C5A-C5-C5T	-3.07	107.57	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	TTD	C3R-C2'-C1'	-2.99	97.20	102.89
2	B	14	TTD	O4P-PB-O3R	2.98	118.82	106.70
2	B	14	TTD	C5M-C5T-C5	-2.95	107.91	116.61
2	B	14	TTD	C5T-C6T-N1T	-2.65	112.14	115.65
2	B	14	TTD	O4R-C4'-C3'	-2.03	101.02	105.65
2	B	14	TTD	O3'-C3'-C4'	-2.00	102.48	110.07

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	14	TTD	O4'-C1'-N1-C2
2	B	14	TTD	C5R-O5R-PB-O4P
2	B	14	TTD	O4'-C1'-N1-C6
2	B	14	TTD	O4R-C4'-C5R-O5R
2	B	14	TTD	C2'-C1'-N1-C6
2	B	14	TTD	C3'-C4'-C5R-O5R
2	B	14	TTD	C3R-O3R-PB-O5P
2	B	14	TTD	O4'-C4R-C5'-O5'
2	B	14	TTD	C2'-C3R-O3R-PB
2	B	14	TTD	C4'-C5R-O5R-PB
2	B	14	TTD	C3R-O3R-PB-O4P
2	B	14	TTD	C3R-C4R-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	14	TTD	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

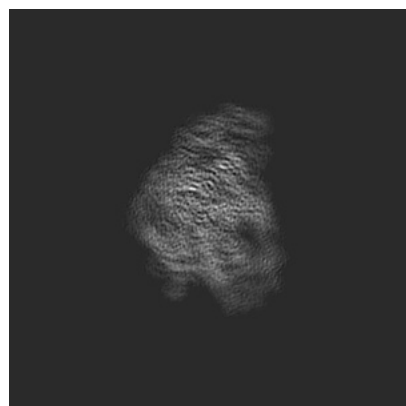
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17586. These allow visual inspection of the internal detail of the map and identification of artifacts.

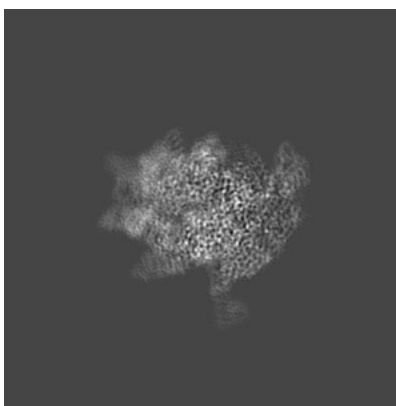
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

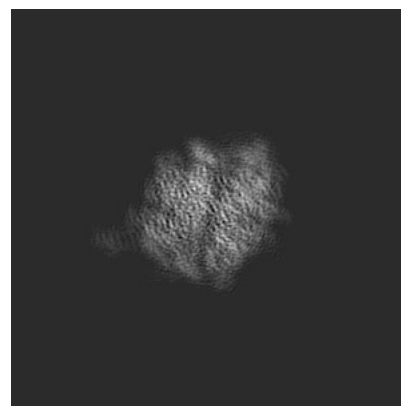
6.1.1 Primary map



X

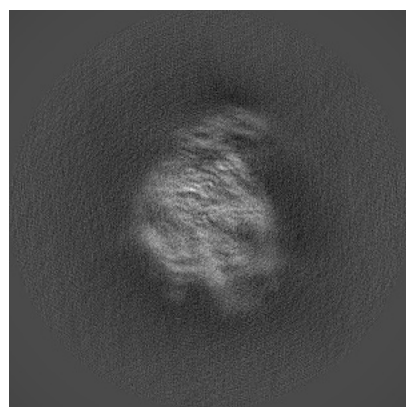


Y

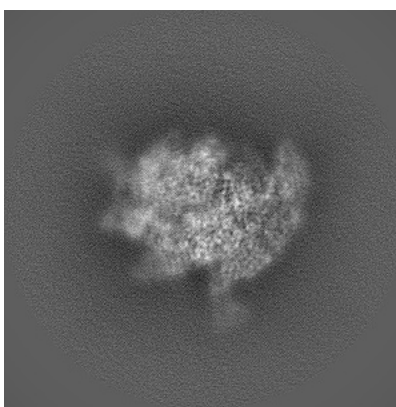


Z

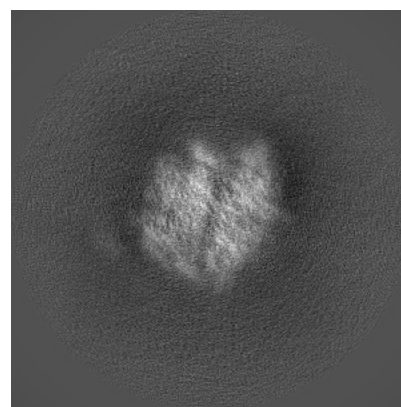
6.1.2 Raw map



X



Y

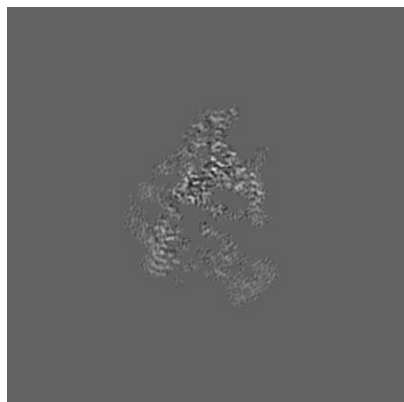


Z

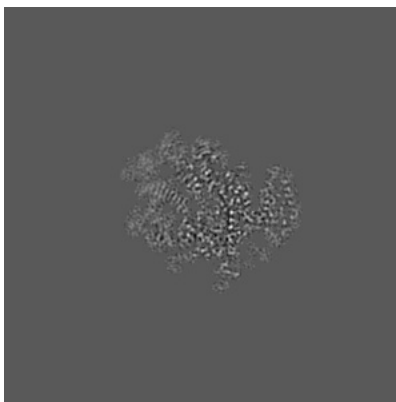
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

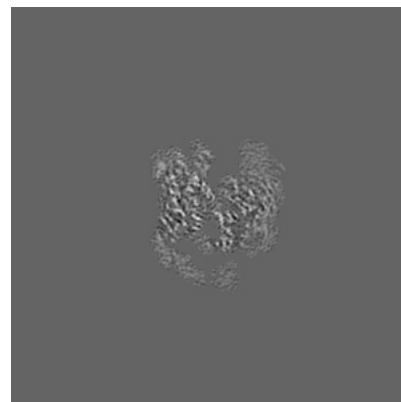
6.2.1 Primary map



X Index: 250

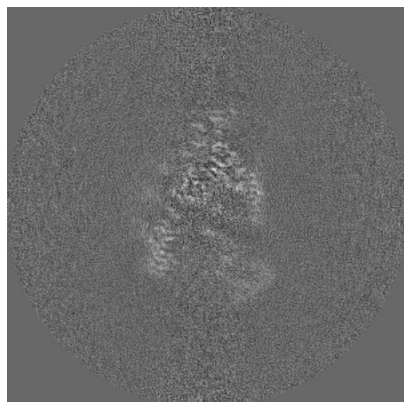


Y Index: 250

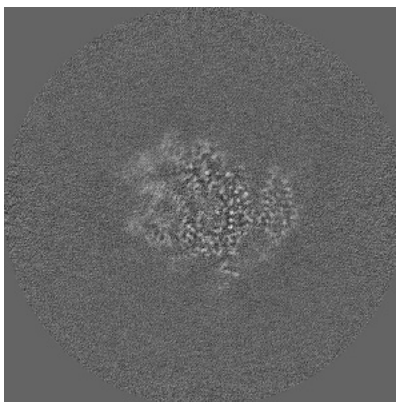


Z Index: 250

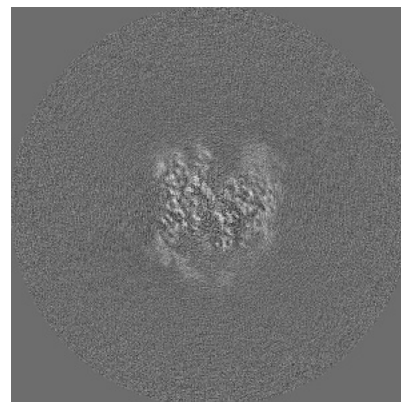
6.2.2 Raw map



X Index: 250



Y Index: 250

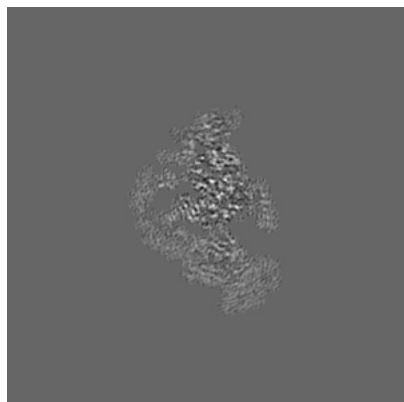


Z Index: 250

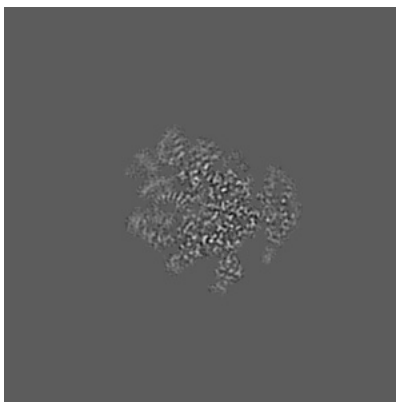
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

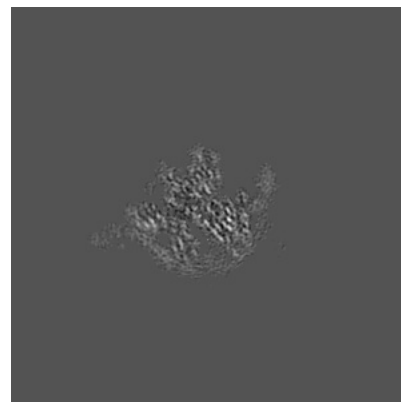
6.3.1 Primary map



X Index: 230

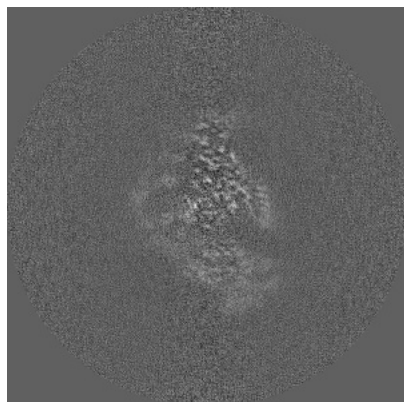


Y Index: 245

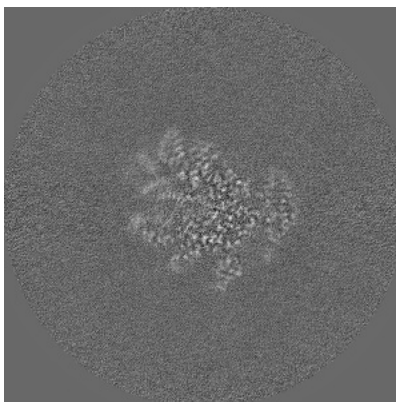


Z Index: 275

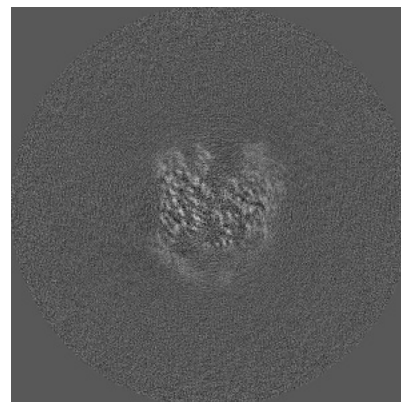
6.3.2 Raw map



X Index: 233



Y Index: 245

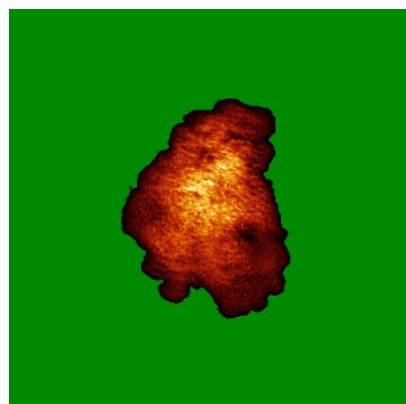


Z Index: 251

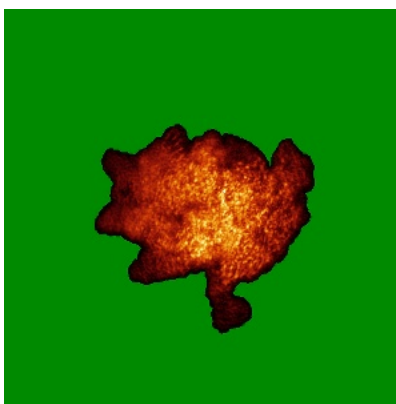
The images above show the largest variance slices of the map in three orthogonal directions.

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

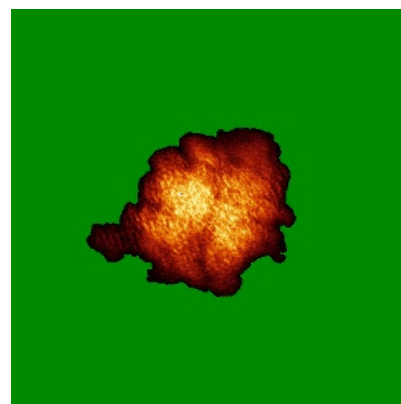
6.4.1 Primary map



X

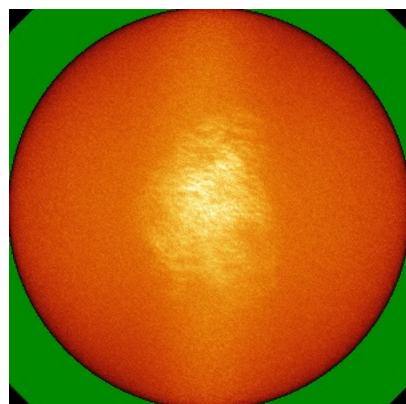


Y

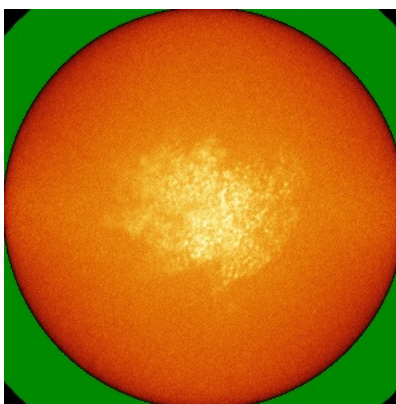


Z

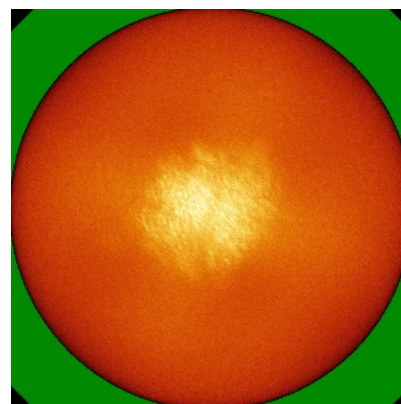
6.4.2 Raw map



X



Y

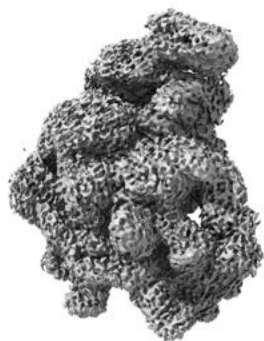


Z

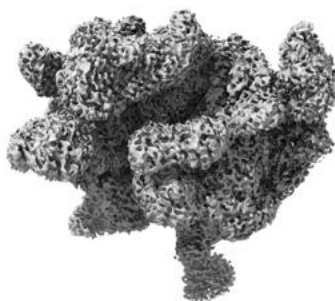
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

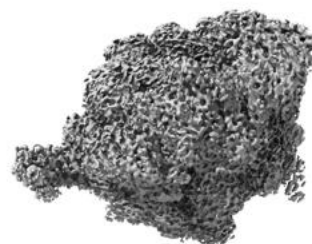
6.5.1 Primary map



X



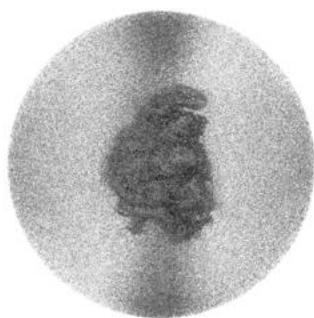
Y



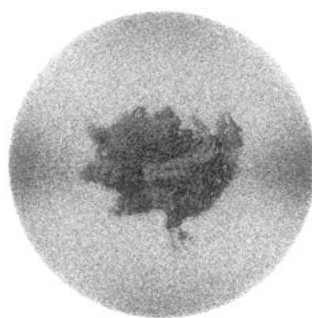
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00102. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

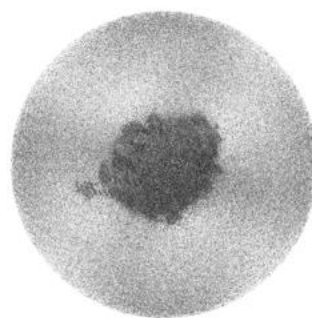
6.5.2 Raw map



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.

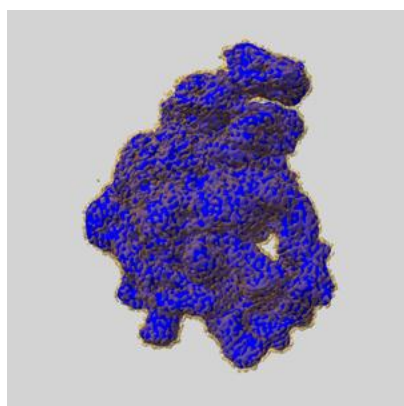
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

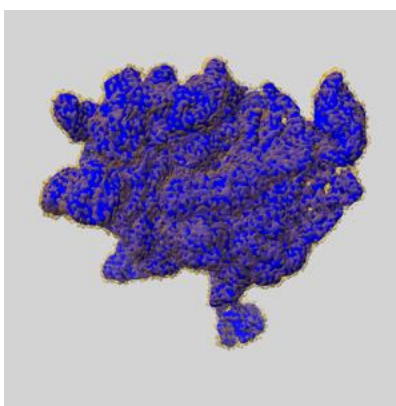
A mask typically either:

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

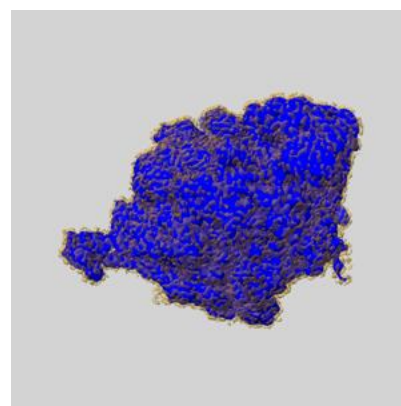
6.6.1 emd_17586_msk_1.map [i](#)



X



Y

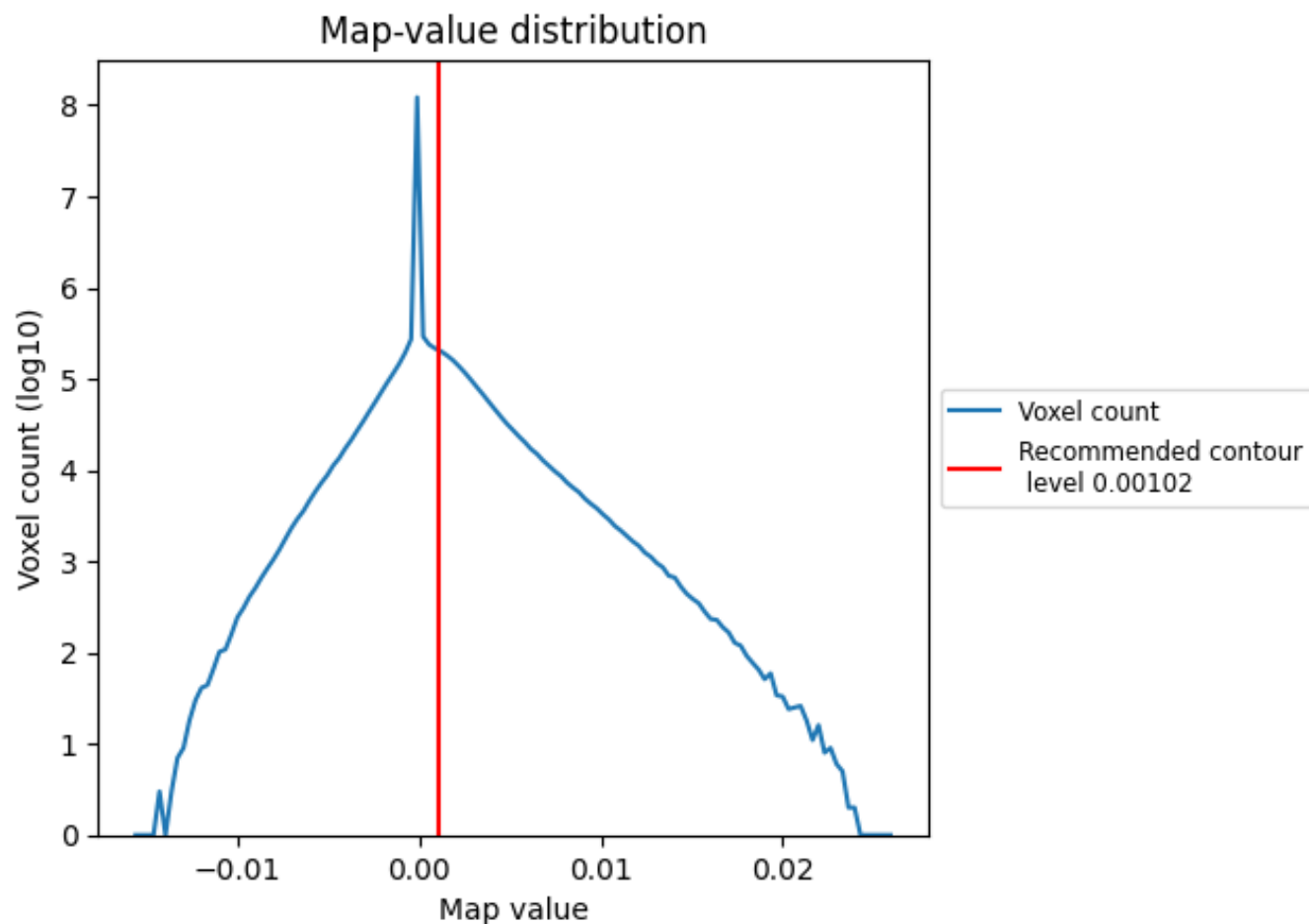


Z

7 Map analysis [i](#)

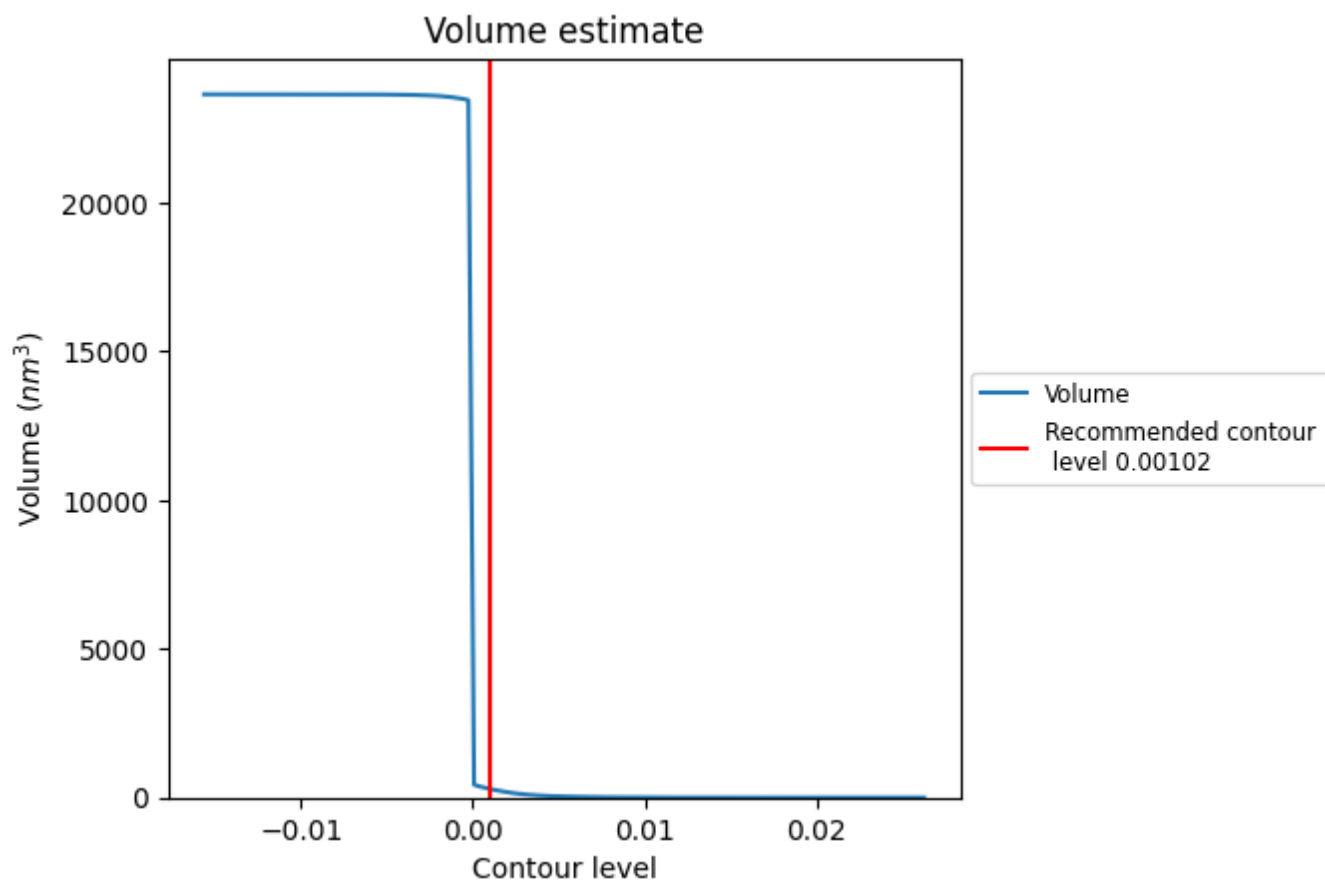
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

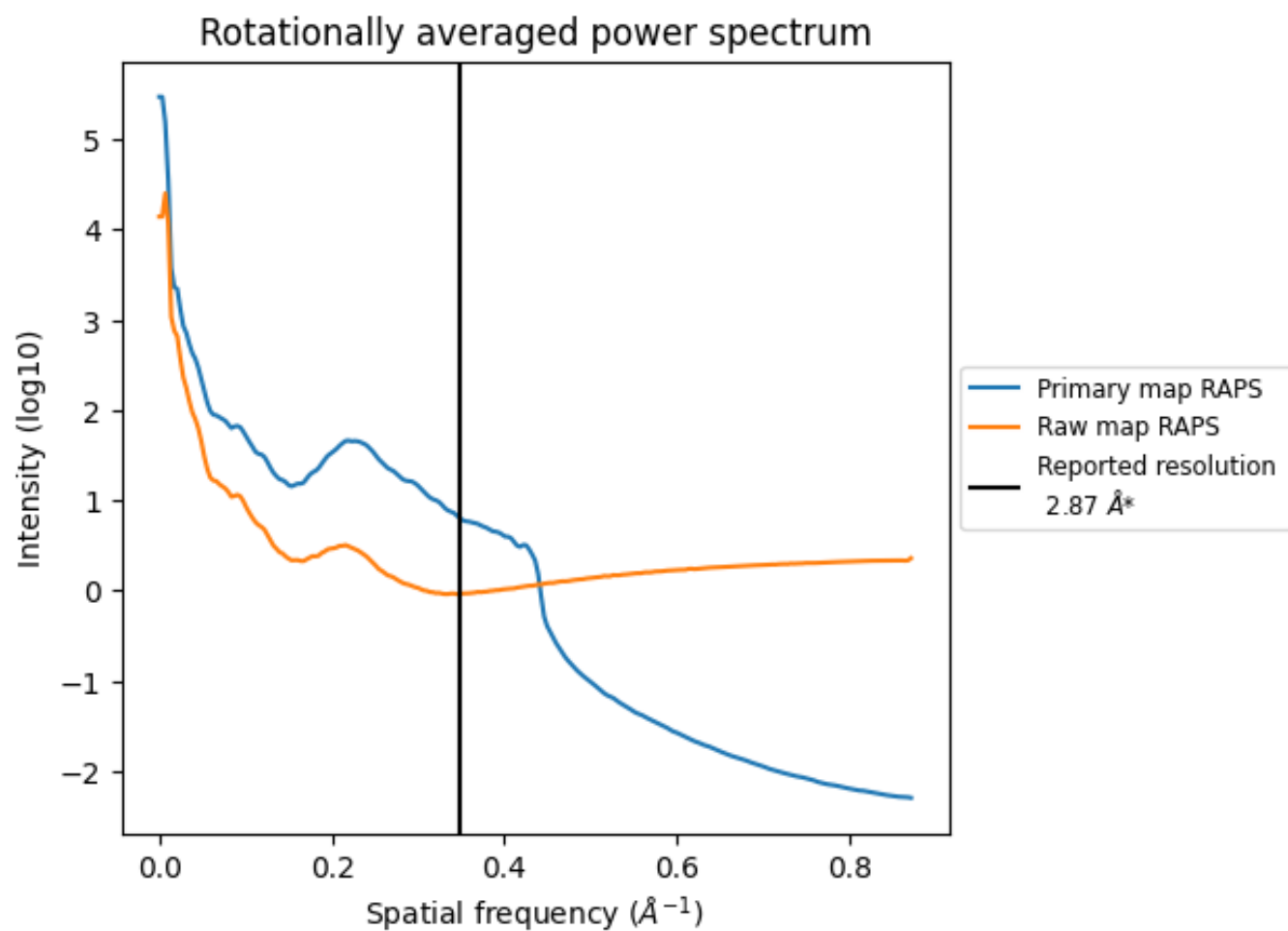
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm³; this corresponds to an approximate mass of 260 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 [i](#)

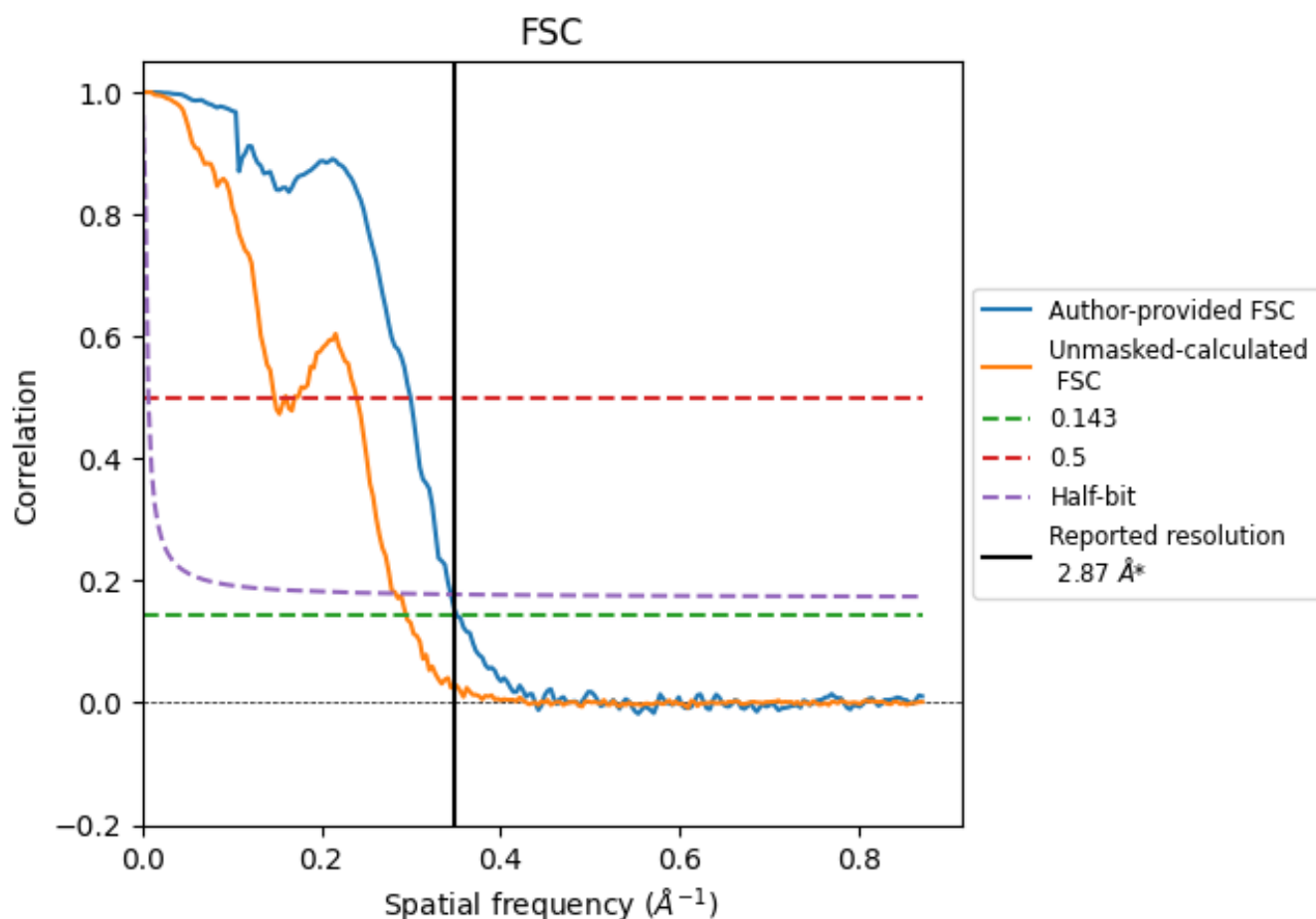


*Reported resolution corresponds to spatial frequency of $0.348 \text{ \AA}^{-1}$

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 $0.348 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

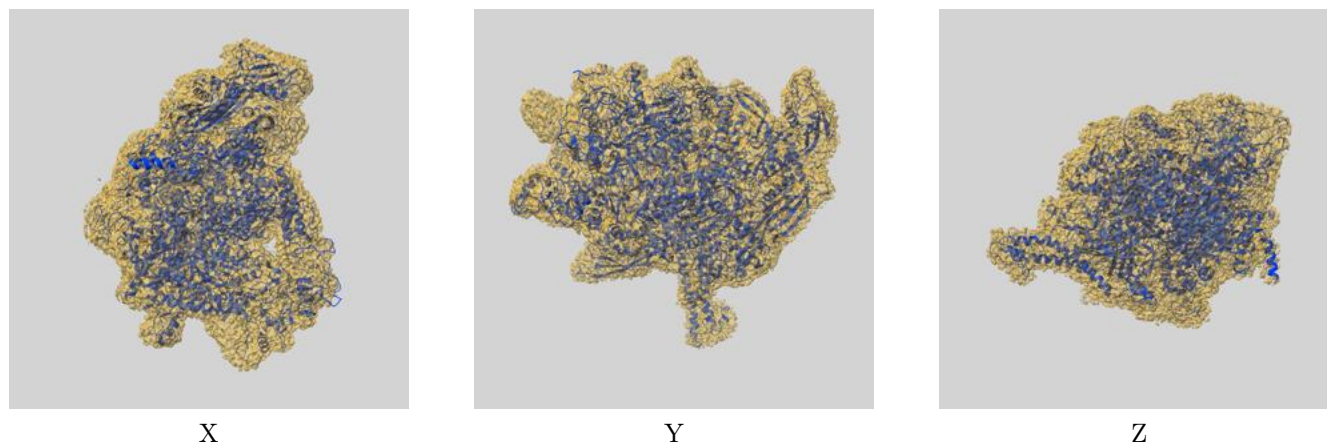
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.84	3.34	2.90
Unmasked-calculated*	3.39	6.78	3.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17586 and PDB model 8PBL. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



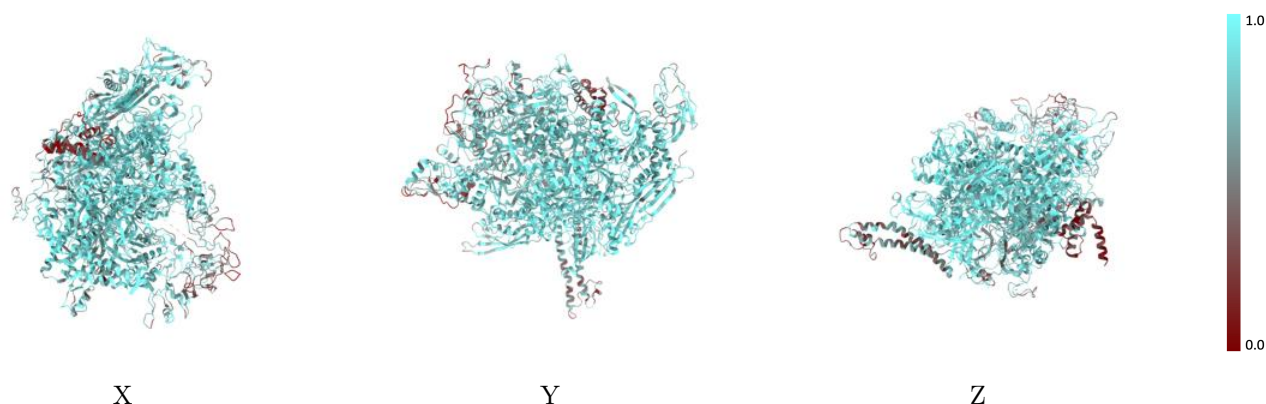
The images above show the 3D surface view of the map at the recommended contour level 0.00102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



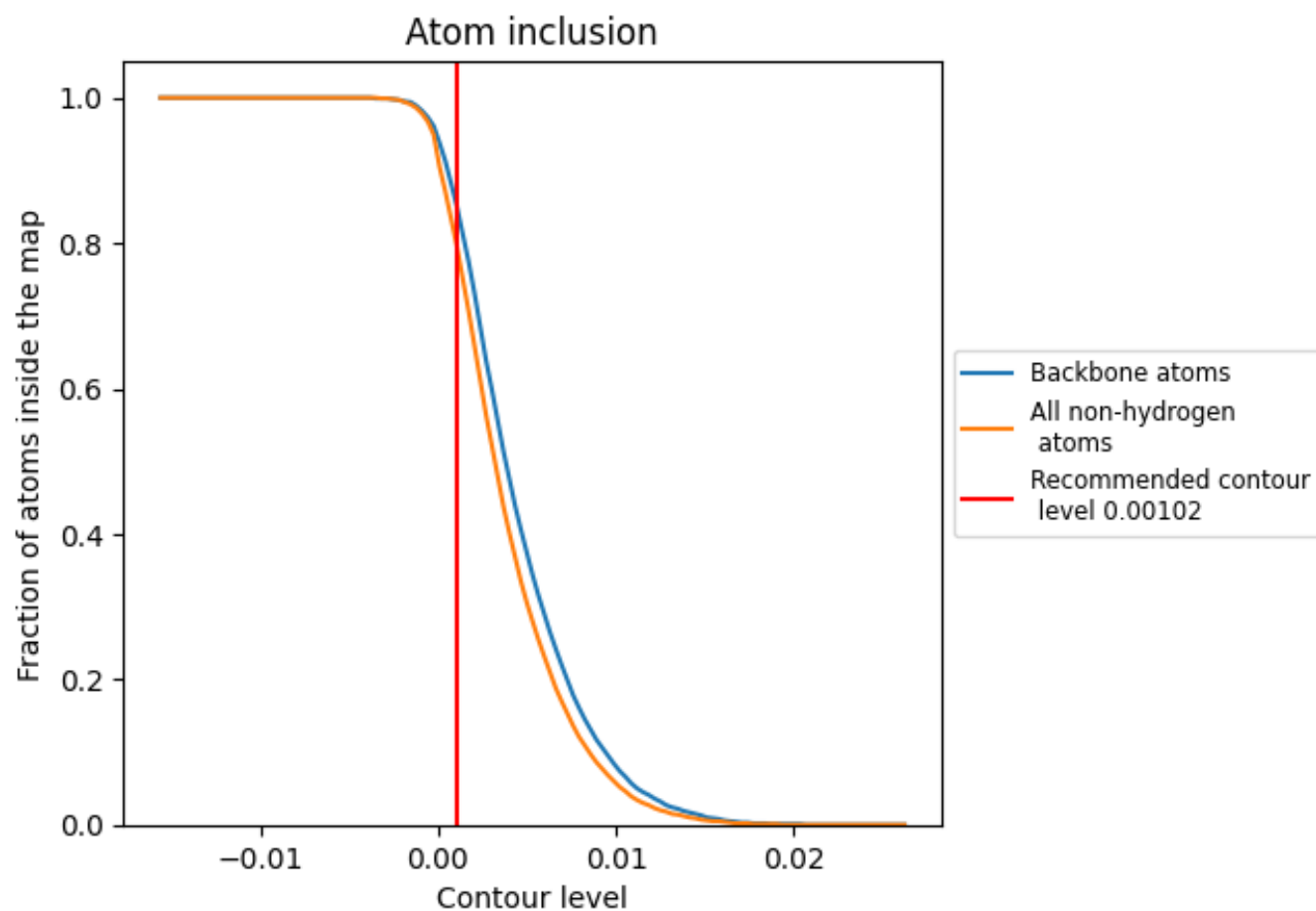
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00102).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.00102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.3460
A	0.7790	0.2090
B	0.8770	0.3560
D	0.8450	0.4290
E	0.7590	0.3170
F	0.8250	0.3710
G	0.8030	0.3360
H	0.2280	0.0400
R	0.8090	0.3460

1.0

0.0

<0.0