



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 05:35 PM EST

PDB ID : 6DBJ
EMDB ID : EMD-7844
Title : Cryo-EM structure of RAG in complex with 12-RSS and 23-RSS nicked DNA intermediates
Authors : Wu, H.; Liao, M.; Ru, H.; Mi, W.
Deposited on : 2018-05-03
Resolution : 2.99 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

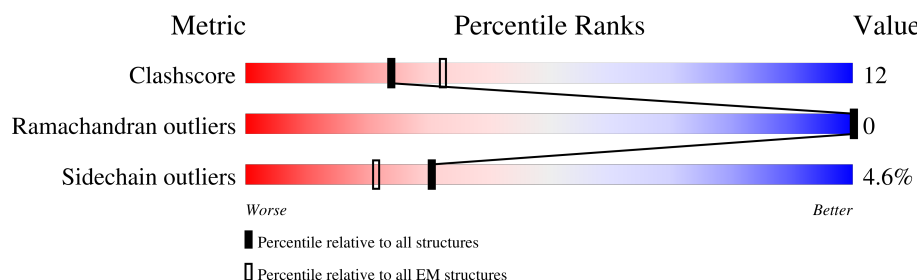
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1159	
1	C	1159	
2	B	533	
2	D	533	
3	E	15	
3	H	15	
4	F	31	
4	G	31	

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Mol	Chain	Length	Quality of chain
5	I	16	<div><div></div><div>12%</div><div>88%</div><div>12%</div></div>
5	J	16	<div><div></div><div>12%</div><div>81%</div><div>19%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Recombination activating gene 1 - MBP chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	552	Total	C	N	O	S	1	0
			4462	2799	792	837	34		
1	C	552	Total	C	N	O	S	1	0
			4462	2799	792	837	34		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP P0AEX9
A	-126	GLY	-	expression tag	UNP P0AEX9
A	-125	SER	-	expression tag	UNP P0AEX9
A	-124	SER	-	expression tag	UNP P0AEX9
A	-123	HIS	-	expression tag	UNP P0AEX9
A	-122	HIS	-	expression tag	UNP P0AEX9
A	-121	HIS	-	expression tag	UNP P0AEX9
A	-120	HIS	-	expression tag	UNP P0AEX9
A	-119	HIS	-	expression tag	UNP P0AEX9
A	-118	HIS	-	expression tag	UNP P0AEX9
A	-117	GLY	-	expression tag	UNP P0AEX9
A	-116	THR	-	expression tag	UNP P0AEX9
A	-115	LYS	-	expression tag	UNP P0AEX9
A	-114	THR	-	expression tag	UNP P0AEX9
A	251	GLY	-	linker	UNP P0AEX9
A	252	THR	-	linker	UNP P0AEX9
A	253	ASP	-	linker	UNP P0AEX9
A	254	TYR	-	linker	UNP P0AEX9
A	255	ASP	-	linker	UNP P0AEX9
A	256	ILE	-	linker	UNP P0AEX9
A	257	PRO	-	linker	UNP P0AEX9
A	258	THR	-	linker	UNP P0AEX9
A	259	THR	-	linker	UNP P0AEX9
A	260	LEU	-	linker	UNP P0AEX9
A	261	GLU	-	linker	UNP P0AEX9
A	262	VAL	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	linker	UNP P0AEX9
A	264	PHE	-	linker	UNP P0AEX9
A	265	GLN	-	linker	UNP P0AEX9
A	266	GLY	-	linker	UNP P0AEX9
A	267	PRO	-	linker	UNP P0AEX9
A	268	LEU	-	linker	UNP P0AEX9
A	269	GLY	-	linker	UNP P0AEX9
A	270	SER	-	linker	UNP P0AEX9
C	-127	MET	-	initiating methionine	UNP P0AEX9
C	-126	GLY	-	expression tag	UNP P0AEX9
C	-125	SER	-	expression tag	UNP P0AEX9
C	-124	SER	-	expression tag	UNP P0AEX9
C	-123	HIS	-	expression tag	UNP P0AEX9
C	-122	HIS	-	expression tag	UNP P0AEX9
C	-121	HIS	-	expression tag	UNP P0AEX9
C	-120	HIS	-	expression tag	UNP P0AEX9
C	-119	HIS	-	expression tag	UNP P0AEX9
C	-118	HIS	-	expression tag	UNP P0AEX9
C	-117	GLY	-	expression tag	UNP P0AEX9
C	-116	THR	-	expression tag	UNP P0AEX9
C	-115	LYS	-	expression tag	UNP P0AEX9
C	-114	THR	-	expression tag	UNP P0AEX9
C	251	GLY	-	linker	UNP P0AEX9
C	252	THR	-	linker	UNP P0AEX9
C	253	ASP	-	linker	UNP P0AEX9
C	254	TYR	-	linker	UNP P0AEX9
C	255	ASP	-	linker	UNP P0AEX9
C	256	ILE	-	linker	UNP P0AEX9
C	257	PRO	-	linker	UNP P0AEX9
C	258	THR	-	linker	UNP P0AEX9
C	259	THR	-	linker	UNP P0AEX9
C	260	LEU	-	linker	UNP P0AEX9
C	261	GLU	-	linker	UNP P0AEX9
C	262	VAL	-	linker	UNP P0AEX9
C	263	LEU	-	linker	UNP P0AEX9
C	264	PHE	-	linker	UNP P0AEX9
C	265	GLN	-	linker	UNP P0AEX9
C	266	GLY	-	linker	UNP P0AEX9
C	267	PRO	-	linker	UNP P0AEX9
C	268	LEU	-	linker	UNP P0AEX9
C	269	GLY	-	linker	UNP P0AEX9
C	270	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Recombination activating gene 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2720	1719	471	511	19		
2	D	352	Total	C	N	O	S	0	0
			2720	1719	471	511	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q1RLW7
B	-1	GLY	-	expression tag	UNP Q1RLW7
B	0	SER	-	expression tag	UNP Q1RLW7
D	-2	GLY	-	expression tag	UNP Q1RLW7
D	-1	GLY	-	expression tag	UNP Q1RLW7
D	0	SER	-	expression tag	UNP Q1RLW7

- Molecule 3 is a DNA chain called Forward stand of RSS signal end.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	15	Total	C	N	O	P	0	0
			306	145	59	87	15		
3	H	15	Total	C	N	O	P	0	0
			306	145	59	87	15		

- Molecule 4 is a DNA chain called Reverse stand of RSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	31	Total	C	N	O	P	0	0
			639	303	120	185	31		
4	G	31	Total	C	N	O	P	0	0
			639	303	120	185	31		

- Molecule 5 is a DNA chain called Forward strand of coding flank.

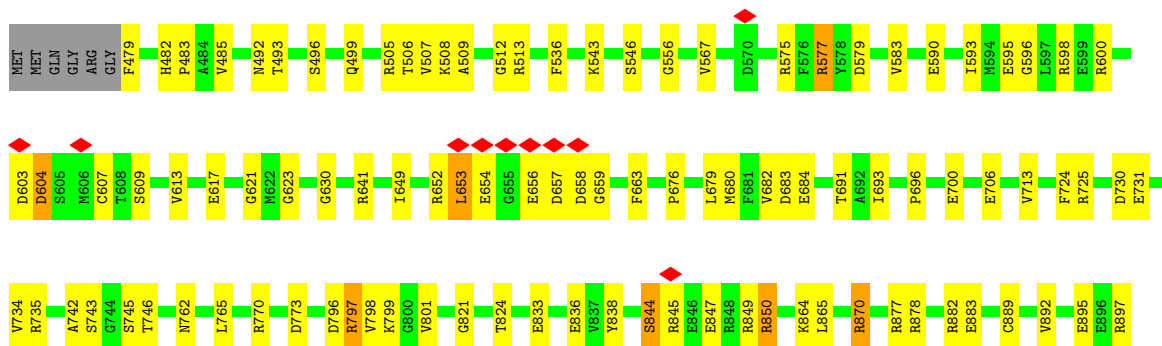
Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	16	Total	C	N	O	P	0	0
			326	156	54	100	16		
5	J	16	Total	C	N	O	P	0	0
			326	156	54	100	16		

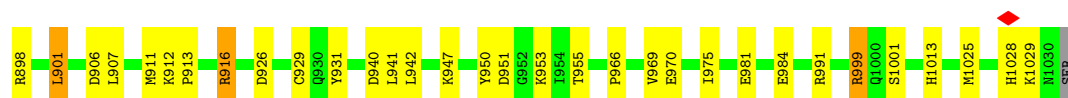
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Zn 1	0
6	C	1	Total 1	Zn 1	0

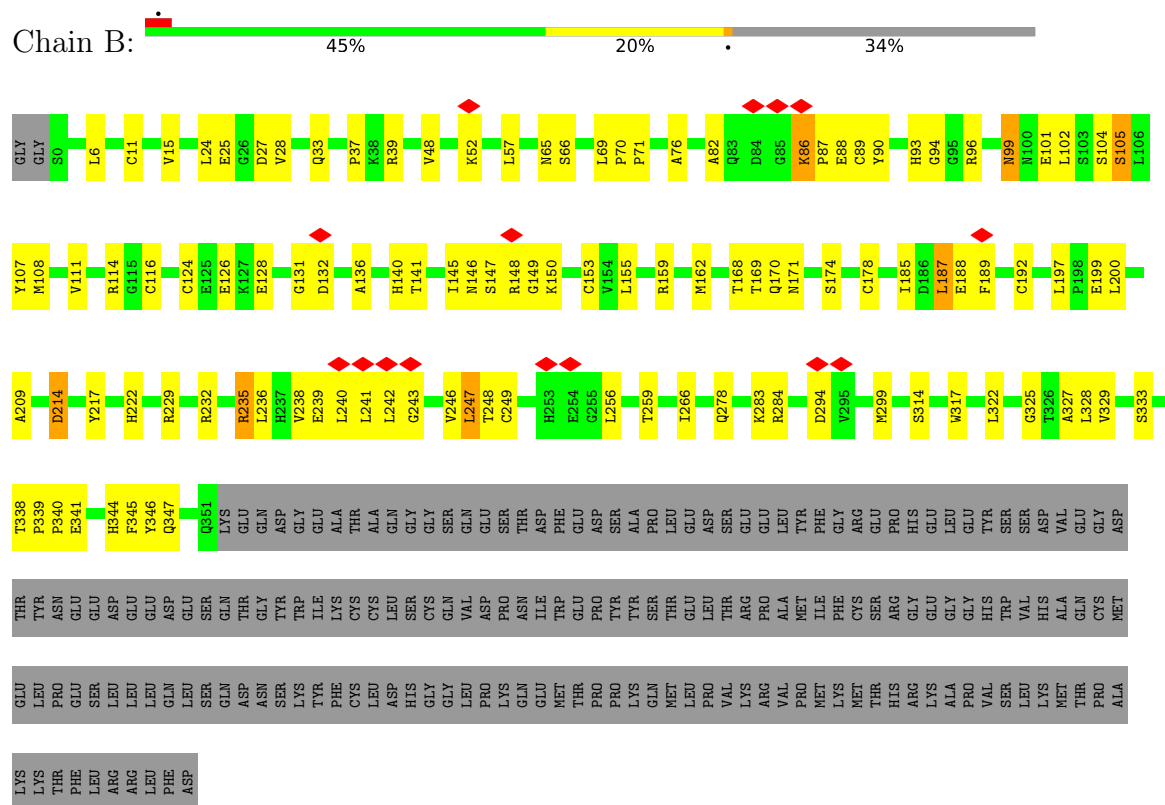
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total 2	Ca 2	0
7	C	2	Total 2	Ca 2	0

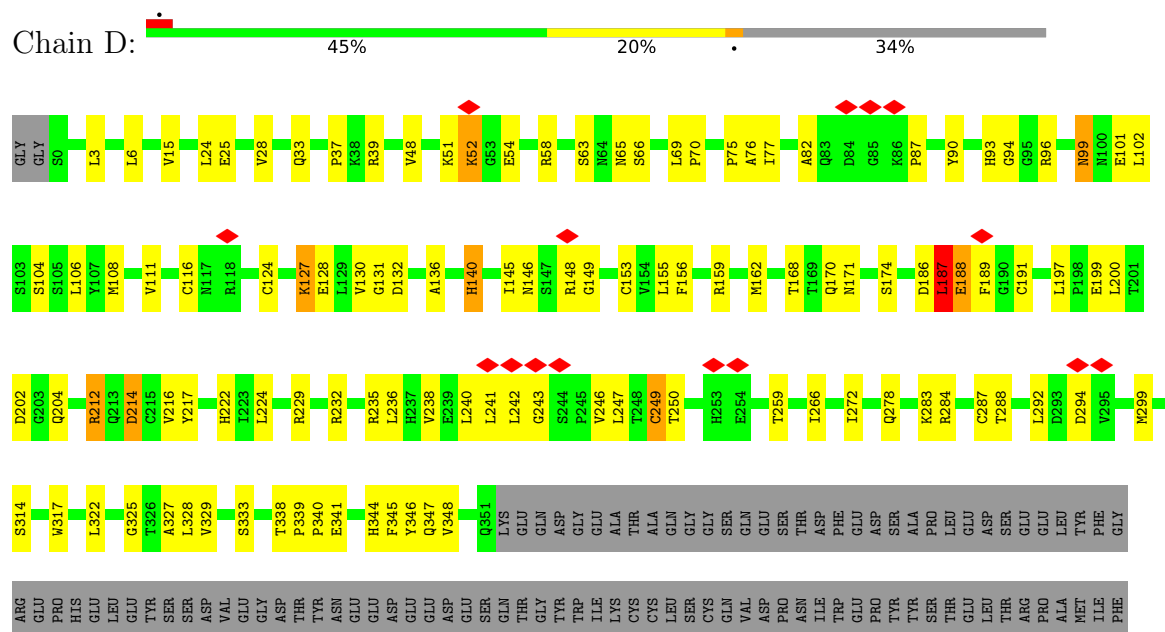




• Molecule 2: Recombination activating gene 2

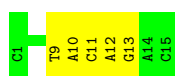


• Molecule 2: Recombination activating gene 2

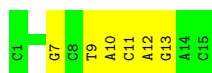


MET THR HIS ARG LYS ALA PRO VAL SER LEU LYS MET THR PRO ALA LYS LYS THR PHE LEU ARG ARG LEU PHE ASP

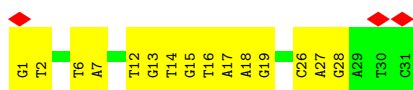
- Chain E:  67% 33%



- Chain H: 60% 40%

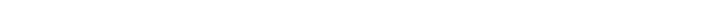


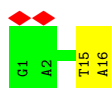
- Chain F:  10% 52% 48%




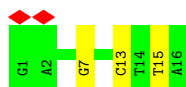
- Chain G: 



- Chain I: 



- Chain J: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	196652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.397	Depositor
Minimum map value	-0.150	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/4557	0.49	1/6136 (0.0%)
1	C	0.27	0/4557	0.49	0/6136
2	B	0.29	0/2790	0.56	1/3792 (0.0%)
2	D	0.31	0/2790	0.56	0/3792
3	E	0.57	0/343	0.90	0/526
3	H	0.57	0/343	0.89	0/526
4	F	0.55	0/717	0.93	0/1105
4	G	0.57	0/717	0.94	0/1105
5	I	0.55	0/363	1.02	0/558
5	J	0.54	0/363	1.02	0/558
All	All	0.34	0/17540	0.62	2/24234 (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
1	A	0	1
2	B	0	1
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	247	LEU	CA-CB-CG	5.49	127.94	115.30
1	A	607	CYS	CA-CB-SG	5.15	123.28	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	606	MET	Peptide
2	B	187	LEU	Peptide
2	D	187	LEU	Peptide
2	D	188	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4462	0	4403	117	0
1	C	4462	0	4405	103	0
2	B	2720	0	2670	75	0
2	D	2720	0	2670	80	0
3	E	306	0	168	5	0
3	H	306	0	168	4	0
4	F	639	0	349	14	0
4	G	639	0	349	14	0
5	I	326	0	183	5	0
5	J	326	0	183	5	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	0	0
7	C	2	0	0	0	0
All	All	16912	0	15548	388	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 (388) 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)
2:B:145:ILE:HD13	2:B:238:VAL:HG21	1.22	1.13
2:D:145:ILE:HD13	2:D:238:VAL:CG2	1.81	1.11
2:B:145:ILE:HD13	2:B:238:VAL:CG2	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:ILE:HD13	2:D:238:VAL:HG21	1.41	1.00
1:A:652:ARG:NE	1:A:658:ASP:O	2.03	0.92
2:B:145:ILE:CD1	2:B:238:VAL:HG21	2.02	0.88
2:D:148:ARG:HH12	2:D:241:LEU:HA	1.37	0.88
1:A:566:ASP:OD2	2:B:159:ARG:NH1	2.06	0.87
2:B:199:GLU:OE2	2:B:199:GLU:N	2.08	0.85
1:A:652:ARG:CZ	1:A:658:ASP:O	2.08	0.84
2:D:199:GLU:OE2	2:D:199:GLU:N	2.09	0.84
1:C:762:ASN:HD21	1:C:765:LEU:HB3	1.43	0.84
4:G:17:DA:H2	5:I:15:DT:H3	1.26	0.83
1:A:708:ARG:HH22	1:A:721:ARG:HG3	1.41	0.82
1:C:653:LEU:HD12	1:C:654:GLU:HA	1.63	0.81
2:D:145:ILE:CD1	2:D:238:VAL:HG21	2.12	0.79
1:A:590:GLU:HG2	1:A:713:VAL:HG23	1.63	0.78
4:F:17:DA:H2	5:J:15:DT:H3	1.32	0.77
2:B:140:HIS:HD2	2:B:155:LEU:HD11	1.49	0.76
1:C:617:GLU:OE2	1:C:724:PHE:HB3	1.85	0.76
2:D:82:ALA:HA	2:D:87:PRO:HB3	1.68	0.75
3:E:12:DA:H2'	3:E:13:DG:C8	2.22	0.74
1:C:947:LYS:HE3	1:C:951:ASP:HA	1.69	0.71
2:D:51:LYS:HG2	2:D:52:LYS:HD3	1.70	0.71
1:A:895:GLU:OE1	1:A:898:ARG:NH1	2.23	0.71
2:D:140:HIS:HD2	2:D:155:LEU:HD11	1.55	0.70
2:B:28:VAL:HG13	2:B:48:VAL:HB	1.74	0.70
2:B:222:HIS:HB2	2:B:259:THR:HG21	1.74	0.69
2:D:148:ARG:HH22	2:D:241:LEU:HG	1.57	0.69
2:D:168:THR:HG22	2:D:170:GLN:H	1.58	0.69
2:D:222:HIS:HB2	2:D:259:THR:HG21	1.75	0.69
1:A:481:LEU:HD11	1:C:507:VAL:HG23	1.75	0.68
1:A:652:ARG:NE	1:A:657:ASP:O	2.27	0.68
2:B:104:SER:HB2	2:B:136:ALA:HB2	1.76	0.68
2:D:216:VAL:HG23	2:D:236:LEU:HB3	1.74	0.68
1:C:847:GLU:HB3	1:C:850[B]:ARG:HH21	1.58	0.68
2:D:28:VAL:HG13	2:D:48:VAL:HB	1.76	0.68
2:B:69:LEU:HD12	2:B:70:PRO:HD2	1.76	0.67
3:H:12:DA:H2'	3:H:13:DG:C8	2.30	0.67
1:C:999:ARG:HH21	1:C:999:ARG:HG3	1.60	0.67
1:C:999:ARG:HG3	1:C:999:ARG:NH2	2.09	0.66
1:C:654:GLU:H	1:C:654:GLU:CD	1.99	0.65
2:D:69:LEU:HD12	2:D:70:PRO:HD2	1.79	0.65
2:B:76:ALA:HB3	2:B:93:HIS:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:ARG:N	2:D:149:GLY:HA2	2.12	0.65
1:A:947:LYS:HE3	1:A:951:ASP:HA	1.79	0.65
1:C:836:GLU:N	1:C:836:GLU:OE1	2.29	0.64
1:A:680:MET:HG2	1:A:693:ILE:HG21	1.79	0.64
2:D:66:SER:HB2	2:D:124:CYS:H	1.62	0.64
1:A:940:ASP:OD1	1:A:941:LEU:N	2.30	0.64
2:D:159:ARG:HH21	2:D:224:LEU:HD13	1.60	0.64
2:B:338:THR:HG22	2:B:340:PRO:HA	1.78	0.64
2:B:66:SER:HB2	2:B:124:CYS:H	1.63	0.64
2:D:106:LEU:HD23	2:D:127:LYS:HB3	1.79	0.64
1:C:940:ASP:OD1	1:C:941:LEU:N	2.31	0.63
2:D:58:ARG:HD2	5:J:7:DG:H5"	1.79	0.63
1:A:652:ARG:CZ	1:A:657:ASP:O	2.46	0.63
1:A:546:SER:O	1:A:577:ARG:NH2	2.32	0.63
1:A:1024:PHE:HD2	1:A:1028:HIS:HE1	1.47	0.63
2:B:15:VAL:HG21	2:B:345:PHE:HZ	1.63	0.63
1:A:897:ARG:NH2	1:A:945:MET:O	2.32	0.63
2:D:338:THR:HG22	2:D:340:PRO:HA	1.80	0.62
1:A:553:ILE:HG21	1:A:1007:GLU:HG3	1.81	0.62
1:C:546:SER:O	1:C:577:ARG:NH2	2.33	0.62
1:C:999:ARG:HH21	1:C:999:ARG:CG	2.13	0.62
2:D:15:VAL:HG21	2:D:345:PHE:HZ	1.64	0.62
2:B:278:GLN:HG3	2:B:284:ARG:HB2	1.80	0.62
2:D:283:LYS:NZ	2:D:314:SER:O	2.29	0.61
1:C:596:GLY:O	1:C:600:ARG:HG2	2.00	0.61
2:D:104:SER:HB2	2:D:136:ALA:HB2	1.83	0.61
2:D:148:ARG:NH1	2:D:240:LEU:O	2.34	0.61
1:C:613:VAL:HG22	1:C:649:ILE:HD12	1.83	0.60
1:C:603:ASP:CG	1:C:604:ASP:H	2.04	0.60
2:D:52:LYS:HE2	2:D:54:GLU:HB2	1.81	0.60
1:A:652:ARG:NE	1:A:658:ASP:C	2.49	0.60
1:C:966:PRO:O	1:C:970:GLU:OE1	2.19	0.59
2:D:76:ALA:HB3	2:D:93:HIS:O	2.01	0.59
1:C:706:GLU:N	1:C:706:GLU:OE1	2.36	0.59
2:D:131:GLY:HA3	2:D:132:ASP:C	2.23	0.59
2:D:217:TYR:CE2	2:D:235:ARG:HG3	2.37	0.59
2:B:283:LYS:NZ	2:B:314:SER:O	2.31	0.59
1:C:590:GLU:HB2	1:C:713:VAL:HG23	1.84	0.59
2:D:278:GLN:HG3	2:D:284:ARG:HB2	1.85	0.59
1:A:882:ARG:HD3	1:A:886:GLU:OE2	2.02	0.58
1:A:814:ASP:OD2	1:A:980:SER:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ALA:HA	2:B:87:PRO:HB3	1.86	0.58
1:C:657:ASP:OD1	1:C:657:ASP:N	2.36	0.58
2:D:24:LEU:HD13	2:D:111:VAL:HG23	1.85	0.58
1:C:882:ARG:NH2	1:C:906:ASP:HB3	2.17	0.58
2:D:236:LEU:HD11	2:D:247:LEU:HD21	1.85	0.58
1:A:933:TYR:CE2	1:A:937:GLN:NE2	2.71	0.58
2:B:148:ARG:N	2:B:149:GLY:HA2	2.17	0.58
2:B:24:LEU:HD13	2:B:111:VAL:HG23	1.86	0.58
1:C:641:ARG:HG3	1:C:679:LEU:HD22	1.85	0.58
2:B:25:GLU:HG2	2:B:114:ARG:HH12	1.69	0.57
1:C:680:MET:HG2	1:C:693:ILE:HG21	1.86	0.57
1:C:865:LEU:HD21	1:C:878:ARG:HD2	1.86	0.57
1:A:490:ARG:NH1	1:A:497:CYS:SG	2.78	0.57
2:B:339:PRO:HB2	2:B:341:GLU:N	2.19	0.57
1:C:745:SER:OG	1:C:746:THR:N	2.38	0.57
2:D:188:GLU:CD	2:D:189:PHE:HA	2.25	0.57
1:A:760:SER:HB3	1:A:954:ILE:HD11	1.86	0.57
2:D:339:PRO:HB2	2:D:341:GLU:N	2.19	0.57
2:D:25:GLU:OE2	2:D:25:GLU:N	2.39	0.56
2:D:148:ARG:NH1	2:D:241:LEU:HA	2.15	0.56
2:B:188:GLU:HA	2:B:189:PHE:C	2.26	0.56
1:A:706:GLU:N	1:A:706:GLU:OE1	2.39	0.56
1:A:836:GLU:N	1:A:836:GLU:OE1	2.38	0.56
1:C:696:PRO:O	1:C:700:GLU:HG3	2.05	0.56
1:C:770:ARG:NH2	1:C:799:LYS:O	2.38	0.56
1:A:865:LEU:HD21	1:A:878:ARG:HD2	1.86	0.56
1:C:870:ARG:NH1	4:F:16:DT:OP1	2.37	0.56
1:C:895:GLU:OE1	1:C:898:ARG:NH1	2.39	0.56
4:G:12:DT:H2'	4:G:13:DG:C8	2.40	0.56
1:A:992:ARG:HH11	1:A:996:MET:CE	2.19	0.55
1:A:770:ARG:NH2	1:A:799:LYS:O	2.40	0.55
1:C:680:MET:SD	1:C:693:ILE:HG21	2.46	0.55
1:A:577:ARG:HD3	1:A:579:ASP:OD1	2.05	0.55
1:A:992:ARG:NH1	1:A:996:MET:HE1	2.21	0.55
4:F:6:DT:H2''	4:F:7:DA:C8	2.42	0.55
2:D:156:PHE:HE2	2:D:204:GLN:HE21	1.55	0.55
1:A:607:CYS:SG	1:A:651:ILE:HD13	2.46	0.55
4:G:6:DT:H2''	4:G:7:DA:C8	2.42	0.54
1:A:912:LYS:HD2	1:A:915:TRP:CZ2	2.42	0.54
1:A:992:ARG:HH11	1:A:996:MET:HE1	1.71	0.54
2:D:188:GLU:HA	2:D:189:PHE:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:LEU:HB2	2:D:136:ALA:HB1	1.90	0.54
1:C:889:CYS:HB3	1:C:898:ARG:HD3	1.90	0.53
1:A:1024:PHE:CD2	1:A:1028:HIS:HE1	2.26	0.53
1:A:652:ARG:HE	1:A:658:ASP:C	2.12	0.53
2:B:162:MET:SD	2:B:174:SER:OG	2.66	0.53
1:C:953:LYS:NZ	5:J:13:DC:OP1	2.42	0.52
1:A:501:HIS:CE1	1:A:505:ARG:HH11	2.28	0.52
1:A:631:SER:HA	1:C:864:LYS:HD2	1.90	0.52
1:C:966:PRO:C	1:C:970:GLU:OE1	2.47	0.52
4:G:26:DC:H2"	4:G:27:DA:C8	2.44	0.52
2:B:238:VAL:HG12	2:B:247:LEU:CD2	2.39	0.52
2:D:145:ILE:CD1	2:D:238:VAL:CG2	2.70	0.52
2:B:140:HIS:CD2	2:B:155:LEU:HD11	2.39	0.52
1:C:844:SER:OG	1:C:845:ARG:N	2.43	0.52
4:F:26:DC:H2"	4:F:27:DA:C8	2.45	0.52
1:A:505:ARG:NH2	1:C:1029:LYS:HD3	2.25	0.52
1:A:696:PRO:O	1:A:700:GLU:HG3	2.09	0.52
1:A:798:VAL:HG13	1:A:801:VAL:H	1.74	0.52
2:B:102:LEU:HB2	2:B:136:ALA:HB1	1.92	0.52
1:C:482:HIS:HB3	1:C:485:VAL:HG23	1.92	0.52
1:C:595:GLU:HA	1:C:598:ARG:HG2	1.92	0.52
1:A:579:ASP:O	1:A:583:VAL:HG13	2.10	0.52
3:H:9:DT:H2"	3:H:10:DA:H5"	1.91	0.51
1:A:906:ASP:OD1	1:A:907:LEU:N	2.43	0.51
1:A:833:GLU:HG3	1:A:901:LEU:HD23	1.92	0.51
2:D:145:ILE:HD13	2:D:238:VAL:HG23	1.83	0.51
2:D:212:ARG:HD3	2:D:292:LEU:HD12	1.91	0.51
2:B:242:LEU:HD12	2:B:243:GLY:HA2	1.91	0.51
1:C:911:MET:HB2	1:C:931:TYR:CE2	2.46	0.51
1:A:653:LEU:HG	1:A:654:GLU:HA	1.92	0.51
2:B:147:SER:HB3	2:B:240:LEU:HD22	1.91	0.51
1:C:621:GLY:HA3	1:C:684:GLU:HG3	1.92	0.51
2:D:189:PHE:C	2:D:191:CYS:H	2.15	0.51
1:C:981:GLU:OE2	4:F:15:DG:N2	2.44	0.50
2:D:284:ARG:NH2	2:D:288:THR:OG1	2.42	0.50
4:G:17:DA:H2	5:I:15:DT:N3	2.04	0.50
2:B:187:LEU:O	2:B:188:GLU:HB3	2.10	0.50
2:D:322:LEU:H	2:D:327:ALA:HA	1.77	0.50
1:A:603:ASP:CG	1:A:604:ASP:H	2.15	0.50
2:B:238:VAL:C	2:B:239:GLU:OE2	2.50	0.50
2:D:108:MET:SD	2:D:127:LYS:HE2	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:ARG:HD3	3:H:7:DG:N3	2.27	0.50
1:C:658:ASP:OD1	1:C:659:GLY:N	2.45	0.49
1:A:861:LYS:HE3	1:A:862:LYS:HZ3	1.77	0.49
1:C:969:VAL:HG12	1:C:975:ILE:HG13	1.94	0.49
2:B:33:GLN:HE22	2:B:37:PRO:HA	1.77	0.49
2:B:141:THR:HG21	2:B:209:ALA:HB2	1.94	0.49
1:C:680:MET:CG	1:C:693:ILE:HG21	2.43	0.49
4:G:18:DA:H2''	4:G:19:DG:C8	2.47	0.49
2:B:197:LEU:HD21	2:B:247:LEU:HD12	1.94	0.49
2:B:236:LEU:HD12	2:B:248:THR:O	2.13	0.49
2:B:256:LEU:HD11	2:B:284:ARG:NH2	2.28	0.49
1:A:911:MET:HB2	1:A:931:TYR:CE2	2.47	0.49
1:C:579:ASP:OD1	1:C:579:ASP:N	2.46	0.49
4:F:27:DA:H2''	4:F:28:DG:C8	2.48	0.49
2:B:148:ARG:HH12	2:B:241:LEU:HD13	1.77	0.49
1:A:654:GLU:H	1:A:654:GLU:CD	2.16	0.49
2:B:25:GLU:OE2	2:B:25:GLU:N	2.46	0.49
1:C:762:ASN:ND2	1:C:765:LEU:HB3	2.21	0.49
1:C:906:ASP:OD1	1:C:907:LEU:N	2.46	0.49
2:D:162:MET:SD	2:D:174:SER:OG	2.71	0.49
2:B:322:LEU:HD11	2:B:328:LEU:HB2	1.95	0.48
1:C:892:VAL:O	1:C:898:ARG:NE	2.44	0.48
2:D:153:CYS:SG	2:D:187:LEU:HD11	2.53	0.48
4:G:18:DA:H2''	4:G:19:DG:H8	1.78	0.48
2:D:197:LEU:HD12	2:D:200:LEU:HD22	1.95	0.48
1:A:617:GLU:HG2	1:A:726:GLY:HA2	1.95	0.48
1:C:577:ARG:HD3	1:C:579:ASP:OD1	2.12	0.48
1:A:940:ASP:OD1	1:A:940:ASP:C	2.52	0.48
1:C:821:GLY:O	1:C:824:THR:HG22	2.13	0.48
4:F:18:DA:H2''	4:F:19:DG:C8	2.49	0.48
2:B:131:GLY:HA3	2:B:132:ASP:C	2.33	0.48
2:D:128:GLU:OE2	2:D:128:GLU:HA	2.13	0.48
1:A:731:GLU:O	1:A:735:ARG:HG3	2.13	0.48
2:B:333:SER:HB3	2:B:344:HIS:CD2	2.49	0.48
2:D:322:LEU:HD11	2:D:328:LEU:HB2	1.96	0.48
1:A:742:ALA:HA	1:A:743:SER:HA	1.60	0.48
2:B:239:GLU:OE2	2:B:239:GLU:N	2.46	0.48
3:E:12:DA:H2'	3:E:13:DG:H8	1.77	0.48
2:D:333:SER:HB3	2:D:344:HIS:CD2	2.48	0.48
4:F:18:DA:H2''	4:F:19:DG:H8	1.78	0.48
1:A:933:TYR:CZ	1:A:937:GLN:NE2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:GLU:OE2	1:C:654:GLU:N	2.28	0.47
1:C:731:GLU:O	1:C:735:ARG:HG3	2.14	0.47
1:C:895:GLU:OE1	1:C:898:ARG:HD2	2.14	0.47
1:A:700:GLU:HG2	2:B:169:THR:HG21	1.97	0.47
2:D:6:LEU:HD11	2:D:347:GLN:HB2	1.95	0.47
2:D:186:ASP:OD1	2:D:187:LEU:N	2.46	0.47
1:A:844:SER:OG	1:A:845:ARG:N	2.47	0.47
1:C:942:LEU:HD22	1:C:950:TYR:HE2	1.80	0.47
1:A:649:ILE:HG23	1:A:663:PHE:HB3	1.96	0.47
2:B:150:LYS:N	2:B:150:LYS:HE2	2.29	0.47
2:B:328:LEU:HD11	2:B:345:PHE:HD2	1.80	0.47
1:C:940:ASP:OD1	1:C:940:ASP:C	2.52	0.47
1:A:604:ASP:OD1	1:A:604:ASP:N	2.47	0.47
1:A:621:GLY:HA3	1:A:684:GLU:HG3	1.97	0.47
1:A:652:ARG:NH2	1:A:657:ASP:O	2.44	0.47
2:B:99:ASN:O	2:B:101:GLU:N	2.46	0.47
1:A:513:ARG:NH2	1:C:479:PHE:HB2	2.30	0.47
1:A:956:ASN:N	5:I:15:DT:OP1	2.48	0.47
2:B:322:LEU:H	2:B:327:ALA:HA	1.78	0.47
1:A:509:ALA:HB3	1:C:1028:HIS:HB3	1.96	0.47
2:B:108:MET:O	2:B:124:CYS:HA	2.15	0.47
1:C:742:ALA:HA	1:C:743:SER:HA	1.61	0.47
1:A:657:ASP:N	1:A:657:ASP:OD1	2.45	0.46
1:A:821:GLY:O	1:A:824:THR:HG22	2.15	0.46
1:C:603:ASP:CG	1:C:604:ASP:N	2.69	0.46
1:A:689:THR:O	1:A:693:ILE:HG12	2.16	0.46
2:B:86:LYS:HE3	2:B:89:CYS:SG	2.54	0.46
2:B:197:LEU:HD13	2:B:249:CYS:HB2	1.97	0.46
1:A:680:MET:HB3	1:A:682:VAL:HG23	1.97	0.46
4:F:12:DT:H2'	4:F:13:DG:C8	2.50	0.46
2:B:146:ASN:O	2:B:214:ASP:HB3	2.15	0.46
2:D:127:LYS:HD3	2:D:187:LEU:O	2.15	0.46
1:A:652:ARG:O	1:A:652:ARG:HG3	2.15	0.46
1:A:969:VAL:HG12	1:A:975:ILE:HG13	1.98	0.46
1:A:984:GLU:O	4:G:14:DT:H2''	2.15	0.46
1:C:833:GLU:HG3	1:C:901:LEU:HD23	1.97	0.46
1:C:981:GLU:OE2	4:F:15:DG:N1	2.47	0.46
3:E:11:DC:H2''	3:E:12:DA:C8	2.51	0.46
2:D:146:ASN:O	2:D:214:ASP:HB3	2.15	0.46
2:D:241:LEU:HD12	2:D:246:VAL:HG11	1.97	0.46
4:G:27:DA:H2''	4:G:28:DG:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HD23	1:A:1010:LEU:HD13	1.96	0.46
1:A:951:ASP:OD1	1:A:951:ASP:N	2.48	0.46
2:B:329:VAL:HG22	2:B:346:TYR:HB2	1.96	0.46
1:C:649:ILE:HG23	1:C:663:PHE:HB3	1.97	0.46
2:D:328:LEU:HD11	2:D:345:PHE:HD2	1.80	0.46
1:A:786:PRO:HG2	1:A:787:PHE:CD1	2.51	0.46
2:B:105:SER:OG	2:B:126:GLU:OE2	2.34	0.46
1:A:698:VAL:HG12	1:A:702:LYS:HE2	1.98	0.46
1:A:870:ARG:HD2	5:I:16:DA:C6	2.50	0.46
1:C:617:GLU:OE2	1:C:724:PHE:CD1	2.69	0.46
5:I:15:DT:H2''	5:I:16:DA:O5'	2.16	0.46
1:A:797:ARG:HE	1:A:797:ARG:HB2	1.41	0.45
1:A:864:LYS:HB3	1:C:630:GLY:O	2.16	0.45
2:B:229:ARG:HD2	2:B:278:GLN:O	2.17	0.45
1:A:675:ARG:HE	1:A:1017:THR:HG23	1.80	0.45
2:B:93:HIS:HA	2:B:94:GLY:HA2	1.67	0.45
1:C:508:LYS:O	1:C:512:GLY:HA2	2.16	0.45
1:A:760:SER:CB	1:A:954:ILE:HD11	2.46	0.45
1:A:762:ASN:OD1	1:A:765:LEU:HB3	2.15	0.45
1:C:590:GLU:O	1:C:593:ILE:HG22	2.15	0.45
1:A:651:ILE:O	1:A:659:GLY:HA2	2.16	0.45
2:D:329:VAL:HG22	2:D:346:TYR:HB2	1.98	0.45
1:A:630:GLY:O	1:C:864:LYS:HB3	2.17	0.45
2:B:217:TYR:CE2	2:B:235:ARG:HG3	2.52	0.45
1:A:926:ASP:OD1	1:A:926:ASP:N	2.50	0.45
1:C:730:ASP:OD1	1:C:730:ASP:N	2.50	0.45
1:A:838:TYR:CZ	1:A:897:ARG:HD2	2.52	0.45
2:B:239:GLU:HG2	2:B:246:VAL:HG13	1.99	0.45
2:D:33:GLN:HE22	2:D:37:PRO:HA	1.81	0.45
3:H:11:DC:H2''	3:H:12:DA:C8	2.52	0.45
1:A:942:LEU:HD22	1:A:950:TYR:HE2	1.81	0.45
1:A:499:GLN:HB3	1:C:493:THR:OG1	2.17	0.44
1:A:741:GLU:H	1:A:741:GLU:CD	2.17	0.44
2:B:153:CYS:SG	2:B:187:LEU:HD11	2.57	0.44
2:D:131:GLY:HA3	2:D:132:ASP:O	2.17	0.44
1:A:583:VAL:HG12	1:A:709:LEU:HD21	2.00	0.44
1:A:686:ASP:OD1	1:A:686:ASP:O	2.35	0.44
2:B:147:SER:HB3	2:B:240:LEU:CD2	2.47	0.44
1:C:926:ASP:OD1	1:C:926:ASP:N	2.50	0.44
1:C:536:PHE:CG	1:C:583:VAL:HG21	2.52	0.44
2:D:93:HIS:HA	2:D:94:GLY:HA2	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ARG:HH21	2:D:339:PRO:HB3	1.82	0.44
2:D:229:ARG:HD2	2:D:278:GLN:O	2.16	0.44
2:B:168:THR:H	2:B:171:ASN:HB2	1.82	0.44
2:D:168:THR:H	2:D:171:ASN:HB2	1.82	0.44
1:A:513:ARG:O	1:A:513:ARG:HG2	2.17	0.44
2:D:82:ALA:CA	2:D:87:PRO:HB3	2.44	0.44
1:A:582:LEU:HD23	1:A:582:LEU:HA	1.83	0.44
1:A:1028:HIS:HB3	1:C:509:ALA:HB3	1.99	0.44
2:B:6:LEU:HD11	2:B:347:GLN:HB2	1.99	0.44
1:C:951:ASP:OD1	1:C:951:ASP:N	2.49	0.44
2:D:249:CYS:SG	2:D:250:THR:N	2.91	0.44
1:A:862:LYS:HE2	1:A:890:GLU:OE1	2.18	0.44
1:C:609:SER:OG	1:C:653:LEU:HD22	2.18	0.43
1:A:543:LYS:HD3	1:A:543:LYS:HA	1.79	0.43
2:B:197:LEU:HD12	2:B:200:LEU:HD22	2.00	0.43
2:B:87:PRO:HA	2:B:88:GLU:HA	1.70	0.43
2:D:3:LEU:HB3	2:D:348:VAL:HG12	2.01	0.43
2:D:242:LEU:HA	2:D:243:GLY:HA2	1.49	0.43
3:E:9:DT:H2"	3:E:10:DA:H5"	2.00	0.43
2:B:70:PRO:HA	2:B:71:PRO:HD3	1.91	0.43
1:C:798:VAL:HG13	1:C:801:VAL:H	1.83	0.43
1:A:721:ARG:HG2	1:A:722:PHE:N	2.33	0.43
1:A:623:GLY:O	1:A:991:ARG:NH1	2.51	0.43
2:B:24:LEU:HD23	2:B:24:LEU:HA	1.93	0.43
2:B:107:TYR:CE1	2:B:126:GLU:HG3	2.54	0.43
1:A:493:THR:OG1	1:C:499:GLN:HB3	2.19	0.42
1:C:543:LYS:HA	1:C:543:LYS:HD3	1.79	0.42
1:C:984:GLU:O	4:F:14:DT:H2"	2.19	0.42
2:D:130:VAL:O	2:D:191:CYS:HA	2.19	0.42
1:A:658:ASP:C	1:A:658:ASP:OD1	2.58	0.42
1:A:886:GLU:HG3	1:A:902:LEU:HD11	2.01	0.42
1:C:955:THR:HG22	5:J:15:DT:OP1	2.19	0.42
2:D:272:ILE:HD11	2:D:287:CYS:SG	2.59	0.42
1:C:877:ARG:HH21	1:C:916:ARG:HH22	1.66	0.42
4:F:17:DA:H2	5:J:15:DT:N3	2.09	0.42
2:D:99:ASN:O	2:D:101:GLU:N	2.49	0.42
2:B:86:LYS:HB3	2:B:86:LYS:HE2	1.89	0.42
1:C:556:GLY:HA2	1:C:575:ARG:HD3	2.02	0.42
1:C:623:GLY:O	1:C:991:ARG:NH1	2.50	0.42
2:D:287:CYS:SG	2:D:288:THR:N	2.93	0.42
1:A:676:PRO:HG3	1:A:1013:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:GLU:HB2	1:A:793:GLU:HB3	2.02	0.42
1:C:590:GLU:HB2	1:C:713:VAL:CG2	2.47	0.42
1:C:652:ARG:NH1	1:C:657:ASP:O	2.53	0.42
1:A:482:HIS:HB3	1:A:485:VAL:HG23	2.01	0.42
1:A:861:LYS:HE3	1:A:862:LYS:NZ	2.34	0.42
2:D:241:LEU:HD12	2:D:246:VAL:CG1	2.49	0.42
1:A:730:ASP:N	1:A:730:ASP:OD1	2.52	0.42
2:B:266:ILE:HG22	2:B:325:GLY:HA2	2.01	0.42
4:G:1:DG:H2''	4:G:2:DT:C5	2.54	0.42
1:A:502:LYS:NZ	1:C:492:ASN:O	2.39	0.42
1:C:883:GLU:H	1:C:883:GLU:CD	2.24	0.42
1:A:642:PHE:HB3	1:A:678:CYS:HB3	2.02	0.41
2:B:149:GLY:H	2:B:150:LYS:HE2	1.84	0.41
1:C:730:ASP:O	1:C:734:VAL:HG23	2.19	0.41
2:D:266:ILE:HG22	2:D:325:GLY:HA2	2.02	0.41
1:C:505:ARG:HG3	1:C:506:THR:N	2.34	0.41
1:C:796:ASP:OD1	1:C:797:ARG:N	2.53	0.41
4:F:1:DG:H2''	4:F:2:DT:C5	2.55	0.41
1:A:730:ASP:O	1:A:734:VAL:HG23	2.20	0.41
2:B:168:THR:HG22	2:B:170:GLN:H	1.85	0.41
1:C:912:LYS:N	1:C:913:PRO:HD2	2.35	0.41
2:D:63:SER:OG	2:D:65:ASN:OD1	2.31	0.41
2:D:108:MET:O	2:D:124:CYS:HA	2.19	0.41
4:G:12:DT:H2'	4:G:13:DG:N7	2.35	0.41
2:B:339:PRO:HB3	1:C:849:ARG:HH21	1.85	0.41
1:C:496:SER:HB2	1:C:499:GLN:HG2	2.03	0.41
1:C:838:TYR:CZ	1:C:897:ARG:HD2	2.55	0.41
2:D:236:LEU:HD11	2:D:247:LEU:CD2	2.51	0.41
1:A:981:GLU:OE2	4:G:15:DG:N1	2.53	0.41
2:B:242:LEU:HA	2:B:243:GLY:HA2	1.65	0.41
2:D:108:MET:HB3	2:D:108:MET:HE2	1.83	0.41
1:A:788:SER:HB2	2:B:65:ASN:HA	2.03	0.41
1:A:882:ARG:HE	1:A:882:ARG:HB2	1.39	0.41
1:A:882:ARG:HG3	1:A:883:GLU:N	2.35	0.41
1:C:682:VAL:HG12	1:C:683:ASP:O	2.20	0.41
1:C:966:PRO:O	1:C:969:VAL:HG22	2.21	0.41
1:C:883:GLU:OE1	1:C:883:GLU:N	2.50	0.41
1:A:653:LEU:HA	1:A:654:GLU:HA	1.89	0.41
1:A:708:ARG:NH2	1:A:721:ARG:HG3	2.23	0.41
1:C:653:LEU:CD1	1:C:654:GLU:HA	2.44	0.41
1:C:676:PRO:HG3	1:C:1013:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:THR:HG21	2:D:99:ASN:HB3	2.03	0.41
4:G:13:DG:H2''	4:G:14:DT:C6	2.56	0.41
1:A:534:HIS:CE1	1:A:587:LYS:HG2	2.56	0.41
2:B:11:CYS:SG	2:B:57:LEU:HG	2.61	0.41
1:A:617:GLU:OE1	1:A:701:ARG:HD2	2.21	0.40
1:A:603:ASP:CG	1:A:604:ASP:N	2.73	0.40
2:B:197:LEU:HD21	2:B:247:LEU:CD1	2.51	0.40
1:C:907:LEU:HD23	1:C:907:LEU:HA	1.92	0.40
2:D:75:PRO:HG2	2:D:77:ILE:HD11	2.02	0.40
1:A:774:GLU:O	1:A:777:GLU:HG3	2.22	0.40
2:B:185:ILE:HG12	2:B:192:CYS:SG	2.62	0.40
1:C:482:HIS:ND1	1:C:483:PRO:HD2	2.36	0.40
1:C:981:GLU:OE2	4:F:15:DG:C2	2.74	0.40
3:E:12:DA:H2''	3:E:13:DG:O5'	2.21	0.40
4:G:1:DG:H2''	4:G:2:DT:C7	2.52	0.40
1:A:999:ARG:HD3	1:A:1008:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/1159 (48%)	525 (95%)	26 (5%)	0	100	100
1	C	551/1159 (48%)	529 (96%)	22 (4%)	0	100	100
2	B	350/533 (66%)	329 (94%)	21 (6%)	0	100	100
2	D	350/533 (66%)	332 (95%)	18 (5%)	0	100	100
All	All	1802/3384 (53%)	1715 (95%)	87 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/1000 (49%)	472 (96%)	20 (4%)	30	67
1	C	492/1000 (49%)	472 (96%)	20 (4%)	30	67
2	B	304/465 (65%)	287 (94%)	17 (6%)	21	56
2	D	304/465 (65%)	287 (94%)	17 (6%)	21	56
All	All	1592/2930 (54%)	1518 (95%)	74 (5%)	31	64

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	PHE
1	A	513	ARG
1	A	567	VAL
1	A	577	ARG
1	A	604	ASP
1	A	607	CYS
1	A	725	ARG
1	A	741	GLU
1	A	752	CYS
1	A	753	ASP
1	A	773	ASP
1	A	797	ARG
1	A	842	ASN
1	A	849	ARG
1	A	882	ARG
1	A	899	GLU
1	A	902	LEU
1	A	929	CYS
1	A	992	ARG
1	A	1025	MET
2	B	27	ASP
2	B	39	ARG
2	B	52	LYS
2	B	86	LYS

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Mol	Chain	Res	Type
2	B	90	TYR
2	B	96	ARG
2	B	99	ASN
2	B	105	SER
2	B	116	CYS
2	B	128	GLU
2	B	178	CYS
2	B	214	ASP
2	B	232	ARG
2	B	235	ARG
2	B	294	ASP
2	B	299	MET
2	B	317	TRP
1	C	513	ARG
1	C	567	VAL
1	C	577	ARG
1	C	604	ASP
1	C	607	CYS
1	C	653	LEU
1	C	656	GLU
1	C	725	ARG
1	C	773	ASP
1	C	797	ARG
1	C	844	SER
1	C	850[A]	ARG
1	C	850[B]	ARG
1	C	870	ARG
1	C	901	LEU
1	C	916	ARG
1	C	929	CYS
1	C	999	ARG
1	C	1001	SER
1	C	1025	MET
2	D	39	ARG
2	D	52	LYS
2	D	90	TYR
2	D	96	ARG
2	D	99	ASN
2	D	116	CYS
2	D	127	LYS
2	D	140	HIS
2	D	187	LEU

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Mol	Chain	Res	Type
2	D	202	ASP
2	D	212	ARG
2	D	214	ASP
2	D	232	ARG
2	D	249	CYS
2	D	294	ASP
2	D	299	MET
2	D	317	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	GLN
1	A	1000	GLN
1	A	1028	HIS
1	C	539	GLN
1	C	762	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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.

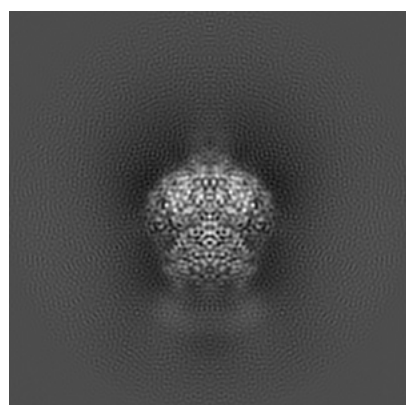
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7844. These allow visual inspection of the internal detail of the map and identification of artifacts.

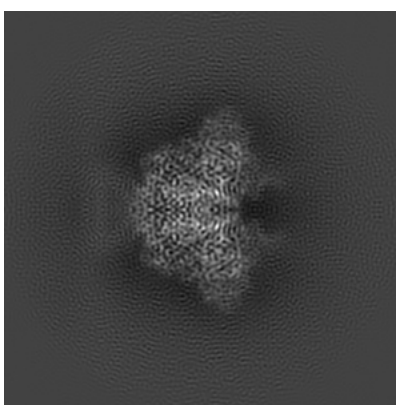
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

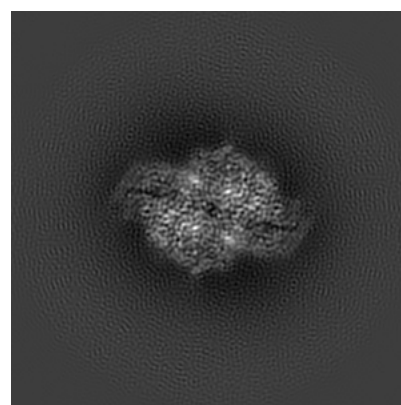
6.1.1 Primary map



X



Y

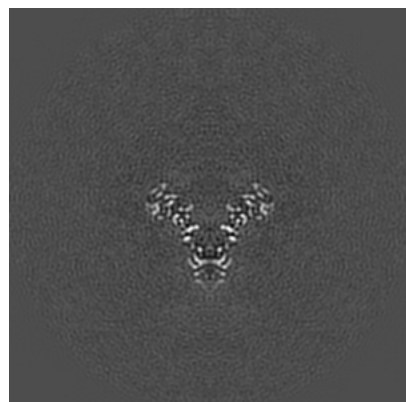


Z

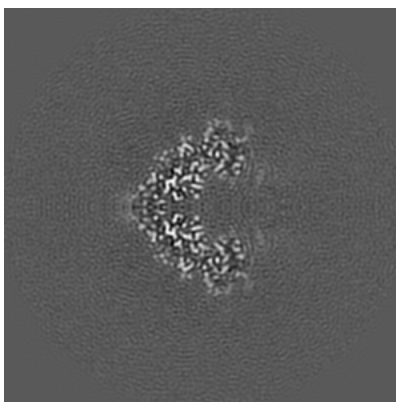
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

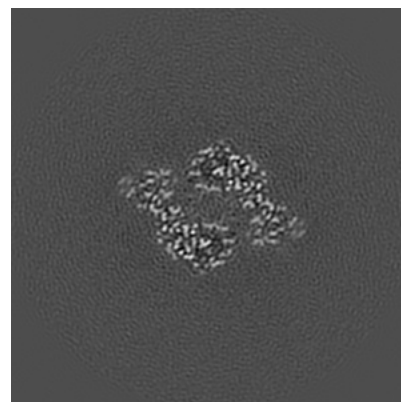
6.2.1 Primary map



X Index: 128



Y Index: 128

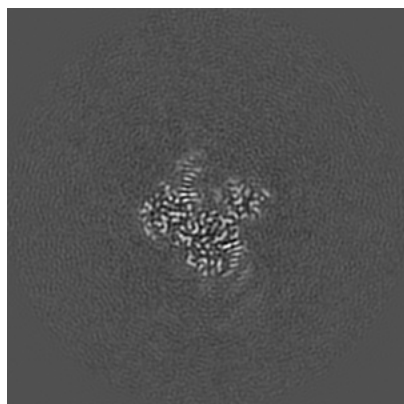


Z Index: 128

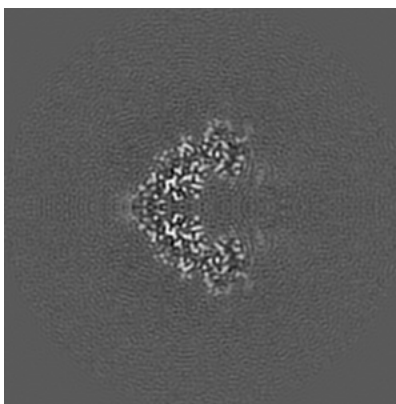
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

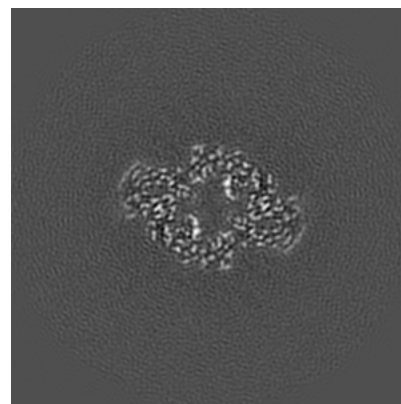
6.3.1 Primary map



X Index: 118



Y Index: 128



Z Index: 136

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

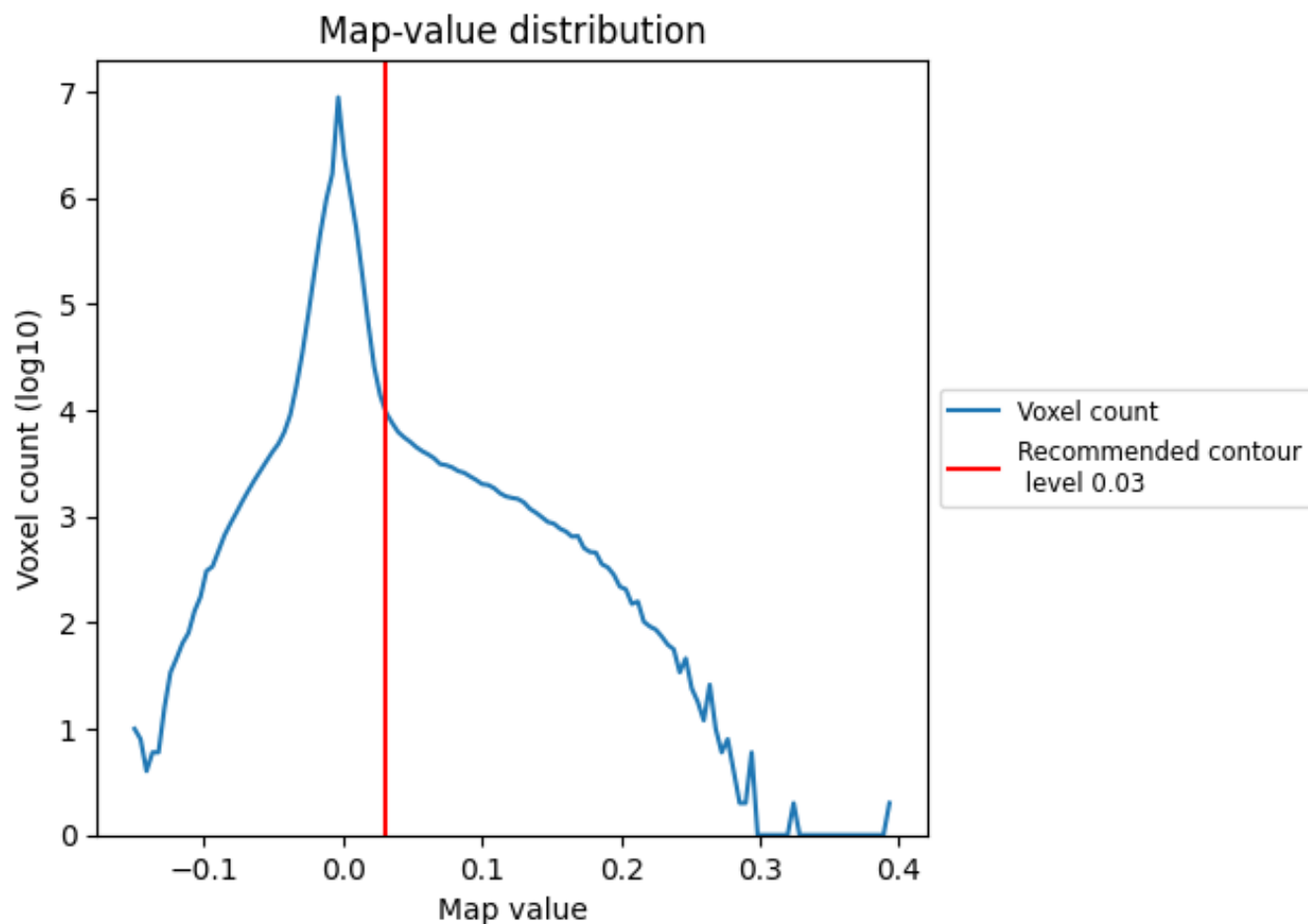
6.5 Mask visualisation

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

7 Map analysis [i](#)

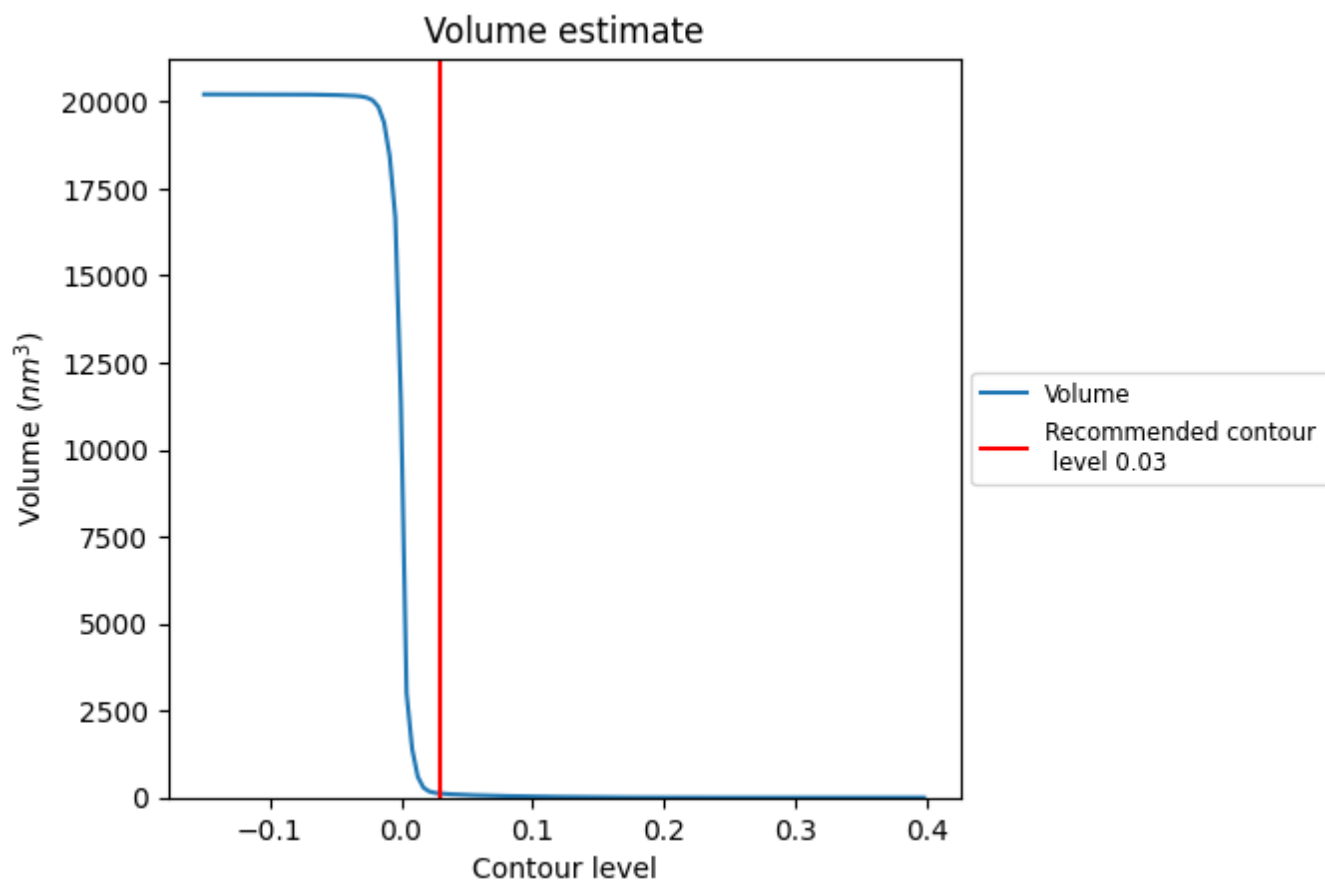
This section contains the results of statistical analysis of the map.

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.

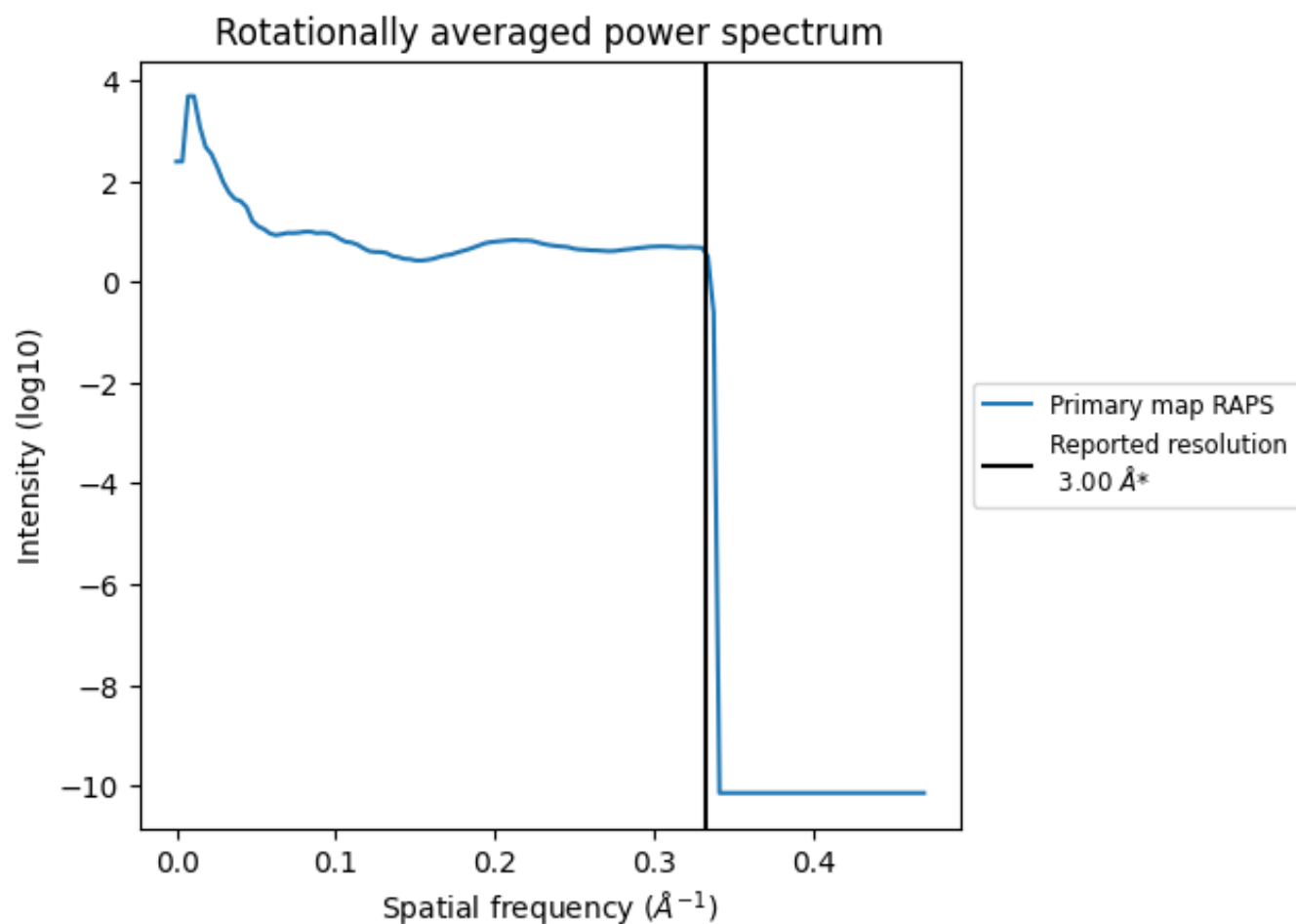
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm^3 ; this corresponds to an approximate mass of 105 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 0.333 Å⁻¹

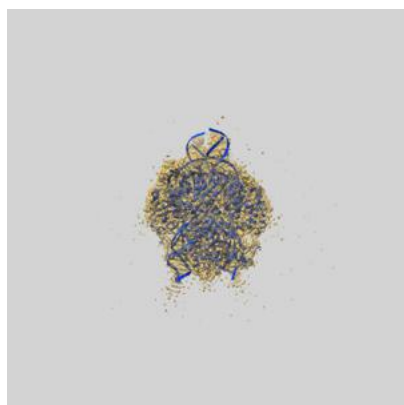
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

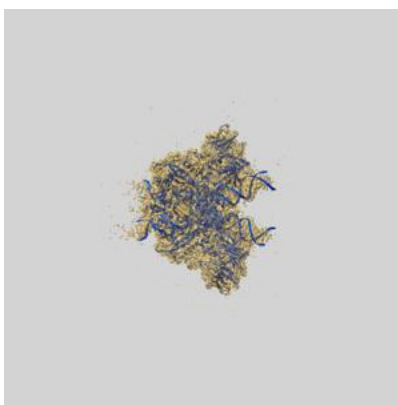
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7844 and PDB model 6DBJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

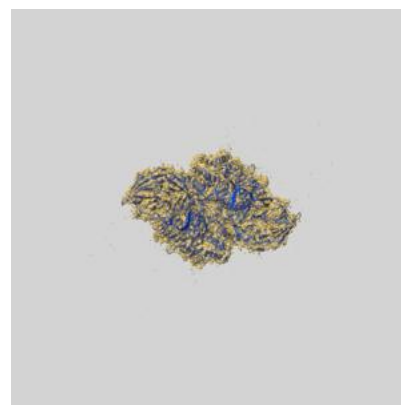
9.1 Map-model overlay [i](#)



X



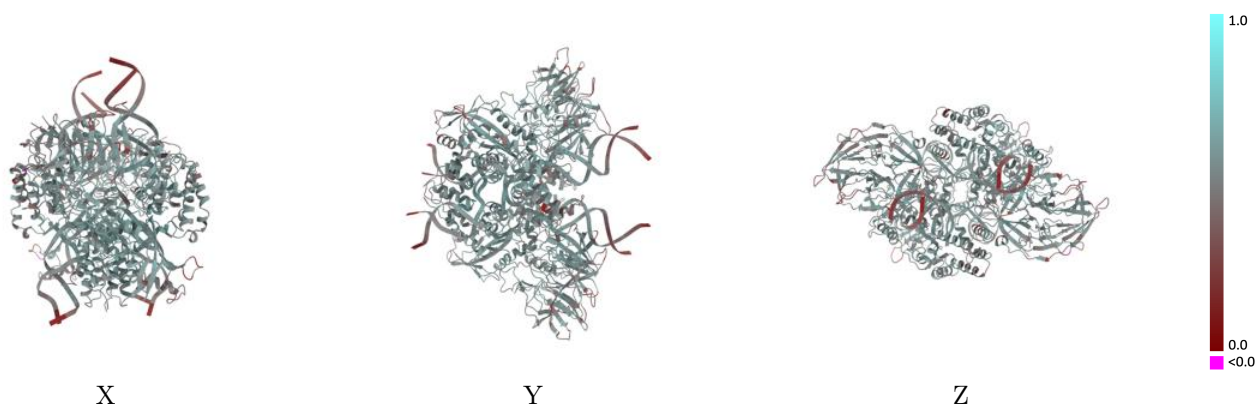
Y



Z

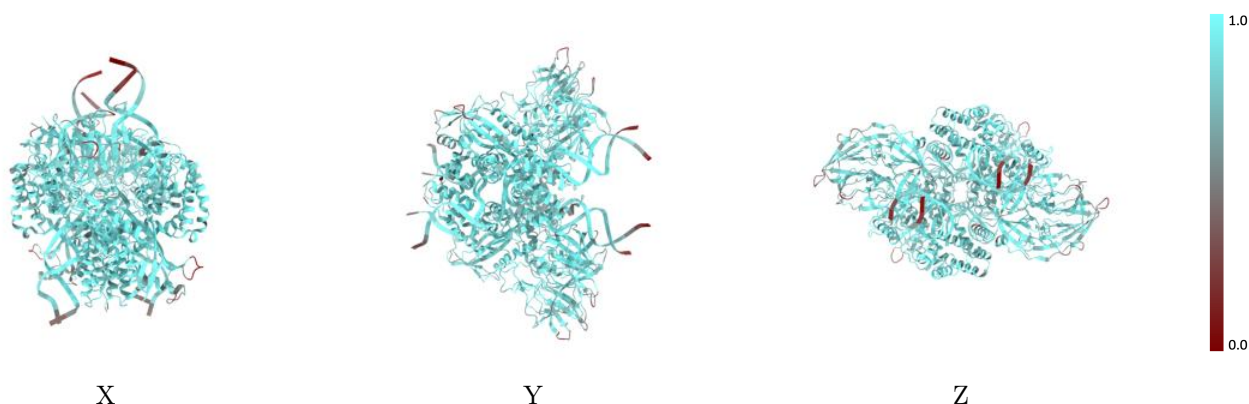
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



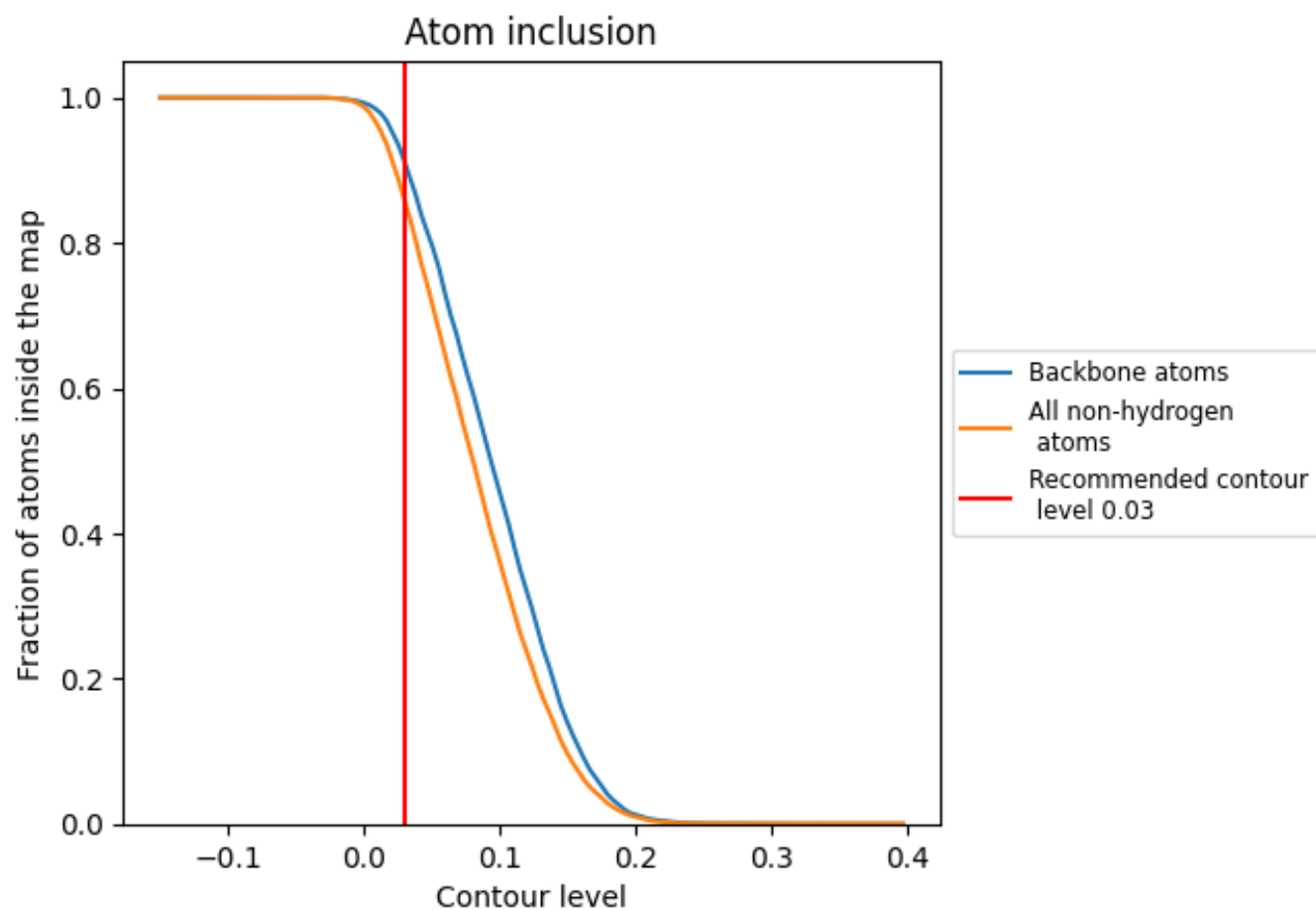
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).























9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8598	 0.5220
A	 0.8805	 0.5370
B	 0.8296	 0.5050
C	 0.8828	 0.5420
D	 0.8337	 0.5060
E	 0.8954	 0.5280
F	 0.8404	 0.4940
G	 0.8466	 0.4870
H	 0.8954	 0.5270
I	 0.7975	 0.4800
J	 0.7975	 0.4770

