Full wwPDB EM Validation Report (i)

Jun 27, 2024 – 03:33 AM JST

PDB ID	:	8GWF
EMDB ID	:	EMD-34311
Title	:	A mechanism for SARS-CoV-2 RNA capping and its inhibition by nucleotide analogue inhibitors
Authors	:	Yan, L.Y.; Huang, Y.C.; Rao, Z.H.; Lou, Z.Y.
Deposited on	:	2022-09-17
Resolution	:	3.39 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 (i) 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 (1)) were used in the production of this report:

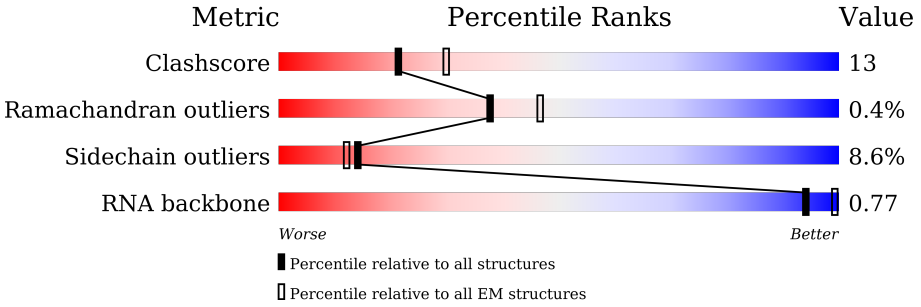
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 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
RNA backbone	4643	859

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 <=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	932	87% 12% •
2	B	198	75% 17% • 6%
2	D	198	64% 27% • 6%
3	C	83	6% 70% 23% • 6%
4	I	25	52% 36% 12%
5	J	33	33% 48% 18%
6	E	601	51% 57% 38% • •

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Mol	Chain	Length	Quality of chain
6	F	601	63% 52% 41% 5%
7	G	117	18% 37% 49% 8%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21955 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	931	7492	4784	1256	1398	54	0	0

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	187	1396	872	240	273	11	0	0
2	D	187	1422	893	244	274	11	0	0

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	78	600	376	98	119	7	0	0

- Molecule 4 is a RNA chain called primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	I	25	545	242	105	173	25	0	0

- Molecule 5 is a RNA chain called template.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	J	27	565	253	94	191	27	0	0

- Molecule 6 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	586	4513	2878	751	849	35	1	0
6	E	586	4513	2878	751	849	35	1	0

- Molecule 7 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	113	868	549	150	164	5	0	0

There are 4 discrepancies between the modelled and reference sequences:

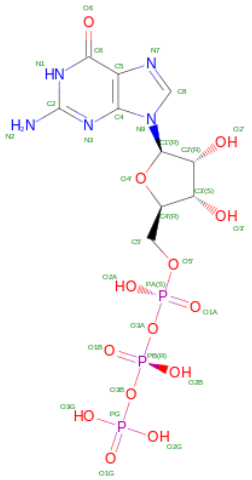
Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	SER	-	expression tag	UNP P0DTD1
G	-2	ASN	-	expression tag	UNP P0DTD1
G	-1	ALA	-	expression tag	UNP P0DTD1
G	0	MET	-	expression tag	UNP P0DTD1

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
8	A	2	2	2	0
8	F	3	3	3	0
8	E	3	3	3	0

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

GTP



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	32	10	5	14	3	0

- Molecule 10 is water.

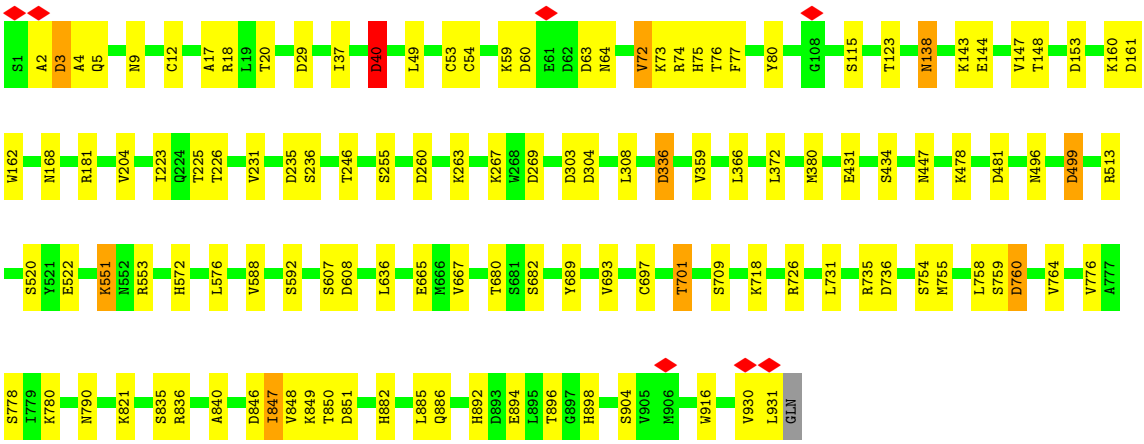
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
10	A	1	1	1	0

3 Residue-property plots (i)

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

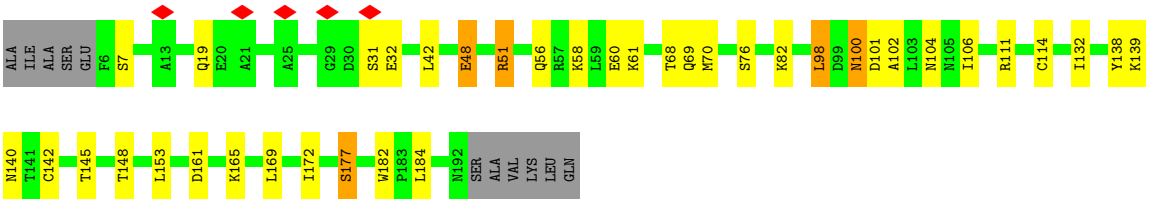
• Molecule 1: RNA-directed RNA polymerase

Chain A: 87% 12%



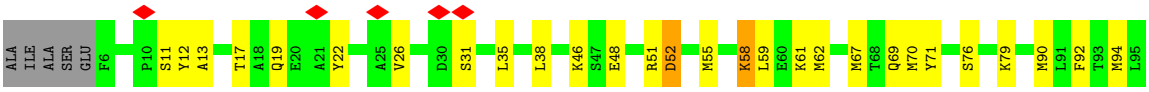
• Molecule 2: Non-structural protein 8

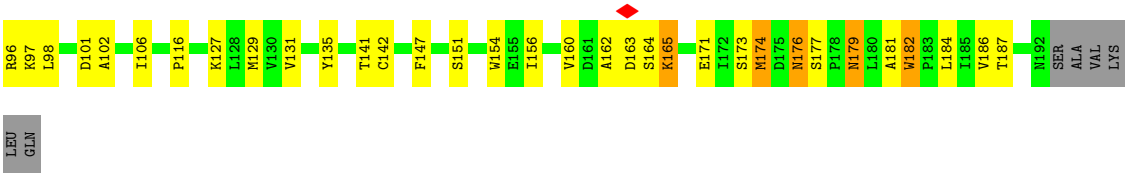
Chain B: 75% 17% 6%



• Molecule 2: Non-structural protein 8

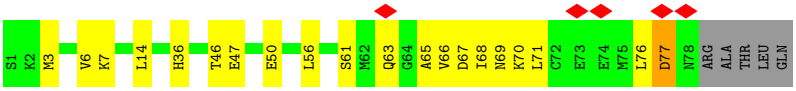
Chain D: 64% 27% 6%





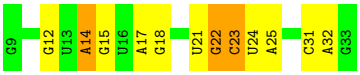
• Molecule 3: Non-structural protein 7

Chain C:



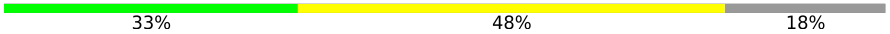
• Molecule 4: primer

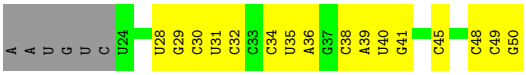
Chain I:



• Molecule 5: template

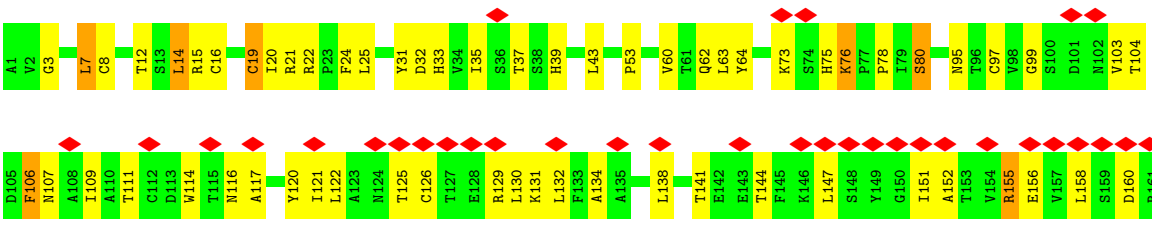
Chain J:





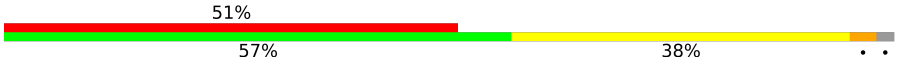
• Molecule 6: Helicase

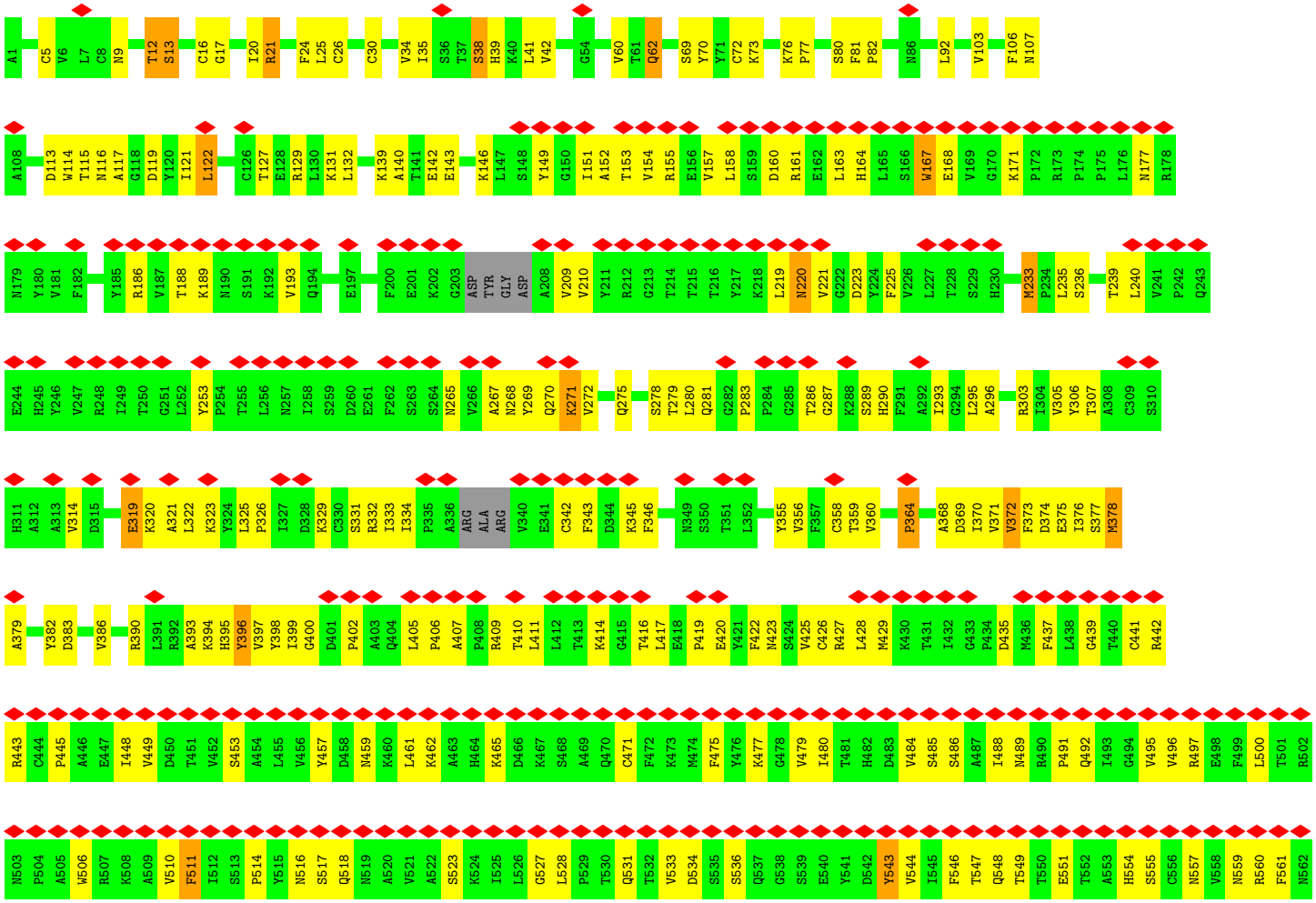
Chain F:

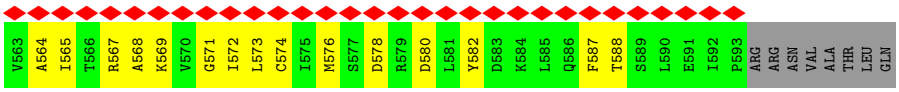


- Molecule 6: Helicase

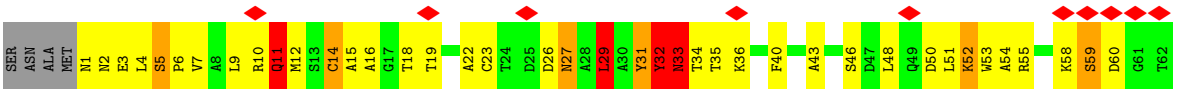
Chain E:

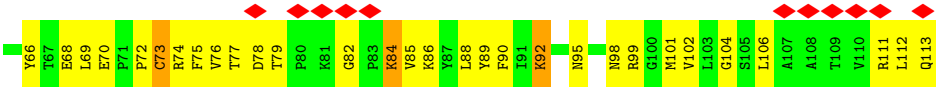






• Molecule 7: Non-structural protein 9





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1485104	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.458	Depositor
Minimum map value	-0.673	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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, GTP

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	0.26	0/7680	0.48	2/10423 (0.0%)
2	B	0.26	0/1414	0.52	0/1922
2	D	0.26	0/1441	0.51	0/1955
3	C	0.25	0/603	0.49	0/812
4	I	0.20	0/611	0.76	0/953
5	J	0.19	0/628	0.77	0/974
6	E	0.30	2/4615 (0.0%)	0.57	3/6290 (0.0%)
6	F	0.57	3/4615 (0.1%)	0.69	5/6290 (0.1%)
7	G	0.49	0/884	0.94	6/1200 (0.5%)
All	All	0.36	5/22491 (0.0%)	0.60	16/30819 (0.1%)

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
6	F	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	491	PRO	CG-CD	-31.95	0.45	1.50
6	F	491	PRO	N-CD	11.27	1.63	1.47
6	E	364	PRO	CG-CD	-7.21	1.26	1.50
6	E	364	PRO	N-CD	6.75	1.57	1.47
6	F	491	PRO	CB-CG	5.77	1.78	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	491	PRO	N-CD-CG	-22.84	68.93	103.20
6	E	364	PRO	CA-N-CD	-15.45	89.87	111.50
6	F	491	PRO	CA-N-CD	-14.84	90.72	111.50
6	F	491	PRO	CA-CB-CG	-12.33	80.58	104.00
7	G	32	TYR	N-CA-C	10.27	138.73	111.00
6	E	364	PRO	N-CD-CG	-9.41	89.09	103.20
6	F	491	PRO	N-CA-CB	-7.94	93.78	103.30
7	G	14	CYS	N-CA-C	7.76	131.95	111.00
7	G	33	ASN	N-CA-C	6.44	128.38	111.00
7	G	11	GLN	N-CA-C	6.35	128.15	111.00
7	G	29	LEU	N-CA-C	-6.17	94.35	111.00
7	G	31	TYR	N-CA-C	5.72	126.44	111.00
6	E	364	PRO	CA-CB-CG	-5.66	93.24	104.00
1	A	40	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	760	ASP	CB-CG-OD2	5.34	123.11	118.30
6	F	147	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	VAL	Mainchain
6	F	76	LYS	Peptide

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	7492	0	7227	56	0
2	B	1396	0	1365	18	0
2	D	1422	0	1422	40	0
3	C	600	0	629	14	0
4	I	545	0	272	13	0
5	J	565	0	291	16	0
6	E	4513	0	4431	169	0
6	F	4513	0	4431	208	0
7	G	868	0	880	46	0
8	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	32	0	12	1	0
10	A	1	0	0	0	0
All	All	21955	0	20960	563	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 13.

All (563) 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)
6:F:371:VAL:HB	6:F:396:TYR:HA	1.53	0.91
6:F:202:LYS:HB3	6:F:210:VAL:HB	1.61	0.81
7:G:53:TRP:HE1	7:G:66:TYR:HB3	1.44	0.81
6:E:443:ARG:HH12	6:E:445:PRO:HD3	1.47	0.79
6:E:278:SER:HB2	6:E:397:VAL:HG12	1.65	0.79
6:E:548:GLN:HE22	6:E:551:GLU:HG2	1.49	0.77
7:G:77:THR:HG21	7:G:86:LYS:NZ	2.00	0.77
6:E:287:GLY:H	6:E:442:ARG:HD2	1.50	0.77
6:E:143:GLU:HA	6:E:146:LYS:HE3	1.67	0.76
2:D:173:SER:O	2:D:177:SER:OG	2.05	0.75
6:E:364:PRO:HD2	6:E:364:PRO:O	1.86	0.75
2:D:176:ASN:O	2:D:176:ASN:ND2	2.21	0.74
6:F:363:LEU:HD12	6:F:364:PRO:HD2	1.70	0.73
6:E:154:VAL:HB	6:E:223:ASP:HB3	1.71	0.73
1:A:5:GLN:O	1:A:9:ASN:ND2	2.22	0.73
6:F:447:GLU:HB3	6:F:467:LYS:HD3	1.70	0.72
6:E:326:PRO:HB2	6:E:329:LYS:HG3	1.73	0.71
6:E:555:SER:HB2	6:E:560:ARG:HD3	1.70	0.71
6:E:306:TYR:HA	6:E:372:VAL:HG22	1.71	0.70
6:F:155:ARG:NH2	6:E:253:TYR:OH	2.24	0.70
4:I:12:G:N1	5:J:48:C:N3	2.29	0.70
6:F:390:ARG:HB3	6:F:391:LEU:HD23	1.72	0.70
7:G:77:THR:HG21	7:G:86:LYS:HZ2	1.56	0.70
7:G:27:ASN:N	7:G:27:ASN:OD1	2.25	0.69
7:G:16:ALA:HA	7:G:54:ALA:HA	1.74	0.69
6:E:371:VAL:HB	6:E:396:TYR:HB3	1.75	0.69
6:F:280:LEU:HD21	6:F:436:MET:HB2	1.73	0.69
6:F:12:THR:HG22	6:F:14:LEU:H	1.57	0.69
6:F:448:ILE:HG21	6:F:566:THR:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:363:LEU:HD23	6:F:390:ARG:HH11	1.57	0.69
6:F:195:ILE:HD11	6:F:223:ASP:HB3	1.73	0.68
6:E:239:THR:HG23	6:E:240:LEU:HD23	1.76	0.68
6:E:546:PHE:HB3	6:E:574:CYS:HA	1.74	0.68
6:F:278:SER:O	6:F:398:TYR:N	2.26	0.68
1:A:226:THR:HG21	7:G:75:PHE:HB3	1.75	0.67
6:F:410:THR:HG23	6:F:411:LEU:H	1.59	0.67
6:E:443:ARG:O	6:E:569:LYS:NZ	2.25	0.67
1:A:930:VAL:HG13	1:A:931:LEU:HD12	1.76	0.66
2:B:100:ASN:O	2:B:104:ASN:ND2	2.25	0.66
6:E:114:TRP:HB3	6:E:411:LEU:HD11	1.77	0.66
6:E:151:ILE:H	6:E:168:GLU:HG2	1.61	0.66
6:E:77:PRO:O	6:E:80:SER:OG	2.14	0.66
6:E:453:SER:HA	6:E:457:TYR:HB2	1.77	0.66
6:E:480:ILE:HD13	6:E:551:GLU:HG3	1.77	0.65
7:G:68:GLU:HG2	7:G:92:LYS:HD2	1.78	0.65
1:A:9:ASN:HA	1:A:12:CYS:HB2	1.78	0.65
6:F:422:PHE:HB2	6:F:426:CYS:HB2	1.76	0.65
6:E:73:LYS:HA	6:E:76:LYS:HE3	1.79	0.65
6:F:132:LEU:HD22	6:F:235:LEU:HD11	1.79	0.65
6:F:558:VAL:HG22	6:F:559:ASN:H	1.62	0.64
6:F:33:HIS:HE1	6:F:39:HIS:CG	2.13	0.64
6:E:576:MET:HG3	6:E:582:TYR:HD2	1.62	0.64
6:E:305:VAL:HB	6:E:371:VAL:HG13	1.77	0.64
6:E:373:PHE:O	6:E:399:ILE:N	2.29	0.64
2:B:101:ASP:OD1	2:B:102:ALA:N	2.30	0.64
6:E:16:CYS:HB2	6:E:25:LEU:HD12	1.79	0.64
6:E:132:LEU:HG	6:E:235:LEU:HD22	1.78	0.64
6:E:286:THR:HG22	6:E:441:CYS:HA	1.78	0.64
4:I:12:G:N2	5:J:48:C:O2	2.15	0.64
6:E:484:VAL:HG22	6:E:485:SER:H	1.61	0.64
6:E:69:SER:OG	6:E:70:TYR:N	2.31	0.63
6:F:248:ARG:HD2	6:F:249:ILE:H	1.62	0.63
6:E:321:ALA:HA	6:E:325:LEU:HD23	1.79	0.63
6:F:109:ILE:HG21	6:F:122:LEU:HD22	1.80	0.63
6:E:510:VAL:H	6:E:544:VAL:HA	1.63	0.63
6:F:8:CYS:HB3	6:F:99:GLY:H	1.63	0.63
6:E:177:ASN:ND2	6:E:516:ASN:OD1	2.32	0.63
6:F:544:VAL:HG21	6:F:567:ARG:HG3	1.81	0.63
6:F:391:LEU:HD12	6:F:393:ALA:HB2	1.81	0.62
6:F:561:PHE:HB2	6:F:564:ALA:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:GLU:OE2	3:C:47:GLU:N	2.33	0.62
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.80	0.62
6:E:219:LEU:HD11	6:E:225:PHE:HE2	1.65	0.62
6:E:471:CYS:O	6:E:588:THR:OG1	2.17	0.62
6:E:523:SER:HA	6:E:527:GLY:HA2	1.82	0.62
1:A:223:ILE:HD13	7:G:104:GLY:HA2	1.82	0.62
2:D:51:ARG:HG3	4:I:17:A:H4'	1.81	0.62
6:F:103:VAL:O	6:F:107:ASN:ND2	2.33	0.62
6:F:134:ALA:O	6:F:138:LEU:HD23	2.00	0.62
6:E:163:LEU:HB3	6:E:209:VAL:HB	1.82	0.61
6:E:407:ALA:HB3	6:E:409:ARG:HE	1.65	0.61
6:F:381:ASN:OD1	6:F:424:SER:OG	2.14	0.61
6:E:358:CYS:SG	6:E:359:THR:N	2.73	0.61
6:E:409:ARG:HD3	6:E:417:LEU:HD13	1.81	0.61
7:G:23:CYS:O	7:G:55:ARG:NH2	2.34	0.61
6:E:17:GLY:HA3	6:E:41:LEU:HG	1.83	0.61
6:F:163:LEU:O	6:F:209:VAL:N	2.33	0.61
6:E:26:CYS:O	6:E:30:CYS:N	2.30	0.61
6:F:277:TYR:HA	6:F:396:TYR:HB2	1.83	0.60
6:F:292:ALA:HB1	6:F:306:TYR:HE2	1.65	0.60
5:J:38:C:H2'	5:J:39:A:H8	1.64	0.60
3:C:56:LEU:HD23	2:D:106:ILE:HD11	1.83	0.60
6:E:279:THR:HG22	6:E:435:ASP:HB2	1.82	0.60
2:B:56:GLN:O	2:B:60:GLU:HG2	2.02	0.60
6:F:278:SER:HB2	6:F:397:VAL:HA	1.83	0.60
6:F:104:THR:HA	6:F:107:ASN:HD22	1.67	0.59
6:F:282:GLY:HA3	6:F:286:THR:HG21	1.84	0.59
7:G:31:TYR:N	7:G:43:ALA:O	2.35	0.59
2:D:127:LYS:NZ	2:D:129:MET:SD	2.76	0.59
6:F:188:THR:HG23	6:F:189:LYS:H	1.66	0.59
6:F:553:ALA:O	6:F:557:ASN:ND2	2.35	0.59
6:F:331:SER:HA	6:F:346:PHE:HB3	1.83	0.59
6:E:564:ALA:HA	6:E:567:ARG:HG2	1.85	0.59
6:E:322:LEU:HD12	6:E:345:LYS:HB3	1.85	0.59
6:F:131:LYS:NZ	6:F:423:ASN:O	2.29	0.59
6:E:153:THR:HG23	6:E:155:ARG:HH21	1.67	0.59
2:D:174:MET:CE	2:D:174:MET:H	2.16	0.58
6:E:157:VAL:HG21	6:E:219:LEU:HB3	1.86	0.58
6:F:168:GLU:OE2	6:F:168:GLU:N	2.37	0.58
6:F:155:ARG:H	6:F:155:ARG:HD3	1.69	0.57
6:E:290:HIS:CD2	6:E:442:ARG:HH22	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:371:VAL:O	6:F:397:VAL:N	2.38	0.57
2:D:171:GLU:OE1	2:D:176:ASN:ND2	2.37	0.57
6:F:318:CYS:HB2	6:F:346:PHE:CE2	2.39	0.57
7:G:84:LYS:HD3	7:G:86:LYS:NZ	2.19	0.57
2:B:132:ILE:HG21	2:B:138:TYR:HB2	1.87	0.57
6:F:37:THR:HG21	6:F:111:THR:HG21	1.85	0.57
6:F:155:ARG:HG2	6:F:156:GLU:OE1	2.03	0.57
6:F:512:ILE:HG13	6:F:531:GLN:HB3	1.84	0.57
6:F:332:ARG:NH1	6:F:346:PHE:H	2.02	0.57
6:F:401:ASP:HB3	6:F:404:GLN:HB2	1.85	0.57
2:D:182:TRP:O	2:D:184:LEU:N	2.38	0.57
6:F:456:VAL:HG21	6:F:559:ASN:ND2	2.20	0.57
6:E:342:CYS:SG	6:E:343:PHE:N	2.78	0.57
2:B:19:GLN:HA	2:B:42:LEU:HD21	1.87	0.56
6:F:358:CYS:SG	6:F:359:THR:N	2.78	0.56
7:G:53:TRP:NE1	7:G:66:TYR:HB3	2.17	0.56
6:F:248:ARG:HD2	6:F:249:ILE:HD12	1.87	0.56
6:F:456:VAL:HG21	6:F:559:ASN:HD22	1.70	0.56
6:E:149:TYR:HA	6:E:171:LYS:HD2	1.86	0.56
6:F:325:LEU:HB2	6:F:329:LYS:HE2	1.87	0.56
6:F:488:ILE:HG23	6:F:490:ARG:HH12	1.71	0.56
1:A:269:ASP:OD1	1:A:269:ASP:N	2.38	0.56
6:E:114:TRP:HE3	6:E:119:ASP:HB3	1.71	0.56
1:A:225:THR:HG22	1:A:226:THR:H	1.70	0.56
1:A:894:GLU:O	1:A:898:HIS:HB3	2.06	0.56
7:G:16:ALA:O	7:G:23:CYS:HA	2.06	0.56
7:G:48:LEU:HB2	7:G:51:LEU:HD11	1.87	0.56
4:I:17:A:H2'	4:I:18:G:C8	2.40	0.56
6:E:20:ILE:HG23	6:E:21:ARG:HG2	1.88	0.56
2:B:161:ASP:OD2	2:B:165:LYS:NZ	2.39	0.56
6:E:578:ASP:O	6:E:580:ASP:N	2.37	0.56
4:I:22:G:O2'	4:I:23:C:OP1	2.23	0.55
6:F:141:THR:HA	6:F:144:THR:HG22	1.87	0.55
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.88	0.55
6:F:305:VAL:HB	6:F:373:PHE:HE1	1.71	0.55
6:E:265:ASN:O	6:E:268:ASN:HB2	2.06	0.55
6:F:31:TYR:O	6:F:35:ILE:HG12	2.06	0.55
6:F:489:ASN:HB2	6:F:549:THR:HG23	1.89	0.55
6:E:536:SER:OG	6:E:536:SER:O	2.23	0.55
6:E:576:MET:HG3	6:E:582:TYR:CD2	2.41	0.55
2:B:169:LEU:HA	2:B:172:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:GLU:OE2	2:D:51:ARG:NH1	2.33	0.55
7:G:53:TRP:HE1	7:G:66:TYR:CB	2.16	0.55
1:A:697:CYS:O	1:A:701:THR:HG22	2.06	0.55
2:B:182:TRP:O	2:B:184:LEU:N	2.40	0.55
6:E:267:ALA:O	6:E:271:LYS:HD3	2.05	0.55
6:E:283:PRO:HB2	6:E:286:THR:HG21	1.88	0.55
5:J:49:C:H2'	5:J:50:G:C8	2.42	0.55
6:F:171:LYS:HG3	6:F:172:PRO:HD2	1.88	0.55
6:E:278:SER:N	6:E:396:TYR:O	2.37	0.55
2:D:173:SER:HB2	2:D:176:ASN:HB3	1.89	0.54
6:F:500:LEU:HD23	6:F:506:TRP:HB3	1.89	0.54
1:A:138:ASN:ND2	1:A:138:ASN:O	2.40	0.54
6:F:175:PRO:HB2	6:F:180:TYR:HE2	1.71	0.54
6:E:332:ARG:HB2	6:E:346:PHE:HB2	1.89	0.54
6:E:38:SER:OG	6:E:38:SER:O	2.24	0.54
6:F:271:LYS:O	6:F:275:GLN:N	2.41	0.54
6:E:161:ARG:HA	6:E:210:VAL:HA	1.90	0.54
6:F:268:ASN:HB3	6:F:291:PHE:HZ	1.73	0.54
6:E:374:ASP:OD1	6:E:375:GLU:N	2.41	0.54
6:E:514:PRO:HD2	6:E:549:THR:HG21	1.90	0.54
7:G:84:LYS:HD3	7:G:86:LYS:HZ2	1.71	0.54
1:A:892:HIS:O	1:A:896:THR:HG23	2.08	0.54
6:F:16:CYS:SG	6:F:19:CYS:HB2	2.48	0.53
6:F:64:TYR:HB3	6:F:80:SER:HB2	1.89	0.53
6:F:297:LEU:HB3	6:F:325:LEU:HD11	1.89	0.53
7:G:15:ALA:HA	7:G:26:ASP:HA	1.90	0.53
1:A:29:ASP:N	1:A:53:CYS:O	2.37	0.53
6:F:151:ILE:HD11	6:F:224:TYR:HB3	1.90	0.53
6:F:448:ILE:HD13	6:F:566:THR:HA	1.89	0.53
6:E:332:ARG:HE	6:E:333:ILE:H	1.55	0.53
5:J:40:U:H2'	5:J:41:G:H8	1.73	0.53
6:F:347:LYS:O	6:F:350:SER:OG	2.25	0.53
6:E:41:LEU:HD12	6:E:42:VAL:N	2.23	0.53
6:E:293:ILE:HG12	6:E:320:LYS:HG2	1.91	0.53
6:F:523:SER:HA	6:F:527:GLY:HA2	1.89	0.53
6:E:369:ASP:OD1	6:E:370:ILE:HG12	2.09	0.53
6:E:374:ASP:HA	6:E:399:ILE:HB	1.90	0.53
6:F:406:PRO:HG2	6:F:560:ARG:HD3	1.91	0.53
6:E:376:ILE:HG22	6:E:400:GLY:HA3	1.91	0.53
1:A:592:SER:HB3	5:J:30:C:H4'	1.90	0.53
6:F:33:HIS:CE1	6:F:39:HIS:CG	2.95	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:104:THR:HA	6:F:107:ASN:HB2	1.91	0.52
1:A:499:ASP:OD1	1:A:513:ARG:NH2	2.35	0.52
2:D:179:ASN:OD1	2:D:179:ASN:N	2.42	0.52
6:F:299:TYR:O	6:F:355:TYR:OH	2.27	0.52
7:G:72:PRO:HB3	7:G:89:TYR:CZ	2.44	0.52
7:G:78:ASP:HB2	7:G:113:GLN:HG3	1.90	0.52
6:F:62:GLN:OE1	6:F:62:GLN:N	2.42	0.52
3:C:14:LEU:HD22	3:C:36:HIS:CG	2.44	0.52
5:J:38:C:H2'	5:J:39:A:C8	2.43	0.52
6:F:239:THR:HG21	6:F:381:ASN:HB3	1.92	0.52
6:F:312:ALA:HB3	6:F:537:GLN:HB2	1.91	0.52
1:A:588:VAL:HG23	1:A:758:LEU:HD12	1.90	0.52
6:F:3:GLY:HA3	6:F:24:PHE:CE2	2.44	0.52
2:B:102:ALA:O	2:B:106:ILE:HG23	2.10	0.52
6:E:233:MET:SD	6:E:233:MET:N	2.83	0.52
2:D:151:SER:O	2:D:151:SER:OG	2.25	0.52
6:E:453:SER:HB3	6:E:459:ASN:HA	1.91	0.52
7:G:59:SER:OG	7:G:60:ASP:N	2.42	0.52
4:I:24:U:H2'	4:I:25:A:H8	1.73	0.52
6:F:203:GLY:HA2	6:F:209:VAL:HA	1.92	0.52
6:E:269:TYR:CD1	6:E:295:LEU:HD13	2.45	0.52
6:E:420:GLU:HB2	6:E:427:ARG:HD3	1.92	0.52
6:E:477:LYS:O	6:E:548:GLN:NE2	2.43	0.52
1:A:846:ASP:O	1:A:847:ILE:HG22	2.10	0.51
6:F:15:ARG:HD3	6:F:22:ARG:HB3	1.91	0.51
6:F:268:ASN:HB3	6:F:291:PHE:CZ	2.45	0.51
6:E:114:TRP:CE3	6:E:119:ASP:HB3	2.45	0.51
6:E:425:VAL:HA	6:E:428:LEU:HB3	1.92	0.51
1:A:303:ASP:N	1:A:303:ASP:OD1	2.43	0.51
6:F:185:TYR:CD1	6:F:192:LYS:HB2	2.46	0.51
6:E:305:VAL:HG13	6:E:356:VAL:HG23	1.91	0.51
2:D:147:PHE:N	2:D:154:TRP:O	2.38	0.51
6:F:60:VAL:HA	6:F:63:LEU:HD12	1.92	0.51
6:F:289:SER:OG	6:F:443:ARG:NH2	2.28	0.51
6:F:493:ILE:HD11	6:F:518:GLN:HG3	1.91	0.51
6:E:81:PHE:HD1	6:E:82:PRO:HD2	1.76	0.51
6:E:186:ARG:O	6:E:193:VAL:N	2.35	0.51
6:F:7:LEU:HD11	6:F:106:PHE:CZ	2.46	0.51
6:F:370:ILE:HG23	6:F:395:HIS:HB2	1.93	0.51
6:E:377:SER:OG	6:E:378:MET:SD	2.67	0.51
4:I:31:C:H2'	4:I:32:A:H8	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:155:ARG:NE	6:F:156:GLU:OE2	2.44	0.51
2:B:177:SER:HB2	2:B:182:TRP:HZ2	1.75	0.51
4:I:17:A:H2'	4:I:18:G:H8	1.76	0.51
6:F:32:ASP:HA	6:F:35:ILE:HG12	1.93	0.50
6:F:378:MET:HA	6:F:407:ALA:HB2	1.92	0.50
6:E:117:ALA:O	6:E:121:ILE:HG13	2.10	0.50
7:G:73:CYS:SG	7:G:74:ARG:N	2.84	0.50
6:F:155:ARG:HH22	6:F:164:HIS:CD2	2.29	0.50
6:E:489:ASN:ND2	6:E:518:GLN:OE1	2.33	0.50
6:F:315:ASP:HA	6:F:318:CYS:SG	2.52	0.50
6:E:383:ASP:HA	6:E:386:VAL:HG12	1.93	0.50
7:G:50:ASP:OD1	7:G:52:LYS:NZ	2.42	0.50
1:A:496:ASN:N	1:A:496:ASN:OD1	2.45	0.50
4:I:22:G:HO2'	4:I:23:C:P	2.34	0.50
6:F:197:GLU:N	6:F:217:TYR:OH	2.41	0.50
6:F:489:ASN:OD1	6:F:492:GLN:HG2	2.11	0.50
6:F:579:ARG:HH12	6:F:582:TYR:HB3	1.76	0.50
4:I:21:U:H2'	4:I:22:G:C8	2.46	0.50
6:F:488:ILE:HG23	6:F:490:ARG:NH1	2.26	0.50
6:F:567:ARG:HB2	6:F:572:ILE:HD11	1.93	0.50
6:F:592:ILE:HD12	6:F:592:ILE:O	2.12	0.50
6:E:484:VAL:HG13	6:E:486:SER:H	1.76	0.50
6:F:121:ILE:O	6:F:125:THR:HG23	2.12	0.50
6:F:276:LYS:O	6:F:396:TYR:N	2.44	0.50
6:F:497:ARG:O	6:F:501:THR:HG23	2.11	0.50
6:E:139:LYS:HD3	6:E:382:TYR:HD2	1.77	0.50
1:A:304:ASP:OD1	1:A:304:ASP:N	2.45	0.49
3:C:46:THR:O	3:C:50:GLU:HG2	2.11	0.49
2:D:174:MET:H	2:D:174:MET:HE2	1.76	0.49
6:F:449:VAL:HA	6:F:452:VAL:HG12	1.94	0.49
6:E:289:SER:HB3	6:E:290:HIS:CE1	2.47	0.49
6:F:369:ASP:O	6:F:394:LYS:N	2.39	0.49
6:F:583:ASP:N	6:F:583:ASP:OD2	2.45	0.49
1:A:304:ASP:HB2	1:A:636:LEU:HD13	1.95	0.49
6:E:139:LYS:HD3	6:E:382:TYR:CD2	2.47	0.49
2:D:90:MET:O	2:D:94:MET:HG3	2.12	0.49
6:F:245:HIS:NE2	6:F:275:GLN:OE1	2.42	0.49
6:F:334:ILE:HG13	6:F:342:CYS:HB3	1.94	0.49
6:E:290:HIS:HA	6:E:293:ILE:HD13	1.93	0.49
7:G:77:THR:HG21	7:G:86:LYS:HZ3	1.77	0.49
6:F:138:LEU:HA	6:F:141:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:292:ALA:HB1	6:F:306:TYR:CE2	2.45	0.49
6:F:316:ALA:HB2	6:F:538:GLY:HA3	1.94	0.49
7:G:98:ASN:O	7:G:102:VAL:HG13	2.13	0.49
6:F:268:ASN:HD21	6:F:436:MET:HB3	1.78	0.49
6:F:269:TYR:HB3	6:F:298:TYR:CZ	2.48	0.49
6:E:305:VAL:O	6:E:372:VAL:N	2.42	0.49
6:E:568:ALA:HB3	6:E:572:ILE:HG13	1.95	0.49
6:F:372:VAL:HA	6:F:397:VAL:HB	1.94	0.49
6:F:373:PHE:CE2	6:F:387:VAL:HB	2.48	0.49
7:G:79:THR:HG21	7:G:84:LYS:HD2	1.95	0.49
1:A:123:THR:HG23	9:A:1003:GTP:HN22	1.78	0.49
6:F:158:LEU:HB2	6:F:163:LEU:HA	1.95	0.49
6:F:322:LEU:HD22	6:F:327:ILE:HD13	1.94	0.49
6:F:383:ASP:OD2	6:F:384:LEU:N	2.45	0.48
6:E:127:THR:O	6:E:131:LYS:HG2	2.13	0.48
6:E:314:VAL:HG21	6:E:342:CYS:SG	2.52	0.48
6:F:15:ARG:HG3	6:F:43:LEU:HB2	1.95	0.48
6:F:275:GLN:HE21	6:F:435:ASP:HB3	1.78	0.48
6:E:543:TYR:CE2	6:E:571:GLY:HA3	2.48	0.48
1:A:40:ASP:HB3	7:G:6:PRO:HG2	1.95	0.48
3:C:63:GLN:OE1	3:C:63:GLN:HA	2.13	0.48
6:F:359:THR:HG22	6:F:361:ASN:H	1.79	0.48
6:F:410:THR:HG23	6:F:411:LEU:N	2.25	0.48
6:F:302:ALA:HA	6:F:303:ARG:NH1	2.29	0.48
6:E:296:ALA:O	6:E:355:TYR:OH	2.25	0.48
6:E:439:GLY:HA2	6:E:461:LEU:HB3	1.94	0.48
1:A:12:CYS:SG	1:A:17:ALA:HB1	2.54	0.47
6:E:265:ASN:ND2	6:E:269:TYR:OH	2.46	0.47
6:E:533:VAL:HG11	6:E:560:ARG:HD2	1.96	0.47
5:J:40:U:H2'	5:J:41:G:C8	2.48	0.47
6:F:464:HIS:HB3	6:F:465:LYS:HZ2	1.78	0.47
6:F:545:ILE:HA	6:F:573:LEU:HD22	1.97	0.47
7:G:76:VAL:HG22	7:G:85:VAL:HG22	1.97	0.47
6:F:243:GLN:HE22	6:F:432:ILE:HD12	1.79	0.47
6:F:278:SER:HB3	6:F:436:MET:SD	2.55	0.47
6:E:419:PRO:HA	6:E:422:PHE:CE2	2.49	0.47
1:A:431:GLU:OE2	1:A:431:GLU:N	2.37	0.47
6:F:374:ASP:HA	6:F:399:ILE:HB	1.97	0.47
3:C:3:MET:O	3:C:6:VAL:HG12	2.15	0.47
6:F:7:LEU:HD11	6:F:106:PHE:HZ	1.79	0.47
6:F:516:ASN:HD21	6:F:530:THR:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:SER:OG	2:B:32:GLU:N	2.47	0.47
6:F:239:THR:HB	6:F:384:LEU:HB3	1.97	0.47
6:F:277:TYR:OH	6:F:428:LEU:HD21	2.13	0.47
6:F:334:ILE:HG23	6:F:342:CYS:HB2	1.96	0.47
6:F:116:ASN:OD1	6:F:117:ALA:N	2.48	0.47
6:F:442:ARG:HA	6:F:465:LYS:NZ	2.30	0.47
6:E:394:LYS:HG2	6:E:395:HIS:CE1	2.49	0.47
1:A:160:LYS:HD3	1:A:161:ASP:H	1.80	0.47
6:E:405:LEU:HD21	6:E:533:VAL:HG12	1.96	0.47
1:A:759:SER:O	1:A:759:SER:OG	2.25	0.47
6:F:371:VAL:N	6:F:395:HIS:O	2.45	0.47
6:F:522:ALA:HB1	6:F:526:LEU:HD21	1.97	0.47
6:E:119:ASP:O	6:E:122:LEU:HD23	2.13	0.47
1:A:849:LYS:O	1:A:850:THR:OG1	2.25	0.46
2:D:58:LYS:HG3	2:D:59:LEU:N	2.30	0.46
2:D:163:ASP:HB2	2:D:165:LYS:HD2	1.97	0.46
6:F:239:THR:OG1	6:F:240:LEU:N	2.48	0.46
6:F:488:ILE:HD12	6:F:489:ASN:H	1.80	0.46
6:E:34:VAL:HG23	6:E:39:HIS:O	2.14	0.46
1:A:851:ASP:HB2	2:D:79:LYS:HE3	1.95	0.46
2:D:101:ASP:OD2	2:D:102:ALA:N	2.48	0.46
6:F:240:LEU:HD23	6:F:424:SER:HB3	1.98	0.46
6:F:450:ASP:OD2	6:F:584:LYS:NZ	2.31	0.46
1:A:882:HIS:O	1:A:886:GLN:HG3	2.15	0.46
2:D:162:ALA:HB3	2:D:181:ALA:HB1	1.97	0.46
6:E:319:GLU:HA	6:E:345:LYS:HZ3	1.80	0.46
6:E:492:GLN:HG3	6:E:518:GLN:NE2	2.31	0.46
2:D:31:SER:O	2:D:35:LEU:HG	2.16	0.46
6:F:268:ASN:O	6:F:272:VAL:HG23	2.15	0.46
6:E:492:GLN:O	6:E:496:VAL:HG23	2.15	0.46
5:J:31:U:H2'	5:J:32:C:H6	1.80	0.46
6:E:492:GLN:HA	6:E:495:VAL:HB	1.98	0.46
7:G:29:LEU:HD12	7:G:29:LEU:HA	1.83	0.46
3:C:70:LYS:O	3:C:70:LYS:HD3	2.16	0.46
4:I:31:C:H2'	4:I:32:A:C8	2.50	0.46
6:F:371:VAL:HG13	6:F:373:PHE:CE1	2.51	0.46
7:G:18:THR:H	7:G:22:ALA:HB3	1.81	0.46
1:A:60:ASP:N	1:A:60:ASP:OD1	2.49	0.46
6:E:332:ARG:NH2	6:E:358:CYS:HA	2.30	0.46
6:E:359:THR:HG22	6:E:360:VAL:H	1.80	0.46
1:A:2:ALA:O	1:A:4:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:479:VAL:HB	6:E:491:PRO:HG2	1.98	0.46
1:A:143:LYS:O	1:A:147:VAL:HG13	2.15	0.46
1:A:551:LYS:HE3	1:A:551:LYS:HB3	1.70	0.46
6:F:331:SER:O	6:F:357:PHE:N	2.49	0.46
6:E:544:VAL:N	6:E:568:ALA:HB2	2.30	0.46
1:A:522:GLU:OE1	1:A:522:GLU:N	2.33	0.45
2:D:177:SER:O	2:D:179:ASN:N	2.41	0.45
6:F:237:ALA:HB3	6:F:389:ALA:HB2	1.97	0.45
1:A:689:TYR:O	1:A:693:VAL:HG23	2.17	0.45
6:F:442:ARG:HA	6:F:465:LYS:HZ1	1.82	0.45
6:E:69:SER:HG	6:E:70:TYR:H	1.63	0.45
1:A:59:LYS:HE2	1:A:59:LYS:HB2	1.63	0.45
2:D:26:VAL:HG22	2:D:35:LEU:HD22	1.99	0.45
6:F:386:VAL:HG22	6:F:390:ARG:HH21	1.82	0.45
7:G:4:LEU:HD12	7:G:4:LEU:HA	1.77	0.45
7:G:95:ASN:O	7:G:99:ARG:HG3	2.16	0.45
6:F:492:GLN:OE1	6:F:577:SER:OG	2.29	0.45
6:F:544:VAL:HG11	6:F:567:ARG:HB3	1.98	0.45
6:E:188:THR:HG23	6:E:189:LYS:H	1.81	0.45
6:E:368:ALA:O	6:E:393:ALA:HA	2.16	0.45
6:F:151:ILE:HG13	6:F:226:VAL:HB	1.99	0.45
6:F:406:PRO:HA	6:F:422:PHE:HZ	1.81	0.45
6:F:452:VAL:HG22	6:F:457:TYR:CE2	2.52	0.45
6:E:12:THR:OG1	6:E:13:SER:N	2.50	0.45
3:C:70:LYS:HD3	3:C:70:LYS:C	2.37	0.45
5:J:48:C:H2'	5:J:49:C:C6	2.51	0.45
6:F:535:SER:HB2	6:F:537:GLN:HE21	1.82	0.45
6:F:114:TRP:HB3	6:F:141:THR:HG21	1.99	0.45
6:F:293:ILE:HG12	6:F:324:TYR:HD2	1.82	0.45
6:F:294:GLY:O	6:F:298:TYR:HB3	2.17	0.45
6:E:269:TYR:HA	6:E:272:VAL:HG22	1.99	0.45
3:C:71:LEU:O	3:C:76:LEU:HB2	2.17	0.44
6:F:20:ILE:HD13	6:F:114:TRP:CD1	2.51	0.44
6:E:116:ASN:N	6:E:119:ASP:OD2	2.48	0.44
6:E:407:ALA:O	6:E:409:ARG:N	2.47	0.44
2:D:13:ALA:O	2:D:17:THR:HG23	2.16	0.44
6:F:3:GLY:HA3	6:F:24:PHE:HE2	1.81	0.44
6:F:489:ASN:ND2	6:F:491:PRO:HD3	2.31	0.44
6:F:562:ASN:HA	6:F:565:ILE:HG13	1.99	0.44
6:E:406:PRO:HB3	6:E:422:PHE:HE1	1.83	0.44
6:E:488:ILE:HG13	6:E:489:ASN:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:SER:HB2	6:F:95:ASN:HB2	1.98	0.44
2:D:160:VAL:HG13	2:D:164:SER:HA	1.97	0.44
6:F:268:ASN:ND2	6:F:436:MET:HB3	2.32	0.44
6:E:290:HIS:CD2	6:E:320:LYS:HD3	2.53	0.44
2:D:52:ASP:OD1	2:D:52:ASP:N	2.50	0.44
5:J:35:U:H2'	5:J:36:A:C8	2.52	0.44
6:F:322:LEU:HB3	6:F:346:PHE:HE1	1.82	0.44
6:E:379:ALA:O	6:E:423:ASN:ND2	2.50	0.44
1:A:162:TRP:HA	1:A:168:ASN:HD22	1.82	0.44
6:F:268:ASN:HD21	6:F:438:LEU:HB2	1.81	0.44
2:D:67:MET:O	2:D:70:MET:HG2	2.17	0.44
6:F:155:ARG:HA	6:F:222:GLY:H	1.81	0.44
6:F:376:ILE:HG12	6:F:376:ILE:O	2.17	0.44
6:E:62:GLN:OE1	6:E:72:CYS:HB2	2.18	0.44
6:F:464:HIS:HB3	6:F:465:LYS:NZ	2.32	0.44
7:G:5:SER:CB	7:G:101:MET:HG2	2.48	0.44
6:F:329:LYS:HD2	6:F:329:LYS:O	2.18	0.44
6:E:220:ASN:ND2	6:E:221:VAL:HG22	2.32	0.44
2:D:147:PHE:O	2:D:154:TRP:N	2.45	0.43
6:F:202:LYS:O	6:F:210:VAL:N	2.51	0.43
6:F:473:LYS:HB2	6:F:587:PHE:HB3	2.00	0.43
6:E:158:LEU:HD21	6:E:164:HIS:CD2	2.53	0.43
2:B:148:THR:HG22	2:B:153:LEU:HD12	1.99	0.43
2:B:48:GLU:HA	2:B:51:ARG:NH2	2.32	0.43
2:D:61:LYS:HG3	2:D:62:MET:N	2.33	0.43
2:D:97:LYS:HB3	2:D:97:LYS:HE2	1.77	0.43
6:E:267:ALA:HA	6:E:270:GLN:HB3	2.00	0.43
3:C:77:ASP:HA	2:D:96:ARG:HD3	2.01	0.43
6:F:305:VAL:HB	6:F:373:PHE:CE1	2.52	0.43
6:F:494:GLY:HA2	6:F:497:ARG:HD2	1.99	0.43
6:F:557:ASN:OD1	6:F:558:VAL:HG12	2.18	0.43
6:E:35:ILE:HD13	6:E:35:ILE:HA	1.85	0.43
6:E:152:ALA:HB2	6:E:167:TRP:HZ3	1.83	0.43
6:E:219:LEU:HD11	6:E:225:PHE:CE2	2.50	0.43
6:E:416:THR:HG21	6:E:557:ASN:HD22	1.83	0.43
2:D:22:TYR:HA	2:D:38:LEU:HD13	2.00	0.43
6:F:332:ARG:HH12	6:F:346:PHE:H	1.66	0.43
6:E:34:VAL:HG21	6:E:60:VAL:HG11	2.00	0.43
6:E:307:THR:HA	6:E:358:CYS:O	2.18	0.43
1:A:478:LYS:HD2	1:A:478:LYS:HA	1.83	0.43
2:D:58:LYS:HE3	2:D:59:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:131:LYS:NZ	6:F:381:ASN:HD21	2.16	0.43
1:A:735:ARG:HA	1:A:735:ARG:HD3	1.84	0.43
3:C:77:ASP:HB2	2:D:92:PHE:HD1	1.82	0.43
2:D:156:ILE:HG23	2:D:186:VAL:HG13	2.01	0.43
6:E:334:ILE:HD12	6:E:342:CYS:HB3	1.99	0.43
6:E:506:TRP:CE2	6:E:573:LEU:HB2	2.53	0.43
7:G:5:SER:O	7:G:5:SER:OG	2.25	0.43
2:B:70:MET:SD	6:E:92:LEU:HG	2.59	0.43
1:A:665:GLU:OE1	1:A:665:GLU:N	2.52	0.43
6:F:126:CYS:HB3	6:F:130:LEU:HB3	2.00	0.43
6:F:197:GLU:OE1	6:F:340:VAL:N	2.52	0.43
6:F:202:LYS:HD2	6:F:202:LYS:HA	1.78	0.43
6:F:394:LYS:HB3	6:F:394:LYS:HE3	1.81	0.43
7:G:95:ASN:OD1	7:G:98:ASN:ND2	2.52	0.43
6:F:152:ALA:HB1	6:F:165:LEU:HD11	2.00	0.43
6:F:371:VAL:HG13	6:F:373:PHE:CZ	2.53	0.43
6:E:280:LEU:HB2	6:E:399:ILE:HA	2.00	0.43
5:J:35:U:H2'	5:J:36:A:H8	1.84	0.42
6:F:518:GLN:OE1	6:F:549:THR:OG1	2.37	0.42
6:E:369:ASP:HA	6:E:394:LYS:H	1.84	0.42
6:E:448:ILE:HG22	6:E:565:ILE:HG23	2.02	0.42
5:J:39:A:H2'	5:J:40:U:H6	1.85	0.42
6:F:368:ALA:HB3	6:F:391:LEU:HD13	2.01	0.42
2:B:68:THR:HG23	6:F:53:PRO:HG2	2.00	0.42
6:F:176:LEU:HD11	6:F:201:GLU:O	2.19	0.42
6:F:186:ARG:O	6:F:193:VAL:N	2.53	0.42
6:E:279:THR:HA	6:E:398:TYR:H	1.84	0.42
6:E:103:VAL:HG12	6:E:107:ASN:ND2	2.33	0.42
2:D:135:TYR:HB2	2:D:182:TRP:CZ2	2.55	0.42
6:F:196:GLY:HA3	6:F:217:TYR:CE1	2.55	0.42
6:F:271:LYS:HA	6:F:274:MET:SD	2.59	0.42
6:E:131:LYS:HG2	6:E:131:LYS:H	1.73	0.42
6:E:419:PRO:HA	6:E:422:PHE:CD2	2.54	0.42
7:G:48:LEU:HD13	7:G:51:LEU:HD21	2.00	0.42
7:G:69:LEU:HD23	7:G:89:TYR:CD2	2.54	0.42
7:G:111:ARG:NH1	7:G:111:ARG:HA	2.34	0.42
6:F:309:CYS:N	6:F:375:GLU:OE2	2.43	0.42
6:E:492:GLN:HG3	6:E:518:GLN:HE22	1.85	0.42
6:E:555:SER:CB	6:E:560:ARG:HD3	2.44	0.42
1:A:836:ARG:NH1	1:A:840:ALA:HB2	2.35	0.42
7:G:70:GLU:OE2	7:G:99:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:LYS:O	6:F:76:LYS:HE2	2.20	0.42
6:F:544:VAL:HG11	6:F:567:ARG:CB	2.49	0.42
6:E:13:SER:O	6:E:13:SER:OG	2.37	0.42
6:E:405:LEU:HD22	6:E:534:ASP:HA	2.02	0.42
6:E:546:PHE:HE2	6:E:560:ARG:NH2	2.17	0.42
6:F:426:CYS:O	6:F:429:MET:HB3	2.20	0.42
6:E:113:ASP:OD1	6:E:115:THR:OG1	2.38	0.42
6:E:319:GLU:HA	6:E:345:LYS:NZ	2.35	0.42
6:E:497:ARG:HA	6:E:500:LEU:HG	2.02	0.42
1:A:847:ILE:HD12	1:A:847:ILE:HA	1.77	0.41
6:E:62:GLN:HE21	6:E:62:GLN:HB3	1.64	0.41
6:E:527:GLY:O	6:E:528:LEU:HD13	2.20	0.41
7:G:79:THR:HG23	7:G:82:GLY:H	1.85	0.41
4:I:14:A:H2'	4:I:15:G:C8	2.55	0.41
6:F:348:VAL:HG12	6:F:349:ASN:OD1	2.20	0.41
6:E:140:ALA:O	6:E:143:GLU:HG3	2.20	0.41
1:A:225:THR:HG22	1:A:226:THR:N	2.35	0.41
6:F:412:LEU:HD13	6:F:554:HIS:NE2	2.35	0.41
6:E:139:LYS:HA	6:E:142:GLU:HG2	2.02	0.41
6:E:280:LEU:HB2	6:E:399:ILE:HG13	2.02	0.41
1:A:64:ASN:OD1	1:A:64:ASN:N	2.53	0.41
5:J:40:U:C2	5:J:41:G:C8	3.08	0.41
6:F:176:LEU:HB2	6:F:485:SER:HB3	2.01	0.41
6:E:281:GLN:HE22	6:E:402:PRO:HD2	1.84	0.41
1:A:572:HIS:O	1:A:576:LEU:HG	2.20	0.41
1:A:608:ASP:OD1	1:A:608:ASP:N	2.54	0.41
6:F:32:ASP:HA	6:F:35:ILE:CG1	2.50	0.41
6:F:188:THR:HG23	6:F:189:LYS:N	2.33	0.41
6:E:544:VAL:H	6:E:568:ALA:HB2	1.85	0.41
1:A:260:ASP:HB3	1:A:263:LYS:HD2	2.03	0.41
7:G:70:GLU:OE2	7:G:90:PHE:HB2	2.20	0.41
1:A:336:ASP:OD1	1:A:336:ASP:N	2.51	0.41
1:A:898:HIS:O	1:A:898:HIS:ND1	2.54	0.41
2:B:139:LYS:HG3	2:B:140:ASN:OD1	2.21	0.41
6:F:291:PHE:O	6:F:295:LEU:HG	2.21	0.41
6:F:491:PRO:HD2	6:F:492:GLN:N	2.35	0.41
6:E:25:LEU:HD21	6:E:106:PHE:CE2	2.55	0.41
6:E:445:PRO:HD2	6:E:569:LYS:O	2.21	0.41
1:A:894:GLU:O	1:A:898:HIS:CB	2.68	0.41
3:C:3:MET:HE3	3:C:7:LYS:HE3	2.03	0.41
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:498:GLU:OE1	6:F:593:PRO:HB2	2.21	0.41
7:G:11:GLN:O	7:G:32:TYR:N	2.49	0.41
2:B:48:GLU:HA	2:B:51:ARG:CZ	2.51	0.41
3:C:61:SER:HB3	2:D:116:PRO:HG2	2.03	0.41
4:I:24:U:H2'	4:I:25:A:C8	2.54	0.41
5:J:34:C:H2'	5:J:35:U:C6	2.56	0.41
6:F:76:LYS:O	6:F:78:PRO:HD3	2.20	0.41
6:F:162:GLU:HG2	6:F:210:VAL:HG22	2.01	0.41
6:F:282:GLY:HA2	6:F:283:PRO:HD3	1.93	0.41
6:F:283:PRO:HA	6:F:563:VAL:HG12	2.03	0.41
6:E:414:LYS:HB3	6:E:414:LYS:HE3	1.74	0.41
6:E:445:PRO:HA	6:E:465:LYS:HB2	2.02	0.41
6:F:373:PHE:N	6:F:373:PHE:CD1	2.89	0.41
6:F:491:PRO:HD2	6:F:492:GLN:H	1.85	0.41
6:E:152:ALA:HB3	6:E:225:PHE:HB2	2.03	0.41
6:E:153:THR:HG23	6:E:155:ARG:HE	1.86	0.41
6:E:511:PHE:O	6:E:531:GLN:HB3	2.21	0.41
1:A:77:PHE:O	1:A:80:TYR:HB3	2.21	0.40
3:C:66:VAL:HG23	3:C:68:ILE:HD12	2.03	0.40
6:F:492:GLN:HE21	6:F:548:GLN:H	1.69	0.40
7:G:31:TYR:HB2	7:G:43:ALA:HB3	2.03	0.40
7:G:106:LEU:HD11	7:G:112:LEU:HD22	2.02	0.40
2:D:141:THR:OG1	2:D:142:CYS:N	2.55	0.40
5:J:28:U:C2	5:J:29:G:C8	3.10	0.40
6:E:275:GLN:O	6:E:395:HIS:ND1	2.54	0.40
6:E:377:SER:OG	6:E:405:LEU:O	2.38	0.40
7:G:16:ALA:O	7:G:27:ASN:ND2	2.54	0.40
7:G:73:CYS:O	7:G:88:LEU:N	2.47	0.40
1:A:37:ILE:HA	7:G:1:ASN:O	2.22	0.40
6:E:544:VAL:HG21	6:E:567:ARG:HB3	2.03	0.40
1:A:144:GLU:O	1:A:148:THR:HG22	2.21	0.40
1:A:885:LEU:HD22	1:A:916:TRP:HA	2.03	0.40
6:F:20:ILE:HG23	6:F:21:ARG:N	2.36	0.40
6:F:404:GLN:O	6:F:563:VAL:HG21	2.22	0.40
6:F:491:PRO:CD	6:F:492:GLN:N	2.84	0.40
6:F:500:LEU:HD13	6:F:507:ARG:NH1	2.37	0.40
6:F:544:VAL:O	6:F:573:LEU:HB3	2.22	0.40
6:E:561:PHE:HA	6:E:564:ALA:HB3	2.03	0.40
2:B:98:LEU:HA	2:B:98:LEU:HD12	1.82	0.40
6:F:293:ILE:HG21	6:F:324:TYR:CD2	2.56	0.40
6:E:449:VAL:O	6:E:453:SER:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:536:SER:O	6:E:567:ARG:NH1	2.54	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	927/932 (100%)	888 (96%)	37 (4%)	2 (0%)	47 78
2	B	185/198 (93%)	176 (95%)	9 (5%)	0	100 100
2	D	185/198 (93%)	174 (94%)	11 (6%)	0	100 100
3	C	76/83 (92%)	68 (90%)	7 (9%)	1 (1%)	12 39
6	E	581/601 (97%)	516 (89%)	64 (11%)	1 (0%)	47 78
6	F	581/601 (97%)	499 (86%)	82 (14%)	0	100 100
7	G	111/117 (95%)	92 (83%)	13 (12%)	6 (5%)	2 13
All	All	2646/2730 (97%)	2413 (91%)	223 (8%)	10 (0%)	38 67

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
3	C	65	ALA
7	G	14	CYS
7	G	33	ASN
7	G	11	GLN
7	G	32	TYR
7	G	59	SER
6	E	220	ASN
7	G	3	GLU
1	A	847	ILE

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	
1	A	821/823 (100%)	766 (93%)	55 (7%)	16	46
2	B	144/167 (86%)	129 (90%)	15 (10%)	7	25
2	D	150/167 (90%)	133 (89%)	17 (11%)	6	21
3	C	73/77 (95%)	70 (96%)	3 (4%)	30	59
6	E	498/523 (95%)	462 (93%)	36 (7%)	14	43
6	F	498/523 (95%)	449 (90%)	49 (10%)	8	28
7	G	94/97 (97%)	73 (78%)	21 (22%)	1	2
All	All	2278/2377 (96%)	2082 (91%)	196 (9%)	14	35

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	18	ARG
1	A	20	THR
1	A	40	ASP
1	A	49	LEU
1	A	54	CYS
1	A	63	ASP
1	A	72	VAL
1	A	73	LYS
1	A	74	ARG
1	A	75	HIS
1	A	76	THR
1	A	115	SER
1	A	138	ASN
1	A	153	ASP
1	A	181	ARG
1	A	204	VAL
1	A	231	VAL
1	A	235	ASP
1	A	236	SER

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Mol	Chain	Res	Type
1	A	246	THR
1	A	255	SER
1	A	267	LYS
1	A	308	LEU
1	A	336	ASP
1	A	359	VAL
1	A	366	LEU
1	A	372	LEU
1	A	380	MET
1	A	434	SER
1	A	447	ASN
1	A	481	ASP
1	A	499	ASP
1	A	520	SER
1	A	551	LYS
1	A	553	ARG
1	A	607	SER
1	A	667	VAL
1	A	680	THR
1	A	682	SER
1	A	701	THR
1	A	709	SER
1	A	718	LYS
1	A	726	ARG
1	A	731	LEU
1	A	736	ASP
1	A	754	SER
1	A	760	ASP
1	A	776	VAL
1	A	778	SER
1	A	780	LYS
1	A	790	ASN
1	A	821	LYS
1	A	835	SER
1	A	848	VAL
2	B	7	SER
2	B	48	GLU
2	B	51	ARG
2	B	58	LYS
2	B	61	LYS
2	B	69	GLN
2	B	76	SER

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Mol	Chain	Res	Type
2	B	82	LYS
2	B	98	LEU
2	B	100	ASN
2	B	111	ARG
2	B	114	CYS
2	B	142	CYS
2	B	145	THR
2	B	177	SER
3	C	67	ASP
3	C	69	ASN
3	C	77	ASP
2	D	11	SER
2	D	12	TYR
2	D	19	GLN
2	D	46	LYS
2	D	52	ASP
2	D	55	MET
2	D	58	LYS
2	D	69	GLN
2	D	71	TYR
2	D	76	SER
2	D	131	VAL
2	D	165	LYS
2	D	174	MET
2	D	176	ASN
2	D	179	ASN
2	D	182	TRP
2	D	187	THR
6	F	7	LEU
6	F	14	LEU
6	F	19	CYS
6	F	25	LEU
6	F	75	HIS
6	F	80	SER
6	F	97	CYS
6	F	106	PHE
6	F	120	TYR
6	F	129	ARG
6	F	155	ARG
6	F	160	ASP
6	F	162	GLU
6	F	173	ARG

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Mol	Chain	Res	Type
6	F	185	TYR
6	F	192	LYS
6	F	199	THR
6	F	202	LYS
6	F	233	MET
6	F	253	TYR
6	F	262	PHE
6	F	274	MET
6	F	291	PHE
6	F	298	TYR
6	F	303	ARG
6	F	318	CYS
6	F	329	LYS
6	F	332	ARG
6	F	344	ASP
6	F	349	ASN
6	F	351	THR
6	F	391	LEU
6	F	414	LYS
6	F	436	MET
6	F	437	PHE
6	F	442	ARG
6	F	447	GLU
6	F	453	SER
6	F	460	LYS
6	F	464	HIS
6	F	490	ARG
6	F	495	VAL
6	F	506	TRP
6	F	515	TYR
6	F	526	LEU
6	F	555	SER
6	F	570	VAL
6	F	576	MET
6	F	584	LYS
6	E	5	CYS
6	E	9	ASN
6	E	12	THR
6	E	13	SER
6	E	21	ARG
6	E	24	PHE
6	E	38	SER

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Mol	Chain	Res	Type
6	E	62	GLN
6	E	122	LEU
6	E	129	ARG
6	E	160	ASP
6	E	167	TRP
6	E	233	MET
6	E	236	SER
6	E	271	LYS
6	E	303	ARG
6	E	319	GLU
6	E	323	LYS
6	E	331	SER
6	E	372	VAL
6	E	378	MET
6	E	390	ARG
6	E	396	TYR
6	E	410	THR
6	E	426	CYS
6	E	429	MET
6	E	437	PHE
6	E	462	LYS
6	E	475	PHE
6	E	511	PHE
6	E	517	SER
6	E	543	TYR
6	E	547	THR
6	E	554	HIS
6	E	559	ASN
6	E	587	PHE
7	G	2	ASN
7	G	5	SER
7	G	7	VAL
7	G	9	LEU
7	G	10	ARG
7	G	11	GLN
7	G	12	MET
7	G	19	THR
7	G	27	ASN
7	G	29	LEU
7	G	33	ASN
7	G	34	THR
7	G	35	THR

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Mol	Chain	Res	Type
7	G	36	LYS
7	G	40	PHE
7	G	46	SER
7	G	52	LYS
7	G	58	LYS
7	G	73	CYS
7	G	84	LYS
7	G	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	HIS
1	A	928	HIS
6	F	33	HIS
6	F	164	HIS
6	F	268	ASN
6	F	516	ASN
6	F	559	ASN
6	E	265	ASN
6	E	290	HIS
7	G	98	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	I	24/25 (96%)	2 (8%)	1 (4%)
5	J	26/33 (78%)	1 (3%)	0
All	All	50/58 (86%)	3 (6%)	1 (2%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	14	A
4	I	23	C
5	J	45	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	I	22	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	GTP	A	1003	-	26,34,34	1.03	1 (3%)	32,54,54	1.34	3 (9%)

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
9	GTP	A	1003	-	-	7/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1003	GTP	C6-N1	-3.52	1.32	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1003	GTP	C3'-C2'-C1'	3.63	106.45	100.98
9	A	1003	GTP	C5-C6-N1	2.85	118.99	113.95
9	A	1003	GTP	C8-N7-C5	2.15	107.09	102.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

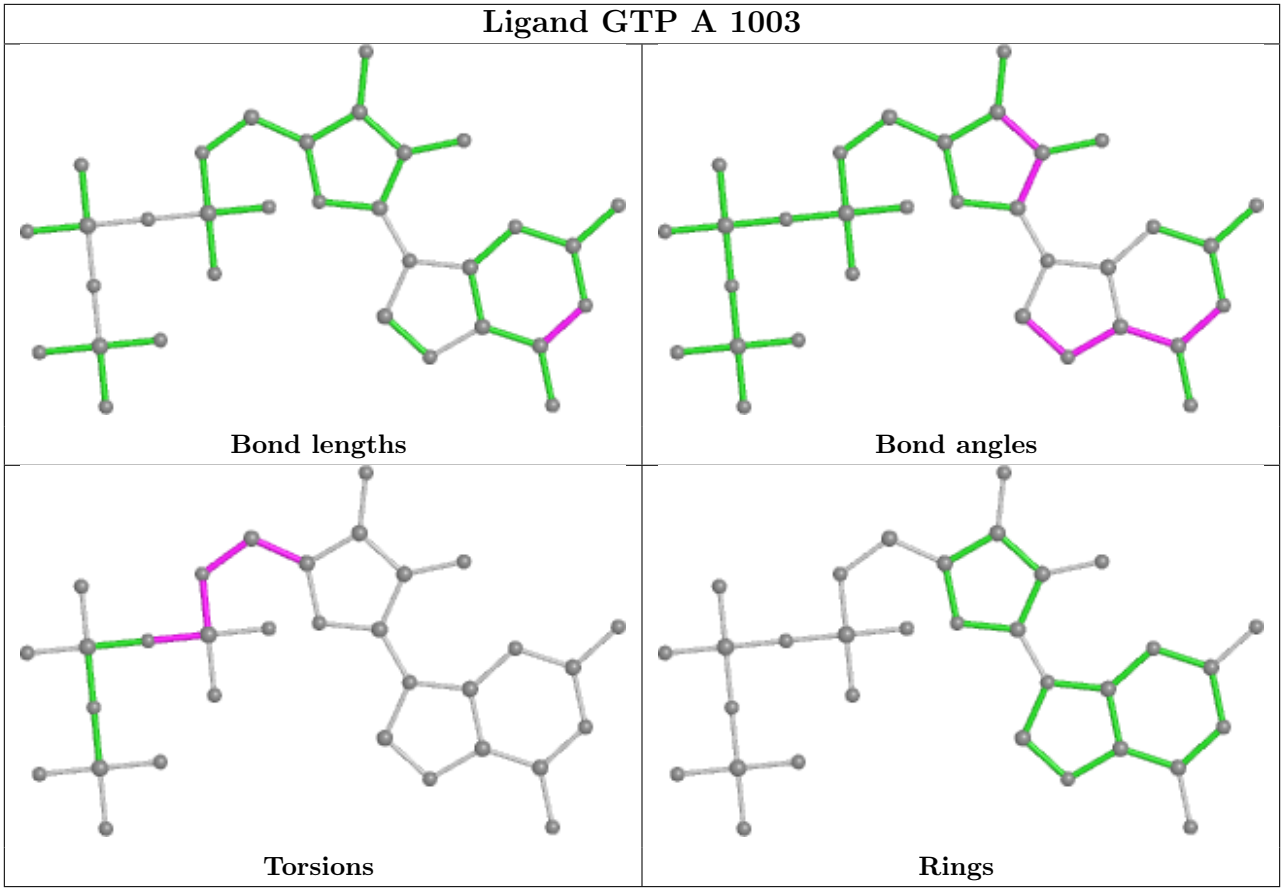
Mol	Chain	Res	Type	Atoms
9	A	1003	GTP	C5'-O5'-PA-O1A
9	A	1003	GTP	C4'-C5'-O5'-PA
9	A	1003	GTP	C5'-O5'-PA-O3A
9	A	1003	GTP	PB-O3A-PA-O1A
9	A	1003	GTP	C5'-O5'-PA-O2A
9	A	1003	GTP	PB-O3A-PA-O2A
9	A	1003	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1003	GTP	1	0

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	929:THR	C	930:VAL	N	3.42

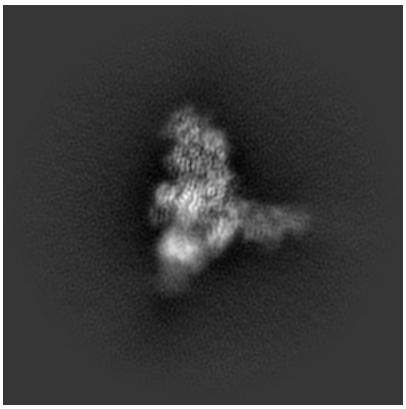
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34311. These allow visual inspection of the internal detail of the map and identification of artifacts.

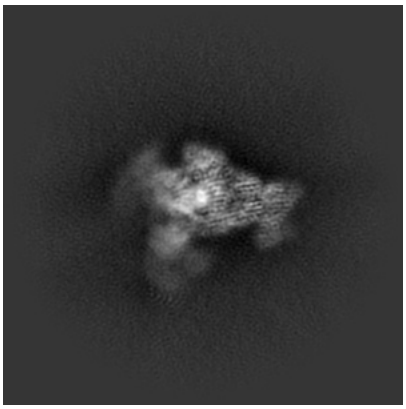
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

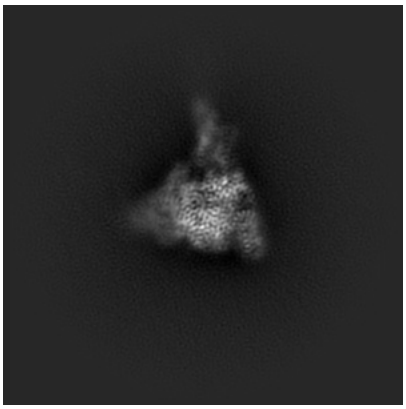
6.1.1 Primary map



X

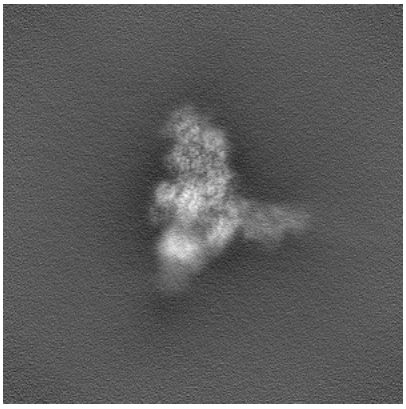


Y

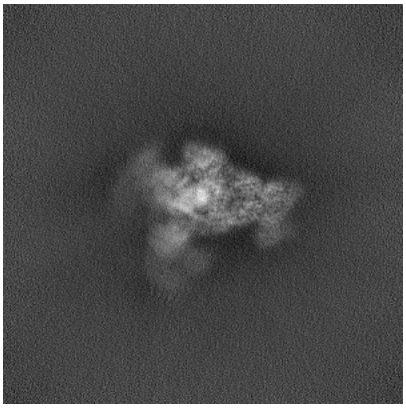


Z

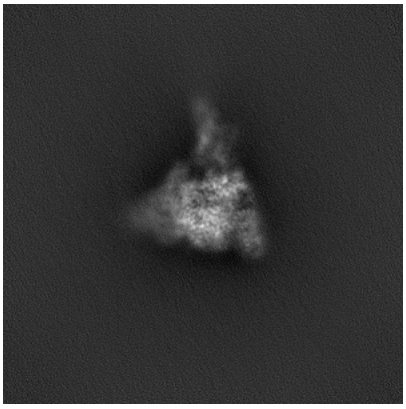
6.1.2 Raw map



X



Y

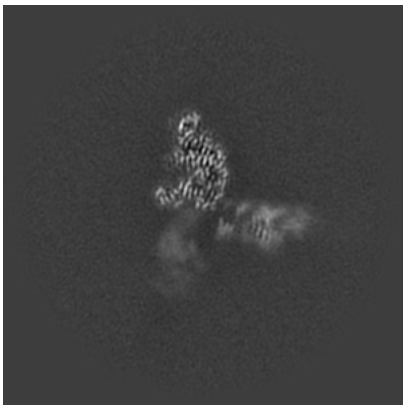


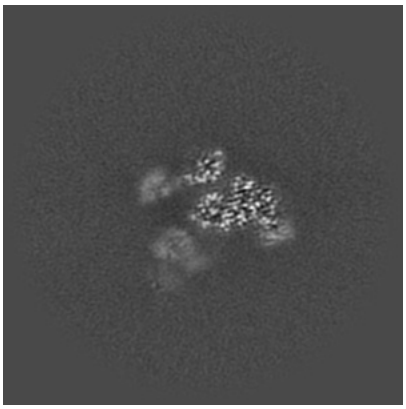
Z

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

6.2 Central slices (i)

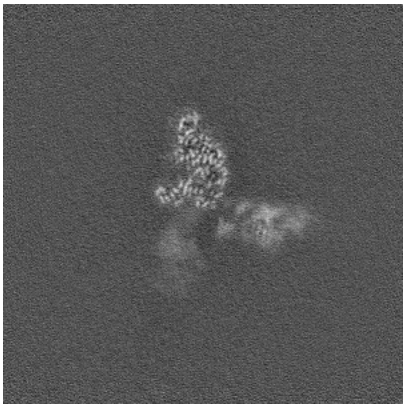
6.2.1 Primary map

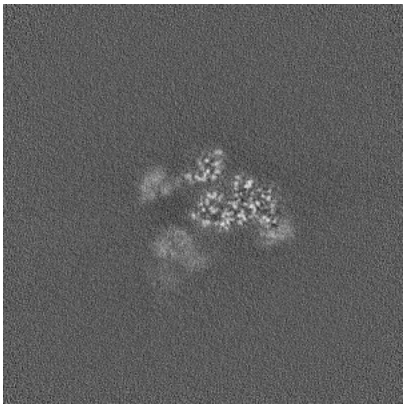

X Index: 224

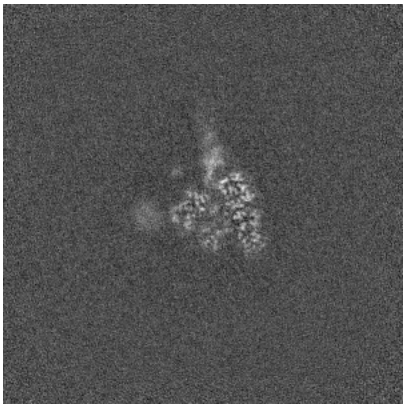

Y Index: 224

Z Index: 224

6.2.2 Raw map


X Index: 224

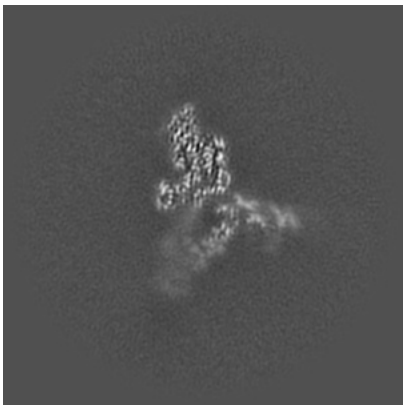

Y Index: 224

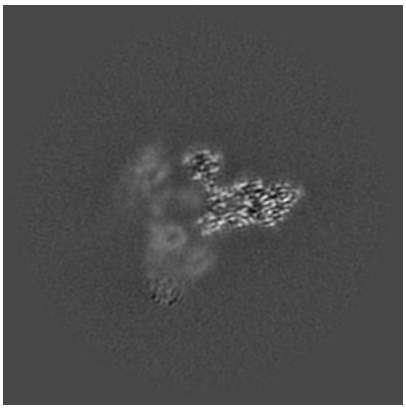

Z Index: 224

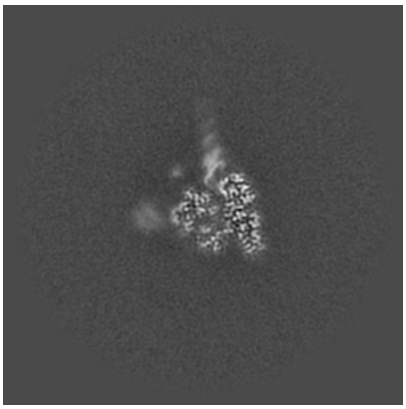
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

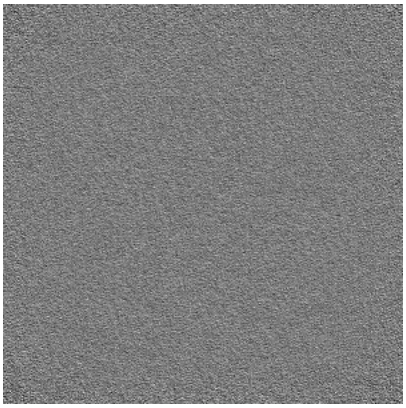
6.3.1 Primary map

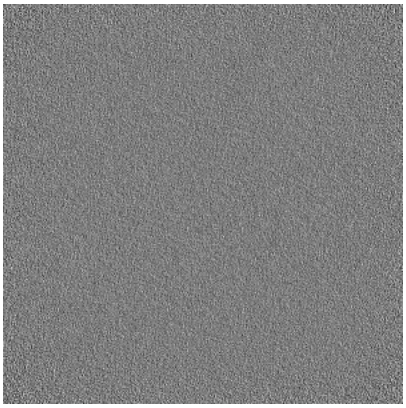

X Index: 236


Y Index: 206


Z Index: 225

6.3.2 Raw map


X Index: 0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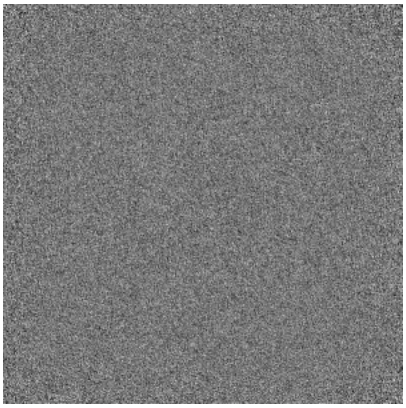
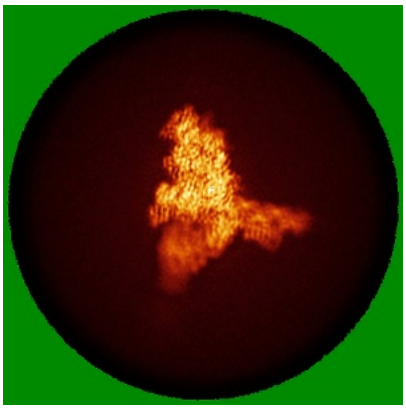
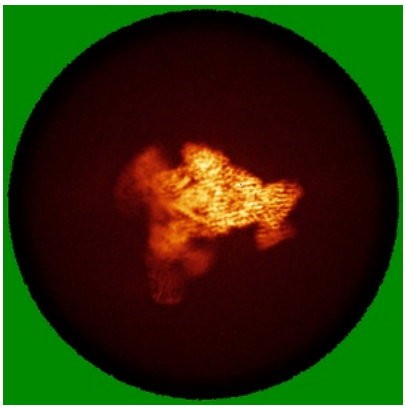

Z Index: 0

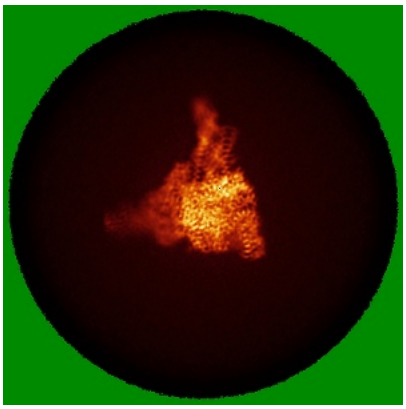
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

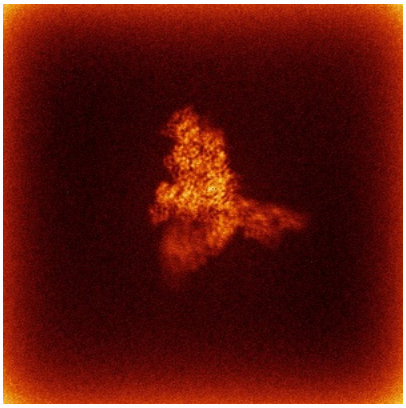
6.4.1 Primary map

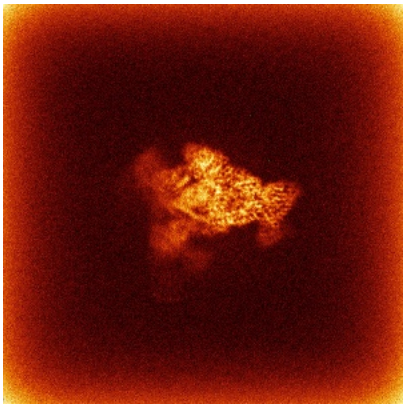

X

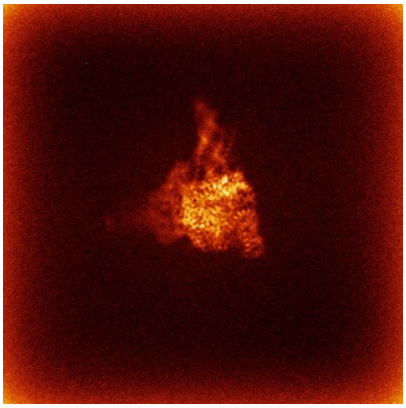

Y


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.

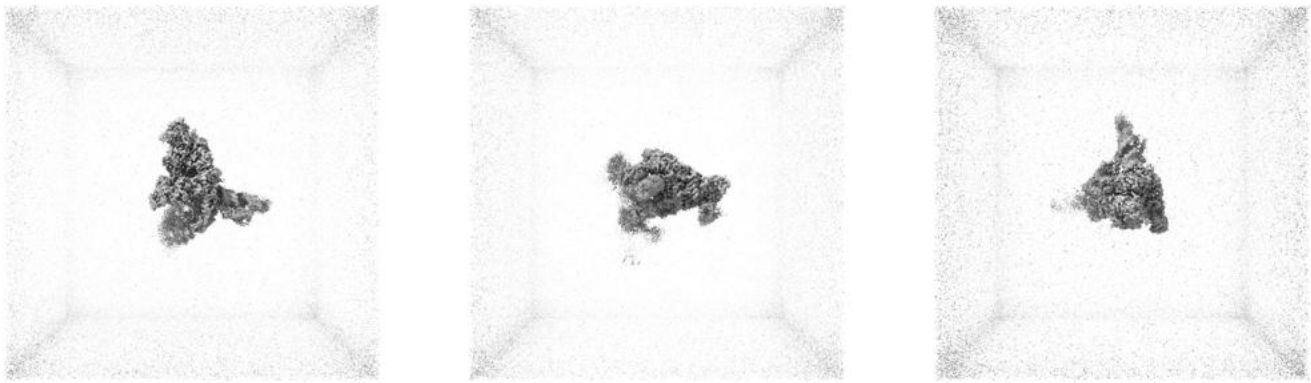
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

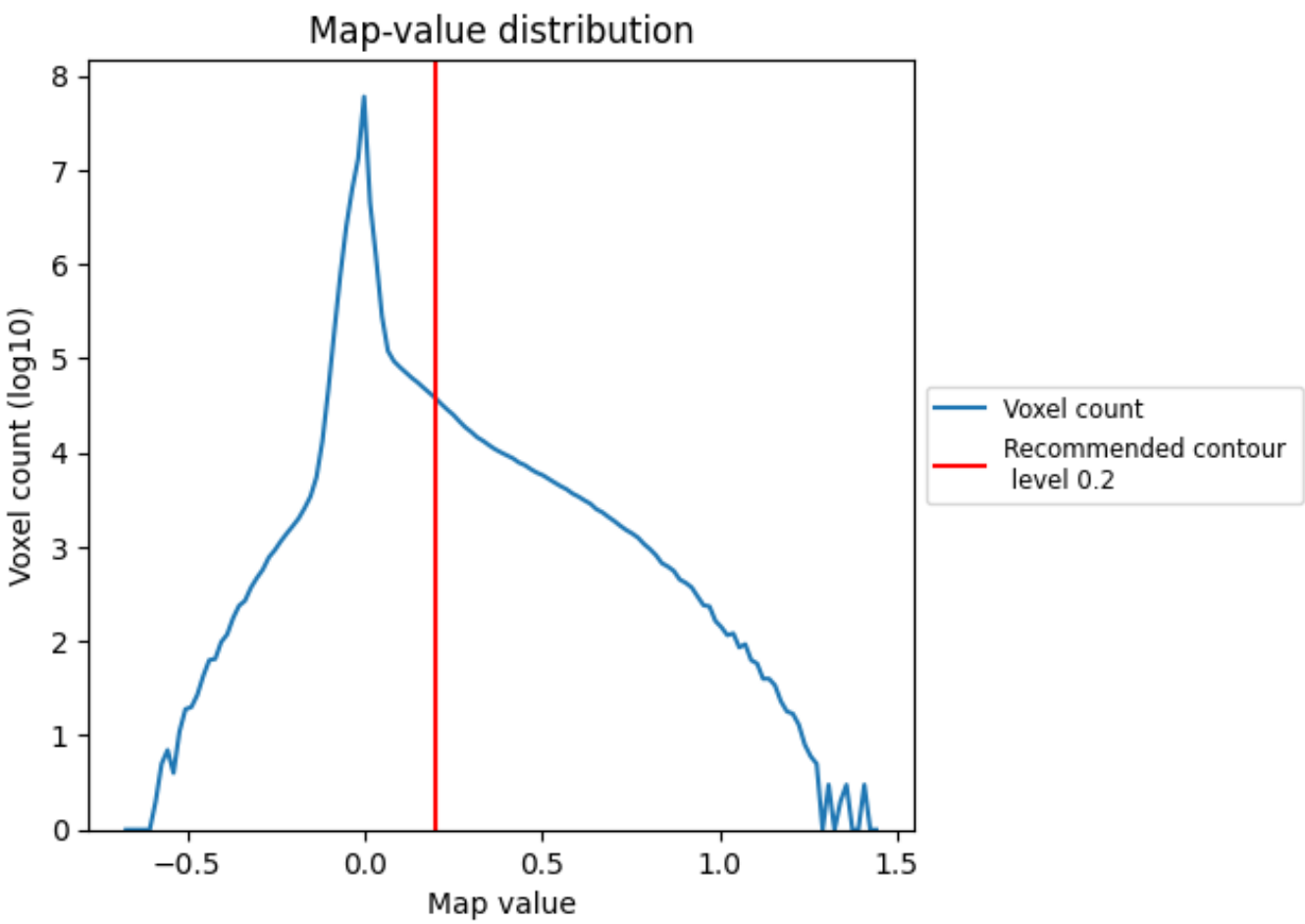
6.6 Mask visualisation (i)

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

7 Map analysis (i)

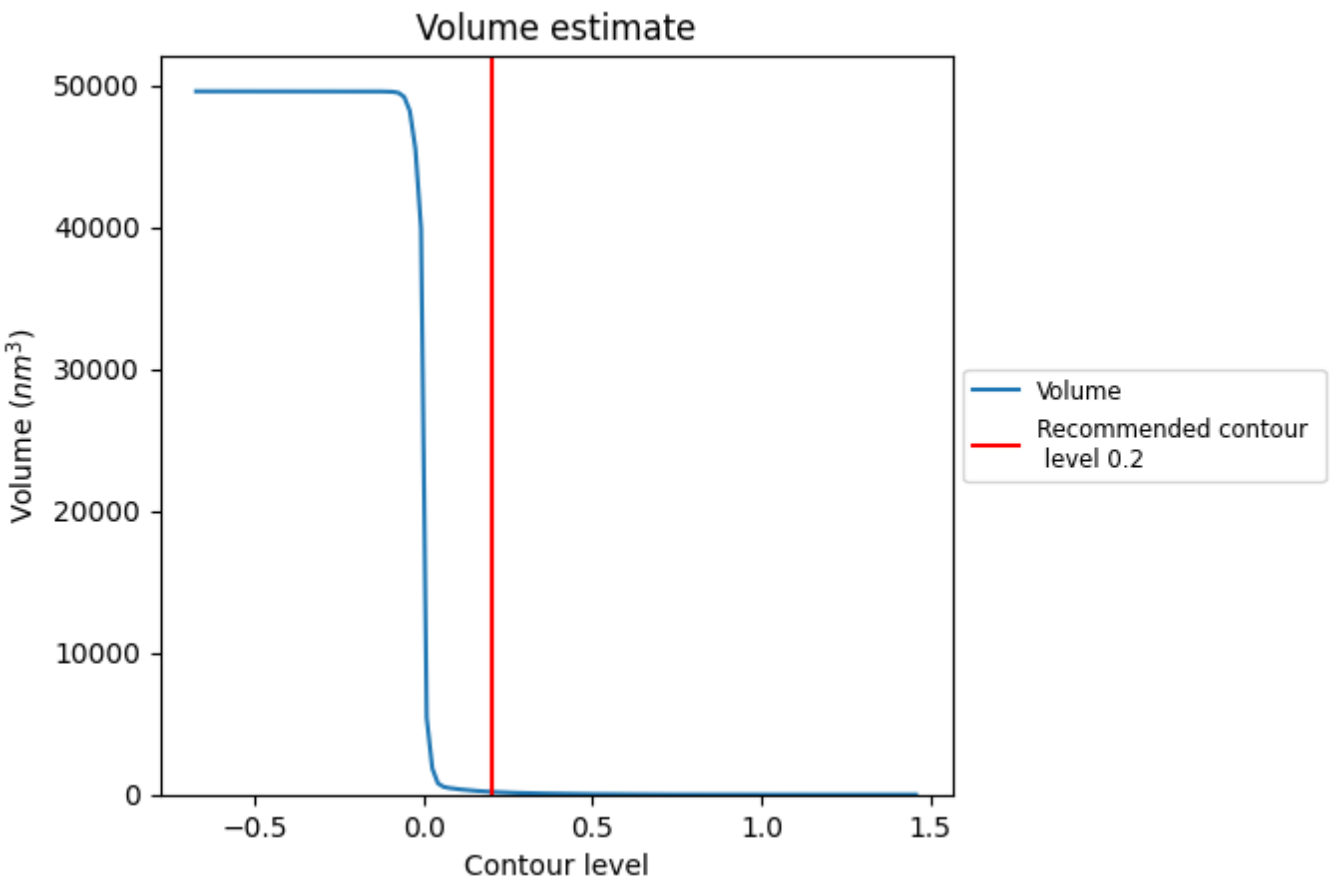
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

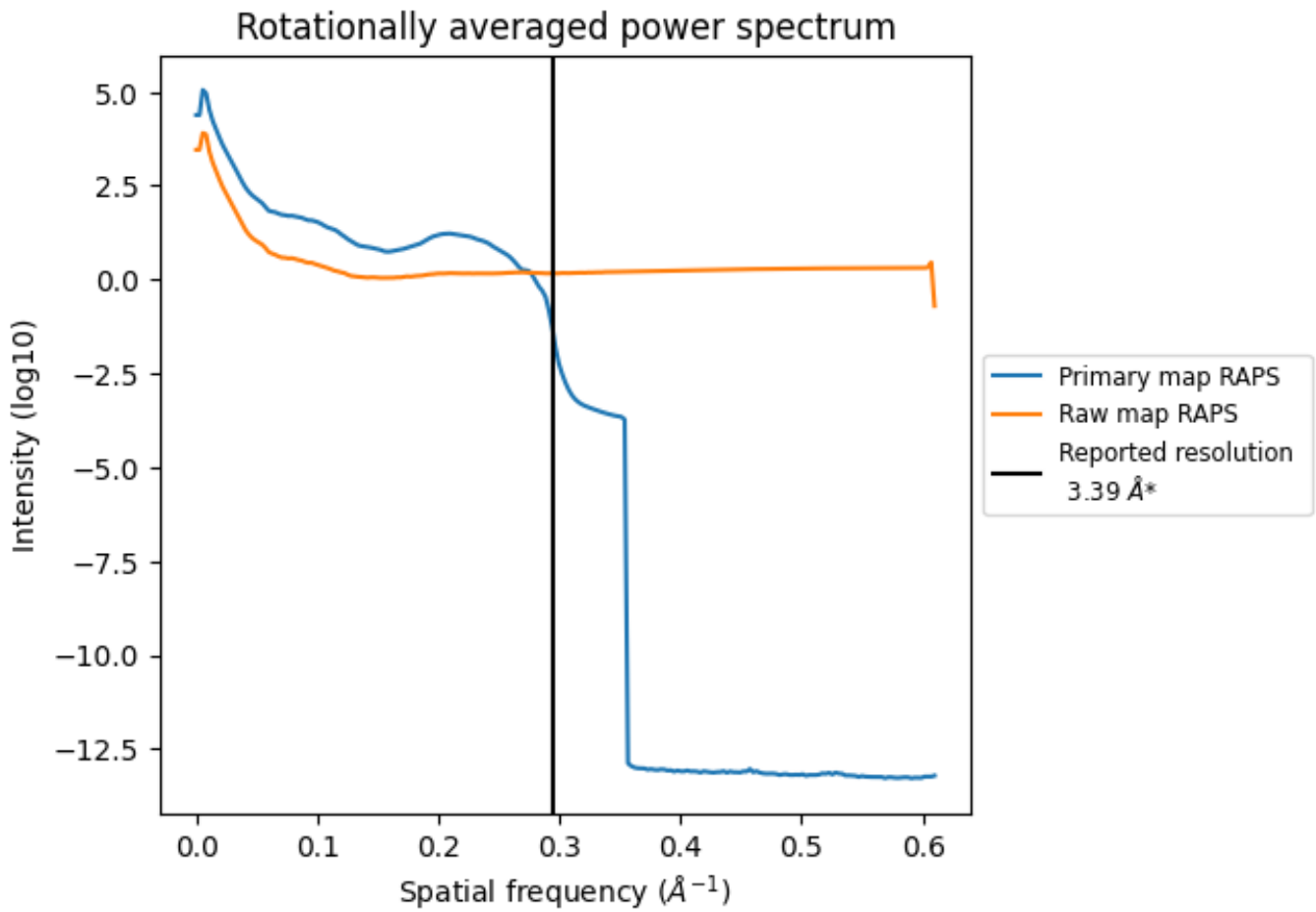
7.2 Volume estimate (i)



The volume at the recommended contour level is 192 nm^3; this corresponds to an approximate mass of 173 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)

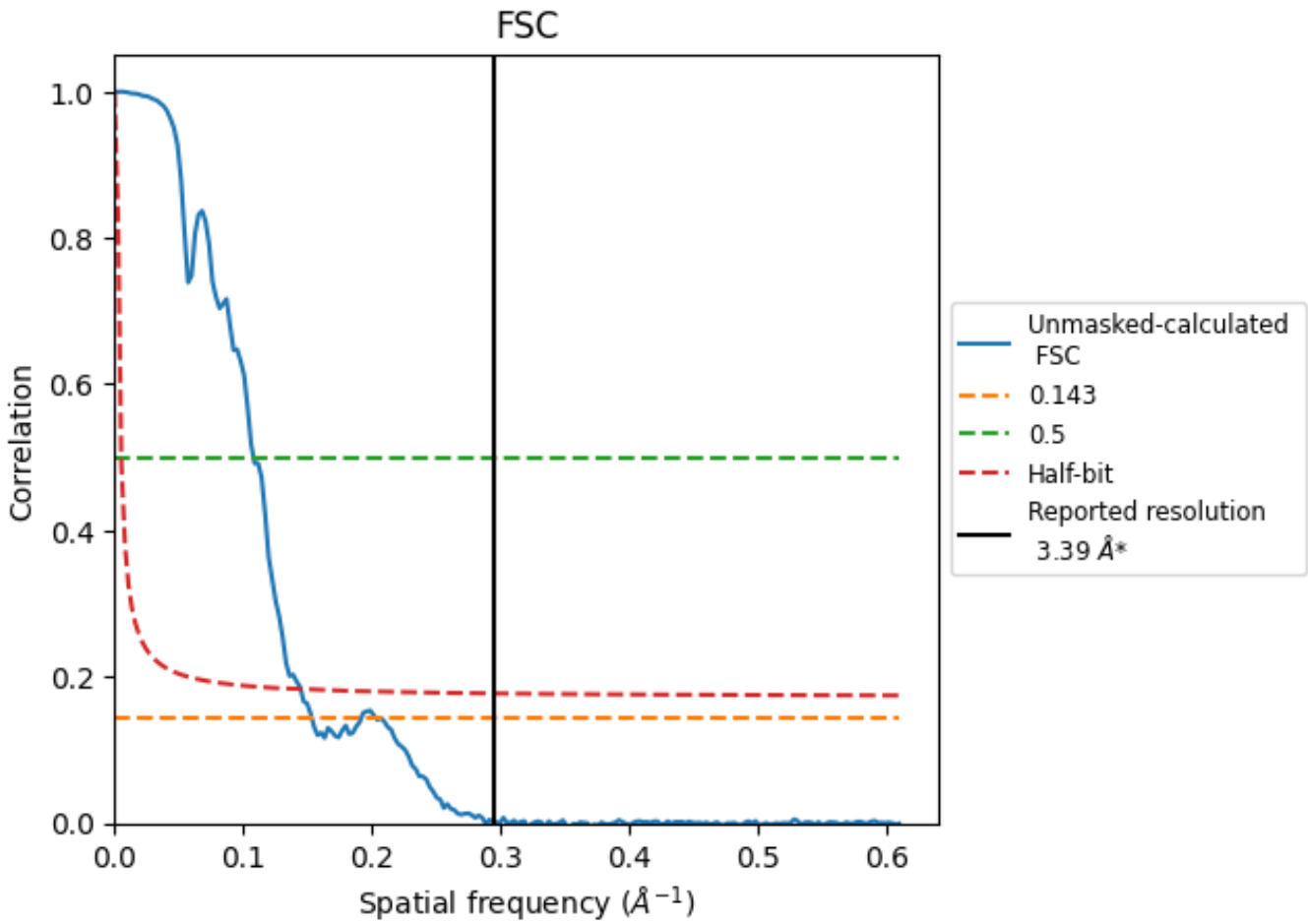


*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

8.2 Resolution estimates (i)

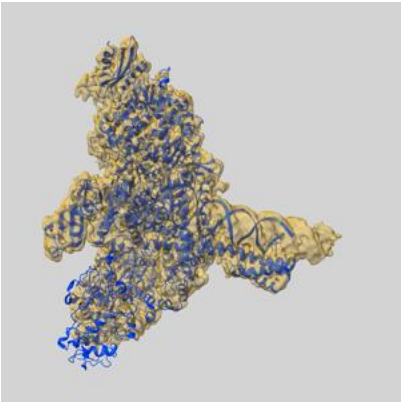
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.52	9.26	6.91

*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 6.52 differs from the reported value 3.39 by more than 10 %

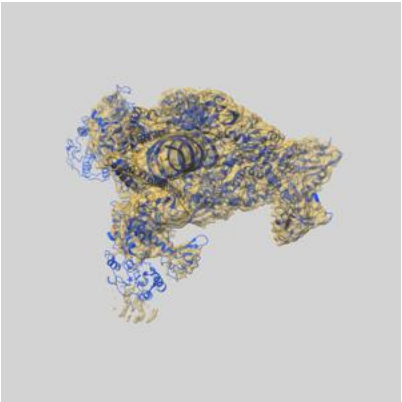
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34311 and PDB model 8GWF. Per-residue inclusion information can be found in section 3 on page 7.

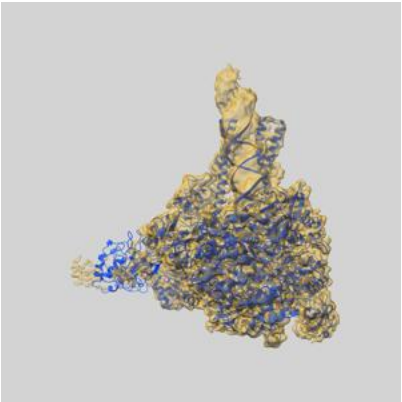
9.1 Map-model overlay (i)



X



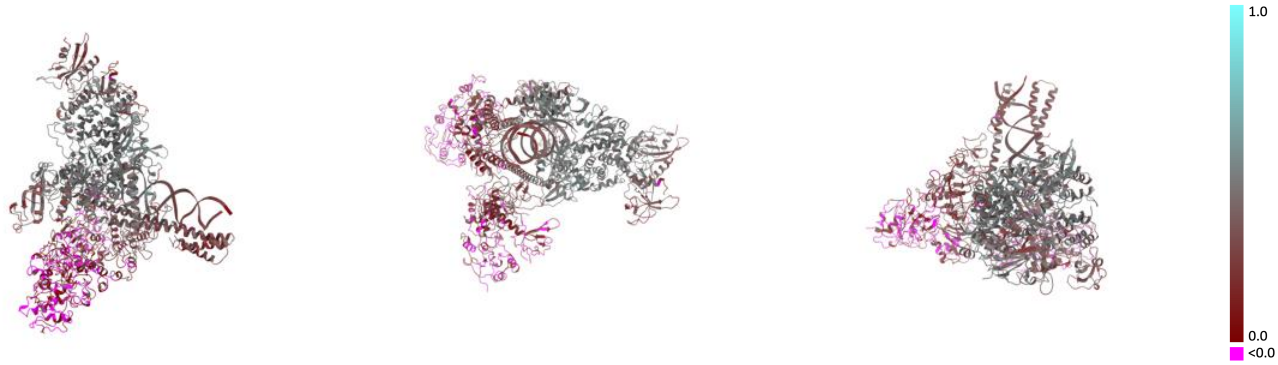
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

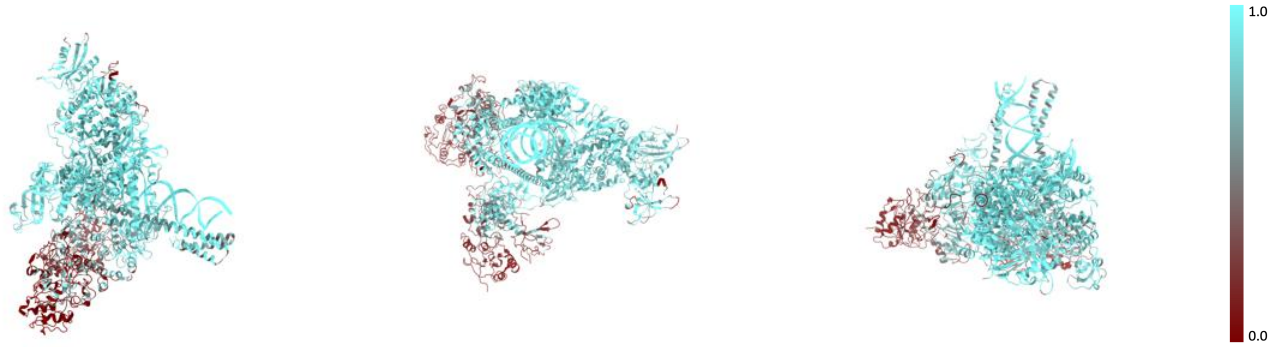
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

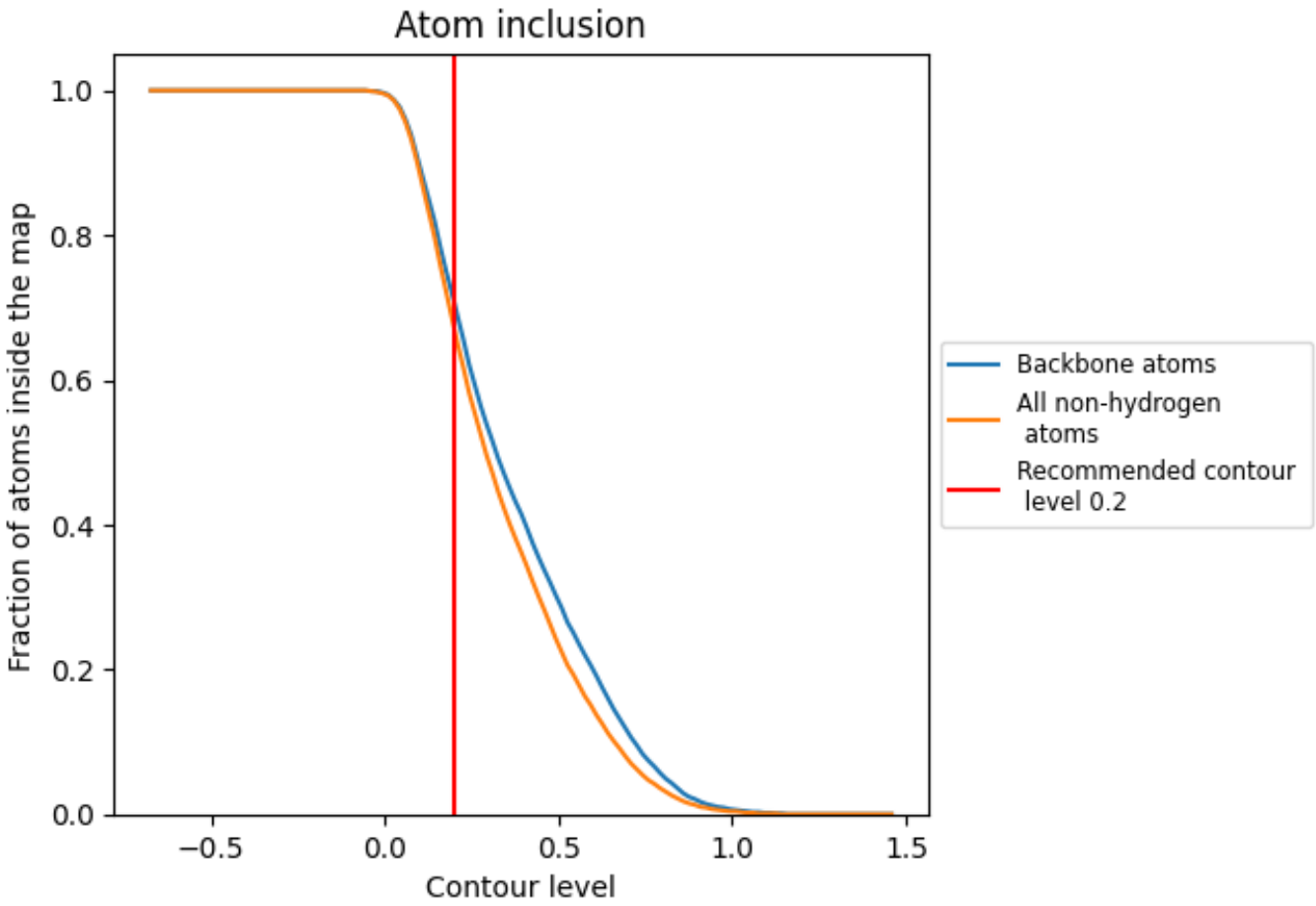
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6700	0.2900
A	0.9160	0.4570
B	0.8640	0.3850
C	0.8340	0.4040
D	0.8320	0.3520
E	0.4020	0.1200
F	0.3190	0.0980
G	0.6910	0.2750
I	0.9930	0.3430
J	0.9820	0.4030