



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:47 PM UTC

PDB ID : 8GWE / pdb_00008gwe
EMDB ID : EMD-34310
Title : SARS-CoV-2 E-RTC complex with RNA-nsp9 and GMPPNP
Authors : Yan, L.M.; Rao, Z.H.; Lou, Z.Y.
Deposited on : 2022-09-16
Resolution : 2.66 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

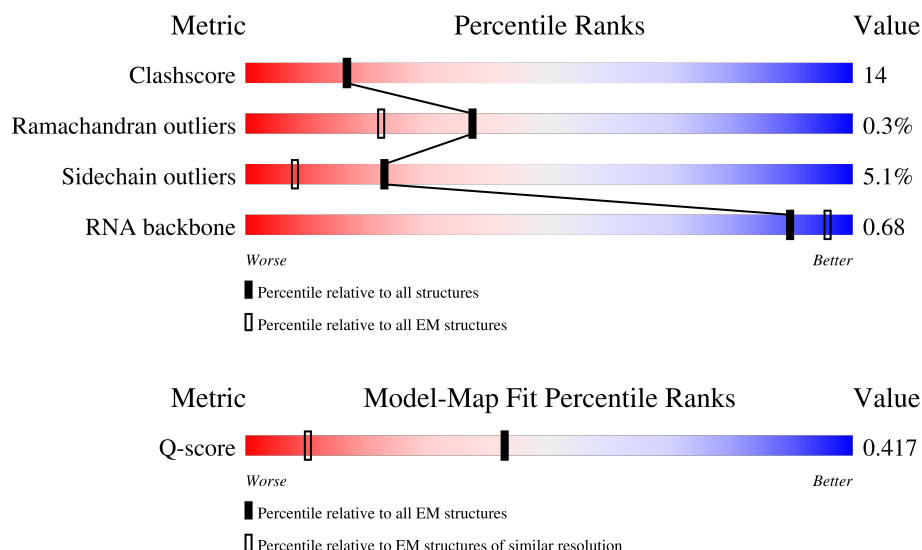
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9119 (2.16 - 3.16)

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	932	
2	B	198	
2	D	198	

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Mol	Chain	Length	Quality of chain
3	C	78	76% 24%
4	E	593	11% 58% 39% ..
4	F	593	19% 53% 44% ..
5	G	113	42% 42% 11% .
6	H	4	25% 25% 50%
7	I	25	52% 36% 12%
8	J	27	37% 63%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22069 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
1	A	931	Total	C	N	O	S	0	0
			7496	4787	1257	1398	54		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	190	Total	C	N	O	S	0	0
			1417	884	244	278	11		
2	D	187	Total	C	N	O	S	0	0
			1426	896	245	274	11		

- Molecule 3 is a protein called Replicase polyprotein 1a.

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

- Molecule 4 is a protein called Helicase nsp13.

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

- Molecule 5 is a protein called Non-structural protein 9.

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

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*UP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	4	Total	C	N	O	P	0	0
			84	38	14	28	4		

- Molecule 7 is a RNA chain called primer.

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

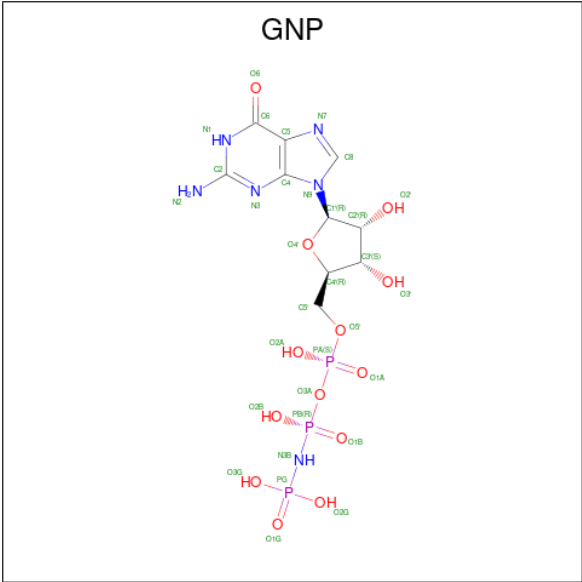
- Molecule 8 is a RNA chain called template.

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

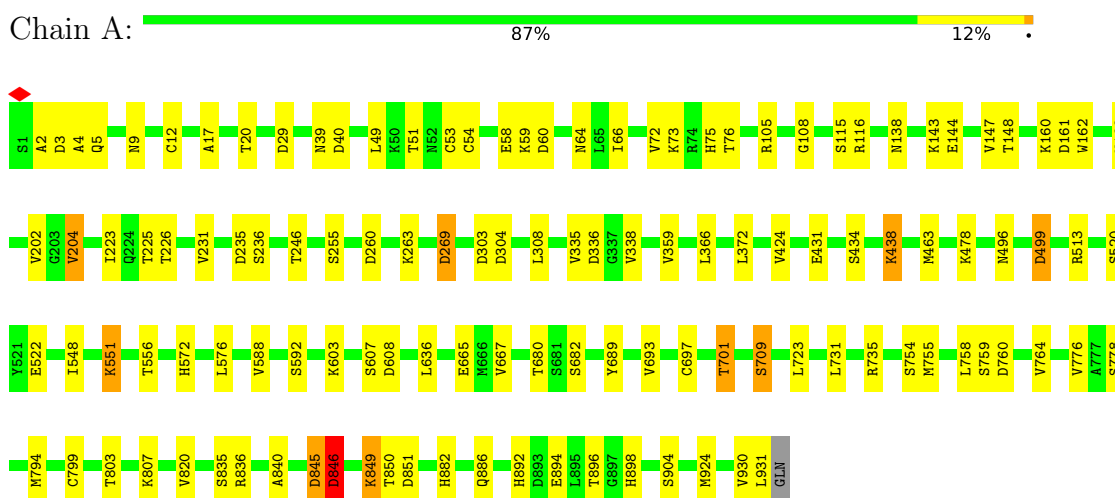
- Molecule 12 is water.

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

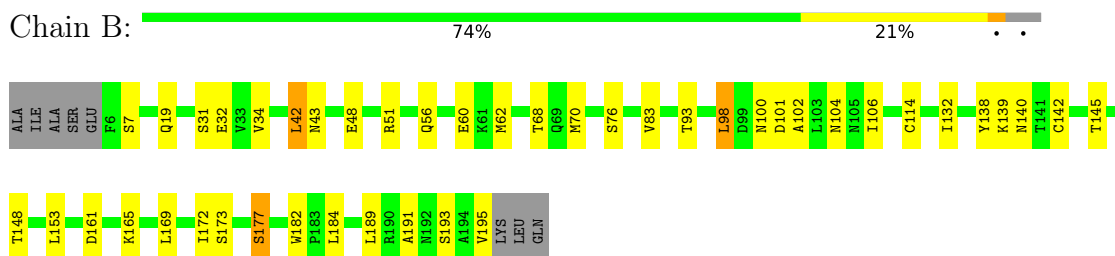
3 Residue-property plots

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

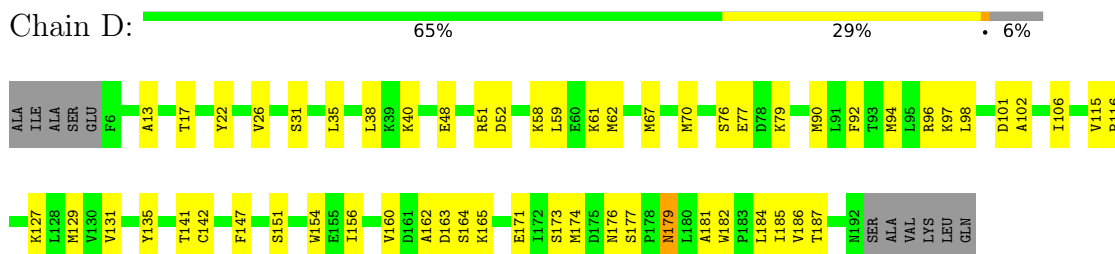
• Molecule 1: RNA-directed RNA polymerase



• Molecule 2: Non-structural protein 8



• Molecule 2: Non-structural protein 8



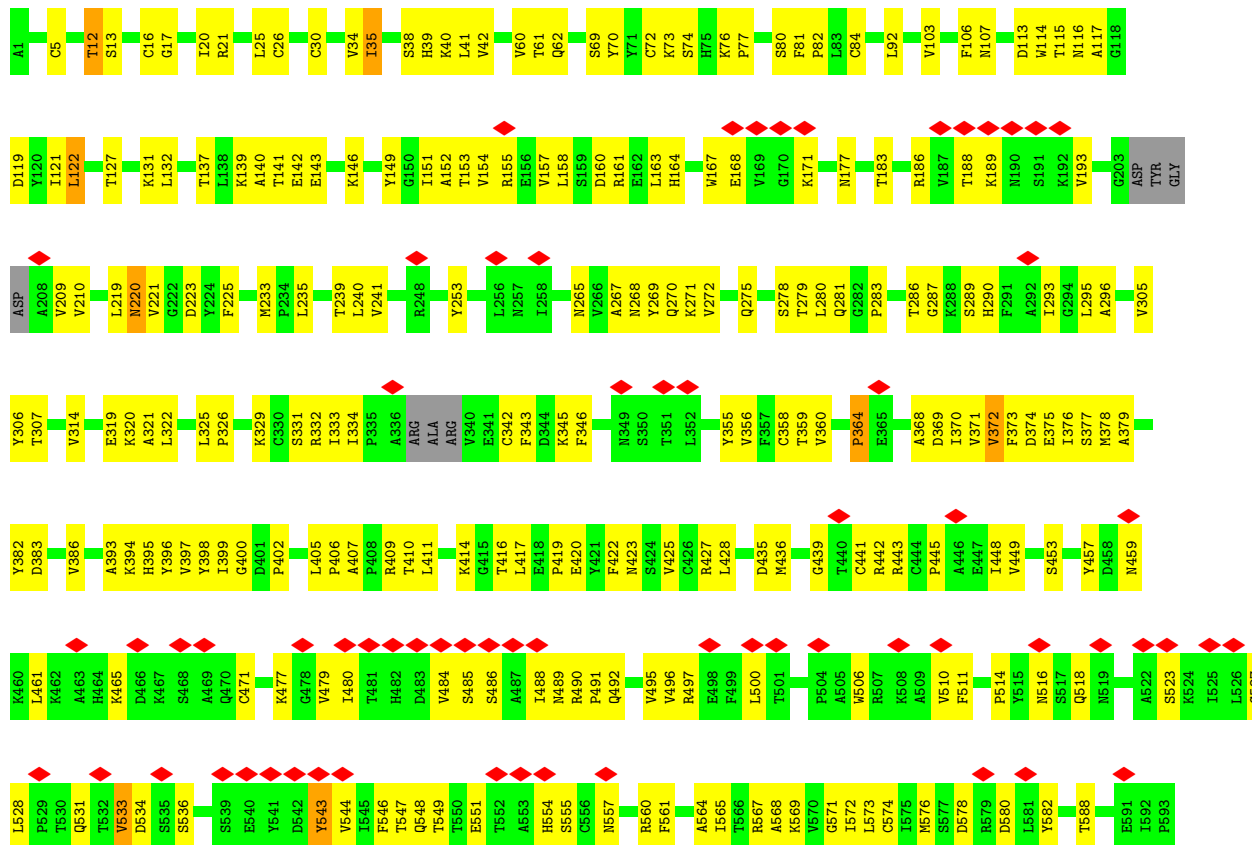
- Molecule 3: Replicase polypeptide 1a

Chain C:  76% 24%



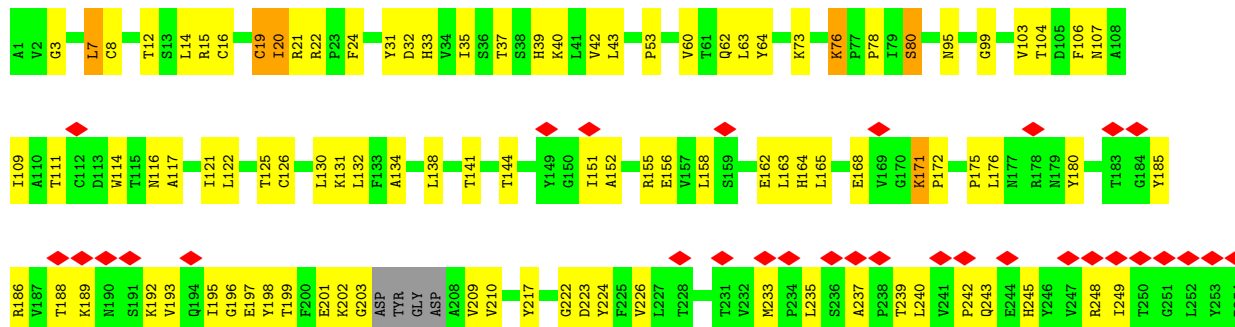
- Molecule 4: Helicase nsp13

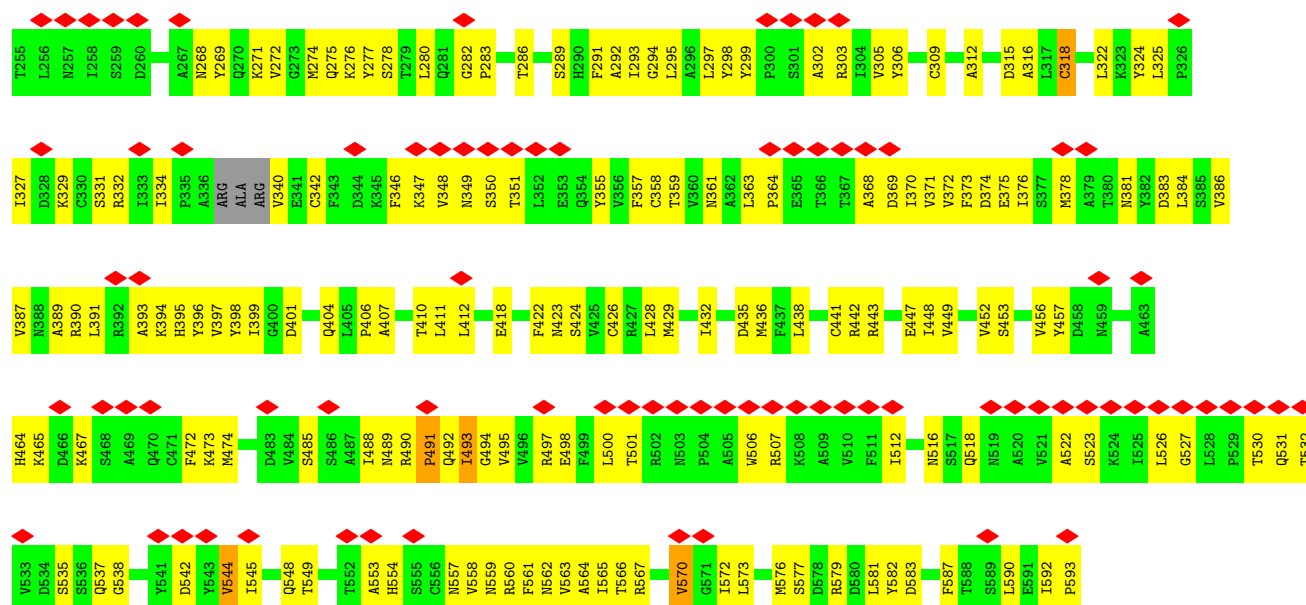
Chain E:  11% 58% 39%



- Molecule 4: Helicase nsp13

Chain F:  19% 53% 44%

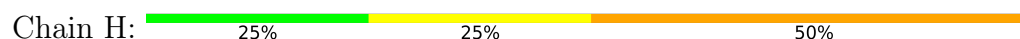




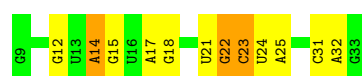
• Molecule 5: Non-structural protein 9



• Molecule 6: RNA (5'-R(P*AP*UP*UP*A)-3')



• Molecule 7: primer



• Molecule 8: template



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1351456	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 ($e^-/\text{\AA}^2$)	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	3.537	Depositor
Minimum map value	-1.547	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	430.08, 430.08, 430.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96, 0.96, 0.96	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, MG, GNP

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	0.21	0/7684	0.45	6/10427 (0.1%)
2	B	0.29	1/1435 (0.1%)	0.46	0/1951
2	D	0.19	0/1445	0.47	0/1959
3	C	0.18	0/603	0.53	0/812
4	E	0.24	2/4615 (0.0%)	0.56	3/6290 (0.0%)
4	F	0.54	4/4615 (0.1%)	0.69	4/6290 (0.1%)
5	G	0.81	4/884 (0.5%)	1.24	16/1200 (1.3%)
6	H	0.98	2/93 (2.2%)	1.30	3/142 (2.1%)
7	I	0.10	0/611	0.23	0/953
8	J	0.10	0/628	0.20	0/974
All	All	0.35	13/22613 (0.1%)	0.58	32/30998 (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
4	F	0	1
5	G	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	491	PRO	CG-CD	-31.08	0.45	1.50
4	F	491	PRO	N-CD	11.24	1.63	1.47
5	G	2	ASN	CA-C	-7.46	1.44	1.53
4	E	364	PRO	CG-CD	-7.00	1.26	1.50
4	E	364	PRO	N-CD	6.86	1.57	1.47
5	G	15	ALA	N-CA	6.68	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1	A	O3'-P	6.67	1.71	1.61
4	F	491	PRO	N-CA	-6.44	1.39	1.47
6	H	1	A	P-OP2	6.38	1.61	1.49
5	G	14	CYS	N-CA	6.23	1.54	1.46
4	F	491	PRO	CB-CG	5.83	1.78	1.49
5	G	4	LEU	CA-C	-5.52	1.47	1.53
2	B	191	ALA	CA-C	-5.16	1.46	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	491	PRO	N-CD-CG	-22.68	69.17	103.20
4	E	364	PRO	CA-N-CD	-15.74	89.97	112.00
4	F	491	PRO	CA-N-CD	-15.22	90.69	112.00
5	G	32	TYR	N-CA-C	13.10	138.71	110.80
4	F	491	PRO	CA-CB-CG	-12.57	80.62	104.50
1	A	850	THR	CA-C-N	12.23	142.69	122.76
1	A	850	THR	C-N-CA	12.23	142.69	122.76
5	G	31	TYR	N-CA-C	10.76	126.41	110.48
5	G	14	CYS	N-CA-C	9.91	131.91	110.80
5	G	15	ALA	N-CA-C	9.53	123.08	107.73
1	A	845	ASP	N-CA-C	-9.51	95.62	110.36
4	E	364	PRO	N-CD-CG	-9.49	88.97	103.20
6	H	1	A	O3'-P-O5'	9.18	117.77	104.00
4	F	491	PRO	N-CA-CB	-9.02	93.78	103.25
5	G	33	ASN	N-CA-C	8.30	128.49	110.80
5	G	11	GLN	N-CA-C	8.16	128.17	110.80
5	G	1	ASN	O-C-N	-7.81	110.51	123.00
6	H	1	A	OP2-P-O3'	-7.72	84.85	108.00
5	G	10	ARG	N-CA-C	7.67	122.27	108.69
5	G	29	LEU	N-CA-C	-7.67	94.35	108.24
5	G	16	ALA	N-CA-C	7.54	120.03	108.42
5	G	1	ASN	N-CA-C	6.90	130.32	111.00
1	A	846	ASP	N-CA-C	6.31	124.24	110.80
5	G	13	SER	N-CA-C	6.11	118.14	108.79
5	G	1	ASN	CB-CA-C	-6.04	98.62	110.10
4	E	364	PRO	CA-CB-CG	-5.94	93.22	104.50
5	G	4	LEU	CA-C-O	-5.61	114.99	122.51
6	H	1	A	P-O3'-C3'	5.54	128.50	120.20
5	G	14	CYS	CA-C-O	-5.22	113.05	120.51
1	A	849	LYS	CA-C-N	5.18	130.90	122.67
1	A	849	LYS	C-N-CA	5.18	130.90	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	13	SER	CA-C-O	-5.07	115.81	121.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	76	LYS	Peptide
5	G	1	ASN	Mainchain

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	7496	0	7238	73	0
2	B	1417	0	1388	25	0
2	D	1426	0	1433	41	0
3	C	600	0	629	16	0
4	E	4513	0	4431	174	0
4	F	4513	0	4431	218	0
5	G	868	0	877	45	0
6	H	84	0	43	5	0
7	I	545	0	272	12	0
8	J	565	0	291	23	0
9	A	2	0	0	0	0
9	E	3	0	0	0	0
9	F	3	0	0	0	0
10	A	32	0	13	1	0
11	A	1	0	0	0	0
12	A	1	0	0	0	0
All	All	22069	0	21046	603	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 14.

All (603) 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)
4:F:371:VAL:HB	4:F:396:TYR:HA	1.53	0.90
1:A:39:ASN:HD21	6:H:1:A:H61	1.23	0.87
4:F:233:MET:H	4:F:233:MET:HE2	1.44	0.83
4:F:202:LYS:HB3	4:F:210:VAL:HB	1.61	0.82
5:G:53:TRP:HE1	5:G:66:TYR:HB3	1.44	0.81
4:E:278:SER:HB2	4:E:397:VAL:HG12	1.65	0.79
4:E:443:ARG:HH12	4:E:445:PRO:HD3	1.47	0.79
1:A:846:ASP:OD1	1:A:849:LYS:CD	2.30	0.79
1:A:39:ASN:HD21	6:H:1:A:N6	1.81	0.78
4:E:548:GLN:HE22	4:E:551:GLU:HG2	1.49	0.77
5:G:77:THR:HG21	5:G:86:LYS:NZ	2.00	0.77
1:A:846:ASP:OD1	1:A:849:LYS:HD2	1.85	0.77
4:E:287:GLY:H	4:E:442:ARG:HD2	1.50	0.77
4:E:143:GLU:HA	4:E:146:LYS:HE3	1.67	0.76
2:D:173:SER:O	2:D:177:SER:OG	2.04	0.74
4:E:364:PRO:HD2	4:E:364:PRO:O	1.86	0.74
2:D:174:MET:H	2:D:174:MET:HE2	1.51	0.74
2:D:176:ASN:O	2:D:176:ASN:ND2	2.21	0.73
4:F:363:LEU:HD12	4:F:364:PRO:HD2	1.71	0.73
1:A:5:GLN:O	1:A:9:ASN:ND2	2.22	0.73
4:E:154:VAL:HB	4:E:223:ASP:HB3	1.71	0.72
4:E:306:TYR:HA	4:E:372:VAL:HG22	1.71	0.72
5:G:77:THR:HG21	5:G:86:LYS:HZ2	1.55	0.72
4:F:447:GLU:HB3	4:F:467:LYS:HD3	1.70	0.71
4:E:555:SER:HB2	4:E:560:ARG:HD3	1.70	0.71
4:E:326:PRO:HB2	4:E:329:LYS:HG3	1.73	0.70
4:F:390:ARG:HB3	4:F:391:LEU:HD23	1.73	0.70
4:E:253:TYR:OH	4:F:155:ARG:NH2	2.24	0.70
5:G:16:ALA:HA	5:G:54:ALA:HA	1.74	0.70
4:F:195:ILE:HD11	4:F:223:ASP:HB3	1.73	0.69
5:G:27:ASN:N	5:G:27:ASN:OD1	2.25	0.69
4:F:12:THR:HG22	4:F:14:LEU:H	1.56	0.69
4:E:371:VAL:HB	4:E:396:TYR:HB3	1.75	0.69
4:F:363:LEU:HD23	4:F:390:ARG:HH11	1.57	0.69
4:F:448:ILE:HG21	4:F:566:THR:HA	1.74	0.69
4:F:280:LEU:HD21	4:F:436:MET:HB2	1.73	0.69
4:E:546:PHE:HB3	4:E:574:CYS:HA	1.74	0.68
7:I:12:G:N1	8:J:48:C:N3	2.29	0.68
4:F:410:THR:HG23	4:F:411:LEU:H	1.59	0.68
2:B:43:ASN:ND2	8:J:47:A:O3'	2.26	0.68
4:F:278:SER:O	4:F:398:TYR:N	2.27	0.68
2:B:100:ASN:O	2:B:104:ASN:ND2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:HG21	5:G:75:PHE:HB3	1.75	0.67
4:E:239:THR:HG23	4:E:240:LEU:HD23	1.76	0.67
7:I:12:G:N2	8:J:48:C:O2	2.15	0.67
1:A:930:VAL:HG13	1:A:931:LEU:HD12	1.76	0.67
4:E:453:SER:HA	4:E:457:TYR:HB2	1.77	0.66
1:A:9:ASN:HA	1:A:12:CYS:HB2	1.78	0.66
4:F:33:HIS:HE1	4:F:39:HIS:CG	2.13	0.66
4:F:131:LYS:NZ	4:F:423:ASN:O	2.29	0.66
4:E:114:TRP:HB3	4:E:411:LEU:HD11	1.77	0.66
4:E:77:PRO:O	4:E:80:SER:OG	2.14	0.65
4:E:151:ILE:H	4:E:168:GLU:HG2	1.61	0.65
4:E:480:ILE:HD13	4:E:551:GLU:HG3	1.77	0.65
4:F:132:LEU:HD22	4:F:235:LEU:HD11	1.79	0.65
5:G:68:GLU:HG2	5:G:92:LYS:HD2	1.78	0.65
4:E:73:LYS:HA	4:E:76:LYS:HE3	1.79	0.65
4:E:305:VAL:HB	4:E:371:VAL:HG13	1.78	0.65
4:E:286:THR:HG22	4:E:441:CYS:HA	1.78	0.65
4:F:422:PHE:HB2	4:F:426:CYS:HB2	1.76	0.65
4:E:576:MET:HG3	4:E:582:TYR:HD2	1.62	0.65
4:E:373:PHE:O	4:E:399:ILE:N	2.29	0.64
4:E:484:VAL:HG22	4:E:485:SER:H	1.61	0.64
4:F:558:VAL:HG22	4:F:559:ASN:H	1.62	0.64
2:B:101:ASP:OD1	2:B:102:ALA:N	2.30	0.64
4:E:132:LEU:HG	4:E:235:LEU:HD22	1.78	0.64
4:F:248:ARG:HD2	4:F:249:ILE:H	1.62	0.64
4:F:233:MET:HE2	4:F:233:MET:N	2.11	0.64
4:E:16:CYS:HB2	4:E:25:LEU:HD12	1.79	0.63
4:E:321:ALA:HA	4:E:325:LEU:HD23	1.80	0.63
4:E:510:VAL:H	4:E:544:VAL:HA	1.62	0.63
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.80	0.63
4:F:8:CYS:HB3	4:F:99:GLY:H	1.63	0.63
4:F:109:ILE:HG21	4:F:122:LEU:HD22	1.80	0.63
4:F:391:LEU:HD12	4:F:393:ALA:HB2	1.81	0.63
4:F:544:VAL:HG21	4:F:567:ARG:HG3	1.81	0.63
3:C:47:GLU:OE2	3:C:47:GLU:N	2.33	0.62
2:D:51:ARG:HG3	7:I:17:A:H4'	1.81	0.62
4:E:69:SER:OG	4:E:70:TYR:N	2.31	0.62
4:E:358:CYS:SG	4:E:359:THR:N	2.73	0.62
4:E:177:ASN:ND2	4:E:516:ASN:OD1	2.32	0.62
4:E:219:LEU:HD11	4:E:225:PHE:HE2	1.65	0.62
4:E:523:SER:HA	4:E:527:GLY:HA2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD13	5:G:104:GLY:HA2	1.82	0.62
4:F:103:VAL:O	4:F:107:ASN:ND2	2.32	0.62
4:F:561:PHE:HB2	4:F:564:ALA:HB3	1.80	0.62
4:E:471:CYS:O	4:E:588:THR:OG1	2.17	0.61
4:F:381:ASN:OD1	4:F:424:SER:OG	2.14	0.61
4:E:407:ALA:HB3	4:E:409:ARG:HE	1.66	0.61
4:F:163:LEU:O	4:F:209:VAL:N	2.33	0.61
4:E:163:LEU:HB3	4:E:209:VAL:HB	1.82	0.61
4:E:409:ARG:HD3	4:E:417:LEU:HD13	1.81	0.61
4:E:279:THR:HG22	4:E:435:ASP:HB2	1.82	0.61
4:E:443:ARG:O	4:E:569:LYS:NZ	2.25	0.61
4:F:134:ALA:O	4:F:138:LEU:HD23	2.00	0.61
4:E:17:GLY:HA3	4:E:41:LEU:HG	1.83	0.60
4:F:277:TYR:HA	4:F:396:TYR:HB2	1.83	0.60
4:F:292:ALA:HB1	4:F:306:TYR:HE2	1.64	0.60
2:B:189:LEU:HD13	2:B:195:VAL:HG12	1.84	0.60
4:F:188:THR:HG23	4:F:189:LYS:H	1.66	0.60
8:J:38:C:H2'	8:J:39:A:H8	1.64	0.60
4:F:553:ALA:O	4:F:557:ASN:ND2	2.35	0.60
2:B:56:GLN:O	2:B:60:GLU:HG2	2.02	0.60
2:D:127:LYS:NZ	2:D:129:MET:SD	2.75	0.59
4:F:282:GLY:HA3	4:F:286:THR:HG21	1.84	0.59
5:G:31:TYR:N	5:G:43:ALA:O	2.35	0.59
3:C:56:LEU:HD23	2:D:106:ILE:HD11	1.83	0.59
4:E:564:ALA:HA	4:E:567:ARG:HG2	1.85	0.59
4:F:104:THR:HA	4:F:107:ASN:HD22	1.67	0.59
4:F:278:SER:HB2	4:F:397:VAL:HA	1.83	0.59
4:F:331:SER:HA	4:F:346:PHE:HB3	1.83	0.59
4:E:26:CYS:O	4:E:30:CYS:N	2.30	0.59
4:E:322:LEU:HD12	4:E:345:LYS:HB3	1.85	0.58
2:D:174:MET:H	2:D:174:MET:CE	2.16	0.58
4:E:157:VAL:HG21	4:E:219:LEU:HB3	1.86	0.58
4:F:168:GLU:OE2	4:F:168:GLU:N	2.37	0.58
4:E:153:THR:HG23	4:E:155:ARG:HH21	1.67	0.57
4:F:512:ILE:HG13	4:F:531:GLN:HB3	1.84	0.57
4:F:37:THR:HG21	4:F:111:THR:HG21	1.85	0.57
4:F:155:ARG:H	4:F:155:ARG:HD3	1.69	0.57
4:F:371:VAL:O	4:F:397:VAL:N	2.37	0.57
5:G:23:CYS:O	5:G:55:ARG:NH2	2.34	0.57
2:B:132:ILE:HG21	2:B:138:TYR:HB2	1.87	0.57
4:E:290:HIS:CD2	4:E:442:ARG:HH22	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:TRP:O	2:D:184:LEU:N	2.38	0.57
4:E:149:TYR:HA	4:E:171:LYS:HD2	1.86	0.57
4:F:456:VAL:HG21	4:F:559:ASN:ND2	2.20	0.57
2:D:171:GLU:OE1	2:D:176:ASN:ND2	2.37	0.57
5:G:84:LYS:HD3	5:G:86:LYS:NZ	2.19	0.57
4:F:155:ARG:HG2	4:F:156:GLU:OE1	2.03	0.57
4:E:342:CYS:SG	4:E:343:PHE:N	2.78	0.57
4:F:401:ASP:HB3	4:F:404:GLN:HB2	1.86	0.56
4:F:464:HIS:HB3	4:F:465:LYS:HZ2	1.69	0.56
4:F:332:ARG:NH1	4:F:346:PHE:H	2.02	0.56
4:F:358:CYS:SG	4:F:359:THR:N	2.79	0.56
4:F:488:ILE:HG23	4:F:490:ARG:HH12	1.71	0.56
4:F:563:VAL:O	4:F:566:THR:OG1	2.21	0.56
5:G:53:TRP:NE1	5:G:66:TYR:HB3	2.17	0.56
4:E:578:ASP:O	4:E:580:ASP:N	2.37	0.56
4:F:318:CYS:HB2	4:F:346:PHE:CE2	2.39	0.56
1:A:225:THR:HG22	1:A:226:THR:H	1.70	0.56
4:F:456:VAL:HG21	4:F:559:ASN:HD22	1.69	0.56
7:I:17:A:H2'	7:I:18:G:C8	2.40	0.56
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.88	0.56
2:B:19:GLN:HA	2:B:42:LEU:HD21	1.86	0.56
4:F:141:THR:HA	4:F:144:THR:HG22	1.87	0.56
5:G:16:ALA:O	5:G:23:CYS:HA	2.06	0.56
1:A:846:ASP:OD1	1:A:849:LYS:CE	2.53	0.56
2:B:161:ASP:OD2	2:B:165:LYS:NZ	2.39	0.56
4:E:20:ILE:HG23	4:E:21:ARG:HG2	1.88	0.56
4:F:325:LEU:HB2	4:F:329:LYS:HE2	1.88	0.56
2:B:169:LEU:HA	2:B:172:ILE:HD12	1.87	0.56
4:F:248:ARG:HD2	4:F:249:ILE:HD12	1.87	0.56
1:A:846:ASP:OD1	1:A:849:LYS:HE3	2.06	0.56
1:A:894:GLU:O	1:A:898:HIS:HB3	2.06	0.56
4:E:114:TRP:HE3	4:E:119:ASP:HB3	1.71	0.56
7:I:22:G:O2'	7:I:23:C:OP1	2.23	0.56
4:E:34:VAL:O	4:E:40:LYS:NZ	2.35	0.56
4:E:283:PRO:HB2	4:E:286:THR:HG21	1.88	0.56
5:G:48:LEU:HB2	5:G:51:LEU:HD11	1.87	0.56
4:E:278:SER:N	4:E:396:TYR:O	2.37	0.55
4:E:267:ALA:O	4:E:271:LYS:HD3	2.05	0.55
4:E:332:ARG:HB2	4:E:346:PHE:HB2	1.88	0.55
4:F:305:VAL:HB	4:F:373:PHE:HE1	1.71	0.55
5:G:53:TRP:HE1	5:G:66:TYR:CB	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:CYS:O	1:A:701:THR:HG22	2.06	0.55
4:E:576:MET:HG3	4:E:582:TYR:CD2	2.41	0.55
2:D:48:GLU:OE2	2:D:51:ARG:NH1	2.33	0.55
4:F:489:ASN:HB2	4:F:549:THR:HG23	1.89	0.55
4:F:31:TYR:O	4:F:35:ILE:HG12	2.05	0.55
4:F:171:LYS:HG3	4:F:172:PRO:HD2	1.88	0.55
4:F:175:PRO:HB2	4:F:180:TYR:HE2	1.71	0.54
4:E:265:ASN:O	4:E:268:ASN:HB2	2.06	0.54
4:F:500:LEU:HD23	4:F:506:TRP:HB3	1.89	0.54
8:J:49:C:H2'	8:J:50:G:C8	2.42	0.54
2:D:173:SER:HB2	2:D:176:ASN:HB3	1.89	0.54
1:A:138:ASN:ND2	1:A:138:ASN:O	2.40	0.54
4:E:374:ASP:OD1	4:E:375:GLU:N	2.41	0.54
4:F:271:LYS:O	4:F:275:GLN:N	2.41	0.54
2:B:182:TRP:O	2:B:184:LEU:N	2.40	0.54
4:E:161:ARG:HA	4:E:210:VAL:HA	1.90	0.54
4:F:268:ASN:HB3	4:F:291:PHE:HZ	1.73	0.54
1:A:892:HIS:O	1:A:896:THR:HG23	2.08	0.54
4:F:523:SER:HA	4:F:527:GLY:HA2	1.89	0.54
4:F:16:CYS:SG	4:F:19:CYS:HB2	2.48	0.53
4:F:297:LEU:HB3	4:F:325:LEU:HD11	1.89	0.53
4:F:448:ILE:HD13	4:F:566:THR:HA	1.90	0.53
4:E:41:LEU:HD12	4:E:42:VAL:N	2.23	0.53
4:E:293:ILE:HG12	4:E:320:LYS:HG2	1.91	0.53
1:A:592:SER:HB3	8:J:30:C:H4'	1.90	0.53
4:F:64:TYR:HB3	4:F:80:SER:HB2	1.89	0.53
4:F:151:ILE:HD11	4:F:224:TYR:HB3	1.90	0.53
4:E:514:PRO:HD2	4:E:549:THR:HG21	1.90	0.53
3:C:14:LEU:HD22	3:C:36:HIS:CG	2.44	0.53
4:E:268:ASN:CG	4:E:436:MET:HE1	2.34	0.53
4:F:33:HIS:CE1	4:F:39:HIS:CG	2.95	0.53
8:J:38:C:H2'	8:J:39:A:C8	2.43	0.53
1:A:29:ASP:N	1:A:53:CYS:O	2.37	0.53
4:F:3:GLY:HA3	4:F:24:PHE:CE2	2.44	0.53
4:F:406:PRO:HG2	4:F:560:ARG:HD3	1.91	0.53
8:J:40:U:H2'	8:J:41:G:H8	1.73	0.53
1:A:588:VAL:HG23	1:A:758:LEU:HD12	1.90	0.52
4:F:62:GLN:OE1	4:F:62:GLN:N	2.42	0.52
4:F:299:TYR:O	4:F:355:TYR:OH	2.28	0.52
5:G:84:LYS:HD3	5:G:86:LYS:HZ2	1.72	0.52
4:E:376:ILE:HG22	4:E:400:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:239:THR:HG21	4:F:381:ASN:HB3	1.92	0.52
4:F:289:SER:OG	4:F:443:ARG:NH2	2.28	0.52
5:G:78:ASP:HB2	5:G:113:GLN:HG3	1.90	0.52
2:D:179:ASN:OD1	2:D:179:ASN:N	2.42	0.52
4:E:374:ASP:HA	4:E:399:ILE:HB	1.90	0.52
5:G:72:PRO:HB3	5:G:89:TYR:CZ	2.44	0.52
4:E:332:ARG:HE	4:E:333:ILE:H	1.56	0.52
4:E:369:ASP:OD1	4:E:370:ILE:HG12	2.09	0.52
4:E:477:LYS:O	4:E:548:GLN:NE2	2.43	0.52
4:E:489:ASN:ND2	4:E:518:GLN:OE1	2.33	0.52
4:E:114:TRP:CE3	4:E:119:ASP:HB3	2.44	0.52
4:E:453:SER:HB3	4:E:459:ASN:HA	1.91	0.52
5:G:15:ALA:HA	5:G:26:ASP:HA	1.90	0.52
4:E:425:VAL:HA	4:E:428:LEU:HB3	1.92	0.52
4:F:312:ALA:HB3	4:F:537:GLN:HB2	1.91	0.52
7:I:24:U:H2'	7:I:25:A:H8	1.73	0.52
4:E:269:TYR:CD1	4:E:295:LEU:HD13	2.45	0.52
4:F:15:ARG:HD3	4:F:22:ARG:HB3	1.91	0.52
4:E:305:VAL:HG13	4:E:356:VAL:HG23	1.91	0.52
4:F:104:THR:HA	4:F:107:ASN:HB2	1.91	0.52
2:B:43:ASN:ND2	8:J:48:C:OP1	2.41	0.51
4:E:233:MET:SD	4:E:233:MET:N	2.83	0.51
4:E:377:SER:OG	4:E:378:MET:SD	2.66	0.51
2:D:151:SER:O	2:D:151:SER:OG	2.25	0.51
1:A:39:ASN:ND2	6:H:1:A:H61	2.01	0.51
1:A:499:ASP:OD1	1:A:513:ARG:NH2	2.35	0.51
1:A:794:MET:HE3	1:A:799:CYS:SG	2.51	0.51
2:B:102:ALA:O	2:B:106:ILE:HG23	2.10	0.51
4:F:60:VAL:HA	4:F:63:LEU:HD12	1.92	0.51
4:F:185:TYR:CD1	4:F:192:LYS:HB2	2.45	0.51
4:F:197:GLU:N	4:F:217:TYR:OH	2.41	0.51
4:F:268:ASN:HB3	4:F:291:PHE:CZ	2.45	0.51
4:F:203:GLY:HA2	4:F:209:VAL:HA	1.92	0.51
4:F:347:LYS:O	4:F:350:SER:OG	2.25	0.51
4:F:378:MET:HA	4:F:407:ALA:HB2	1.92	0.51
4:E:81:PHE:HD1	4:E:82:PRO:HD2	1.76	0.51
5:G:73:CYS:SG	5:G:74:ARG:N	2.84	0.51
4:E:117:ALA:O	4:E:121:ILE:HG13	2.11	0.51
4:E:420:GLU:HB2	4:E:427:ARG:HD3	1.92	0.51
4:F:493:ILE:HD11	4:F:518:GLN:HG3	1.91	0.51
7:I:31:C:H2'	7:I:32:A:H8	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:SER:HB2	2:B:182:TRP:HZ2	1.75	0.51
4:F:7:LEU:HD11	4:F:106:PHE:CZ	2.46	0.51
4:F:369:ASP:O	4:F:394:LYS:N	2.39	0.51
4:F:370:ILE:HG23	4:F:395:HIS:HB2	1.93	0.51
4:F:32:ASP:HA	4:F:35:ILE:HG12	1.93	0.50
4:F:155:ARG:NE	4:F:156:GLU:OE2	2.44	0.50
4:F:472:PHE:HZ	4:F:474[B]:MET:HE2	1.76	0.50
1:A:73:LYS:NZ	10:A:1003:GNP:O1G	2.44	0.50
4:E:536:SER:O	4:E:536:SER:OG	2.23	0.50
1:A:303:ASP:N	1:A:303:ASP:OD1	2.43	0.50
1:A:496:ASN:N	1:A:496:ASN:OD1	2.45	0.50
4:E:305:VAL:O	4:E:372:VAL:N	2.41	0.50
4:E:383:ASP:HA	4:E:386:VAL:HG12	1.93	0.50
7:I:17:A:H2'	7:I:18:G:H8	1.77	0.50
4:F:315:ASP:HA	4:F:318:CYS:SG	2.52	0.50
4:F:472:PHE:HZ	4:F:474[A]:MET:HE2	1.76	0.50
4:F:567:ARG:HB2	4:F:572:ILE:HD11	1.93	0.50
5:G:59:SER:OG	5:G:60:ASP:N	2.42	0.50
2:D:147:PHE:N	2:D:154:TRP:O	2.38	0.50
4:F:155:ARG:HH22	4:F:164:HIS:CD2	2.29	0.50
4:F:292:ALA:HB1	4:F:306:TYR:CE2	2.45	0.50
4:F:449:VAL:HA	4:F:452:VAL:HG12	1.94	0.50
4:F:583:ASP:N	4:F:583:ASP:OD2	2.45	0.50
3:C:70:LYS:HD3	3:C:70:LYS:C	2.37	0.50
4:E:268:ASN:OD1	4:E:436:MET:HE1	2.12	0.50
4:F:579:ARG:HH12	4:F:582:TYR:HB3	1.76	0.50
4:E:290:HIS:HA	4:E:293:ILE:HD13	1.93	0.49
4:F:489:ASN:OD1	4:F:492:GLN:HG2	2.11	0.49
1:A:269:ASP:OD1	1:A:269:ASP:N	2.38	0.49
2:D:90:MET:O	2:D:94:MET:HG3	2.12	0.49
4:E:139:LYS:HD3	4:E:382:TYR:HD2	1.77	0.49
4:F:121:ILE:O	4:F:125:THR:HG23	2.12	0.49
4:F:276:LYS:O	4:F:396:TYR:N	2.44	0.49
4:F:488:ILE:HG23	4:F:490:ARG:NH1	2.26	0.49
7:I:21:U:H2'	7:I:22:G:C8	2.46	0.49
4:E:289:SER:HB3	4:E:290:HIS:CE1	2.47	0.49
4:F:592:ILE:HD12	4:F:592:ILE:O	2.12	0.49
1:A:304:ASP:HB2	1:A:636:LEU:HD13	1.94	0.49
4:E:484:VAL:HG13	4:E:486:SER:H	1.76	0.49
4:F:245:HIS:NE2	4:F:275:GLN:OE1	2.42	0.49
1:A:304:ASP:OD1	1:A:304:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:THR:O	3:C:50:GLU:HG2	2.11	0.49
4:E:139:LYS:HD3	4:E:382:TYR:CD2	2.47	0.49
4:F:268:ASN:HD21	4:F:436:MET:HB3	1.77	0.49
4:F:15:ARG:HG3	4:F:43:LEU:HB2	1.95	0.49
4:F:497:ARG:O	4:F:501:THR:HG23	2.11	0.49
5:G:98:ASN:O	5:G:102:VAL:HG13	2.13	0.49
4:F:269:TYR:HB3	4:F:298:TYR:CZ	2.48	0.49
4:F:410:THR:HG23	4:F:411:LEU:N	2.25	0.49
4:F:158:LEU:HB2	4:F:163:LEU:HA	1.95	0.49
4:F:322:LEU:HD22	4:F:327:ILE:HD13	1.94	0.49
4:F:138:LEU:HA	4:F:141:THR:HG22	1.95	0.48
4:F:275:GLN:HE21	4:F:435:ASP:HB3	1.78	0.48
5:G:79:THR:HG21	5:G:84:LYS:HD2	1.95	0.48
1:A:40:ASP:HB3	5:G:6:PRO:HG2	1.95	0.48
4:E:439:GLY:HA2	4:E:461:LEU:HB3	1.95	0.48
4:E:568:ALA:HB3	4:E:572:ILE:HG13	1.94	0.48
4:F:316:ALA:HB2	4:F:538:GLY:HA3	1.94	0.48
4:F:372:VAL:HA	4:F:397:VAL:HB	1.94	0.48
4:F:195:ILE:O	4:F:198:TYR:OH	2.28	0.48
4:E:407:ALA:O	4:E:409:ARG:N	2.47	0.48
4:F:359:THR:HG22	4:F:361:ASN:H	1.79	0.48
1:A:759:SER:O	1:A:759:SER:OG	2.25	0.48
4:E:127:THR:O	4:E:131:LYS:HG2	2.13	0.48
4:F:334:ILE:HG13	4:F:342:CYS:HB3	1.94	0.48
4:F:373:PHE:CE2	4:F:387:VAL:HB	2.48	0.48
5:G:77:THR:HG21	5:G:86:LYS:HZ3	1.78	0.48
4:F:277:TYR:OH	4:F:428:LEU:HD21	2.13	0.48
2:B:43:ASN:ND2	8:J:48:C:P	2.86	0.48
4:E:314:VAL:HG21	4:E:342:CYS:SG	2.53	0.48
4:E:533:VAL:HG11	4:E:560:ARG:HD2	1.96	0.48
4:F:243:GLN:HE22	4:F:432:ILE:HD12	1.79	0.48
4:F:334:ILE:HG23	4:F:342:CYS:HB2	1.96	0.48
8:J:40:U:H2'	8:J:41:G:C8	2.48	0.48
4:F:383:ASP:OD2	4:F:384:LEU:N	2.45	0.47
4:F:545:ILE:HA	4:F:573:LEU:HD22	1.96	0.47
5:G:76:VAL:HG22	5:G:85:VAL:HG22	1.96	0.47
1:A:12:CYS:SG	1:A:17:ALA:HB1	2.54	0.47
4:E:543:TYR:CE2	4:E:571:GLY:HA3	2.49	0.47
1:A:431:GLU:OE2	1:A:431:GLU:N	2.37	0.47
4:F:302:ALA:HA	4:F:303:ARG:NH1	2.29	0.47
1:A:851:ASP:HB2	2:D:79:LYS:HE3	1.95	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	2.48	0.47
3:C:3:MET:O	3:C:6:VAL:HG12	2.15	0.47
4:E:405:LEU:HD21	4:E:533:VAL:HG12	1.96	0.47
4:E:419:PRO:HA	4:E:422:PHE:CE2	2.49	0.47
1:A:709:SER:O	1:A:709:SER:OG	2.33	0.47
3:C:63:GLN:OE1	3:C:63:GLN:HA	2.13	0.47
4:F:278:SER:HB3	4:F:436:MET:SD	2.55	0.47
4:F:374:ASP:HA	4:F:399:ILE:HB	1.97	0.47
2:D:162:ALA:HB3	2:D:181:ALA:HB1	1.97	0.47
4:E:34:VAL:HG23	4:E:39:HIS:O	2.14	0.47
4:E:265:ASN:ND2	4:E:269:TYR:OH	2.47	0.47
4:E:492:GLN:O	4:E:496:VAL:HG23	2.14	0.47
4:F:522:ALA:HB1	4:F:526:LEU:HD21	1.97	0.47
4:E:119:ASP:O	4:E:122:LEU:HD23	2.13	0.47
4:F:7:LEU:HD11	4:F:106:PHE:HZ	1.79	0.47
4:F:239:THR:HB	4:F:384:LEU:HB3	1.97	0.47
4:F:239:THR:OG1	4:F:240:LEU:N	2.48	0.47
4:F:268:ASN:O	4:F:272:VAL:HG23	2.15	0.47
4:F:516:ASN:HD21	4:F:530:THR:HG23	1.80	0.47
1:A:160:LYS:HD3	1:A:161:ASP:H	1.80	0.47
4:F:271:LYS:HG2	4:F:436:MET:HE3	1.97	0.47
4:F:371:VAL:N	4:F:395:HIS:O	2.45	0.47
1:A:846:ASP:OD1	1:A:849:LYS:CG	2.63	0.46
2:D:58:LYS:HG3	2:D:59:LEU:N	2.31	0.46
4:E:394:LYS:HG2	4:E:395:HIS:CE1	2.49	0.46
4:F:442:ARG:HA	4:F:465:LYS:NZ	2.30	0.46
1:A:882:HIS:O	1:A:886:GLN:HG3	2.15	0.46
2:D:163:ASP:HB2	2:D:165:LYS:HD2	1.97	0.46
7:I:31:C:H2'	7:I:32:A:C8	2.50	0.46
3:C:70:LYS:HD3	3:C:70:LYS:O	2.16	0.46
2:D:31:SER:O	2:D:35:LEU:HG	2.16	0.46
4:E:359:THR:HG22	4:E:360:VAL:H	1.80	0.46
4:E:479:VAL:HB	4:E:491:PRO:HG2	1.98	0.46
1:A:51:THR:OG1	6:H:2:U:OP1	2.32	0.46
4:F:371:VAL:HG13	4:F:373:PHE:CE1	2.51	0.46
1:A:39:ASN:ND2	6:H:1:A:N6	2.56	0.46
1:A:522:GLU:OE1	1:A:522:GLU:N	2.33	0.46
4:E:332:ARG:NH2	4:E:358:CYS:HA	2.30	0.46
4:E:492:GLN:HG3	4:E:518:GLN:NE2	2.31	0.46
4:F:240:LEU:HD23	4:F:424:SER:HB3	1.98	0.46
5:G:11:GLN:O	5:G:32:TYR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:449:VAL:O	4:E:453:SER:OG	2.30	0.46
5:G:18:THR:H	5:G:22:ALA:HB3	1.81	0.46
1:A:846:ASP:OD1	1:A:849:LYS:HG3	2.16	0.46
1:A:73:LYS:HE2	1:A:116:ARG:HH12	1.81	0.46
1:A:2:ALA:O	1:A:4:ALA:N	2.49	0.45
2:D:97:LYS:HB3	2:D:97:LYS:HE2	1.77	0.45
2:D:101:ASP:OD2	2:D:102:ALA:N	2.48	0.45
4:F:488:ILE:HD12	4:F:489:ASN:H	1.80	0.45
8:J:31:U:H2'	8:J:32:C:H6	1.80	0.45
2:B:62:MET:HE2	2:B:62:MET:HB3	1.85	0.45
2:D:160:VAL:HG13	2:D:164:SER:HA	1.97	0.45
4:E:116:ASN:N	4:E:119:ASP:OD2	2.48	0.45
4:E:492:GLN:HA	4:E:495:VAL:HB	1.98	0.45
4:E:544:VAL:N	4:E:568:ALA:HB2	2.30	0.45
1:A:603:LYS:HD2	1:A:603:LYS:HA	1.64	0.45
4:E:188:THR:HG23	4:E:189:LYS:H	1.81	0.45
4:E:368:ALA:O	4:E:393:ALA:HA	2.16	0.45
4:E:271:LYS:HE2	4:E:436:MET:HE3	1.97	0.45
4:F:237:ALA:HB3	4:F:389:ALA:HB2	1.97	0.45
4:F:268:ASN:HD21	4:F:438:LEU:HB2	1.81	0.45
4:F:406:PRO:HA	4:F:422:PHE:HZ	1.81	0.45
4:F:492:GLN:OE1	4:F:577:SER:OG	2.29	0.45
4:F:386:VAL:HG22	4:F:390:ARG:HH21	1.82	0.45
8:J:48:C:H2'	8:J:49:C:C6	2.52	0.45
1:A:689:TYR:O	1:A:693:VAL:HG23	2.17	0.45
4:E:269:TYR:HA	4:E:272:VAL:HG22	1.99	0.45
4:F:116:ASN:OD1	4:F:117:ALA:N	2.48	0.45
4:F:155:ARG:HA	4:F:222:GLY:H	1.81	0.45
4:F:309:CYS:SG	4:F:378:MET:HE2	2.57	0.45
1:A:143:LYS:O	1:A:147:VAL:HG13	2.16	0.45
4:E:186:ARG:O	4:E:193:VAL:N	2.35	0.45
4:F:114:TRP:HB3	4:F:141:THR:HG21	1.99	0.45
5:G:95:ASN:O	5:G:99:ARG:HG3	2.17	0.45
4:F:202:LYS:HD2	4:F:202:LYS:HA	1.78	0.45
4:F:535:SER:HB2	4:F:537:GLN:HE21	1.82	0.45
4:F:562:ASN:HA	4:F:565:ILE:HG13	1.99	0.45
2:D:52:ASP:OD1	2:D:52:ASP:N	2.50	0.45
1:A:904:SER:HB2	4:F:95:ASN:HB2	1.99	0.44
2:D:13:ALA:O	2:D:17:THR:HG23	2.16	0.44
2:D:26:VAL:HG22	2:D:35:LEU:HD22	1.99	0.44
4:F:20:ILE:HD13	4:F:114:TRP:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:293:ILE:HG12	4:F:324:TYR:HD2	1.82	0.44
4:F:452:VAL:HG22	4:F:457:TYR:CE2	2.52	0.44
4:F:489:ASN:ND2	4:F:491:PRO:HD3	2.32	0.44
2:D:177:SER:O	2:D:179:ASN:N	2.41	0.44
4:F:464:HIS:HB3	4:F:465:LYS:NZ	2.31	0.44
4:F:544:VAL:HG11	4:F:567:ARG:HB3	1.99	0.44
3:C:71:LEU:O	3:C:76:LEU:HB2	2.17	0.44
4:F:151:ILE:HG13	4:F:226:VAL:HB	1.99	0.44
4:E:488:ILE:HG13	4:E:489:ASN:H	1.82	0.44
4:E:62:GLN:OE1	4:E:72:CYS:HB2	2.18	0.44
4:E:12:THR:OG1	4:E:13:SER:N	2.50	0.44
4:E:220:ASN:ND2	4:E:221:VAL:HG22	2.32	0.44
4:E:290:HIS:CD2	4:E:320:LYS:HD3	2.53	0.44
4:E:406:PRO:HB3	4:E:422:PHE:HE1	1.83	0.44
4:F:294:GLY:O	4:F:298:TYR:HB3	2.17	0.44
4:F:376:ILE:HG12	4:F:376:ILE:O	2.17	0.44
8:J:35:U:H2'	8:J:36:A:C8	2.52	0.44
4:F:494:GLY:HA2	4:F:497:ARG:HD2	1.99	0.44
5:G:5:SER:CB	5:G:101:MET:HG2	2.48	0.44
2:B:43:ASN:CG	8:J:47:A:O3'	2.61	0.44
4:E:62:GLN:HE21	4:E:62:GLN:HB3	1.64	0.44
4:F:202:LYS:O	4:F:210:VAL:N	2.51	0.44
4:E:219:LEU:HD11	4:E:225:PHE:CE2	2.50	0.44
4:F:3:GLY:HA3	4:F:24:PHE:HE2	1.81	0.44
4:F:126:CYS:HB3	4:F:130:LEU:HB3	2.00	0.44
4:F:331:SER:O	4:F:357:PHE:N	2.49	0.44
4:F:473:LYS:HB2	4:F:587:PHE:HB3	2.00	0.44
2:B:148:THR:HG22	2:B:153:LEU:HD12	1.99	0.43
2:D:22:TYR:HA	2:D:38:LEU:HD13	1.99	0.43
4:E:158:LEU:HD21	4:E:164:HIS:CD2	2.53	0.43
4:E:267:ALA:HA	4:E:270:GLN:HB3	2.00	0.43
3:C:77:ASP:HA	2:D:96:ARG:HD3	2.00	0.43
4:E:379:ALA:O	4:E:423:ASN:ND2	2.50	0.43
4:E:414:LYS:HB3	4:E:414:LYS:HE3	1.74	0.43
4:E:506:TRP:CE2	4:E:573:LEU:HB2	2.53	0.43
4:F:242:PRO:C	4:F:276:LYS:HZ2	2.25	0.43
4:F:268:ASN:ND2	4:F:436:MET:HB3	2.32	0.43
1:A:162:TRP:HA	1:A:168:ASN:HD22	1.82	0.43
3:C:77:ASP:HB2	2:D:92:PHE:HD1	1.82	0.43
4:F:322:LEU:HB3	4:F:346:PHE:HE1	1.82	0.43
4:F:329:LYS:HD2	4:F:329:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:332:ARG:HH12	4:F:346:PHE:H	1.67	0.43
2:D:58:LYS:HE3	2:D:59:LEU:HD12	2.00	0.43
4:E:280:LEU:HB2	4:E:399:ILE:HA	2.00	0.43
4:F:368:ALA:HB3	4:F:391:LEU:HD13	2.00	0.43
4:E:416:THR:HG21	4:E:557:ASN:HD22	1.84	0.43
4:F:305:VAL:HB	4:F:373:PHE:CE1	2.52	0.43
2:D:67:MET:O	2:D:70:MET:HG2	2.17	0.43
4:F:371:VAL:HG13	4:F:373:PHE:CZ	2.53	0.43
4:F:542:ASP:CG	4:F:570:VAL:H	2.26	0.43
5:G:111:ARG:NH1	5:G:111:ARG:HA	2.34	0.43
7:I:22:G:HO2'	7:I:23:C:P	2.40	0.43
1:A:924:MET:HE3	1:A:924:MET:HB3	1.83	0.43
2:B:48:GLU:HA	2:B:51:ARG:NH2	2.32	0.43
2:B:68:THR:HG23	4:F:53:PRO:HG2	2.00	0.43
2:D:156:ILE:HG23	2:D:186:VAL:HG13	2.01	0.43
4:F:152:ALA:HB1	4:F:165:LEU:HD11	2.00	0.43
4:F:557:ASN:OD1	4:F:558:VAL:HG12	2.18	0.43
5:G:29:LEU:HD12	5:G:29:LEU:HA	1.83	0.43
4:E:307:THR:HA	4:E:358:CYS:O	2.18	0.43
1:A:202:VAL:HG12	5:G:4:LEU:HD21	2.01	0.43
1:A:665:GLU:OE1	1:A:665:GLU:N	2.52	0.43
2:B:70:MET:SD	4:E:92:LEU:HG	2.59	0.43
4:E:152:ALA:HB2	4:E:167:TRP:HZ3	1.82	0.43
4:E:296:ALA:O	4:E:355:TYR:OH	2.25	0.43
4:F:131:LYS:NZ	4:F:381:ASN:HD21	2.16	0.43
4:F:518:GLN:OE1	4:F:549:THR:OG1	2.37	0.43
5:G:95:ASN:OD1	5:G:98:ASN:ND2	2.52	0.43
1:A:60:ASP:N	1:A:60:ASP:OD1	2.49	0.42
4:E:103:VAL:HG12	4:E:107:ASN:ND2	2.33	0.42
5:G:5:SER:O	5:G:5:SER:OG	2.25	0.42
5:G:48:LEU:HD13	5:G:51:LEU:HD21	2.00	0.42
4:E:34:VAL:HG21	4:E:60:VAL:HG11	2.01	0.42
5:G:69:LEU:HD23	5:G:89:TYR:CD2	2.54	0.42
8:J:39:A:H2'	8:J:40:U:H6	1.85	0.42
1:A:438:LYS:HE2	1:A:438:LYS:HB3	1.90	0.42
2:D:61:LYS:HG3	2:D:62:MET:N	2.33	0.42
2:D:135:TYR:HB2	2:D:182:TRP:CZ2	2.55	0.42
4:E:334:ILE:HD12	4:E:342:CYS:HB3	2.00	0.42
4:E:369:ASP:HA	4:E:394:LYS:H	1.84	0.42
4:F:186:ARG:O	4:F:193:VAL:N	2.53	0.42
5:G:50:ASP:OD1	5:G:52:LYS:NZ	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ARG:NH1	1:A:840:ALA:HB2	2.35	0.42
2:B:98:LEU:HD12	2:B:98:LEU:HA	1.82	0.42
4:E:279:THR:HA	4:E:398:TYR:H	1.84	0.42
4:E:448:ILE:HG22	4:E:565:ILE:HG23	2.02	0.42
4:E:546:PHE:HE2	4:E:560:ARG:NH2	2.17	0.42
4:F:176:LEU:HD11	4:F:201:GLU:O	2.19	0.42
4:F:271:LYS:HA	4:F:274:MET:SD	2.59	0.42
4:F:544:VAL:HG11	4:F:567:ARG:CB	2.49	0.42
8:J:35:U:H2'	8:J:36:A:H8	1.85	0.42
1:A:40:ASP:OD1	1:A:40:ASP:C	2.62	0.42
4:E:544:VAL:H	4:E:568:ALA:HB2	1.85	0.42
4:F:188:THR:HG23	4:F:189:LYS:N	2.33	0.42
4:F:197:GLU:OE1	4:F:340:VAL:N	2.52	0.42
4:E:113:ASP:OD1	4:E:115:THR:OG1	2.38	0.42
4:E:139:LYS:HA	4:E:142:GLU:HG2	2.02	0.42
4:E:281:GLN:HE22	4:E:402:PRO:HD2	1.84	0.42
4:F:32:ASP:HA	4:F:35:ILE:CG1	2.50	0.42
4:F:196:GLY:HA3	4:F:217:TYR:CE1	2.55	0.42
1:A:204:VAL:HG12	5:G:4:LEU:HD13	2.02	0.42
1:A:551:LYS:HB3	1:A:551:LYS:HE3	1.70	0.42
1:A:572:HIS:O	1:A:576:LEU:HG	2.20	0.42
1:A:894:GLU:O	1:A:898:HIS:CB	2.68	0.42
4:F:176:LEU:HB2	4:F:485:SER:HB3	2.01	0.42
4:F:348:VAL:HG12	4:F:349:ASN:OD1	2.20	0.42
5:G:70:GLU:OE2	5:G:99:ARG:NH2	2.53	0.42
5:G:73:CYS:O	5:G:88:LEU:N	2.47	0.42
5:G:79:THR:HG23	5:G:82:GLY:H	1.85	0.42
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.85	0.41
4:E:405:LEU:HD22	4:E:534:ASP:HA	2.02	0.41
4:F:399:ILE:H	4:F:399:ILE:HG13	1.71	0.41
4:F:426:CYS:O	4:F:429:MET:HB3	2.20	0.41
7:I:14:A:H2'	7:I:15:G:C8	2.55	0.41
1:A:260:ASP:HB3	1:A:263:LYS:HD2	2.02	0.41
1:A:760:ASP:OD2	1:A:760:ASP:C	2.63	0.41
4:E:140:ALA:O	4:E:143:GLU:HG3	2.20	0.41
4:E:319:GLU:HA	4:E:345:LYS:NZ	2.35	0.41
4:E:419:PRO:HA	4:E:422:PHE:CD2	2.54	0.41
4:E:527:GLY:O	4:E:528:LEU:HD13	2.20	0.41
4:F:73:LYS:O	4:F:76:LYS:HE2	2.20	0.41
4:E:25:LEU:HD21	4:E:106:PHE:CE2	2.55	0.41
4:F:491:PRO:HD2	4:F:492:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:OD1	1:A:336:ASP:N	2.51	0.41
4:F:40:LYS:HB2	4:F:40:LYS:HE2	1.69	0.41
4:F:76:LYS:O	4:F:78:PRO:HD3	2.20	0.41
1:A:225:THR:HG22	1:A:226:THR:N	2.35	0.41
4:E:131:LYS:HG2	4:E:131:LYS:H	1.74	0.41
5:G:70:GLU:OE2	5:G:90:PHE:HB2	2.20	0.41
4:E:280:LEU:HB2	4:E:399:ILE:HG13	2.01	0.41
4:E:445:PRO:HA	4:E:465:LYS:HB2	2.02	0.41
4:F:309:CYS:N	4:F:375:GLU:OE2	2.43	0.41
8:J:40:U:C2	8:J:41:G:C8	3.08	0.41
2:B:43:ASN:HD22	8:J:48:C:P	2.44	0.41
2:B:48:GLU:HA	2:B:51:ARG:CZ	2.51	0.41
4:E:492:GLN:HG3	4:E:518:GLN:HE22	1.85	0.41
4:E:497:ARG:HA	4:E:500:LEU:HG	2.02	0.41
4:F:489:ASN:CG	4:F:492:GLN:HG2	2.45	0.41
1:A:59:LYS:HE2	1:A:59:LYS:HB2	1.63	0.41
2:B:139:LYS:HG3	2:B:140:ASN:OD1	2.20	0.41
3:C:66:VAL:HG23	3:C:68:ILE:HD12	2.03	0.41
3:C:76:LEU:C	2:D:96:ARG:HD3	2.46	0.41
4:E:275:GLN:O	4:E:395:HIS:ND1	2.54	0.41
4:F:412:LEU:HD13	4:F:554:HIS:NE2	2.35	0.41
5:G:16:ALA:O	5:G:27:ASN:ND2	2.54	0.41
1:A:64:ASN:OD1	1:A:64:ASN:N	2.53	0.41
1:A:608:ASP:OD1	1:A:608:ASP:N	2.54	0.41
1:A:898:HIS:O	1:A:898:HIS:ND1	2.54	0.41
3:C:3:MET:HG2	3:C:45:THR:HB	2.03	0.41
3:C:45:THR:O	3:C:45:THR:OG1	2.36	0.41
3:C:61:SER:HB3	2:D:116:PRO:HG2	2.03	0.41
4:E:72:CYS:SG	4:E:74:SER:OG	2.71	0.41
4:E:377:SER:OG	4:E:405:LEU:O	2.39	0.41
4:F:162:GLU:HG2	4:F:210:VAL:HG22	2.01	0.41
4:F:282:GLY:HA2	4:F:283:PRO:HD3	1.93	0.41
4:F:283:PRO:HA	4:F:563:VAL:HG12	2.03	0.41
4:F:291:PHE:O	4:F:295:LEU:HG	2.21	0.41
4:F:418:GLU:CD	4:F:418:GLU:H	2.28	0.41
4:F:498:GLU:OE1	4:F:593:PRO:HB2	2.21	0.41
2:D:22:TYR:HD2	2:D:38:LEU:HB3	1.86	0.41
4:F:20:ILE:HG23	4:F:21:ARG:H	1.85	0.41
4:F:576:MET:HE3	4:F:581:LEU:HD12	2.02	0.41
1:A:478:LYS:HA	1:A:478:LYS:HD2	1.83	0.40
4:E:153:THR:HG23	4:E:155:ARG:HE	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:445:PRO:HD2	4:E:569:LYS:O	2.21	0.40
4:E:490:ARG:C	4:E:492:GLN:H	2.29	0.40
4:E:511:PHE:O	4:E:531:GLN:HB3	2.21	0.40
4:F:492:GLN:HE21	4:F:548:GLN:H	1.69	0.40
8:J:34:C:H2'	8:J:35:U:C6	2.56	0.40
8:J:47:A:H2'	8:J:48:C:C6	2.56	0.40
4:E:35:ILE:HD13	4:E:35:ILE:HA	1.85	0.40
4:E:61:THR:HG22	4:E:84:CYS:SG	2.62	0.40
4:F:491:PRO:HD2	4:F:492:GLN:H	1.85	0.40
1:A:105:ARG:NH2	1:A:108:GLY:O	2.49	0.40
1:A:144:GLU:O	1:A:148:THR:HG22	2.21	0.40
2:D:141:THR:OG1	2:D:142:CYS:N	2.55	0.40
4:E:152:ALA:HB3	4:E:225:PHE:HB2	2.04	0.40
4:E:536:SER:O	4:E:567:ARG:NH1	2.54	0.40
4:E:561:PHE:HA	4:E:564:ALA:HB3	2.03	0.40
4:F:441:CYS:HB2	4:F:464:HIS:HD1	1.86	0.40
8:J:28:U:C2	8:J:29:G:C8	3.10	0.40
8:J:31:U:H2'	8:J:32:C:C6	2.56	0.40
1:A:58:GLU:O	1:A:66:ILE:HG22	2.22	0.40
1:A:735:ARG:HA	1:A:735:ARG:HD3	1.84	0.40
4:E:137:THR:O	4:E:141:THR:HG22	2.21	0.40
4:E:544:VAL:HG21	4:E:567:ARG:HB3	2.03	0.40
4:E:555:SER:CB	4:E:560:ARG:HD3	2.44	0.40
4:E:152:ALA:HB2	4:E:167:TRP:CZ3	2.57	0.40
4:F:20:ILE:HG23	4:F:21:ARG:N	2.36	0.40
4:F:500:LEU:HD13	4:F:507:ARG:NH1	2.37	0.40
4:F:544:VAL:O	4:F:573:LEU:HB3	2.22	0.40
5:G:92:LYS:HE2	5:G:92:LYS:HB2	1.84	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%)	890 (96%)	35 (4%)	2 (0%)	43	60
2	B	188/198 (95%)	177 (94%)	11 (6%)	0	100	100
2	D	185/198 (93%)	175 (95%)	10 (5%)	0	100	100
3	C	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	9	16
4	E	581/593 (98%)	515 (89%)	65 (11%)	1 (0%)	43	60
4	F	581/593 (98%)	499 (86%)	82 (14%)	0	100	100
5	G	111/113 (98%)	93 (84%)	13 (12%)	5 (4%)	2	2
All	All	2649/2705 (98%)	2417 (91%)	223 (8%)	9 (0%)	37	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	846	ASP
3	C	65	ALA
5	G	14	CYS
5	G	33	ASN
5	G	11	GLN
5	G	32	TYR
5	G	59	SER
4	E	220	ASN

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	822/823 (100%)	776 (94%)	46 (6%)	19	32
2	B	147/167 (88%)	134 (91%)	13 (9%)	9	15
2	D	151/167 (90%)	143 (95%)	8 (5%)	20	35
3	C	73/73 (100%)	72 (99%)	1 (1%)	59	76
4	E	498/516 (96%)	483 (97%)	15 (3%)	36	57
4	F	498/516 (96%)	482 (97%)	16 (3%)	34	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	94/94 (100%)	77 (82%)	17 (18%)	2	2
All	All	2283/2356 (97%)	2167 (95%)	116 (5%)	23	36

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	49	LEU
1	A	54	CYS
1	A	72	VAL
1	A	75	HIS
1	A	76	THR
1	A	115	SER
1	A	204	VAL
1	A	231	VAL
1	A	235	ASP
1	A	236	SER
1	A	246	THR
1	A	255	SER
1	A	269	ASP
1	A	308	LEU
1	A	335	VAL
1	A	338	VAL
1	A	359	VAL
1	A	366	LEU
1	A	372	LEU
1	A	424	VAL
1	A	434	SER
1	A	438	LYS
1	A	463	MET
1	A	499	ASP
1	A	520	SER
1	A	548	ILE
1	A	551	LYS
1	A	556	THR
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	723	LEU

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Mol	Chain	Res	Type
1	A	731	LEU
1	A	754	SER
1	A	776	VAL
1	A	778	SER
1	A	803	THR
1	A	807	LYS
1	A	820	VAL
1	A	835	SER
1	A	845	ASP
1	A	846	ASP
2	B	7	SER
2	B	34	VAL
2	B	42	LEU
2	B	76	SER
2	B	83	VAL
2	B	93	THR
2	B	98	LEU
2	B	114	CYS
2	B	142	CYS
2	B	145	THR
2	B	173	SER
2	B	177	SER
2	B	193	SER
3	C	59	LEU
2	D	40	LYS
2	D	76	SER
2	D	77	GLU
2	D	115	VAL
2	D	131	VAL
2	D	179	ASN
2	D	185	ILE
2	D	187	THR
4	E	5	CYS
4	E	12	THR
4	E	35	ILE
4	E	38	SER
4	E	122	LEU
4	E	160	ASP
4	E	183	THR
4	E	241	VAL
4	E	331	SER
4	E	372	VAL

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Mol	Chain	Res	Type
4	E	410	THR
4	E	533	VAL
4	E	543	TYR
4	E	547	THR
4	E	554	HIS
4	F	7	LEU
4	F	19	CYS
4	F	20	ILE
4	F	42	VAL
4	F	80	SER
4	F	171	LYS
4	F	199	THR
4	F	318	CYS
4	F	351	THR
4	F	453	SER
4	F	493	ILE
4	F	495	VAL
4	F	532	THR
4	F	544	VAL
4	F	570	VAL
4	F	590	LEU
5	G	4	LEU
5	G	5	SER
5	G	7	VAL
5	G	9	LEU
5	G	10	ARG
5	G	11	GLN
5	G	12	MET
5	G	19	THR
5	G	27	ASN
5	G	29	LEU
5	G	33	ASN
5	G	34	THR
5	G	35	THR
5	G	46	SER
5	G	73	CYS
5	G	84	LYS
5	G	102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	191	GLN
1	A	297	ASN
1	A	543	ASN
1	A	698	GLN
1	A	713	ASN
1	A	789	GLN
1	A	882	HIS
2	B	19	GLN
2	B	65	GLN
3	C	69	ASN
2	D	108	ASN
4	E	243	GLN
4	E	265	ASN
4	E	290	HIS
4	E	557	ASN
4	F	33	HIS
4	F	46	ASN
4	F	51	ASN
4	F	164	HIS
4	F	230	HIS
4	F	268	ASN
4	F	354	GLN
4	F	516	ASN
4	F	559	ASN
5	G	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	H	3/4 (75%)	2 (66%)	0
7	I	24/25 (96%)	2 (8%)	1 (4%)
8	J	26/27 (96%)	1 (3%)	0
All	All	53/56 (94%)	5 (9%)	1 (1%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	H	2	U
6	H	4	A
7	I	14	A
7	I	23	C

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Mol	Chain	Res	Type
8	J	45	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	$\# Z > 2$
10	GNP	A	1003	11	34,34,34	1.75	5 (14%)	47,54,54	2.02	8 (17%)

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
10	GNP	A	1003	11	-	9/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1003	GNP	PG-N3B	5.20	1.76	1.63
10	A	1003	GNP	PB-N3B	4.88	1.76	1.63
10	A	1003	GNP	C5-C4	3.44	1.48	1.38
10	A	1003	GNP	C6-N1	-3.07	1.33	1.38
10	A	1003	GNP	C5-N7	-2.27	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1003	GNP	C5-C4-N3	-7.16	117.00	128.39
10	A	1003	GNP	C2-N3-C4	5.92	122.50	112.30
10	A	1003	GNP	N9-C4-N3	5.73	137.40	125.95
10	A	1003	GNP	O2G-PG-O1G	-3.46	104.77	113.45
10	A	1003	GNP	C6-C5-N7	2.80	135.38	130.29
10	A	1003	GNP	O2G-PG-O3G	2.56	114.48	107.59
10	A	1003	GNP	C3'-C2'-C1'	2.08	105.41	101.46
10	A	1003	GNP	C4-C5-N7	-2.03	107.45	110.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1003	GNP	PB-N3B-PG-O1G
10	A	1003	GNP	C5'-O5'-PA-O3A
10	A	1003	GNP	C5'-O5'-PA-O1A
10	A	1003	GNP	C2'-C1'-N9-C4
10	A	1003	GNP	C4'-C5'-O5'-PA
10	A	1003	GNP	C2'-C1'-N9-C8
10	A	1003	GNP	PG-N3B-PB-O3A
10	A	1003	GNP	C5'-O5'-PA-O2A
10	A	1003	GNP	PB-O3A-PA-O2A

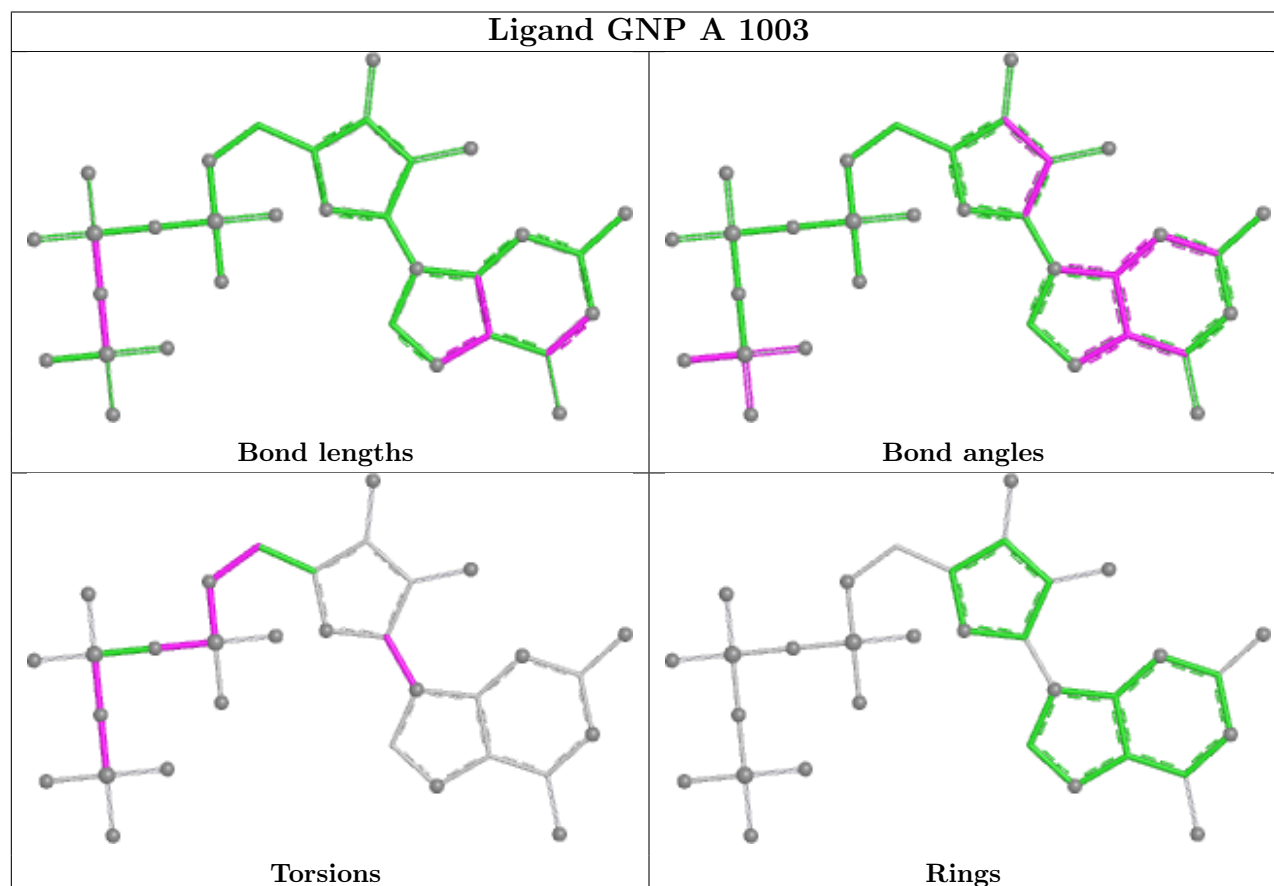
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1003	GNP	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 than 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

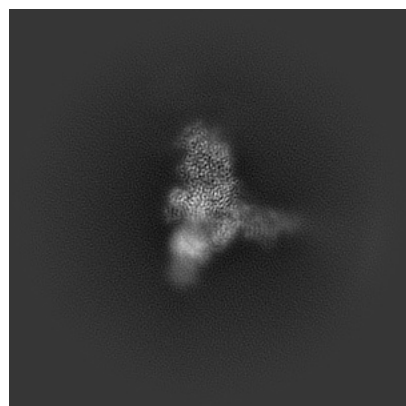
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34310. These allow visual inspection of the internal detail of the map and identification of artifacts.

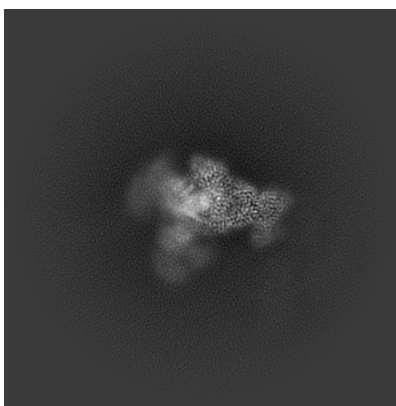
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

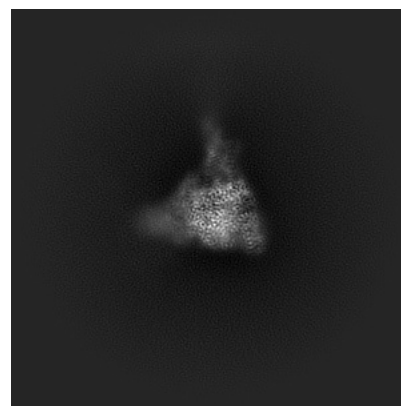
6.1.1 Primary map



X

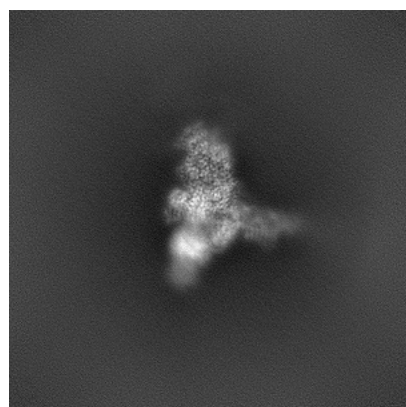


Y

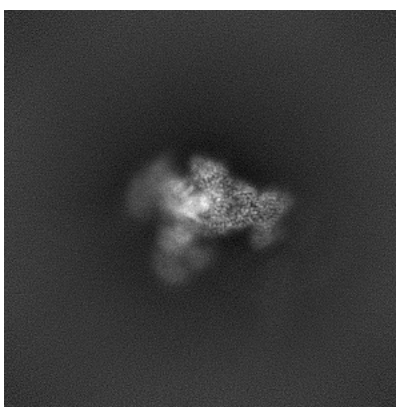


Z

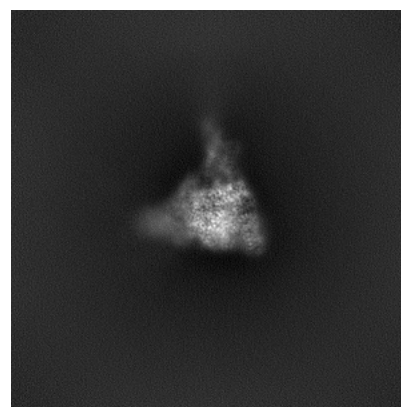
6.1.2 Raw map



X



Y

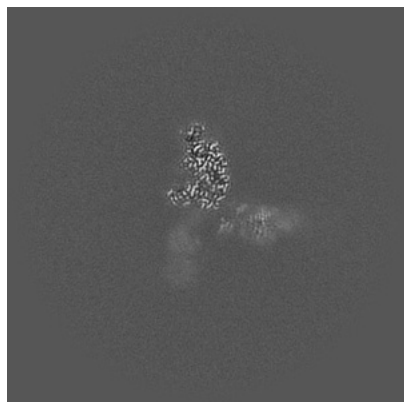


Z

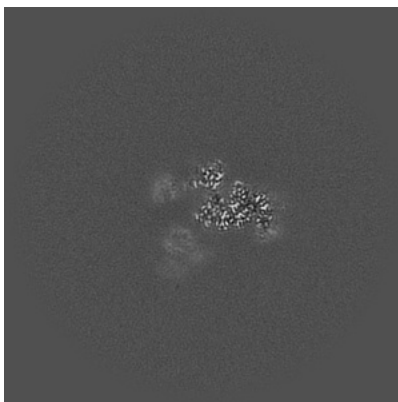
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

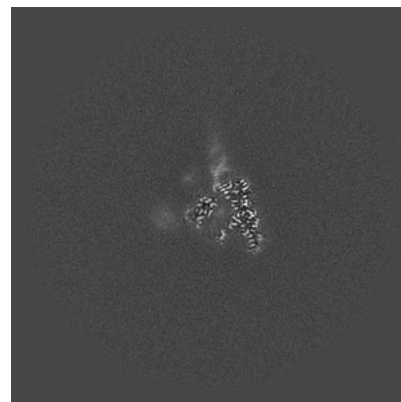
6.2.1 Primary map



X Index: 224



Y Index: 224

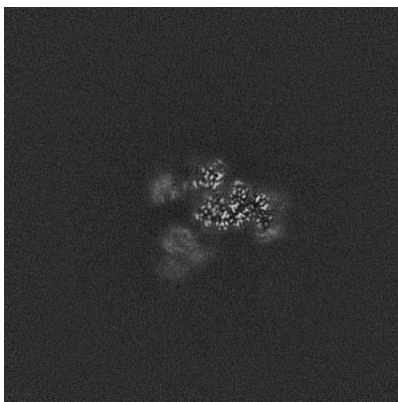


Z Index: 224

6.2.2 Raw map



X Index: 224



Y Index: 224

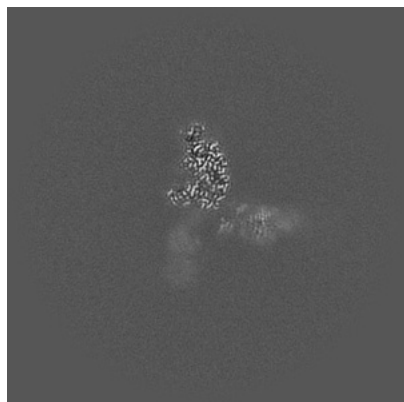


Z Index: 224

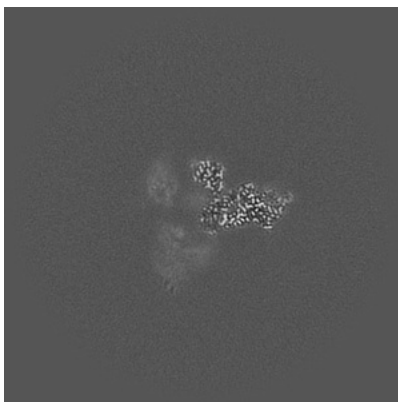
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

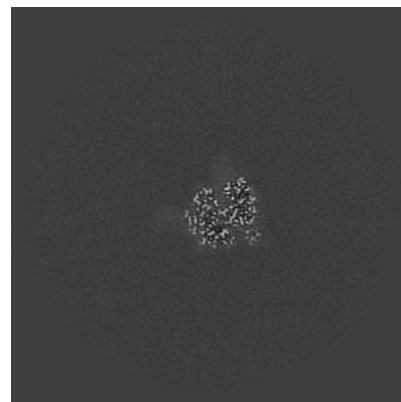
6.3.1 Primary map



X Index: 224



Y Index: 215

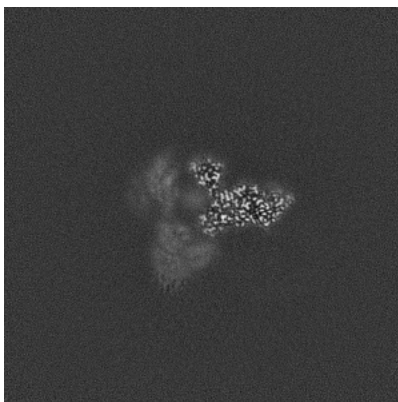


Z Index: 235

6.3.2 Raw map



X Index: 233



Y Index: 211

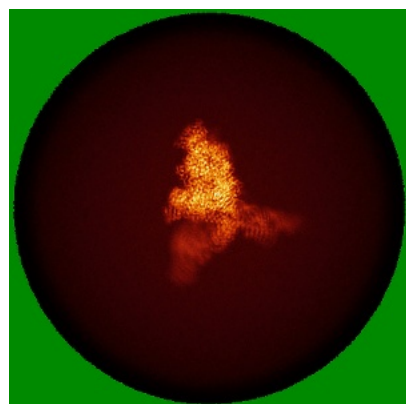


Z Index: 235

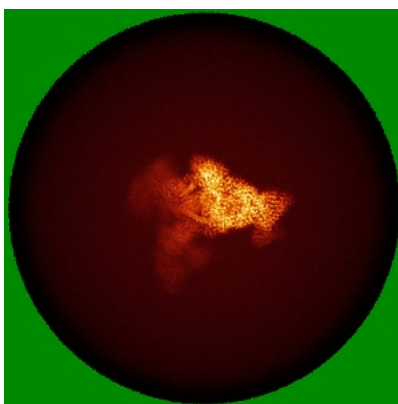
The images above show the largest variance slices of the map in three orthogonal directions.

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

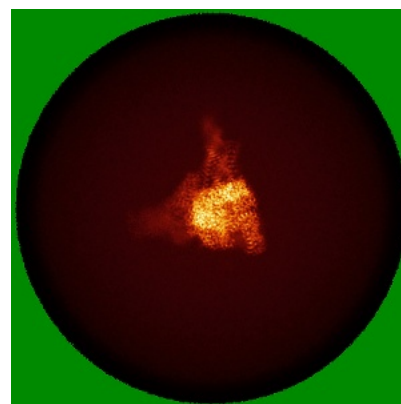
6.4.1 Primary map



X

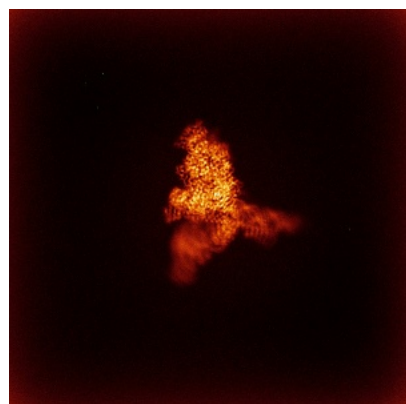


Y

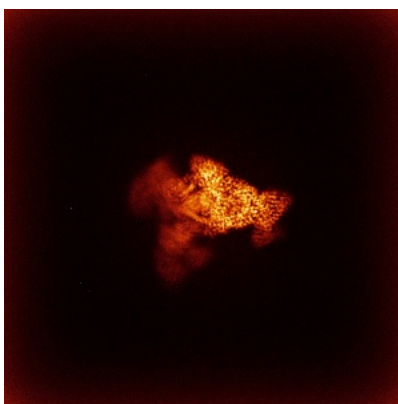


Z

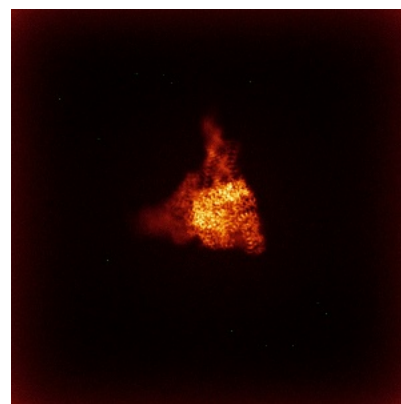
6.4.2 Raw map



X



Y

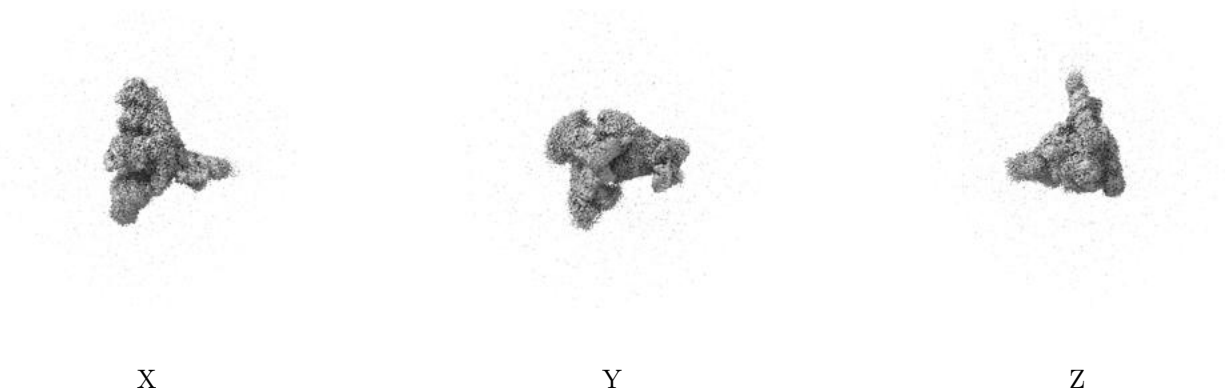


Z

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.

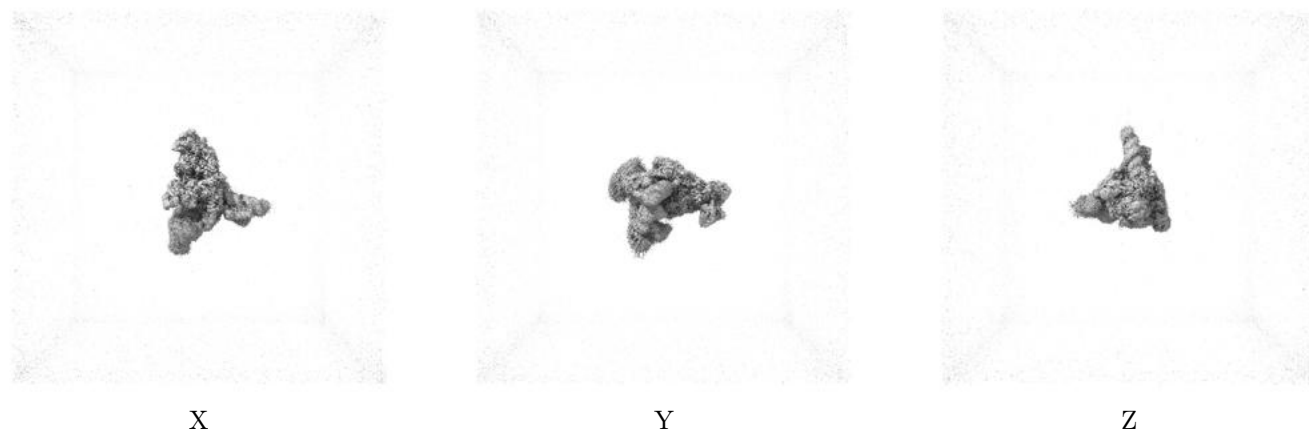
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

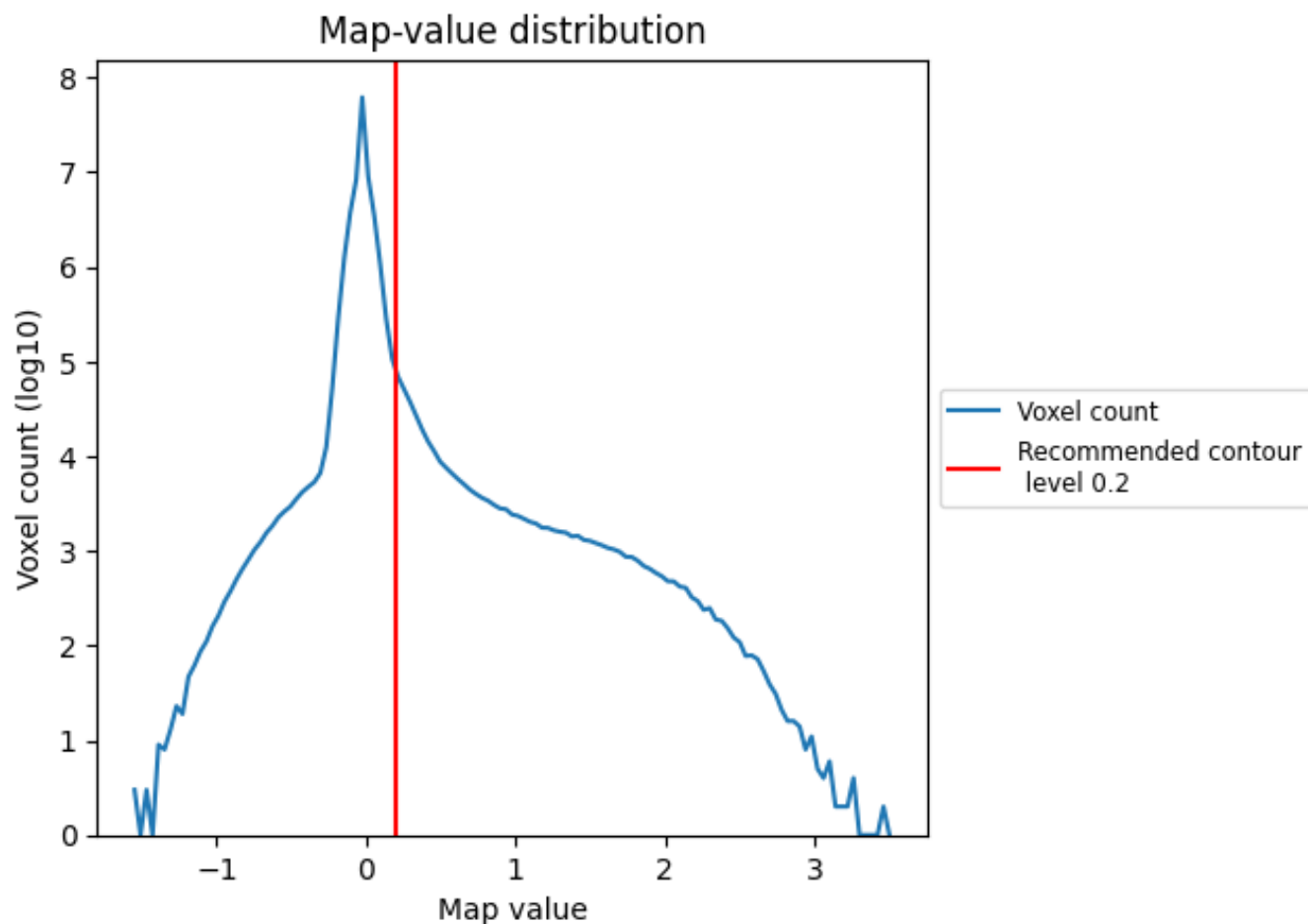
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

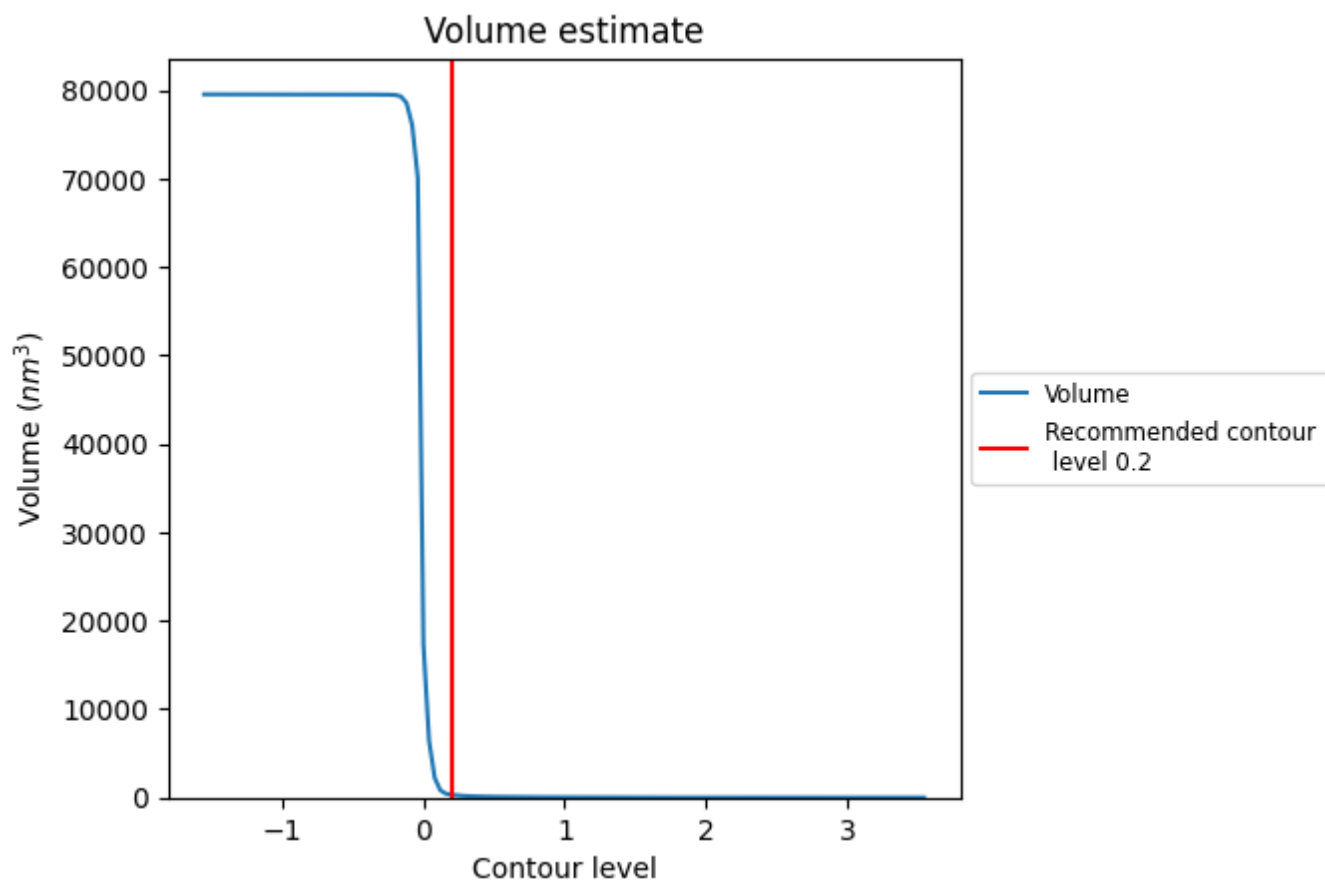
This section contains the results of statistical analysis of the map.

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.

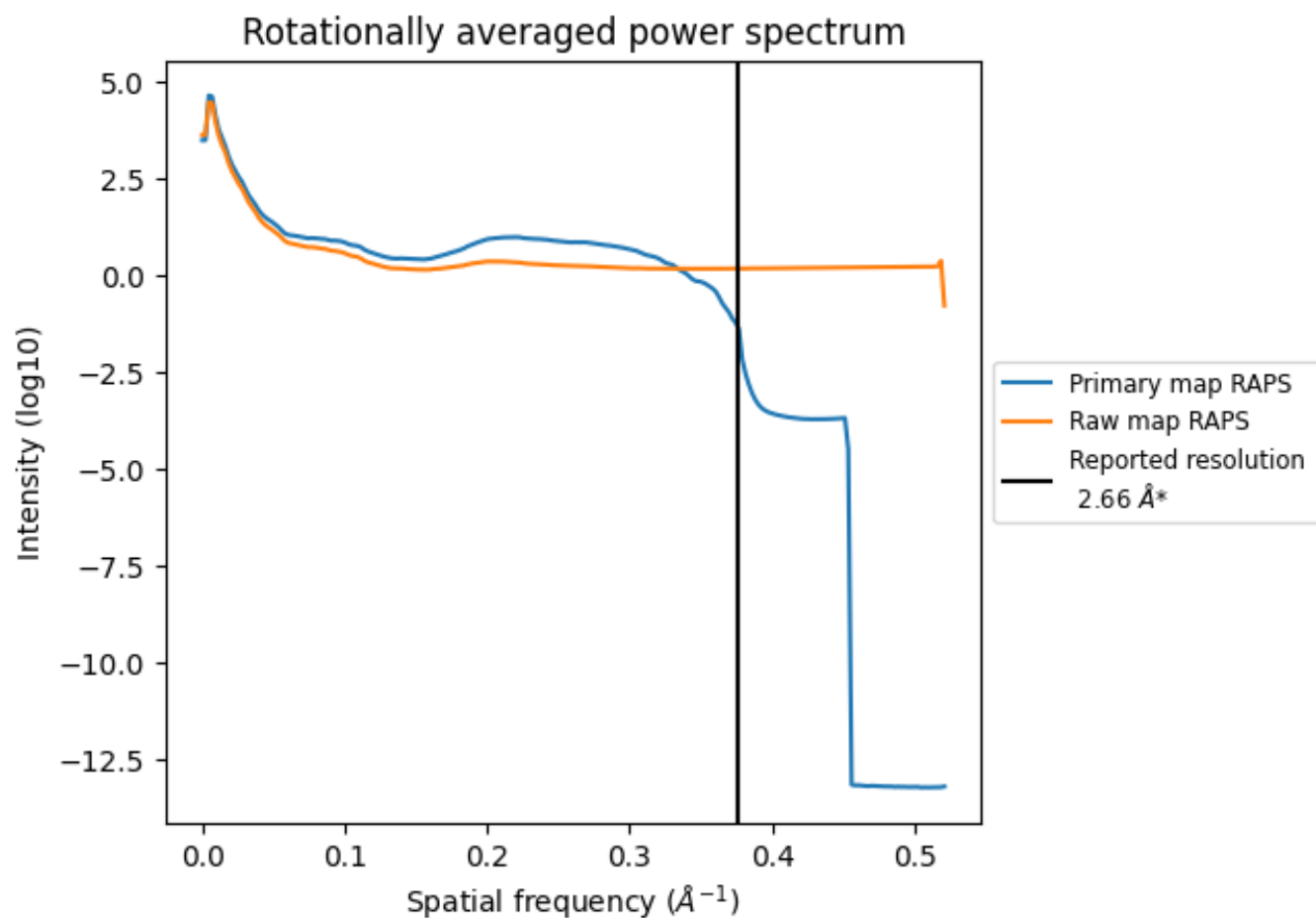
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 287 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 ⓘ

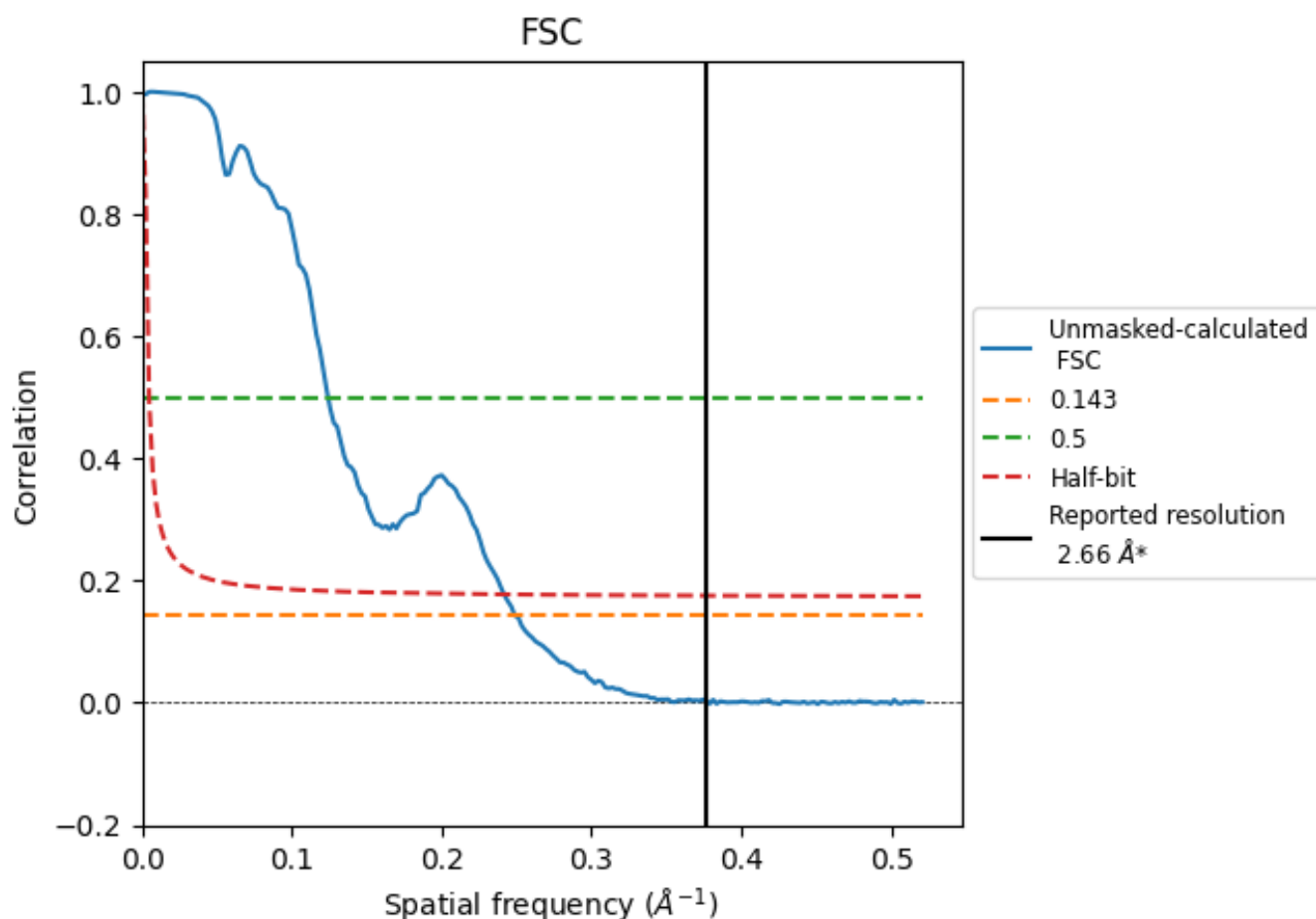


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

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 0.376 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

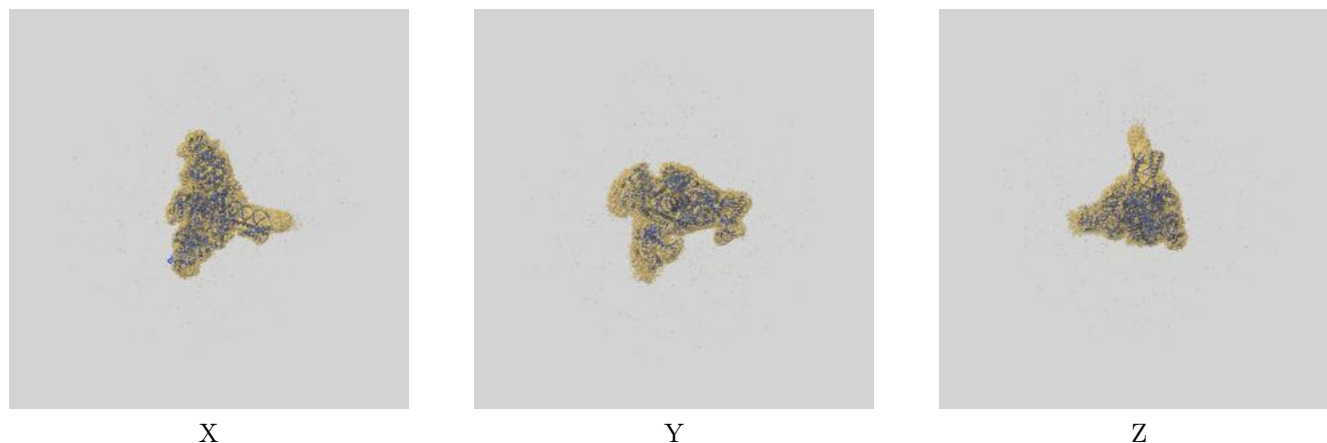
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	8.06	4.14

*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 4.02 differs from the reported value 2.66 by more than 10 %

9 Map-model fit [i](#)

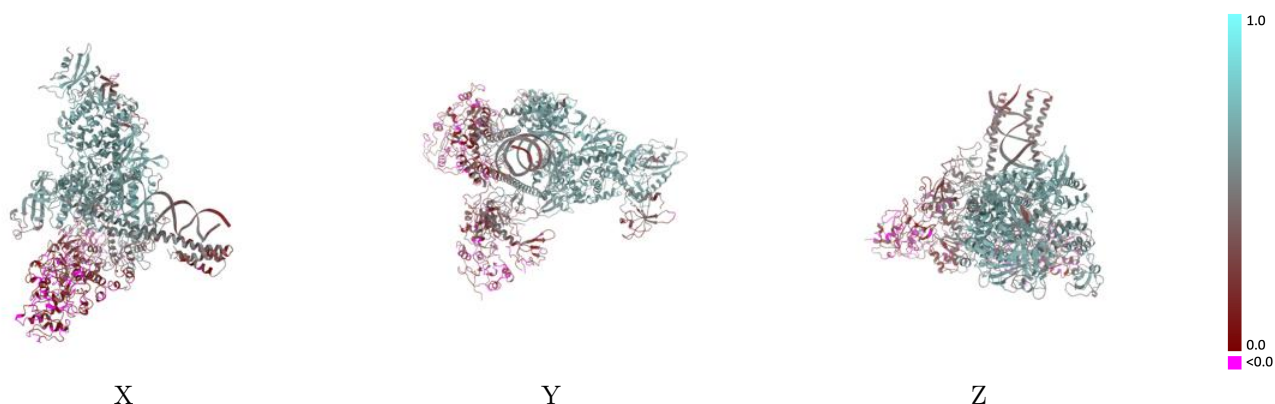
This section contains information regarding the fit between EMDB map EMD-34310 and PDB model 8GWE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



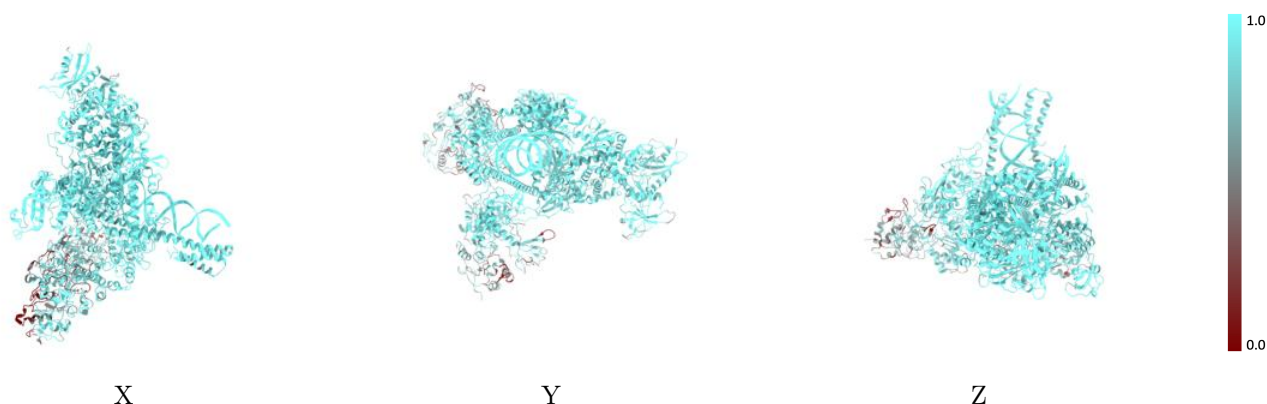
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



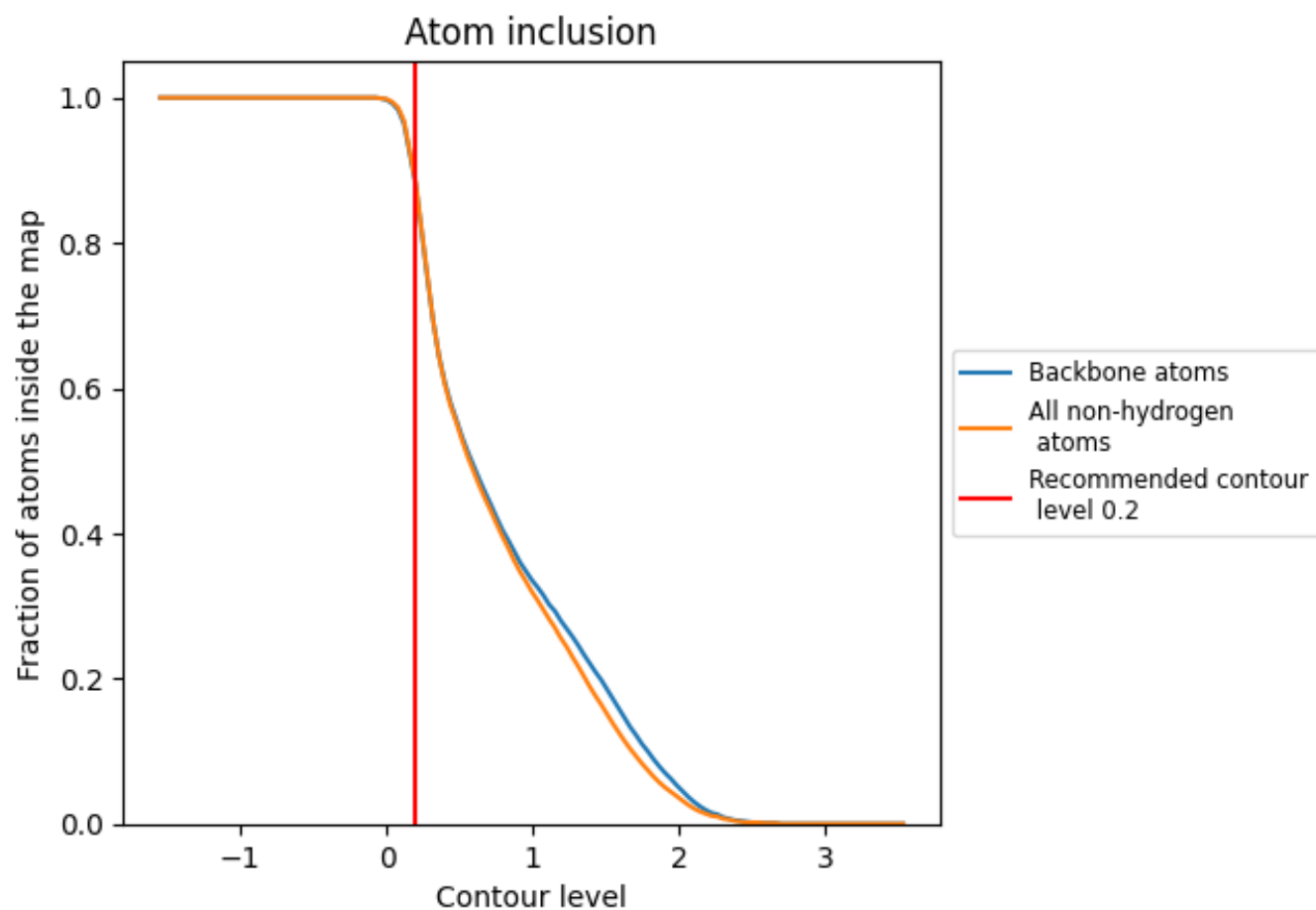
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.4170
A	0.9920	0.6140
B	0.9640	0.5110
C	0.9680	0.5740
D	0.9740	0.5020
E	0.7760	0.2250
F	0.7250	0.1940
G	0.8950	0.3730
H	0.7980	0.3770
I	1.0000	0.4630
J	0.9970	0.5030

1.0

0.0

<0.0