



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 8CXI / pdb_00008cxi
EMDB ID : EMD-27058
Title : Structures of Zika Virus in Complex with Antibodies Targeting E Dimer Epitopes and Basis for Neutralization Efficacy
Authors : Liu, W.; Zhang, X.K.; Gong, D.Y.; Dai, X.H.; Sharma, A.; Zhang, T.H.; Rey, F.; Zhou, Z.H.
Deposited on : 2022-05-21
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

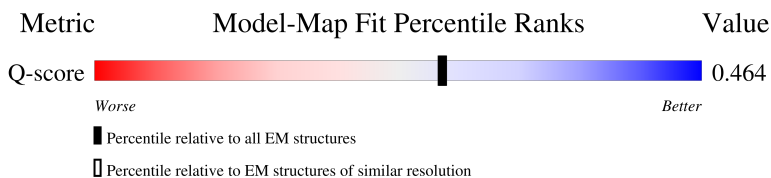
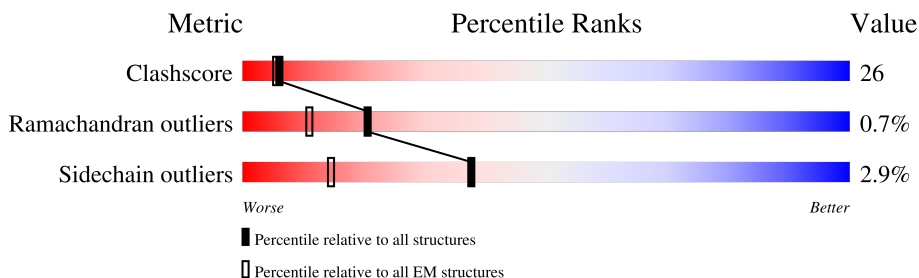
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



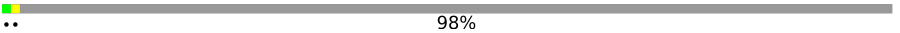
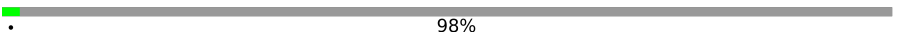
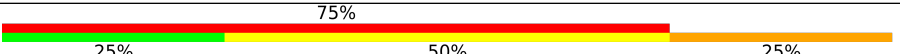
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	639	
1	B	639	
1	C	639	
2	D	3423	

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Mol	Chain	Length	Quality of chain
2	E	3423	 98%
2	F	3423	 98%
3	H	133	 52% 75% 24%
3	h	133	 50% 68% 31%
4	L	111	 73% 69% 23% 6%
4	l	111	 68% 63% 28% 9%
5	G	4	 100% 25% 50% 25%
5	I	4	 75% 25% 50% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	X	-	X	-
5	NAG	G	2	-	-	X	-
5	NAG	I	1	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16832 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 Ankyrin repeat family A protein 2,Envelope E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	501	Total	C	N	O	S	0	0
			3790	2384	657	718	31		
1	B	501	Total	C	N	O	S	0	0
			3790	2384	657	718	31		
1	C	501	Total	C	N	O	S	0	0
			3790	2384	657	718	31		

- Molecule 2 is a protein called Membrane M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

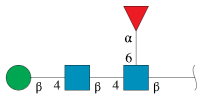
- Molecule 3 is a protein called A11 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	132	Total	C	N	O	S	0	0
			1036	655	179	197	5		
3	h	131	Total	C	N	O	S	0	0
			1024	646	178	195	5		

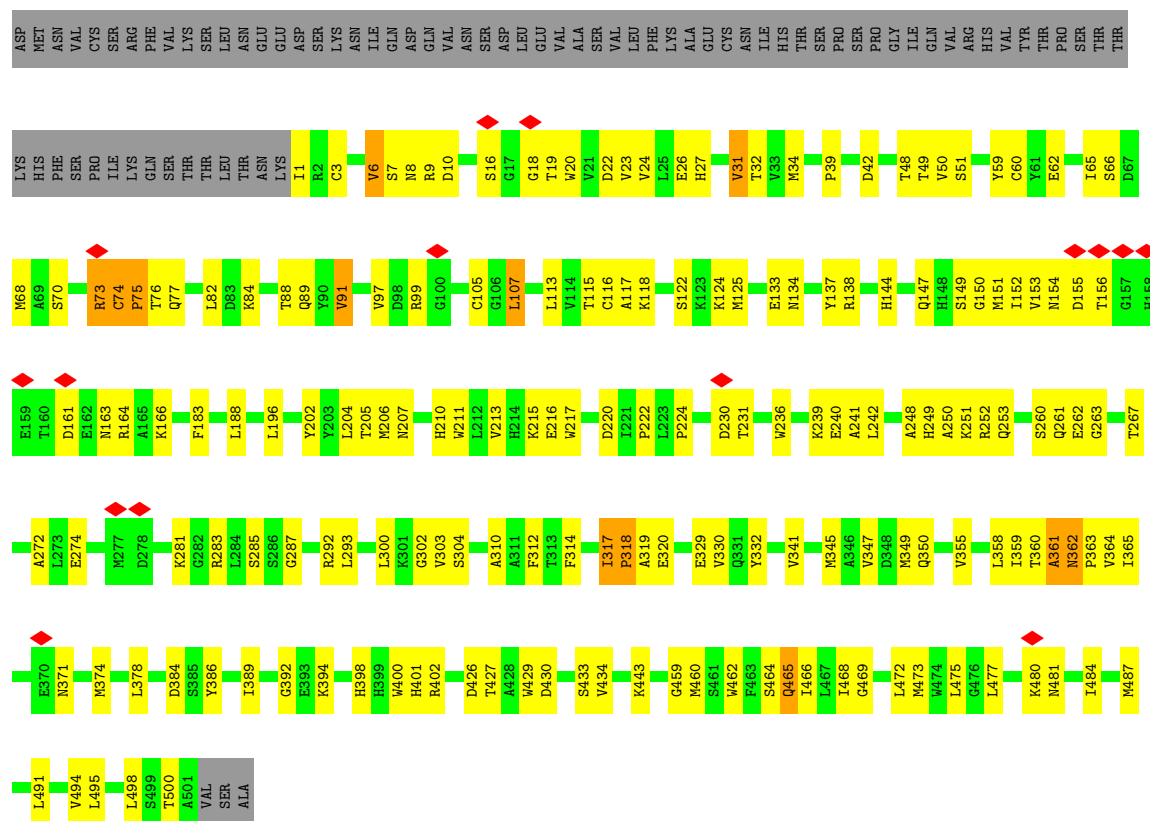
- Molecule 4 is a protein called A11 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	104	Total	C	N	O	S	0	0
			761	471	129	157	4		
4	l	101	Total	C	N	O	S	0	0
			743	459	126	154	4		

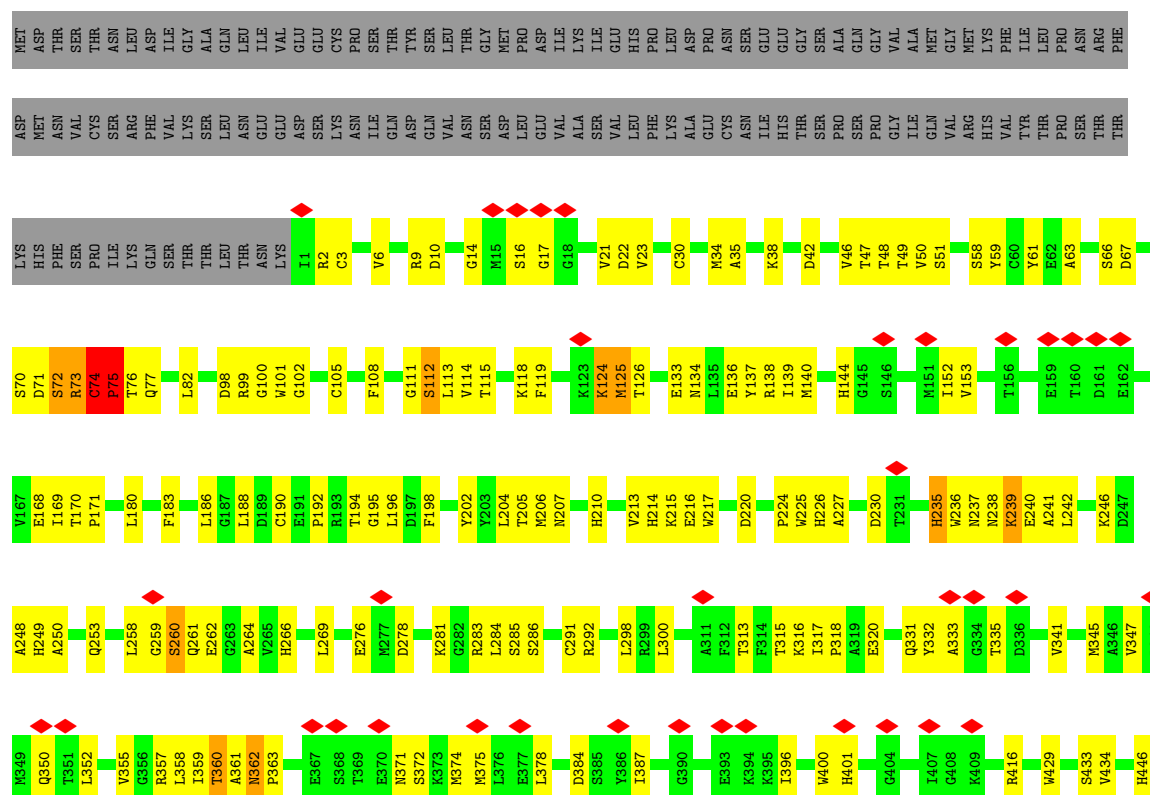
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	4	Total	C	N	O	0	0
			49	28	2	19		
5	I	4	Total	C	N	O	0	0
			49	28	2	19		



• Molecule 1: Ankyrin repeat family A protein 2,Envelope E protein







- Molecule 2: Membrane M protein





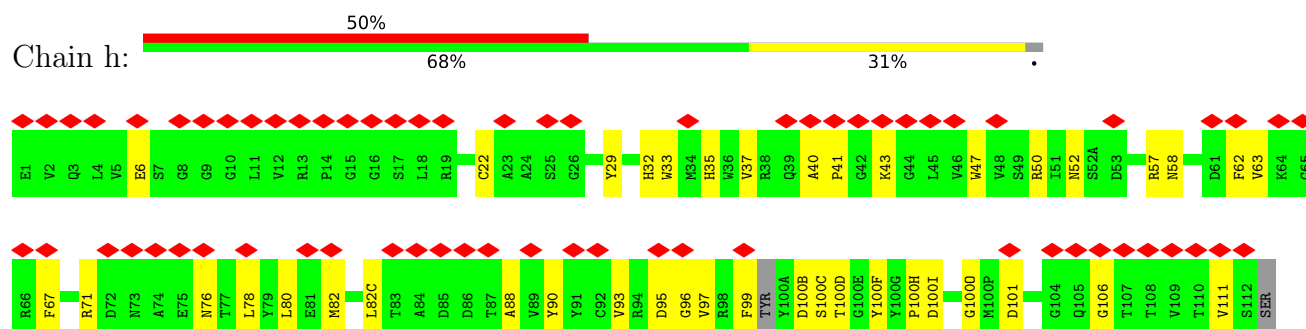




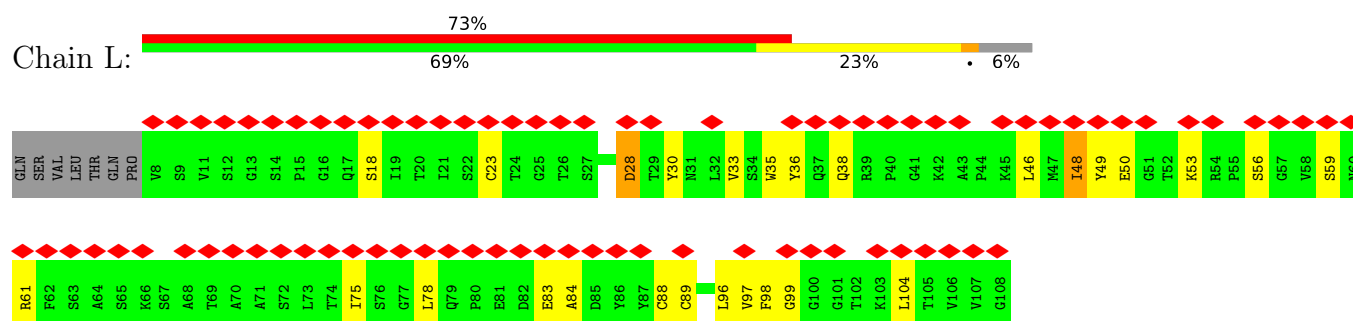




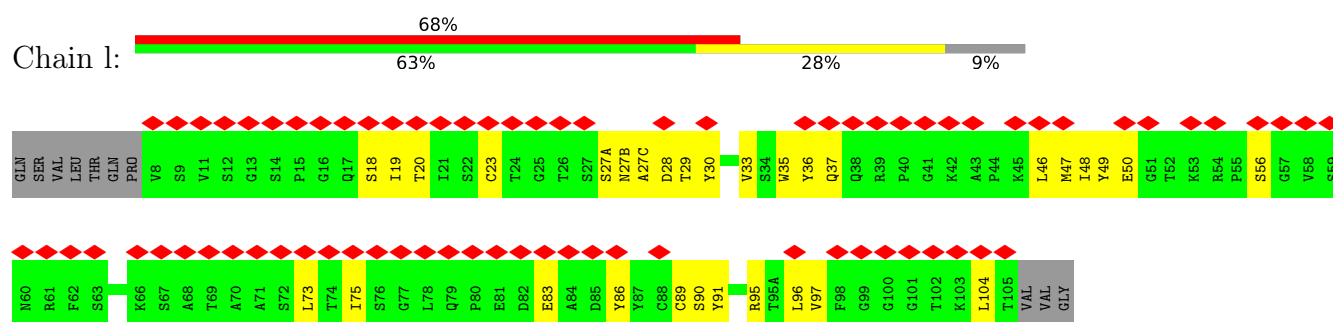
- Molecule 3: A11 heavy chain



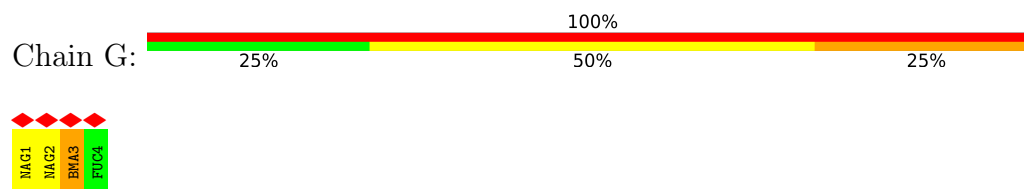
- Molecule 4: A11 light chain



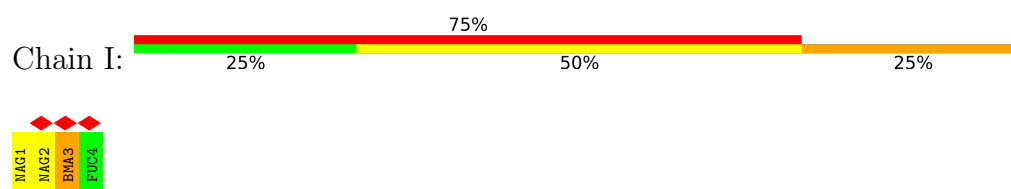
- Molecule 4: A11 light chain



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1124970	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 ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.247	Depositor
Minimum map value	-12.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, FUC

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	0.53	5/3869 (0.1%)	0.73	14/5236 (0.3%)
1	B	0.35	0/3869	0.62	4/5236 (0.1%)
1	C	0.48	4/3869 (0.1%)	0.70	11/5236 (0.2%)
2	D	0.38	0/615	0.51	0/838
2	E	0.37	0/615	0.49	0/838
2	F	0.36	0/615	0.50	0/838
3	H	0.15	0/1064	0.35	0/1445
3	h	0.16	0/1050	0.36	0/1424
4	L	0.13	0/775	0.32	0/1052
4	l	0.14	0/757	0.44	2/1027 (0.2%)
All	All	0.40	9/17098 (0.1%)	0.61	31/23170 (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	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	SER	CA-C	-8.74	1.42	1.52
1	A	125	MET	CA-C	-8.23	1.43	1.52
1	C	73	ARG	C-O	-7.92	1.14	1.23
1	A	125	MET	C-O	-7.26	1.15	1.24
1	A	316	LYS	CA-C	-6.95	1.43	1.52
1	A	124	LYS	C-O	-6.75	1.15	1.23
1	A	123	LYS	C-O	-6.51	1.15	1.24
1	C	73	ARG	CA-C	-6.46	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	PRO	CA-CB	-6.32	1.44	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	CYS	CA-C-N	12.53	135.50	119.84
1	B	74	CYS	C-N-CA	12.53	135.50	119.84
1	A	316	LYS	N-CA-C	-10.61	100.08	113.23
1	B	73	ARG	N-CA-C	10.12	125.37	112.92
1	A	315	THR	N-CA-C	9.62	123.14	111.40
1	C	74	CYS	CA-C-N	9.56	131.79	119.84
1	C	74	CYS	C-N-CA	9.56	131.79	119.84
1	C	361	ALA	N-CA-C	9.16	120.96	110.97
1	A	78	GLY	CA-C-N	-7.68	109.91	122.81
1	A	78	GLY	C-N-CA	-7.68	109.91	122.81
1	A	77	GLN	N-CA-C	7.46	121.83	112.87
1	A	316	LYS	CA-C-N	-6.43	110.23	122.13
1	A	316	LYS	C-N-CA	-6.43	110.23	122.13
1	C	74	CYS	N-CA-C	6.37	123.89	109.81
1	C	124	LYS	N-CA-C	6.08	117.54	108.31
1	C	359	ILE	O-C-N	5.97	126.97	121.96
1	C	362	ASN	N-CA-C	-5.91	96.75	109.81
1	A	122	SER	CA-C-N	5.88	132.77	121.54
1	A	122	SER	C-N-CA	5.88	132.77	121.54
1	C	359	ILE	CA-C-N	5.84	132.70	121.54
1	C	359	ILE	C-N-CA	5.84	132.70	121.54
1	A	241	ALA	CA-C-N	-5.84	113.06	122.23
1	A	241	ALA	C-N-CA	-5.84	113.06	122.23
1	C	124	LYS	CB-CA-C	-5.79	109.88	116.54
1	C	360	THR	N-CA-C	-5.69	98.68	110.80
1	A	498	LEU	N-CA-C	5.50	117.36	111.36
1	B	362	ASN	N-CA-C	-5.08	98.58	109.81
4	l	28	ASP	CA-C-N	5.03	128.36	120.82
4	l	28	ASP	C-N-CA	5.03	128.36	120.82
1	A	122	SER	N-CA-C	-5.02	100.34	108.52
1	A	362	ASN	N-CA-C	-5.01	99.50	108.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	239	LYS	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	3790	0	3744	293	0
1	B	3790	0	3746	211	0
1	C	3790	0	3748	249	0
2	D	600	0	624	22	0
2	E	600	0	624	27	0
2	F	600	0	624	20	0
3	H	1036	0	965	34	0
3	h	1024	0	954	63	0
4	L	761	0	743	20	0
4	l	743	0	722	43	0
5	G	49	0	43	23	0
5	I	49	0	43	14	0
All	All	16832	0	16580	874	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 26.

All (874) 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)
1:A:314:PHE:CD2	1:A:396:ILE:HD12	1.32	1.62
1:A:1:ILE:CG1	1:A:147:GLN:HE21	1.06	1.58
1:A:1:ILE:HG12	1:A:147:GLN:NE2	1.25	1.49
1:C:101:TRP:CD1	1:C:108:PHE:CZ	2.02	1.47
1:C:101:TRP:HD1	1:C:108:PHE:CE1	1.33	1.46
1:A:314:PHE:CE2	1:A:396:ILE:HD12	1.47	1.45
1:A:314:PHE:CE2	1:A:396:ILE:CD1	1.98	1.44
1:A:1:ILE:CG2	1:A:147:GLN:HE22	1.31	1.39
1:B:473:MET:HB2	1:B:491:LEU:CD2	1.50	1.39
1:A:15:MET:HG2	1:A:21:VAL:CG2	1.51	1.38
1:A:1:ILE:HG21	1:A:147:GLN:NE2	1.37	1.37
3:h:101:ASP:OD1	4:l:46:LEU:CB	1.74	1.35
1:B:469:GLY:O	1:B:491:LEU:HD13	1.19	1.35
1:A:175:ARG:HG3	1:A:189:ASP:OD1	1.17	1.33
1:C:101:TRP:HD1	1:C:108:PHE:CZ	1.40	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ALA:CB	1:C:73:ARG:HH22	1.40	1.31
1:B:473:MET:CB	1:B:491:LEU:HD22	1.60	1.31
3:H:100:TYR:CE1	5:G:2:NAG:H4	1.64	1.30
1:A:475:LEU:O	1:A:479:THR:HG23	1.19	1.30
1:A:150:GLY:C	5:G:1:NAG:O7	1.75	1.30
1:C:63:ALA:HB2	1:C:242:LEU:CD2	1.60	1.30
1:A:15:MET:SD	1:A:21:VAL:HG23	1.72	1.29
1:A:74:CYS:HB2	1:A:77:GLN:CG	1.62	1.29
1:A:74:CYS:CB	1:A:77:GLN:HG2	1.61	1.29
1:C:469:GLY:O	1:C:491:LEU:HD22	1.32	1.28
1:C:316:LYS:O	1:C:317:ILE:HG13	1.29	1.28
1:A:229:ALA:HB2	1:C:73:ARG:NH2	1.49	1.28
1:A:15:MET:CG	1:A:21:VAL:CG2	2.12	1.27
1:A:314:PHE:CE2	1:A:396:ILE:CG1	2.21	1.24
1:A:314:PHE:HE2	1:A:396:ILE:CG1	1.51	1.22
1:B:150:GLY:HA3	5:I:1:NAG:O7	1.31	1.22
1:A:262:GLU:O	1:A:266:HIS:CD2	1.90	1.22
1:C:101:TRP:CD1	1:C:108:PHE:CE1	2.23	1.21
1:A:317:ILE:HG12	1:A:318:PRO:CD	1.71	1.20
1:A:1:ILE:CG2	1:A:147:GLN:NE2	1.93	1.19
1:A:317:ILE:CG1	1:A:318:PRO:HD2	1.72	1.19
1:A:125:MET:CE	1:A:204:LEU:HD11	1.72	1.18
1:C:63:ALA:CB	1:C:242:LEU:HD21	1.74	1.18
1:A:175:ARG:CG	1:A:189:ASP:OD1	1.92	1.17
1:A:241:ALA:HB1	2:D:1:ALA:HB2	1.26	1.17
1:A:302:GLY:H	1:A:362:ASN:ND2	1.41	1.17
1:A:72:SER:HB2	1:A:251:LYS:NZ	1.58	1.16
3:h:58:ASN:ND2	4:l:95:ARG:HH21	1.41	1.16
2:D:26:THR:HG22	2:D:30:ILE:CD1	1.74	1.16
3:H:93:VAL:HG11	3:H:100(P):MET:HB3	1.25	1.15
1:A:314:PHE:HE2	1:A:396:ILE:HG13	1.13	1.13
1:A:150:GLY:CA	5:G:1:NAG:O7	1.96	1.13
1:B:460:MET:CE	1:B:468:ILE:HD12	1.78	1.13
3:h:58:ASN:ND2	4:l:95:ARG:HE	1.47	1.12
1:C:74:CYS:HB3	1:C:75:PRO:HD2	1.23	1.12
1:C:119:PHE:CZ	1:C:242:LEU:HD23	1.83	1.12
1:C:119:PHE:CE1	1:C:242:LEU:HD23	1.84	1.11
1:A:97:VAL:HG22	1:A:251:LYS:HA	1.16	1.11
1:A:475:LEU:O	1:A:479:THR:CG2	1.98	1.11
1:A:1:ILE:CG1	1:A:147:GLN:NE2	1.90	1.10
2:D:26:THR:HG22	2:D:30:ILE:HD11	1.21	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:HB3	1:A:252:ARG:HB2	1.34	1.09
1:B:469:GLY:O	1:B:491:LEU:CD1	1.99	1.09
3:h:101:ASP:OD1	4:l:46:LEU:HB2	0.92	1.09
1:C:238:ASN:OD1	1:C:240:GLU:HB2	1.48	1.09
1:A:314:PHE:CE2	1:A:396:ILE:HG13	1.85	1.09
1:B:473:MET:CA	1:B:491:LEU:HD22	1.82	1.09
1:C:61:TYR:O	1:C:260:SER:O	1.71	1.09
1:B:460:MET:HE3	1:B:468:ILE:HD12	1.14	1.09
1:A:150:GLY:O	5:G:1:NAG:O7	1.71	1.08
1:A:262:GLU:O	1:A:266:HIS:HD2	1.24	1.08
1:A:302:GLY:N	1:A:362:ASN:HD22	1.50	1.08
1:B:473:MET:CB	1:B:491:LEU:CD2	2.20	1.08
1:A:314:PHE:CD2	1:A:396:ILE:CD1	2.27	1.05
1:A:125:MET:HE3	1:A:204:LEU:HD11	1.05	1.04
1:C:48:THR:HG22	1:C:137:TYR:HD1	1.22	1.04
1:A:363:PRO:O	1:A:364:VAL:HG23	1.55	1.04
1:C:241:ALA:HB1	2:F:1:ALA:HB2	1.32	1.04
1:B:150:GLY:CA	5:I:1:NAG:O7	2.06	1.03
1:A:229:ALA:HB2	1:C:73:ARG:HH22	0.87	1.02
1:A:15:MET:SD	1:A:21:VAL:CG2	2.44	1.02
1:A:15:MET:CG	1:A:21:VAL:HG22	1.79	1.02
1:A:1:ILE:CB	1:A:147:GLN:NE2	2.21	1.02
1:B:317:ILE:HB	1:B:318:PRO:CD	1.90	1.02
3:h:58:ASN:ND2	4:l:95:ARG:NH2	2.06	1.01
1:B:473:MET:HB2	1:B:491:LEU:HD21	1.37	1.01
1:A:479:THR:O	1:A:480:LYS:HG2	1.59	1.01
1:B:473:MET:HB2	1:B:491:LEU:HD22	1.17	1.01
1:C:205:THR:HG22	1:C:210:HIS:ND1	1.74	1.01
1:A:72:SER:CB	1:A:251:LYS:HZ1	1.73	1.00
1:B:358:LEU:HA	1:B:378:LEU:HD22	1.42	1.00
1:A:60:CYS:SG	1:A:236:TRP:CZ2	2.54	1.00
1:C:225:TRP:CZ2	1:C:237:ASN:ND2	2.30	0.99
1:A:72:SER:HB2	1:A:251:LYS:HZ1	0.83	0.99
1:A:48:THR:HG22	1:A:137:TYR:HD1	1.23	0.98
1:A:150:GLY:O	5:G:1:NAG:C7	2.12	0.97
3:h:58:ASN:ND2	4:l:95:ARG:NE	2.12	0.97
1:A:97:VAL:HG22	1:A:251:LYS:CA	1.95	0.96
1:B:319:ALA:CB	1:C:101:TRP:HE1	1.79	0.96
1:C:469:GLY:O	1:C:491:LEU:CD2	2.13	0.96
1:A:479:THR:OG1	1:A:484:ILE:HG22	1.65	0.96
3:h:67:PHE:CZ	3:h:82:MET:HE2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:HG22	1:C:137:TYR:CD1	2.00	0.95
1:C:74:CYS:CB	1:C:75:PRO:HD2	1.93	0.95
2:D:26:THR:CG2	2:D:30:ILE:HD11	1.95	0.95
1:A:1:ILE:CB	1:A:147:GLN:HE21	1.80	0.95
3:h:67:PHE:CE2	3:h:82:MET:HE2	2.02	0.94
1:C:472:LEU:HB2	1:C:491:LEU:HD21	1.46	0.94
1:A:99:ARG:NE	1:A:251:LYS:HZ2	1.64	0.94
1:A:241:ALA:HB1	2:D:1:ALA:CB	1.99	0.93
1:A:72:SER:CB	1:A:251:LYS:NZ	2.28	0.93
1:A:48:THR:HG22	1:A:137:TYR:CD1	2.03	0.92
1:C:74:CYS:HB3	1:C:75:PRO:CD	1.98	0.92
1:A:460:MET:SD	1:A:468:ILE:HD12	2.09	0.92
3:H:93:VAL:CG1	3:H:100(P):MET:HB3	1.99	0.92
1:C:472:LEU:CB	1:C:491:LEU:HD21	1.99	0.92
1:A:248:ALA:CB	1:A:252:ARG:HB2	1.99	0.92
1:A:288:HIS:CE1	1:A:424:LEU:CD2	2.54	0.91
1:B:302:GLY:HA3	1:B:362:ASN:ND2	1.84	0.91
1:A:316:LYS:O	1:A:317:ILE:HG22	1.71	0.91
3:h:58:ASN:HD22	4:l:95:ARG:HH21	1.04	0.91
3:h:99:PHE:CE2	5:I:2:NAG:O7	2.24	0.90
3:H:100:TYR:CE1	5:G:2:NAG:C4	2.54	0.90
3:h:58:ASN:HD22	4:l:95:ARG:NH2	1.62	0.90
1:B:358:LEU:HA	1:B:378:LEU:CD2	2.01	0.90
1:C:472:LEU:HB2	1:C:491:LEU:CD2	2.03	0.89
1:C:3:CYS:HG	1:C:30:CYS:HG	1.06	0.89
1:B:317:ILE:HB	1:B:318:PRO:HD3	1.53	0.89
1:A:288:HIS:CE1	1:A:424:LEU:HD22	2.08	0.88
1:A:314:PHE:CE1	1:A:389:ILE:HD12	2.07	0.88
1:A:99:ARG:HE	1:A:251:LYS:HZ2	1.13	0.88
1:A:493:GLY:O	1:A:497:PHE:CD2	2.27	0.87
1:B:152:ILE:HD11	1:C:101:TRP:C	1.99	0.87
1:C:66:SER:HB3	1:C:118:LYS:HB3	1.56	0.87
1:C:362:ASN:OD1	1:C:362:ASN:O	1.92	0.87
1:B:465:GLN:HB3	1:B:498:LEU:HD21	1.55	0.86
1:A:15:MET:HG2	1:A:21:VAL:HG22	0.87	0.86
1:B:319:ALA:HB2	1:C:101:TRP:HE1	1.41	0.86
1:B:430:ASP:OD2	1:B:443:LYS:HE3	1.76	0.86
1:B:152:ILE:HD11	1:C:101:TRP:O	1.74	0.86
1:B:263:GLY:C	1:C:261:GLN:OE1	2.18	0.86
1:A:1:ILE:HG21	1:A:147:GLN:HE22	0.69	0.86
1:B:473:MET:HA	1:B:491:LEU:HD22	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LEU:HD12	1:C:378:LEU:CD1	2.06	0.85
1:A:60:CYS:SG	1:A:236:TRP:CH2	2.68	0.85
1:C:59:TYR:HB2	1:C:125:MET:SD	2.15	0.85
1:A:479:THR:OG1	1:A:484:ILE:CG2	2.24	0.85
1:B:62:GLU:HB3	1:B:122:SER:OG	1.75	0.85
1:A:1:ILE:HG12	1:A:147:GLN:CD	2.01	0.84
1:A:99:ARG:NH2	1:A:251:LYS:HZ3	1.75	0.84
3:h:58:ASN:ND2	4:l:95:ARG:CZ	2.41	0.84
1:B:263:GLY:HA3	1:C:261:GLN:CD	2.03	0.84
1:B:205:THR:HG22	1:B:210:HIS:ND1	1.93	0.83
1:B:480:LYS:O	1:B:481:ASN:OD1	1.97	0.83
2:E:39:ASN:OD1	2:F:10:ARG:NH1	2.12	0.83
1:A:262:GLU:HG2	1:A:266:HIS:NE2	1.94	0.83
1:A:66:SER:HB3	1:A:118:LYS:HB3	1.61	0.82
1:C:119:PHE:HZ	1:C:242:LEU:HD23	1.44	0.82
1:A:469:GLY:O	1:A:473:MET:HG2	1.78	0.82
1:A:125:MET:HE3	1:A:204:LEU:CD1	2.01	0.82
1:A:302:GLY:N	1:A:362:ASN:ND2	2.17	0.82
1:A:97:VAL:CG2	1:A:251:LYS:HA	2.06	0.81
1:B:466:ILE:HG13	1:B:498:LEU:HD22	1.60	0.81
1:C:101:TRP:CD1	1:C:108:PHE:HZ	1.90	0.81
1:A:241:ALA:CB	2:D:1:ALA:HB2	2.09	0.81
1:B:73:ARG:HG3	1:B:77:GLN:HB2	1.61	0.80
1:A:125:MET:CE	1:A:204:LEU:CD1	2.59	0.80
1:A:63:ALA:HB1	1:A:119:PHE:CE1	2.16	0.80
1:A:308:CYS:N	1:A:339:CYS:SG	2.54	0.80
1:C:316:LYS:O	1:C:317:ILE:CG1	2.22	0.80
1:C:332:TYR:O	1:C:371:ASN:HA	1.82	0.79
4:L:83:GLU:HA	4:L:104:LEU:O	1.81	0.79
1:C:466:ILE:HG13	1:C:498:LEU:HD13	1.64	0.79
1:B:48:THR:HG22	1:B:137:TYR:CD1	2.17	0.79
1:C:63:ALA:HB2	1:C:242:LEU:CG	2.13	0.79
1:A:60:CYS:SG	1:A:236:TRP:CE2	2.75	0.79
1:B:312:PHE:HD2	1:B:330:VAL:HG11	1.48	0.79
1:A:426:ASP:OD2	1:A:447:GLN:HA	1.83	0.79
1:C:22:ASP:HB3	1:C:433:SER:HB3	1.64	0.79
1:C:119:PHE:CZ	1:C:242:LEU:CD2	2.65	0.79
1:B:473:MET:CG	1:B:491:LEU:CD2	2.61	0.79
3:h:99:PHE:CD2	5:I:2:NAG:O7	2.35	0.79
1:A:239:LYS:O	1:A:240:GLU:HG3	1.84	0.78
1:B:302:GLY:CA	1:B:362:ASN:ND2	2.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:MET:N	1:C:491:LEU:HD21	1.99	0.78
1:A:222:PRO:HD2	2:D:4:LEU:HD23	1.63	0.78
1:C:63:ALA:HB2	1:C:242:LEU:HD21	0.81	0.78
1:A:479:THR:O	1:A:480:LYS:CG	2.32	0.77
1:B:317:ILE:CB	1:B:318:PRO:CD	2.61	0.77
1:B:267:THR:HG23	1:C:261:GLN:HE22	1.47	0.77
1:C:224:PRO:HA	1:C:238:ASN:HB3	1.66	0.77
1:C:358:LEU:HD12	1:C:378:LEU:HD11	1.66	0.77
1:A:27:HIS:CE1	1:A:45:LEU:HD23	2.20	0.77
1:A:309:THR:HG22	1:A:391:VAL:HG21	1.65	0.77
3:h:99:PHE:HE2	5:I:2:NAG:O7	1.68	0.77
1:C:3:CYS:SG	1:C:42:ASP:HB3	2.24	0.77
1:C:206:MET:HE1	1:C:262:GLU:HG3	1.67	0.76
1:B:216:GLU:OE2	2:E:10:ARG:NH2	2.19	0.76
1:C:188:LEU:HD11	1:C:291:CYS:HB3	1.67	0.76
3:h:67:PHE:CE2	3:h:82:MET:CE	2.67	0.76
1:B:263:GLY:CA	1:C:261:GLN:CD	2.59	0.76
3:h:58:ASN:HD21	4:l:95:ARG:HE	1.30	0.76
4:l:95:ARG:HH11	1:C:82:LEU:HD22	1.49	0.76
1:A:300:LEU:HD22	1:A:362:ASN:HB3	1.68	0.75
1:A:58:SER:CB	1:A:126:THR:HG22	2.16	0.75
1:B:312:PHE:HD2	1:B:330:VAL:CG1	2.00	0.75
1:A:288:HIS:CE1	1:A:424:LEU:CD1	2.69	0.75
3:h:58:ASN:HD21	4:l:95:ARG:NE	1.82	0.75
1:C:119:PHE:CE1	1:C:242:LEU:CD2	2.67	0.75
1:C:119:PHE:HE1	1:C:242:LEU:HD23	1.47	0.74
1:A:58:SER:HB2	1:A:126:THR:HG22	1.70	0.74
1:C:74:CYS:CB	1:C:75:PRO:CD	2.62	0.74
1:A:77:GLN:HE21	1:A:77:GLN:N	1.84	0.74
1:A:260:SER:O	1:A:262:GLU:N	2.21	0.74
3:H:99:PHE:CD2	5:G:2:NAG:O7	2.40	0.74
1:B:161:ASP:OD2	1:B:164:ARG:NH1	2.21	0.74
1:B:222:PRO:HG3	2:E:3:THR:OG1	1.87	0.74
1:C:74:CYS:O	1:C:111:GLY:HA2	1.87	0.74
1:A:150:GLY:HA3	5:G:1:NAG:O7	1.86	0.73
1:A:99:ARG:NE	1:A:251:LYS:NZ	2.35	0.73
1:A:3:CYS:HG	1:A:30:CYS:HG	1.29	0.73
1:A:339:CYS:SG	1:A:340:LYS:N	2.61	0.73
1:C:63:ALA:CB	1:C:242:LEU:CD2	2.51	0.73
1:A:3:CYS:SG	1:A:42:ASP:HB3	2.28	0.73
1:C:48:THR:CG2	1:C:137:TYR:CD1	2.72	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:HIS:CD2	1:B:285:SER:O	2.42	0.73
1:C:72:SER:HB3	1:C:113:LEU:HD12	1.69	0.73
1:B:312:PHE:CD2	1:B:330:VAL:HG11	2.24	0.72
3:H:100:TYR:CZ	5:G:2:NAG:H4	2.23	0.72
2:E:74:TYR:HH	2:F:9:THR:HG1	1.34	0.72
1:A:248:ALA:HB3	1:A:252:ARG:CB	2.18	0.72
1:A:14:GLY:O	1:A:15:MET:HG3	1.89	0.72
4:L:78:LEU:HD11	4:L:104:LEU:HD21	1.70	0.72
1:B:473:MET:CG	1:B:491:LEU:HD21	2.19	0.72
1:B:263:GLY:HA3	1:C:261:GLN:HA	1.72	0.72
1:B:358:LEU:CA	1:B:378:LEU:CD2	2.63	0.72
1:B:153:VAL:HG11	1:C:102:GLY:O	1.90	0.71
1:C:262:GLU:HG2	1:C:266:HIS:NE2	2.06	0.71
1:B:263:GLY:HA3	1:C:261:GLN:OE1	1.90	0.71
1:B:320:GLU:HB2	1:B:400:TRP:HZ2	1.55	0.71
1:B:473:MET:CB	1:B:491:LEU:HD21	2.05	0.71
1:C:76:THR:O	1:C:77:GLN:NE2	2.23	0.71
1:C:202:TYR:HE1	1:C:215:LYS:HG2	1.55	0.71
1:A:229:ALA:HB3	1:C:73:ARG:HH22	1.49	0.71
1:A:288:HIS:HE1	1:A:424:LEU:CD1	2.05	0.70
1:A:288:HIS:CE1	1:A:424:LEU:HD13	2.26	0.70
1:B:330:VAL:HG21	1:B:389:ILE:HD13	1.73	0.70
1:B:48:THR:HG22	1:B:137:TYR:HD1	1.56	0.70
1:C:462:TRP:HA	1:C:498:LEU:HD22	1.73	0.70
1:A:288:HIS:NE2	1:A:424:LEU:HD22	2.06	0.70
1:A:314:PHE:CZ	1:A:389:ILE:HD12	2.25	0.70
1:B:97:VAL:HG13	1:B:251:LYS:HA	1.74	0.70
1:A:150:GLY:O	5:G:1:NAG:C8	2.39	0.69
3:h:101:ASP:OD1	4:l:46:LEU:CD1	2.40	0.69
1:B:465:GLN:HG2	1:B:494:VAL:HG13	1.74	0.69
1:C:241:ALA:CB	2:F:1:ALA:HB2	2.18	0.69
1:C:473:MET:N	1:C:491:LEU:CD2	2.54	0.69
1:A:214:HIS:ND1	1:A:215:LYS:O	2.25	0.69
1:B:1:ILE:HG13	1:B:152:ILE:HG22	1.75	0.69
1:B:263:GLY:CA	1:C:261:GLN:OE1	2.40	0.69
1:C:472:LEU:CA	1:C:491:LEU:HD21	2.23	0.69
1:C:58:SER:HB2	1:C:125:MET:O	1.93	0.69
4:l:56:SER:HB3	5:I:3:BMA:O4	1.91	0.69
1:A:99:ARG:NH2	1:A:251:LYS:NZ	2.41	0.69
1:B:27:HIS:HE2	1:C:249:HIS:CE1	2.12	0.68
1:C:460:MET:HG3	1:C:465:GLN:HE21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:101:ASP:OD1	4:l:46:LEU:HD12	1.93	0.68
1:A:15:MET:CG	1:A:21:VAL:HG21	2.20	0.68
1:C:363:PRO:HB3	1:C:374:MET:HE1	1.75	0.68
1:B:48:THR:CG2	1:B:137:TYR:CD1	2.76	0.68
3:h:52:ASN:O	3:h:71:ARG:NH1	2.27	0.68
3:h:62:PHE:CE1	3:h:63:VAL:HG23	2.28	0.68
3:h:101:ASP:OD1	4:l:46:LEU:CG	2.39	0.68
1:A:358:LEU:CD2	1:A:360:THR:OG1	2.41	0.68
1:B:469:GLY:C	1:B:491:LEU:CD1	2.66	0.68
1:A:1:ILE:HG12	1:A:147:GLN:HE21	0.51	0.68
3:H:100:TYR:HE1	5:G:2:NAG:H4	1.48	0.68
1:A:229:ALA:CB	1:C:73:ARG:NH2	2.23	0.67
1:A:75:PRO:HG2	1:A:107:LEU:HB3	1.76	0.67
2:D:26:THR:HG22	2:D:30:ILE:HD12	1.76	0.67
1:B:317:ILE:HB	1:B:318:PRO:HD2	1.76	0.67
1:A:63:ALA:CB	1:A:119:PHE:CE1	2.78	0.67
1:A:316:LYS:O	1:A:317:ILE:CG2	2.42	0.67
1:B:32:THR:HG22	1:B:42:ASP:OD1	1.94	0.67
1:B:205:THR:CG2	1:B:210:HIS:ND1	2.57	0.67
1:C:48:THR:CG2	1:C:137:TYR:HD1	2.03	0.67
1:C:100:GLY:C	1:C:108:PHE:HE1	2.03	0.67
1:A:294:LYS:HE2	1:B:350:GLN:HG2	1.77	0.67
2:E:38:ARG:NH2	1:C:220:ASP:OD2	2.28	0.67
3:h:99:PHE:HE2	5:I:2:NAG:C7	2.08	0.66
1:A:99:ARG:CZ	1:A:251:LYS:NZ	2.58	0.66
1:C:202:TYR:CE1	1:C:215:LYS:HG2	2.30	0.66
1:C:205:THR:CG2	1:C:210:HIS:ND1	2.55	0.66
1:B:27:HIS:NE2	1:C:249:HIS:CE1	2.63	0.66
1:A:1:ILE:HG12	1:A:147:GLN:CG	2.26	0.66
1:C:472:LEU:C	1:C:491:LEU:HD21	2.20	0.66
1:B:6:VAL:HG12	1:B:8:ASN:H	1.60	0.66
1:B:220:ASP:OD2	2:F:38:ARG:NE	2.25	0.66
1:A:152:ILE:HD11	1:A:375:MET:HE1	1.77	0.66
1:B:460:MET:HE3	1:B:468:ILE:CD1	2.08	0.66
1:A:288:HIS:CE1	1:A:424:LEU:HD21	2.31	0.65
1:B:302:GLY:CA	1:B:362:ASN:HD21	2.09	0.65
1:A:48:THR:CG2	1:A:137:TYR:CD1	2.80	0.65
3:H:99:PHE:CE2	5:G:2:NAG:O7	2.49	0.65
1:A:317:ILE:HG12	1:A:318:PRO:HD2	0.80	0.64
1:C:152:ILE:HG22	1:C:153:VAL:HG23	1.79	0.64
1:A:24:VAL:HG11	1:A:288:HIS:CE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:HD2	1:A:396:ILE:HD12	1.48	0.64
3:h:33:TRP:HB2	3:h:95:ASP:HB3	1.79	0.64
1:C:188:LEU:CD1	1:C:291:CYS:HB3	2.26	0.64
1:C:74:CYS:HG	1:C:105:CYS:HG	1.45	0.64
3:h:101:ASP:CG	4:l:46:LEU:HB2	2.06	0.64
1:C:71:ASP:OD1	1:C:72:SER:N	2.31	0.64
1:A:197:ASP:O	1:A:199:SER:N	2.29	0.64
1:B:460:MET:HE1	1:B:468:ILE:HD12	1.77	0.64
1:A:63:ALA:HB1	1:A:119:PHE:HE1	1.60	0.64
1:C:276:GLU:OE1	1:C:283:ARG:NH2	2.31	0.64
1:B:27:HIS:NE2	1:C:249:HIS:ND1	2.45	0.63
1:C:72:SER:HB3	1:C:113:LEU:CD1	2.28	0.63
1:A:363:PRO:O	1:A:364:VAL:CG2	2.39	0.63
1:A:460:MET:SD	1:A:468:ILE:CD1	2.84	0.63
1:A:97:VAL:CG2	1:A:251:LYS:CA	2.69	0.63
1:C:63:ALA:CB	1:C:242:LEU:CG	2.74	0.63
1:A:239:LYS:O	1:A:240:GLU:CG	2.46	0.63
4:L:49:TYR:OH	4:L:53:LYS:NZ	2.30	0.63
1:B:319:ALA:CB	1:C:101:TRP:NE1	2.57	0.63
1:C:358:LEU:CD1	1:C:378:LEU:HD11	2.28	0.63
1:C:188:LEU:HD11	1:C:291:CYS:CB	2.28	0.63
1:A:314:PHE:CE2	1:A:396:ILE:HD11	2.24	0.62
1:A:99:ARG:CZ	1:A:251:LYS:HZ3	2.11	0.62
1:B:26:GLU:OE1	2:E:15:ARG:NH1	2.32	0.62
1:A:2:ARG:NH2	1:A:140:MET:SD	2.73	0.62
1:A:99:ARG:HE	1:A:251:LYS:NZ	1.92	0.62
1:B:473:MET:HG3	1:B:491:LEU:CD2	2.29	0.62
1:C:238:ASN:O	1:C:240:GLU:HG2	1.99	0.62
1:A:462:TRP:CD1	1:A:498:LEU:HD22	2.33	0.62
1:B:317:ILE:CG1	1:B:318:PRO:HD2	2.30	0.62
3:h:90:TYR:O	3:h:106:GLY:HA2	1.98	0.62
1:A:127:GLY:HA3	1:A:218:PHE:CE2	2.35	0.62
3:H:94:ARG:NH2	3:H:101:ASP:OD2	2.30	0.61
4:l:35:TRP:HB2	4:l:48:ILE:HB	1.82	0.61
1:C:10:ASP:CG	1:C:416:ARG:HE	2.07	0.61
1:C:169:ILE:HD11	1:C:188:LEU:HD23	1.83	0.61
1:A:314:PHE:HE2	1:A:396:ILE:CB	2.11	0.61
1:B:302:GLY:N	1:B:362:ASN:HD21	1.96	0.61
1:A:479:THR:C	1:A:480:LYS:HG2	2.25	0.61
1:B:150:GLY:C	5:I:1:NAG:O7	2.44	0.61
1:A:22:ASP:HB2	1:A:433:SER:OG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG11	1:A:288:HIS:HE1	1.66	0.61
3:h:63:VAL:HG13	3:h:67:PHE:HD1	1.66	0.61
1:A:27:HIS:ND1	1:A:45:LEU:HD23	2.16	0.60
2:E:9:THR:OG1	2:F:74:TYR:OH	2.13	0.60
1:B:319:ALA:HB2	1:C:101:TRP:NE1	2.16	0.60
1:C:262:GLU:HG2	1:C:266:HIS:CD2	2.35	0.60
1:B:314:PHE:HE2	1:B:398:HIS:HB2	1.66	0.60
3:h:63:VAL:HG22	3:h:67:PHE:CE1	2.36	0.60
1:A:213:VAL:CG1	1:A:217:TRP:CE3	2.84	0.60
1:A:251:LYS:HG2	1:A:251:LYS:O	2.01	0.60
3:h:22:CYS:HB3	3:h:78:LEU:HB3	1.83	0.60
1:A:97:VAL:CG2	1:A:251:LYS:CB	2.68	0.60
1:B:16:SER:HB2	1:B:434:VAL:HG11	1.84	0.60
1:B:267:THR:HG23	1:C:261:GLN:NE2	2.16	0.60
1:C:138:ARG:NH1	1:C:168:GLU:OE2	2.34	0.60
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.83	0.60
1:B:133:GLU:HG3	1:B:134:ASN:HD22	1.66	0.60
1:B:302:GLY:H	1:B:362:ASN:HD21	1.47	0.60
1:B:73:ARG:HG3	1:B:73:ARG:O	2.02	0.60
1:B:91:VAL:O	1:B:116:CYS:HA	2.02	0.60
1:A:32:THR:HG22	1:A:42:ASP:CG	2.27	0.59
3:h:63:VAL:HG11	3:h:67:PHE:HB2	1.82	0.59
1:B:152:ILE:CD1	1:C:101:TRP:O	2.48	0.59
1:A:58:SER:HB3	1:A:126:THR:HG22	1.84	0.59
1:B:32:THR:HG22	1:B:42:ASP:CG	2.27	0.59
1:A:426:ASP:CG	1:A:447:GLN:HA	2.27	0.59
1:B:138:ARG:HH11	1:B:166:LYS:HD2	1.68	0.59
3:h:100(C):SER:HB3	5:I:1:NAG:HN2	1.67	0.59
1:A:22:ASP:CB	1:A:433:SER:OG	2.50	0.59
1:A:63:ALA:CB	1:A:119:PHE:HE1	2.14	0.59
1:B:125:MET:HE3	1:B:204:LEU:HD11	1.84	0.59
1:A:213:VAL:CG1	1:A:217:TRP:HE3	2.16	0.59
1:A:460:MET:HE1	1:A:468:ILE:HD13	1.85	0.59
1:A:493:GLY:O	1:A:497:PHE:HD2	1.82	0.59
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.85	0.58
1:A:358:LEU:HD23	1:A:360:THR:OG1	2.02	0.58
2:E:2:VAL:HG11	2:F:27:LYS:HE2	1.85	0.58
3:h:50:ARG:NE	3:h:58:ASN:OD1	2.28	0.58
1:B:97:VAL:HG13	1:B:250:ALA:O	2.04	0.58
1:C:74:CYS:HB2	1:C:77:GLN:HG2	1.85	0.58
1:A:14:GLY:O	1:A:15:MET:CG	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:CG1	1:A:288:HIS:CE1	2.87	0.58
1:A:222:PRO:HG3	2:D:3:THR:OG1	2.03	0.58
1:A:481:ASN:OD1	1:A:482:GLY:N	2.29	0.58
1:B:260:SER:O	1:B:262:GLU:N	2.37	0.58
1:B:430:ASP:OD2	1:B:443:LYS:CE	2.50	0.58
2:E:10:ARG:NH1	2:F:39:ASN:OD1	2.36	0.58
3:h:82(C):LEU:HD22	3:h:111:VAL:HG21	1.85	0.58
1:B:360:THR:O	1:B:361:ALA:HB2	2.03	0.57
1:C:241:ALA:HB1	2:F:1:ALA:CB	2.21	0.57
1:C:358:LEU:HD23	1:C:360:THR:O	2.05	0.57
1:B:88:THR:O	1:B:239:LYS:NZ	2.27	0.57
4:l:18:SER:HA	4:l:75:ILE:O	2.05	0.57
1:A:99:ARG:HH21	1:A:251:LYS:HD3	1.69	0.57
1:A:288:HIS:HE1	1:A:424:LEU:HD11	1.70	0.57
4:l:19:ILE:HG21	4:l:104:LEU:HD11	1.85	0.57
1:C:63:ALA:CB	1:C:242:LEU:HD11	2.34	0.57
1:B:97:VAL:HG21	1:B:113:LEU:HD22	1.86	0.57
1:C:46:VAL:HG12	1:C:47:THR:HG23	1.85	0.57
1:A:246:LYS:HG3	1:A:254:THR:OG1	2.05	0.57
1:C:316:LYS:C	1:C:317:ILE:HG13	2.19	0.57
1:A:99:ARG:HH21	1:A:251:LYS:NZ	2.02	0.57
1:A:479:THR:HG1	1:A:484:ILE:HG22	1.69	0.56
1:B:19:THR:HG1	1:B:20:TRP:CD1	2.22	0.56
1:B:34:MET:SD	1:B:359:ILE:HD13	2.45	0.56
2:E:27:LYS:HE2	2:F:2:VAL:HG11	1.86	0.56
1:C:49:THR:HG22	1:C:283:ARG:HG2	1.86	0.56
3:H:100:TYR:CD1	5:G:2:NAG:O5	2.58	0.56
1:B:76:THR:O	1:B:77:GLN:NE2	2.38	0.56
3:h:58:ASN:HD21	4:l:95:ARG:CZ	2.13	0.56
1:C:59:TYR:CE1	1:C:225:TRP:HB3	2.40	0.56
1:C:115:THR:OG1	1:C:253:GLN:OE1	2.13	0.56
1:A:307:LEU:CD1	1:A:340:LYS:HD3	2.35	0.56
1:B:462:TRP:O	1:B:466:ILE:HD12	2.04	0.56
1:B:97:VAL:CG1	1:B:251:LYS:HA	2.35	0.56
1:A:493:GLY:C	1:A:497:PHE:CE2	2.83	0.56
1:B:300:LEU:HD22	1:B:362:ASN:OD1	2.05	0.56
1:C:119:PHE:HE1	1:C:242:LEU:CD2	2.14	0.56
1:A:276:GLU:OE2	1:A:283:ARG:NH2	2.39	0.56
3:H:35:HIS:NE2	3:H:95:ASP:OD2	2.39	0.56
2:E:26:THR:O	2:E:30:ILE:HB	2.06	0.55
1:A:99:ARG:HH21	1:A:251:LYS:CE	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LYS:O	1:A:317:ILE:CB	2.50	0.55
1:B:430:ASP:CG	1:B:443:LYS:HE3	2.30	0.55
1:B:460:MET:HE2	1:B:465:GLN:HA	1.87	0.55
1:A:8:ASN:HD21	2:D:15:ARG:HD3	1.71	0.55
1:A:74:CYS:CB	1:A:77:GLN:CG	2.47	0.55
1:A:314:PHE:HE1	1:A:389:ILE:HD12	1.69	0.55
1:C:225:TRP:HZ2	1:C:237:ASN:ND2	1.99	0.55
1:C:363:PRO:CB	1:C:374:MET:HE1	2.36	0.55
1:B:48:THR:CG2	1:B:137:TYR:HD1	2.17	0.55
4:L:88:CYS:O	4:L:99:GLY:N	2.37	0.55
1:B:196:LEU:HD22	1:B:287:GLY:HA2	1.89	0.55
1:A:213:VAL:HG11	1:A:217:TRP:CE3	2.42	0.54
1:C:194:THR:O	1:C:194:THR:OG1	2.25	0.54
1:C:384:ASP:OD1	1:C:401:HIS:ND1	2.34	0.54
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.89	0.54
1:B:364:VAL:HG12	1:B:365:ILE:N	2.22	0.54
1:C:3:CYS:O	1:C:9:ARG:HD3	2.07	0.54
1:C:133:GLU:HA	1:C:171:PRO:HG2	1.90	0.54
1:C:472:LEU:HB2	1:C:491:LEU:HD23	1.88	0.54
1:C:472:LEU:CB	1:C:491:LEU:CD2	2.72	0.54
1:A:27:HIS:CE1	1:A:45:LEU:CD2	2.88	0.54
1:B:147:GLN:NE2	1:B:163:ASN:OD1	2.41	0.54
1:A:59:TYR:CE1	1:A:225:TRP:HB3	2.42	0.54
1:B:154:ASN:HD21	1:B:164:ARG:HH22	1.55	0.54
1:A:148:HIS:CD2	1:A:150:GLY:H	2.25	0.54
1:C:466:ILE:CG1	1:C:498:LEU:HD13	2.35	0.54
1:A:125:MET:HE2	1:A:204:LEU:HD11	1.81	0.54
1:C:119:PHE:HZ	1:C:242:LEU:CD2	2.09	0.54
1:A:172:ASN:OD1	1:B:317:ILE:HG22	2.08	0.53
2:F:26:THR:O	2:F:30:ILE:HB	2.08	0.53
1:A:224:PRO:N	1:A:238:ASN:HD22	2.06	0.53
2:D:26:THR:O	2:D:30:ILE:HG13	2.09	0.53
1:B:475:LEU:HD23	1:B:487:MET:HE2	1.91	0.53
1:A:150:GLY:O	5:G:1:NAG:H81	2.09	0.53
1:B:426:ASP:O	1:B:429:TRP:N	2.41	0.53
1:C:238:ASN:OD1	1:C:240:GLU:CB	2.41	0.53
1:B:24:VAL:HG21	1:B:427:THR:HG22	1.90	0.53
3:h:58:ASN:HD21	4:l:95:ARG:NH2	1.99	0.53
1:C:63:ALA:HB3	1:C:242:LEU:HD11	1.89	0.53
1:A:376:LEU:HD13	1:A:378:LEU:HD21	1.90	0.52
1:B:144:HIS:HB3	1:B:360:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:ASN:OD1	1:C:482:GLY:N	2.32	0.52
1:C:126:THR:OG1	1:C:205:THR:OG1	2.27	0.52
1:A:307:LEU:HD23	1:A:342:PRO:HB3	1.91	0.52
1:A:493:GLY:O	1:A:497:PHE:CE2	2.62	0.52
1:B:480:LYS:O	1:B:481:ASN:CG	2.51	0.52
1:C:74:CYS:HB2	1:C:77:GLN:CG	2.40	0.52
1:A:466:ILE:N	1:A:498:LEU:HD11	2.24	0.52
2:E:38:ARG:HD2	1:C:216:GLU:HB3	1.92	0.52
1:C:358:LEU:CD1	1:C:378:LEU:CD1	2.84	0.52
4:L:30:TYR:HA	4:L:33:VAL:HG23	1.92	0.52
4:I:83:GLU:HA	4:I:104:LEU:O	2.08	0.52
1:A:426:ASP:OD2	1:A:447:GLN:HG3	2.10	0.52
1:B:70:SER:HB3	1:B:115:THR:HG22	1.92	0.52
4:I:95:ARG:NH1	1:C:82:LEU:HD22	2.20	0.52
1:C:240:GLU:O	1:C:241:ALA:HB3	2.09	0.52
1:A:460:MET:CE	1:A:468:ILE:CD1	2.87	0.52
1:C:61:TYR:CD2	1:C:262:GLU:HB2	2.45	0.52
1:B:66:SER:HB3	1:B:118:LYS:HB3	1.92	0.51
1:B:358:LEU:CA	1:B:378:LEU:HD22	2.03	0.51
1:C:61:TYR:HB3	1:C:125:MET:HE3	1.91	0.51
1:B:330:VAL:HG21	1:B:389:ILE:CD1	2.39	0.51
1:B:481:ASN:H	1:B:484:ILE:HG23	1.75	0.51
1:C:235:HIS:O	1:C:235:HIS:ND1	2.43	0.51
1:C:317:ILE:HG23	1:C:318:PRO:HD2	1.92	0.51
1:A:74:CYS:SG	1:A:77:GLN:CG	2.98	0.51
1:A:207:ASN:OD1	1:A:207:ASN:N	2.43	0.51
1:A:77:GLN:HE21	1:A:77:GLN:CA	2.23	0.51
1:A:302:GLY:H	1:A:362:ASN:HD22	0.66	0.51
1:B:248:ALA:HB3	1:B:252:ARG:HB2	1.92	0.51
1:A:239:LYS:C	1:A:240:GLU:HG3	2.34	0.51
1:C:152:ILE:HD11	1:C:375:MET:HE1	1.92	0.51
1:C:188:LEU:HG	1:C:190:CYS:SG	2.51	0.51
1:A:307:LEU:HD11	1:A:340:LYS:HD3	1.92	0.51
1:A:58:SER:O	1:A:236:TRP:HZ3	1.93	0.51
1:A:175:ARG:CD	1:A:189:ASP:OD1	2.56	0.51
1:C:100:GLY:O	1:C:108:PHE:HE1	1.93	0.51
2:F:24:GLU:O	2:F:27:LYS:HB3	2.11	0.51
1:C:34:MET:HE1	1:C:357:ARG:HD2	1.93	0.50
2:F:3:THR:OG1	2:F:4:LEU:N	2.44	0.50
1:A:247:ASP:OD1	1:A:248:ALA:N	2.45	0.50
1:B:202:TYR:CE1	1:B:215:LYS:HE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:ARG:HG2	3:H:58:ASN:HB2	1.93	0.50
2:E:74:TYR:OH	2:F:9:THR:OG1	2.10	0.50
1:A:1:ILE:HG23	1:A:147:GLN:HE22	1.57	0.50
1:A:460:MET:HE1	1:A:468:ILE:CD1	2.41	0.50
1:B:3:CYS:SG	1:B:42:ASP:HB3	2.51	0.50
1:B:222:PRO:HG3	2:E:3:THR:HG1	1.76	0.50
1:C:2:ARG:NH2	1:C:140:MET:HB2	2.25	0.50
1:B:317:ILE:HD12	1:B:318:PRO:HD2	1.93	0.50
1:C:124:LYS:O	1:C:125:MET:HB2	2.11	0.50
1:C:473:MET:H	1:C:491:LEU:CD2	2.23	0.50
1:C:317:ILE:CG2	1:C:318:PRO:HD2	2.42	0.50
1:A:45:LEU:HD12	1:A:139:ILE:HG12	1.93	0.50
1:B:62:GLU:CB	1:B:122:SER:OG	2.55	0.50
1:A:48:THR:CG2	1:A:137:TYR:CE1	2.95	0.50
1:A:70:SER:HB3	1:A:115:THR:HG22	1.93	0.50
1:A:341:VAL:HG11	1:A:374:MET:HE1	1.93	0.50
1:C:169:ILE:HD11	1:C:188:LEU:CD2	2.41	0.50
1:A:20:TRP:HZ3	1:A:22:ASP:OD1	1.94	0.50
2:E:51:TRP:HA	2:E:60:LYS:HD2	1.94	0.50
1:A:60:CYS:SG	1:A:236:TRP:CZ3	3.03	0.49
1:A:74:CYS:SG	1:A:77:GLN:HG3	2.51	0.49
1:B:460:MET:CE	1:B:468:ILE:CD1	2.70	0.49
3:h:63:VAL:HG22	3:h:67:PHE:CD1	2.47	0.49
1:A:345:MET:HE2	1:A:378:LEU:HD12	1.93	0.49
1:B:49:THR:HG22	1:B:283:ARG:HG2	1.95	0.49
1:C:230:ASP:N	1:C:230:ASP:OD1	2.39	0.49
1:C:236:TRP:O	1:C:239:LYS:HG3	2.12	0.49
1:B:59:TYR:O	1:B:124:LYS:HB2	2.11	0.49
1:B:426:ASP:N	1:B:426:ASP:OD1	2.45	0.49
1:C:70:SER:HB3	1:C:115:THR:HG22	1.95	0.49
1:B:384:ASP:OD1	1:B:401:HIS:ND1	2.39	0.49
3:h:32:HIS:HD2	3:h:96:GLY:HA2	1.77	0.49
1:A:204:LEU:HD22	1:A:213:VAL:HG21	1.94	0.49
1:B:155:ASP:OD1	1:B:156:THR:N	2.42	0.49
1:B:466:ILE:CG1	1:B:498:LEU:HD13	2.42	0.49
3:h:37:VAL:HG13	3:h:47:TRP:HA	1.94	0.49
1:C:101:TRP:CG	1:C:108:PHE:CZ	2.87	0.49
1:B:462:TRP:HA	1:B:498:LEU:CD2	2.43	0.49
1:C:144:HIS:HB3	1:C:360:THR:HG23	1.94	0.49
1:A:175:ARG:HG3	1:A:189:ASP:CG	2.20	0.49
1:C:10:ASP:OD1	1:C:416:ARG:NE	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:HIS:CD2	1:A:287:GLY:O	2.63	0.48
4:L:59:SER:CB	4:L:61:ARG:NH1	2.76	0.48
1:B:272:ALA:HB2	2:E:7:HIS:CD2	2.47	0.48
1:C:61:TYR:HB3	1:C:125:MET:CE	2.43	0.48
1:C:169:ILE:HD13	1:C:190:CYS:SG	2.53	0.48
1:A:127:GLY:HA3	1:A:218:PHE:CZ	2.47	0.48
1:A:300:LEU:HD22	1:A:362:ASN:CB	2.41	0.48
1:A:314:PHE:CZ	1:A:396:ILE:HG13	2.44	0.48
4:L:56:SER:CB	5:I:3:BMA:O4	2.60	0.48
1:C:136:GLU:HB3	1:C:170:THR:HG22	1.95	0.48
1:C:213:VAL:CG1	1:C:217:TRP:CE3	2.96	0.48
3:H:100(P):MET:HE1	4:L:98:PHE:HZ	1.78	0.48
4:L:56:SER:HB3	5:G:3:BMA:O4	2.13	0.48
1:B:88:THR:C	1:B:239:LYS:HZ3	2.17	0.48
1:B:207:ASN:N	1:B:207:ASN:OD1	2.46	0.48
4:L:23:CYS:HB2	4:L:35:TRP:CH2	2.49	0.48
1:A:91:VAL:O	1:A:116:CYS:HA	2.13	0.48
3:H:47:TRP:HZ2	3:H:50:ARG:HB3	1.78	0.48
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.95	0.48
3:H:52:ASN:O	3:H:71:ARG:NH1	2.41	0.48
1:C:484:ILE:HG13	1:C:485:SER:H	1.77	0.48
1:A:61:TYR:O	1:A:261:GLN:HB2	2.14	0.48
1:A:320:GLU:HB2	1:A:400:TRP:CH2	2.48	0.48
1:C:6:VAL:HG21	1:C:30:CYS:SG	2.53	0.48
3:h:63:VAL:CG2	3:h:67:PHE:CD1	2.97	0.48
4:L:37:GLN:HB2	4:L:47:MET:SD	2.53	0.48
1:A:314:PHE:CE2	1:A:396:ILE:CB	2.93	0.48
1:A:320:GLU:HB2	1:A:400:TRP:CZ2	2.49	0.48
1:B:312:PHE:CD2	1:B:330:VAL:CG1	2.88	0.48
1:C:462:TRP:O	1:C:466:ILE:HD12	2.14	0.48
1:B:263:GLY:C	1:C:261:GLN:CD	2.79	0.47
1:A:99:ARG:HH21	1:A:251:LYS:CD	2.27	0.47
3:H:82:MET:HB3	3:H:82(C):LEU:HD21	1.96	0.47
1:B:263:GLY:HA3	1:C:261:GLN:CA	2.41	0.47
2:E:49:ILE:HG12	1:C:472:LEU:HD21	1.96	0.47
1:A:479:THR:OG1	1:A:484:ILE:HG23	2.13	0.47
1:B:222:PRO:HG2	2:E:1:ALA:HB3	1.97	0.47
1:C:315:THR:CG2	1:C:331:GLN:HB2	2.45	0.47
4:L:36:TYR:HE1	4:L:89:CYS:HB3	1.79	0.47
1:A:462:TRP:CE2	1:A:466:ILE:HD11	2.49	0.47
1:C:241:ALA:O	1:C:258:LEU:CD1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TYR:O	1:A:371:ASN:HA	2.13	0.47
1:B:262:GLU:OE1	1:C:259:GLY:HA3	2.14	0.47
1:B:317:ILE:CG1	1:B:318:PRO:CD	2.92	0.47
2:E:10:ARG:NH1	2:F:39:ASN:HD21	2.12	0.47
1:C:14:GLY:HA3	1:C:21:VAL:HG21	1.97	0.47
1:C:317:ILE:CG2	1:C:318:PRO:CD	2.93	0.47
2:E:14:THR:OG1	2:E:15:ARG:N	2.47	0.47
1:C:100:GLY:C	1:C:108:PHE:CE1	2.88	0.47
1:A:224:PRO:CA	1:A:238:ASN:HD22	2.28	0.47
1:A:317:ILE:CG1	1:A:318:PRO:CD	2.58	0.47
1:A:430:ASP:HA	1:A:433:SER:HB3	1.96	0.47
3:h:58:ASN:HD22	4:l:95:ARG:CZ	2.15	0.47
1:C:429:TRP:CD1	1:C:446:HIS:HD1	2.33	0.47
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.76	0.47
1:A:213:VAL:HG11	1:A:217:TRP:HE3	1.78	0.47
1:B:22:ASP:HB2	1:B:433:SER:OG	2.14	0.47
4:l:20:THR:HA	4:l:73:LEU:O	2.15	0.47
1:C:35:ALA:HB3	1:C:38:LYS:HB2	1.96	0.47
1:C:341:VAL:HB	1:C:363:PRO:HB2	1.97	0.47
1:A:473:MET:HG2	1:A:491:LEU:HD22	1.96	0.46
1:B:7:SER:OG	1:C:98:ASP:OD2	2.30	0.46
4:l:30:TYR:HA	4:l:33:VAL:HG23	1.96	0.46
1:C:269:LEU:O	2:F:19:TRP:HD1	1.99	0.46
1:B:150:GLY:O	1:B:152:ILE:N	2.49	0.46
1:B:263:GLY:O	1:C:261:GLN:NE2	2.49	0.46
3:h:35:HIS:HB2	3:h:93:VAL:HB	1.96	0.46
1:B:115:THR:HG21	1:B:253:GLN:HB2	1.96	0.46
1:B:459:GLY:C	1:B:460:MET:HG3	2.39	0.46
3:h:100(B):ASP:OD1	3:h:100(D):THR:OG1	2.29	0.46
1:C:213:VAL:HG11	1:C:217:TRP:CE3	2.51	0.46
1:B:20:TRP:HA	1:B:293:LEU:O	2.15	0.46
1:A:340:LYS:HA	1:A:364:VAL:HG22	1.97	0.46
1:C:205:THR:HG22	1:C:210:HIS:CE1	2.46	0.46
1:A:14:GLY:C	1:A:15:MET:HG3	2.40	0.46
2:E:52:LEU:HB2	1:C:475:LEU:HD21	1.98	0.46
1:C:100:GLY:O	1:C:108:PHE:CE1	2.67	0.46
1:A:62:GLU:HB3	1:A:122:SER:O	2.16	0.46
1:A:77:GLN:CA	1:A:77:GLN:NE2	2.79	0.46
1:B:74:CYS:O	1:B:105:CYS:SG	2.74	0.46
1:B:89:GLN:C	1:B:239:LYS:HZ2	2.23	0.46
3:h:63:VAL:CG1	3:h:67:PHE:CD1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:HG3	1:C:134:ASN:HD22	1.81	0.46
1:B:358:LEU:HA	1:B:378:LEU:HD23	1.89	0.46
1:C:196:LEU:O	1:C:198:PHE:N	2.48	0.46
1:A:213:VAL:HG13	1:A:217:TRP:CE3	2.50	0.46
4:L:23:CYS:HB2	4:L:35:TRP:CH2	2.50	0.46
4:L:28:ASP:N	4:L:28:ASP:OD1	2.47	0.46
4:L:96:LEU:HD23	4:L:96:LEU:HA	1.84	0.46
1:B:430:ASP:OD1	1:B:443:LYS:HD2	2.15	0.46
1:C:206:MET:CE	1:C:262:GLU:HG3	2.43	0.46
1:B:392:GLY:C	1:B:394:LYS:H	2.24	0.46
1:A:384:ASP:OD1	1:A:401:HIS:ND1	2.43	0.45
1:A:493:GLY:C	1:A:497:PHE:CD2	2.93	0.45
3:H:100(C):SER:HB3	5:G:1:NAG:HN2	1.81	0.45
1:B:466:ILE:HG12	1:B:498:LEU:HD13	1.97	0.45
3:h:29:TYR:CD2	3:h:76:ASN:HA	2.51	0.45
1:C:317:ILE:HG22	1:C:318:PRO:N	2.31	0.45
1:A:294:LYS:NZ	1:B:349:MET:HB2	2.31	0.45
1:B:153:VAL:HG12	5:I:1:NAG:H82	1.98	0.45
1:B:400:TRP:HZ3	1:B:402:ARG:HB2	1.80	0.45
1:A:53:MET:HE3	1:A:53:MET:HB2	1.87	0.45
1:A:473:MET:CG	1:A:491:LEU:HD22	2.46	0.45
1:B:74:CYS:C	1:B:105:CYS:SG	2.99	0.45
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.68	0.45
4:l:47:MET:HE1	4:l:86:TYR:HD2	1.82	0.45
1:B:48:THR:HG21	1:B:137:TYR:CD1	2.52	0.45
1:B:473:MET:HB2	1:B:491:LEU:CD1	2.45	0.45
1:C:72:SER:HA	1:C:112:SER:O	2.16	0.45
3:H:17:SER:HA	3:H:82:MET:O	2.17	0.45
1:B:364:VAL:CG1	1:B:365:ILE:N	2.80	0.45
1:C:2:ARG:NH2	1:C:140:MET:CB	2.79	0.45
1:A:492:GLY:O	1:A:493:GLY:C	2.58	0.45
1:B:68:MET:SD	1:B:68:MET:N	2.90	0.45
3:h:100(H):PRO:HG2	1:C:71:ASP:HA	1.98	0.45
1:A:48:THR:HG21	1:A:137:TYR:CE1	2.52	0.45
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.85	0.45
1:A:238:ASN:ND2	1:A:240:GLU:O	2.50	0.45
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.77	0.45
1:C:215:LYS:C	1:C:217:TRP:H	2.25	0.45
1:A:214:HIS:H	2:D:7:HIS:HE1	1.65	0.45
1:A:345:MET:HE3	1:A:380:PRO:HB3	1.99	0.45
2:D:68:LEU:HA	2:D:68:LEU:HD23	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:SER:HB2	2:F:74:TYR:HD1	1.82	0.45
1:A:74:CYS:CB	1:A:105:CYS:SG	3.05	0.45
1:A:358:LEU:HD21	1:A:360:THR:OG1	2.16	0.45
1:B:317:ILE:CB	1:B:318:PRO:HD2	2.38	0.45
1:A:161:ASP:OD1	1:A:162:GLU:N	2.49	0.44
2:D:29:LEU:HD23	2:D:29:LEU:HA	1.80	0.44
3:H:22:CYS:HB3	3:H:78:LEU:HB3	1.99	0.44
3:H:99:PHE:HD2	5:G:2:NAG:O7	1.94	0.44
1:B:472:LEU:HA	1:B:472:LEU:HD23	1.63	0.44
1:C:22:ASP:C	1:C:23:VAL:HG23	2.42	0.44
1:A:48:THR:HG21	1:A:137:TYR:HE1	1.82	0.44
1:B:9:ARG:O	1:B:10:ASP:OD1	2.36	0.44
1:B:22:ASP:C	1:B:23:VAL:HG23	2.42	0.44
1:B:206:MET:HG3	1:B:211:TRP:HZ3	1.83	0.44
3:h:63:VAL:HG13	3:h:67:PHE:CD1	2.49	0.44
4:l:27(A):SER:O	4:l:27(C):ALA:N	2.50	0.44
1:C:3:CYS:CB	1:C:30:CYS:HG	2.30	0.44
1:C:362:ASN:OD1	1:C:362:ASN:C	2.55	0.44
1:A:462:TRP:CZ3	2:D:25:TYR:HB3	2.53	0.44
3:H:100:TYR:HA	5:G:1:NAG:O3	2.17	0.44
2:E:23:ARG:HH22	1:C:241:ALA:HA	1.82	0.44
3:h:40:ALA:HB3	3:h:43:LYS:HG3	2.00	0.44
3:h:57:ARG:O	4:l:95:ARG:NH2	2.50	0.44
1:C:63:ALA:CB	1:C:242:LEU:CD1	2.96	0.44
1:A:49:THR:HG22	1:A:283:ARG:HG2	2.00	0.44
1:A:272:ALA:HB2	2:D:7:HIS:CD2	2.52	0.44
1:A:288:HIS:HE1	1:A:424:LEU:HD13	1.74	0.44
1:A:1:ILE:HG12	1:A:147:GLN:HG3	2.00	0.44
1:B:39:PRO:HG3	1:B:183:PHE:HD2	1.83	0.44
2:E:52:LEU:HB3	1:C:475:LEU:HD11	2.00	0.44
3:h:41:PRO:HD3	3:h:88:ALA:HA	1.99	0.44
4:l:90:SER:OG	4:l:91:TYR:N	2.50	0.44
1:C:139:ILE:HD12	1:C:188:LEU:HD21	1.98	0.44
1:A:488:CYS:HA	1:A:491:LEU:CD1	2.47	0.44
1:B:374:MET:HE3	1:B:374:MET:HB2	1.81	0.44
1:C:59:TYR:O	1:C:125:MET:HB3	2.17	0.44
2:D:26:THR:O	2:D:30:ILE:CG1	2.66	0.44
4:L:49:TYR:HD2	4:L:50:GLU:HG3	1.82	0.44
4:l:49:TYR:HD1	4:l:50:GLU:HG3	1.82	0.44
1:A:269:LEU:O	2:D:19:TRP:HD1	2.00	0.44
1:C:333:ALA:HA	1:C:371:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:100:TYR:CD1	5:G:2:NAG:H62	2.53	0.43
4:l:36:TYR:HE1	4:l:89:CYS:HB3	1.83	0.43
1:B:224:PRO:HD3	1:B:242:LEU:HD23	2.00	0.43
1:B:310:ALA:HB3	1:B:332:TYR:CZ	2.53	0.43
1:B:495:LEU:HA	1:B:498:LEU:HD12	2.00	0.43
1:A:66:SER:OG	1:A:67:ASP:N	2.52	0.43
1:A:392:GLY:C	1:A:394:LYS:H	2.26	0.43
1:B:18:GLY:C	1:B:19:THR:HG23	2.43	0.43
1:A:72:SER:CB	1:A:251:LYS:HZ3	2.21	0.43
3:h:67:PHE:HB3	3:h:80:LEU:HD11	1.99	0.43
3:h:100(I):ASP:OD1	1:C:99:ARG:NH1	2.39	0.43
1:C:180:LEU:HB2	1:C:183:PHE:HB2	2.01	0.43
1:C:241:ALA:O	1:C:258:LEU:HD12	2.18	0.43
1:C:465:GLN:HG2	1:C:498:LEU:HD11	1.99	0.43
1:C:473:MET:H	1:C:491:LEU:HD21	1.75	0.43
1:A:125:MET:O	1:A:125:MET:CG	2.66	0.43
3:h:99:PHE:HD2	5:I:2:NAG:O7	1.93	0.43
1:C:214:HIS:ND1	1:C:215:LYS:O	2.30	0.43
1:C:358:LEU:HD12	1:C:378:LEU:HD13	1.96	0.43
1:A:27:HIS:HE1	1:A:48:THR:HG23	1.83	0.43
1:A:242:LEU:HD11	1:A:261:GLN:HG3	1.99	0.43
1:B:9:ARG:NH1	1:B:32:THR:HG21	2.34	0.43
1:B:65:ILE:HG23	1:B:117:ALA:HB1	2.01	0.43
3:h:101:ASP:CG	4:l:46:LEU:HD12	2.44	0.43
4:l:29:THR:HG23	4:l:90:SER:OG	2.18	0.43
1:C:248:ALA:O	1:C:250:ALA:N	2.49	0.43
1:C:262:GLU:CG	1:C:266:HIS:NE2	2.78	0.43
1:C:352:LEU:HD23	1:C:352:LEU:HA	1.89	0.43
1:A:196:LEU:O	1:A:198:PHE:N	2.52	0.43
1:B:22:ASP:OD1	1:B:292:ARG:HB3	2.19	0.43
1:B:60:CYS:HB2	1:B:236:TRP:CH2	2.53	0.43
1:B:466:ILE:CG1	1:B:498:LEU:HD22	2.42	0.43
2:E:67:ILE:HA	2:E:70:ILE:HG22	2.00	0.43
3:h:50:ARG:HG2	3:h:58:ASN:HB2	2.00	0.43
1:C:226:HIS:HB2	1:C:236:TRP:CZ3	2.54	0.43
1:C:347:VAL:HG23	1:C:355:VAL:HG11	2.01	0.43
1:A:60:CYS:SG	1:A:236:TRP:CD2	3.11	0.43
1:A:358:LEU:HG	1:A:378:LEU:HD22	1.99	0.43
1:B:1:ILE:HG12	1:B:147:GLN:HG3	2.01	0.43
1:B:213:VAL:CG1	1:B:217:TRP:CE3	3.01	0.43
1:B:274:GLU:HB2	1:C:246:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:CG	1:A:254:THR:OG1	2.67	0.43
1:B:360:THR:O	1:B:361:ALA:CB	2.67	0.43
1:C:204:LEU:HD22	1:C:213:VAL:HG21	2.01	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.72	0.43
1:A:288:HIS:CD2	1:A:424:LEU:HD22	2.53	0.43
1:B:149:SER:HB2	1:B:329:GLU:CD	2.44	0.43
1:B:473:MET:SD	1:B:491:LEU:HD21	2.58	0.43
3:h:52:ASN:ND2	3:h:100(F):TYR:O	2.52	0.43
1:C:63:ALA:CB	1:C:242:LEU:HG	2.47	0.43
1:C:264:ALA:HB1	2:F:4:LEU:HD13	2.00	0.43
1:C:313:THR:OG1	1:C:331:GLN:HB3	2.19	0.43
1:C:320:GLU:HB2	1:C:400:TRP:CZ2	2.54	0.43
1:C:350:GLN:HE21	1:C:350:GLN:HB2	1.57	0.43
1:C:61:TYR:HD1	1:C:124:LYS:O	2.01	0.42
1:C:138:ARG:HH11	1:C:166:LYS:HD2	1.84	0.42
1:B:23:VAL:HG11	1:B:31:VAL:HG11	2.00	0.42
1:B:74:CYS:HA	1:B:75:PRO:HD2	1.54	0.42
1:C:207:ASN:OD1	1:C:207:ASN:N	2.51	0.42
1:C:226:HIS:CG	1:C:227:ALA:H	2.37	0.42
1:B:345:MET:HB2	1:B:355:VAL:O	2.19	0.42
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.74	0.42
4:L:18:SER:HA	4:L:75:ILE:O	2.20	0.42
3:h:82:MET:SD	3:h:82(C):LEU:HG	2.59	0.42
1:A:248:ALA:HB3	1:A:252:ARG:O	2.18	0.42
1:A:491:LEU:O	1:A:492:GLY:C	2.61	0.42
1:C:16:SER:HA	1:C:434:VAL:HG13	2.02	0.42
1:B:153:VAL:CG1	5:I:1:NAG:H82	2.49	0.42
1:C:16:SER:OG	1:C:17:GLY:N	2.52	0.42
1:C:66:SER:OG	1:C:67:ASP:N	2.52	0.42
3:H:100(P):MET:HE1	4:L:98:PHE:CZ	2.54	0.42
1:B:303:VAL:O	1:B:304:SER:OG	2.31	0.42
2:E:35:TRP:CE3	2:E:72:PRO:HG3	2.55	0.42
3:h:47:TRP:CD2	4:I:96:LEU:HB2	2.54	0.42
2:F:53:LEU:HD23	2:F:53:LEU:HA	1.79	0.42
1:A:72:SER:CB	1:A:251:LYS:CE	2.97	0.42
3:H:101:ASP:HA	4:L:46:LEU:HD22	2.01	0.42
1:B:48:THR:HG21	1:B:137:TYR:CE1	2.54	0.42
1:B:349:MET:HE2	1:B:386:TYR:CG	2.55	0.42
1:C:42:ASP:N	1:C:42:ASP:OD1	2.53	0.42
1:C:63:ALA:HB2	1:C:242:LEU:CD1	2.49	0.42
1:A:59:TYR:CZ	1:A:221:ILE:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:67:PHE:HB3	3:H:80:LEU:HD11	2.02	0.42
1:B:320:GLU:O	1:C:108:PHE:HB2	2.20	0.42
1:B:332:TYR:O	1:B:371:ASN:HA	2.20	0.42
1:C:72:SER:O	1:C:72:SER:OG	2.29	0.42
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.83	0.42
1:C:480:LYS:HE2	1:C:480:LYS:HB3	1.77	0.42
1:A:369:THR:OG1	1:A:370:GLU:N	2.51	0.42
1:B:22:ASP:OD1	1:B:292:ARG:CB	2.68	0.42
1:B:153:VAL:HG13	3:h:100(C):SER:OG	2.19	0.42
1:B:317:ILE:CD1	1:B:318:PRO:HD2	2.49	0.42
1:C:492:GLY:O	1:C:493:GLY:C	2.63	0.42
1:A:335:THR:HG22	1:A:370:GLU:HA	2.02	0.41
4:l:36:TYR:HA	4:l:46:LEU:HA	2.02	0.41
1:C:59:TYR:CB	1:C:125:MET:SD	2.97	0.41
1:A:288:HIS:ND1	1:A:424:LEU:HD21	2.35	0.41
3:H:100:TYR:HE1	5:G:2:NAG:H2	1.85	0.41
1:B:75:PRO:CG	1:B:99:ARG:HB2	2.49	0.41
1:B:230:ASP:O	1:B:231:THR:OG1	2.28	0.41
1:C:317:ILE:HG23	1:C:318:PRO:CD	2.50	0.41
1:C:331:GLN:HA	1:C:372:SER:O	2.20	0.41
1:C:467:LEU:HD23	1:C:467:LEU:HA	1.87	0.41
1:A:85:GLN:HE22	1:A:94:ARG:NH1	2.19	0.41
3:H:66:ARG:HD3	3:H:82(B):SER:HB2	2.02	0.41
3:H:100:TYR:CD1	5:G:2:NAG:C6	3.03	0.41
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.87	0.41
1:C:22:ASP:HA	1:C:292:ARG:HA	2.02	0.41
1:A:150:GLY:HA2	5:G:1:NAG:O7	2.04	0.41
1:A:307:LEU:HD12	1:A:340:LYS:HD3	2.02	0.41
1:A:382:PHE:CE2	1:A:406:THR:HG22	2.55	0.41
1:C:286:SER:HB2	2:F:14:THR:HG21	2.02	0.41
1:C:484:ILE:HG13	1:C:485:SER:N	2.35	0.41
1:A:360:THR:HB	1:A:361:ALA:H	1.69	0.41
2:D:4:LEU:HD23	2:D:4:LEU:HA	1.91	0.41
3:H:100:TYR:CD1	5:G:2:NAG:C5	3.04	0.41
4:L:36:TYR:CE1	4:L:89:CYS:HB3	2.56	0.41
1:B:240:GLU:C	1:B:242:LEU:H	2.27	0.41
4:L:38:GLN:O	4:L:84:ALA:HB1	2.21	0.41
3:h:67:PHE:HD2	3:h:80:LEU:HD11	1.86	0.41
1:C:465:GLN:HG2	1:C:494:VAL:HG13	2.02	0.41
1:A:231:THR:OG1	1:A:232:GLY:N	2.54	0.41
1:A:271:GLY:HA2	2:D:18:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HG13	1:B:318:PRO:N	2.36	0.41
3:h:100(C):SER:HB3	5:I:1:NAG:N2	2.35	0.41
4:l:33:VAL:HG22	4:l:90:SER:HB2	2.01	0.41
4:l:48:ILE:HD13	4:l:48:ILE:HA	1.97	0.41
1:C:70:SER:HA	1:C:114:VAL:O	2.20	0.41
1:C:238:ASN:C	1:C:240:GLU:N	2.77	0.41
1:A:113:LEU:HD13	1:A:251:LYS:HE2	2.03	0.41
1:A:260:SER:C	1:A:262:GLU:H	2.28	0.41
1:A:374:MET:HB3	1:A:374:MET:HE2	1.79	0.41
2:D:56:SER:O	2:D:60:LYS:HG3	2.20	0.41
3:h:6:GLU:OE1	3:h:6:GLU:N	2.54	0.41
1:C:186:LEU:HD12	1:C:298:LEU:HD11	2.02	0.41
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.55	0.41
3:H:90:TYR:O	3:H:106:GLY:HA2	2.20	0.41
1:B:241:ALA:HB1	2:E:1:ALA:HB2	2.02	0.41
1:C:51:SER:HB3	1:C:281:LYS:HG2	2.02	0.41
1:A:226:HIS:N	1:A:236:TRP:CE3	2.89	0.40
1:A:484:ILE:HG13	1:A:485:SER:N	2.36	0.40
3:H:103:TRP:HE1	4:L:46:LEU:HD11	1.86	0.40
1:B:341:VAL:HB	1:B:363:PRO:HB2	2.03	0.40
1:C:278:ASP:OD1	1:C:278:ASP:N	2.54	0.40
1:A:248:ALA:CB	1:A:252:ARG:CB	2.85	0.40
1:A:472:LEU:HD23	1:A:475:LEU:HD12	2.03	0.40
3:H:6:GLU:N	3:H:6:GLU:OE1	2.54	0.40
1:B:249:HIS:CE1	1:C:285:SER:HG	2.39	0.40
1:C:137:TYR:HE2	1:C:192:PRO:HB3	1.86	0.40
1:B:22:ASP:HA	1:B:292:ARG:HA	2.03	0.40
1:B:51:SER:HB3	1:B:281:LYS:HG2	2.03	0.40
2:E:53:LEU:O	2:E:60:LYS:HG2	2.22	0.40
3:h:100(O):GLY:C	4:l:46:LEU:HD13	2.41	0.40
1:A:214:HIS:H	2:D:7:HIS:CE1	2.40	0.40
1:A:345:MET:CE	1:A:380:PRO:HB3	2.52	0.40
1:C:460:MET:HE2	1:C:460:MET:HB3	1.66	0.40
1:A:210:HIS:CD2	1:A:210:HIS:N	2.90	0.40
1:A:278:ASP:OD1	1:A:278:ASP:N	2.53	0.40
1:B:27:HIS:CE1	1:C:249:HIS:CE1	3.10	0.40
3:h:62:PHE:CD1	3:h:63:VAL:HG23	2.57	0.40
1:C:345:MET:SD	1:C:387:ILE:HG12	2.62	0.40
1:C:465:GLN:OE1	1:C:498:LEU:HD21	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/639 (78%)	437 (88%)	59 (12%)	3 (1%)	21	50
1	B	499/639 (78%)	443 (89%)	50 (10%)	6 (1%)	10	35
1	C	499/639 (78%)	436 (87%)	58 (12%)	5 (1%)	12	40
2	D	73/3423 (2%)	63 (86%)	10 (14%)	0	100	100
2	E	73/3423 (2%)	67 (92%)	6 (8%)	0	100	100
2	F	73/3423 (2%)	62 (85%)	11 (15%)	0	100	100
3	H	130/133 (98%)	125 (96%)	5 (4%)	0	100	100
3	h	127/133 (96%)	124 (98%)	3 (2%)	0	100	100
4	L	102/111 (92%)	99 (97%)	3 (3%)	0	100	100
4	l	99/111 (89%)	95 (96%)	3 (3%)	1 (1%)	12	40
All	All	2174/12674 (17%)	1951 (90%)	208 (10%)	15 (1%)	20	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	PRO
1	B	317	ILE
1	B	361	ALA
1	C	125	MET
1	A	261	GLN
1	A	361	ALA
1	B	261	GLN
1	C	260	SER
4	l	27(B)	ASN
1	C	74	CYS
1	B	151	MET
1	B	318	PRO
1	C	75	PRO
1	C	195	GLY

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Mol	Chain	Res	Type
1	A	364	VAL

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	408/534 (76%)	392 (96%)	16 (4%)	28	53
1	B	408/534 (76%)	397 (97%)	11 (3%)	39	60
1	C	408/534 (76%)	401 (98%)	7 (2%)	53	67
2	D	64/2832 (2%)	63 (98%)	1 (2%)	55	68
2	E	64/2832 (2%)	59 (92%)	5 (8%)	11	37
2	F	64/2832 (2%)	58 (91%)	6 (9%)	8	29
3	H	108/111 (97%)	107 (99%)	1 (1%)	70	76
3	h	107/111 (96%)	106 (99%)	1 (1%)	70	76
4	L	85/92 (92%)	82 (96%)	3 (4%)	32	56
4	l	83/92 (90%)	82 (99%)	1 (1%)	63	72
All	All	1799/10504 (17%)	1747 (97%)	52 (3%)	38	60

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	23	VAL
1	A	50	VAL
1	A	65	ILE
1	A	77	GLN
1	A	97	VAL
1	A	124	LYS
1	A	152	ILE
1	A	221	ILE
1	A	235	HIS
1	A	277	MET
1	A	317	ILE

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Mol	Chain	Res	Type
1	A	330	VAL
1	A	359	ILE
1	A	364	VAL
1	A	495	LEU
2	D	25	TYR
3	H	63	VAL
4	L	28	ASP
4	L	48	ILE
4	L	97	VAL
1	B	6	VAL
1	B	31	VAL
1	B	50	VAL
1	B	84	LYS
1	B	91	VAL
1	B	107	LEU
1	B	188	LEU
1	B	347	VAL
1	B	465	GLN
1	B	477	LEU
1	B	500	THR
2	E	2	VAL
2	E	14	THR
2	E	25	TYR
2	E	30	ILE
2	E	38	ARG
3	h	97	VAL
4	l	97	VAL
1	C	50	VAL
1	C	112	SER
1	C	235	HIS
1	C	284	LEU
1	C	335	THR
1	C	396	ILE
1	C	487	MET
2	F	2	VAL
2	F	25	TYR
2	F	30	ILE
2	F	38	ARG
2	F	61	VAL
2	F	65	VAL

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	27	HIS
1	A	77	GLN
1	A	85	GLN
1	A	134	ASN
1	A	147	GLN
1	A	148	HIS
1	A	163	ASN
1	A	238	ASN
1	A	266	HIS
1	A	288	HIS
1	A	362	ASN
2	D	7	HIS
4	L	60	ASN
1	B	77	GLN
1	B	85	GLN
1	B	134	ASN
1	B	147	GLN
1	B	163	ASN
1	B	219	HIS
1	B	226	HIS
1	B	344	GLN
1	B	350	GLN
1	B	465	GLN
2	E	7	HIS
3	h	35	HIS
3	h	58	ASN
1	C	154	ASN
1	C	163	ASN
1	C	288	HIS
1	C	350	GLN
1	C	362	ASN
1	C	465	GLN
2	F	7	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1	1,5	14,14,15	0.36	0	17,19,21	0.65	0
5	NAG	G	2	5	14,14,15	0.33	0	17,19,21	0.63	0
5	BMA	G	3	5	11,11,12	0.50	0	15,15,17	1.66	1 (6%)
5	FUC	G	4	5	10,10,11	0.42	0	14,14,16	0.79	0
5	NAG	I	1	5	14,14,15	0.35	0	17,19,21	0.65	0
5	NAG	I	2	5	14,14,15	0.34	0	17,19,21	0.63	0
5	BMA	I	3	5	11,11,12	0.49	0	15,15,17	1.66	1 (6%)
5	FUC	I	4	5	10,10,11	0.41	0	14,14,16	0.79	0

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
5	NAG	G	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	1/1/1/1
5	FUC	G	4	5	-	-	0/1/1/1
5	NAG	I	1	5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	1/1/1/1
5	FUC	I	4	5	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3	BMA	C1-O5-C5	6.15	120.43	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C1-O5-C5	6.12	120.39	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	1	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6

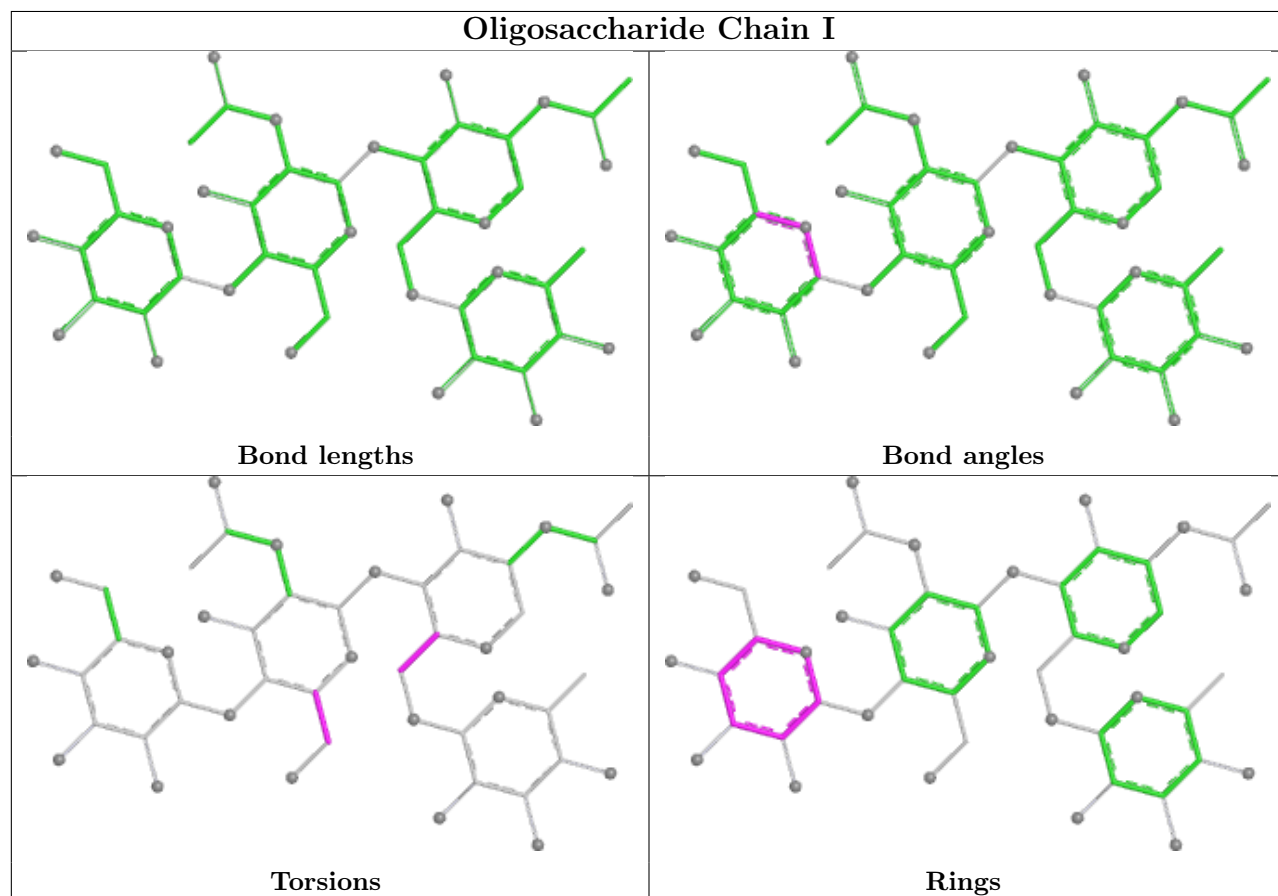
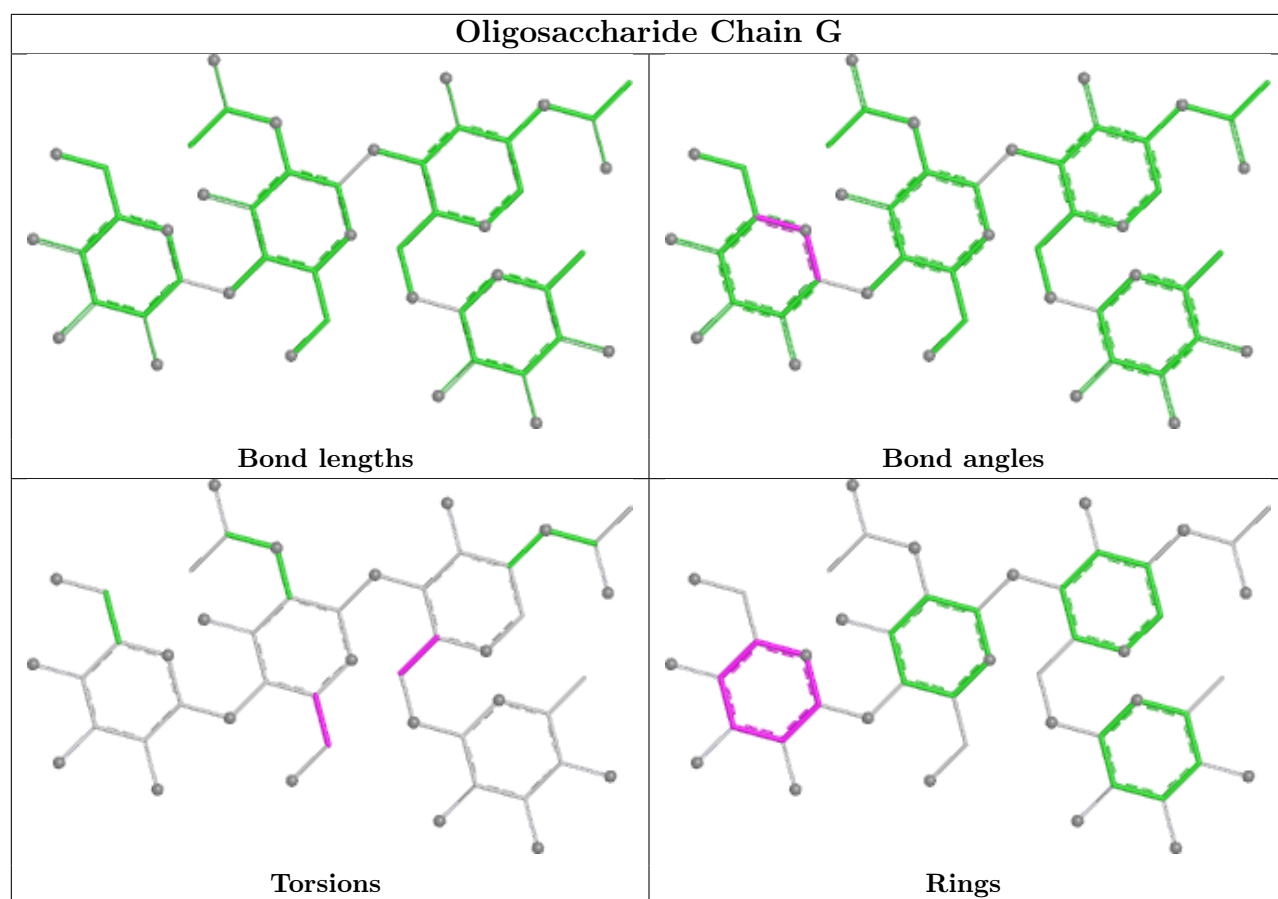
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	C1-C2-C3-C4-C5-O5
5	I	3	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3	BMA	1	0
5	I	2	NAG	5	0
5	G	1	NAG	10	0
5	I	1	NAG	7	0
5	G	2	NAG	12	0
5	I	3	BMA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

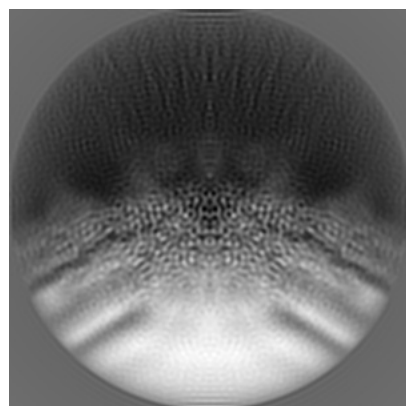
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27058. These allow visual inspection of the internal detail of the map and identification of artifacts.

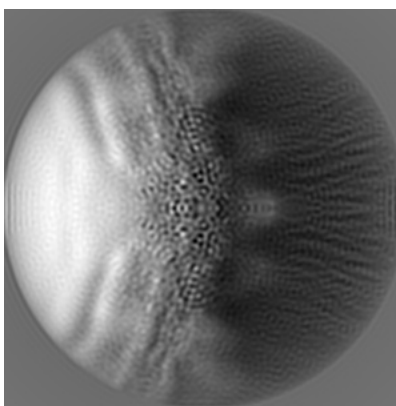
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

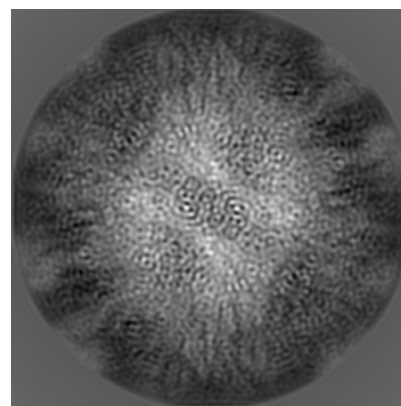
6.1.1 Primary map



X

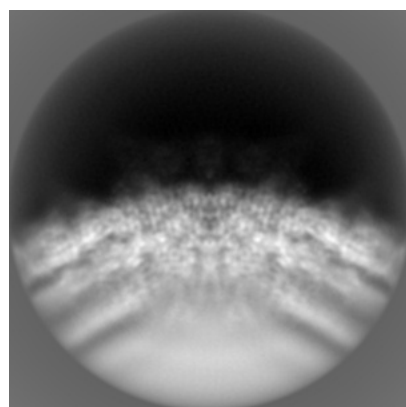


Y

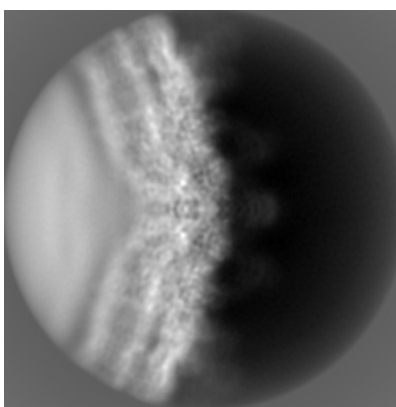


Z

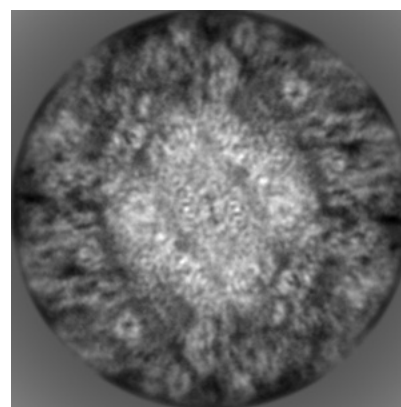
6.1.2 Raw map



X



Y

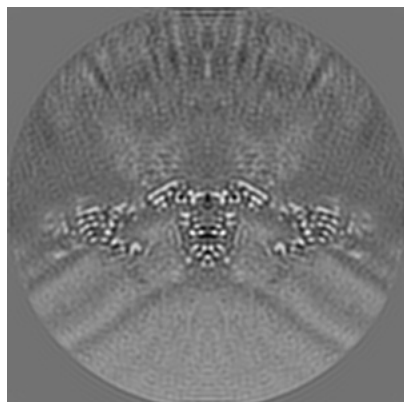


Z

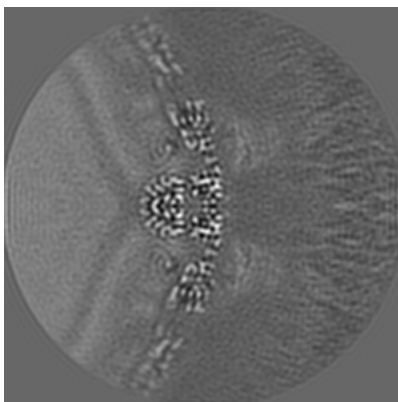
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

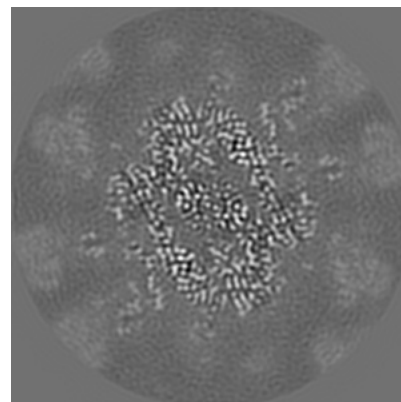
6.2.1 Primary map



X Index: 125

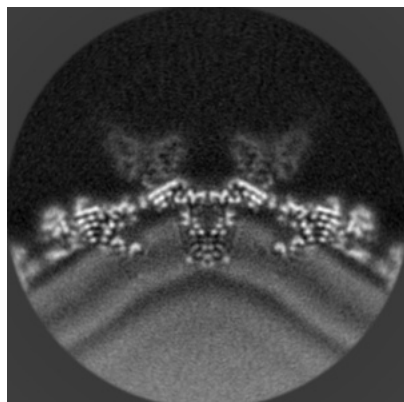


Y Index: 125

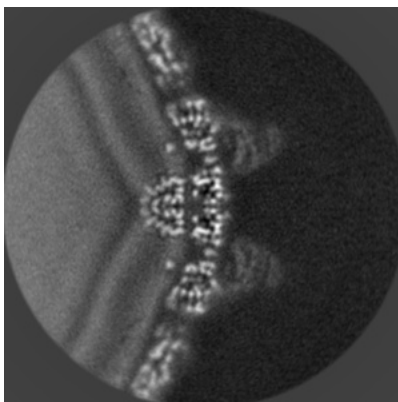


Z Index: 125

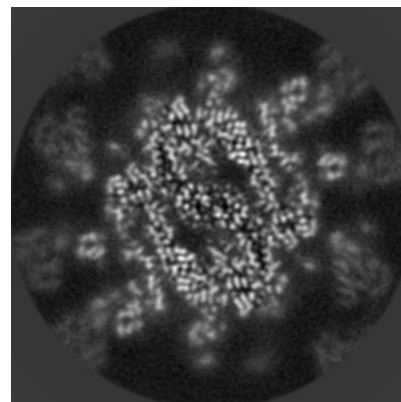
6.2.2 Raw map



X Index: 125



Y Index: 125

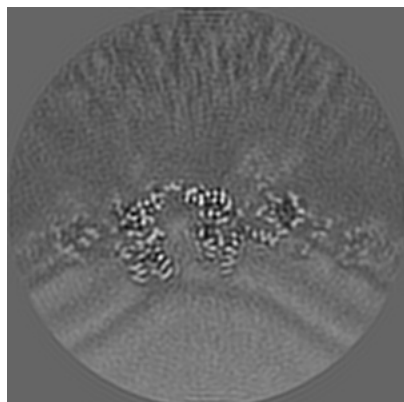


Z Index: 125

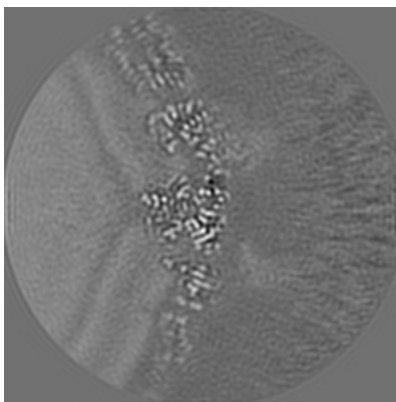
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

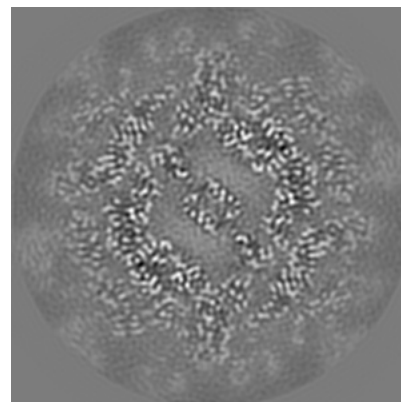
6.3.1 Primary map



X Index: 112

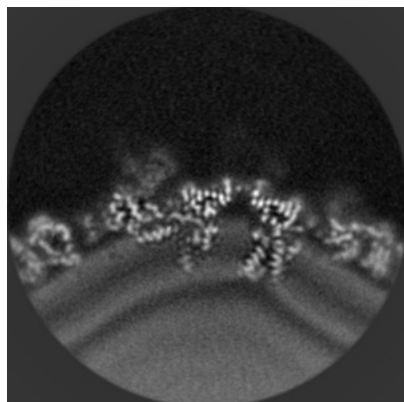


Y Index: 131

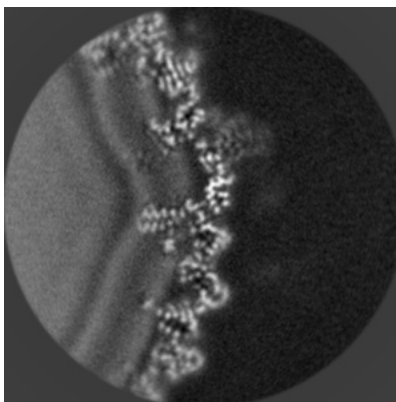


Z Index: 114

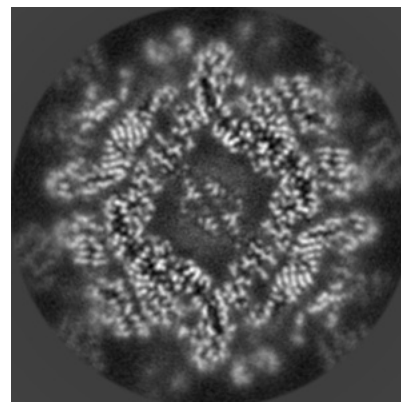
6.3.2 Raw map



X Index: 140



Y Index: 138

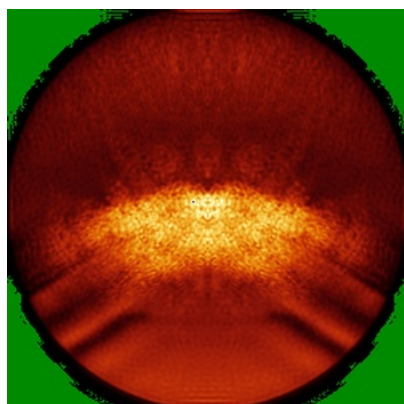


Z Index: 116

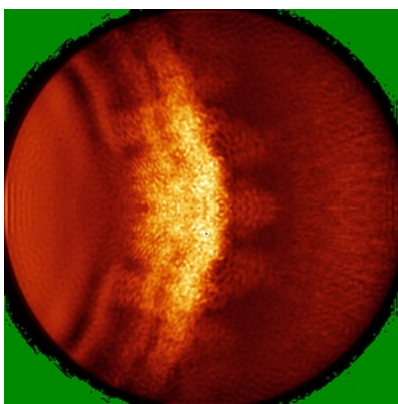
The images above show the largest variance slices of the map in three orthogonal directions.

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

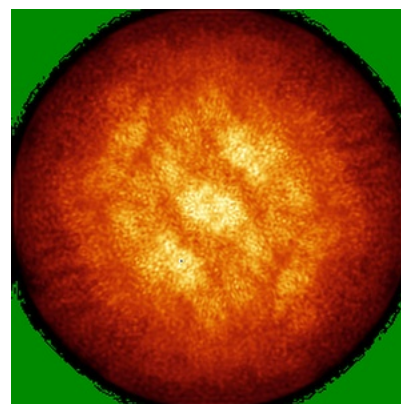
6.4.1 Primary map



X

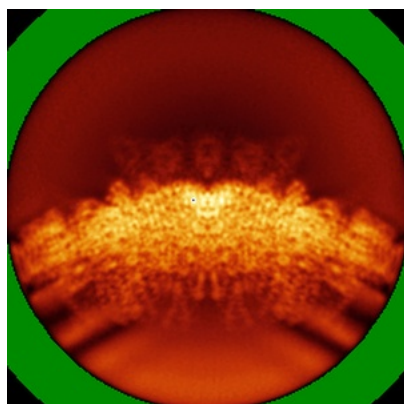


Y

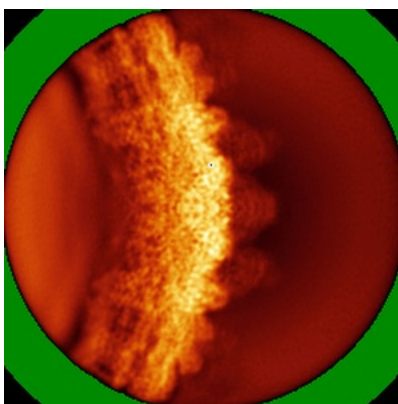


Z

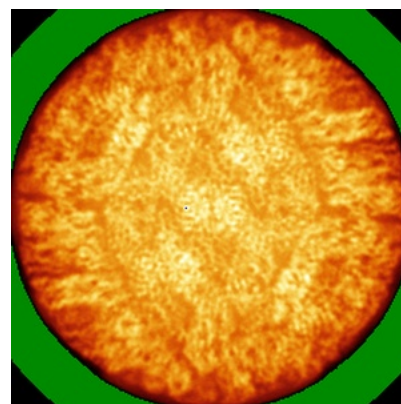
6.4.2 Raw map



X



Y

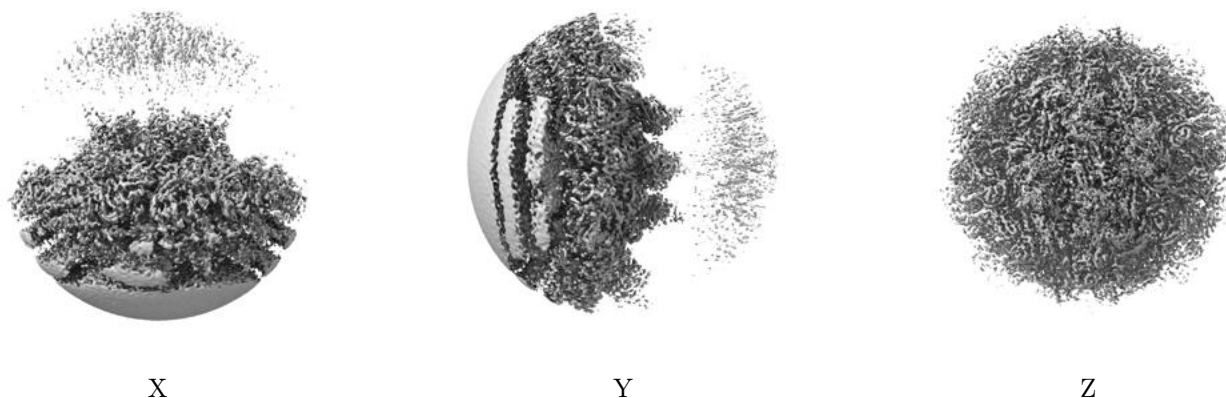


Z

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.

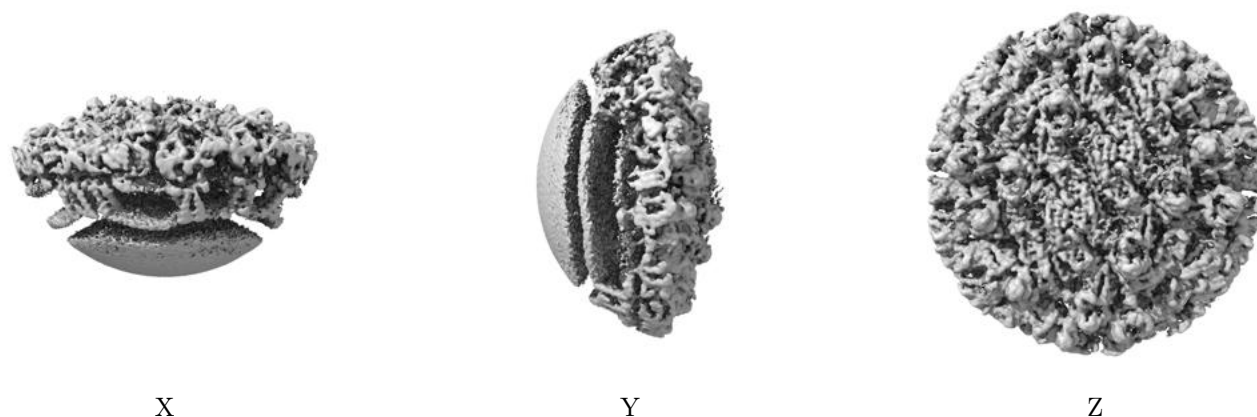
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. 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.

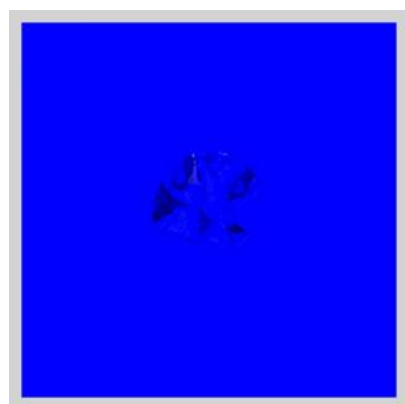
6.6 Mask visualisation [i](#)

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

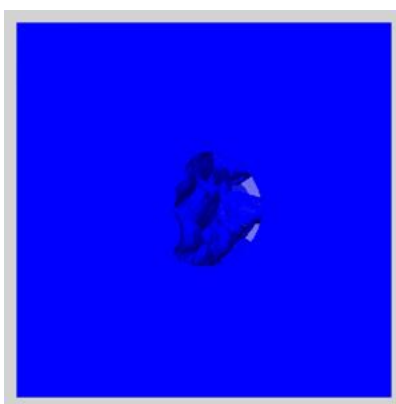
A mask typically either:

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

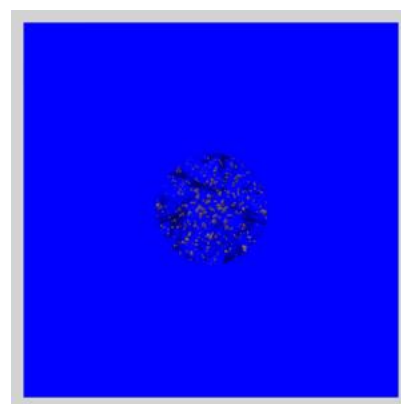
6.6.1 emd_27058_msk_1.map [i](#)



X



Y

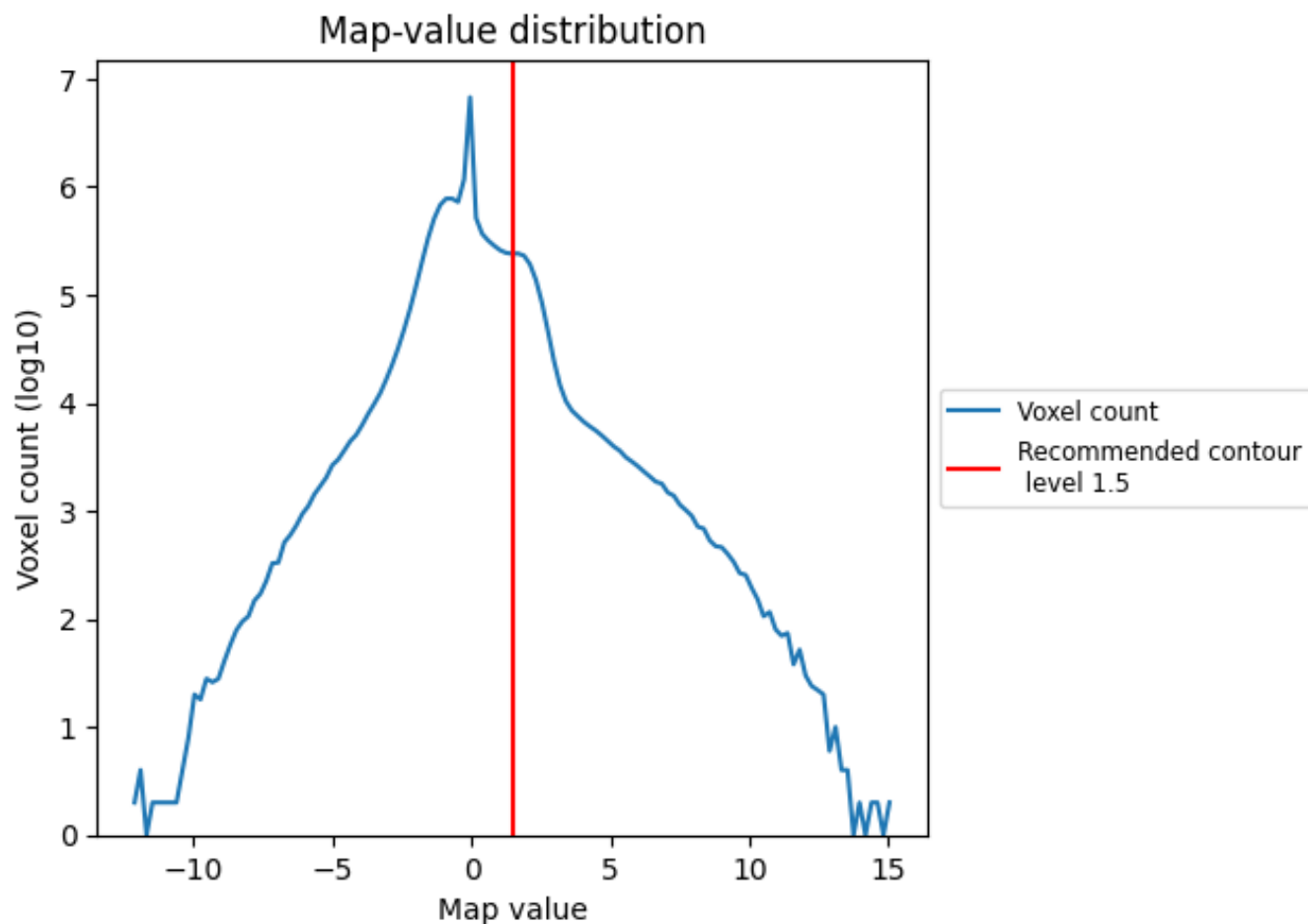


Z

7 Map analysis [i](#)

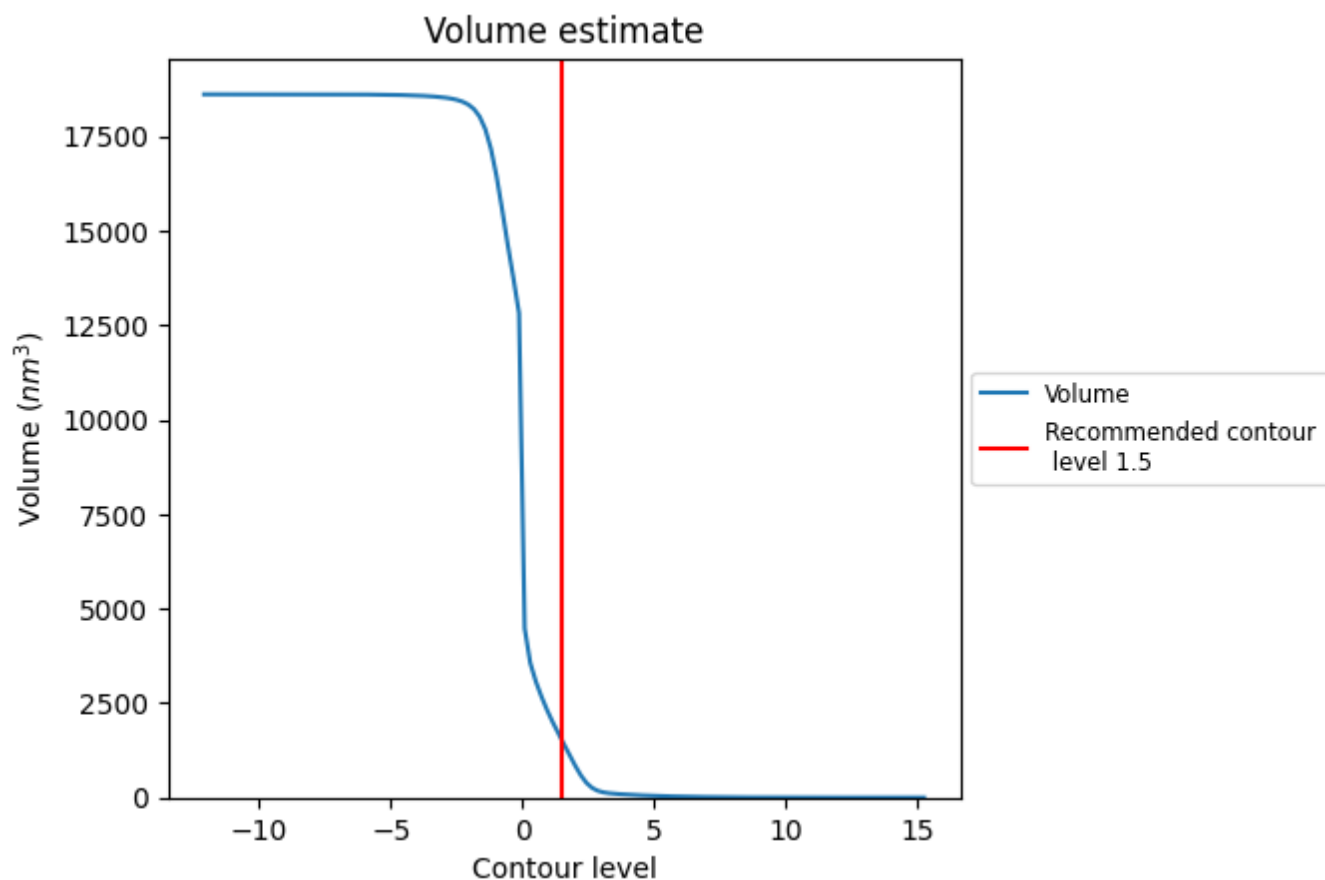
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

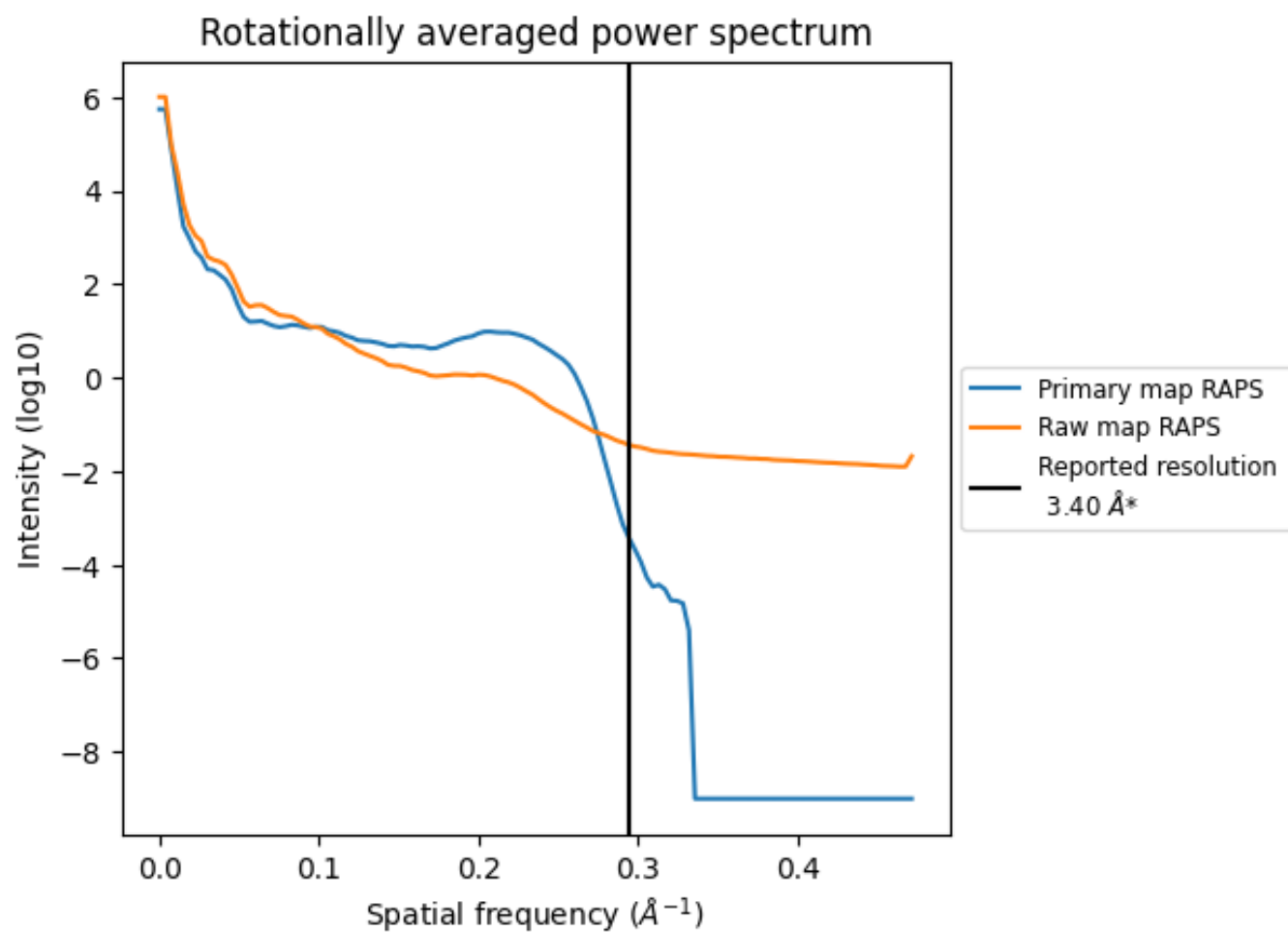
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1507 nm³; this corresponds to an approximate mass of 1361 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 ⓘ

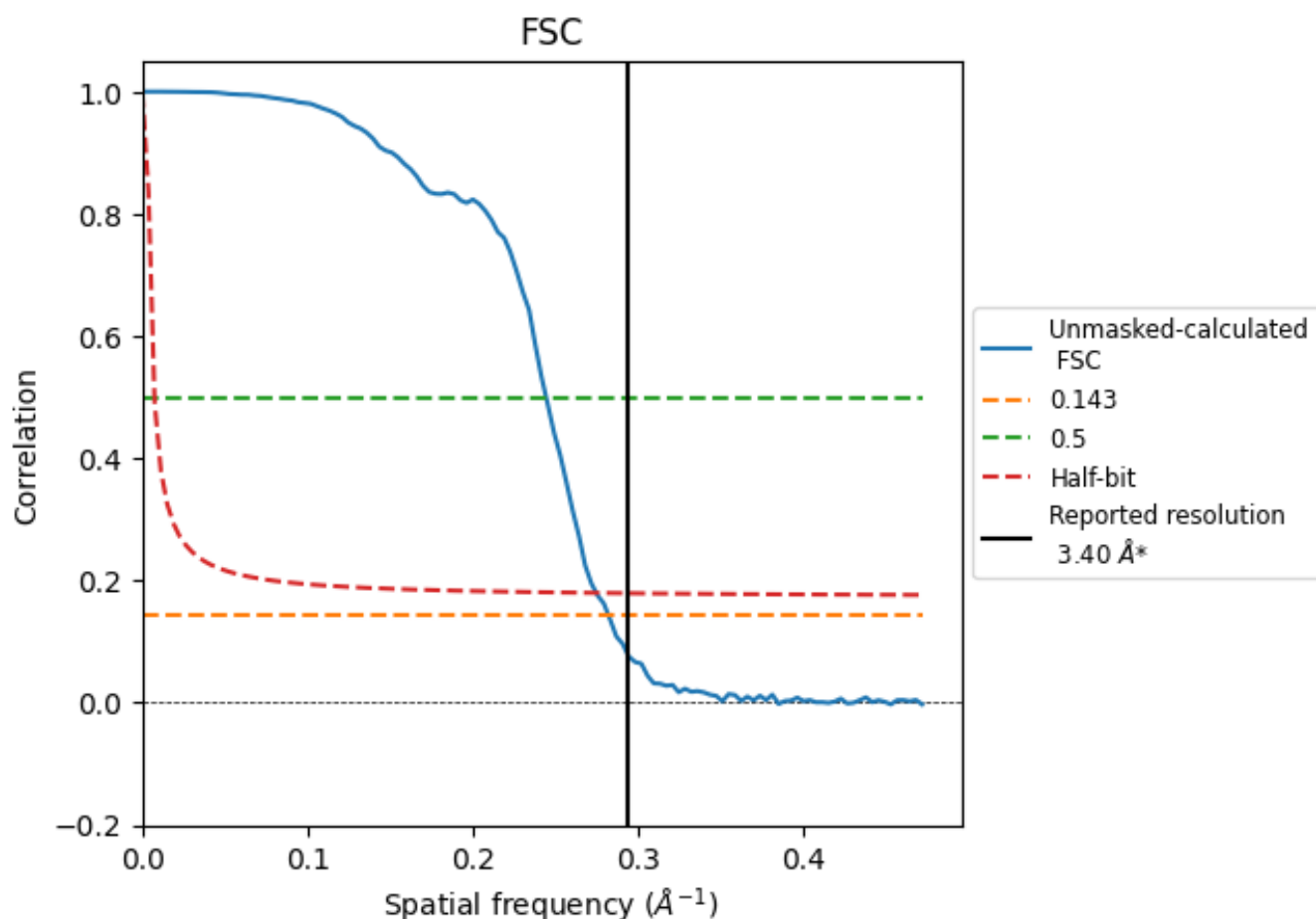


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	4.09	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27058 and PDB model 8CXI. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

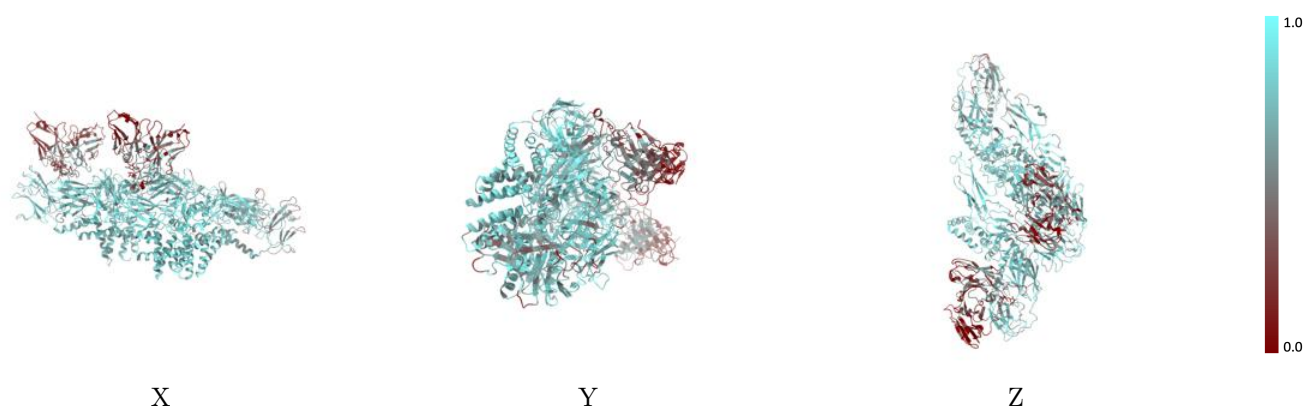
This section was not generated.

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



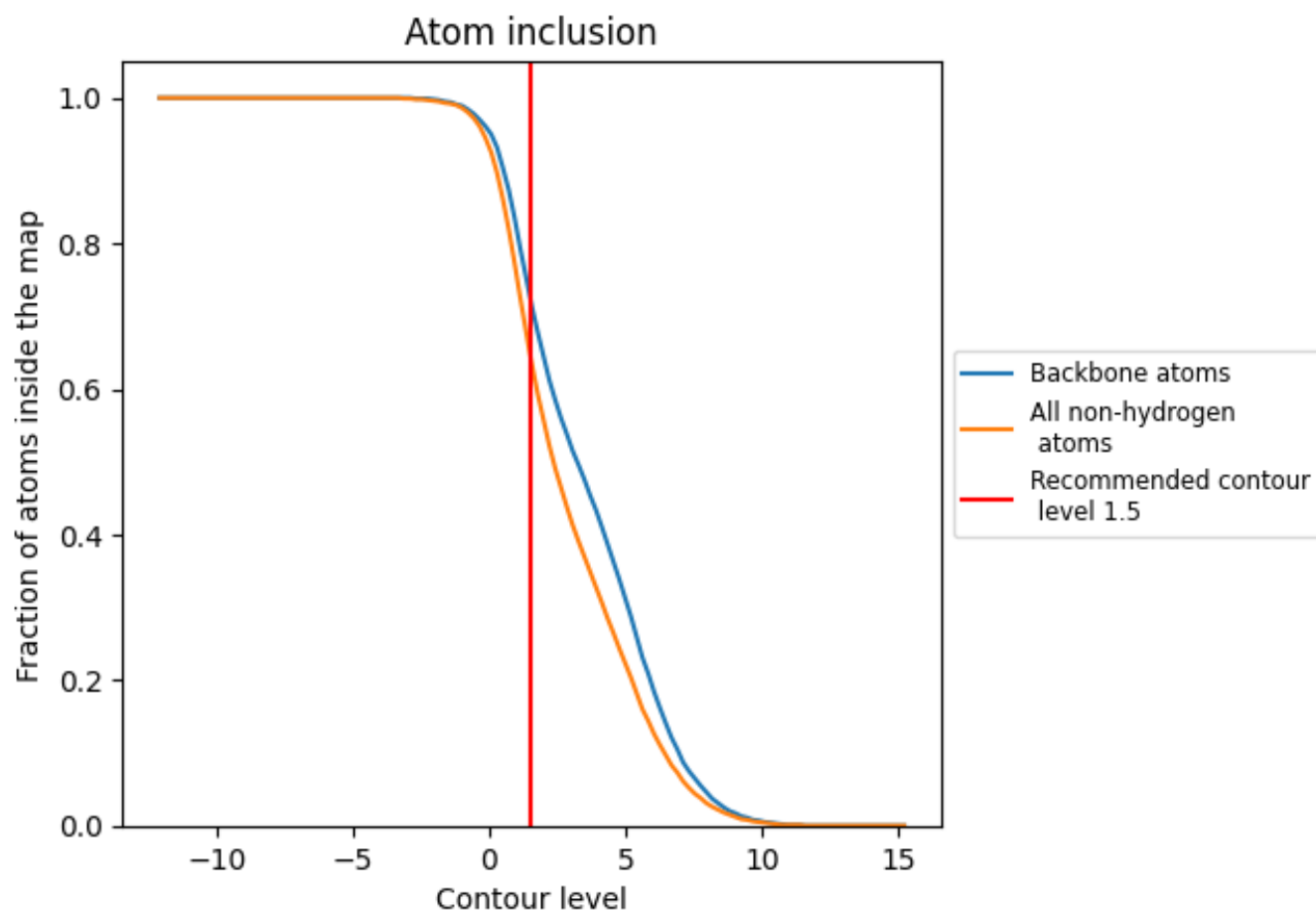
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 65% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.4640
A	0.7500	0.4940
B	0.7440	0.4930
C	0.6940	0.4840
D	0.8150	0.5220
E	0.8240	0.5110
F	0.8010	0.5020
G	0.1840	0.2820
H	0.3650	0.4030
I	0.2250	0.1980
L	0.2230	0.3280
h	0.3900	0.3820
l	0.2380	0.3250

