



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 10:51 AM JST

PDB ID : 5XSY
EMDB ID : EMD-6770
Title : Structure of the Nav1.4-beta1 complex from electric eel
Authors : Yan, Z.; Zhou, Q.; Wu, J.P.; Yan, N.
Deposited on : 2017-06-15
Resolution : 4.00 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

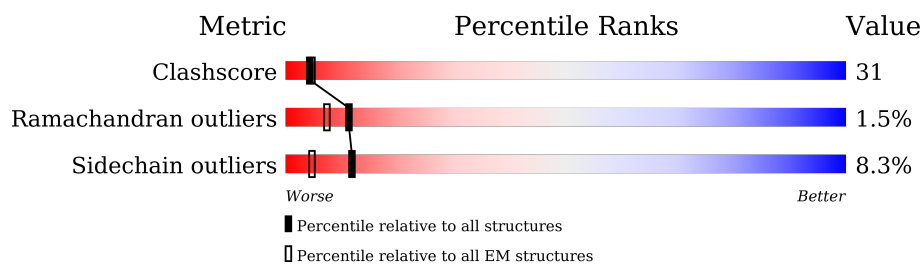
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1820	<div> <div>25%</div> <div>40%</div> <div>19%</div> <div>•</div> <div>37%</div> </div>
2	B	209	<div> <div>31%</div> <div>41%</div> <div>32%</div> <div>7%</div> <div>•</div> <div>18%</div> </div>
3	C	5	<div> <div>20%</div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
4	D	3	<div> <div>67%</div> <div>33%</div> <div>67%</div> </div>
4	E	3	<div> <div>67%</div> <div>67%</div> <div>33%</div> </div>
4	F	3	<div> <div>67%</div> <div>33%</div> <div>67%</div> </div>
5	G	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10634 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.

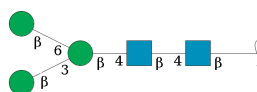
- Molecule 1 is a protein called Sodium channel protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0
			9057	5992	1436	1551	78		

- Molecule 2 is a protein called Voltage-gated sodium channel beta subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	172	Total	C	N	O	S	0	0
			1371	874	223	261	13		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

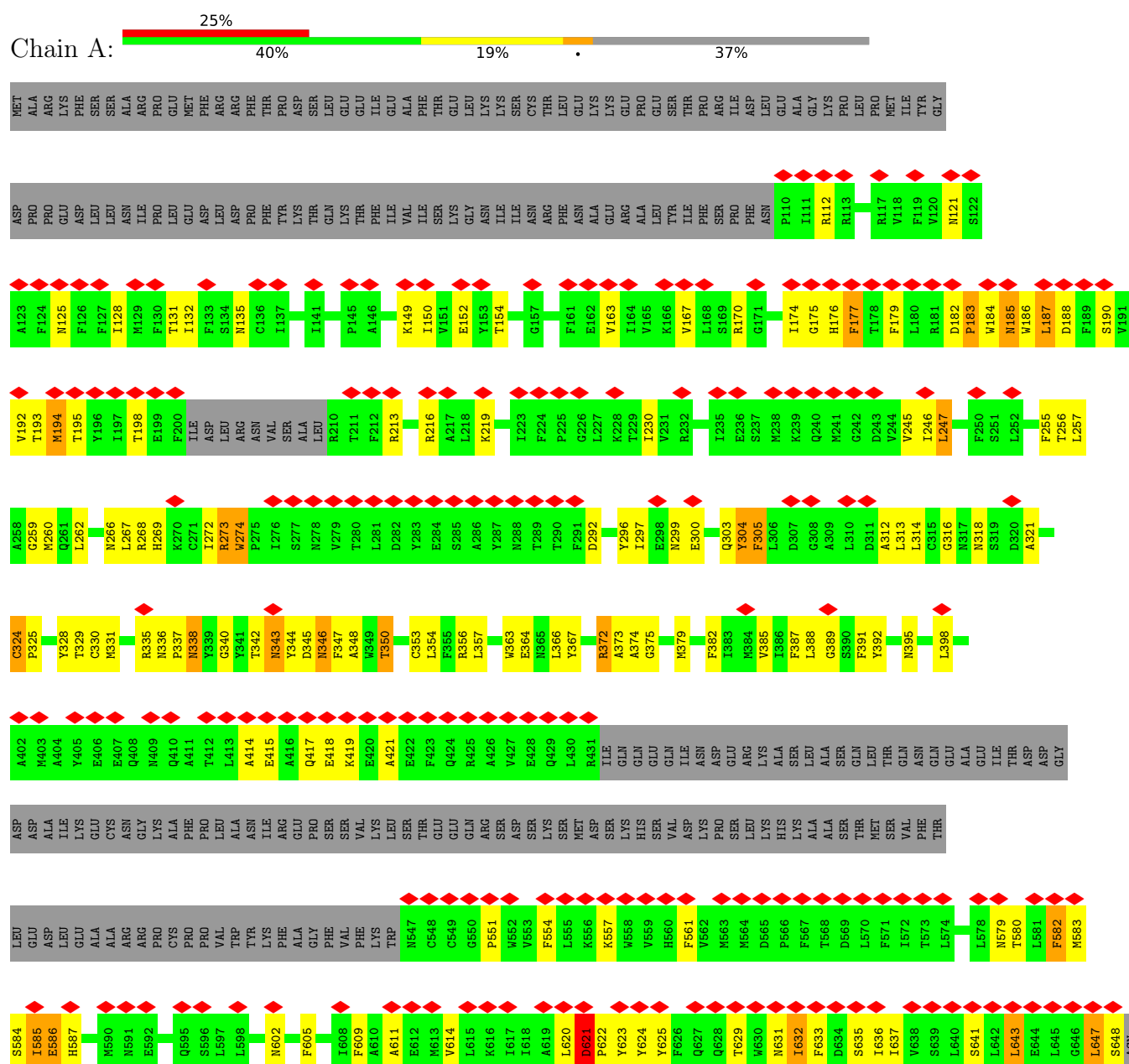


Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

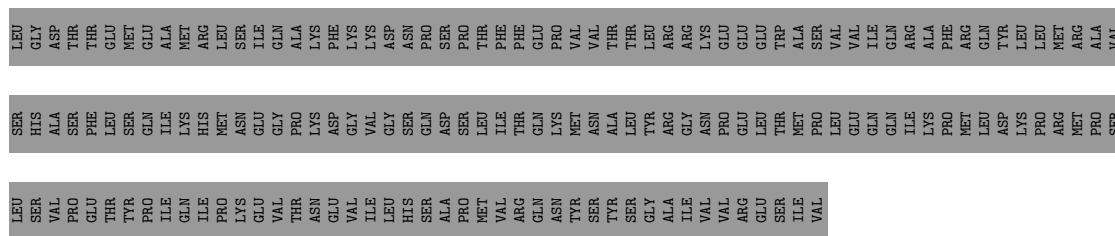
3 Residue-property plots

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.

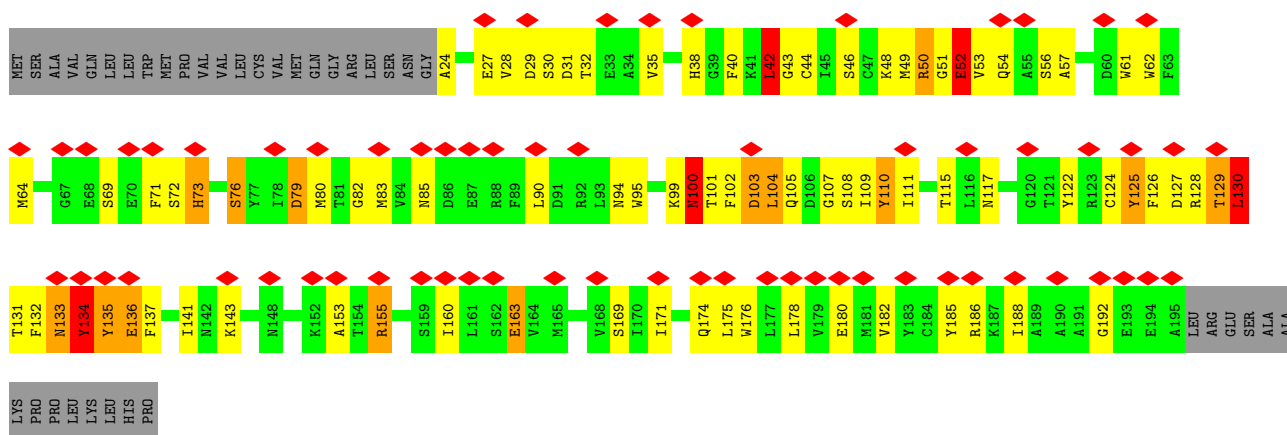
- Molecule 1: Sodium channel protein



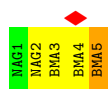




• Molecule 2: Voltage-gated sodium channel beta subunit 1



• Molecule 3: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	123431	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 ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.334	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	267.6, 267.6, 267.6	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	6/9269 (0.1%)	0.67	11/12571 (0.1%)
2	B	0.51	1/1399 (0.1%)	1.07	12/1894 (0.6%)
All	All	0.54	7/10668 (0.1%)	0.73	23/14465 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	136	GLU	CA-C	6.02	1.68	1.52
1	A	1520	PRO	N-CD	5.70	1.55	1.47
1	A	183	PRO	N-CD	5.43	1.55	1.47
1	A	1519	PRO	N-CD	5.27	1.55	1.47
1	A	622	PRO	N-CD	5.15	1.55	1.47
1	A	1513	PRO	N-CD	5.10	1.54	1.47
1	A	1127	PRO	N-CD	5.05	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	SER	CB-CA-C	-14.61	82.35	110.10
2	B	110	TYR	CB-CA-C	-13.68	83.04	110.40
2	B	130	LEU	CB-CA-C	12.86	134.63	110.20
2	B	130	LEU	N-CA-C	-11.00	81.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	MET	CB-CA-C	-9.08	92.25	110.40
2	B	129	THR	N-CA-C	-7.96	89.52	111.00
2	B	125	TYR	N-CA-C	-6.52	93.40	111.00
2	B	54	GLN	CB-CA-C	-6.51	97.37	110.40
1	A	1528	ASN	C-N-CD	6.28	141.59	128.40
2	B	29	ASP	CB-CA-C	-6.08	98.24	110.40
1	A	1383	VAL	C-N-CA	-5.98	109.75	122.30
1	A	1518	GLY	C-N-CD	5.97	140.95	128.40
1	A	1126	ILE	C-N-CD	5.76	140.50	128.40
1	A	621	ASP	C-N-CD	5.73	140.42	128.40
2	B	42	LEU	N-CA-C	-5.71	95.59	111.00
1	A	1512	LEU	C-N-CD	5.68	140.33	128.40
1	A	586	GLU	N-CA-C	-5.61	95.85	111.00
1	A	1256	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	335	ARG	C-N-CA	5.54	135.55	121.70
2	B	136	GLU	C-N-CA	5.45	135.34	121.70
2	B	32	THR	CB-CA-C	-5.36	97.12	111.60
1	A	1106	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	1573	ALA	CB-CA-C	5.11	117.77	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1524	PRO	Peptide
1	A	213	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	726	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9057	0	9064	559	0
2	B	1371	0	1326	121	0
3	C	61	0	52	1	0
4	D	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	39	0	34	0	0
4	F	39	0	34	0	0
5	G	28	0	25	0	0
All	All	10634	0	10569	663	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 31.

All (663) 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:1383:VAL:CG1	1:A:1386:ASN:HB2	1.64	1.28
2:B:76:SER:O	2:B:82:GLY:HA3	1.33	1.23
1:A:324:CYS:SG	1:A:325:PRO:HD2	1.83	1.17
1:A:664:ILE:HD12	1:A:1142:ILE:HD11	1.27	1.16
1:A:1376:LEU:CB	1:A:1380:PHE:HB3	1.76	1.16
1:A:273:ARG:HG2	1:A:328:TYR:CE1	1.80	1.14
1:A:1022:ILE:HD13	2:B:24:ALA:HB3	1.28	1.14
1:A:1383:VAL:HG12	1:A:1386:ASN:HB2	1.19	1.13
1:A:629:THR:O	1:A:632:ILE:HG22	1.47	1.13
1:A:661:LEU:O	1:A:664:ILE:HG13	1.47	1.13
1:A:247:LEU:HD23	1:A:1437:ILE:HG13	1.14	1.12
1:A:1522:CYS:C	1:A:1524:PRO:CD	2.18	1.11
1:A:1376:LEU:CD1	1:A:1380:PHE:HB3	1.81	1.11
1:A:1188:ARG:HH21	1:A:1190:VAL:HG21	1.10	1.09
2:B:43:GLY:HA2	2:B:108:SER:HB3	1.31	1.09
1:A:1123:LEU:O	1:A:1126:ILE:HG22	1.51	1.08
1:A:247:LEU:CD2	1:A:1437:ILE:HG13	1.83	1.07
1:A:1383:VAL:CG1	1:A:1386:ASN:CB	2.33	1.07
1:A:1383:VAL:HG13	1:A:1386:ASN:H	1.18	1.06
2:B:35:VAL:CG2	2:B:153:ALA:HB2	1.86	1.05
1:A:629:THR:C	1:A:632:ILE:HG22	1.76	1.05
1:A:1522:CYS:O	1:A:1524:PRO:HD2	1.54	1.04
1:A:304:TYR:HD1	1:A:305:PHE:N	1.55	1.03
1:A:629:THR:CA	1:A:632:ILE:HG22	1.87	1.03
1:A:1188:ARG:HD2	1:A:1190:VAL:CG2	1.89	1.03
1:A:1376:LEU:CD1	1:A:1380:PHE:CB	2.36	1.02
1:A:1376:LEU:HD12	1:A:1380:PHE:CB	1.90	1.02
1:A:629:THR:HA	1:A:632:ILE:HG22	1.43	1.01
1:A:1522:CYS:C	1:A:1524:PRO:HD3	1.81	1.01
1:A:1188:ARG:CD	1:A:1190:VAL:CG2	2.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:SER:O	1:A:193:THR:HG22	1.61	1.00
1:A:273:ARG:HG2	1:A:328:TYR:HE1	1.17	0.99
1:A:671:TRP:HD1	1:A:672:PRO:N	1.61	0.98
1:A:643:LEU:HD22	1:A:656:LEU:HD13	1.44	0.98
1:A:1522:CYS:HB3	1:A:1524:PRO:HD3	1.44	0.98
1:A:247:LEU:HD23	1:A:1437:ILE:CG1	1.92	0.97
1:A:1188:ARG:HD2	1:A:1190:VAL:HG23	1.44	0.97
1:A:1346:GLN:H	1:A:1346:GLN:HE21	1.09	0.96
2:B:43:GLY:CA	2:B:108:SER:HB3	1.95	0.96
1:A:1188:ARG:HD3	1:A:1190:VAL:HG22	1.43	0.96
1:A:629:THR:O	1:A:632:ILE:CG2	2.14	0.96
1:A:583:MET:HE1	1:A:661:LEU:HG	1.46	0.95
2:B:35:VAL:HG21	2:B:153:ALA:HB2	1.48	0.95
1:A:176:HIS:O	1:A:179:PHE:HB3	1.63	0.95
1:A:1376:LEU:HB3	1:A:1380:PHE:HB3	1.46	0.95
1:A:1522:CYS:C	1:A:1524:PRO:HD2	1.83	0.95
1:A:367:TYR:HD1	1:A:382:PHE:CD2	1.85	0.95
1:A:1434:ALA:CB	1:A:1437:ILE:HG22	1.97	0.95
1:A:1402:LEU:HD23	1:A:1419:ILE:HG13	1.47	0.94
1:A:1171:GLU:O	1:A:1172:VAL:HB	1.64	0.94
1:A:1529:PRO:CG	2:B:105:GLN:HE21	1.81	0.93
1:A:1383:VAL:HG12	1:A:1386:ASN:CB	1.98	0.92
1:A:629:THR:HA	1:A:632:ILE:CG2	1.98	0.92
1:A:1315:VAL:HG12	1:A:1375:ALA:HB2	1.50	0.92
1:A:1172:VAL:HG13	1:A:1172:VAL:O	1.65	0.92
1:A:1529:PRO:HG3	2:B:105:GLN:HE21	1.35	0.92
1:A:367:TYR:CD1	1:A:382:PHE:HD2	1.87	0.91
1:A:664:ILE:HA	1:A:667:LEU:HD12	1.52	0.91
1:A:784:LEU:O	1:A:788:LEU:HD23	1.70	0.91
1:A:1066:TRP:CH2	1:A:1119:VAL:HG11	2.06	0.90
1:A:325:PRO:HG2	1:A:328:TYR:HD2	1.36	0.90
2:B:43:GLY:HA2	2:B:108:SER:CB	2.00	0.90
1:A:321:ALA:HB2	1:A:375:GLY:HA2	1.54	0.90
1:A:1522:CYS:HB3	1:A:1524:PRO:CD	2.01	0.90
1:A:367:TYR:HD1	1:A:382:PHE:HD2	1.19	0.90
2:B:134:TYR:HB2	2:B:135:TYR:CD1	2.06	0.90
1:A:1113:GLU:CG	1:A:1282:THR:HG21	2.02	0.89
1:A:1376:LEU:HD12	1:A:1380:PHE:HB2	1.50	0.89
1:A:583:MET:HE1	1:A:661:LEU:CG	2.01	0.89
1:A:1515:LEU:HD11	1:A:1544:ILE:HD11	1.53	0.89
1:A:1529:PRO:CG	2:B:105:GLN:NE2	2.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:ARG:HH21	1:A:1190:VAL:CG2	1.87	0.88
1:A:1498:LEU:O	1:A:1501:ILE:HG22	1.72	0.88
1:A:1527:GLU:OE1	1:A:1534:ARG:HG3	1.73	0.88
1:A:1346:GLN:O	1:A:1347:SER:OG	1.92	0.88
1:A:187:LEU:HD23	1:A:188:ASP:N	1.89	0.87
1:A:643:LEU:CD2	1:A:656:LEU:HD13	2.03	0.87
1:A:671:TRP:CD1	1:A:672:PRO:HD2	2.09	0.87
2:B:134:TYR:HB2	2:B:135:TYR:CE1	2.07	0.87
2:B:42:LEU:HD13	2:B:122:TYR:CE2	2.08	0.87
1:A:643:LEU:CD2	1:A:656:LEU:CD1	2.52	0.87
1:A:174:ILE:HG23	1:A:177:PHE:CE2	2.10	0.87
1:A:1475:TYR:OH	1:A:1533:VAL:HG21	1.75	0.86
1:A:664:ILE:HD12	1:A:1142:ILE:CD1	2.06	0.86
1:A:1169:VAL:HG21	1:A:1226:ARG:NH1	1.90	0.86
1:A:1361:PHE:O	1:A:1364:ILE:HG22	1.76	0.85
1:A:1188:ARG:HD3	1:A:1190:VAL:CG2	2.05	0.85
1:A:1524:PRO:HA	1:A:1535:GLY:HA2	1.59	0.85
1:A:1529:PRO:HG3	2:B:105:GLN:NE2	1.92	0.85
1:A:195:THR:O	1:A:198:THR:HG22	1.77	0.85
1:A:1402:LEU:CD2	1:A:1419:ILE:HD12	2.06	0.85
1:A:661:LEU:O	1:A:664:ILE:CG1	2.24	0.84
2:B:35:VAL:HG22	2:B:153:ALA:HB2	1.58	0.84
1:A:1123:LEU:O	1:A:1123:LEU:HD22	1.78	0.84
2:B:57:ALA:HB1	2:B:104:LEU:HD12	1.58	0.83
1:A:1523:ASP:N	1:A:1524:PRO:CD	2.40	0.83
2:B:42:LEU:HD11	2:B:111:ILE:HD11	1.58	0.83
1:A:324:CYS:SG	1:A:325:PRO:CD	2.67	0.83
1:A:1383:VAL:HG11	1:A:1386:ASN:ND2	1.93	0.83
1:A:174:ILE:HG23	1:A:177:PHE:HE2	1.42	0.82
1:A:367:TYR:CD1	1:A:382:PHE:CD2	2.66	0.82
1:A:989:LEU:O	1:A:992:THR:HG22	1.79	0.82
1:A:1022:ILE:HD13	2:B:24:ALA:CB	2.07	0.82
1:A:1383:VAL:HG13	1:A:1386:ASN:N	1.95	0.82
1:A:1379:TYR:O	1:A:1382:THR:HG23	1.80	0.81
1:A:305:PHE:HB3	1:A:312:ALA:HA	1.60	0.81
1:A:632:ILE:HD13	1:A:632:ILE:O	1.79	0.81
1:A:1346:GLN:HE21	1:A:1346:GLN:N	1.78	0.81
1:A:1383:VAL:CG1	1:A:1386:ASN:ND2	2.43	0.81
1:A:357:LEU:HD21	1:A:366:LEU:HD23	1.61	0.81
1:A:1123:LEU:O	1:A:1127:PRO:HD3	1.81	0.81
1:A:1188:ARG:NH2	1:A:1190:VAL:HG21	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:LEU:HD23	1:A:1419:ILE:CG1	2.11	0.81
1:A:1066:TRP:CZ2	1:A:1119:VAL:HG11	2.16	0.80
1:A:1312:GLN:NE2	1:A:1375:ALA:HA	1.96	0.80
1:A:1434:ALA:HB1	1:A:1437:ILE:HG22	1.63	0.80
1:A:304:TYR:CD1	1:A:305:PHE:N	2.45	0.80
1:A:1353:ILE:O	1:A:1357:ILE:HG13	1.82	0.80
1:A:300:GLU:HA	1:A:303:GLN:HE21	1.46	0.80
1:A:671:TRP:CD1	1:A:672:PRO:N	2.48	0.80
1:A:1516:ASN:HD22	1:A:1517:THR:N	1.80	0.80
1:A:273:ARG:HA	1:A:328:TYR:HD1	1.46	0.80
1:A:620:LEU:O	1:A:621:ASP:O	1.99	0.80
1:A:1434:ALA:HB3	1:A:1437:ILE:HG22	1.62	0.80
1:A:1522:CYS:CB	1:A:1524:PRO:HD3	2.11	0.80
1:A:583:MET:HE3	1:A:661:LEU:HD11	1.63	0.79
1:A:1402:LEU:CD2	1:A:1419:ILE:CD1	2.59	0.79
1:A:1517:THR:HG21	1:A:1540:PRO:HD3	1.64	0.79
1:A:664:ILE:CD1	1:A:1142:ILE:HD11	2.09	0.79
1:A:582:PHE:HD2	1:A:605:PHE:CE2	2.01	0.79
1:A:1113:GLU:HG3	1:A:1282:THR:HG21	1.63	0.78
1:A:1113:GLU:HG2	1:A:1282:THR:HG21	1.65	0.78
1:A:1188:ARG:HG2	1:A:1189:TRP:N	1.99	0.78
1:A:1515:LEU:HD11	1:A:1544:ILE:CD1	2.14	0.78
1:A:1383:VAL:HG13	1:A:1386:ASN:HB2	1.60	0.78
1:A:671:TRP:HD1	1:A:672:PRO:CD	1.96	0.78
1:A:671:TRP:CD1	1:A:672:PRO:CD	2.66	0.78
2:B:50:ARG:HH11	2:B:50:ARG:HG2	1.49	0.77
1:A:583:MET:CE	1:A:661:LEU:HD11	2.14	0.77
1:A:1172:VAL:O	1:A:1172:VAL:CG1	2.30	0.77
1:A:582:PHE:HD2	1:A:605:PHE:HE2	1.32	0.77
1:A:1526:VAL:HG12	1:A:1535:GLY:CA	2.15	0.77
1:A:1113:GLU:HG3	1:A:1282:THR:CG2	2.15	0.77
1:A:1376:LEU:CG	1:A:1380:PHE:HB3	2.14	0.77
1:A:1376:LEU:HD13	1:A:1380:PHE:CB	2.15	0.76
1:A:1383:VAL:HG11	1:A:1386:ASN:CG	2.05	0.76
1:A:274:TRP:CZ3	1:A:331:MET:CE	2.68	0.76
1:A:602:ASN:HB3	1:A:660:ARG:HH12	1.50	0.76
1:A:664:ILE:HG22	1:A:667:LEU:HD13	1.67	0.76
1:A:1511:LEU:HG	1:A:1515:LEU:HD13	1.67	0.76
1:A:1335:ASN:HB2	1:A:1361:PHE:CE1	2.21	0.76
2:B:42:LEU:CD1	2:B:122:TYR:CE2	2.69	0.76
1:A:1129:ILE:HD12	1:A:1259:PHE:HE1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:TYR:CE1	1:A:631:ASN:HB3	2.20	0.75
1:A:247:LEU:O	1:A:247:LEU:HD22	1.85	0.75
1:A:304:TYR:CE2	1:A:325:PRO:HG3	2.21	0.75
1:A:1526:VAL:HG12	1:A:1535:GLY:HA2	1.68	0.75
1:A:1022:ILE:CD1	2:B:24:ALA:HB3	2.14	0.74
1:A:1434:ALA:HB3	1:A:1437:ILE:CG2	2.16	0.74
2:B:62:TRP:CH2	2:B:73:HIS:HD2	2.05	0.74
1:A:738:SER:O	1:A:741:ILE:HG22	1.87	0.74
1:A:1383:VAL:CG1	1:A:1386:ASN:CG	2.55	0.74
2:B:42:LEU:HD13	2:B:122:TYR:CD2	2.20	0.74
1:A:195:THR:HG21	1:A:216:ARG:HH21	1.53	0.74
1:A:345:ASP:O	1:A:346:ASN:HB3	1.85	0.74
2:B:130:LEU:O	2:B:130:LEU:HD23	1.86	0.74
1:A:1523:ASP:HB3	1:A:1526:VAL:HB	1.69	0.74
1:A:1501:ILE:HD12	1:A:1510:LEU:HD12	1.69	0.74
1:A:987:TRP:CE3	1:A:987:TRP:HA	2.23	0.74
1:A:1529:PRO:HG2	2:B:105:GLN:NE2	2.01	0.73
1:A:274:TRP:HA	1:A:274:TRP:CE3	2.24	0.73
1:A:629:THR:CA	1:A:632:ILE:CG2	2.62	0.73
1:A:1124:GLY:O	1:A:1127:PRO:HD2	1.88	0.73
1:A:1111:ARG:N	1:A:1111:ARG:HD2	2.02	0.73
1:A:379:MET:SD	1:A:1496:ILE:HD13	2.29	0.72
1:A:751:ILE:HG23	1:A:755:TRP:CZ2	2.24	0.72
2:B:61:TRP:CZ3	2:B:124:CYS:HB3	2.23	0.72
1:A:986:TRP:HH2	1:A:990:ARG:HH11	1.36	0.72
1:A:1188:ARG:HG2	1:A:1189:TRP:H	1.55	0.72
1:A:1517:THR:CG2	1:A:1540:PRO:HD3	2.20	0.72
1:A:583:MET:CE	1:A:661:LEU:HD21	2.20	0.71
1:A:379:MET:SD	1:A:1496:ILE:CD1	2.78	0.71
1:A:1434:ALA:CB	1:A:1437:ILE:CG2	2.68	0.71
1:A:1113:GLU:CG	1:A:1282:THR:CG2	2.68	0.71
1:A:1349:VAL:O	1:A:1353:ILE:HG13	1.91	0.71
1:A:1376:LEU:HB2	1:A:1380:PHE:HB3	1.72	0.71
1:A:1516:ASN:HD22	1:A:1517:THR:H	1.38	0.71
1:A:987:TRP:HA	1:A:987:TRP:HE3	1.55	0.71
1:A:1415:LEU:O	1:A:1419:ILE:HG12	1.90	0.71
2:B:99:LYS:O	2:B:100:ASN:CB	2.39	0.71
1:A:273:ARG:HA	1:A:328:TYR:CD1	2.27	0.70
1:A:620:LEU:O	1:A:624:TYR:HB2	1.92	0.70
1:A:664:ILE:CA	1:A:667:LEU:HD12	2.22	0.70
1:A:1123:LEU:HD13	1:A:1124:GLY:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:TYR:HB3	2:B:24:ALA:N	2.07	0.69
1:A:1376:LEU:HD13	1:A:1380:PHE:CA	2.22	0.69
2:B:57:ALA:HB3	2:B:104:LEU:HG	1.73	0.69
1:A:751:ILE:CG2	1:A:755:TRP:CZ2	2.75	0.69
2:B:99:LYS:O	2:B:100:ASN:HB3	1.90	0.69
1:A:657:ARG:O	1:A:660:ARG:HG3	1.92	0.69
1:A:273:ARG:CG	1:A:328:TYR:HE1	2.01	0.69
1:A:321:ALA:CB	1:A:375:GLY:HA2	2.23	0.69
1:A:1125:ALA:O	1:A:1129:ILE:HG12	1.93	0.69
1:A:1522:CYS:CA	1:A:1524:PRO:HD3	2.23	0.69
1:A:1523:ASP:N	1:A:1524:PRO:HD3	2.06	0.69
1:A:174:ILE:HA	1:A:177:PHE:HD2	1.58	0.69
1:A:664:ILE:CG2	1:A:667:LEU:HD13	2.22	0.68
1:A:1315:VAL:CG1	1:A:1375:ALA:HB2	2.21	0.68
1:A:584:SER:HA	1:A:1145:ILE:HD12	1.75	0.68
1:A:1510:LEU:O	1:A:1513:PRO:HD2	1.91	0.68
1:A:247:LEU:CD2	1:A:1437:ILE:CG1	2.64	0.68
1:A:664:ILE:HA	1:A:667:LEU:CD1	2.23	0.68
1:A:1066:TRP:HH2	1:A:1119:VAL:HG11	1.54	0.67
1:A:999:HIS:CE1	1:A:1001:TYR:HD2	2.12	0.67
1:A:1116:LYS:CE	1:A:1120:ARG:HE	2.08	0.67
1:A:1123:LEU:HD13	1:A:1123:LEU:C	2.15	0.67
1:A:1475:TYR:CZ	1:A:1533:VAL:HG21	2.30	0.67
1:A:664:ILE:O	1:A:667:LEU:HB2	1.94	0.67
1:A:666:LYS:O	1:A:669:LYS:HD3	1.95	0.67
1:A:304:TYR:HE2	1:A:325:PRO:HG3	1.58	0.67
1:A:262:LEU:O	1:A:1417:ARG:HD2	1.95	0.67
2:B:57:ALA:CB	2:B:104:LEU:HD12	2.25	0.67
1:A:1319:VAL:HG13	1:A:1320:THR:HG23	1.76	0.67
1:A:272:ILE:HD12	1:A:331:MET:HB2	1.75	0.67
1:A:986:TRP:HH2	1:A:990:ARG:NH1	1.92	0.66
1:A:1133:LEU:O	1:A:1137:LEU:HD13	1.93	0.66
2:B:50:ARG:O	2:B:52:GLU:N	2.29	0.66
1:A:643:LEU:HD22	1:A:656:LEU:CD1	2.17	0.66
1:A:347:PHE:O	1:A:350:THR:HG23	1.96	0.66
1:A:187:LEU:HD23	1:A:187:LEU:C	2.15	0.66
1:A:318:ASN:ND2	1:A:374:ALA:O	2.29	0.66
1:A:247:LEU:C	1:A:247:LEU:HD13	2.16	0.65
1:A:274:TRP:CZ3	1:A:331:MET:HE1	2.31	0.65
1:A:1115:MET:HE2	1:A:1456:LEU:HG	1.79	0.65
1:A:190:SER:C	1:A:193:THR:HG22	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:ILE:CD1	2:B:24:ALA:CB	2.74	0.65
1:A:1486:PHE:HB3	1:A:1497:CYS:SG	2.36	0.65
1:A:1188:ARG:CD	1:A:1190:VAL:HG23	2.13	0.65
1:A:744:ARG:NH1	1:A:752:GLU:OE1	2.29	0.64
1:A:1123:LEU:O	1:A:1126:ILE:CG2	2.37	0.64
1:A:1376:LEU:O	1:A:1377:ARG:C	2.36	0.64
1:A:1376:LEU:HB3	1:A:1380:PHE:CB	2.25	0.64
1:A:1376:LEU:HD13	1:A:1380:PHE:HB3	1.76	0.64
1:A:1157:ARG:HH11	1:A:1192:LEU:CD2	2.11	0.64
1:A:329:THR:HG22	1:A:330:CYS:N	2.12	0.64
1:A:673:THR:CG2	1:A:1135:VAL:HG21	2.27	0.64
1:A:663:ARG:O	1:A:666:LYS:HB3	1.97	0.64
1:A:1523:ASP:CB	1:A:1526:VAL:HB	2.28	0.64
1:A:1383:VAL:HG12	1:A:1386:ASN:HD22	1.63	0.64
1:A:300:GLU:HA	1:A:303:GLN:NE2	2.13	0.63
1:A:583:MET:CE	1:A:661:LEU:CG	2.77	0.63
1:A:274:TRP:CZ3	1:A:331:MET:HE3	2.33	0.63
1:A:337:PRO:O	1:A:338:ASN:HB2	1.96	0.63
1:A:582:PHE:CD2	1:A:605:PHE:HE2	2.17	0.62
1:A:1402:LEU:HD22	1:A:1419:ILE:HD12	1.81	0.62
1:A:1529:PRO:HG2	2:B:105:GLN:HE21	1.58	0.62
1:A:1483:ASP:O	1:A:1484:ASP:OD1	2.18	0.62
2:B:104:LEU:O	2:B:105:GLN:HB2	1.99	0.62
1:A:1145:ILE:O	1:A:1148:VAL:CG2	2.48	0.62
1:A:1522:CYS:HB3	1:A:1524:PRO:CG	2.29	0.62
1:A:1379:TYR:O	1:A:1382:THR:CG2	2.48	0.62
1:A:187:LEU:O	1:A:190:SER:N	2.33	0.61
1:A:256:THR:HG23	1:A:354:LEU:HD23	1.80	0.61
1:A:342:THR:HG22	1:A:342:THR:O	2.00	0.61
1:A:1194:VAL:HG13	1:A:1515:LEU:CD2	2.30	0.61
1:A:625:TYR:CD1	1:A:631:ASN:HB3	2.36	0.61
1:A:1168:PRO:O	1:A:1169:VAL:HG12	2.01	0.61
2:B:132:PHE:O	2:B:133:ASN:HB2	2.01	0.61
1:A:1364:ILE:HG23	1:A:1365:PHE:CD1	2.36	0.61
2:B:103:ASP:O	2:B:104:LEU:HB2	2.00	0.61
1:A:1169:VAL:HG21	1:A:1226:ARG:HH11	1.65	0.60
1:A:1519:PRO:HA	1:A:1520:PRO:C	2.22	0.60
1:A:190:SER:O	1:A:193:THR:CG2	2.44	0.60
2:B:62:TRP:CH2	2:B:73:HIS:CD2	2.89	0.60
1:A:357:LEU:CD2	1:A:366:LEU:HD23	2.30	0.60
1:A:625:TYR:CE1	1:A:631:ASN:CB	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:ILE:CD1	1:A:1510:LEU:HD12	2.32	0.60
2:B:46:SER:HB2	2:B:126:PHE:CD2	2.36	0.60
2:B:155:ARG:HH11	2:B:155:ARG:CG	2.15	0.60
1:A:274:TRP:HZ3	1:A:331:MET:CE	2.14	0.59
1:A:1352:ASP:O	1:A:1356:GLN:HG2	2.01	0.59
1:A:1376:LEU:CB	1:A:1380:PHE:CB	2.69	0.59
1:A:1518:GLY:C	1:A:1522:CYS:HB2	2.23	0.59
1:A:1534:ARG:H	1:A:1534:ARG:CD	2.15	0.59
1:A:183:PRO:O	1:A:186:TRP:HB3	2.02	0.59
1:A:585:ILE:HG13	1:A:585:ILE:O	2.02	0.59
1:A:1383:VAL:HG12	1:A:1386:ASN:ND2	2.15	0.59
1:A:1511:LEU:HD11	1:A:1544:ILE:HD13	1.83	0.59
1:A:272:ILE:HD13	1:A:297:ILE:HB	1.85	0.59
1:A:999:HIS:CE1	1:A:1001:TYR:CD2	2.90	0.59
1:A:1376:LEU:HD12	1:A:1380:PHE:HB3	1.60	0.59
1:A:266:ASN:O	1:A:269:HIS:HD2	1.84	0.59
1:A:583:MET:CE	1:A:661:LEU:CD1	2.80	0.59
1:A:1312:GLN:HE21	1:A:1375:ALA:HA	1.65	0.59
1:A:602:ASN:HB3	1:A:660:ARG:NH1	2.18	0.59
1:A:256:THR:CG2	1:A:354:LEU:HD23	2.33	0.58
1:A:1373:LEU:HD12	1:A:1380:PHE:CE1	2.38	0.58
1:A:1511:LEU:CG	1:A:1515:LEU:HD13	2.33	0.58
2:B:42:LEU:HD13	2:B:122:TYR:HE2	1.67	0.58
1:A:661:LEU:O	1:A:664:ILE:CD1	2.51	0.58
1:A:1348:GLN:O	1:A:1352:ASP:N	2.32	0.58
1:A:1376:LEU:HD13	1:A:1380:PHE:HA	1.84	0.58
2:B:40:PHE:HD2	2:B:42:LEU:CD2	2.15	0.58
1:A:1101:ARG:O	1:A:1104:ARG:HG2	2.03	0.58
1:A:1383:VAL:CG1	1:A:1386:ASN:HD22	2.13	0.58
1:A:1385:TRP:HA	1:A:1385:TRP:CE3	2.38	0.58
1:A:1383:VAL:CG1	1:A:1386:ASN:H	2.04	0.58
2:B:132:PHE:HE1	2:B:137:PHE:HB3	1.68	0.58
1:A:1145:ILE:O	1:A:1148:VAL:HG23	2.04	0.58
1:A:245:VAL:HG12	1:A:246:ILE:N	2.18	0.58
1:A:188:ASP:OD2	1:A:219:LYS:NZ	2.36	0.58
1:A:255:PHE:CB	1:A:354:LEU:HD21	2.33	0.58
2:B:178:LEU:O	2:B:182:VAL:HG23	2.03	0.58
2:B:100:ASN:C	2:B:100:ASN:HD22	2.06	0.58
1:A:1169:VAL:HG21	1:A:1226:ARG:HH12	1.68	0.57
1:A:673:THR:HG22	1:A:1135:VAL:HG21	1.84	0.57
1:A:1511:LEU:CD1	1:A:1515:LEU:HD13	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:SER:OG	2:B:31:ASP:N	2.37	0.57
1:A:305:PHE:O	1:A:305:PHE:HD1	1.87	0.57
1:A:316:GLY:HA3	1:A:373:ALA:O	2.04	0.57
2:B:35:VAL:HG21	2:B:153:ALA:CB	2.30	0.57
1:A:632:ILE:O	1:A:636:ILE:HG12	2.05	0.57
1:A:1208:GLN:OE1	1:A:1218:ILE:HD11	2.03	0.57
1:A:1009:MET:HG3	1:A:1044:VAL:HG11	1.85	0.57
1:A:1377:ARG:O	1:A:1380:PHE:CD1	2.57	0.57
1:A:1123:LEU:HD22	1:A:1123:LEU:C	2.24	0.57
1:A:673:THR:HG22	1:A:1135:VAL:CG2	2.35	0.57
1:A:1194:VAL:CG1	1:A:1515:LEU:HD21	2.34	0.57
2:B:62:TRP:CZ2	2:B:73:HIS:HD2	2.23	0.56
2:B:134:TYR:CB	2:B:135:TYR:CE1	2.85	0.56
1:A:347:PHE:O	1:A:350:THR:CG2	2.53	0.56
1:A:1373:LEU:HD12	1:A:1380:PHE:CZ	2.41	0.56
1:A:1385:TRP:HA	1:A:1385:TRP:HE3	1.69	0.56
1:A:1402:LEU:HD23	1:A:1419:ILE:CD1	2.31	0.56
2:B:62:TRP:CZ2	2:B:73:HIS:CD2	2.93	0.56
2:B:125:TYR:CE2	2:B:127:ASP:HB2	2.41	0.56
2:B:50:ARG:HH11	2:B:50:ARG:CG	2.15	0.56
2:B:57:ALA:HB2	2:B:128:ARG:HG2	1.88	0.56
1:A:1550:TYR:O	1:A:1554:SER:N	2.39	0.56
1:A:1129:ILE:HD12	1:A:1259:PHE:CE1	2.38	0.56
1:A:1373:LEU:HA	1:A:1380:PHE:CE1	2.40	0.56
2:B:180:GLU:OE2	2:B:180:GLU:HA	2.03	0.56
1:A:1116:LYS:HG2	1:A:1120:ARG:HD2	1.87	0.56
2:B:48:LYS:O	2:B:50:ARG:N	2.39	0.56
1:A:273:ARG:HH12	2:B:135:TYR:HB2	1.70	0.55
1:A:313:LEU:HD13	1:A:313:LEU:C	2.26	0.55
1:A:256:THR:O	1:A:260:MET:N	2.39	0.55
1:A:367:TYR:HA	1:A:382:PHE:CE2	2.41	0.55
1:A:1194:VAL:CG1	1:A:1515:LEU:CD2	2.84	0.55
1:A:625:TYR:CE1	1:A:631:ASN:CG	2.80	0.55
1:A:751:ILE:HG23	1:A:755:TRP:CH2	2.41	0.55
2:B:43:GLY:HA3	2:B:108:SER:HB3	1.86	0.55
1:A:299:ASN:O	1:A:303:GLN:HG2	2.07	0.55
1:A:325:PRO:HG2	1:A:328:TYR:CD2	2.27	0.55
1:A:346:ASN:O	1:A:350:THR:HG22	2.06	0.55
1:A:1522:CYS:HB3	1:A:1524:PRO:HG3	1.86	0.55
1:A:1377:ARG:HG3	1:A:1378:GLN:H	1.71	0.55
1:A:343:ASN:ND2	1:A:345:ASP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ARG:NH1	2:B:155:ARG:HG2	2.20	0.54
2:B:35:VAL:O	2:B:38:HIS:HB3	2.06	0.54
1:A:583:MET:HE1	1:A:661:LEU:CD1	2.36	0.54
1:A:664:ILE:CG2	1:A:667:LEU:CD1	2.86	0.54
1:A:583:MET:CE	1:A:661:LEU:CD2	2.85	0.54
1:A:1454:ILE:HG21	1:A:1561:MET:HB2	1.88	0.54
2:B:64:MET:HB2	2:B:71:PHE:HE1	1.73	0.54
1:A:551:PRO:HA	1:A:554:PHE:HB3	1.88	0.53
1:A:1335:ASN:HB2	1:A:1361:PHE:CD1	2.43	0.53
2:B:42:LEU:N	2:B:42:LEU:HD23	2.23	0.53
1:A:1115:MET:CE	1:A:1456:LEU:HG	2.37	0.53
1:A:1170:GLU:OE1	1:A:1170:GLU:HA	2.08	0.53
1:A:1373:LEU:HA	1:A:1380:PHE:CZ	2.43	0.53
1:A:1434:ALA:O	1:A:1435:LYS:HB3	2.08	0.53
1:A:602:ASN:CB	1:A:660:ARG:HH12	2.18	0.53
1:A:273:ARG:HH12	2:B:135:TYR:CB	2.22	0.53
2:B:40:PHE:CD2	2:B:42:LEU:CD2	2.92	0.53
1:A:163:VAL:CG2	1:A:188:ASP:OD1	2.57	0.52
1:A:274:TRP:HZ3	1:A:331:MET:HE1	1.74	0.52
1:A:1457:LEU:O	1:A:1461:ILE:HG13	2.09	0.52
1:A:1534:ARG:NH1	1:A:1534:ARG:HG2	2.23	0.52
1:A:167:VAL:HG11	1:A:176:HIS:ND1	2.25	0.52
1:A:1116:LYS:HE2	1:A:1120:ARG:HE	1.72	0.52
1:A:1136:CYS:SG	1:A:1255:THR:HG23	2.50	0.52
1:A:1116:LYS:HE2	1:A:1120:ARG:NE	2.25	0.52
1:A:1169:VAL:HG11	1:A:1233:ILE:HG13	1.92	0.52
1:A:1534:ARG:CD	1:A:1534:ARG:N	2.73	0.52
1:A:343:ASN:HB2	1:A:345:ASP:OD2	2.10	0.52
1:A:993:CYS:SG	1:A:1054:VAL:CG2	2.98	0.52
1:A:344:TYR:HA	1:A:350:THR:HB	1.91	0.52
2:B:132:PHE:HB3	2:B:134:TYR:CE1	2.45	0.52
1:A:417:GLN:O	1:A:421:ALA:N	2.43	0.51
1:A:1377:ARG:O	1:A:1380:PHE:CE1	2.63	0.51
1:A:1116:LYS:HE3	1:A:1120:ARG:HE	1.73	0.51
2:B:79:ASP:O	2:B:80:MET:HG3	2.10	0.51
2:B:115:THR:HG23	2:B:117:ASN:H	1.74	0.51
1:A:304:TYR:HD1	1:A:305:PHE:H	1.49	0.51
1:A:990:ARG:HG3	1:A:1054:VAL:O	2.10	0.51
1:A:580:THR:HG23	1:A:661:LEU:HD22	1.92	0.51
1:A:632:ILE:HD13	1:A:632:ILE:C	2.30	0.51
1:A:1173:ASN:H	4:D:1:NAG:H82	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:PHE:HE1	1:A:1248:ILE:HD11	1.76	0.51
1:A:1383:VAL:O	1:A:1387:VAL:HG23	2.10	0.51
1:A:1273:LYS:N	1:A:1273:LYS:CD	2.73	0.51
1:A:1534:ARG:HG2	1:A:1534:ARG:HH11	1.75	0.51
1:A:1120:ARG:CG	1:A:1120:ARG:HH11	2.22	0.51
1:A:1247:PHE:O	1:A:1251:GLY:N	2.38	0.51
1:A:353:CYS:O	1:A:356:ARG:HB3	2.11	0.51
2:B:104:LEU:O	2:B:105:GLN:CB	2.60	0.50
1:A:150:ILE:O	1:A:154:THR:N	2.44	0.50
1:A:625:TYR:O	1:A:631:ASN:HB2	2.11	0.50
1:A:664:ILE:O	1:A:667:LEU:HD12	2.11	0.50
2:B:50:ARG:CG	2:B:50:ARG:NH1	2.73	0.50
1:A:329:THR:CG2	1:A:330:CYS:N	2.74	0.50
1:A:128:ILE:HA	1:A:131:THR:HG22	1.93	0.50
1:A:1250:PHE:HA	1:A:1254:PHE:HD2	1.75	0.50
1:A:1359:VAL:O	1:A:1363:ILE:HG12	2.11	0.50
2:B:134:TYR:C	2:B:135:TYR:CG	2.85	0.50
1:A:1013:SER:HB3	1:A:1041:PHE:CD1	2.47	0.50
1:A:1483:ASP:N	1:A:1483:ASP:OD1	2.44	0.50
2:B:133:ASN:C	2:B:134:TYR:CG	2.85	0.50
1:A:121:ASN:O	1:A:125:ASN:ND2	2.44	0.50
1:A:347:PHE:CD1	1:A:347:PHE:C	2.85	0.50
1:A:757:CYS:SG	1:A:770:TYR:HE2	2.34	0.50
1:A:1527:GLU:OE1	1:A:1534:ARG:CG	2.55	0.50
1:A:751:ILE:CG2	1:A:755:TRP:CE2	2.95	0.50
1:A:1388:PHE:C	1:A:1388:PHE:CD1	2.85	0.50
1:A:1273:LYS:N	1:A:1273:LYS:HD3	2.26	0.50
1:A:1516:ASN:OD1	1:A:1521:ASP:HB3	2.12	0.50
1:A:1528:ASN:HB3	2:B:24:ALA:O	2.11	0.50
2:B:76:SER:O	2:B:82:GLY:CA	2.28	0.49
2:B:133:ASN:C	2:B:134:TYR:CD1	2.85	0.49
1:A:304:TYR:CD2	1:A:325:PRO:HG3	2.46	0.49
1:A:1332:ILE:O	1:A:1336:MET:N	2.45	0.49
1:A:346:ASN:ND2	1:A:348:ALA:N	2.60	0.49
1:A:367:TYR:CE1	1:A:382:PHE:HD2	2.29	0.49
1:A:985:ILE:HG23	2:B:185:TYR:OH	2.11	0.49
1:A:1027:ARG:HG3	1:A:1030:ILE:HD12	1.94	0.49
1:A:1489:GLU:HG2	2:B:24:ALA:HB2	1.95	0.49
1:A:1534:ARG:H	1:A:1534:ARG:HD2	1.77	0.49
1:A:149:LYS:HG2	1:A:152:GLU:OE1	2.12	0.49
2:B:124:CYS:SG	2:B:143:LYS:HB2	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:TYR:CD1	1:A:304:TYR:C	2.86	0.49
1:A:255:PHE:HB3	1:A:354:LEU:HD21	1.95	0.49
1:A:1377:ARG:HG3	1:A:1378:GLN:N	2.28	0.49
2:B:57:ALA:HB3	2:B:104:LEU:CG	2.42	0.49
1:A:602:ASN:HB3	1:A:660:ARG:HH22	1.78	0.49
1:A:170:ARG:O	1:A:175:GLY:C	2.51	0.49
1:A:1120:ARG:HH11	1:A:1120:ARG:CB	2.26	0.49
1:A:629:THR:O	1:A:633:PHE:N	2.44	0.48
1:A:1157:ARG:HH11	1:A:1192:LEU:HD23	1.77	0.48
1:A:643:LEU:CD2	1:A:656:LEU:HD12	2.41	0.48
2:B:57:ALA:CB	2:B:104:LEU:CD1	2.90	0.48
1:A:583:MET:HE3	1:A:661:LEU:HD21	1.93	0.48
2:B:61:TRP:CH2	2:B:124:CYS:HB3	2.47	0.48
1:A:314:LEU:O	1:A:372:ARG:CG	2.62	0.48
1:A:1483:ASP:C	1:A:1484:ASP:OD1	2.52	0.48
1:A:177:PHE:CD1	1:A:177:PHE:C	2.85	0.48
1:A:247:LEU:CD2	1:A:1437:ILE:CD1	2.91	0.48
1:A:1039:LYS:O	1:A:1042:THR:OG1	2.25	0.48
1:A:1534:ARG:N	1:A:1534:ARG:HD2	2.28	0.48
1:A:1402:LEU:HD21	1:A:1419:ILE:CD1	2.41	0.48
2:B:43:GLY:HA2	2:B:108:SER:CA	2.43	0.48
2:B:130:LEU:HD23	2:B:130:LEU:C	2.34	0.48
2:B:171:ILE:O	2:B:175:LEU:HG	2.13	0.47
1:A:179:PHE:CE1	1:A:185:ASN:OD1	2.67	0.47
1:A:255:PHE:O	1:A:259:GLY:N	2.45	0.47
1:A:1376:LEU:HB2	1:A:1380:PHE:CD1	2.49	0.47
1:A:267:LEU:HG	1:A:344:TYR:CD2	2.49	0.47
1:A:1373:LEU:CD1	1:A:1380:PHE:HZ	2.27	0.47
1:A:583:MET:HE1	1:A:661:LEU:CD2	2.44	0.47
1:A:1524:PRO:HA	1:A:1535:GLY:CA	2.38	0.47
1:A:163:VAL:HG21	1:A:192:VAL:HG21	1.95	0.47
1:A:346:ASN:ND2	1:A:348:ALA:H	2.12	0.47
1:A:755:TRP:CE3	1:A:755:TRP:CA	2.97	0.47
1:A:582:PHE:CD2	1:A:605:PHE:CE2	2.92	0.47
2:B:155:ARG:CG	2:B:155:ARG:NH1	2.73	0.47
1:A:167:VAL:CG1	1:A:176:HIS:ND1	2.78	0.47
1:A:643:LEU:HD21	1:A:656:LEU:CD1	2.41	0.47
1:A:717:TYR:HB2	1:A:760:VAL:HG23	1.97	0.47
1:A:755:TRP:CE3	1:A:755:TRP:HA	2.49	0.47
1:A:1326:ILE:O	1:A:1329:MET:HB2	2.15	0.47
2:B:107:GLY:H	2:B:126:PHE:HZ	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:GLN:N	1:A:1356:GLN:OE1	2.48	0.47
1:A:267:LEU:HD12	1:A:342:THR:O	2.15	0.47
1:A:415:GLU:O	1:A:419:LYS:N	2.47	0.47
1:A:671:TRP:CD1	1:A:671:TRP:C	2.88	0.47
1:A:1298:LYS:O	1:A:1299:LYS:CB	2.63	0.47
1:A:1383:VAL:HG13	1:A:1386:ASN:CB	2.25	0.47
1:A:1520:PRO:O	1:A:1521:ASP:HB2	2.15	0.47
2:B:188:ILE:O	2:B:192:GLY:N	2.47	0.47
1:A:609:PHE:CD1	1:A:663:ARG:CZ	2.98	0.46
2:B:50:ARG:HG2	2:B:50:ARG:NH1	2.24	0.46
1:A:663:ARG:O	1:A:666:LYS:CB	2.63	0.46
2:B:155:ARG:HH11	2:B:155:ARG:HG2	1.79	0.46
1:A:1373:LEU:CD1	1:A:1380:PHE:CZ	2.98	0.46
1:A:364:GLU:O	1:A:367:TYR:HB3	2.16	0.46
1:A:255:PHE:HZ	1:A:388:LEU:HD22	1.81	0.46
1:A:372:ARG:HH21	1:A:1485:ILE:HD13	1.79	0.46
1:A:664:ILE:CD1	1:A:1142:ILE:CD1	2.81	0.46
1:A:1021:ASP:OD1	1:A:1022:ILE:N	2.49	0.46
2:B:160:ILE:O	2:B:163:GLU:HB3	2.15	0.46
1:A:273:ARG:HH21	1:A:273:ARG:HG3	1.81	0.46
1:A:1022:ILE:HG23	1:A:1531:THR:HG21	1.97	0.46
1:A:1212:PHE:CE1	1:A:1248:ILE:HD11	2.51	0.46
1:A:1160:ASN:HA	1:A:1187:VAL:HG23	1.98	0.46
2:B:174:GLN:HA	2:B:174:GLN:NE2	2.31	0.46
1:A:273:ARG:HG3	1:A:273:ARG:NH2	2.32	0.45
1:A:655:VAL:HG12	1:A:655:VAL:O	2.16	0.45
1:A:754:MET:HA	1:A:757:CYS:HB3	1.97	0.45
1:A:719:CYS:O	1:A:720:LYS:C	2.54	0.45
1:A:1209:VAL:HG12	1:A:1215:TRP:HB2	1.98	0.45
3:C:5:BMA:O6	3:C:5:BMA:O4	2.28	0.45
1:A:724:ASP:O	1:A:725:CYS:HB2	2.14	0.45
1:A:1098:ARG:HD2	1:A:1101:ARG:NH1	2.32	0.45
1:A:1376:LEU:CB	1:A:1380:PHE:CD1	3.00	0.45
1:A:193:THR:HG23	1:A:194:MET:N	2.31	0.45
1:A:1066:TRP:HZ2	1:A:1119:VAL:HG11	1.78	0.45
1:A:1134:LEU:HD23	1:A:1134:LEU:HA	1.72	0.45
1:A:1171:GLU:O	1:A:1172:VAL:CB	2.51	0.45
1:A:1388:PHE:C	1:A:1388:PHE:HD1	2.19	0.45
1:A:1511:LEU:HD11	1:A:1515:LEU:CD1	2.47	0.45
1:A:1376:LEU:HB3	1:A:1380:PHE:H	1.82	0.45
1:A:1518:GLY:O	1:A:1522:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:GLY:N	1:A:1537:CYS:SG	2.83	0.45
2:B:131:THR:O	2:B:131:THR:OG1	2.29	0.45
1:A:584:SER:O	1:A:586:GLU:N	2.50	0.45
1:A:718:VAL:HG13	1:A:719:CYS:N	2.32	0.45
1:A:1021:ASP:CG	1:A:1022:ILE:H	2.20	0.45
1:A:163:VAL:HG22	1:A:188:ASP:OD1	2.17	0.45
1:A:1387:VAL:O	1:A:1391:ALA:N	2.46	0.45
1:A:1435:LYS:CD	1:A:1435:LYS:C	2.85	0.45
1:A:313:LEU:C	1:A:313:LEU:CD1	2.85	0.45
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.78	0.45
1:A:346:ASN:HD21	1:A:348:ALA:H	1.64	0.45
1:A:584:SER:CB	1:A:1145:ILE:HD11	2.47	0.45
1:A:1200:GLY:HA2	1:A:1203:TYR:HB2	1.99	0.45
2:B:46:SER:OG	2:B:141:ILE:HD13	2.17	0.45
1:A:580:THR:HA	1:A:661:LEU:HD21	1.99	0.44
1:A:664:ILE:HD11	1:A:1142:ILE:HG12	1.99	0.44
1:A:1216:MET:HB3	1:A:1220:TYR:CZ	2.53	0.44
1:A:1475:TYR:CZ	1:A:1533:VAL:CG2	2.98	0.44
2:B:134:TYR:CD1	2:B:134:TYR:N	2.85	0.44
1:A:174:ILE:O	1:A:177:PHE:CD2	2.70	0.44
1:A:367:TYR:HA	1:A:382:PHE:HE2	1.82	0.44
1:A:398:LEU:HD11	1:A:1566:ILE:HG12	1.99	0.44
1:A:664:ILE:HG23	1:A:667:LEU:CD1	2.47	0.44
1:A:1380:PHE:C	1:A:1382:THR:N	2.68	0.44
2:B:102:PHE:O	2:B:102:PHE:CG	2.70	0.44
1:A:770:TYR:HA	1:A:773:VAL:HG12	2.00	0.44
1:A:1167:LEU:HD23	1:A:1167:LEU:HA	1.87	0.44
1:A:1120:ARG:CG	1:A:1120:ARG:NH1	2.79	0.44
1:A:387:PHE:HZ	1:A:1451:LEU:HD21	1.83	0.44
1:A:1321:GLN:HG2	1:A:1323:PHE:H	1.83	0.44
2:B:132:PHE:CE1	2:B:137:PHE:HB3	2.52	0.44
1:A:292:ASP:O	1:A:296:TYR:N	2.50	0.44
2:B:40:PHE:CD2	2:B:42:LEU:HD23	2.52	0.44
2:B:57:ALA:CB	2:B:128:ARG:HG2	2.46	0.44
2:B:95:TRP:HE3	2:B:109:ILE:HG22	1.82	0.44
2:B:102:PHE:O	2:B:102:PHE:CD2	2.70	0.44
2:B:134:TYR:O	2:B:135:TYR:CD2	2.71	0.44
2:B:101:THR:O	2:B:102:PHE:CD1	2.70	0.44
1:A:184:TRP:HA	1:A:184:TRP:CE3	2.52	0.44
1:A:1010:ILE:HD11	1:A:1111:ARG:HH11	1.83	0.44
1:A:1223:VAL:HG13	1:A:1238:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:SER:OG	2:B:141:ILE:HG21	2.17	0.44
2:B:48:LYS:C	2:B:50:ARG:H	2.21	0.44
2:B:130:LEU:O	2:B:137:PHE:O	2.35	0.44
1:A:247:LEU:HD11	1:A:392:TYR:CE1	2.53	0.43
1:A:336:ASN:HB2	1:A:340:GLY:HA2	1.99	0.43
1:A:1213:LYS:HE2	1:A:1505:ALA:HA	2.00	0.43
1:A:391:PHE:O	1:A:395:ASN:ND2	2.51	0.43
1:A:664:ILE:HG13	1:A:664:ILE:H	1.62	0.43
1:A:986:TRP:CH2	1:A:990:ARG:NH1	2.73	0.43
1:A:1155:PHE:HD1	1:A:1221:ALA:HB1	1.83	0.43
1:A:629:THR:HA	1:A:632:ILE:HG21	1.91	0.43
1:A:1140:TRP:O	1:A:1143:PHE:N	2.51	0.43
1:A:1522:CYS:CB	1:A:1524:PRO:CD	2.80	0.43
1:A:1022:ILE:HG23	1:A:1531:THR:CG2	2.47	0.43
1:A:1373:LEU:HD13	1:A:1380:PHE:HZ	1.84	0.43
2:B:94:ASN:HB3	2:B:110:TYR:HD2	1.84	0.43
1:A:305:PHE:O	1:A:305:PHE:CD1	2.70	0.43
1:A:637:ILE:O	1:A:641:SER:N	2.48	0.43
1:A:1122:LEU:HD23	1:A:1122:LEU:HA	1.81	0.43
1:A:1168:PRO:HB2	1:A:1170:GLU:HG2	2.00	0.43
2:B:85:ASN:HA	2:B:90:LEU:HD13	1.99	0.43
1:A:629:THR:O	1:A:632:ILE:HG23	2.08	0.43
2:B:42:LEU:CD1	2:B:122:TYR:HE2	2.26	0.43
2:B:56:SER:OG	2:B:102:PHE:HE2	2.02	0.43
1:A:273:ARG:NH1	2:B:135:TYR:HB2	2.32	0.43
1:A:704:LEU:HD23	1:A:704:LEU:HA	1.87	0.43
1:A:1046:ILE:HD13	1:A:1046:ILE:HA	1.92	0.43
1:A:664:ILE:O	1:A:667:LEU:N	2.50	0.43
1:A:1109:LEU:HD21	1:A:1460:LEU:HD23	2.01	0.43
1:A:357:LEU:HD23	1:A:363:TRP:HB2	2.01	0.42
2:B:28:VAL:HG13	2:B:28:VAL:O	2.18	0.42
1:A:273:ARG:CA	1:A:328:TYR:HD1	2.25	0.42
1:A:1140:TRP:O	1:A:1143:PHE:HB2	2.19	0.42
1:A:1315:VAL:HA	1:A:1318:ILE:HD12	2.02	0.42
1:A:1364:ILE:HG23	1:A:1365:PHE:N	2.34	0.42
2:B:42:LEU:CD1	2:B:122:TYR:CD2	2.95	0.42
2:B:85:ASN:OD1	2:B:85:ASN:N	2.52	0.42
2:B:129:THR:HG22	2:B:136:GLU:HG3	2.00	0.42
1:A:187:LEU:HD23	1:A:188:ASP:CA	2.48	0.42
1:A:230:ILE:HG21	1:A:694:VAL:HG21	2.02	0.42
1:A:346:ASN:HD21	1:A:348:ALA:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:TYR:O	1:A:631:ASN:CB	2.67	0.42
1:A:671:TRP:HA	1:A:672:PRO:HD3	1.82	0.42
1:A:1331:LEU:HD23	1:A:1331:LEU:HA	1.88	0.42
2:B:43:GLY:HA2	2:B:108:SER:HA	2.00	0.42
1:A:1034:LEU:HD12	1:A:1034:LEU:HA	1.86	0.42
1:A:1167:LEU:HB3	1:A:1168:PRO:HD2	2.01	0.42
1:A:1516:ASN:OD1	1:A:1521:ASP:CB	2.68	0.42
2:B:43:GLY:CA	2:B:108:SER:CB	2.78	0.42
1:A:247:LEU:O	1:A:247:LEU:HD13	2.20	0.42
1:A:665:PHE:O	1:A:668:ALA:HB3	2.20	0.42
1:A:1167:LEU:HD11	1:A:1187:VAL:HG21	2.01	0.42
1:A:1270:GLN:O	1:A:1275:GLY:N	2.53	0.42
1:A:1145:ILE:O	1:A:1148:VAL:HG22	2.20	0.42
1:A:343:ASN:ND2	1:A:343:ASN:O	2.52	0.42
2:B:44:CYS:HB2	2:B:61:TRP:HH2	1.85	0.42
1:A:1028:ARG:NH2	2:B:31:ASP:OD1	2.53	0.41
1:A:1120:ARG:NH1	1:A:1120:ARG:HG2	2.35	0.41
1:A:1123:LEU:C	1:A:1126:ILE:HG22	2.32	0.41
1:A:1498:LEU:HD12	1:A:1498:LEU:HA	1.76	0.41
1:A:1511:LEU:CD1	1:A:1515:LEU:CD1	2.98	0.41
2:B:42:LEU:HD21	2:B:111:ILE:HD12	2.01	0.41
1:A:257:LEU:HB3	1:A:1424:ILE:HD12	2.01	0.41
1:A:300:GLU:CA	1:A:303:GLN:HE21	2.26	0.41
1:A:346:ASN:ND2	1:A:346:ASN:C	2.73	0.41
1:A:730:TRP:HZ3	1:A:740:LEU:HB3	1.85	0.41
1:A:1151:PHE:CE1	1:A:1222:ALA:HB1	2.55	0.41
2:B:48:LYS:C	2:B:50:ARG:N	2.73	0.41
1:A:379:MET:SD	1:A:1496:ILE:HD12	2.56	0.41
1:A:611:ALA:HA	1:A:614:VAL:HG12	2.02	0.41
1:A:621:ASP:OD2	1:A:624:TYR:CE2	2.73	0.41
1:A:1248:ILE:HD13	1:A:1248:ILE:HG21	1.87	0.41
1:A:1126:ILE:CG2	1:A:1127:PRO:HD3	2.50	0.41
2:B:126:PHE:HB2	2:B:141:ILE:HG22	2.02	0.41
1:A:583:MET:HG2	1:A:1145:ILE:CG2	2.51	0.41
1:A:655:VAL:HG21	1:A:1150:LEU:HD11	2.01	0.41
1:A:665:PHE:HD1	1:A:674:LEU:HD21	1.86	0.41
1:A:1123:LEU:C	1:A:1123:LEU:CD1	2.86	0.41
1:A:1474:ALA:O	1:A:1475:TYR:CD1	2.73	0.41
1:A:414:ALA:O	1:A:418:GLU:N	2.44	0.41
1:A:1434:ALA:O	1:A:1436:GLY:N	2.44	0.41
1:A:262:LEU:O	1:A:1417:ARG:CD	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HG2	1:A:328:TYR:CD1	2.48	0.41
1:A:385:VAL:O	1:A:389:GLY:N	2.47	0.41
1:A:557:LYS:O	1:A:561:PHE:N	2.51	0.41
1:A:1335:ASN:OD1	1:A:1426:ARG:NH1	2.53	0.41
1:A:132:ILE:HD11	1:A:219:LYS:HB3	2.02	0.41
1:A:1122:LEU:HD11	1:A:1557:VAL:HG22	2.03	0.41
1:A:1388:PHE:HD1	1:A:1388:PHE:O	2.03	0.41
1:A:314:LEU:HD23	1:A:373:ALA:HB2	2.02	0.40
1:A:398:LEU:HA	1:A:398:LEU:HD23	1.87	0.40
1:A:781:MET:HE3	1:A:781:MET:HB3	1.90	0.40
2:B:100:ASN:C	2:B:100:ASN:ND2	2.73	0.40
2:B:64:MET:HG3	2:B:69:SER:HA	2.03	0.40
1:A:766:CYS:O	1:A:770:TYR:HD2	2.04	0.40
1:A:1066:TRP:CE3	1:A:1066:TRP:HA	2.56	0.40
1:A:1098:ARG:HD2	1:A:1101:ARG:HH12	1.86	0.40
1:A:734:ASP:O	1:A:738:SER:HB2	2.22	0.40
1:A:1216:MET:HB3	1:A:1220:TYR:OH	2.20	0.40
1:A:582:PHE:HD1	1:A:582:PHE:HA	1.72	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	1126/1820 (62%)	1041 (92%)	73 (6%)	12 (1%)	12	45
2	B	170/209 (81%)	149 (88%)	13 (8%)	8 (5%)	2	20
All	All	1296/2029 (64%)	1190 (92%)	86 (7%)	20 (2%)	11	40

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1169	VAL
1	A	1172	VAL
1	A	1299	LYS
1	A	1305	PRO
1	A	1307	PRO
2	B	51	GLY
2	B	100	ASN
2	B	133	ASN
1	A	1022	ILE
2	B	79	ASP
1	A	338	ASN
1	A	621	ASP
1	A	1377	ARG
2	B	49	MET
2	B	104	LEU
2	B	134	TYR
1	A	585	ILE
2	B	52	GLU
1	A	1523	ASP
1	A	1519	PRO

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	965/1628 (59%)	889 (92%)	76 (8%)	10	33
2	B	149/181 (82%)	132 (89%)	17 (11%)	4	20
All	All	1114/1809 (62%)	1021 (92%)	93 (8%)	12	31

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	135	ASN
1	A	177	PHE
1	A	182	ASP

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Mol	Chain	Res	Type
1	A	185	ASN
1	A	187	LEU
1	A	194	MET
1	A	247	LEU
1	A	273	ARG
1	A	274	TRP
1	A	304	TYR
1	A	305	PHE
1	A	324	CYS
1	A	343	ASN
1	A	346	ASN
1	A	350	THR
1	A	372	ARG
1	A	579	ASN
1	A	582	PHE
1	A	587	HIS
1	A	623	TYR
1	A	632	ILE
1	A	635	SER
1	A	643	LEU
1	A	647	LEU
1	A	648	SER
1	A	667	LEU
1	A	669	LYS
1	A	673	THR
1	A	690	ASN
1	A	719	CYS
1	A	733	ASN
1	A	738	SER
1	A	755	TRP
1	A	771	MET
1	A	772	MET
1	A	779	LEU
1	A	781	MET
1	A	793	PHE
1	A	987	TRP
1	A	999	HIS
1	A	1027	ARG
1	A	1111	ARG
1	A	1120	ARG
1	A	1123	LEU
1	A	1130	MET

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Mol	Chain	Res	Type
1	A	1133	LEU
1	A	1144	SER
1	A	1148	VAL
1	A	1169	VAL
1	A	1171	GLU
1	A	1172	VAL
1	A	1175	ARG
1	A	1178	CYS
1	A	1203	TYR
1	A	1230	ASP
1	A	1295	LEU
1	A	1335	ASN
1	A	1346	GLN
1	A	1354	LEU
1	A	1356	GLN
1	A	1381	PHE
1	A	1385	TRP
1	A	1388	PHE
1	A	1435	LYS
1	A	1475	TYR
1	A	1497	CYS
1	A	1498	LEU
1	A	1516	ASN
1	A	1525	ASP
1	A	1527	GLU
1	A	1532	ASP
1	A	1533	VAL
1	A	1534	ARG
1	A	1537	CYS
1	A	1539	ASN
2	B	27	GLU
2	B	42	LEU
2	B	50	ARG
2	B	52	GLU
2	B	53	VAL
2	B	72	SER
2	B	73	HIS
2	B	100	ASN
2	B	103	ASP
2	B	130	LEU
2	B	134	TYR
2	B	135	TYR

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Mol	Chain	Res	Type
2	B	155	ARG
2	B	163	GLU
2	B	169	SER
2	B	176	TRP
2	B	186	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	269	HIS
1	A	303	GLN
1	A	343	ASN
1	A	346	ASN
1	A	365	ASN
1	A	395	ASN
1	A	409	ASN
1	A	587	HIS
1	A	628	GLN
1	A	690	ASN
1	A	999	HIS
1	A	1312	GLN
1	A	1346	GLN
1	A	1386	ASN
1	A	1516	ASN
1	A	1528	ASN
2	B	73	HIS
2	B	100	ASN
2	B	105	GLN
2	B	174	GLN

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 ⓘ

16 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$
3	NAG	C	1	3,1	14,14,15	0.47	0	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.46	0	17,19,21	1.02	1 (5%)
3	BMA	C	3	3	11,11,12	0.84	0	15,15,17	2.11	3 (20%)
3	BMA	C	4	3	11,11,12	0.79	0	15,15,17	1.42	3 (20%)
3	BMA	C	5	3	11,11,12	0.86	1 (9%)	15,15,17	0.84	0
4	NAG	D	1	4,1	14,14,15	0.46	0	17,19,21	0.59	0
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.54	0
4	BMA	D	3	4	11,11,12	0.58	0	15,15,17	1.29	2 (13%)
4	NAG	E	1	4,1	14,14,15	0.41	0	17,19,21	0.60	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.62	0
4	BMA	E	3	4	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
4	NAG	F	1	2,4	14,14,15	1.26	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	F	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.57	0
4	BMA	F	3	4	11,11,12	0.94	0	15,15,17	0.82	0
5	NAG	G	1	2,5	14,14,15	0.64	1 (7%)	17,19,21	0.69	0
5	NAG	G	2	5	14,14,15	0.53	0	17,19,21	0.54	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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	BMA	C	4	3	-	2/2/19/22	0/1/1/1
3	BMA	C	5	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	NAG	F	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-4.45	1.36	1.43
4	F	2	NAG	O5-C1	2.31	1.47	1.43
5	G	1	NAG	O5-C1	-2.13	1.40	1.43
3	C	5	BMA	C1-C2	2.11	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	5.80	120.05	112.19
4	D	3	BMA	C1-O5-C5	3.92	117.50	112.19
4	F	1	NAG	C4-C3-C2	3.75	116.52	111.02
3	C	3	BMA	C3-C4-C5	-3.67	103.69	110.24
3	C	4	BMA	C1-O5-C5	3.54	116.99	112.19
3	C	2	NAG	C1-O5-C5	3.51	116.95	112.19
3	C	3	BMA	O2-C2-C3	-2.95	104.22	110.14
4	E	3	BMA	C1-O5-C5	2.47	115.53	112.19
3	C	4	BMA	O2-C2-C3	-2.37	105.40	110.14
4	F	1	NAG	O3-C3-C2	-2.15	105.02	109.47
4	D	3	BMA	O2-C2-C3	-2.09	105.96	110.14
3	C	4	BMA	C3-C4-C5	-2.06	106.56	110.24
4	E	3	BMA	O2-C2-C3	-2.06	106.01	110.14

There are no chirality outliers.

All (26) torsion outliers are listed below:

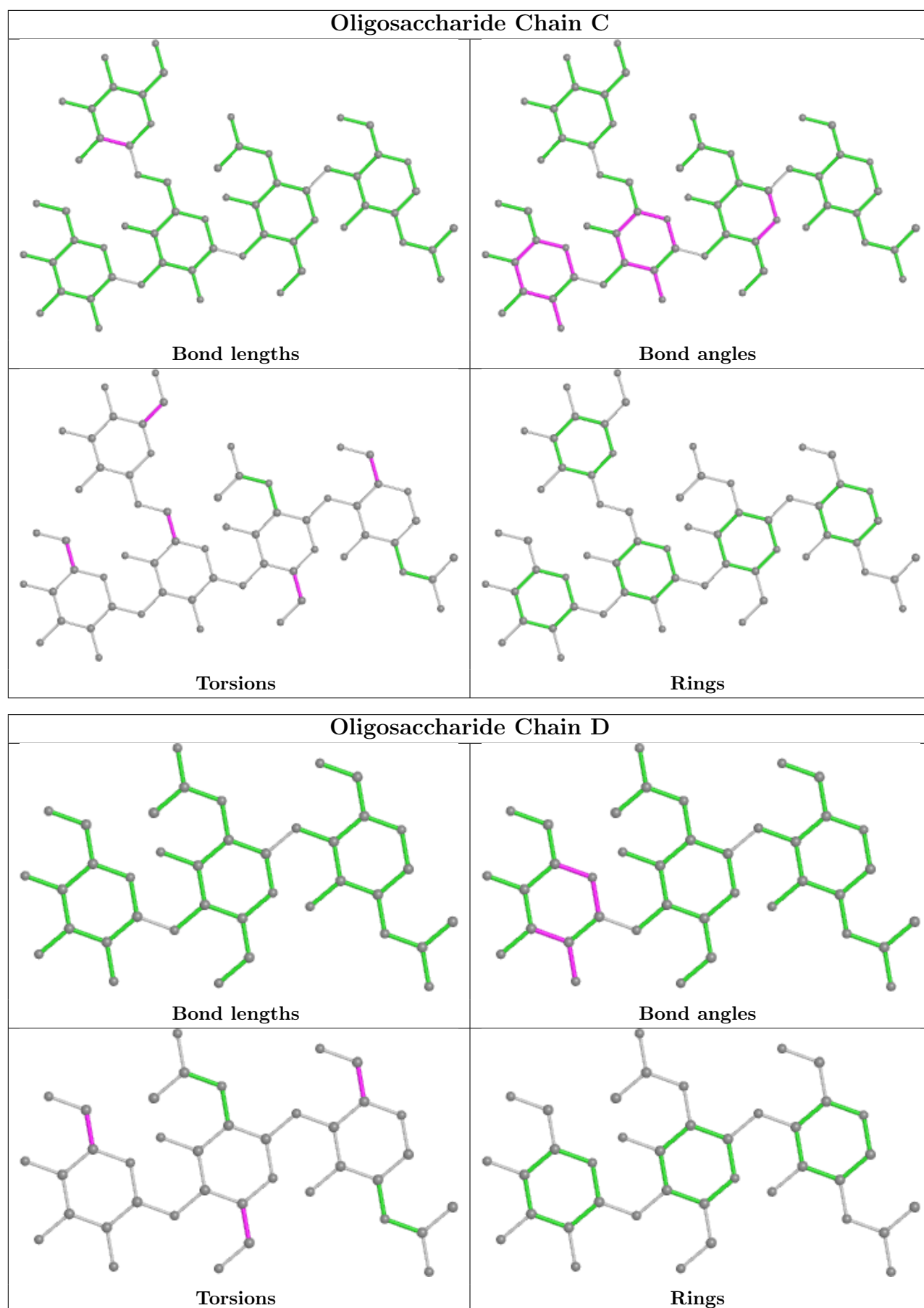
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	5	BMA	O5-C5-C6-O6
3	C	4	BMA	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	4	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7

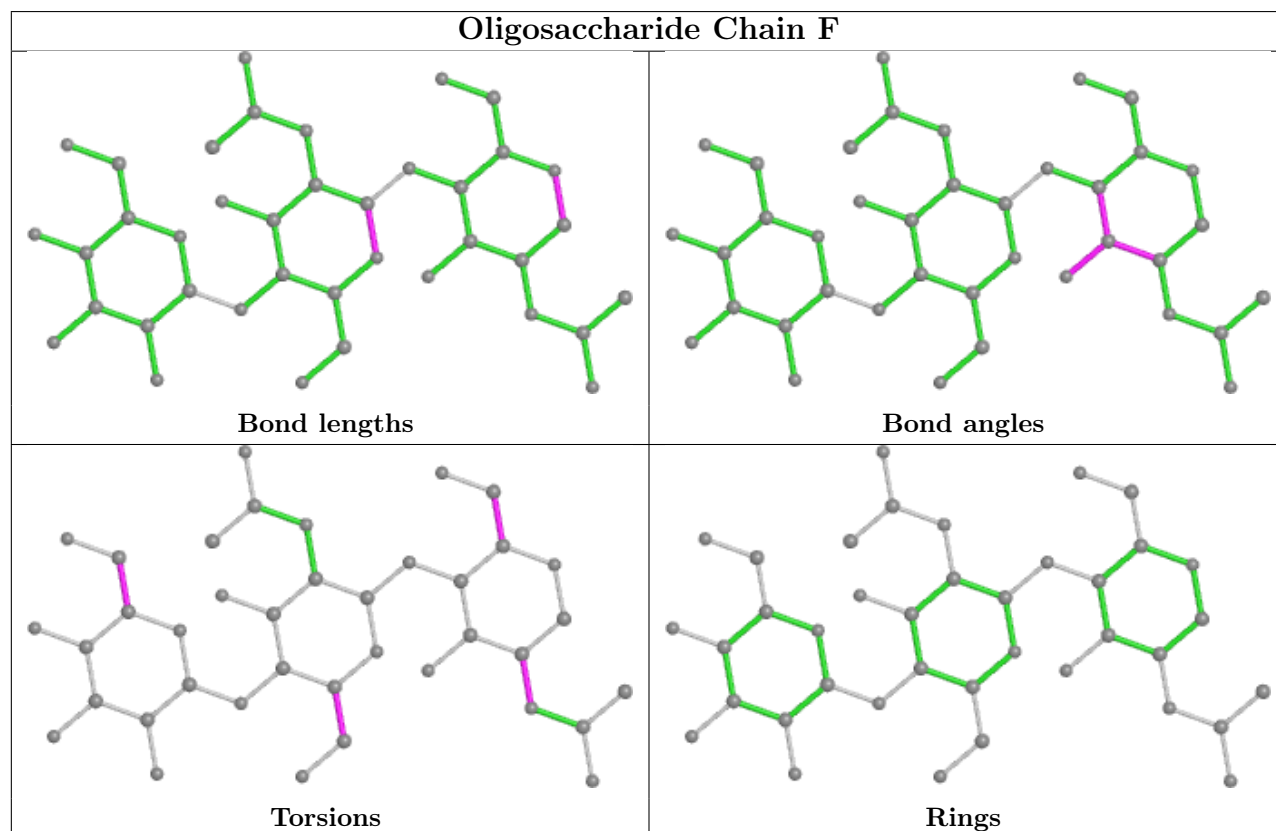
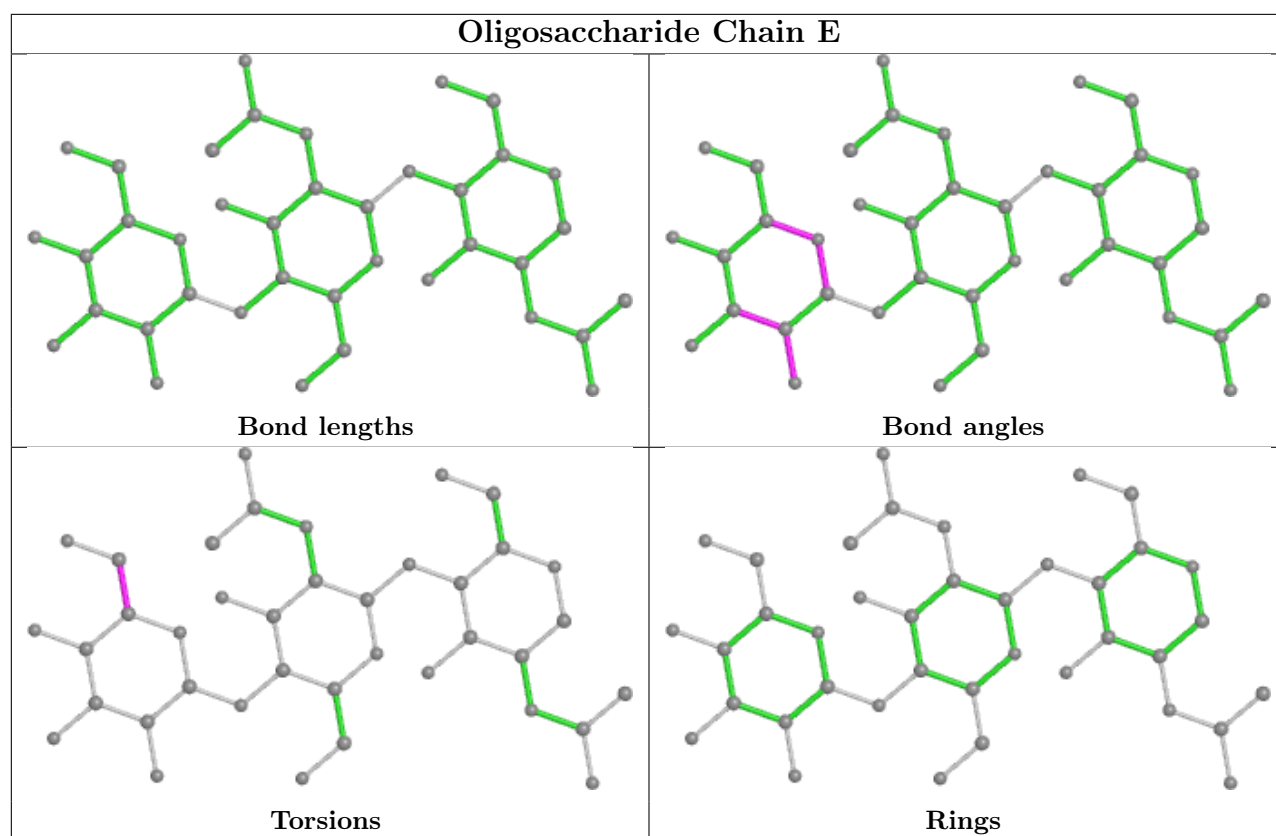
There are no ring outliers.

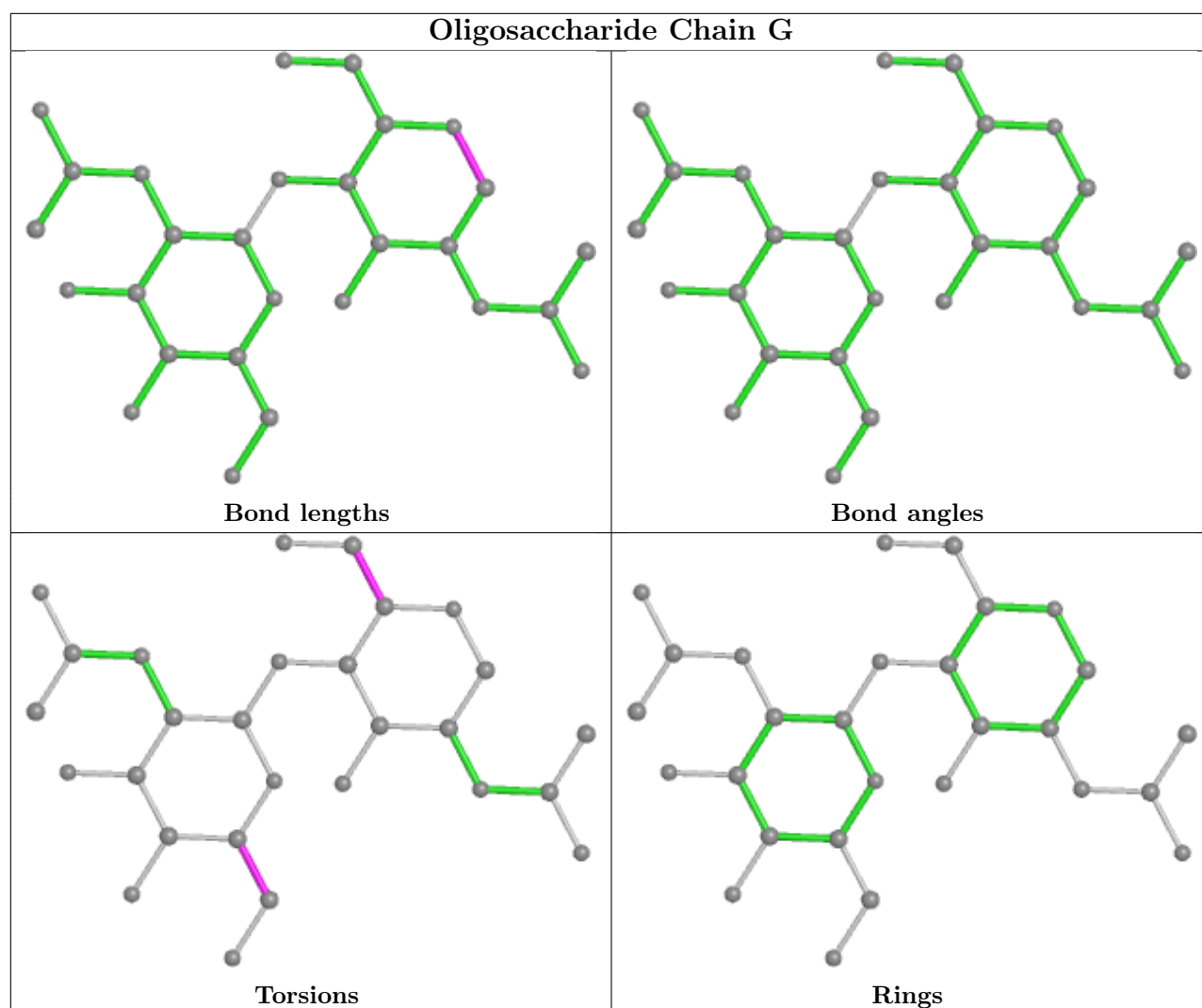
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	BMA	1	0
4	D	1	NAG	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 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.

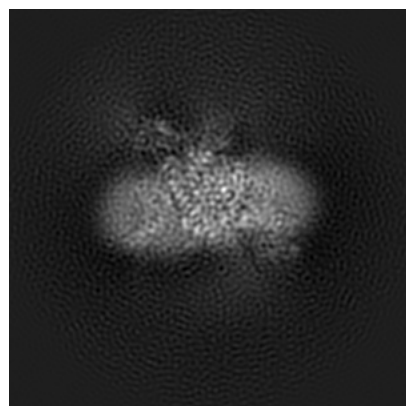
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6770. These allow visual inspection of the internal detail of the map and identification of artifacts.

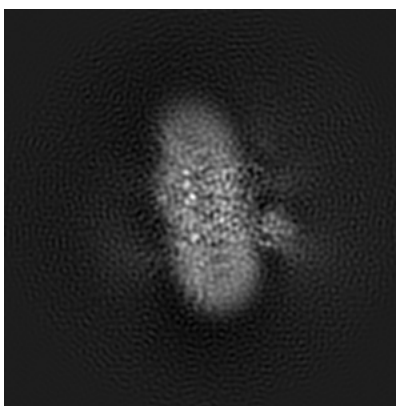
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

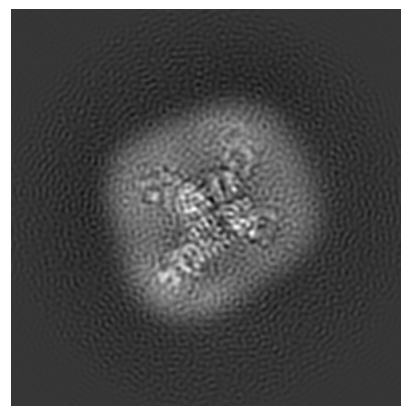
6.1.1 Primary map



X

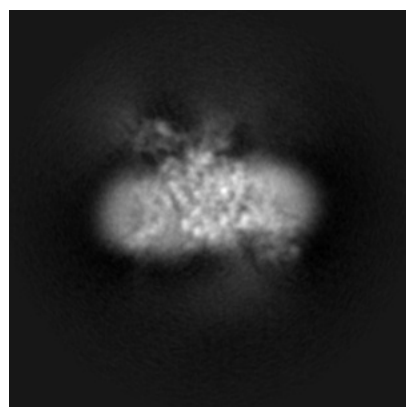


Y

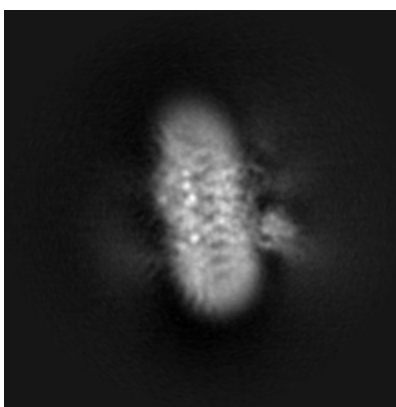


Z

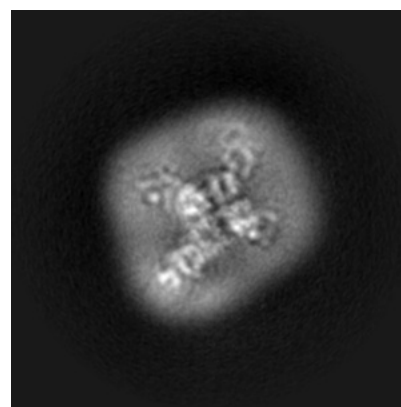
6.1.2 Raw map



X



Y

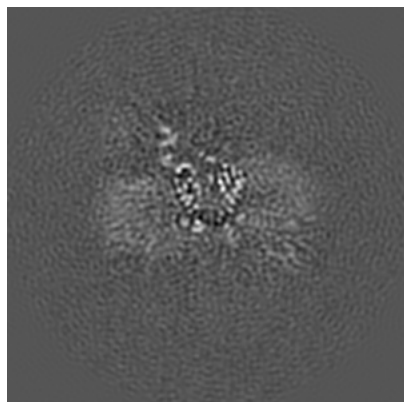


Z

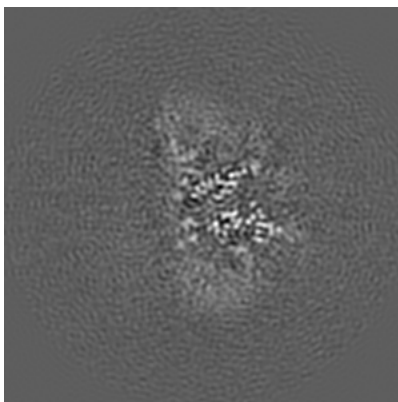
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

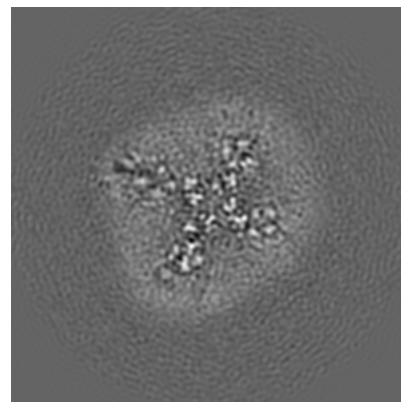
6.2.1 Primary map



X Index: 100

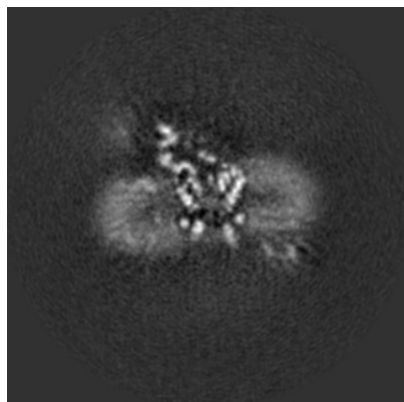


Y Index: 100

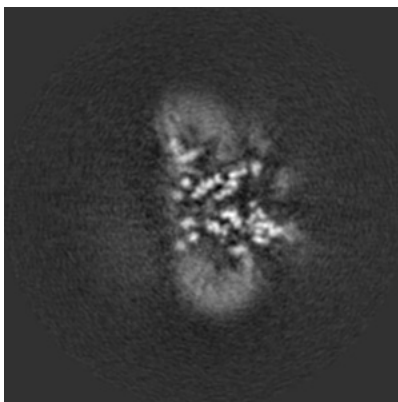


Z Index: 100

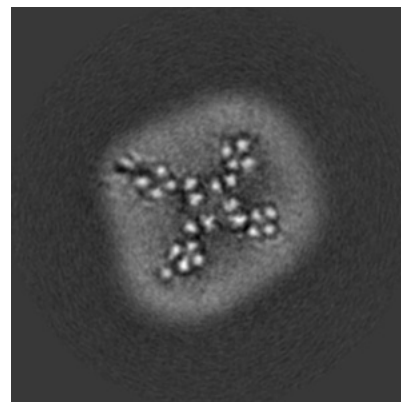
6.2.2 Raw map



X Index: 100



Y Index: 100

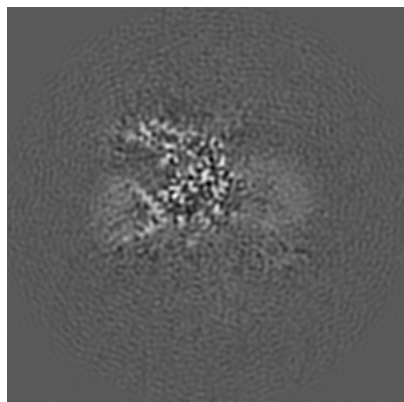


Z Index: 100

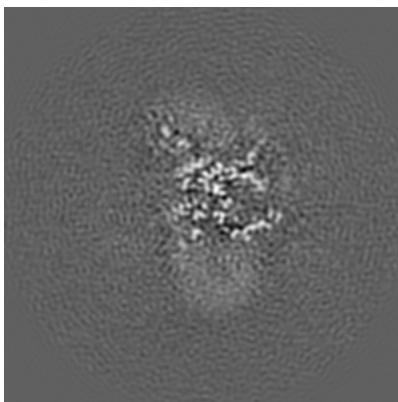
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

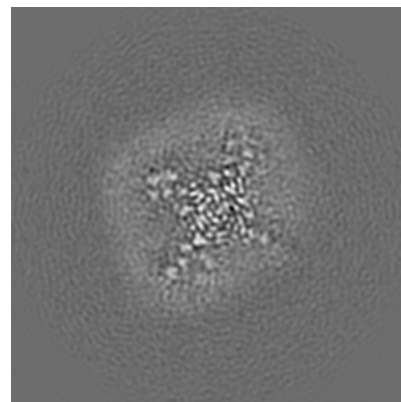
6.3.1 Primary map



X Index: 93

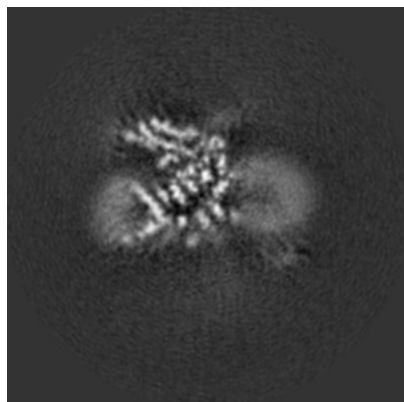


Y Index: 94

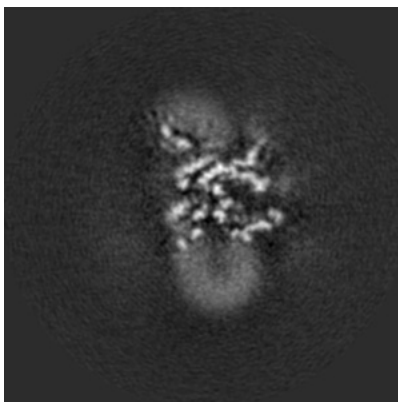


Z Index: 109

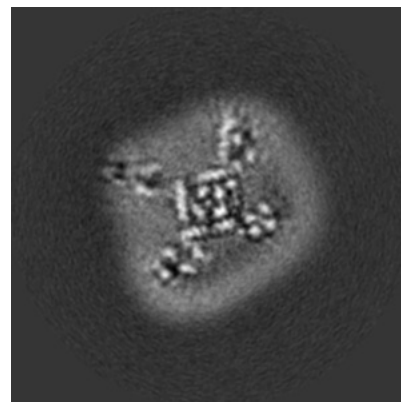
6.3.2 Raw map



X Index: 93



Y Index: 94

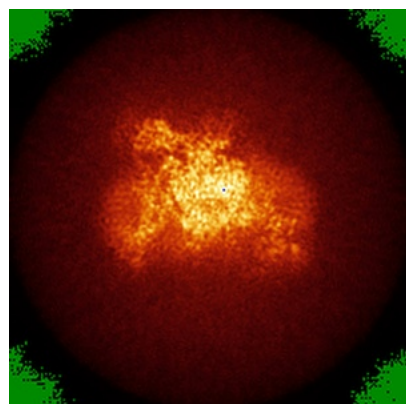


Z Index: 94

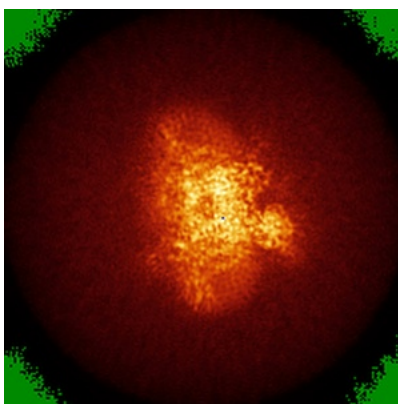
The images above show the largest variance slices of the map in three orthogonal directions.

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

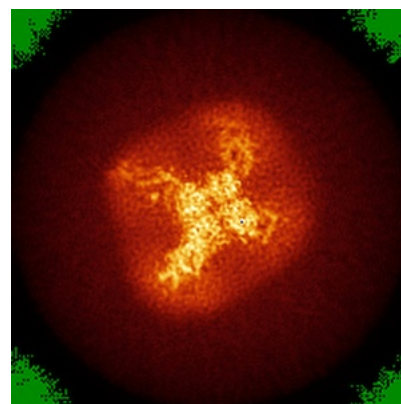
6.4.1 Primary map



X

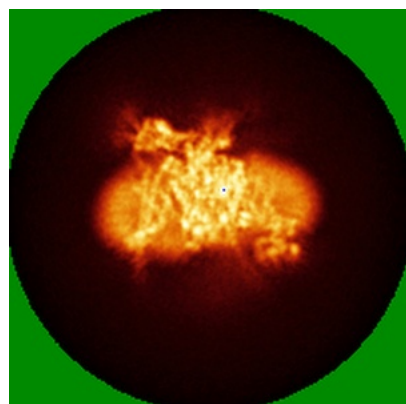


Y

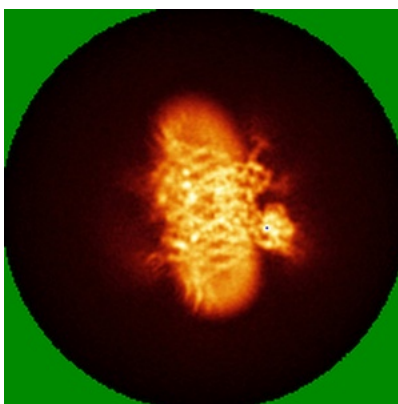


Z

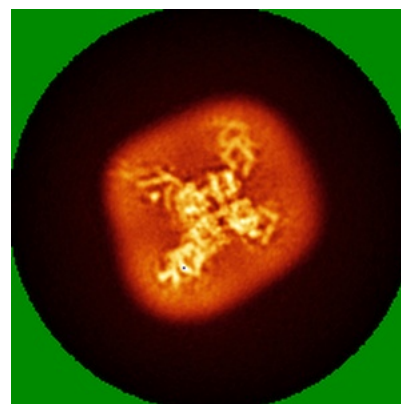
6.4.2 Raw map



X



Y

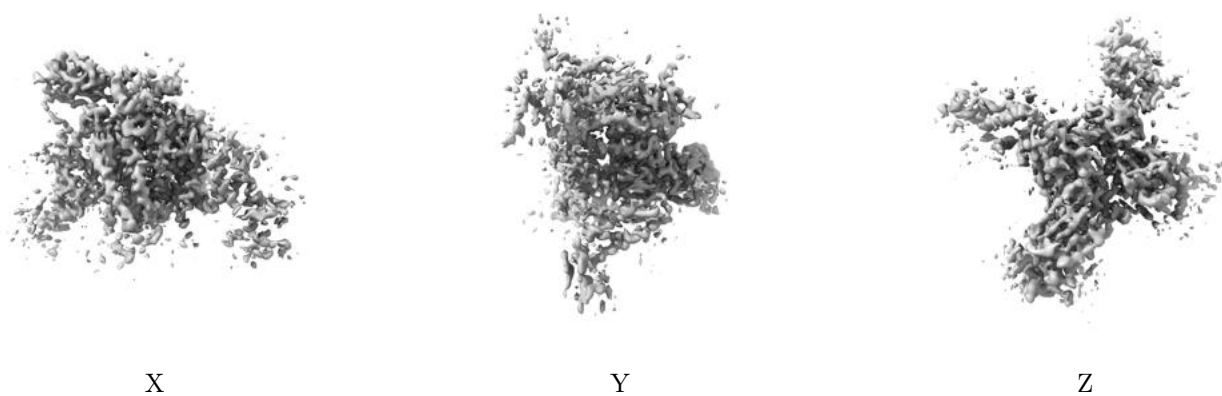


Z

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.

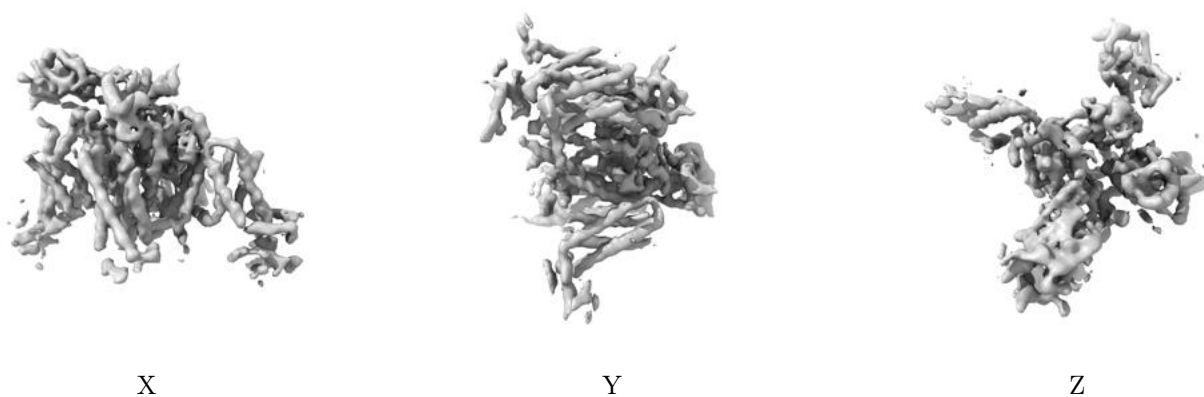
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

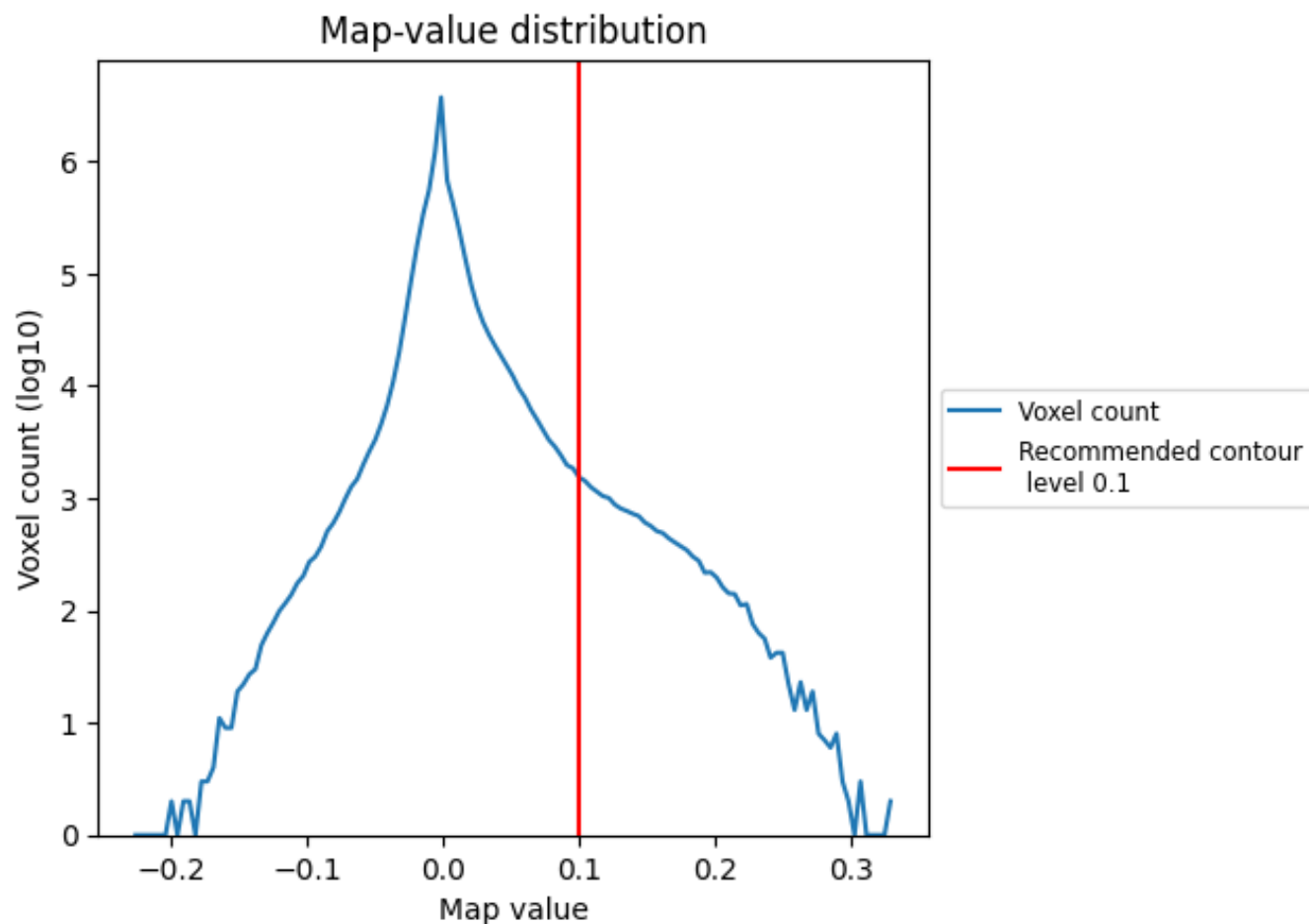
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

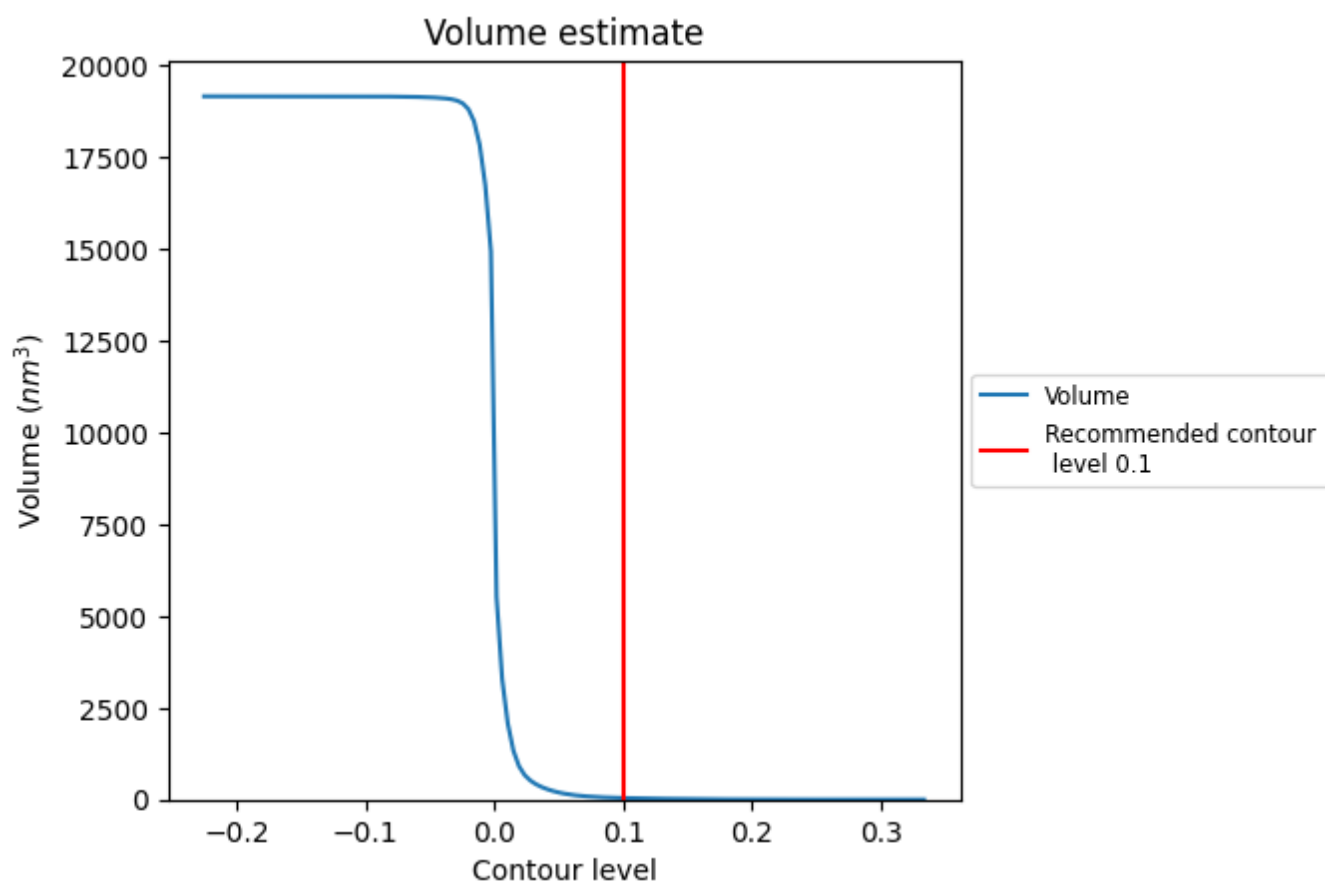
This section contains the results of statistical analysis of the map.

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.

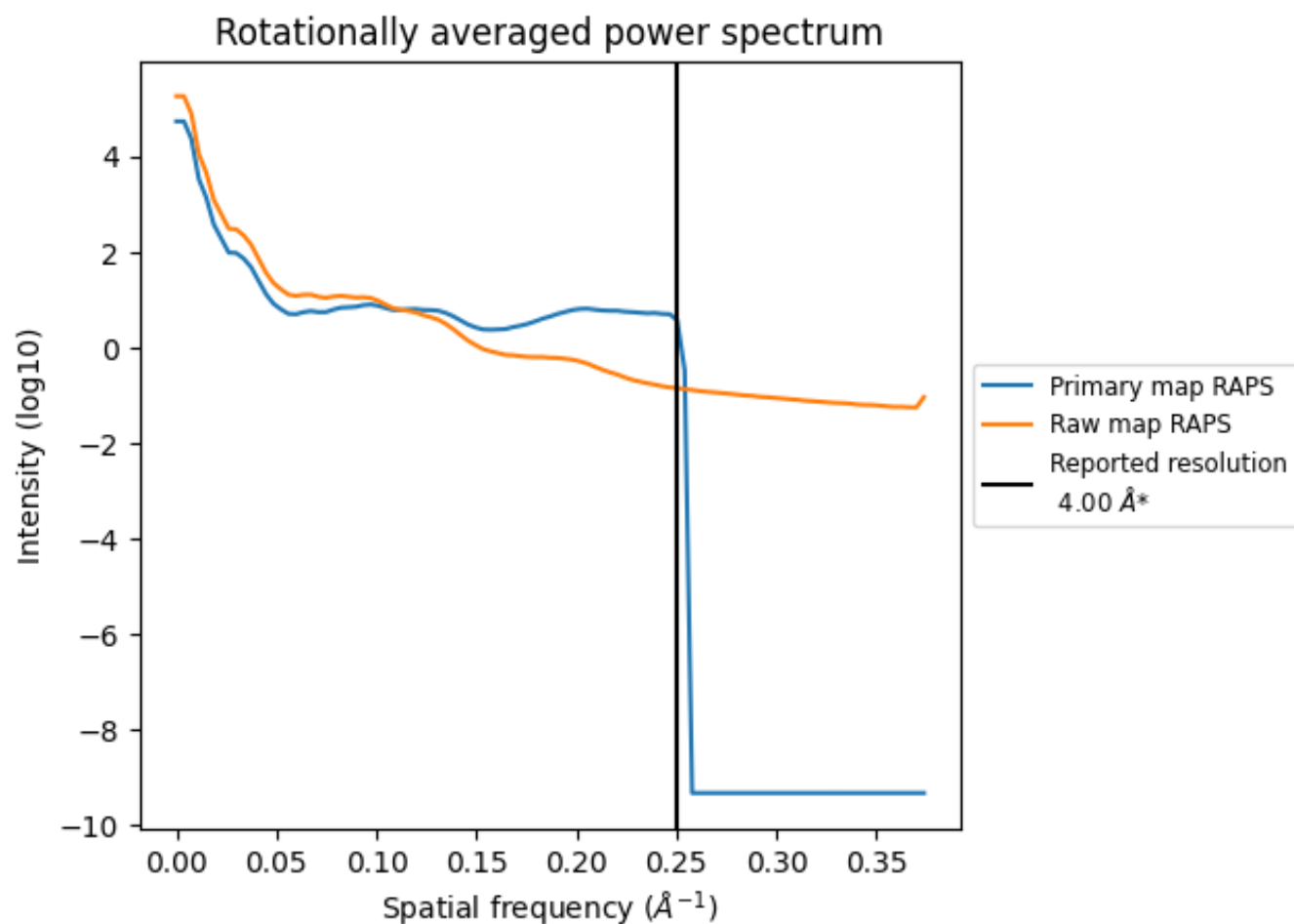
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm³; this corresponds to an approximate mass of 38 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 ⓘ

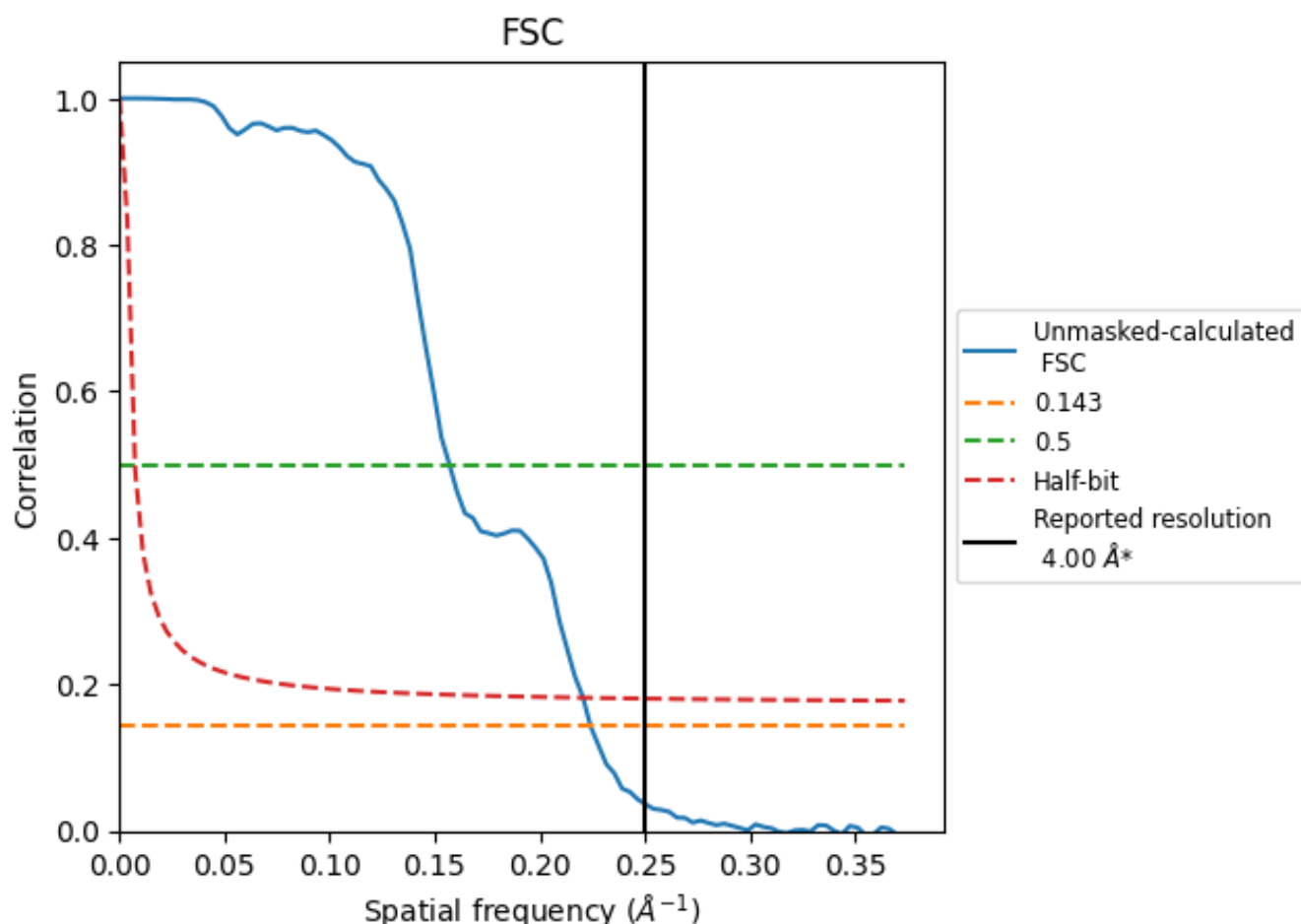


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

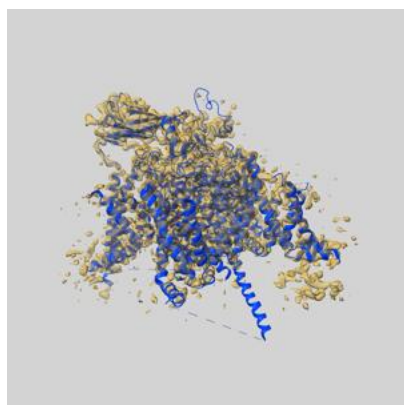
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.46	6.37	4.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.46 differs from the reported value 4.0 by more than 10 %

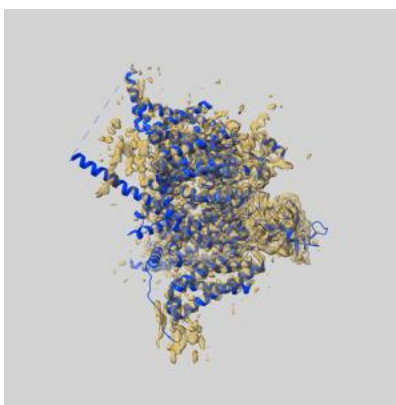
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6770 and PDB model 5XSY. Per-residue inclusion information can be found in section 3 on page 5.

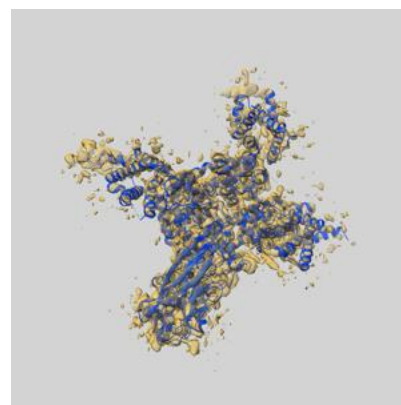
9.1 Map-model overlay [i](#)



X



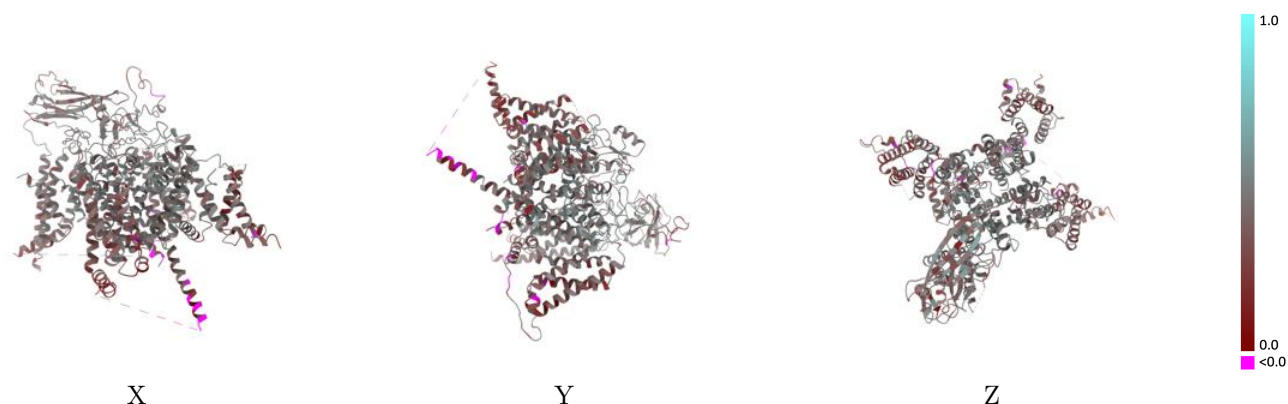
Y



Z

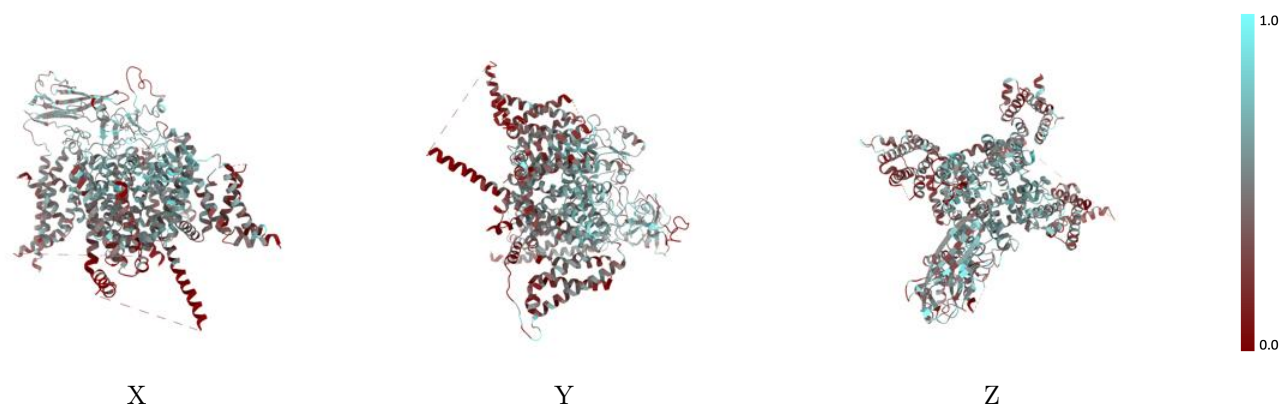
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



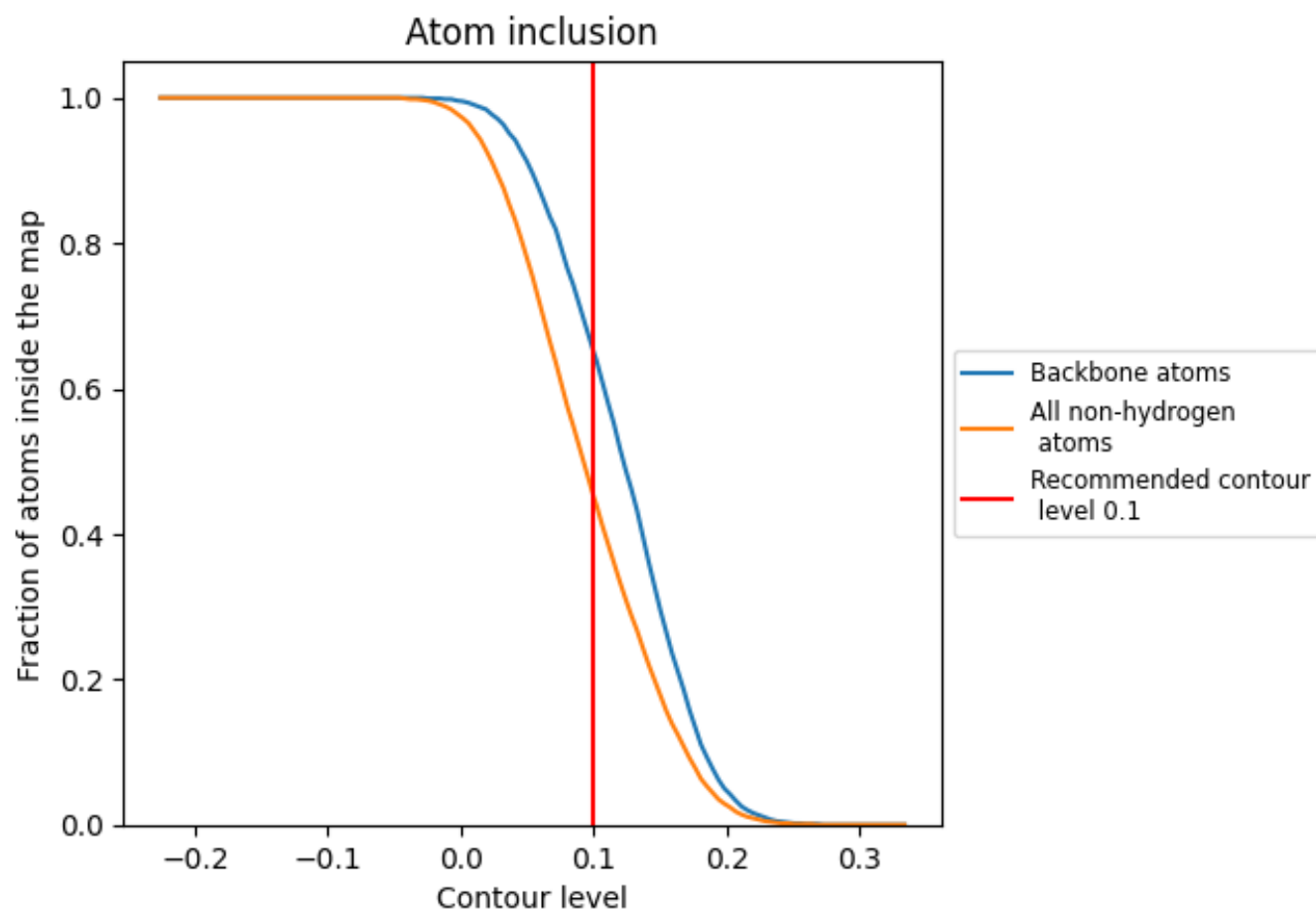
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 45% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4510	<div></div> 0.4030
A	<div></div> 0.4510	<div></div> 0.4030
B	<div></div> 0.4730	<div></div> 0.4040
C	<div></div> 0.5410	<div></div> 0.4620
D	<div></div> 0.3590	<div></div> 0.3830
E	<div></div> 0.2310	<div></div> 0.3220
F	<div></div> 0.1540	<div></div> 0.2480
G	<div></div> 0.1430	<div></div> 0.3210

1.0

0.0

<0.0