



# Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 03:53 PM JST

PDB ID : 7XMF / pdb\_00007xmf  
EMDB ID : EMD-33295  
Title : Cryo-EM structure of human NaV1.7/beta1/beta2-Nav1.7-IN2  
Authors : Zhang, J.T.; Jiang, D.H.  
Deposited on : 2022-04-25  
Resolution : 3.07 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.44

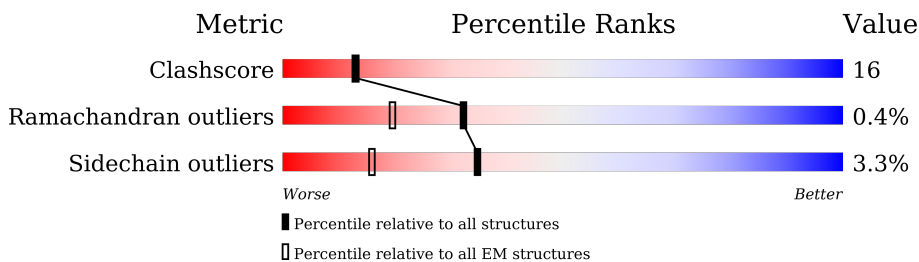
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.07 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  $\geq 3$ , 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	2250	
2	B	481	
3	C	215	
4	D	2	
4	E	2	

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
6	G2W	A	2303	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11709 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 Isoform 3 of Sodium channel protein type 9 subunit alpha, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1140	9185	6103	1437	1569	76	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1161	ARG	TRP	engineered mutation	UNP Q15858
A	1989	ALA	-	linker	UNP Q15858
A	1990	ALA	-	linker	UNP Q15858
A	1991	ALA	-	linker	UNP Q15858
A	1992	LEU	-	linker	UNP Q15858
A	1993	GLU	-	linker	UNP Q15858
A	1994	VAL	-	linker	UNP Q15858
A	1995	LEU	-	linker	UNP Q15858
A	1996	PHE	-	linker	UNP Q15858
A	1997	GLN	-	linker	UNP Q15858
A	1998	GLY	-	linker	UNP Q15858
A	1999	PRO	-	linker	UNP Q15858
A	2000	SER	-	linker	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	173	1416	902	232	272	10	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	ALA	-	linker	UNP Q07699
B	220	ALA	-	linker	UNP Q07699
B	221	ALA	-	linker	UNP Q07699

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	LEU	-	linker	UNP Q07699
B	223	GLU	-	linker	UNP Q07699
B	224	VAL	-	linker	UNP Q07699
B	225	LEU	-	linker	UNP Q07699
B	226	PHE	-	linker	UNP Q07699
B	227	GLN	-	linker	UNP Q07699
B	228	GLY	-	linker	UNP Q07699
B	229	PRO	-	linker	UNP Q07699
B	230	SER	-	linker	UNP Q07699

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	120	Total	C	N	O	S	0	0
			938	583	167	178	10		

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



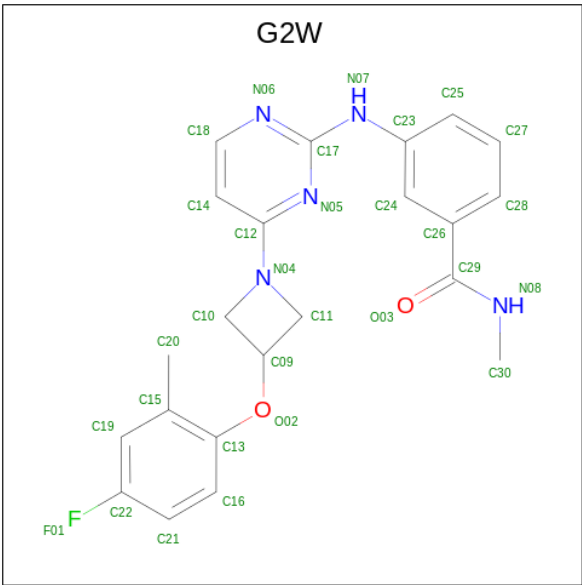
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 3-[[4-[3-(4-fluoranyl-2-methyl-phenoxy)azetidin-1-yl]pyrimidin-2-yl]amino] - {N}-methyl-benzamide (CCD ID: G2W) (formula: C<sub>22</sub>H<sub>22</sub>FN<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	F	N	O	0
			30	22	1	5	2	

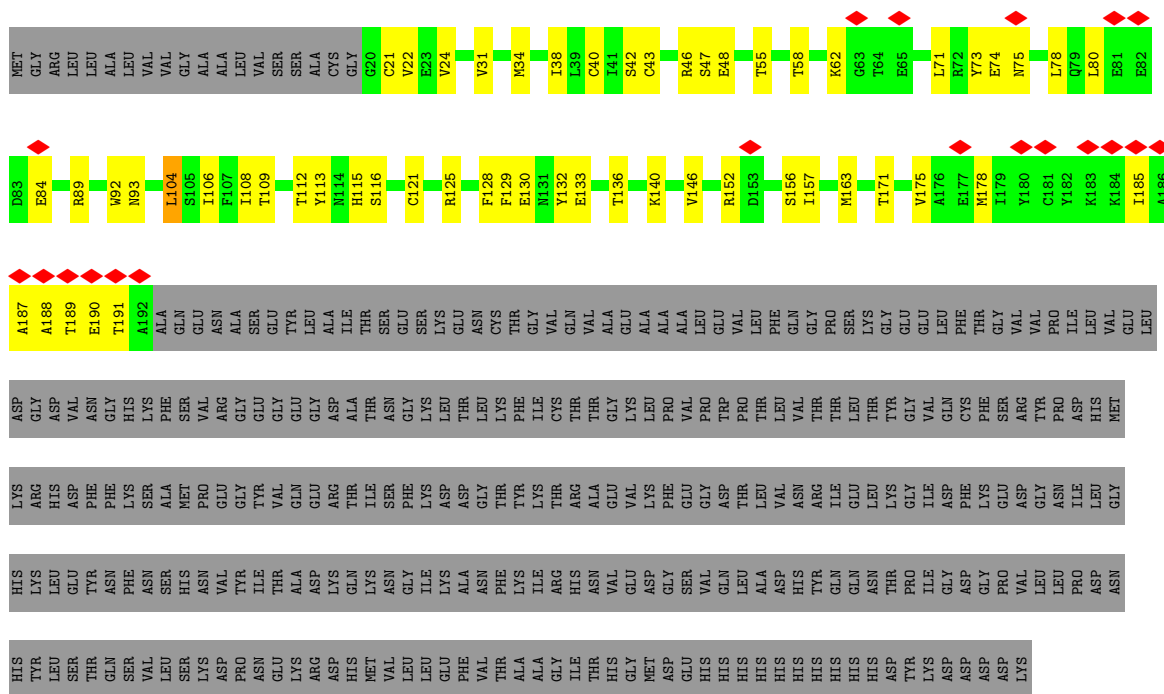




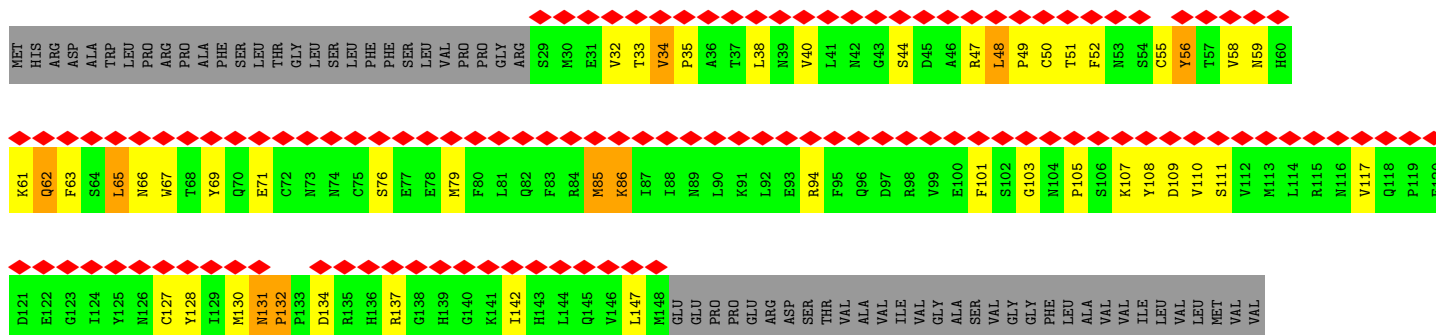
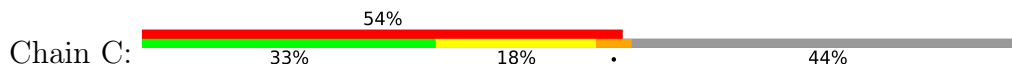


GLY	VAL	ASP	ARG	PRO
SER	LEU	GLY	TYR	ILE
ALA	LEU	ASN	PRO	LEU
TRP	PRO	ILE	ASP	GLU
SER	ASP	LEU	HIS	MET
HIS	ASN	GLY	LEU	ASP
PRO	HIS	HIS	LYS	ASP
GLN	TYR	LYS	ARG	GLY
PHE	LEU	LEU	HIS	ASP
GLU	SER	GLU	ASP	VAL
LYS	THR	TYR	PHE	ASN
	GLN	ASN	PHE	GLY
	SER	PHE	LYS	HIS
	VAL	ASN	SER	LYS
	LEU	SER	ALA	PHE
	SER	HIS	MET	SER
	LYS	ASN	PRO	VAL
	ASP	VAL	GLU	ARG
	PRO	TYR	GLY	GLY
	ASN	ILE	TYR	GLU
	GLU	THR	VAL	GLU
	LYS	ALA	GLN	GLU
	ARG	ASP	GLU	GLY
	ASP	LYS	ARG	ASP
	HIS	GLN	THR	ALA
	MET	LYS	ILE	ASN
	VAL	ASN	SER	THR
	LEU	GLY	PHE	GLY
	LEU	ILE	LYS	LYS
	GLU	LYS	ASP	LEU
	PHE	ALA	ASP	THR
	VAL	ASN	GLY	LEU
	THR	PHE	THR	LYS
	ALA	ILE	LYS	ILE
	GLY	ARG	THR	CYS
	ILE	HIS	ARG	THR
	THR	ASN	ALA	THR
	HIS	VAL	GLU	GLY
	GLY	GLU	VAL	LYS
	MET	ASP	LYS	LEU
	ASP	GLY	PHE	PRO
	GLU	SER	GLU	VAL
	TRP	VAL	GLY	PRO
	SER	GLN	ASP	TRP
	HIS	LEU	THR	PRO
	PRO	ALA	LEU	THR
	GLN	ASP	VAL	LEU
	PHE	HIS	ASN	VAL
	GLU	TYR	ILE	THR
	LYS	GLN	ARG	THR
	GLY	GLN	GLU	THR
	GLY	ASN	LEU	THR
	GLY	THR	LYS	TYR
	SER	PRO	GLY	VAL
	GLY	ILE	ILE	VAL
	GLY	GLY	ASP	CYS
	GLY	ASP	PHE	CYS
	SER	GLY	LYS	PHE
	GLY	PRO	GLU	SER

- Molecule 2: Sodium channel subunit beta-1, Green fluorescent protein



- Molecule 3: Sodium channel subunit beta-2




LYS  
CYS  
VAL  
ARG  
ARG  
LYS  
LYS  
GLN  
GLN  
LYS  
LEU  
SER  
THR  
ASP  
ASP  
LEU  
LYS  
THR  
GLU  
GLU  
GLY  
LYS  
THR  
ASP  
GLY  
GLY  
GLY  
ASN  
PRO  
ASP  
ASP  
GLY  
ALA  
LYS

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

Chain D:  100%

NAG1  
NAG2

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

Chain E:  50%  50%

NAG1  
NAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	206251	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.322	Depositor
Minimum map value	-2.352	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.607	Depositor
Map size ( $\text{\AA}$ )	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	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, G2W

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	0.23	0/9409	0.46	6/12751 (0.0%)
2	B	0.19	0/1442	0.38	0/1949
3	C	0.46	1/958 (0.1%)	0.90	7/1300 (0.5%)
All	All	0.25	1/11809 (0.0%)	0.51	13/16000 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	127	CYS	CB-SG	6.04	2.01	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	ASP	CB-CA-C	13.15	136.07	110.17
1	A	799	ASP	N-CA-C	-12.97	81.14	109.81
3	C	85	MET	CB-CA-C	-10.13	94.71	111.23
3	C	131	ASN	CA-C-N	-7.77	114.07	119.66
3	C	131	ASN	C-N-CA	-7.77	114.07	119.66
3	C	127	CYS	CA-CB-SG	5.99	128.18	114.40
3	C	132	PRO	O-C-N	5.71	123.83	121.15
1	A	799	ASP	CA-C-N	5.66	126.92	119.84
1	A	799	ASP	C-N-CA	5.66	126.92	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	VAL	N-CA-C	-5.44	107.98	113.20
3	C	86	LYS	N-CA-CB	5.44	119.68	110.49
1	A	800	PRO	CB-CA-C	-5.14	103.08	111.56
3	C	62	GLN	N-CA-C	5.10	116.92	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	799	ASP	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9185	0	9408	264	0
2	B	1416	0	1380	33	0
3	C	938	0	867	85	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	28	0	26	1	0
5	B	56	0	52	0	0
6	A	30	0	0	9	0
All	All	11709	0	11783	379	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 16.

All (379) 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)
3:C:65:LEU:CD1	3:C:110:VAL:HB	1.58	1.31
1:A:1496:PRO:O	1:A:1497:ILE:HG13	1.32	1.29
3:C:128:TYR:CD2	3:C:137:ARG:NH2	2.09	1.21
3:C:128:TYR:CD2	3:C:137:ARG:CZ	2.27	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:THR:HB	3:C:51:THR:HB	1.28	1.12
3:C:59:ASN:HB2	3:C:62:GLN:HB2	1.15	1.09
1:A:1347:PHE:HB3	1:A:1385:LEU:HD13	1.26	1.06
3:C:63:PHE:HE2	3:C:105:PRO:HB3	1.21	1.06
3:C:101:PHE:CE2	3:C:103:GLY:O	2.11	1.03
3:C:65:LEU:HD11	3:C:110:VAL:HB	1.38	1.03
1:A:289:ILE:CG2	1:A:293:LEU:HD23	1.90	1.01
3:C:65:LEU:CD1	3:C:110:VAL:CB	2.39	1.01
1:A:1449:LEU:HD12	6:A:2303:G2W:C27	1.91	1.00
1:A:289:ILE:HG23	1:A:293:LEU:HD23	1.42	0.99
3:C:52:PHE:O	3:C:108:TYR:HB3	1.63	0.98
3:C:62:GLN:O	3:C:132:PRO:CD	2.11	0.98
1:A:1508:ILE:HG22	1:A:1568:SER:OG	1.66	0.95
1:A:1449:LEU:HD12	6:A:2303:G2W:C25	1.99	0.93
3:C:128:TYR:HD2	3:C:137:ARG:CZ	1.75	0.93
1:A:1449:LEU:CD1	6:A:2303:G2W:C25	2.49	0.91
3:C:62:GLN:O	3:C:132:PRO:HD3	1.71	0.90
3:C:66:ASN:ND2	3:C:79:MET:HE2	1.85	0.90
3:C:59:ASN:CB	3:C:62:GLN:HB2	2.03	0.89
3:C:34:VAL:HG12	3:C:50:CYS:SG	2.13	0.88
1:A:289:ILE:CG2	1:A:293:LEU:CD2	2.53	0.87
1:A:839:LEU:O	1:A:842:VAL:HG12	1.76	0.86
3:C:66:ASN:ND2	3:C:79:MET:CE	2.40	0.85
3:C:69:TYR:HE2	3:C:94:ARG:NH1	1.75	0.85
3:C:63:PHE:CE2	3:C:105:PRO:HB3	2.10	0.85
1:A:251:LEU:HD13	1:A:1630:ILE:HG23	1.59	0.84
3:C:59:ASN:HB2	3:C:62:GLN:CB	2.03	0.84
3:C:33:THR:O	3:C:50:CYS:HA	1.79	0.83
3:C:65:LEU:HD12	3:C:110:VAL:CB	2.07	0.83
1:A:1496:PRO:O	1:A:1497:ILE:CG1	2.23	0.82
3:C:32:VAL:CG1	3:C:50:CYS:SG	2.66	0.82
1:A:1340:VAL:O	1:A:1344:ALA:HB2	1.79	0.81
1:A:289:ILE:HG22	1:A:293:LEU:CD2	2.12	0.80
3:C:128:TYR:CG	3:C:137:ARG:NH2	2.49	0.80
3:C:66:ASN:HD21	3:C:79:MET:CE	1.95	0.80
3:C:33:THR:O	3:C:51:THR:N	2.15	0.79
3:C:47:ARG:O	3:C:49:PRO:HD3	1.81	0.79
1:A:1347:PHE:CD2	1:A:1385:LEU:HD22	2.19	0.78
3:C:62:GLN:O	3:C:132:PRO:HD2	1.85	0.77
1:A:1315:ILE:O	1:A:1318:ILE:HG22	1.85	0.76
3:C:32:VAL:HA	3:C:51:THR:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:THR:HB	3:C:51:THR:CB	2.14	0.75
3:C:69:TYR:CE2	3:C:94:ARG:NH1	2.52	0.75
3:C:101:PHE:HE2	3:C:103:GLY:O	1.69	0.74
3:C:103:GLY:O	3:C:105:PRO:HD3	1.87	0.74
1:A:139:ASN:ND2	1:A:220:ARG:HD3	2.03	0.74
1:A:394:ILE:HD13	6:A:2303:G2W:C19	2.18	0.74
3:C:58:VAL:HG13	3:C:63:PHE:HB2	1.69	0.74
1:A:892:TYR:O	1:A:896:VAL:HG13	1.88	0.74
1:A:275:CYS:N	1:A:315:CYS:SG	2.60	0.73
1:A:1738:PHE:O	1:A:1742:SER:OG	2.07	0.73
1:A:357:LEU:HD23	1:A:363:TRP:HB2	1.70	0.73
3:C:71:GLU:HG3	3:C:94:ARG:HH12	1.53	0.72
1:A:1496:PRO:C	1:A:1497:ILE:HG13	2.13	0.72
3:C:65:LEU:HD13	3:C:110:VAL:HB	1.67	0.72
3:C:65:LEU:HD12	3:C:110:VAL:CG1	2.19	0.72
3:C:65:LEU:C	3:C:65:LEU:HD23	2.15	0.71
3:C:59:ASN:HD22	3:C:62:GLN:HG3	1.55	0.71
1:A:388:LEU:O	1:A:392:TYR:HB3	1.90	0.71
1:A:798:MET:C	1:A:799:ASP:O	2.13	0.70
3:C:33:THR:CB	3:C:51:THR:HB	2.14	0.70
3:C:71:GLU:CG	3:C:94:ARG:HH12	2.06	0.69
1:A:1661:PHE:O	1:A:1665:ASN:ND2	2.25	0.69
1:A:922:ARG:HG2	1:A:927:GLU:HB2	1.73	0.69
1:A:1636:ALA:HB2	1:A:1765:VAL:HG11	1.75	0.69
1:A:784:THR:HG21	1:A:823:LEU:HD21	1.75	0.68
1:A:285:THR:HG22	1:A:286:LEU:N	2.08	0.68
2:B:38:ILE:HD11	2:B:108:ILE:HD11	1.75	0.68
3:C:33:THR:N	3:C:51:THR:O	2.27	0.68
2:B:89:ARG:NH1	2:B:112:THR:OG1	2.27	0.68
1:A:289:ILE:HG22	1:A:293:LEU:HD21	1.76	0.67
3:C:34:VAL:HG23	3:C:142:ILE:HG12	1.76	0.67
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.58	0.67
1:A:1324:VAL:HG21	1:A:1455:VAL:HG11	1.77	0.67
3:C:32:VAL:HG12	3:C:50:CYS:SG	2.33	0.66
1:A:1595:LEU:HD22	1:A:1612:ILE:HG21	1.76	0.66
3:C:65:LEU:CD1	3:C:110:VAL:CG1	2.74	0.66
3:C:66:ASN:HD21	3:C:79:MET:HE1	1.59	0.66
1:A:1444:GLY:O	1:A:1448:THR:OG1	2.04	0.65
2:B:113:TYR:HA	2:B:146:VAL:HG11	1.78	0.65
3:C:62:GLN:C	3:C:132:PRO:HD2	2.21	0.65
1:A:1508:ILE:CG2	1:A:1568:SER:OG	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:NZ	1:A:1537:GLU:OE1	2.30	0.64
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.79	0.64
1:A:379:MET:HG3	1:A:1689:ILE:HG12	1.79	0.64
2:B:121:CYS:HB3	2:B:140:LYS:HB2	1.79	0.64
3:C:65:LEU:HD12	3:C:110:VAL:HG11	1.77	0.64
1:A:209:ASN:HB3	1:A:212:ALA:HB3	1.79	0.64
1:A:139:ASN:HD21	1:A:220:ARG:CD	2.11	0.64
1:A:1364:VAL:HG21	1:A:1373:LEU:HD22	1.79	0.64
1:A:898:LYS:HE3	3:C:56:TYR:HA	1.80	0.63
1:A:804:PHE:HD1	1:A:810:ILE:HG22	1.64	0.62
1:A:812:ASP:OD1	1:A:844:LYS:NZ	2.25	0.62
1:A:1755:TYR:O	1:A:1759:ILE:HG12	2.00	0.62
1:A:321:SER:HB3	1:A:375:GLY:HA2	1.79	0.62
3:C:34:VAL:CG2	3:C:142:ILE:HG12	2.30	0.62
2:B:188:ALA:O	2:B:191:THR:OG1	2.18	0.62
3:C:103:GLY:HA3	3:C:109:ASP:OD1	1.99	0.61
1:A:1709:ASN:HB2	1:A:1714:ASP:HB3	1.80	0.61
1:A:802:GLU:HA	1:A:805:GLN:HG2	1.81	0.61
3:C:65:LEU:HD21	3:C:67:TRP:CD1	2.35	0.61
3:C:105:PRO:HA	3:C:109:ASP:O	2.01	0.61
1:A:214:ARG:HG2	1:A:217:ARG:HH21	1.66	0.61
1:A:360:GLN:NE2	1:A:390:SER:OG	2.25	0.60
2:B:125:ARG:HB3	2:B:136:THR:OG1	2.01	0.60
1:A:1751:VAL:HG21	6:A:2303:G2W:C11	2.31	0.60
1:A:1694:ILE:HD11	1:A:1703:LEU:HD13	1.85	0.59
1:A:1347:PHE:HB3	1:A:1385:LEU:CD1	2.17	0.59
3:C:59:ASN:O	3:C:63:PHE:N	2.30	0.59
1:A:170:LYS:HD3	1:A:183:PHE:HE1	1.68	0.59
1:A:1752:VAL:O	1:A:1756:ILE:HG12	2.03	0.59
3:C:65:LEU:HD21	3:C:67:TRP:HD1	1.67	0.58
1:A:272:LYS:NZ	1:A:345:ASP:OD2	2.35	0.58
1:A:1529:MET:HG2	1:A:1533:MET:HE3	1.86	0.58
1:A:396:LEU:HD11	1:A:1633:LEU:HB3	1.85	0.58
1:A:120:ILE:HD12	1:A:173:ALA:HB1	1.86	0.58
1:A:1234:THR:HG21	1:A:1273:LEU:HD12	1.86	0.58
3:C:101:PHE:CZ	3:C:103:GLY:O	2.56	0.58
1:A:1528:ASN:ND2	1:A:1619:ARG:HE	2.02	0.57
1:A:192:ASP:O	1:A:196:ILE:HG12	2.05	0.57
1:A:1585:VAL:HA	1:A:1588:ILE:HG22	1.86	0.57
1:A:180:GLU:HG3	1:A:184:LEU:HD12	1.86	0.57
1:A:322:GLY:HA3	1:A:323:GLN:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ILE:HD11	2:B:163:MET:HA	1.87	0.57
1:A:1453:ILE:O	1:A:1457:ILE:HG13	2.05	0.57
4:E:1:NAG:H3	4:E:1:NAG:H83	1.87	0.57
1:A:1180:ASN:O	1:A:1184:THR:HG23	2.05	0.57
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.87	0.56
1:A:1601:THR:HG22	1:A:1602:TYR:CE1	2.40	0.56
1:A:1748:PHE:HB2	6:A:2303:G2W:C18	2.36	0.56
3:C:65:LEU:HD23	3:C:65:LEU:O	2.04	0.56
1:A:1329:LEU:O	1:A:1396:TYR:OH	2.22	0.56
3:C:32:VAL:HG13	3:C:50:CYS:SG	2.44	0.56
2:B:74:GLU:HG3	2:B:75:ASN:H	1.71	0.56
2:B:78:LEU:HD13	2:B:92:TRP:HB2	1.87	0.55
3:C:107:LYS:O	3:C:108:TYR:HB2	2.06	0.55
1:A:1275:ALA:O	1:A:1281:SER:OG	2.25	0.55
1:A:285:THR:HG22	1:A:286:LEU:H	1.71	0.55
1:A:747:ASP:OD2	1:A:748:LEU:N	2.39	0.55
1:A:1491:LYS:O	1:A:1491:LYS:HG2	2.07	0.55
2:B:40:CYS:HB3	2:B:104:LEU:O	2.06	0.55
3:C:44:SER:O	3:C:117:VAL:HG22	2.07	0.55
1:A:245:LEU:HD21	1:A:401:VAL:HG23	1.89	0.54
1:A:1449:LEU:HD11	6:A:2303:G2W:C25	2.36	0.54
6:A:2303:G2W:C09	6:A:2303:G2W:C20	2.85	0.54
1:A:295:SER:OG	1:A:298:ASP:OD1	2.14	0.54
1:A:1672:GLU:HB2	1:A:1706:PRO:HB3	1.89	0.54
1:A:191:LEU:HD21	1:A:219:LEU:HB3	1.89	0.54
1:A:1185:CYS:HB3	1:A:1247:ALA:HB2	1.90	0.54
2:B:112:THR:HG22	2:B:113:TYR:H	1.73	0.54
2:B:42:SER:O	2:B:125:ARG:NH2	2.40	0.54
1:A:820:LEU:HA	1:A:823:LEU:HD23	1.90	0.54
1:A:1651:LEU:HD13	1:A:1750:VAL:HG21	1.88	0.54
1:A:778:ILE:HA	1:A:781:LEU:HG	1.89	0.53
3:C:33:THR:O	3:C:50:CYS:CA	2.55	0.53
1:A:733:PHE:CE2	1:A:796:ILE:HD13	2.43	0.53
3:C:62:GLN:HB3	3:C:132:PRO:HD2	1.90	0.53
1:A:213:LEU:HA	1:A:216:PHE:HD2	1.73	0.53
1:A:908:TRP:NE1	1:A:1413:TYR:OH	2.36	0.53
1:A:1230:ASP:O	1:A:1234:THR:HG22	2.09	0.53
1:A:1676:ASN:O	1:A:1680:ASN:ND2	2.42	0.53
1:A:1656:PHE:O	1:A:1660:ILE:HG12	2.09	0.53
2:B:84:GLU:CD	2:B:84:GLU:H	2.16	0.53
1:A:285:THR:CG2	1:A:286:LEU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ILE:O	1:A:758:THR:HG23	2.08	0.53
1:A:1601:THR:HG22	1:A:1602:TYR:CD1	2.44	0.53
1:A:120:ILE:O	1:A:124:VAL:HG22	2.09	0.52
1:A:1581:PHE:O	1:A:1585:VAL:HG23	2.08	0.52
1:A:289:ILE:CG2	1:A:293:LEU:HD21	2.36	0.52
1:A:1340:VAL:O	1:A:1344:ALA:CB	2.56	0.52
1:A:1546:VAL:O	1:A:1550:ILE:HG13	2.09	0.52
1:A:1712:PRO:HG3	1:A:1717:PRO:HD3	1.91	0.52
1:A:1564:LEU:HA	1:A:1567:ILE:HG13	1.92	0.52
1:A:1582:ASP:OD1	1:A:1622:ARG:NH1	2.42	0.52
1:A:235:VAL:O	1:A:239:ILE:HG12	2.09	0.52
1:A:293:LEU:HD12	1:A:293:LEU:O	2.10	0.52
1:A:315:CYS:HB2	1:A:330:CYS:SG	2.50	0.52
1:A:166:GLU:O	1:A:170:LYS:HG2	2.10	0.52
1:A:800:PRO:O	1:A:804:PHE:HD2	1.93	0.51
3:C:47:ARG:NH2	3:C:111:SER:OG	2.43	0.51
1:A:218:VAL:HG11	1:A:883:VAL:HG23	1.93	0.51
1:A:1508:ILE:HG22	1:A:1568:SER:HG	1.69	0.51
1:A:238:LEU:HD21	1:A:958:VAL:HG23	1.91	0.51
1:A:1238:ILE:HD11	1:A:1270:LEU:HD13	1.92	0.51
1:A:749:ALA:O	1:A:752:ILE:HG13	2.11	0.51
1:A:1442:ILE:O	1:A:1446:PHE:HB3	2.10	0.51
3:C:34:VAL:HG21	3:C:142:ILE:HG13	1.93	0.51
1:A:290:MET:HG3	1:A:333:ILE:HG12	1.93	0.50
1:A:1588:ILE:HA	1:A:1591:VAL:HG22	1.93	0.50
1:A:1675:ILE:HD12	1:A:1706:PRO:HG2	1.93	0.50
2:B:112:THR:H	2:B:115:HIS:CD2	2.29	0.50
1:A:733:PHE:HE2	1:A:796:ILE:HD13	1.77	0.50
1:A:807:GLY:HA2	1:A:810:ILE:HG12	1.92	0.50
1:A:1426:LYS:HB2	1:A:1429:TYR:HB2	1.92	0.50
2:B:55:THR:HG22	2:B:73:TYR:HB3	1.93	0.49
1:A:285:THR:CG2	1:A:286:LEU:H	2.25	0.49
1:A:1295:LEU:HD22	1:A:1298:LEU:HD22	1.94	0.49
1:A:1747:SER:HA	1:A:1750:VAL:HG22	1.93	0.49
1:A:1219:LYS:HB2	1:A:1222:ILE:HG22	1.94	0.49
1:A:1520:SER:O	1:A:1524:LEU:HG	2.13	0.49
1:A:842:VAL:CG1	1:A:1334:ILE:HD11	2.42	0.49
3:C:128:TYR:HB3	3:C:137:ARG:HE	1.77	0.49
1:A:1408:TRP:H	1:A:1408:TRP:CD1	2.30	0.49
1:A:286:LEU:HD11	1:A:333:ILE:HG21	1.95	0.49
1:A:1443:PHE:O	1:A:1447:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:VAL:HG21	3:C:142:ILE:CG1	2.43	0.49
1:A:188:TRP:CD1	1:A:232:LYS:HE3	2.48	0.48
3:C:128:TYR:CE2	3:C:137:ARG:NH2	2.74	0.48
1:A:1680:ASN:O	1:A:1686:ASN:HB3	2.14	0.48
1:A:1497:ILE:HG21	1:A:1569:LEU:HD22	1.95	0.48
1:A:758:THR:HG21	1:A:842:VAL:HB	1.95	0.48
1:A:1221:THR:O	1:A:1225:ILE:HD12	2.13	0.48
1:A:191:LEU:O	1:A:195:VAL:HG23	2.14	0.48
1:A:367:TYR:OH	1:A:1689:ILE:HG23	2.14	0.48
1:A:909:HIS:HD2	1:A:911:ASN:H	1.60	0.48
1:A:1558:PHE:O	1:A:1561:GLU:HG3	2.14	0.48
1:A:1572:TYR:O	1:A:1575:THR:HG22	2.14	0.48
3:C:34:VAL:CG2	3:C:142:ILE:CG1	2.91	0.48
1:A:1587:ILE:O	1:A:1591:VAL:HG13	2.14	0.48
3:C:61:LYS:HA	3:C:85:MET:SD	2.54	0.48
2:B:55:THR:HB	2:B:104:LEU:HG	1.96	0.47
3:C:34:VAL:CG1	3:C:50:CYS:SG	2.96	0.47
1:A:923:VAL:HG13	1:A:928:TRP:HB3	1.96	0.47
1:A:1508:ILE:O	1:A:1512:VAL:HG13	2.14	0.47
1:A:1457:ILE:HG12	1:A:1756:ILE:CD1	2.44	0.47
1:A:361:ASP:OD2	1:A:929:ILE:N	2.43	0.47
1:A:1707:ILE:HD13	1:A:1740:PHE:HE2	1.80	0.47
1:A:1460:PHE:HD2	1:A:1756:ILE:HG13	1.80	0.47
3:C:34:VAL:HG23	3:C:35:PRO:N	2.29	0.47
3:C:103:GLY:C	3:C:105:PRO:HD3	2.40	0.47
2:B:152:ARG:HD2	2:B:157:ILE:HB	1.97	0.47
2:B:46:ARG:NE	2:B:48:GLU:OE2	2.22	0.47
1:A:889:GLY:O	1:A:911:ASN:ND2	2.46	0.47
1:A:249:MET:HA	1:A:252:THR:HG22	1.97	0.46
1:A:1195:GLU:O	1:A:1199:VAL:HG23	2.16	0.46
1:A:228:ILE:HB	1:A:231:LEU:HD22	1.97	0.46
1:A:760:PHE:HE2	1:A:776:LEU:HA	1.81	0.46
1:A:150:ASP:N	1:A:150:ASP:OD1	2.48	0.46
1:A:896:VAL:O	1:A:899:ILE:N	2.48	0.46
1:A:357:LEU:HD13	1:A:385:VAL:HG11	1.96	0.46
2:B:71:LEU:HD21	2:B:106:ILE:HG21	1.96	0.46
1:A:167:SER:O	1:A:171:ILE:HG12	2.15	0.46
1:A:1524:LEU:HD13	1:A:1557:LEU:HD13	1.97	0.46
1:A:394:ILE:CD1	6:A:2303:G2W:C19	2.90	0.46
1:A:891:SER:HA	1:A:894:GLU:HB2	1.98	0.46
2:B:171:THR:O	2:B:175:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:ND2	1:A:220:ARG:CD	2.73	0.45
1:A:300:ARG:HG2	2:B:130:GLU:HG2	1.98	0.45
1:A:798:MET:O	1:A:799:ASP:C	2.57	0.45
1:A:873:LEU:HD13	1:A:958:VAL:HG13	1.99	0.45
1:A:286:LEU:HG	1:A:333:ILE:HD13	1.98	0.45
1:A:804:PHE:CD1	1:A:810:ILE:HG22	2.49	0.45
1:A:1347:PHE:HD2	1:A:1385:LEU:HD22	1.72	0.45
1:A:1528:ASN:HD21	1:A:1619:ARG:HH11	1.64	0.45
2:B:62:LYS:N	2:B:116:SER:O	2.49	0.45
1:A:1449:LEU:HA	1:A:1452:PHE:HB2	1.98	0.45
1:A:1559:THR:O	1:A:1563:VAL:HG22	2.16	0.45
1:A:1412:MET:O	1:A:1416:VAL:HG13	2.17	0.45
1:A:793:LEU:O	1:A:796:ILE:HG13	2.17	0.45
1:A:1416:VAL:HG11	1:A:1434:TYR:CE2	2.52	0.45
1:A:1707:ILE:HD13	1:A:1740:PHE:CE2	2.51	0.45
1:A:248:VAL:O	1:A:252:THR:HG22	2.17	0.44
1:A:812:ASP:O	1:A:816:VAL:HG22	2.18	0.44
3:C:65:LEU:C	3:C:65:LEU:CD2	2.86	0.44
1:A:364:GLU:O	1:A:368:GLN:HG3	2.17	0.44
3:C:128:TYR:HD2	3:C:137:ARG:NE	2.12	0.44
1:A:310:LYS:HE3	1:A:310:LYS:HB2	1.65	0.44
1:A:1251:LYS:O	1:A:1255:THR:HG23	2.18	0.44
1:A:293:LEU:HD12	1:A:299:PHE:CE1	2.52	0.44
1:A:1530:VAL:O	1:A:1534:VAL:HG13	2.18	0.44
3:C:131:ASN:O	3:C:134:ASP:N	2.51	0.44
1:A:1526:CYS:O	1:A:1530:VAL:HG23	2.17	0.44
1:A:278:ASN:HD22	1:A:327:GLY:C	2.26	0.44
1:A:1529:MET:HG3	1:A:1620:ILE:HD13	2.00	0.44
3:C:34:VAL:HG23	3:C:35:PRO:O	2.18	0.44
1:A:399:ALA:HB2	1:A:1759:ILE:HD12	1.99	0.44
1:A:1270:LEU:O	1:A:1274:VAL:HG23	2.17	0.44
1:A:1492:LYS:HE2	1:A:1493:PRO:O	2.18	0.44
1:A:1298:LEU:HD12	1:A:1298:LEU:HA	1.87	0.44
1:A:1566:LEU:O	1:A:1569:LEU:N	2.51	0.44
1:A:815:ILE:HG21	1:A:841:ARG:HG3	2.00	0.43
1:A:1443:PHE:HA	1:A:1447:PHE:HD2	1.82	0.43
1:A:1710:SER:O	1:A:1714:ASP:HB2	2.18	0.43
1:A:283:ASN:HB3	5:A:2302:NAG:O5	2.18	0.43
1:A:1624:VAL:O	1:A:1631:ARG:HG3	2.18	0.43
3:C:47:ARG:C	3:C:49:PRO:HD3	2.43	0.43
3:C:55:CYS:SG	3:C:56:TYR:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1516:ALA:HA	1:A:1519:ILE:HG12	2.01	0.43
3:C:101:PHE:CZ	3:C:105:PRO:HD3	2.54	0.43
1:A:213:LEU:O	1:A:216:PHE:HB2	2.19	0.43
1:A:247:ASP:OD1	1:A:1629:GLY:HA3	2.18	0.43
1:A:737:ILE:HG21	1:A:796:ILE:HD11	2.00	0.43
1:A:781:LEU:HD12	1:A:782:VAL:N	2.34	0.43
1:A:806:VAL:O	1:A:810:ILE:HG23	2.18	0.43
1:A:914:PHE:HE2	1:A:1431:LEU:O	2.02	0.43
1:A:1502:ASN:OD1	1:A:1504:ILE:HG12	2.19	0.43
3:C:108:TYR:N	3:C:108:TYR:CD1	2.86	0.43
1:A:406:GLU:O	1:A:410:GLN:HG2	2.19	0.43
1:A:742:MET:HB2	1:A:746:VAL:HG23	1.99	0.43
1:A:1430:SER:HB3	1:A:1433:MET:HG2	1.99	0.43
1:A:1258:TRP:HB3	1:A:1302:SER:OG	2.19	0.43
2:B:71:LEU:HB3	2:B:80:LEU:HD23	2.01	0.43
1:A:398:LEU:HG	1:A:960:LEU:HD11	2.00	0.42
1:A:1305:GLU:OE2	1:A:1308:ARG:NH1	2.51	0.42
1:A:1528:ASN:HD21	1:A:1619:ARG:NH1	2.17	0.42
1:A:293:LEU:CD1	1:A:299:PHE:CE1	3.02	0.42
1:A:399:ALA:CB	1:A:1762:ASN:HD22	2.32	0.42
1:A:910:MET:HE3	1:A:919:ILE:HG21	2.01	0.42
3:C:40:VAL:HG22	3:C:44:SER:OG	2.19	0.42
3:C:58:VAL:HG13	3:C:63:PHE:CB	2.46	0.42
1:A:1745:ILE:O	1:A:1749:LEU:HG	2.18	0.42
2:B:185:ILE:O	2:B:189:THR:HG22	2.19	0.42
1:A:1609:PHE:CZ	1:A:1613:ARG:HD2	2.54	0.42
1:A:1763:PHE:O	1:A:1767:THR:HG23	2.18	0.42
1:A:1198:ILE:HD13	1:A:1198:ILE:HA	1.88	0.42
1:A:1497:ILE:HG23	1:A:1498:PRO:HD2	2.01	0.42
1:A:170:LYS:HB3	1:A:170:LYS:HE2	1.80	0.42
1:A:181:PHE:O	1:A:185:ARG:HG2	2.19	0.42
1:A:185:ARG:HA	1:A:185:ARG:HD2	1.80	0.42
1:A:1593:MET:HE3	1:A:1593:MET:HB2	1.90	0.42
2:B:21:CYS:SG	2:B:22:VAL:N	2.92	0.42
1:A:734:LYS:HE3	1:A:734:LYS:HB2	1.77	0.42
2:B:89:ARG:HB2	2:B:109:THR:O	2.19	0.42
1:A:762:ALA:HB2	1:A:1337:ILE:HD11	2.02	0.42
1:A:791:MET:HG2	1:A:816:VAL:HG21	2.01	0.42
1:A:1457:ILE:HG12	1:A:1756:ILE:HD12	2.01	0.42
1:A:1508:ILE:CG2	1:A:1568:SER:HG	2.30	0.42
1:A:1678:MET:HE3	1:A:1679:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:ARG:HA	1:A:907:ARG:HD2	1.84	0.42
1:A:115:LEU:O	1:A:119:SER:HB3	2.20	0.42
1:A:132:ILE:O	1:A:136:ILE:HG23	2.20	0.42
1:A:1703:LEU:O	1:A:1707:ILE:HD12	2.20	0.42
1:A:799:ASP:O	1:A:803:TYR:CB	2.68	0.41
2:B:128:PHE:HD1	2:B:133:GLU:HG2	1.85	0.41
1:A:276:PHE:HE2	1:A:280:LEU:HD11	1.84	0.41
1:A:836:SER:HB3	1:A:1338:MET:HG3	2.01	0.41
1:A:1528:ASN:HD21	1:A:1619:ARG:HE	1.68	0.41
1:A:356:ARG:HG3	1:A:361:ASP:O	2.21	0.41
1:A:1256:ASN:HB3	1:A:1259:CYS:HB2	2.02	0.41
1:A:1359:PHE:CZ	1:A:1373:LEU:HD21	2.53	0.41
1:A:893:LYS:HD3	1:A:905:LEU:HD21	2.03	0.41
1:A:1588:ILE:HG12	1:A:1615:ALA:HB1	2.03	0.41
2:B:31:VAL:HG23	2:B:34:MET:HG3	2.03	0.41
1:A:810:ILE:O	1:A:814:LEU:HG	2.20	0.41
1:A:1458:ASP:O	1:A:1462:GLN:HG2	2.21	0.41
1:A:275:CYS:HB3	1:A:328:TYR:HB3	2.03	0.41
1:A:1315:ILE:HD13	1:A:1315:ILE:HA	1.87	0.41
1:A:289:ILE:HG22	1:A:293:LEU:HD23	1.78	0.41
1:A:844:LYS:C	1:A:846:ALA:H	2.29	0.41
1:A:919:ILE:O	1:A:923:VAL:HG23	2.20	0.41
1:A:1355:ASP:OD1	1:A:1355:ASP:N	2.39	0.41
1:A:1358:ARG:NH2	1:A:1417:ASP:OD2	2.48	0.41
1:A:1553:VAL:O	1:A:1556:ILE:HG22	2.21	0.41
1:A:838:ARG:HG2	1:A:841:ARG:NH1	2.36	0.41
1:A:1318:ILE:N	1:A:1319:PRO:HD2	2.36	0.41
3:C:32:VAL:CA	3:C:51:THR:O	2.64	0.41
1:A:771:GLU:HA	1:A:774:ASN:OD1	2.21	0.41
1:A:1224:ILE:HG21	2:B:156:SER:HA	2.03	0.41
2:B:75:ASN:N	2:B:75:ASN:OD1	2.53	0.41
1:A:123:LEU:HD23	1:A:124:VAL:HG13	2.02	0.40
1:A:300:ARG:HA	1:A:305:TYR:CD2	2.56	0.40
1:A:1719:LYS:H	1:A:1728:GLY:H	1.68	0.40
2:B:187:ALA:O	2:B:191:THR:HG23	2.21	0.40
3:C:38:LEU:HD23	3:C:48:LEU:HD22	2.03	0.40
1:A:200:TYR:HD1	1:A:200:TYR:HA	1.76	0.40
1:A:765:HIS:HD2	1:A:767:PRO:O	2.03	0.40
1:A:1204:LEU:HB3	1:A:1233:PHE:CZ	2.56	0.40
1:A:1217:GLU:HB3	2:B:24:VAL:HG21	2.03	0.40
1:A:1343:PHE:HB3	1:A:1347:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:SER:C	1:A:1432:TYR:H	2.29	0.40
3:C:103:GLY:O	3:C:105:PRO:CD	2.64	0.40
1:A:396:LEU:HD13	1:A:1633:LEU:HD13	2.04	0.40
1:A:1497:ILE:HD13	1:A:1569:LEU:HD22	2.03	0.40
1:A:1512:VAL:HG12	1:A:1564:LEU:HD12	2.03	0.40
1:A:211:SER:O	1:A:215:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1132/2250 (50%)	1068 (94%)	63 (6%)	1 (0%)	48	77
2	B	171/481 (36%)	160 (94%)	11 (6%)	0	100	100
3	C	118/215 (55%)	109 (92%)	5 (4%)	4 (3%)	3	15
All	All	1421/2946 (48%)	1337 (94%)	79 (6%)	5 (0%)	32	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	56	TYR
3	C	76	SER
3	C	86	LYS
3	C	147	LEU
1	A	800	PRO

### 5.3.2 Protein sidechains [i](#)

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



entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1017/1998 (51%)	986 (97%)	31 (3%)	36	62
2	B	157/419 (38%)	150 (96%)	7 (4%)	23	51
3	C	103/193 (53%)	99 (96%)	4 (4%)	27	56
All	All	1277/2610 (49%)	1235 (97%)	42 (3%)	35	60

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ILE
1	A	131	LEU
1	A	146	ASN
1	A	191	LEU
1	A	348	SER
1	A	354	LEU
1	A	362	TYR
1	A	364	GLU
1	A	379	MET
1	A	839	LEU
1	A	851	THR
1	A	900	ASN
1	A	944	CYS
1	A	1188	ILE
1	A	1195	GLU
1	A	1225	ILE
1	A	1256	ASN
1	A	1272	THR
1	A	1330	ILE
1	A	1336	SER
1	A	1380	VAL
1	A	1388	ASN
1	A	1424	GLN
1	A	1514	ASN
1	A	1572	TYR
1	A	1675	ILE
1	A	1677	ASP
1	A	1683	THR
1	A	1691	LEU
1	A	1720	VAL

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Mol	Chain	Res	Type
1	A	1726	VAL
2	B	43	CYS
2	B	47	SER
2	B	58	THR
2	B	93	ASN
2	B	104	LEU
2	B	178	MET
2	B	190	GLU
3	C	34	VAL
3	C	48	LEU
3	C	65	LEU
3	C	130	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	265	GLN
1	A	278	ASN
1	A	282	ASN
1	A	365	ASN
1	A	395	ASN
1	A	765	HIS
1	A	766	HIS
1	A	853	ASN
1	A	941	GLN
1	A	956	ASN
1	A	961	ASN
1	A	1341	ASN
1	A	1528	ASN
1	A	1721	HIS
1	A	1762	ASN
2	B	50	ASN
2	B	102	GLN
2	B	115	HIS
2	B	134	HIS
3	C	59	ASN
3	C	145	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 ⓘ

4 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$
4	NAG	D	1	4,1	14,14,15	0.32	0	17,19,21	0.42	0
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	E	1	4,1	14,14,15	0.57	0	17,19,21	1.41	2 (11%)
4	NAG	E	2	4	14,14,15	0.90	1 (7%)	17,19,21	1.07	1 (5%)

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
4	NAG	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	3.16	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C2-N2-C7	4.44	129.23	122.90
4	E	2	NAG	C1-O5-C5	4.16	117.83	112.19
4	E	1	NAG	C1-C2-N2	2.19	114.23	110.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

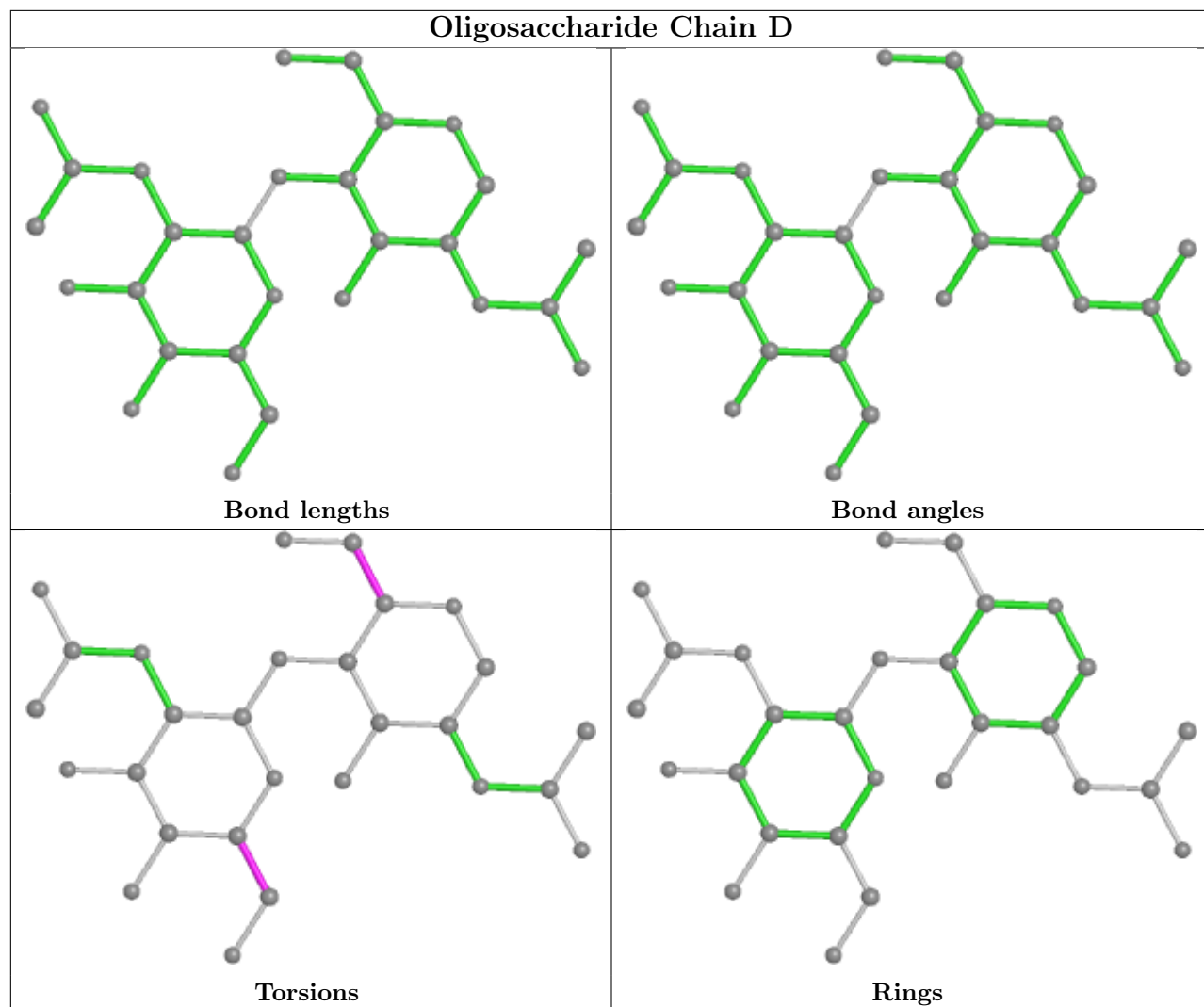
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7

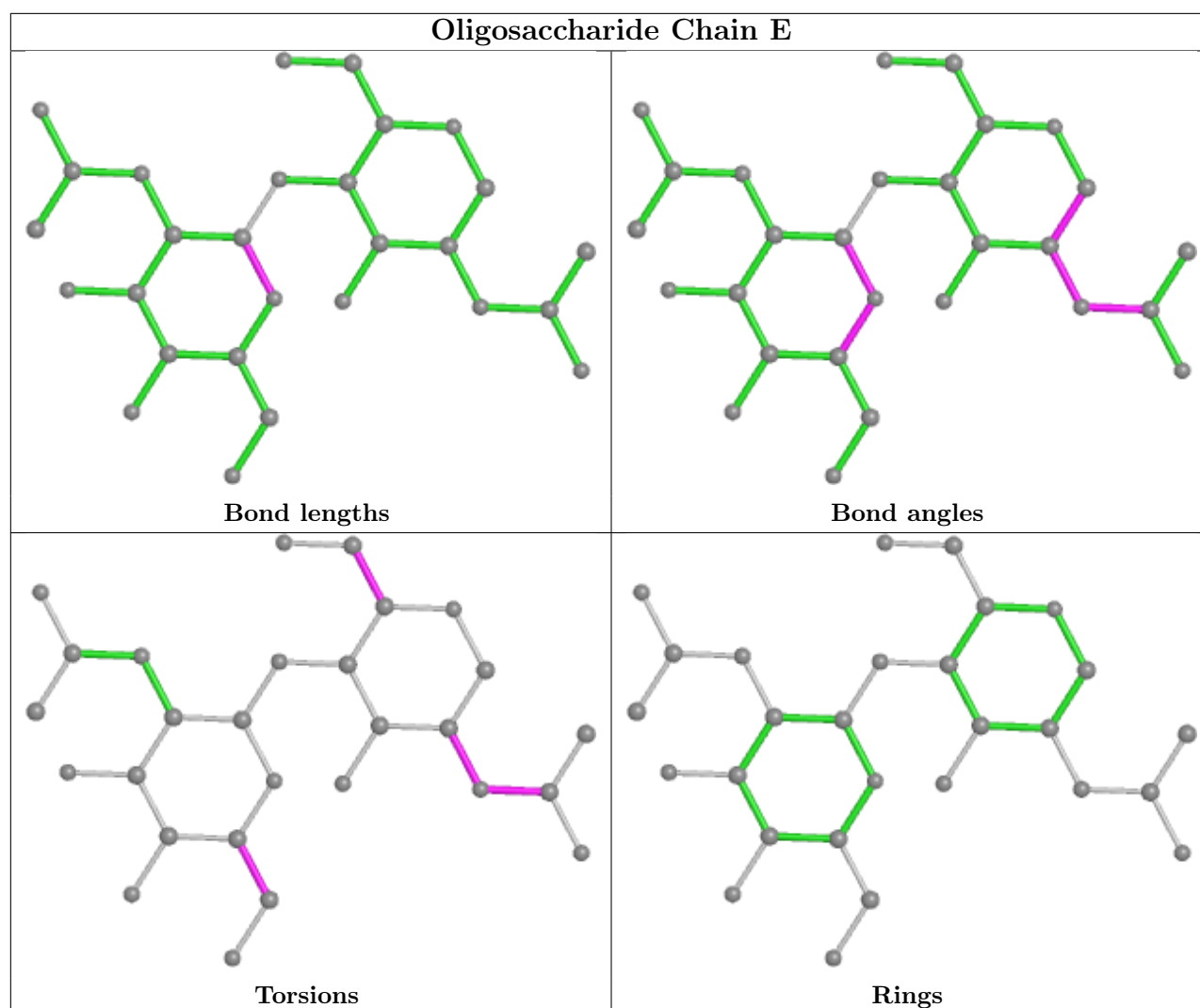
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	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](#)

7 ligands 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	A	2301	1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	B	502	2	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	B	504	2	14,14,15	0.24	0	17,19,21	0.37	0
5	NAG	B	501	2	14,14,15	0.17	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	G2W	A	2303	-	31,33,33	5.98	24 (77%)	41,46,46	2.03	5 (12%)
5	NAG	B	503	2	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	2302	1	14,14,15	0.36	0	17,19,21	0.62	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	A	2301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	502	2	-	2/6/23/26	0/1/1/1
5	NAG	B	504	2	-	1/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
6	G2W	A	2303	-	-	6/14/26/26	0/4/4/4
5	NAG	B	503	2	-	2/6/23/26	0/1/1/1
5	NAG	A	2302	1	-	2/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2303	G2W	C17-N06	9.82	1.48	1.34
6	A	2303	G2W	C24-C26	9.77	1.53	1.39
6	A	2303	G2W	C29-N08	9.68	1.46	1.33
6	A	2303	G2W	C19-C22	8.92	1.52	1.37
6	A	2303	G2W	C19-C15	8.87	1.52	1.39
6	A	2303	G2W	C24-C23	8.61	1.53	1.39
6	A	2303	G2W	C25-C23	8.18	1.53	1.39
6	A	2303	G2W	C28-C26	7.97	1.52	1.39
6	A	2303	G2W	C21-C22	7.81	1.52	1.37
6	A	2303	G2W	C16-C21	7.77	1.52	1.38
6	A	2303	G2W	C27-C25	6.56	1.52	1.38
6	A	2303	G2W	C27-C28	6.52	1.52	1.38
6	A	2303	G2W	C12-N05	6.51	1.44	1.34
6	A	2303	G2W	C16-C13	6.21	1.52	1.39
6	A	2303	G2W	C13-C15	5.54	1.51	1.39
6	A	2303	G2W	C14-C18	5.26	1.49	1.38
6	A	2303	G2W	C18-N06	5.24	1.45	1.34
6	A	2303	G2W	C17-N07	4.39	1.45	1.36
6	A	2303	G2W	C17-N05	4.28	1.47	1.34
6	A	2303	G2W	C14-C12	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2303	G2W	C12-N04	3.24	1.44	1.37
6	A	2303	G2W	C23-N07	2.28	1.45	1.40
6	A	2303	G2W	O03-C29	-2.15	1.18	1.23
6	A	2303	G2W	C10-N04	2.02	1.49	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2303	G2W	N06-C17-N05	-7.86	119.11	126.55
6	A	2303	G2W	C18-N06-C17	6.20	120.95	115.45
6	A	2303	G2W	C13-O02-C09	-3.52	108.30	120.21
6	A	2303	G2W	C14-C18-N06	-3.23	119.94	123.96
6	A	2303	G2W	C26-C29-N08	2.51	120.22	116.89

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2302	NAG	O5-C5-C6-O6
5	B	503	NAG	O5-C5-C6-O6
5	A	2302	NAG	C4-C5-C6-O6
5	B	503	NAG	C4-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
6	A	2303	G2W	C15-C13-O02-C09
6	A	2303	G2W	C25-C23-N07-C17
5	B	501	NAG	C4-C5-C6-O6
6	A	2303	G2W	C24-C23-N07-C17
6	A	2303	G2W	C16-C13-O02-C09
5	B	502	NAG	C4-C5-C6-O6
5	B	504	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
6	A	2303	G2W	N05-C17-N07-C23
6	A	2303	G2W	N06-C17-N07-C23

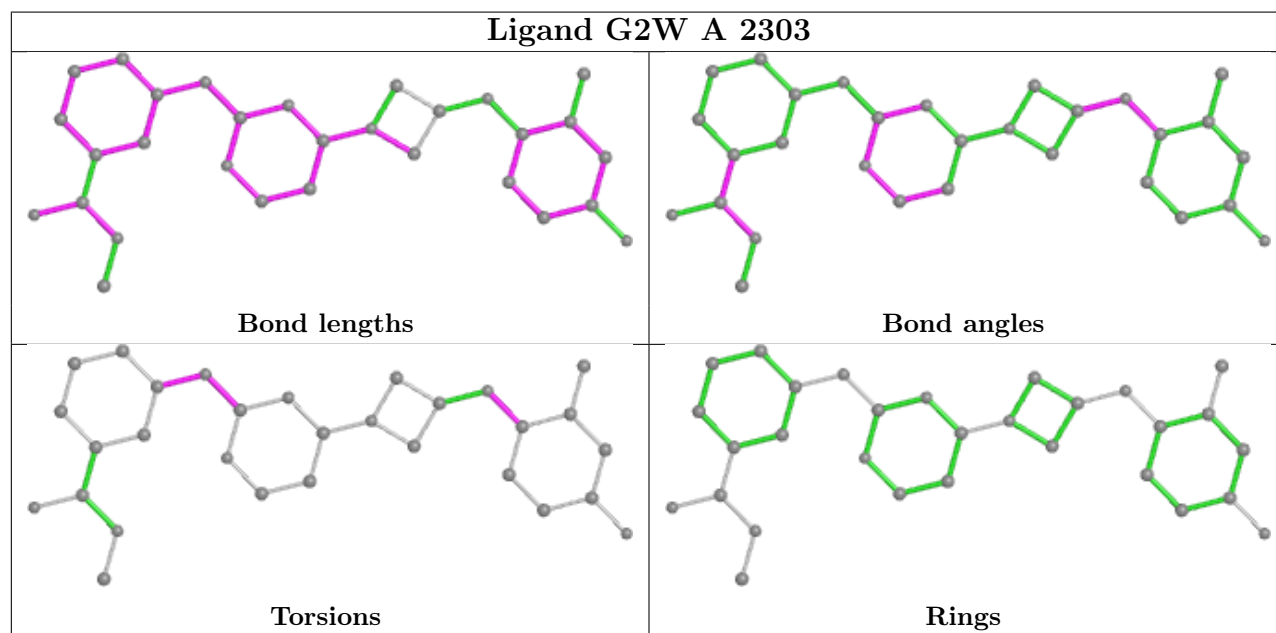
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2303	G2W	9	0
5	A	2302	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

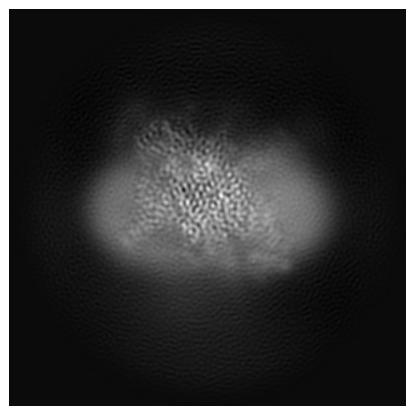
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33295. These allow visual inspection of the internal detail of the map and identification of artifacts.

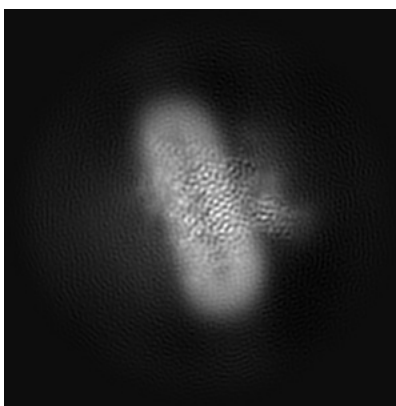
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

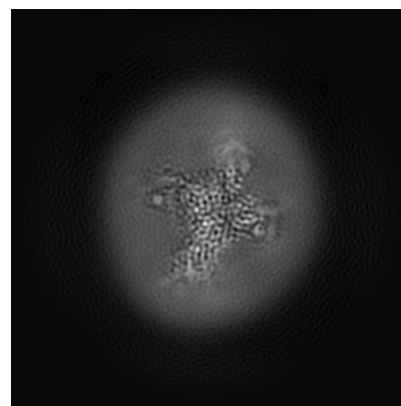
#### 6.1.1 Primary map



X

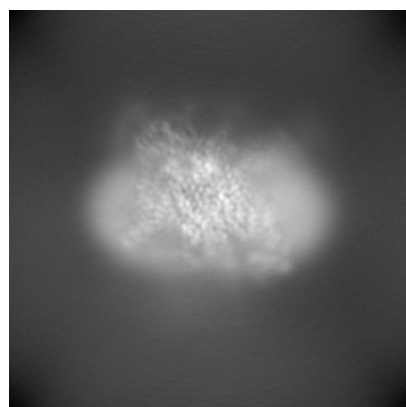


Y

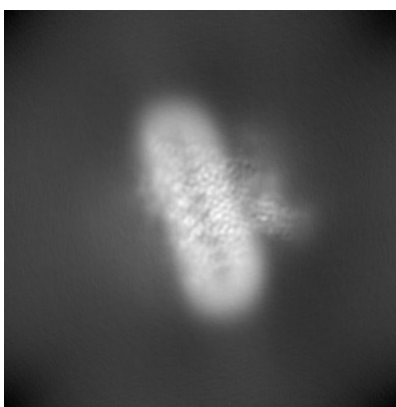


Z

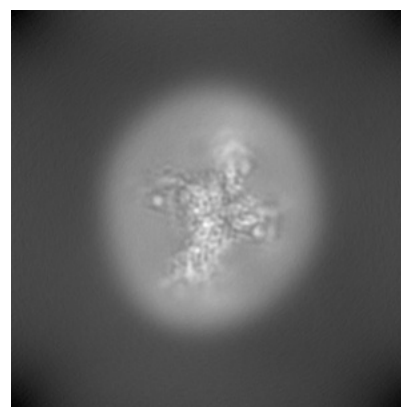
#### 6.1.2 Raw map



X



Y

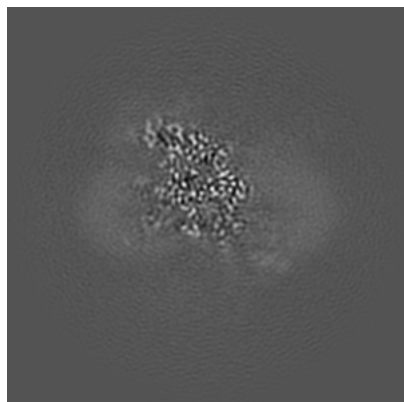


Z

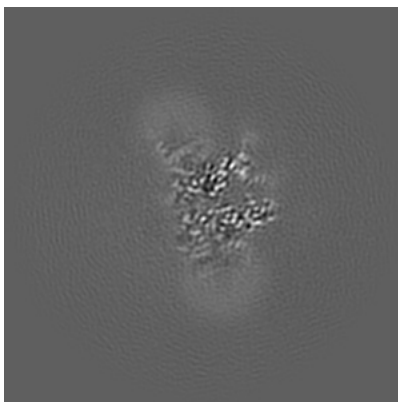
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

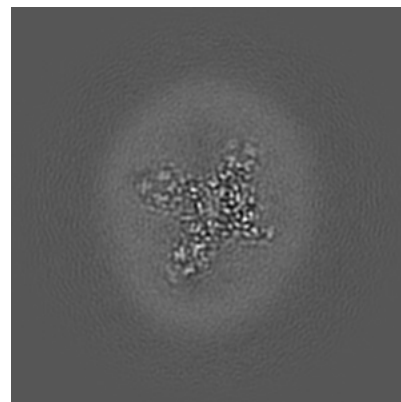
### 6.2.1 Primary map



X Index: 128

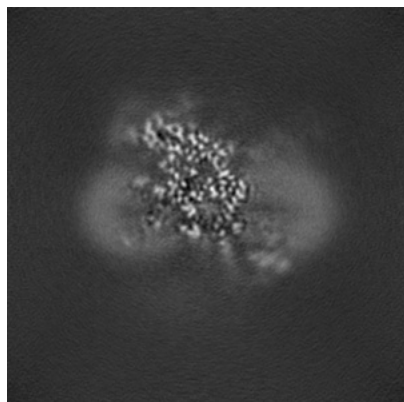


Y Index: 128

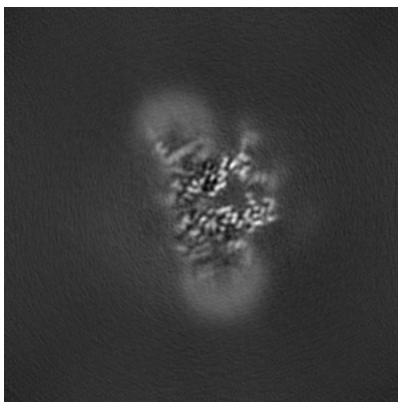


Z Index: 128

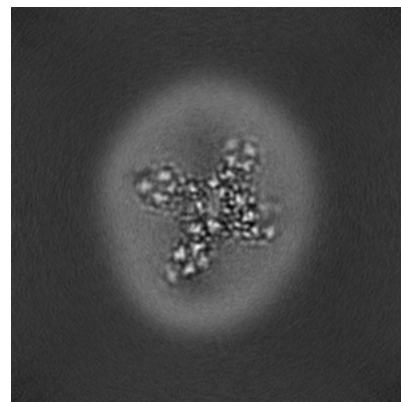
### 6.2.2 Raw map



X Index: 128



Y Index: 128

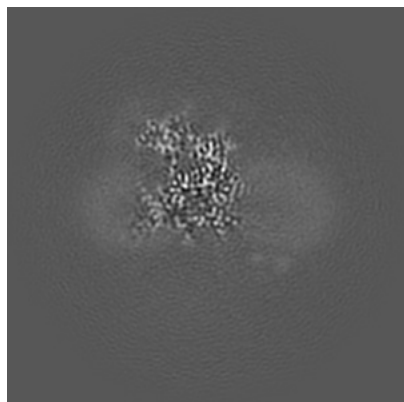


Z Index: 128

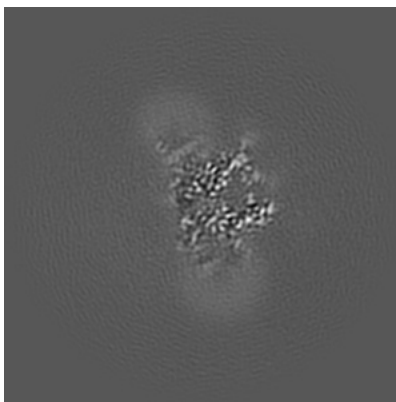
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

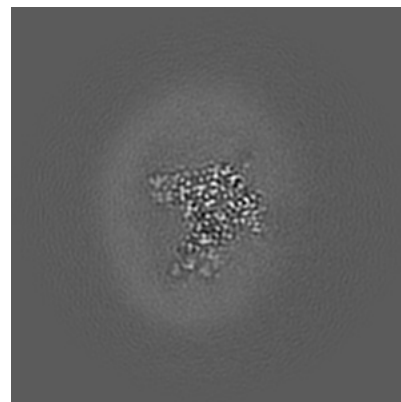
### 6.3.1 Primary map



X Index: 122

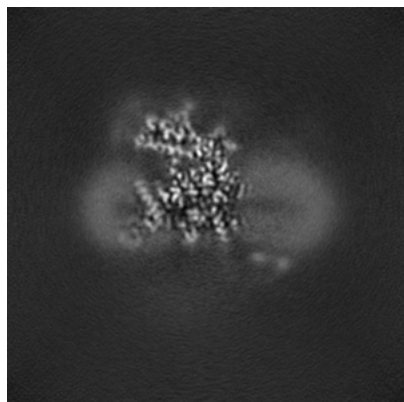


Y Index: 127

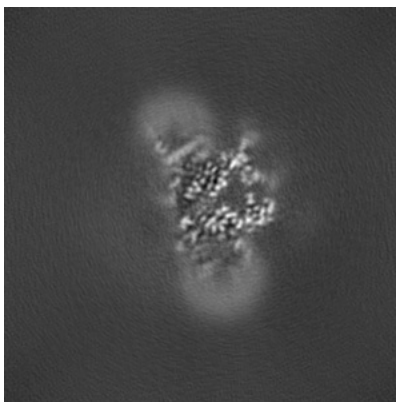


Z Index: 139

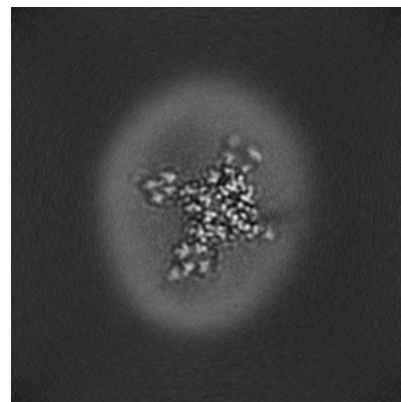
### 6.3.2 Raw map



X Index: 123



Y Index: 127

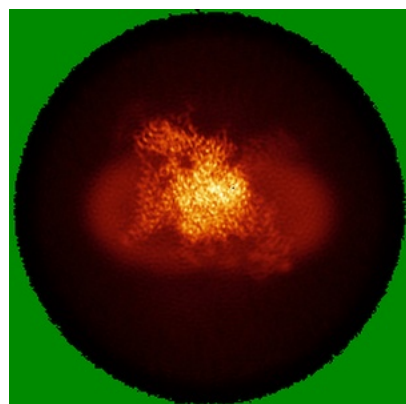


Z Index: 133

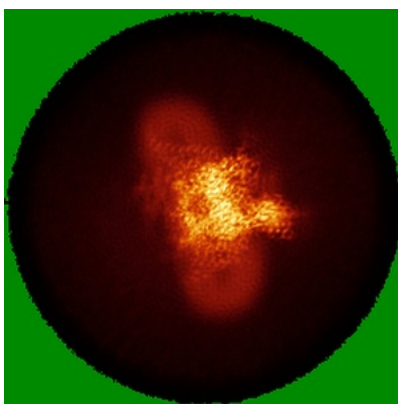
The images above show the largest variance slices of the map in three orthogonal directions.

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

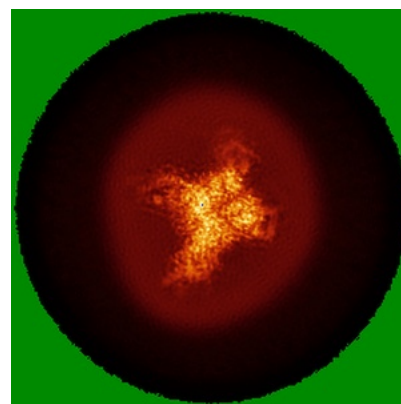
### 6.4.1 Primary map



X

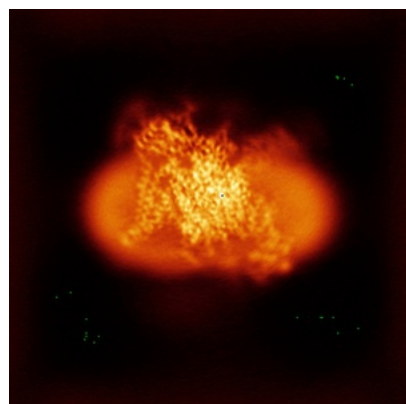


Y

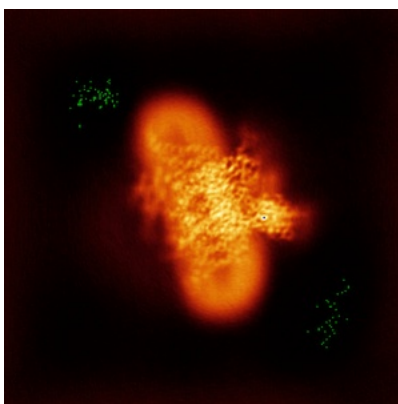


Z

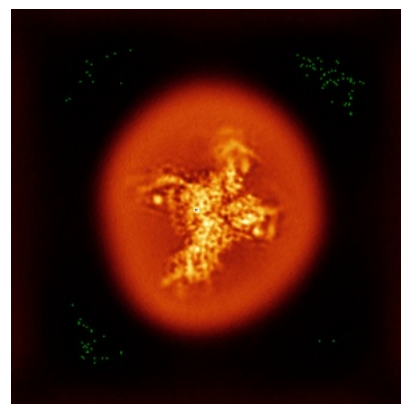
### 6.4.2 Raw map



X



Y

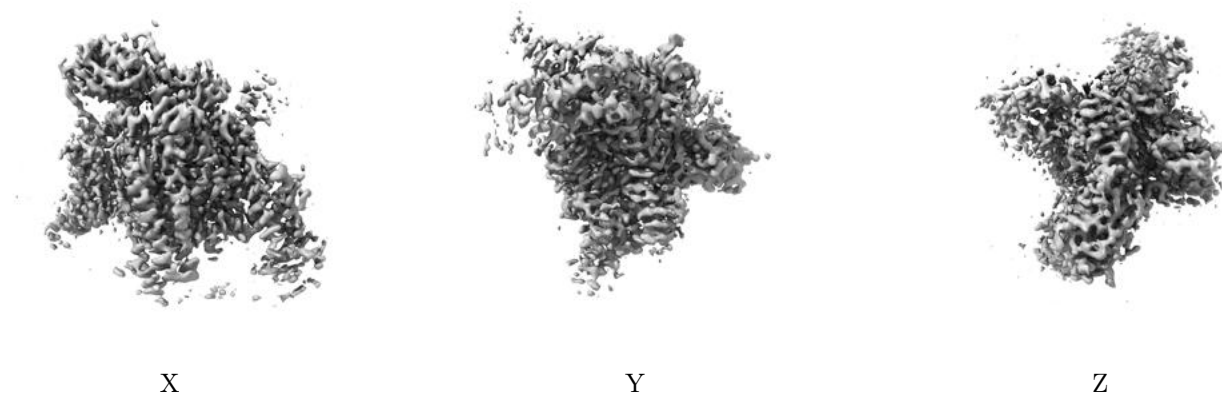


Z

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 0.607. 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](#)

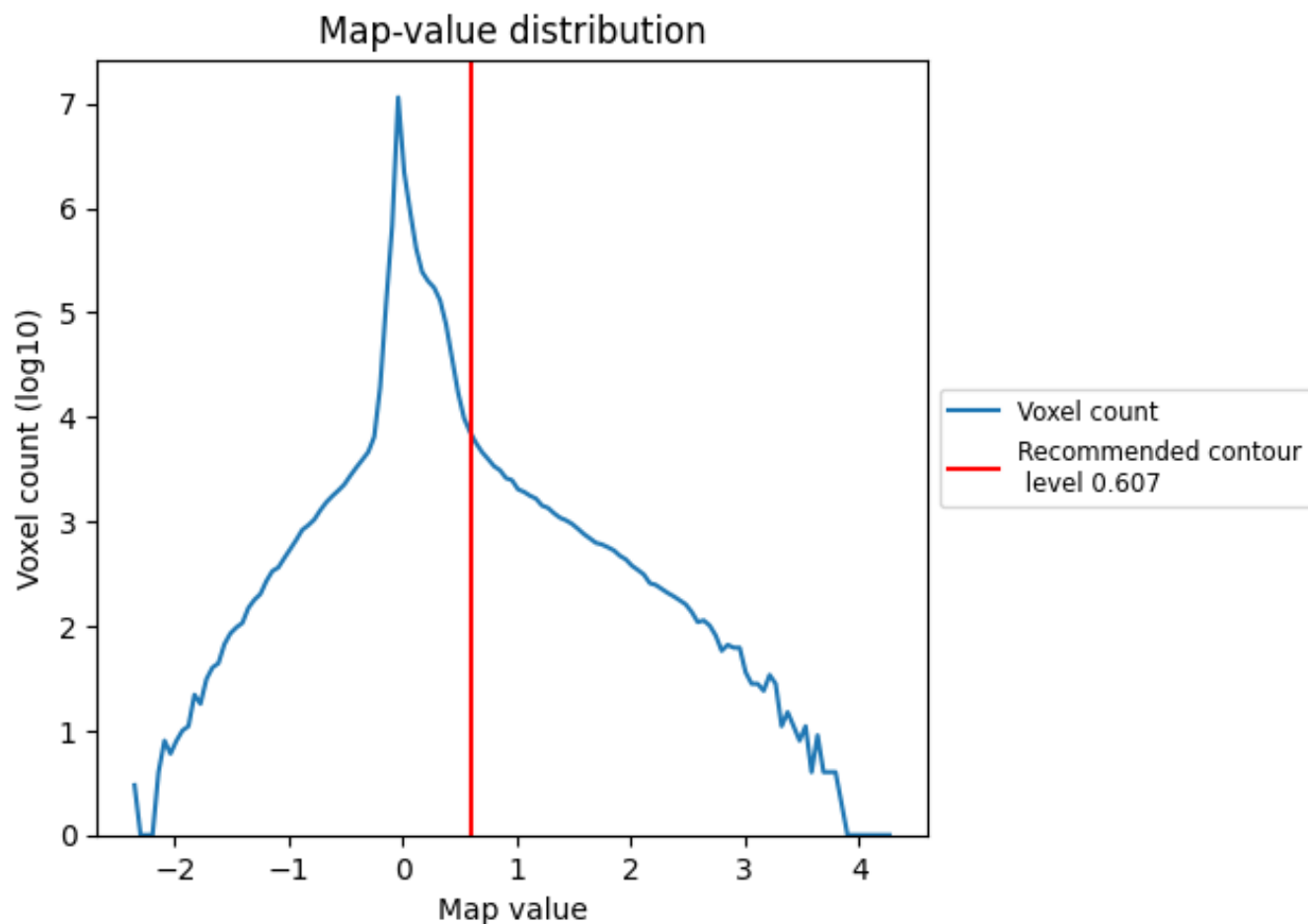
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

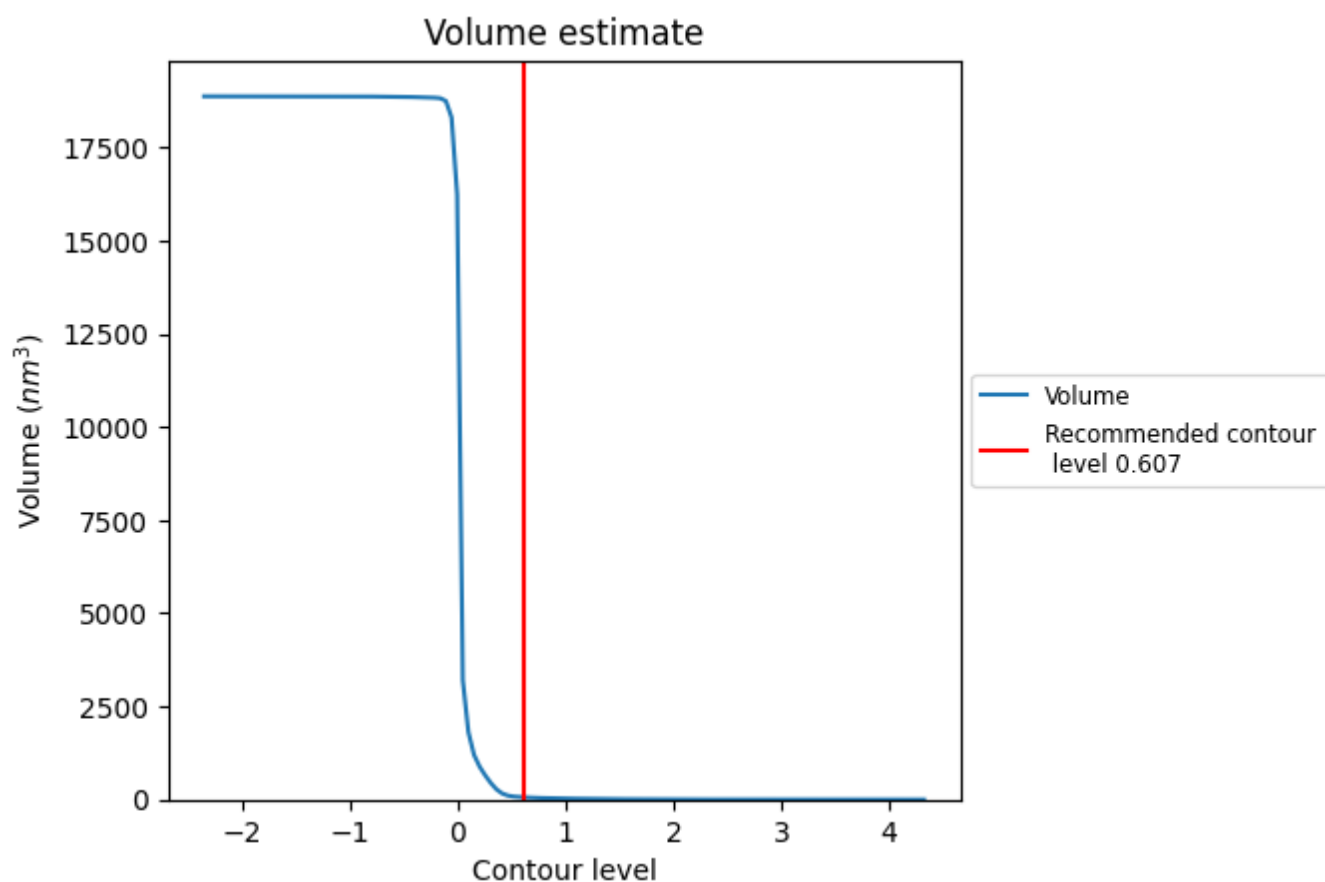
This section contains the results of statistical analysis of the map.

### 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](#)

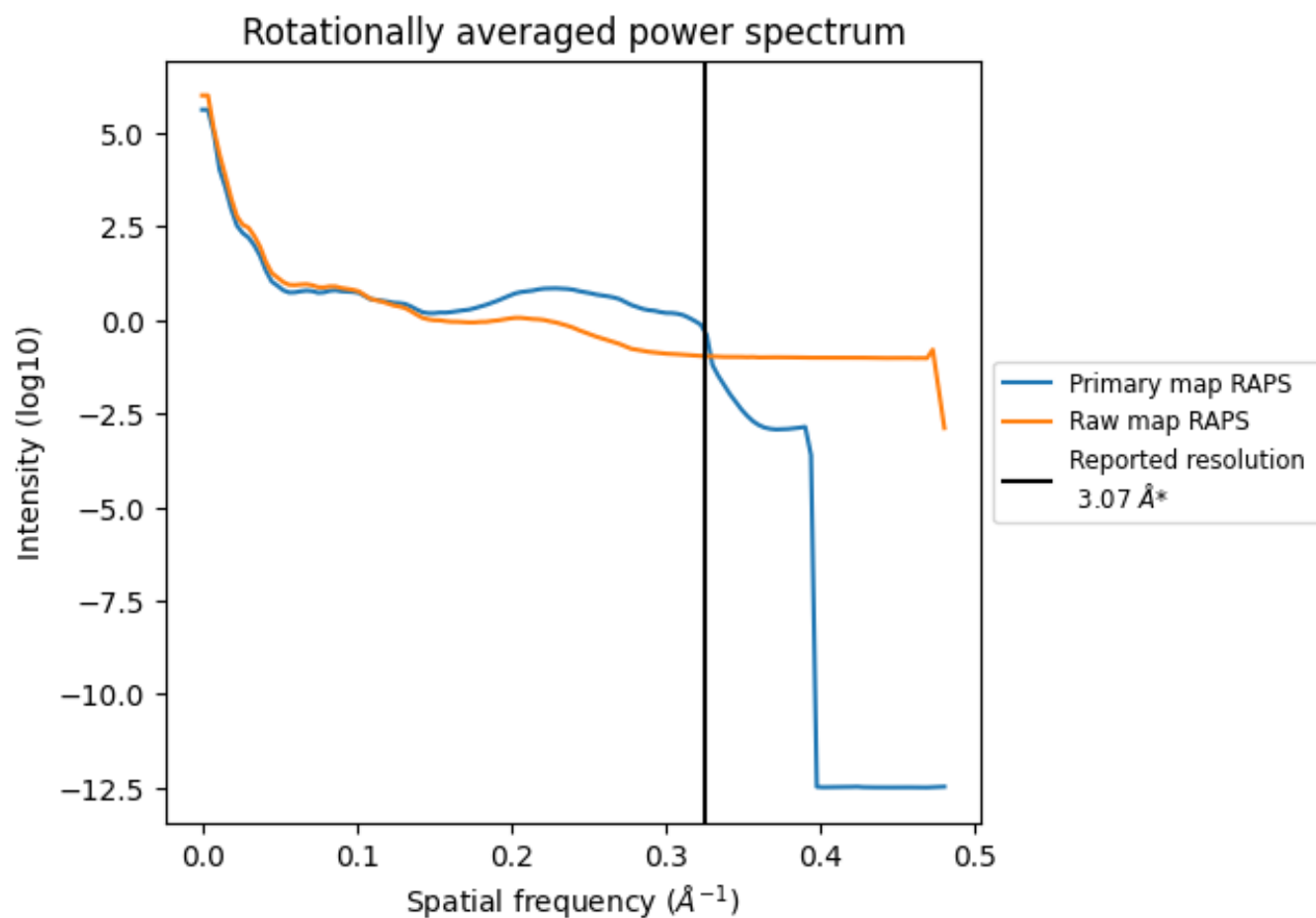


The volume at the recommended contour level is 61  $\text{nm}^3$ ; this corresponds to an approximate mass of 55 kDa.

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 ⓘ

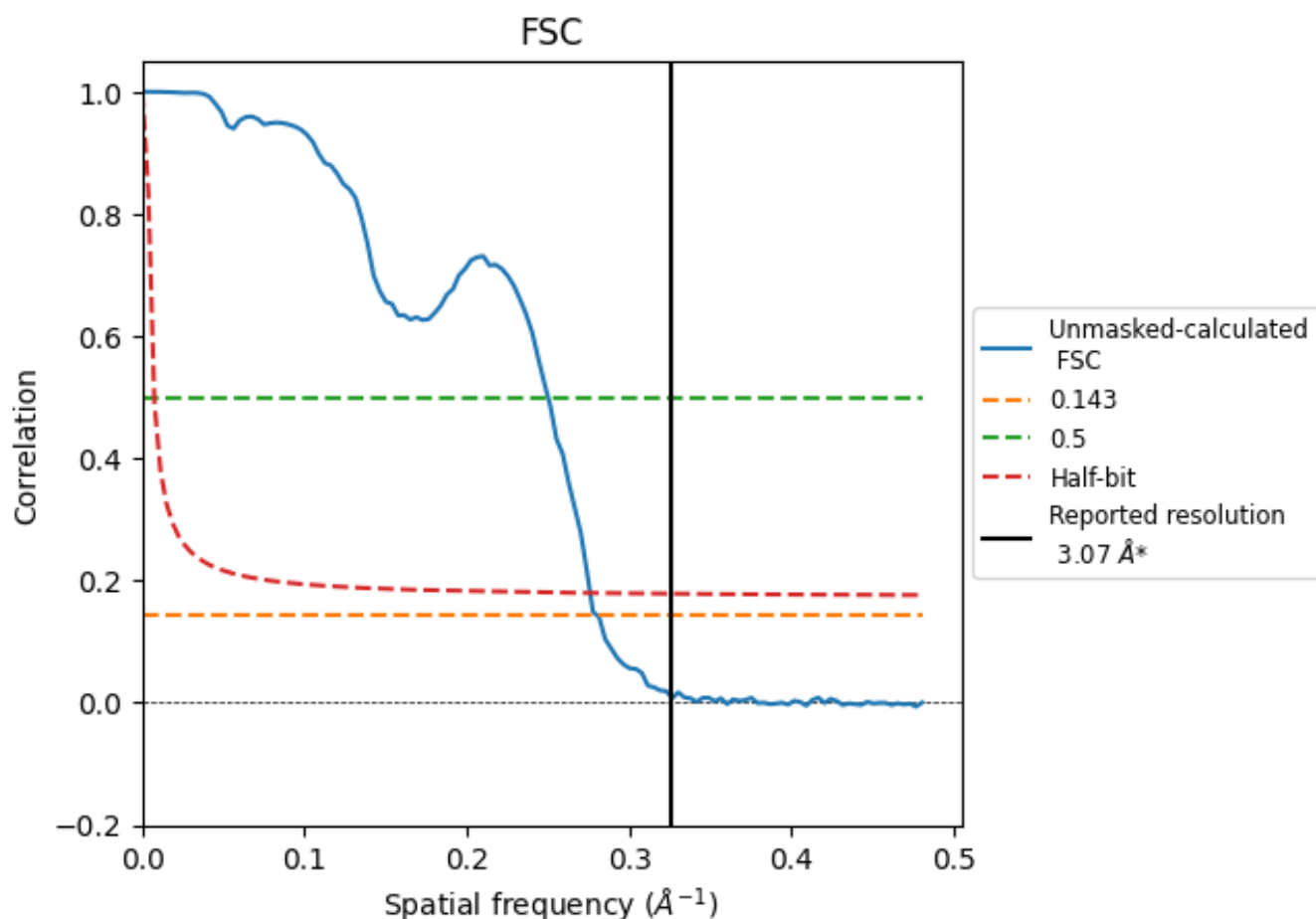


\*Reported resolution corresponds to spatial frequency of 0.326  $\text{\AA}^{-1}$

## 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  $0.326 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

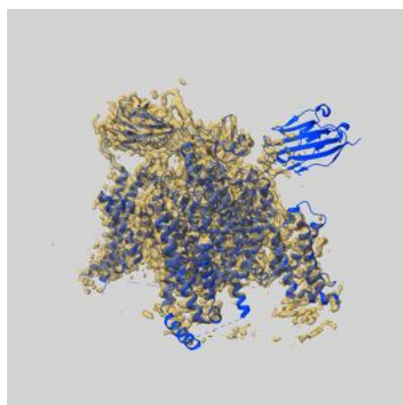
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.00	3.62

\*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 3.57 differs from the reported value 3.07 by more than 10 %

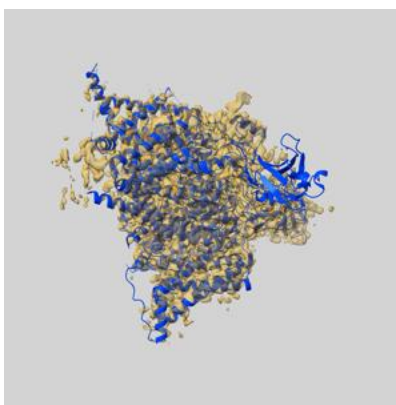
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33295 and PDB model 7XMF. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

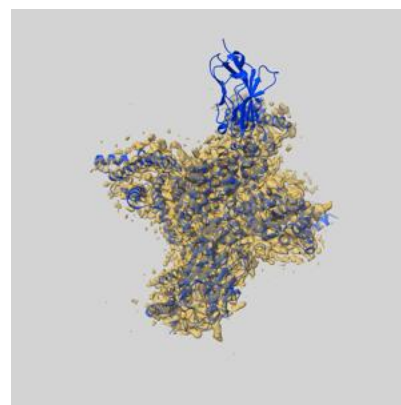
### 9.1 Map-model overlay [i](#)



X



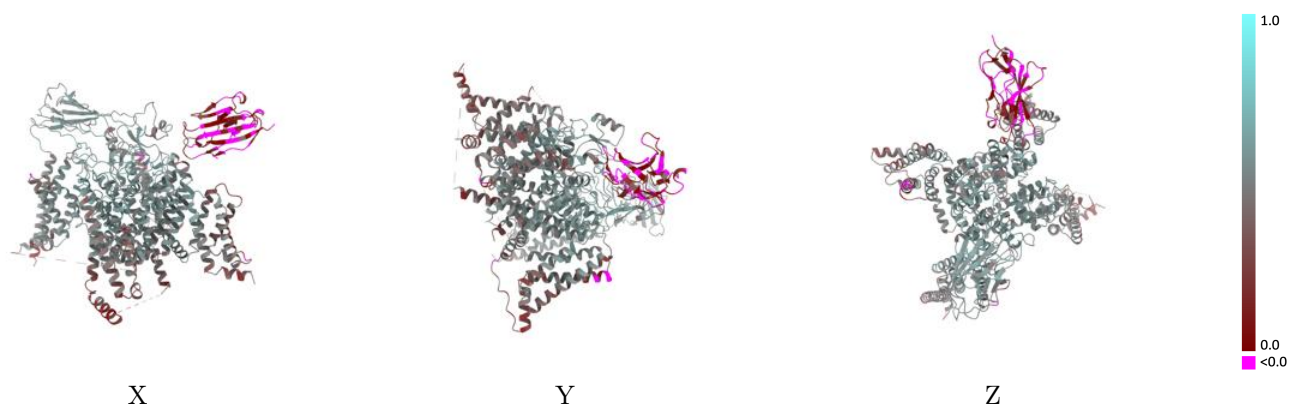
Y



Z

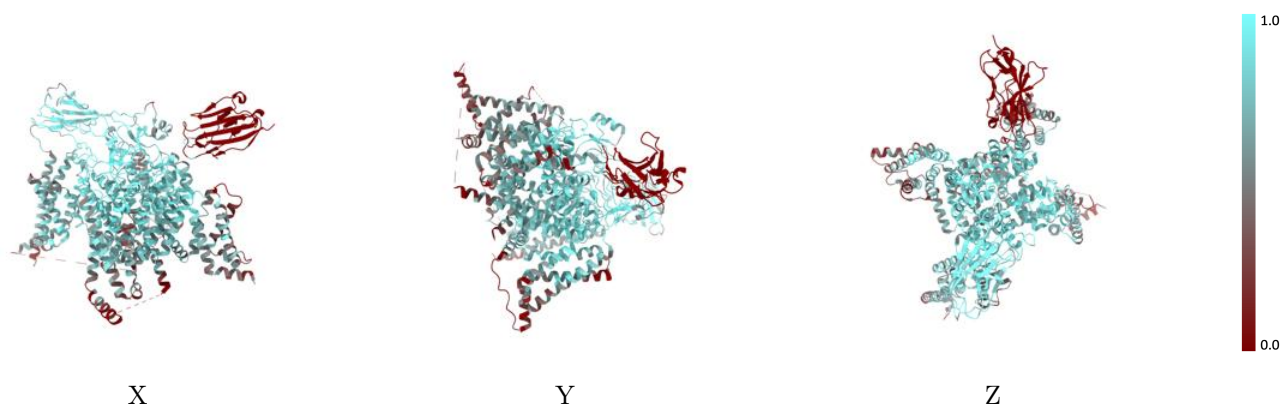
The images above show the 3D surface view of the map at the recommended contour level 0.607 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



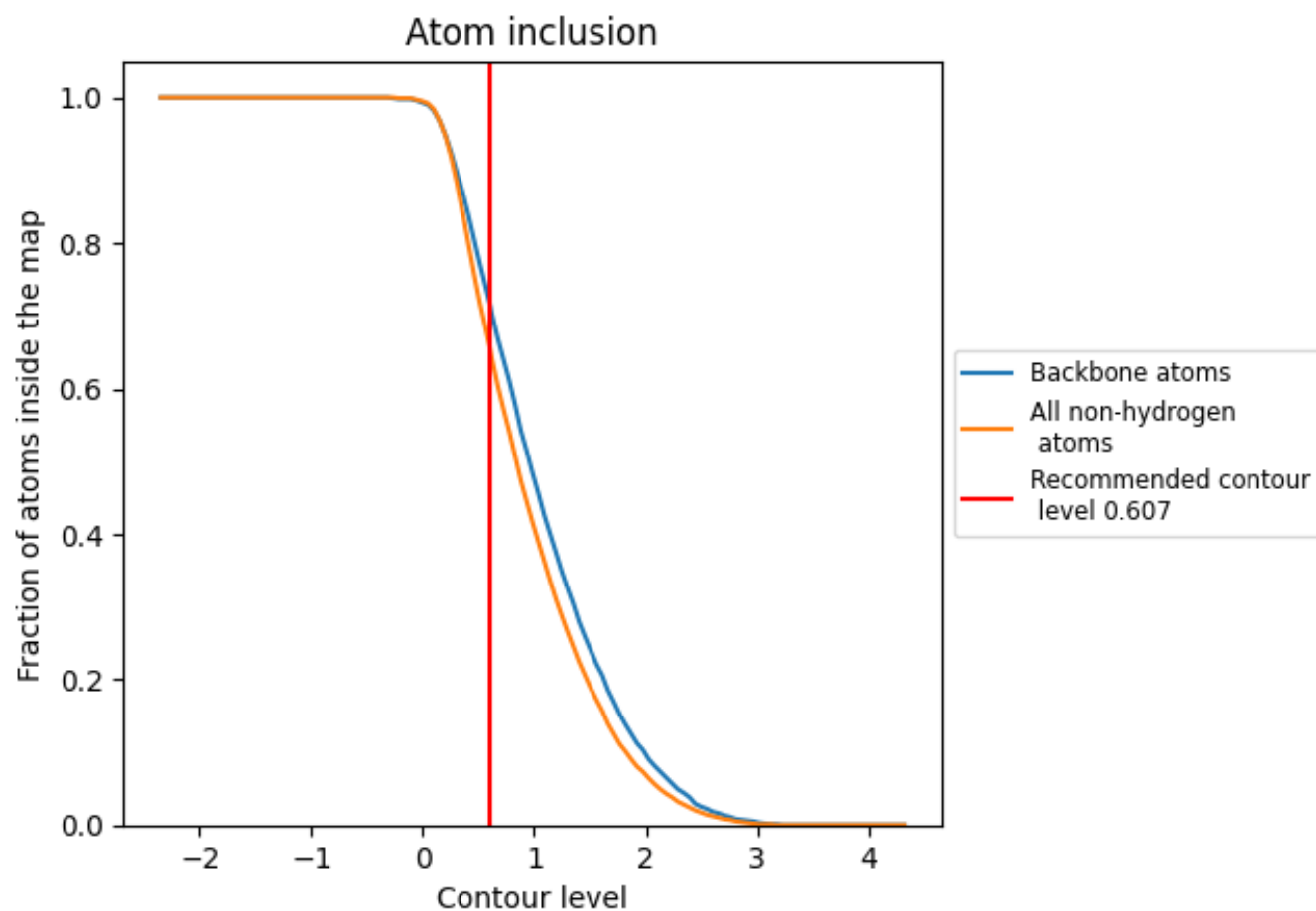
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.607).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% 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 (0.607) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6540	<div></div> 0.4570
A	<div></div> 0.7040	<div></div> 0.4910
B	<div></div> 0.7390	<div></div> 0.5030
C	<div></div> 0.0240	<div></div> 0.0500
D	<div></div> 0.5710	<div></div> 0.4180
E	<div></div> 0.7500	<div></div> 0.4710

