



Full wwPDB EM Validation Report ⓘ

Dec 20, 2022 – 02:15 PM JST

PDB ID : 7XM9
EMDB ID : EMD-33292
Title : Cryo-EM structure of human NaV1.7/beta1/beta2-XEN907
Authors : zhang, J.T.; Jiang, D.H.
Deposited on : 2022-04-25
Resolution : 3.22 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:

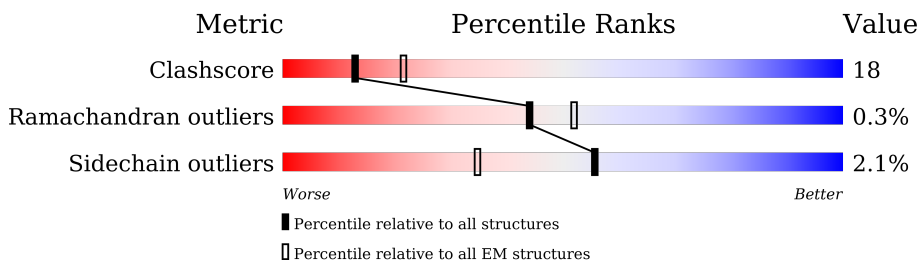
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.22 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2250	
2	B	481	
3	C	215	
4	D	2	
4	E	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12490 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	1230	9896	6569	1549	1701	77	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
			Total	C	N	O	S		
3	C	120	977	612	173	182	10	0	0

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



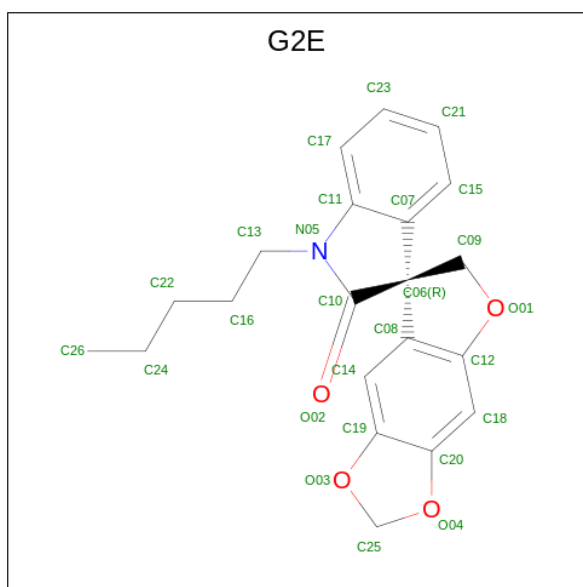
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



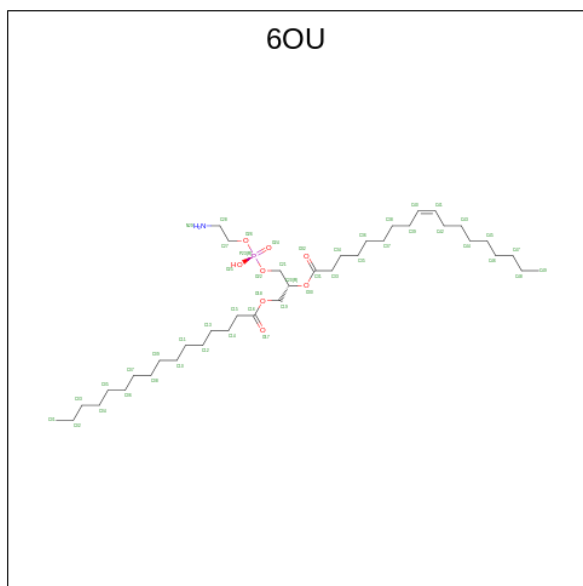
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	1	5	0
5	B	1	56	32	4	20	0
5	B	1	56	32	4	20	0
5	B	1	56	32	4	20	0
5	B	1	56	32	4	20	0

- Molecule 6 is (7 {R})-1'-pentylspiro[6 {H}-furo[3,2-f][1,3]benzodioxole-7,3'-indole]-2'-one (three-letter code: G2E) (formula: C₂₁H₂₁NO₄) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	26	21	1	4	0

- Molecule 7 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C₃₉H₇₆NO₈P).




Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	49	39	1	8	1	0

Chain D:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175883	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 IS (4k x 4k)	Depositor
Maximum map value	4.299	Depositor
Minimum map value	-3.071	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.402	Depositor
Map size (\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 (\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, 6OU, G2E

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	0.31	0/10142	0.45	2/13748 (0.0%)
2	B	0.27	0/1442	0.47	0/1949
3	C	0.50	1/999 (0.1%)	0.70	2/1351 (0.1%)
All	All	0.32	1/12583 (0.0%)	0.48	4/17048 (0.0%)

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	11.06	2.01	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	127	CYS	CA-CB-SG	7.90	128.22	114.00
3	C	85	MET	CB-CA-C	-6.32	97.76	110.40
1	A	801	TYR	N-CA-C	5.27	125.24	111.00
1	A	801	TYR	CB-CA-C	-5.13	100.15	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9896	0	10104	324	0
2	B	1416	0	1382	38	0
3	C	977	0	937	102	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	14	0	13	0	0
5	B	56	0	52	0	0
6	A	26	0	0	6	0
7	A	49	0	0	1	0
All	All	12490	0	12538	460	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 18.

All (460) 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
3:C:128:TYR:CD2	3:C:137:ARG:NH2	2.09	1.20
1:A:1497:ILE:HD13	1:A:1569:LEU:HD22	1.18	1.17
3:C:128:TYR:CD2	3:C:137:ARG:CZ	2.27	1.17
1:A:361:ASP:OD1	1:A:927:GLU:HA	1.43	1.15
1:A:286:LEU:HD11	1:A:333:ILE:HD13	1.14	1.13
3:C:33:THR:HB	3:C:51:THR:HB	1.28	1.12
1:A:1497:ILE:CD1	1:A:1569:LEU:HD22	1.79	1.11
3:C:59:ASN:HB2	3:C:62:GLN:HB2	1.15	1.09
1:A:1305:GLU:HG2	1:A:1308:ARG:NH1	1.67	1.08
1:A:89:ILE:CG2	1:A:99:ARG:HD3	1.82	1.08
1:A:799:ASP:O	1:A:803:TYR:HB3	1.54	1.06
1:A:967:LEU:HD21	1:A:1454:GLY:CA	1.86	1.05
3:C:63:PHE:HE2	3:C:105:PRO:HB3	1.21	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG23	1:A:293:LEU:HD23	1.31	1.04
1:A:799:ASP:HB3	1:A:800:PRO:CD	1.87	1.04
1:A:286:LEU:CD1	1:A:333:ILE:HD13	1.87	1.04
3:C:65:LEU:HD11	3:C:110:VAL:HB	1.38	1.03
1:A:89:ILE:HG22	1:A:99:ARG:HD3	1.39	1.03
3:C:101:PHE:CE2	3:C:103:GLY:O	2.11	1.03
1:A:273:HIS:HB3	1:A:315:CYS:SG	1.99	1.02
1:A:403:MET:CE	1:A:1767:THR:HG21	1.90	1.02
3:C:65:LEU:CD1	3:C:110:VAL:CB	2.39	1.01
1:A:290:MET:HG3	1:A:333:ILE:HD11	1.39	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:289:ILE:CG2	1:A:293:LEU:CD2	2.44	0.95
1:A:289:ILE:CG2	1:A:293:LEU:HD23	1.95	0.95
1:A:799:ASP:HB3	1:A:800:PRO:HD2	1.48	0.94
1:A:795:LEU:O	1:A:799:ASP:HA	1.69	0.92
1:A:967:LEU:HD21	1:A:1454:GLY:HA2	1.50	0.92
3:C:128:TYR:HD2	3:C:137:ARG:CZ	1.75	0.92
3:C:63:PHE:HE1	3:C:129:ILE:HG23	1.33	0.91
1:A:967:LEU:C	1:A:967:LEU:HD13	1.89	0.91
1:A:890:LYS:O	1:A:894:GLU:HG3	1.70	0.90
3:C:62:GLN:O	3:C:132:PRO:HD3	1.71	0.90
1:A:799:ASP:O	1:A:803:TYR:CB	2.21	0.89
3:C:59:ASN:CB	3:C:62:GLN:HB2	2.03	0.89
1:A:795:LEU:O	1:A:799:ASP:N	2.04	0.89
1:A:967:LEU:HD21	1:A:1454:GLY:HA3	1.55	0.88
1:A:1606:PRO:O	1:A:1610:ARG:HG3	1.74	0.88
1:A:290:MET:HG3	1:A:333:ILE:CD1	2.03	0.87
3:C:32:VAL:CG1	3:C:50:CYS:SG	2.63	0.87
1:A:1748:PHE:HB2	6:A:2302:G2E:C17	2.05	0.86
1:A:321:SER:HB3	1:A:375:GLY:HA2	1.55	0.86
3:C:66:ASN:HD21	3:C:79:MET:HE1	1.38	0.86
1:A:275:CYS:SG	1:A:315:CYS:HB3	2.17	0.85
1:A:361:ASP:OD1	1:A:926:GLY:O	1.93	0.85
3:C:66:ASN:ND2	3:C:79:MET:CE	2.40	0.85
3:C:63:PHE:CE2	3:C:105:PRO:HB3	2.10	0.85
3:C:69:TYR:HE2	3:C:94:ARG:NH1	1.75	0.85
1:A:286:LEU:HD11	1:A:333:ILE:CD1	2.05	0.85
3:C:59:ASN:HB2	3:C:62:GLN:CB	2.03	0.84
1:A:1305:GLU:HG2	1:A:1308:ARG:HH12	1.44	0.83
3:C:33:THR:O	3:C:50:CYS:HA	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:HD21	1:A:220:ARG:CD	1.90	0.82
1:A:139:ASN:ND2	1:A:220:ARG:HD3	1.93	0.82
3:C:65:LEU:HD12	3:C:110:VAL:CB	2.08	0.82
1:A:372:ARG:HA	1:A:1678:MET:HE1	1.60	0.82
1:A:795:LEU:O	1:A:799:ASP:CA	2.27	0.81
1:A:403:MET:HE3	1:A:1767:THR:HG21	1.62	0.81
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.43	0.81
1:A:379:MET:SD	1:A:1689:ILE:HG12	2.21	0.81
1:A:59:LEU:HD21	1:A:63:TYR:HB2	1.63	0.81
1:A:1497:ILE:HD13	1:A:1569:LEU:CD2	2.06	0.81
3:C:128:TYR:CG	3:C:137:ARG:NH2	2.49	0.80
1:A:290:MET:CG	1:A:333:ILE:HD11	2.11	0.80
3:C:47:ARG:O	3:C:49:PRO:HD3	1.81	0.79
3:C:66:ASN:HD21	3:C:79:MET:CE	1.95	0.79
3:C:33:THR:O	3:C:51:THR:N	2.15	0.79
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.65	0.78
3:C:110:VAL:HG21	3:C:129:ILE:HD11	1.65	0.77
1:A:361:ASP:OD1	1:A:927:GLU:CA	2.30	0.76
3:C:62:GLN:O	3:C:132:PRO:HD2	1.85	0.76
3:C:32:VAL:HA	3:C:51:THR:O	1.85	0.76
3:C:69:TYR:CE2	3:C:94:ARG:NH1	2.53	0.75
1:A:388:LEU:O	1:A:392:TYR:HB3	1.86	0.75
3:C:33:THR:HB	3:C:51:THR:CB	2.14	0.75
1:A:289:ILE:CG2	1:A:293:LEU:HD21	2.14	0.75
1:A:293:LEU:CD1	1:A:299:PHE:CE1	2.69	0.74
1:A:1340:VAL:O	1:A:1344:ALA:HB2	1.87	0.74
3:C:58:VAL:HG13	3:C:63:PHE:HB2	1.69	0.74
3:C:101:PHE:HE2	3:C:103:GLY:O	1.70	0.74
3:C:103:GLY:O	3:C:105:PRO:HD3	1.87	0.74
1:A:293:LEU:HD12	1:A:299:PHE:CE1	2.23	0.73
1:A:967:LEU:HD13	1:A:967:LEU:O	1.88	0.73
3:C:71:GLU:HG3	3:C:94:ARG:HH12	1.53	0.72
1:A:967:LEU:CD2	1:A:1454:GLY:HA3	2.18	0.72
3:C:65:LEU:HD13	3:C:110:VAL:HB	1.67	0.72
3:C:66:ASN:ND2	3:C:79:MET:HE1	2.04	0.72
3:C:59:ASN:HD22	3:C:62:GLN:HG3	1.55	0.72
3:C:65:LEU:HD12	3:C:110:VAL:CG1	2.20	0.72
1:A:251:LEU:HD13	1:A:1630:ILE:HG23	1.72	0.71
1:A:289:ILE:HG22	1:A:293:LEU:CD2	2.20	0.71
1:A:289:ILE:HG22	1:A:293:LEU:HD21	1.73	0.70
1:A:1384:ASN:HD22	1:A:1385:LEU:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:LEU:HD12	1:A:960:LEU:O	1.91	0.70
1:A:967:LEU:C	1:A:967:LEU:CD1	2.61	0.70
1:A:1602:TYR:HD2	1:A:1603:PHE:CE2	2.10	0.69
3:C:33:THR:CB	3:C:51:THR:HB	2.14	0.69
3:C:55:CYS:SG	3:C:56:TYR:CZ	2.85	0.69
3:C:66:ASN:ND2	3:C:79:MET:HE2	2.07	0.69
3:C:52:PHE:CD2	3:C:129:ILE:HD13	2.26	0.69
3:C:71:GLU:CG	3:C:94:ARG:HH12	2.06	0.69
1:A:784:THR:HB	1:A:838:ARG:HH21	1.58	0.69
1:A:1324:VAL:HG21	1:A:1455:VAL:HG11	1.75	0.69
3:C:33:THR:N	3:C:51:THR:O	2.27	0.68
1:A:1358:ARG:NH2	1:A:1417:ASP:OD2	2.26	0.68
1:A:405:TYR:CD2	1:A:968:LEU:HD12	2.29	0.67
1:A:1625:LYS:O	1:A:1631:ARG:NH2	2.27	0.67
3:C:34:VAL:HG23	3:C:142:ILE:HG12	1.76	0.67
3:C:34:VAL:HG12	3:C:50:CYS:SG	2.34	0.67
3:C:65:LEU:C	3:C:65:LEU:HD23	2.15	0.67
3:C:32:VAL:HG13	3:C:50:CYS:SG	2.33	0.66
1:A:1719:LYS:H	1:A:1728:GLY:H	1.44	0.66
1:A:799:ASP:HB3	1:A:800:PRO:HD3	1.75	0.66
1:A:403:MET:HE1	1:A:1767:THR:HG21	1.77	0.66
3:C:65:LEU:CD1	3:C:110:VAL:CG1	2.74	0.66
1:A:293:LEU:HD13	1:A:299:PHE:CD1	2.29	0.66
1:A:1584:VAL:O	1:A:1588:ILE:HG13	1.95	0.66
1:A:1676:ASN:OD1	1:A:1676:ASN:N	2.23	0.66
1:A:403:MET:CE	1:A:1767:THR:CG2	2.71	0.65
1:A:1672:GLU:HB2	1:A:1706:PRO:HB3	1.78	0.65
1:A:1381:ARG:NH2	1:A:1714:ASP:OD1	2.30	0.65
1:A:166:GLU:OE1	1:A:223:LYS:NZ	2.30	0.65
1:A:909:HIS:HD2	1:A:911:ASN:H	1.45	0.64
3:C:65:LEU:HD12	3:C:110:VAL:HG11	1.77	0.64
1:A:231:LEU:HD22	1:A:872:VAL:HG23	1.78	0.64
1:A:908:TRP:HE1	1:A:1413:TYR:HH	1.45	0.64
1:A:1614:LEU:HD23	1:A:1614:LEU:O	1.96	0.64
1:A:293:LEU:CD1	1:A:299:PHE:CD1	2.80	0.64
2:B:42:SER:O	2:B:125:ARG:NH2	2.31	0.64
1:A:410:GLN:O	1:A:414:GLU:HG2	1.97	0.64
1:A:927:GLU:OE2	1:A:1408:TRP:NE1	2.29	0.64
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.80	0.64
1:A:273:HIS:CE1	1:A:317:PHE:HE2	2.16	0.63
1:A:372:ARG:CA	1:A:1678:MET:HE1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:THR:HB	1:A:838:ARG:NH2	2.14	0.63
1:A:285:THR:HG22	1:A:286:LEU:N	2.14	0.63
3:C:32:VAL:HG12	3:C:50:CYS:SG	2.37	0.63
1:A:866:LEU:HD12	1:A:966:LEU:HD23	1.80	0.63
1:A:25:GLN:HE21	1:A:29:GLU:HG3	1.64	0.62
1:A:54:GLU:HB2	1:A:57:LYS:HD2	1.81	0.62
1:A:1675:ILE:HG22	1:A:1675:ILE:O	2.00	0.62
3:C:34:VAL:CG2	3:C:142:ILE:HG12	2.30	0.62
1:A:286:LEU:CD1	1:A:333:ILE:CD1	2.71	0.62
1:A:1718:LYS:O	1:A:1718:LYS:HG3	2.00	0.62
1:A:372:ARG:NH2	1:A:1676:ASN:HD22	1.98	0.62
3:C:103:GLY:HA3	3:C:109:ASP:OD1	1.99	0.62
1:A:405:TYR:HD2	1:A:968:LEU:HD12	1.65	0.61
1:A:1350:CYS:H	1:A:1424:GLN:HE22	1.47	0.61
1:A:799:ASP:CB	1:A:800:PRO:CD	2.65	0.61
3:C:65:LEU:HD21	3:C:67:TRP:CD1	2.35	0.61
1:A:403:MET:HE1	1:A:1767:THR:CG2	2.30	0.61
3:C:105:PRO:HA	3:C:109:ASP:O	2.01	0.61
2:B:71:LEU:HA	2:B:80:LEU:HA	1.81	0.61
1:A:271:LEU:HD21	1:A:370:THR:HG22	1.81	0.61
1:A:1631:ARG:NE	7:A:2303:6OU:O25	2.34	0.60
2:B:44:LYS:NZ	2:B:100:ASP:OD2	2.30	0.60
3:C:62:GLN:C	3:C:132:PRO:HD2	2.21	0.60
3:C:55:CYS:SG	3:C:56:TYR:CE1	2.95	0.59
3:C:59:ASN:O	3:C:63:PHE:N	2.30	0.59
1:A:1180:ASN:O	1:A:1184:THR:HG23	2.03	0.59
1:A:139:ASN:ND2	1:A:220:ARG:CD	2.60	0.59
3:C:65:LEU:HD21	3:C:67:TRP:HD1	1.67	0.59
1:A:120:ILE:O	1:A:124:VAL:HG22	2.03	0.58
1:A:101:ASN:HD22	1:A:180:GLU:H	1.51	0.58
1:A:1697:SER:HB3	6:A:2302:G2E:C09	2.32	0.58
1:A:888:PHE:O	1:A:892:TYR:HD1	1.86	0.58
1:A:1588:ILE:HG22	1:A:1615:ALA:HB1	1.84	0.58
1:A:1661:PHE:O	1:A:1665:ASN:ND2	2.36	0.58
1:A:967:LEU:HD11	1:A:971:PHE:CZ	2.39	0.58
1:A:89:ILE:HG23	1:A:99:ARG:HD3	1.83	0.58
1:A:1651:LEU:HD22	1:A:1751:VAL:CG2	2.34	0.58
3:C:101:PHE:CZ	3:C:103:GLY:O	2.56	0.58
1:A:1449:LEU:O	1:A:1453:ILE:HG12	2.04	0.58
4:E:1:NAG:H3	4:E:1:NAG:H83	1.86	0.58
1:A:889:GLY:O	1:A:911:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:SER:HB2	1:A:1459:ASN:HD22	1.68	0.57
1:A:1679:PHE:CD1	1:A:1689:ILE:HG21	2.39	0.57
1:A:367:TYR:OH	1:A:379:MET:HG3	2.04	0.57
1:A:371:LEU:HD12	1:A:1679:PHE:CE1	2.39	0.57
1:A:357:LEU:HD23	1:A:363:TRP:HB2	1.87	0.57
1:A:832:SER:OG	1:A:835:ARG:NH2	2.38	0.57
1:A:890:LYS:O	1:A:894:GLU:CG	2.49	0.57
1:A:1329:LEU:O	1:A:1396:TYR:OH	2.19	0.57
1:A:274:LYS:N	1:A:315:CYS:SG	2.78	0.57
1:A:411:ALA:O	1:A:415:GLU:HG2	2.05	0.57
1:A:1186:TYR:HA	1:A:1247:ALA:HB1	1.87	0.57
3:C:65:LEU:HD23	3:C:65:LEU:O	2.04	0.56
1:A:24:GLU:HA	1:A:27:ILE:HD12	1.88	0.56
1:A:761:MET:HE1	1:A:838:ARG:HD3	1.87	0.56
1:A:967:LEU:CD2	1:A:1454:GLY:CA	2.70	0.56
1:A:281:GLU:OE2	1:A:281:GLU:N	2.38	0.56
1:A:1305:GLU:CG	1:A:1308:ARG:HH12	2.17	0.56
1:A:1602:TYR:CD2	1:A:1603:PHE:CZ	2.94	0.56
2:B:21:CYS:HG	2:B:43:CYS:HG	0.95	0.55
3:C:63:PHE:CE1	3:C:129:ILE:HG23	2.25	0.55
3:C:107:LYS:O	3:C:108:TYR:HB2	2.06	0.55
2:B:116:SER:HB3	2:B:146:VAL:HG12	1.88	0.55
1:A:881:ALA:O	1:A:916:SER:OG	2.23	0.55
1:A:1624:VAL:O	1:A:1631:ARG:HG3	2.07	0.55
1:A:1232:ILE:HD11	2:B:163:MET:HA	1.89	0.55
1:A:139:ASN:HD21	1:A:220:ARG:HD2	1.69	0.55
1:A:1408:TRP:HD1	1:A:1408:TRP:H	1.55	0.55
1:A:1577:GLY:HA2	1:A:1580:ILE:HD12	1.89	0.55
1:A:371:LEU:HD12	1:A:1679:PHE:HE1	1.69	0.55
1:A:354:LEU:N	1:A:354:LEU:HD12	2.22	0.54
1:A:1384:ASN:ND2	1:A:1385:LEU:H	2.04	0.54
3:C:44:SER:O	3:C:117:VAL:HG22	2.07	0.54
3:C:61:LYS:HG2	3:C:85:MET:CE	2.38	0.54
1:A:238:LEU:CD2	1:A:958:VAL:HG22	2.37	0.54
1:A:1343:PHE:HE1	1:A:1433:MET:HG3	1.72	0.54
1:A:1709:ASN:HB2	1:A:1714:ASP:HB3	1.90	0.54
1:A:350:ALA:O	1:A:354:LEU:HD13	2.07	0.54
1:A:733:PHE:HE2	1:A:796:ILE:HD12	1.73	0.54
1:A:1679:PHE:O	1:A:1690:CYS:SG	2.65	0.54
1:A:290:MET:HG3	1:A:333:ILE:CG1	2.38	0.54
1:A:322:GLY:HA3	1:A:323:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HG22	1:A:797:ALA:HB2	1.89	0.53
1:A:1597:ASP:O	1:A:1601:THR:HG23	2.07	0.53
3:C:33:THR:O	3:C:50:CYS:CA	2.55	0.53
1:A:1377:SER:OG	1:A:1378:GLN:N	2.41	0.53
1:A:1467:LEU:HD22	1:A:1472:ILE:HG22	1.91	0.53
1:A:1679:PHE:CE1	1:A:1689:ILE:HG21	2.44	0.53
1:A:321:SER:HB3	1:A:375:GLY:CA	2.31	0.53
1:A:833:VAL:HG22	1:A:1342:LEU:HD21	1.90	0.53
1:A:882:VAL:HG23	1:A:885:MET:HE3	1.91	0.53
1:A:1499:ARG:HD3	1:A:1509:PHE:CE2	2.43	0.53
1:A:1707:ILE:HD13	1:A:1740:PHE:HE2	1.72	0.53
3:C:62:GLN:HB3	3:C:132:PRO:HD2	1.90	0.53
1:A:1426:LYS:HB2	1:A:1429:TYR:HB2	1.89	0.53
2:B:71:LEU:HD21	2:B:106:ILE:HD12	1.90	0.53
1:A:101:ASN:O	1:A:116:ARG:NH2	2.41	0.53
1:A:1184:THR:HG21	2:B:182:TYR:HA	1.91	0.53
1:A:1542:HIS:O	1:A:1546:VAL:HG23	2.09	0.53
6:A:2302:G2E:C17	6:A:2302:G2E:C16	2.86	0.53
1:A:1602:TYR:HD2	1:A:1603:PHE:CZ	2.27	0.53
3:C:131:ASN:O	3:C:134:ASP:HB3	2.09	0.52
1:A:1679:PHE:CD1	1:A:1689:ILE:CG2	2.92	0.52
1:A:1712:PRO:HG3	1:A:1717:PRO:HD3	1.91	0.52
1:A:396:LEU:HD11	1:A:1633:LEU:HB3	1.91	0.52
1:A:1221:THR:O	1:A:1225:ILE:HG23	2.09	0.52
3:C:41:LEU:HD23	3:C:147:LEU:HB2	1.90	0.52
1:A:389:GLY:O	1:A:393:LEU:HB2	2.10	0.52
1:A:967:LEU:HD11	1:A:971:PHE:CE1	2.45	0.52
1:A:366:LEU:O	1:A:370:THR:HG23	2.10	0.51
1:A:800:PRO:O	1:A:804:PHE:HD2	1.92	0.51
1:A:1679:PHE:HD1	1:A:1689:ILE:CG2	2.23	0.51
1:A:1497:ILE:HD11	1:A:1569:LEU:HD22	1.83	0.51
2:B:113:TYR:HA	2:B:146:VAL:HG11	1.91	0.51
3:C:47:ARG:NH2	3:C:111:SER:OG	2.43	0.51
3:C:61:LYS:HG2	3:C:85:MET:HE1	1.92	0.51
1:A:799:ASP:O	1:A:803:TYR:HB2	2.09	0.51
1:A:1458:ASP:O	1:A:1462:GLN:HG2	2.11	0.51
1:A:1595:LEU:O	1:A:1599:ILE:HG13	2.11	0.51
1:A:360:GLN:NE2	1:A:390:SER:OG	2.44	0.51
1:A:1211:PHE:HB2	1:A:1226:LEU:HD11	1.93	0.51
1:A:1605:SER:OG	1:A:1608:LEU:HB3	2.10	0.51
3:C:52:PHE:CG	3:C:129:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1558:PHE:O	1:A:1561:GLU:HG3	2.11	0.51
1:A:1607:THR:O	1:A:1611:VAL:HG23	2.10	0.51
3:C:34:VAL:HG21	3:C:142:ILE:HG13	1.93	0.51
1:A:101:ASN:ND2	1:A:180:GLU:H	2.09	0.50
1:A:1673:ASP:N	1:A:1673:ASP:OD1	2.43	0.50
1:A:1679:PHE:HD1	1:A:1689:ILE:HG22	1.76	0.50
1:A:923:VAL:HG13	1:A:928:TRP:HB3	1.93	0.50
1:A:1753:ASN:HA	1:A:1756:ILE:CG2	2.42	0.50
1:A:1578:TRP:HH2	1:A:1624:VAL:HG23	1.75	0.50
1:A:74:PRO:HA	1:A:90:VAL:HG22	1.92	0.50
1:A:344:PHE:HE2	1:A:354:LEU:HD11	1.75	0.50
1:A:1522:MET:HA	1:A:1525:ILE:HD12	1.94	0.50
2:B:83:ASP:OD2	2:B:83:ASP:N	2.43	0.50
2:B:32:TYR:N	2:B:147:VAL:O	2.44	0.49
1:A:248:VAL:HG21	1:A:400:VAL:HG21	1.94	0.49
1:A:290:MET:CG	1:A:333:ILE:CD1	2.78	0.49
1:A:1668:TYR:CE2	1:A:1726:VAL:HG11	2.47	0.49
2:B:21:CYS:CB	2:B:43:CYS:HG	2.24	0.49
1:A:1640:SER:HB2	1:A:1758:VAL:HG12	1.94	0.49
2:B:40:CYS:HB3	2:B:104:LEU:O	2.11	0.49
3:C:128:TYR:HB3	3:C:137:ARG:HE	1.76	0.49
1:A:89:ILE:CG2	1:A:99:ARG:CD	2.74	0.49
1:A:1502:ASN:HB3	1:A:1505:GLN:HB2	1.93	0.49
1:A:286:LEU:HD11	1:A:333:ILE:HG21	1.93	0.49
3:C:52:PHE:CD1	3:C:52:PHE:C	2.85	0.49
1:A:801:TYR:O	1:A:805:GLN:HG2	2.13	0.49
1:A:1753:ASN:HA	1:A:1756:ILE:HG22	1.95	0.49
3:C:34:VAL:HG21	3:C:142:ILE:CG1	2.43	0.49
3:C:128:TYR:CE2	3:C:137:ARG:NH2	2.74	0.49
1:A:332:LYS:NZ	1:A:1537:GLU:OE2	2.33	0.49
1:A:1576:VAL:O	1:A:1580:ILE:HG13	2.13	0.48
2:B:112:THR:HG22	2:B:113:TYR:H	1.77	0.48
1:A:1384:ASN:HD21	1:A:1388:ASN:ND2	2.11	0.48
1:A:892:TYR:O	1:A:896:VAL:HG22	2.13	0.48
1:A:269:GLY:O	1:A:272:LYS:HB2	2.13	0.48
1:A:1588:ILE:HA	1:A:1591:VAL:HG22	1.95	0.48
2:B:89:ARG:O	2:B:89:ARG:HG3	2.13	0.48
1:A:146:ASN:ND2	1:A:911:ASN:O	2.47	0.48
1:A:1578:TRP:CH2	1:A:1624:VAL:HG23	2.48	0.48
1:A:762:ALA:HB2	1:A:1337:ILE:HD11	1.95	0.48
1:A:1580:ILE:O	1:A:1584:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:HG22	1:A:18:GLN:H	1.79	0.48
1:A:285:THR:CG2	1:A:286:LEU:N	2.76	0.48
1:A:371:LEU:HB2	1:A:1679:PHE:HZ	1.79	0.48
1:A:892:TYR:O	1:A:896:VAL:CG2	2.62	0.48
1:A:1442:ILE:O	1:A:1446:PHE:HB3	2.14	0.48
1:A:1757:ALA:O	1:A:1761:GLU:HG2	2.14	0.48
3:C:34:VAL:CG2	3:C:142:ILE:CG1	2.91	0.48
1:A:165:PHE:O	1:A:169:VAL:HG13	2.14	0.47
1:A:175:GLY:O	1:A:182:THR:OG1	2.28	0.47
1:A:182:THR:HG22	1:A:185:ARG:HG2	1.96	0.47
3:C:61:LYS:HA	3:C:85:MET:SD	2.54	0.47
1:A:238:LEU:HD21	1:A:958:VAL:HG22	1.96	0.47
1:A:936:MET:HG2	1:A:941:GLN:HA	1.97	0.47
2:B:21:CYS:SG	2:B:43:CYS:HB3	2.54	0.47
1:A:209:ASN:HB2	1:A:212:ALA:HB3	1.95	0.47
1:A:791:MET:HG2	1:A:816:VAL:HG11	1.96	0.47
1:A:403:MET:SD	1:A:1767:THR:HG21	2.55	0.47
1:A:163:TYR:O	1:A:166:GLU:HG3	2.13	0.47
1:A:265:GLN:HE21	1:A:1613:ARG:HB3	1.78	0.47
1:A:1602:TYR:CG	1:A:1602:TYR:O	2.68	0.47
3:C:34:VAL:HG23	3:C:35:PRO:N	2.29	0.47
1:A:90:VAL:HG21	1:A:120:ILE:HG21	1.96	0.47
2:B:58:THR:HG1	2:B:67:PHE:HD1	1.62	0.47
1:A:53:LEU:HD23	1:A:79:ASP:HB2	1.96	0.46
1:A:78:LEU:HD13	1:A:89:ILE:HD11	1.95	0.46
1:A:166:GLU:O	1:A:170:LYS:HG2	2.15	0.46
1:A:1286:ILE:HD13	1:A:1289:LEU:HD21	1.97	0.46
1:A:402:ALA:HB2	1:A:964:LEU:HD11	1.96	0.46
1:A:1651:LEU:HD22	1:A:1751:VAL:HG22	1.97	0.46
1:A:19:SER:O	1:A:23:ILE:HG12	2.16	0.46
1:A:234:ILE:HG13	1:A:868:ASN:HB3	1.97	0.46
1:A:361:ASP:OD1	1:A:926:GLY:C	2.54	0.46
1:A:896:VAL:HG11	1:A:904:THR:C	2.36	0.46
1:A:866:LEU:HD12	1:A:966:LEU:CD2	2.45	0.46
1:A:1502:ASN:HD22	1:A:1505:GLN:H	1.64	0.46
2:B:21:CYS:SG	2:B:43:CYS:CB	3.04	0.46
1:A:1232:ILE:HG13	2:B:163:MET:HG3	1.97	0.46
1:A:1258:TRP:HH2	1:A:1311:VAL:HG11	1.80	0.46
1:A:733:PHE:CE2	1:A:796:ILE:HD12	2.50	0.45
1:A:1529:MET:HG3	1:A:1620:ILE:HD13	1.98	0.45
1:A:1412:MET:O	1:A:1416:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:ILE:HD13	1:A:1740:PHE:CE2	2.51	0.45
1:A:164:THR:HG21	1:A:200:TYR:CZ	2.51	0.45
2:B:21:CYS:CB	2:B:43:CYS:SG	3.04	0.45
2:B:31:VAL:HG23	2:B:34:MET:HB2	1.98	0.45
3:C:41:LEU:HA	3:C:147:LEU:HB2	1.97	0.45
3:C:55:CYS:O	3:C:56:TYR:CG	2.70	0.45
1:A:286:LEU:CG	1:A:333:ILE:CD1	2.95	0.45
1:A:922:ARG:HG2	1:A:927:GLU:HB2	1.98	0.45
2:B:86:PHE:HB3	2:B:90:VAL:HG21	1.98	0.45
1:A:59:LEU:HD23	1:A:60:PRO:O	2.17	0.45
2:B:46:ARG:NE	2:B:48:GLU:OE2	2.26	0.45
1:A:276:PHE:CE2	1:A:280:LEU:HD11	2.52	0.45
3:C:52:PHE:CB	3:C:129:ILE:CD1	2.94	0.45
3:C:55:CYS:C	3:C:56:TYR:CG	2.90	0.45
1:A:1177:ILE:HD12	1:A:1177:ILE:H	1.82	0.45
3:C:128:TYR:HD2	3:C:137:ARG:NE	2.12	0.44
2:B:21:CYS:HB3	2:B:43:CYS:SG	2.57	0.44
1:A:919:ILE:O	1:A:923:VAL:HG23	2.18	0.44
3:C:131:ASN:O	3:C:134:ASP:N	2.51	0.44
3:C:63:PHE:HE1	3:C:129:ILE:CG2	2.16	0.44
1:A:286:LEU:HG	1:A:333:ILE:CD1	2.47	0.44
1:A:1216:ILE:HD12	1:A:1216:ILE:HA	1.89	0.44
1:A:1478:GLN:HE21	1:A:1642:PRO:HB3	1.83	0.44
3:C:52:PHE:CB	3:C:129:ILE:HD12	2.48	0.44
1:A:53:LEU:HD21	1:A:78:LEU:HB2	2.00	0.44
1:A:278:ASN:HD22	1:A:327:GLY:C	2.21	0.44
1:A:346:THR:HG22	1:A:1536:LYS:HB2	2.00	0.44
1:A:109:LEU:HD22	1:A:113:SER:OG	2.18	0.44
1:A:1764:SER:O	1:A:1768:GLU:HG3	2.17	0.44
3:C:34:VAL:HG23	3:C:35:PRO:O	2.18	0.44
3:C:55:CYS:O	3:C:56:TYR:CD2	2.70	0.44
1:A:82:TYR:CD2	1:A:99:ARG:NH2	2.85	0.44
1:A:1262:ASP:O	1:A:1266:VAL:HG23	2.18	0.44
1:A:1492:LYS:HE3	1:A:1492:LYS:HB3	1.75	0.44
1:A:71:VAL:HG21	1:A:93:LYS:HG3	2.00	0.43
1:A:896:VAL:HG11	1:A:904:THR:O	2.18	0.43
1:A:51:SER:HA	1:A:54:GLU:HG2	1.99	0.43
1:A:300:ARG:HA	1:A:305:TYR:CD2	2.53	0.43
1:A:1211:PHE:O	1:A:1216:ILE:HD13	2.18	0.43
1:A:1529:MET:O	1:A:1533:MET:HG3	2.19	0.43
1:A:1748:PHE:N	6:A:2302:G2E:C23	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HG22	1:A:1630:ILE:HD11	2.00	0.43
2:B:21:CYS:HG	2:B:43:CYS:CB	2.25	0.43
3:C:101:PHE:CZ	3:C:105:PRO:HD3	2.54	0.43
1:A:274:LYS:HD2	1:A:333:ILE:O	2.18	0.43
1:A:952:MET:O	1:A:956:ASN:HB2	2.17	0.43
2:B:134:HIS:CD2	2:B:136:THR:HG23	2.52	0.43
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.83	0.43
1:A:405:TYR:CE2	1:A:968:LEU:HD12	2.54	0.43
1:A:764:GLU:OE2	1:A:1341:ASN:ND2	2.52	0.43
1:A:960:LEU:HD12	1:A:960:LEU:C	2.28	0.43
1:A:1444:GLY:O	1:A:1448:THR:OG1	2.16	0.43
2:B:38:ILE:HD11	2:B:108:ILE:HD11	1.99	0.43
1:A:907:ARG:HA	1:A:907:ARG:HD2	1.55	0.43
1:A:910:MET:HG3	1:A:919:ILE:HD12	2.00	0.43
2:B:85:ARG:O	2:B:115:HIS:HE1	2.02	0.43
3:C:108:TYR:N	3:C:108:TYR:CD1	2.86	0.43
1:A:1656:PHE:O	1:A:1660:ILE:HG12	2.19	0.42
3:C:40:VAL:HG22	3:C:44:SER:OG	2.19	0.42
1:A:1443:PHE:O	1:A:1447:PHE:HB2	2.19	0.42
2:B:26:SER:OG	2:B:39:LEU:N	2.48	0.42
1:A:116:ARG:O	1:A:120:ILE:HG13	2.19	0.42
2:B:172:ILE:HA	2:B:175:VAL:HG22	2.01	0.42
3:C:103:GLY:C	3:C:105:PRO:HD3	2.40	0.42
1:A:799:ASP:CB	1:A:800:PRO:HD3	2.40	0.42
1:A:1590:ILE:HG13	1:A:1591:VAL:N	2.35	0.42
1:A:236:GLY:O	1:A:240:GLN:HG2	2.19	0.42
1:A:300:ARG:HG2	2:B:130:GLU:HG2	2.00	0.42
1:A:332:LYS:HG3	1:A:332:LYS:O	2.19	0.42
1:A:1416:VAL:HG11	1:A:1434:TYR:CD2	2.54	0.42
3:C:58:VAL:HG13	3:C:63:PHE:CB	2.46	0.42
1:A:92:ASN:OD1	1:A:93:LYS:N	2.52	0.42
1:A:734:LYS:HE3	1:A:734:LYS:HB2	1.78	0.42
1:A:1317:ALA:O	1:A:1321:ILE:HG12	2.20	0.42
1:A:1566:LEU:HD13	1:A:1566:LEU:HA	1.84	0.42
1:A:276:PHE:HE2	1:A:280:LEU:HD11	1.84	0.42
1:A:737:ILE:HD13	1:A:740:ILE:HD11	2.01	0.42
1:A:1485:MET:O	1:A:1488:LEU:HB2	2.19	0.42
1:A:1748:PHE:HB2	6:A:2302:G2E:C16	2.50	0.42
1:A:1224:ILE:HD13	1:A:1224:ILE:HA	1.97	0.42
1:A:22:LEU:O	1:A:26:ARG:NH1	2.53	0.41
1:A:1243:LEU:HD11	2:B:174:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1712:PRO:CG	1:A:1717:PRO:HD3	2.50	0.41
2:B:26:SER:HB2	2:B:39:LEU:O	2.20	0.41
1:A:1262:ASP:OD2	1:A:1303:ARG:NH2	2.53	0.41
1:A:1511:LEU:HD11	1:A:1564:LEU:HD21	2.03	0.41
3:C:52:PHE:HB3	3:C:129:ILE:CD1	2.50	0.41
1:A:274:LYS:HB3	1:A:303:PHE:HD2	1.86	0.41
3:C:107:LYS:O	3:C:107:LYS:HG2	2.21	0.41
1:A:315:CYS:CB	1:A:324:CYS:SG	3.09	0.41
1:A:1410:ILE:H	1:A:1410:ILE:HG13	1.70	0.41
1:A:1531:THR:O	1:A:1534:VAL:HG12	2.21	0.41
1:A:1756:ILE:HG23	1:A:1757:ALA:N	2.35	0.41
1:A:248:VAL:CG2	1:A:400:VAL:HG21	2.50	0.41
1:A:293:LEU:HD12	1:A:293:LEU:O	2.19	0.41
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.83	0.41
1:A:1354:THR:OG1	1:A:1355:ASP:N	2.53	0.41
1:A:325:PRO:HD3	2:B:46:ARG:HD3	2.03	0.41
1:A:838:ARG:H	1:A:838:ARG:HG3	1.49	0.41
2:B:64:THR:HG22	2:B:66:GLU:OE1	2.20	0.41
2:B:152:ARG:HD2	2:B:157:ILE:HB	2.03	0.41
1:A:273:HIS:CE1	1:A:317:PHE:CE2	3.04	0.41
3:C:103:GLY:O	3:C:105:PRO:CD	2.64	0.41
1:A:235:VAL:O	1:A:239:ILE:HG12	2.20	0.41
1:A:403:MET:O	1:A:407:GLU:HG2	2.21	0.41
1:A:1715:CYS:SG	1:A:1716:ASP:N	2.94	0.41
1:A:1748:PHE:CB	6:A:2302:G2E:C17	2.90	0.41
3:C:32:VAL:CA	3:C:51:THR:O	2.64	0.41
1:A:88:PHE:CE1	1:A:100:PHE:HB2	2.56	0.40
1:A:238:LEU:HD23	1:A:958:VAL:HG22	2.03	0.40
1:A:274:LYS:HG2	1:A:312:ALA:HB3	2.03	0.40
1:A:1348:TYR:HB3	1:A:1382:TRP:CE2	2.56	0.40
1:A:1581:PHE:O	1:A:1585:VAL:HG22	2.22	0.40
3:C:38:LEU:HD23	3:C:48:LEU:HD22	2.03	0.40
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.91	0.40
1:A:259:PHE:HB3	1:A:354:LEU:HD23	2.02	0.40
1:A:1350:CYS:N	1:A:1424:GLN:HE22	2.14	0.40
1:A:832:SER:HA	1:A:835:ARG:HB3	2.03	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	1220/2250 (54%)	1165 (96%)	54 (4%)	1 (0%)	51	83
2	B	171/481 (36%)	160 (94%)	11 (6%)	0	100	100
3	C	118/215 (55%)	109 (92%)	6 (5%)	3 (2%)	5	31
All	All	1509/2946 (51%)	1434 (95%)	71 (5%)	4 (0%)	44	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	56	TYR
3	C	76	SER
3	C	147	LEU
1	A	799	ASP

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	1094/1998 (55%)	1070 (98%)	24 (2%)	52	78
2	B	157/419 (38%)	154 (98%)	3 (2%)	57	80
3	C	112/193 (58%)	111 (99%)	1 (1%)	78	90
All	All	1363/2610 (52%)	1335 (98%)	28 (2%)	56	79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	166	GLU
1	A	217	ARG
1	A	311	ASP
1	A	362	TYR
1	A	364	GLU
1	A	772	PHE
1	A	838	ARG
1	A	907	ARG
1	A	935	CYS
1	A	944	CYS
1	A	961	ASN
1	A	1191	HIS
1	A	1331	PHE
1	A	1383	LYS
1	A	1384	ASN
1	A	1408	TRP
1	A	1452	PHE
1	A	1631	ARG
1	A	1676	ASN
1	A	1677	ASP
1	A	1701	ASP
1	A	1730	CYS
1	A	1755	TYR
2	B	93	ASN
2	B	113	TYR
2	B	132	TYR
3	C	52	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	139	ASN
1	A	146	ASN
1	A	278	ASN
1	A	323	GLN
1	A	360	GLN
1	A	395	ASN
1	A	412	ASN
1	A	757	ASN
1	A	909	HIS
1	A	911	ASN

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Mol	Chain	Res	Type
1	A	941	GLN
1	A	1256	ASN
1	A	1384	ASN
1	A	1424	GLN
1	A	1459	ASN
1	A	1502	ASN
1	A	1528	ASN
1	A	1579	ASN
1	A	1709	ASN
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	66	ASN
3	C	82	GLN
3	C	118	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.24	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	E	1	4,1	14,14,15	0.63	1 (7%)	17,19,21	1.38	2 (11%)
4	NAG	E	2	4	14,14,15	1.02	1 (7%)	17,19,21	1.19	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	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	3.60	1.49	1.43
4	E	1	NAG	O5-C1	-2.13	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C1-O5-C5	4.66	118.51	112.19
4	E	1	NAG	C2-N2-C7	4.35	129.10	122.90
4	E	1	NAG	C1-C2-N2	2.04	113.97	110.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-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	D	1	NAG	C4-C5-C6-O6

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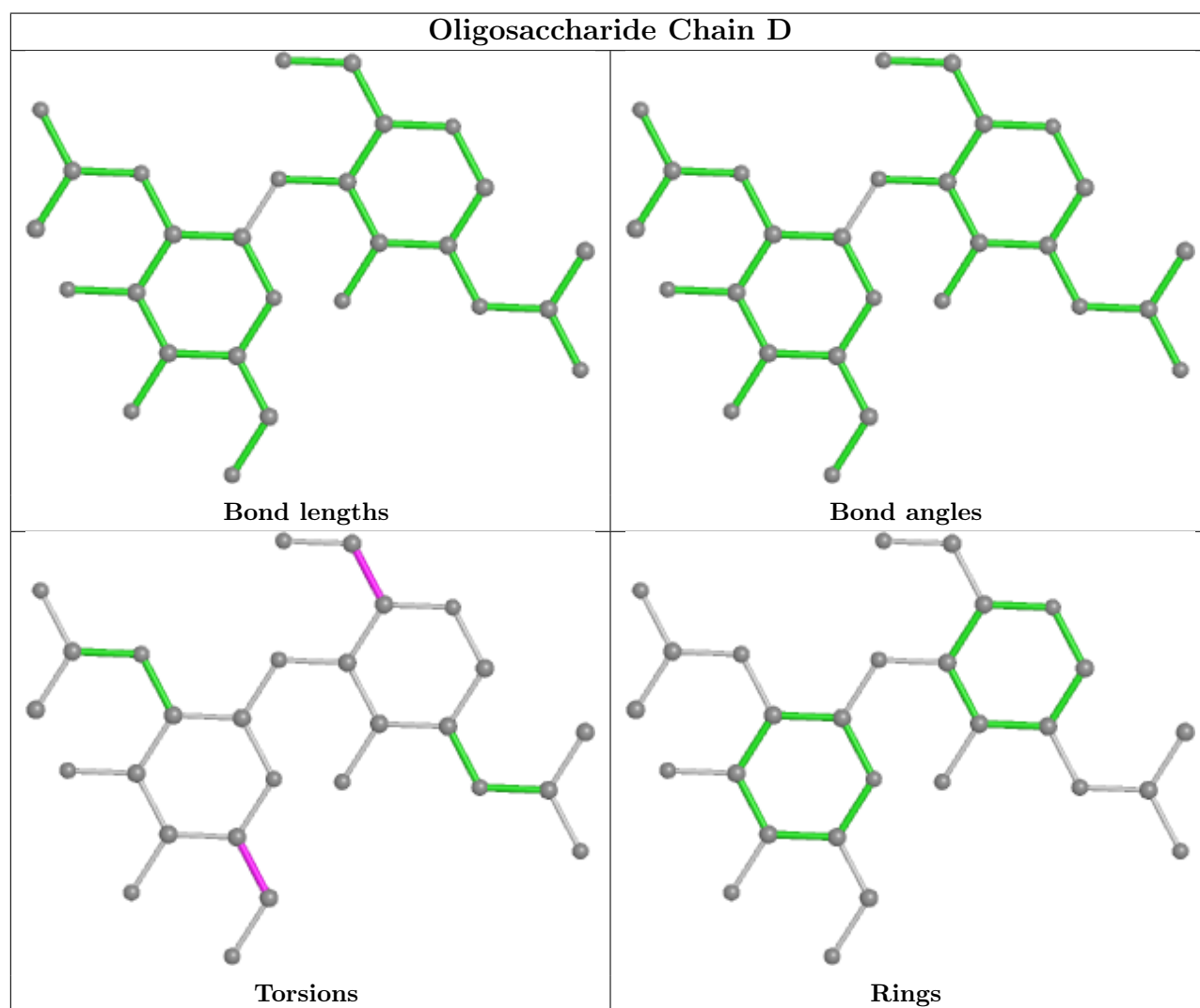
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C3-C2-N2-C7

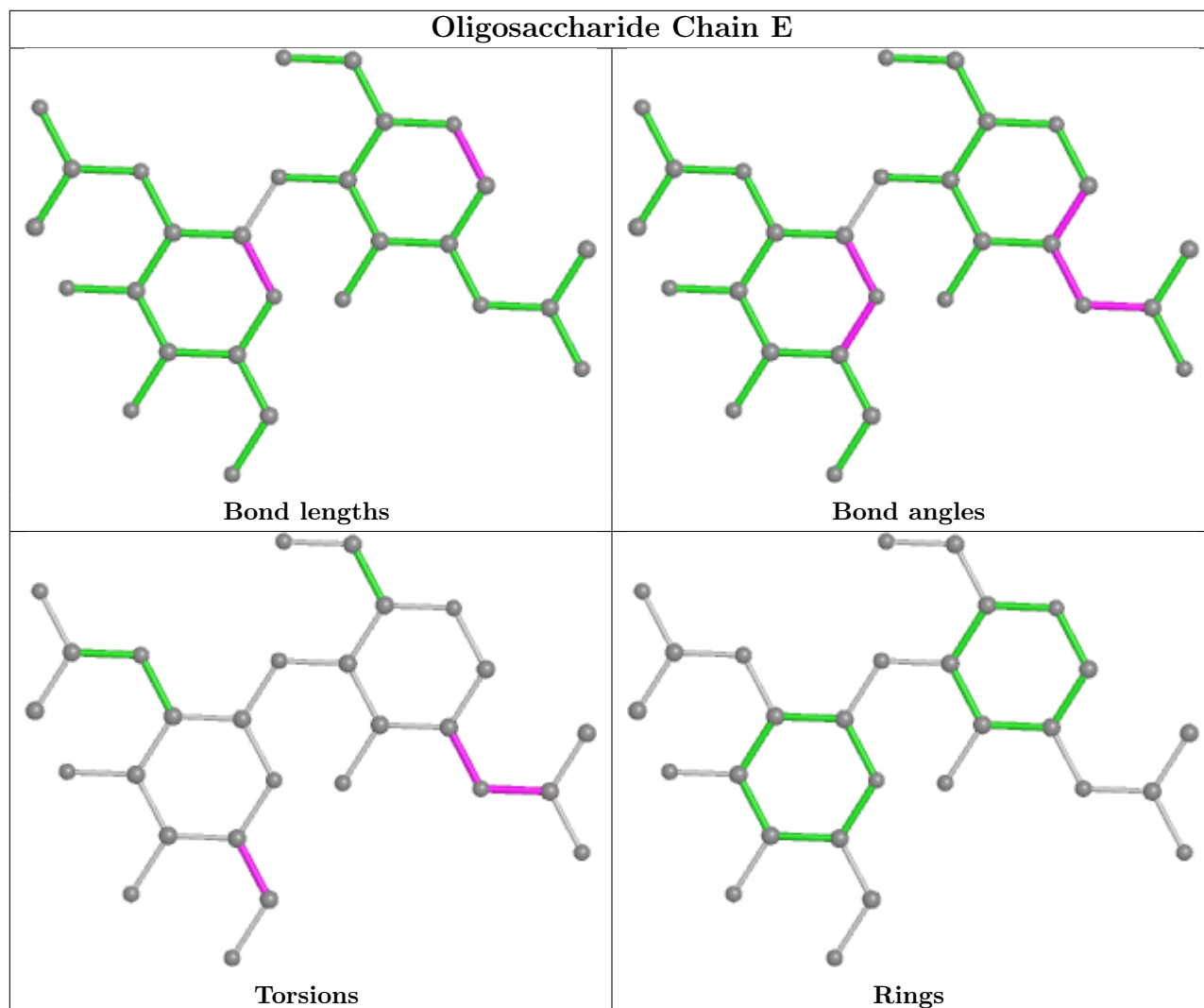
There are no ring outliers.

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	B	502	2	14,14,15	0.18	0	17,19,21	0.40	0
5	NAG	B	503	2	14,14,15	0.19	0	17,19,21	0.38	0
5	NAG	A	2301	1	14,14,15	0.31	0	17,19,21	0.47	0
5	NAG	B	504	2	14,14,15	0.19	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	6OU	A	2303	-	48,48,48	0.88	4 (8%)	51,53,53	1.19	2 (3%)
6	G2E	A	2302	-	29,30,30	6.71	21 (72%)	41,45,45	2.79	12 (29%)
5	NAG	B	501	2	14,14,15	0.19	0	17,19,21	0.40	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	B	502	2	-	0/6/23/26	0/1/1/1
5	NAG	B	503	2	-	2/6/23/26	0/1/1/1
5	NAG	A	2301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	504	2	-	1/6/23/26	0/1/1/1
7	6OU	A	2303	-	-	27/52/52/52	-
6	G2E	A	2302	-	-	4/5/43/43	0/5/5/5
5	NAG	B	501	2	-	1/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2302	G2E	C14-C08	13.24	1.59	1.39
6	A	2302	G2E	O01-C12	13.10	1.57	1.38
6	A	2302	G2E	C18-C12	11.98	1.60	1.38
6	A	2302	G2E	C10-N05	11.82	1.49	1.36
6	A	2302	G2E	C15-C07	10.58	1.53	1.39
6	A	2302	G2E	C11-C07	8.82	1.50	1.39
6	A	2302	G2E	C23-C17	8.07	1.55	1.38
6	A	2302	G2E	C17-C11	8.02	1.53	1.39
6	A	2302	G2E	C21-C15	7.61	1.54	1.38
6	A	2302	G2E	C14-C19	7.16	1.51	1.38
6	A	2302	G2E	O01-C09	-6.53	1.35	1.46
6	A	2302	G2E	C18-C20	6.29	1.50	1.38
6	A	2302	G2E	C11-N05	5.58	1.50	1.39
6	A	2302	G2E	O04-C20	5.33	1.46	1.38
6	A	2302	G2E	C23-C21	5.24	1.51	1.38
6	A	2302	G2E	C12-C08	-4.95	1.31	1.38
6	A	2302	G2E	O04-C25	-4.19	1.35	1.43
6	A	2302	G2E	C06-C10	-3.64	1.51	1.54
6	A	2302	G2E	O03-C25	2.62	1.48	1.43
7	A	2303	6OU	O18-C19	-2.55	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2303	6OU	O30-C20	-2.51	1.40	1.46
6	A	2302	G2E	C06-C07	-2.34	1.49	1.52
7	A	2303	6OU	O18-C16	2.23	1.39	1.33
6	A	2302	G2E	O03-C19	-2.16	1.34	1.38
7	A	2303	6OU	O30-C31	2.02	1.40	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2302	G2E	C07-C06-C10	12.01	107.97	101.67
6	A	2302	G2E	O01-C12-C08	-6.55	108.99	112.99
6	A	2302	G2E	C11-N05-C10	-5.25	108.17	111.16
7	A	2303	6OU	O30-C31-C33	4.13	120.40	111.50
6	A	2302	G2E	O04-C20-C18	3.53	132.57	127.85
6	A	2302	G2E	O03-C19-C14	3.52	132.55	127.85
6	A	2302	G2E	C09-C06-C07	3.42	120.68	114.16
6	A	2302	G2E	C08-C06-C10	3.28	116.99	110.44
6	A	2302	G2E	C07-C11-N05	-3.00	107.82	109.76
6	A	2302	G2E	C18-C12-C08	-2.82	119.88	123.39
7	A	2303	6OU	O18-C16-C15	2.75	120.55	111.91
6	A	2302	G2E	O01-C12-C18	2.45	131.13	127.85
6	A	2302	G2E	O04-C20-C19	-2.39	107.07	109.78
6	A	2302	G2E	C13-N05-C10	2.20	125.91	123.14

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2302	G2E	C16-C13-N05-C10
6	A	2302	G2E	C16-C13-N05-C11
7	A	2303	6OU	O30-C20-C21-O22
5	B	503	NAG	O5-C5-C6-O6
5	B	503	NAG	C4-C5-C6-O6
7	A	2303	6OU	C45-C46-C47-C48
7	A	2303	6OU	C15-C16-O18-C19
7	A	2303	6OU	C03-C04-C05-C06
7	A	2303	6OU	C33-C34-C35-C36
7	A	2303	6OU	C31-C33-C34-C35
7	A	2303	6OU	C05-C06-C07-C08
7	A	2303	6OU	C13-C14-C15-C16
7	A	2303	6OU	O17-C16-O18-C19
6	A	2302	G2E	C13-C16-C22-C24

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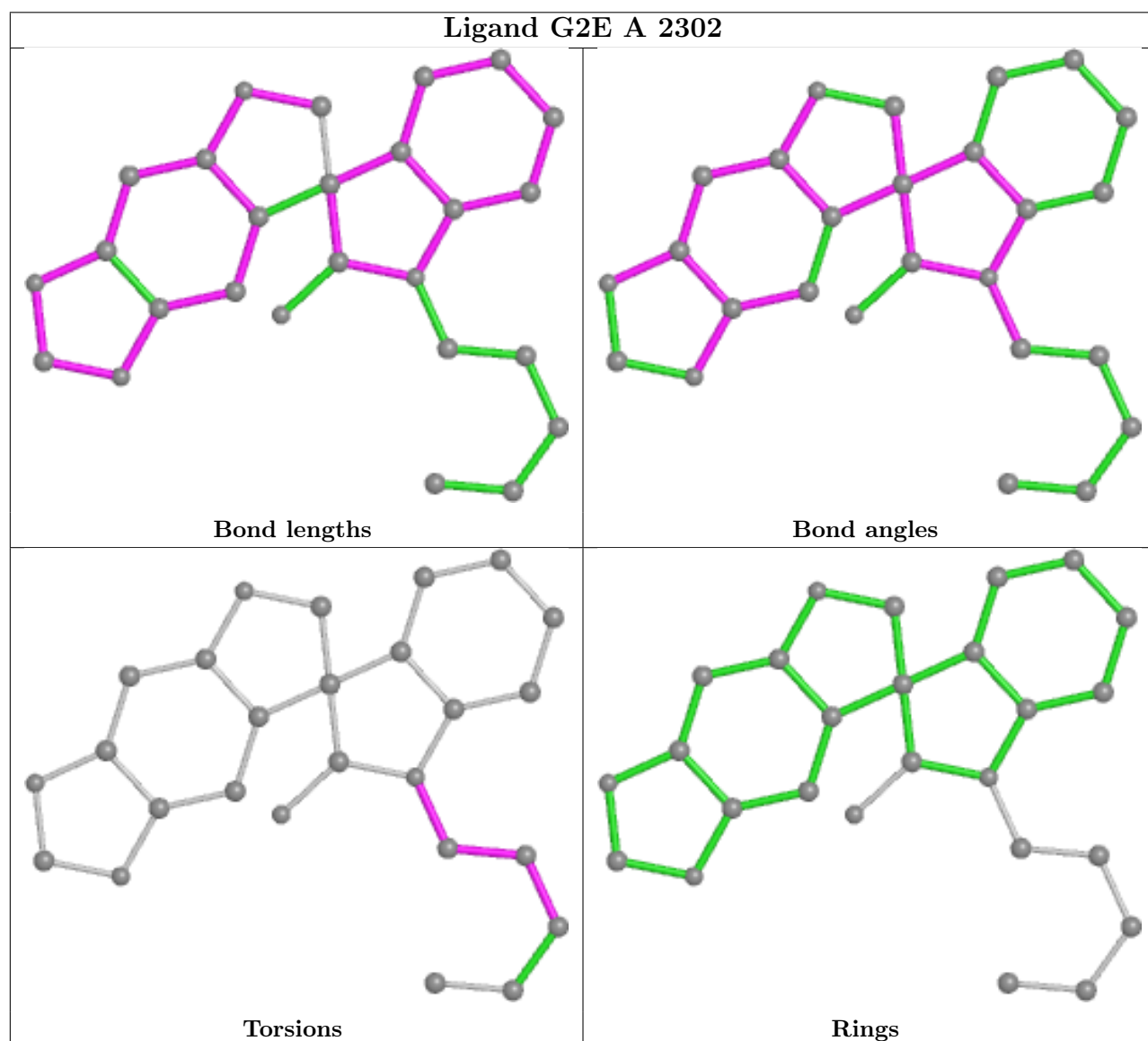
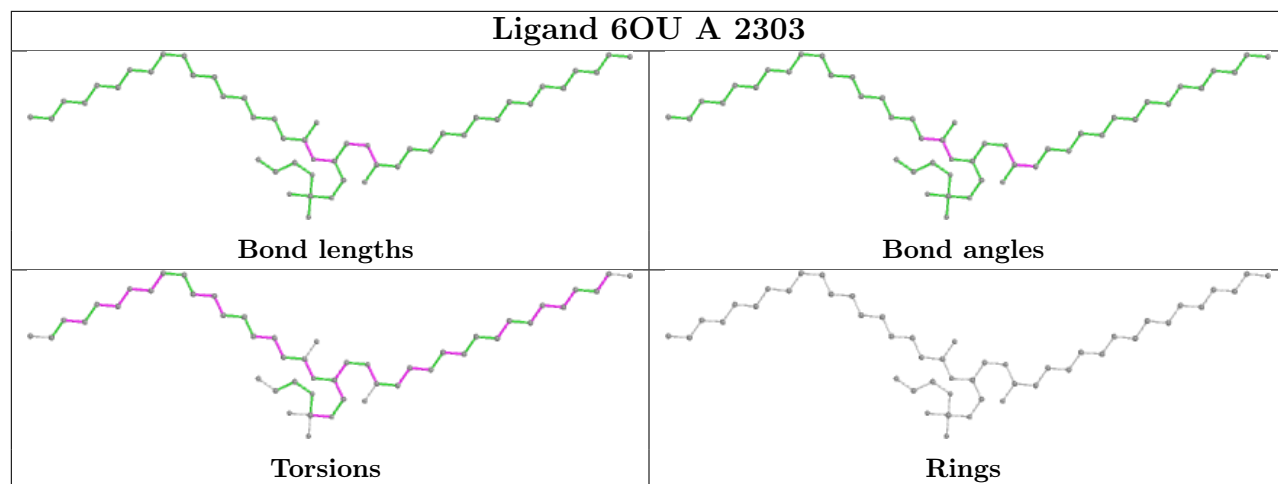
Mol	Chain	Res	Type	Atoms
7	A	2303	6OU	C41-C42-C43-C44
7	A	2303	6OU	C33-C31-O30-C20
7	A	2303	6OU	O32-C31-O30-C20
7	A	2303	6OU	C12-C13-C14-C15
7	A	2303	6OU	C01-C02-C03-C04
7	A	2303	6OU	C04-C05-C06-C07
7	A	2303	6OU	C43-C44-C45-C46
7	A	2303	6OU	C19-C20-C21-O22
7	A	2303	6OU	C36-C37-C38-C39
7	A	2303	6OU	C42-C43-C44-C45
7	A	2303	6OU	O18-C19-C20-C21
6	A	2302	G2E	N05-C13-C16-C22
7	A	2303	6OU	O18-C19-C20-O30
7	A	2303	6OU	C10-C11-C12-C13
7	A	2303	6OU	C07-C08-C09-C10
7	A	2303	6OU	C21-O22-P23-O26
7	A	2303	6OU	C37-C38-C39-C40
5	B	504	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
7	A	2303	6OU	C40-C41-C42-C43
7	A	2303	6OU	C21-O22-P23-O24

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2303	6OU	1	0
6	A	2302	G2E	6	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

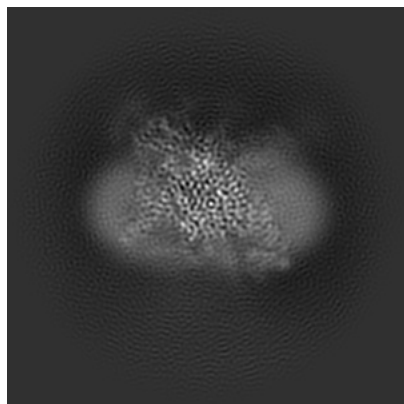
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33292. These allow visual inspection of the internal detail of the map and identification of artifacts.

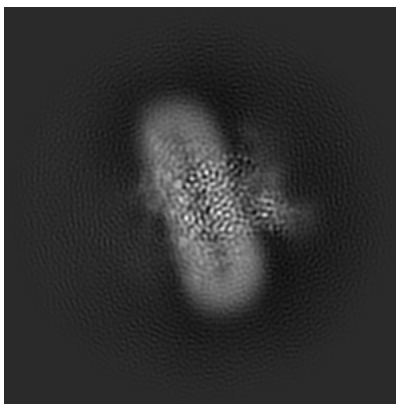
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

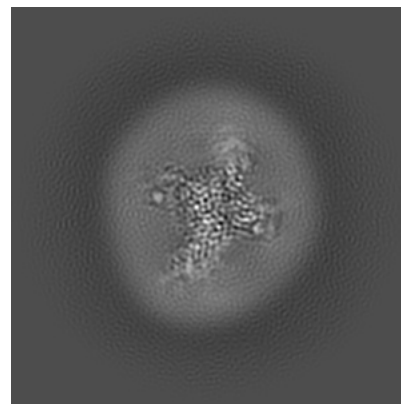
6.1.1 Primary map



X

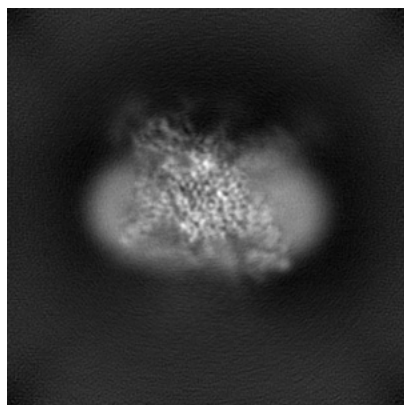


Y

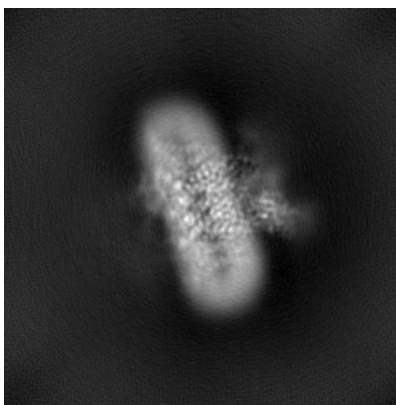


Z

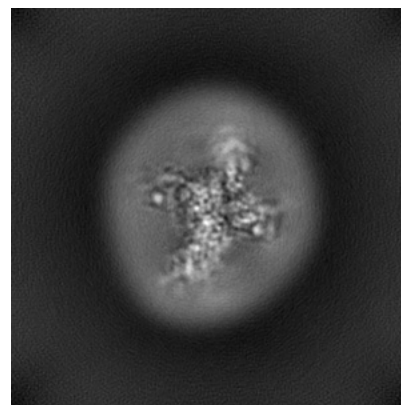
6.1.2 Raw map



X



Y

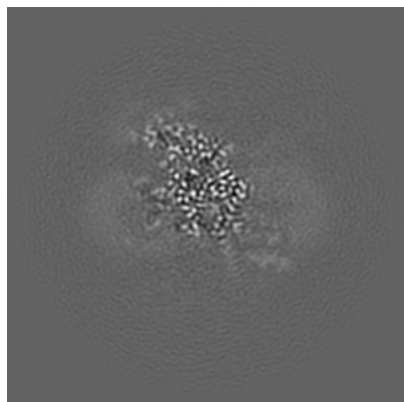


Z

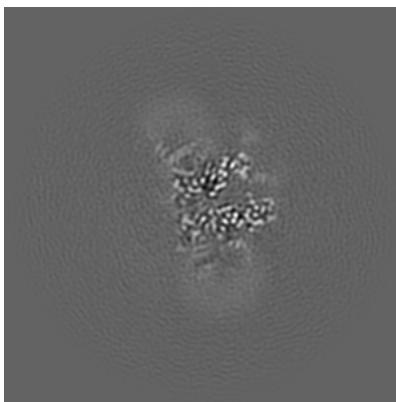
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

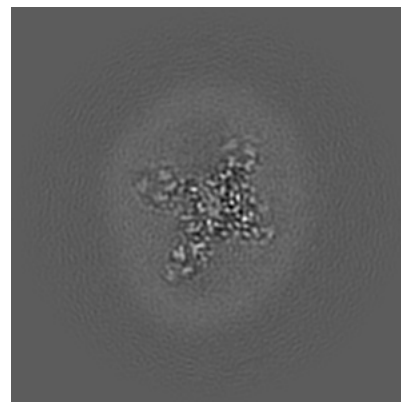
6.2.1 Primary map



X Index: 128

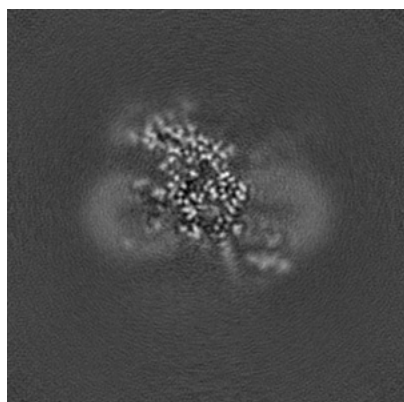


Y Index: 128

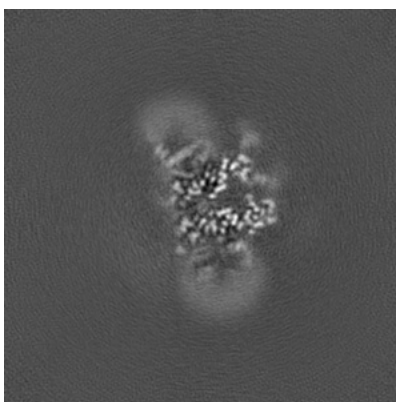


Z Index: 128

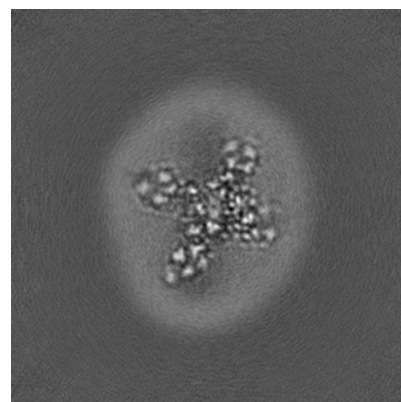
6.2.2 Raw map



X Index: 128



Y Index: 128

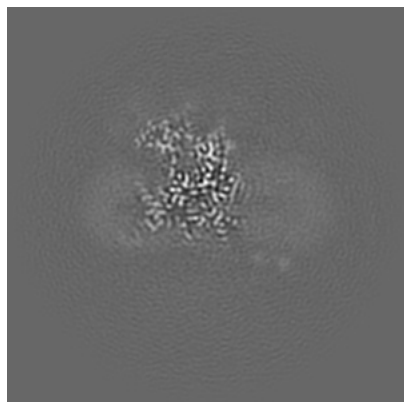


Z Index: 128

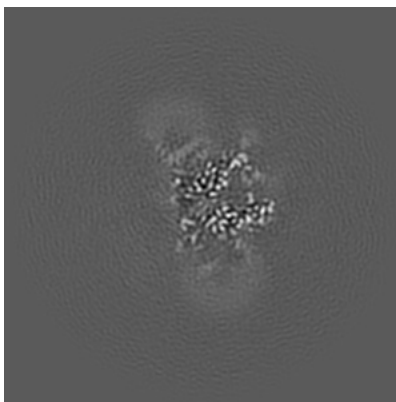
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

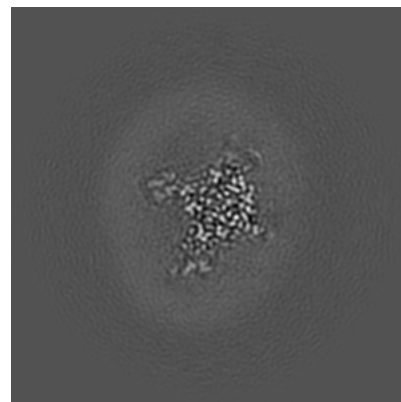
6.3.1 Primary map



X Index: 122

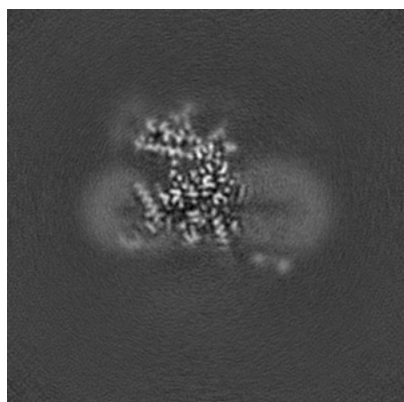


Y Index: 127

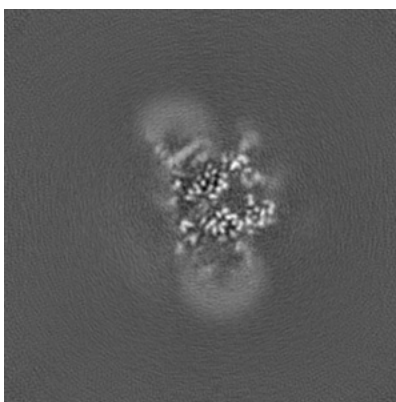


Z Index: 134

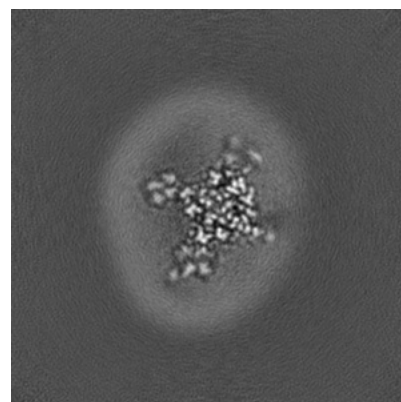
6.3.2 Raw map



X Index: 123



Y Index: 127

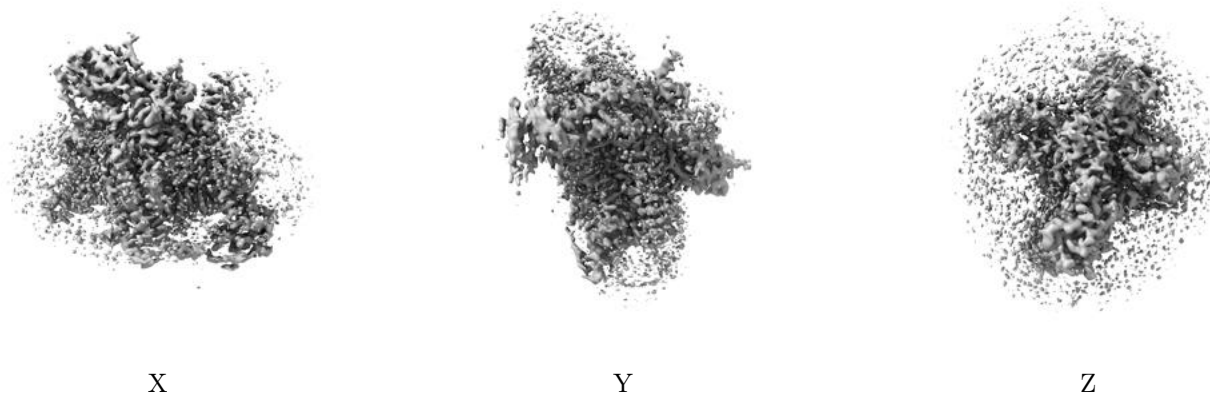


Z Index: 134

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.402. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

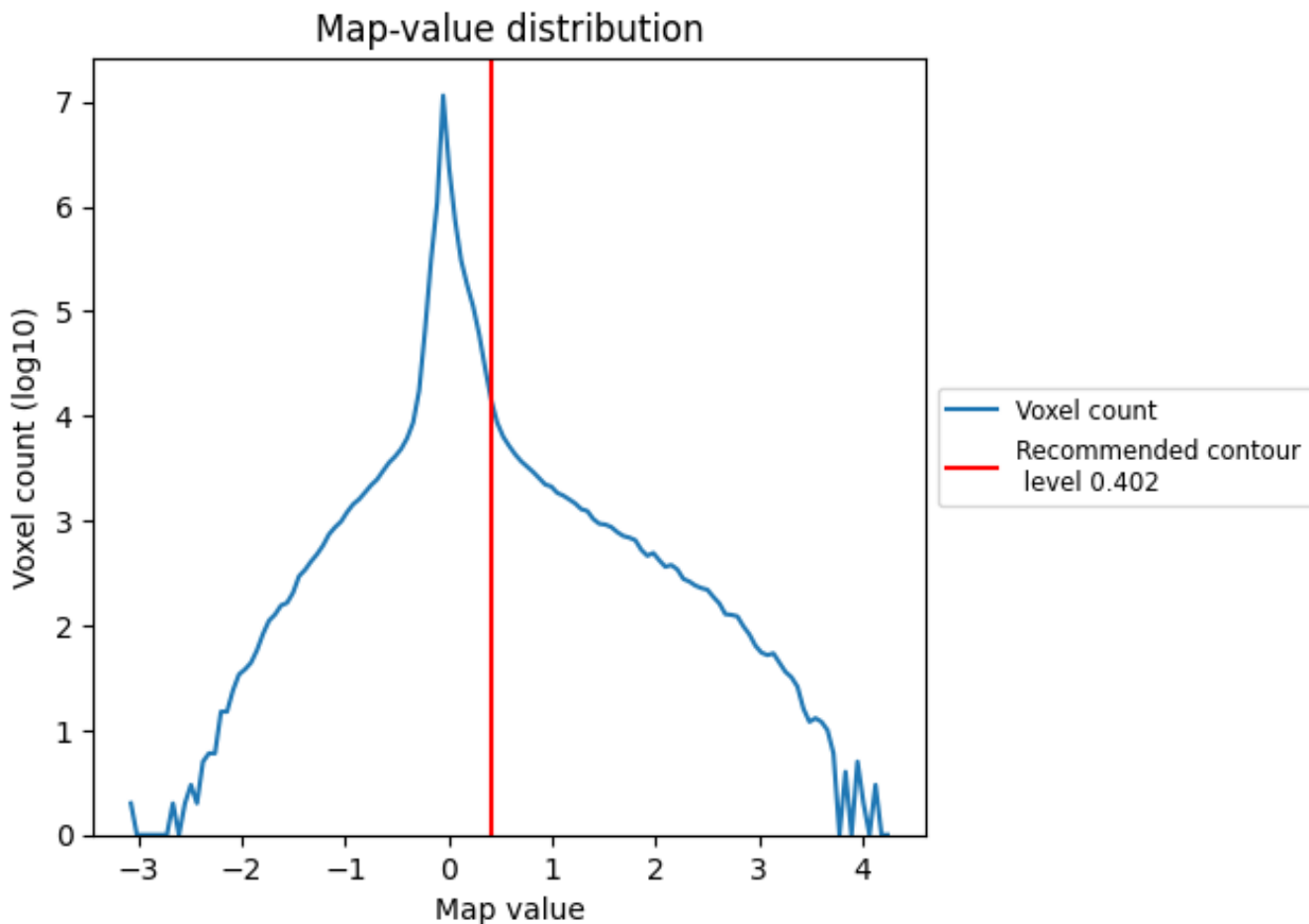
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

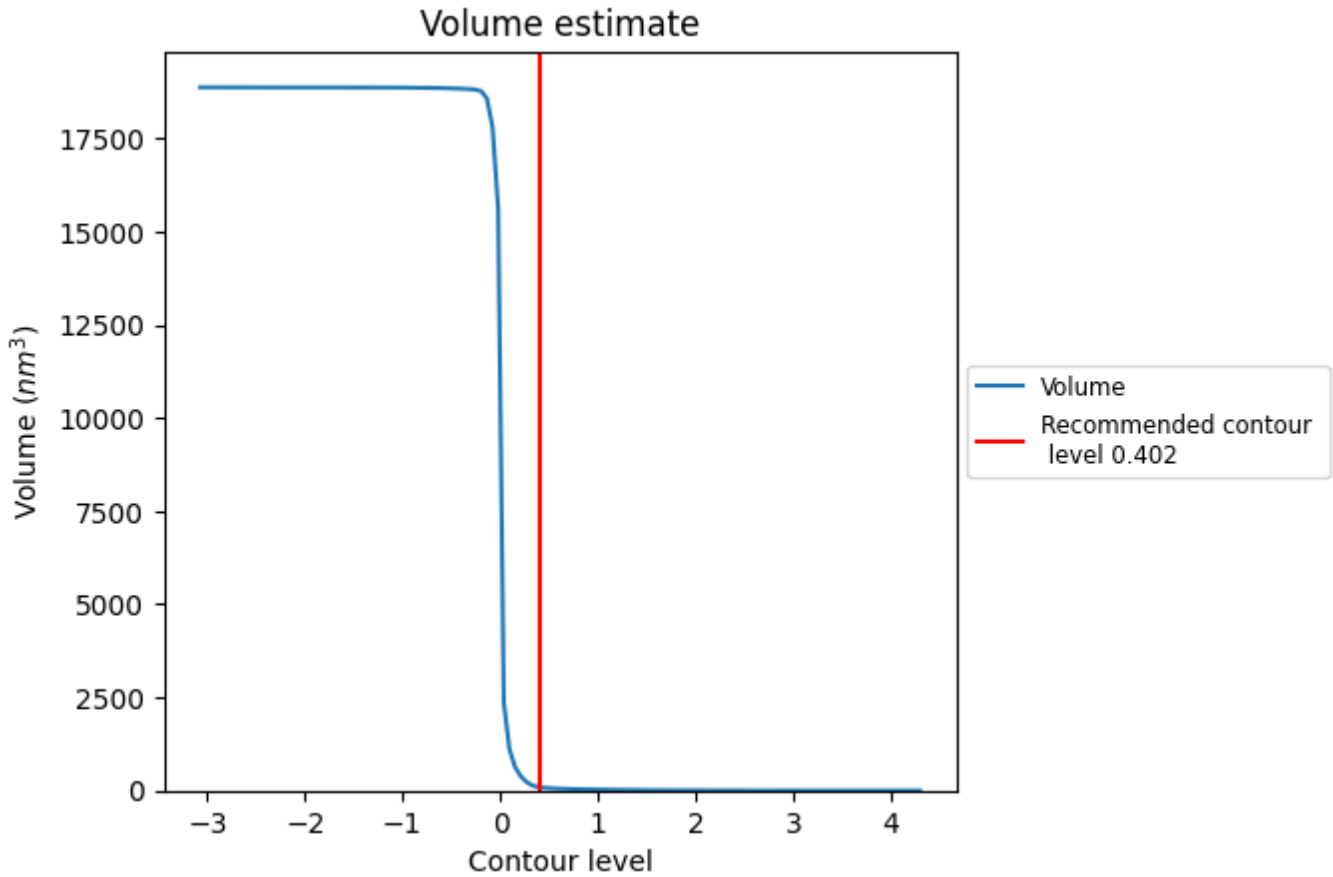
This section contains the results of statistical analysis of the map.

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.

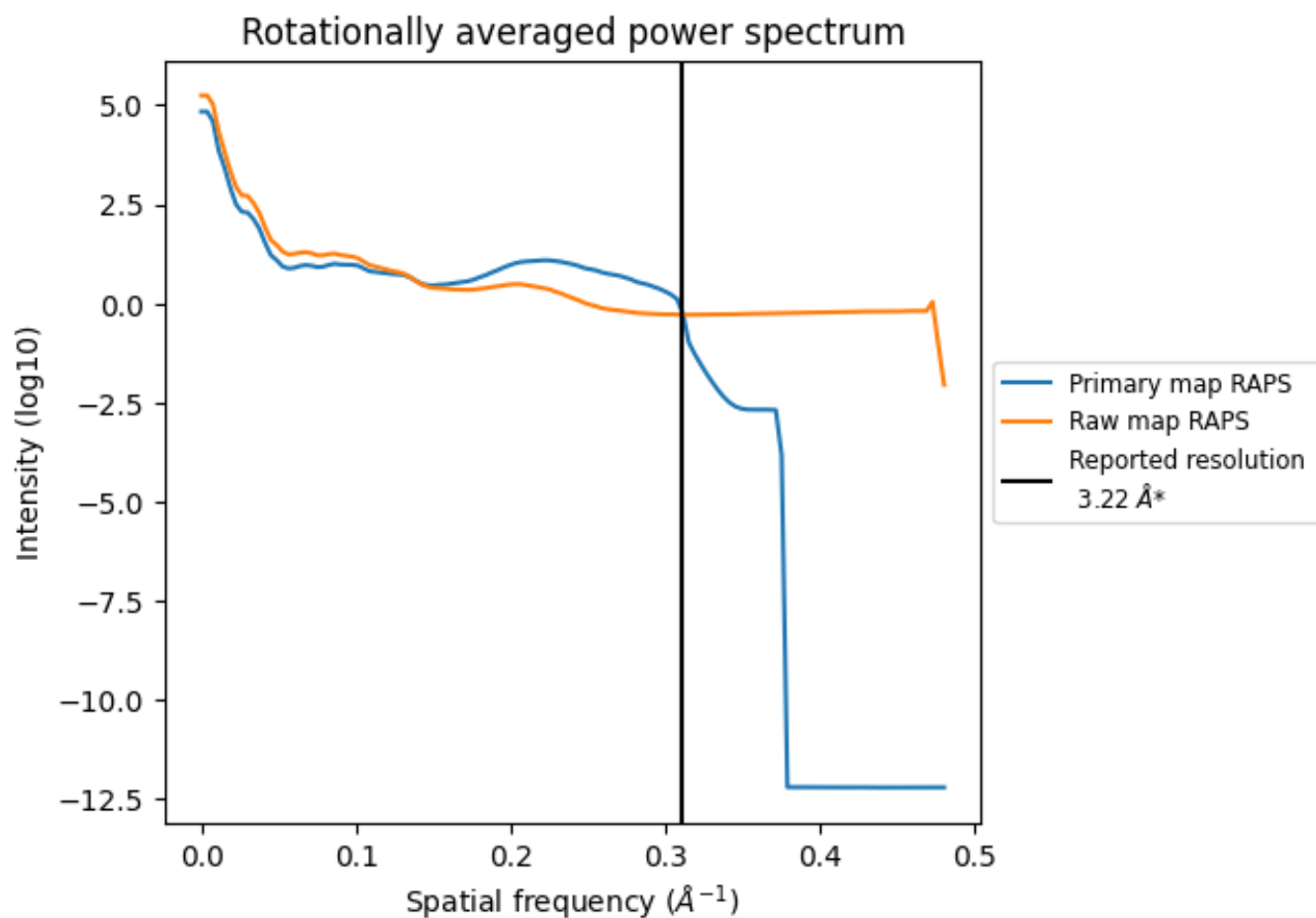
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 82 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

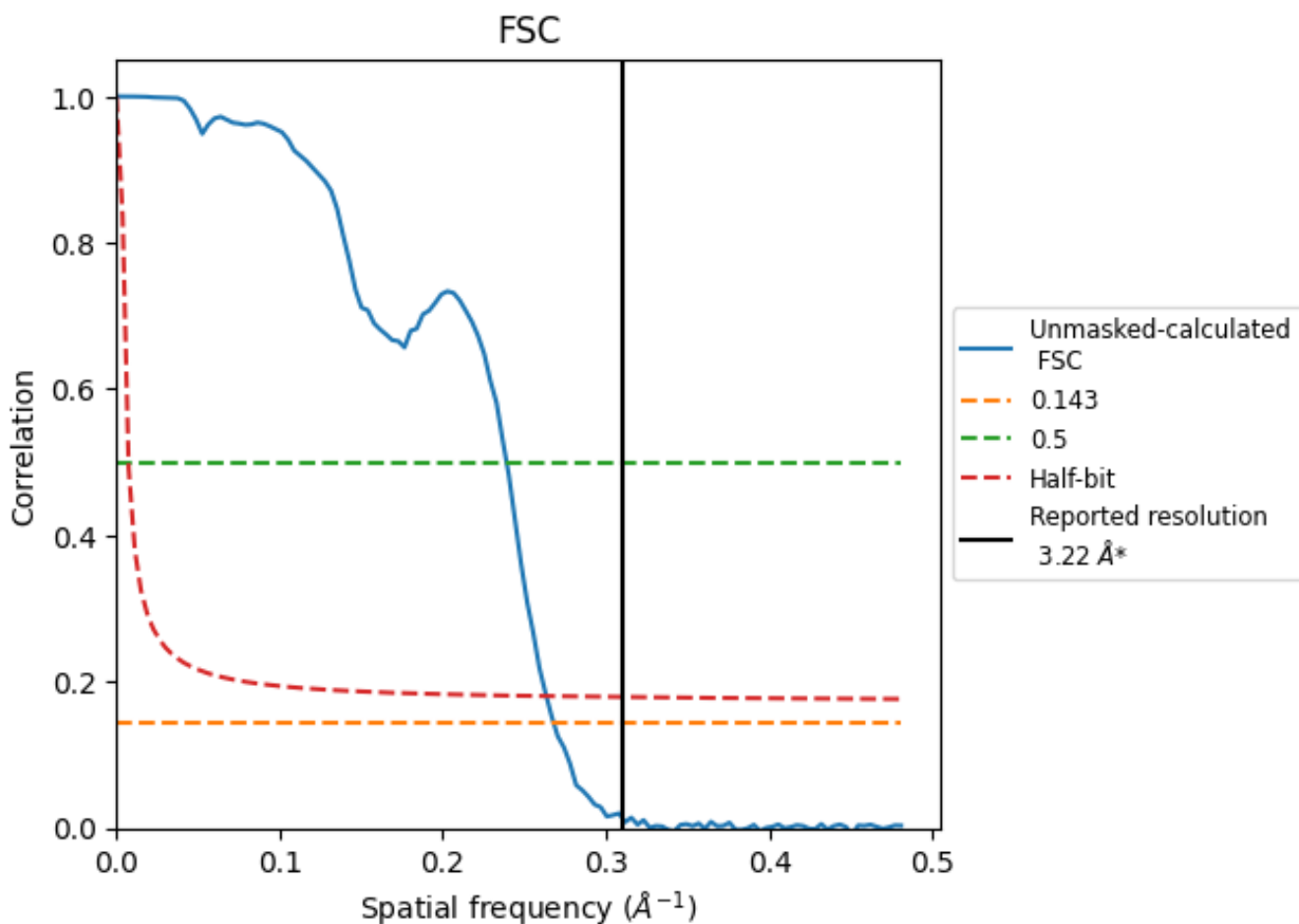


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

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 0.311 Å⁻¹

8.2 Resolution estimates [i](#)

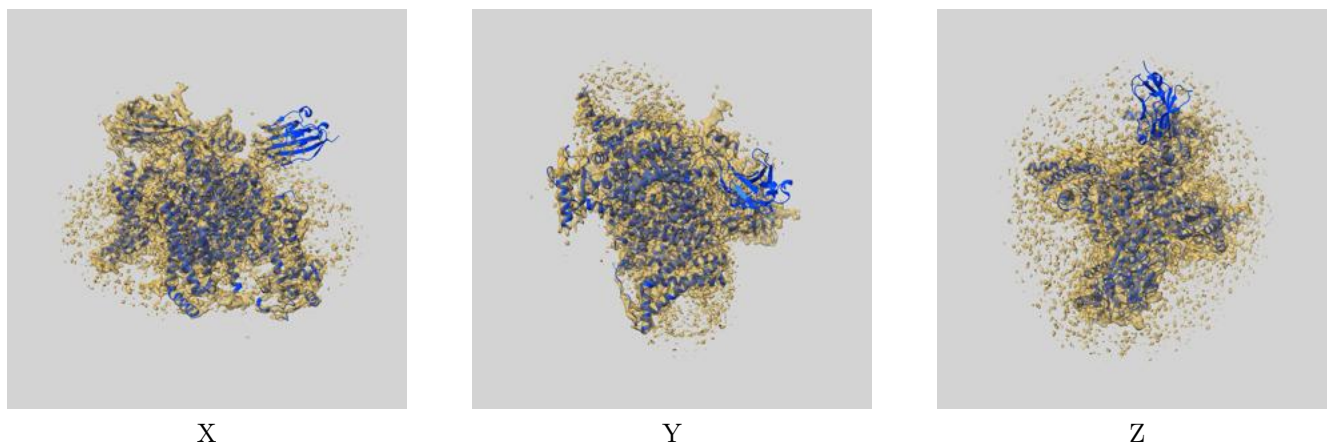
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.18	3.80

*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 3.73 differs from the reported value 3.22 by more than 10 %

9 Map-model fit [i](#)

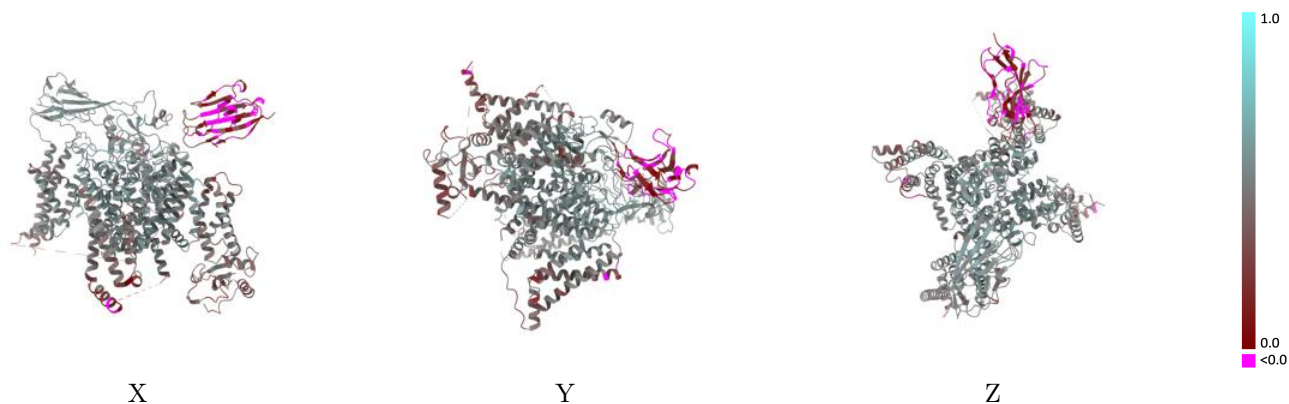
This section contains information regarding the fit between EMDB map EMD-33292 and PDB model 7XM9. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



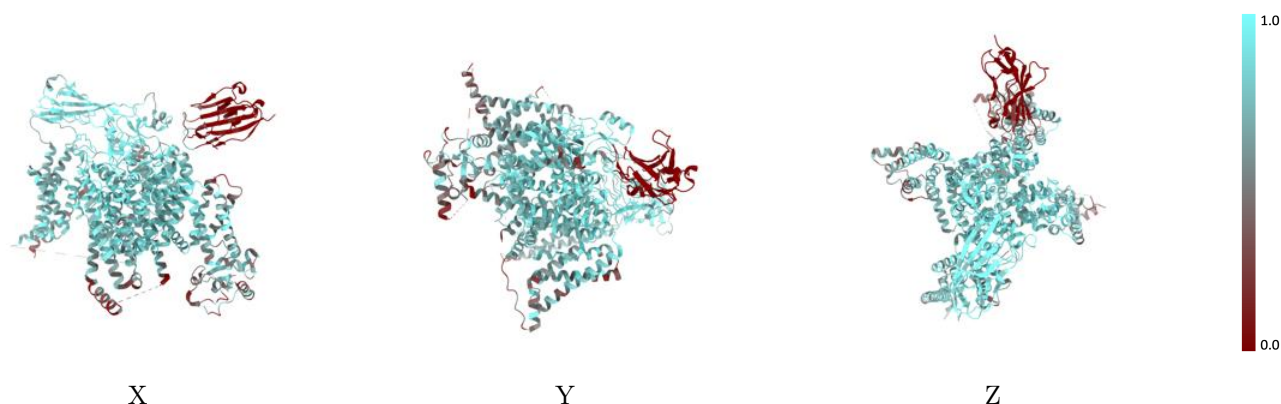
The images above show the 3D surface view of the map at the recommended contour level 0.402 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



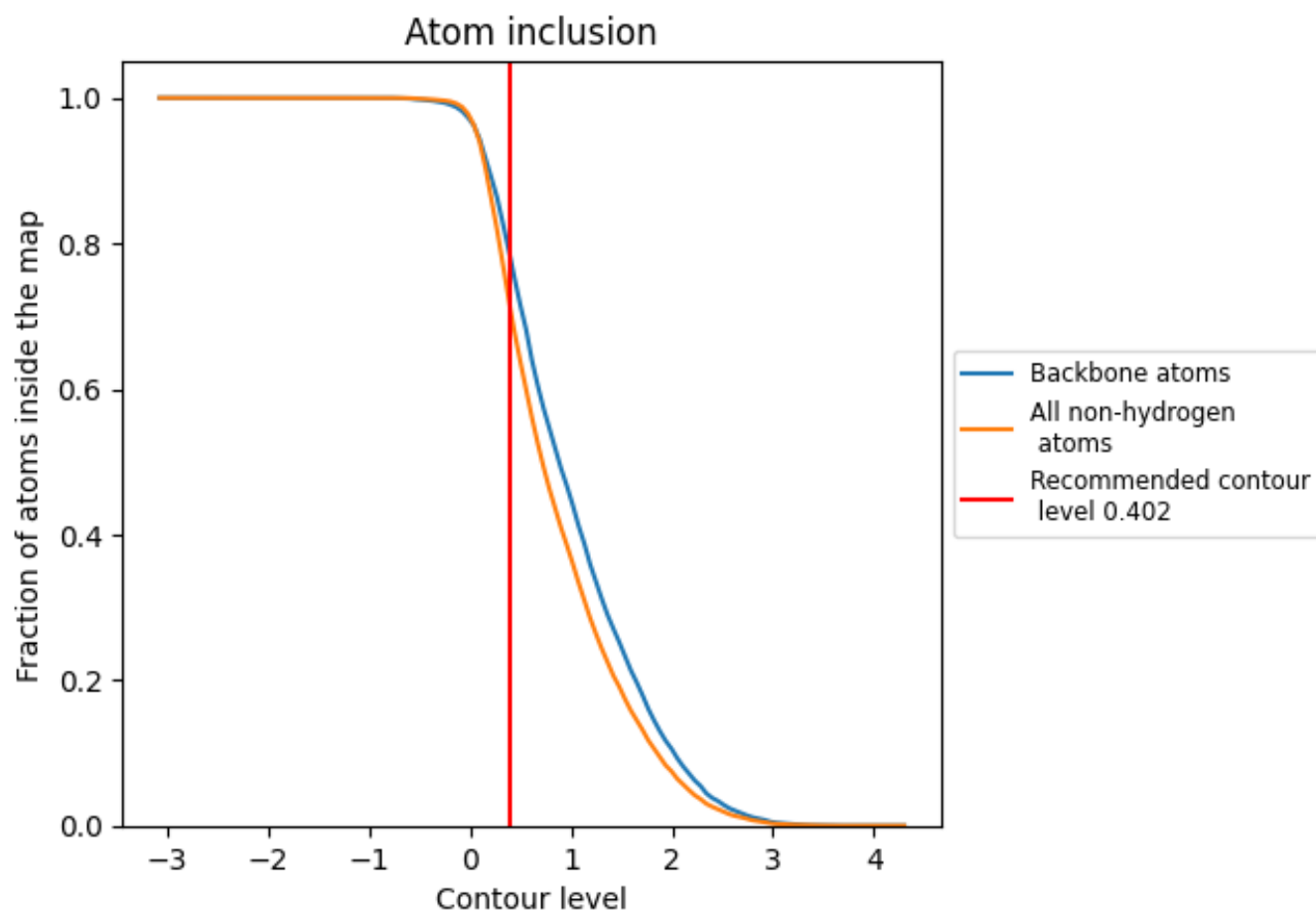
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.402).













9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.402) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7083	 0.4490
A	 0.7581	 0.4800
B	 0.7864	 0.4950
C	 0.0784	 0.0740
D	 0.7500	 0.4270
E	 0.7143	 0.4340

