



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 02:02 AM EDT

PDB ID : 8D87
EMDB ID : EMD-27248
Title : Fitted crystal structure of the homotrimer of fusion glycoprotein E1 from SFV into subtomogram averaged CHIKV E1 glycoprotein density
Authors : Mangala Prasad, V.; Lee, K.K.
Deposited on : 2022-06-08
Resolution : 27.20 Å(reported)
Based on initial model : 1RER

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

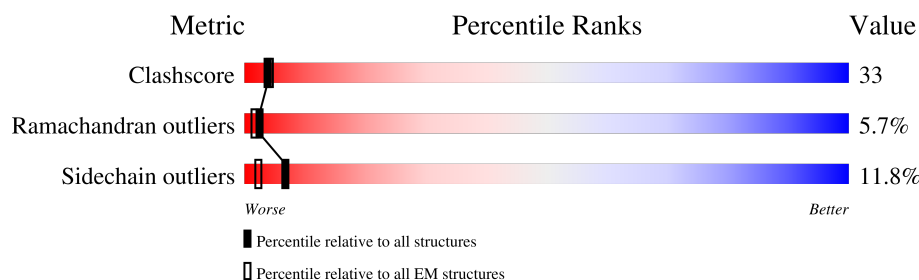
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 27.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	<div> <div>21%</div> <div>51%</div> <div>40%</div> <div>8%</div> </div>
1	B	391	<div> <div>19%</div> <div>50%</div> <div>39%</div> <div>9%</div> </div>
1	C	391	<div> <div>15%</div> <div>51%</div> <div>40%</div> <div>8%</div> </div>
2	D	6	<div> <div>83%</div> <div>50%</div> <div>50%</div> </div>
3	E	7	<div> <div>86%</div> <div>29%</div> <div>71%</div> </div>
4	F	2	<div> <div>50%</div> <div>100%</div> </div>

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
3	FUC	E	7	X	-	-	-

2 Entry composition [i](#)

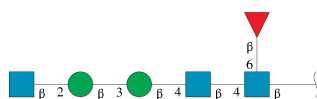
There are 8 unique types of molecules in this entry. The entry contains 9317 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Spike glycoprotein E1.

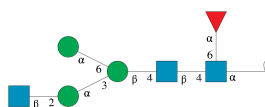
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	391	Total	C	N	O	S	0	0
			2993	1891	501	578	23		
1	B	391	Total	C	N	O	S	0	0
			2993	1891	501	578	23		
1	C	391	Total	C	N	O	S	0	0
			2993	1891	501	578	23		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	6	Total	C	N	O	0	0
			74	42	3	29		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	7	Total	C	N	O	0	0
			85	48	3	34		

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

cetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Br	0
			1	1	
5	B	1	Total	Br	0
			1	1	
5	C	1	Total	Br	0
			1	1	

- Molecule 6 is HOLMIUM ATOM (three-letter code: HO) (formula: Ho).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Ho	0
			2	2	
6	B	1	Total	Ho	0
			1	1	
6	C	1	Total	Ho	0
			1	1	

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	O	P	0
			5	4	1	

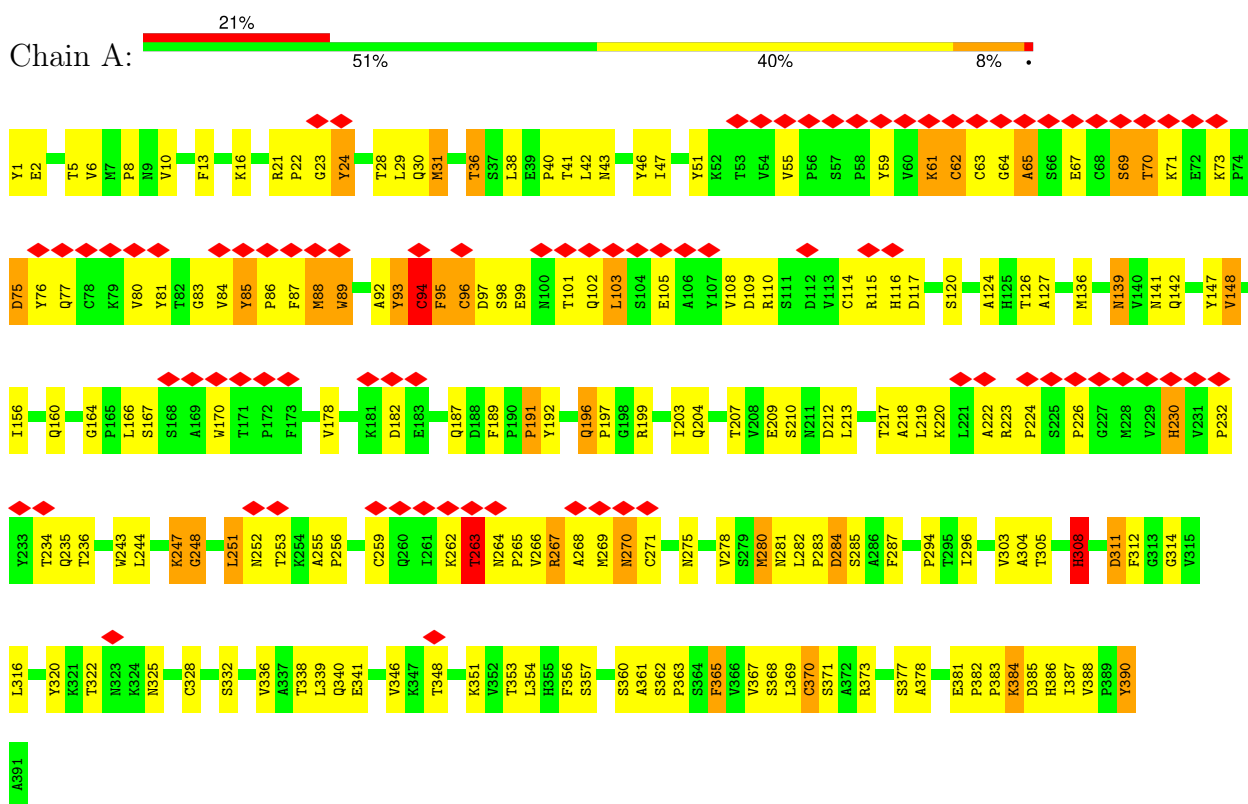
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	54	Total	O	0
			54	54	
8	B	46	Total	O	0
			46	46	
8	C	39	Total	O	0
			39	39	

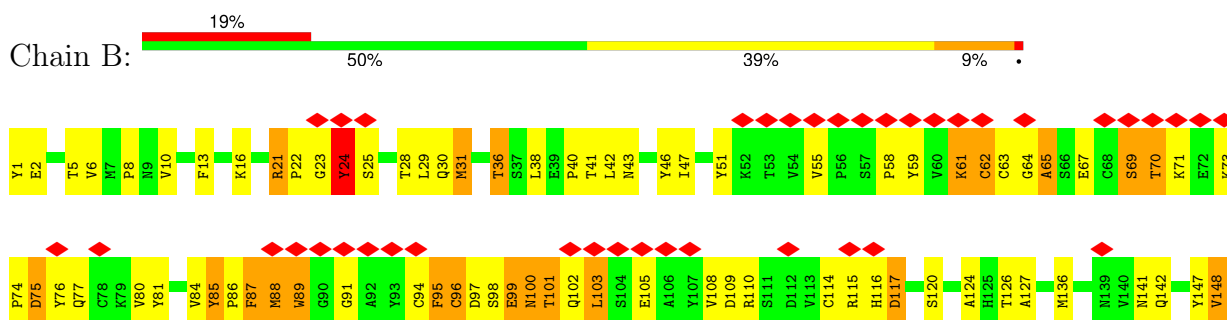
3 Residue-property plots

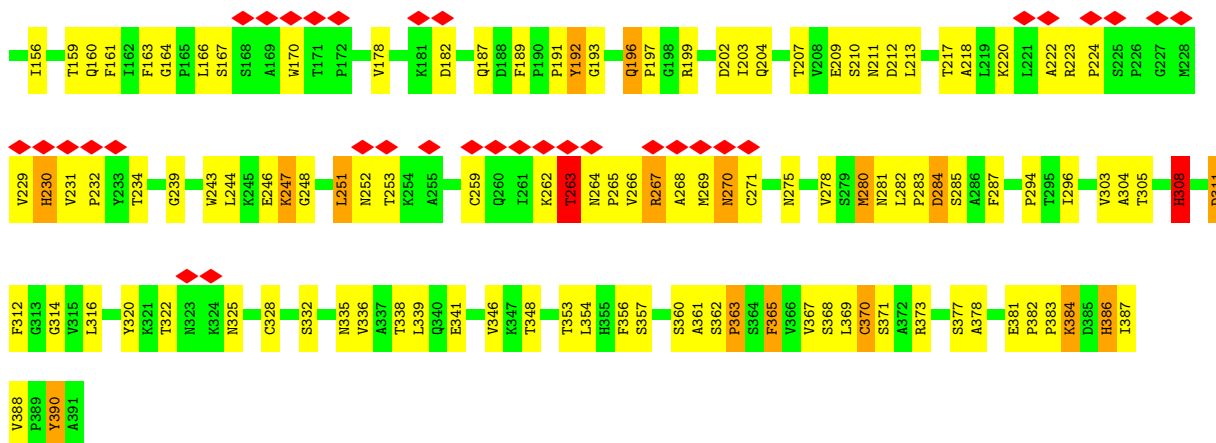
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike glycoprotein E1

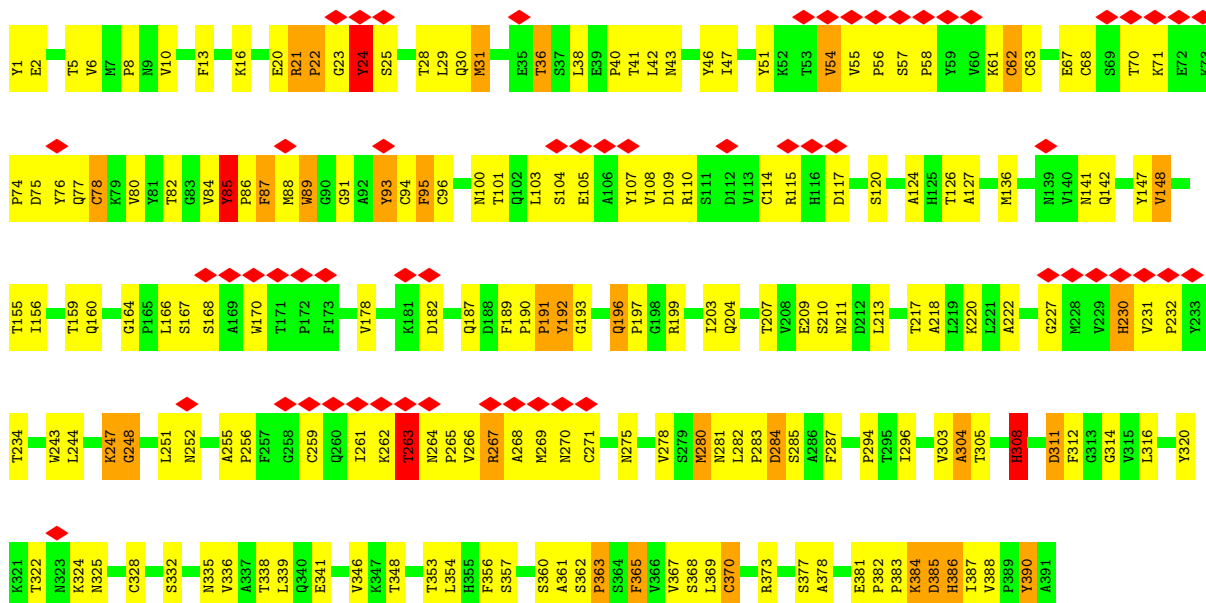


- Molecule 1: Spike glycoprotein E1

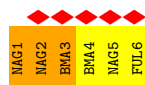
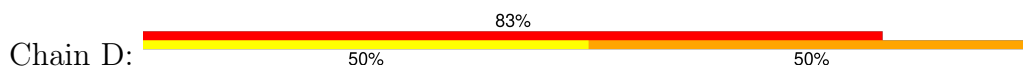




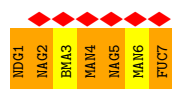
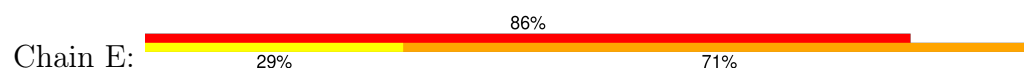
• Molecule 1: Spike glycoprotein E1



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	590	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	53000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.381	Depositor
Minimum map value	-5.755	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.55	Depositor
Map size (Å)	264.48, 264.48, 264.48	wwPDB
Map dimensions	40, 40, 40	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.6120005, 6.6120005, 6.6120005	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: FUL, BR, BMA, FUC, HO, PO4, NAG, MAN, NDG

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	0.70	0/3073	0.76	3/4193 (0.1%)
1	B	0.73	0/3073	0.75	2/4193 (0.0%)
1	C	0.69	0/3073	0.74	2/4193 (0.0%)
All	All	0.71	0/9219	0.75	7/12579 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	C	21	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	A	21	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	A	94	CYS	CA-CB-SG	5.74	124.33	114.00
1	B	263	THR	N-CA-C	5.34	125.42	111.00
1	A	263	THR	N-CA-C	5.29	125.30	111.00
1	C	263	THR	N-CA-C	5.25	125.19	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2993	0	2889	193	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2993	0	2888	223	0
1	C	2993	0	2889	192	0
2	D	74	0	64	6	0
3	E	85	0	72	5	0
4	F	28	0	25	5	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	5	0	0	1	0
8	A	54	0	0	2	0
8	B	46	0	0	8	0
8	C	39	0	0	6	0
All	All	9317	0	8827	601	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 33.

All (601) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:NH2	1:C:24:TYR:CE2	2.08	1.22
1:C:21:ARG:NH2	1:C:24:TYR:CZ	2.17	1.11
1:B:84:VAL:HG13	1:B:223:ARG:HH11	1.17	1.10
1:C:21:ARG:NH2	1:C:24:TYR:OH	1.84	1.10
1:B:65:ALA:HA	1:B:101:THR:HG21	1.39	1.03
1:B:61:LYS:HZ2	1:B:62:CYS:H	1.03	1.00
1:A:65:ALA:HA	1:A:101:THR:HG21	1.42	0.98
1:A:265:PRO:HG2	1:A:267:ARG:HD2	1.45	0.98
1:C:265:PRO:HG2	1:C:267:ARG:HD2	1.43	0.97
1:B:265:PRO:HG2	1:B:267:ARG:HD2	1.44	0.97
1:C:316:LEU:HD11	1:C:365:PHE:CZ	2.01	0.96
1:A:5:THR:HG22	1:A:6:VAL:H	1.32	0.95
1:A:316:LEU:HD11	1:A:365:PHE:CZ	2.01	0.95
1:C:5:THR:HG22	1:C:6:VAL:H	1.30	0.95
2:D:1:NAG:H61	2:D:2:NAG:HN2	1.28	0.95
1:B:303:VAL:HG22	1:B:316:LEU:CD2	1.97	0.94
1:C:303:VAL:HG22	1:C:316:LEU:CD2	1.97	0.93
1:B:5:THR:HG22	1:B:6:VAL:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:HG22	1:A:316:LEU:CD2	1.99	0.93
1:B:316:LEU:HD11	1:B:365:PHE:CZ	2.03	0.93
1:A:316:LEU:HD11	1:A:365:PHE:CE1	2.04	0.91
1:C:316:LEU:HD11	1:C:365:PHE:CE1	2.05	0.91
1:B:59:TYR:HB3	1:B:103:LEU:HD23	1.53	0.91
1:B:316:LEU:HD11	1:B:365:PHE:CE1	2.06	0.90
1:A:61:LYS:HZ2	1:A:62:CYS:H	1.10	0.88
1:A:59:TYR:HB3	1:A:103:LEU:HD23	1.55	0.87
1:C:61:LYS:HB2	1:C:101:THR:O	1.75	0.87
1:C:21:ARG:NH2	1:C:24:TYR:HE2	1.66	0.86
1:B:303:VAL:HG22	1:B:316:LEU:HD23	1.59	0.83
1:C:303:VAL:HG22	1:C:316:LEU:HD23	1.59	0.83
1:C:304:ALA:HB2	8:C:511:HOH:O	1.79	0.82
1:B:384:LYS:H	1:B:384:LYS:HD3	1.43	0.82
1:B:84:VAL:HG13	1:B:223:ARG:NH1	1.95	0.82
1:A:303:VAL:HG22	1:A:316:LEU:HD23	1.60	0.82
2:D:1:NAG:H61	2:D:2:NAG:N2	1.94	0.82
1:B:61:LYS:NZ	1:B:62:CYS:H	1.78	0.81
1:C:332:SER:HB2	1:C:339:LEU:HD13	1.61	0.81
1:C:141:ASN:HB2	4:F:1:NAG:H83	1.63	0.81
1:A:61:LYS:HB3	1:A:101:THR:HG23	1.62	0.80
1:C:160:GLN:H	1:C:281:ASN:ND2	1.79	0.80
1:B:160:GLN:H	1:B:281:ASN:ND2	1.79	0.79
1:A:160:GLN:H	1:A:281:ASN:ND2	1.79	0.79
1:C:187:GLN:HE22	1:C:243:TRP:HE1	1.31	0.79
1:B:100:ASN:N	1:B:100:ASN:HD22	1.80	0.78
1:A:61:LYS:NZ	1:A:62:CYS:H	1.81	0.78
1:C:54:VAL:HG21	1:C:107:TYR:CE1	2.18	0.78
1:B:332:SER:HB2	1:B:339:LEU:HD13	1.64	0.78
1:B:61:LYS:HB3	1:B:101:THR:HG23	1.64	0.78
1:B:84:VAL:HG11	1:B:224:PRO:HD2	1.66	0.77
1:A:332:SER:HB2	1:A:339:LEU:HD13	1.65	0.77
3:E:2:NAG:H5	3:E:7:FUC:H5	1.66	0.76
1:C:54:VAL:HG23	1:C:107:TYR:O	1.87	0.75
1:C:104:SER:HB2	1:C:231:VAL:HG13	1.67	0.75
1:B:187:GLN:HE22	1:B:243:TRP:HE1	1.34	0.74
1:C:294:PRO:HA	1:C:324:LYS:HE2	1.68	0.74
1:B:61:LYS:HZ1	1:B:62:CYS:HB2	1.52	0.74
1:A:170:TRP:CH2	1:C:126:THR:HB	2.23	0.73
1:B:141:ASN:CG	3:E:1:NDG:HA	1.91	0.73
4:F:1:NAG:H62	4:F:2:NAG:N2	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PRO:HG2	1:B:267:ARG:CD	2.18	0.73
1:A:187:GLN:HE22	1:A:243:TRP:HE1	1.34	0.73
1:C:16:LYS:HE3	1:C:30:GLN:NE2	2.04	0.73
1:A:126:THR:HB	1:B:170:TRP:CH2	2.23	0.73
1:A:265:PRO:HG2	1:A:267:ARG:CD	2.18	0.72
1:C:308:HIS:HB3	1:C:383:PRO:HD3	1.71	0.72
1:B:10:VAL:HA	8:B:507:HOH:O	1.87	0.72
1:A:126:THR:HB	1:B:170:TRP:CZ3	2.25	0.72
1:C:265:PRO:HG2	1:C:267:ARG:CD	2.19	0.72
1:A:16:LYS:HE3	1:A:30:GLN:NE2	2.04	0.72
1:A:61:LYS:HZ1	1:A:62:CYS:HB2	1.54	0.72
1:B:16:LYS:HE3	1:B:30:GLN:NE2	2.05	0.71
1:C:86:PRO:HG2	1:C:227:GLY:H	1.55	0.71
1:B:308:HIS:HB3	1:B:383:PRO:HD3	1.71	0.71
1:C:316:LEU:HD11	1:C:365:PHE:HZ	1.56	0.71
1:A:308:HIS:HB3	1:A:383:PRO:HD3	1.71	0.71
1:B:110:ARG:HB2	1:B:114:CYS:SG	2.31	0.70
1:A:170:TRP:CZ3	1:C:126:THR:HB	2.26	0.70
1:B:142:GLN:HB3	1:B:156:ILE:HD12	1.72	0.70
1:B:86:PRO:HG2	1:B:229:VAL:CG1	2.22	0.69
1:A:142:GLN:HB3	1:A:156:ILE:HD12	1.73	0.69
1:C:110:ARG:HB2	1:C:114:CYS:SG	2.33	0.69
1:C:316:LEU:HG	1:C:356:PHE:CD2	2.28	0.69
1:C:21:ARG:O	1:C:21:ARG:HG3	1.90	0.69
1:B:84:VAL:O	1:B:86:PRO:HD3	1.92	0.69
1:C:142:GLN:HB3	1:C:156:ILE:HD12	1.74	0.69
1:A:88:MET:HG3	1:A:89:TRP:H	1.57	0.69
1:B:21:ARG:HG3	1:B:21:ARG:O	1.92	0.69
1:B:316:LEU:HG	1:B:356:PHE:CD2	2.28	0.69
1:B:84:VAL:CG1	1:B:224:PRO:HD2	2.23	0.68
1:A:308:HIS:HB2	1:A:382:PRO:HA	1.75	0.68
1:C:308:HIS:HB2	1:C:382:PRO:HA	1.76	0.68
1:A:61:LYS:HB3	1:A:101:THR:CG2	2.23	0.68
1:B:63:CYS:HA	1:B:100:ASN:HA	1.76	0.68
1:B:384:LYS:HD3	1:B:384:LYS:N	2.09	0.68
1:A:88:MET:HG2	1:A:92:ALA:HA	1.75	0.68
1:A:351:LYS:HE3	8:A:546:HOH:O	1.94	0.67
1:A:88:MET:SD	1:A:92:ALA:HA	2.35	0.67
1:A:43:ASN:HB2	1:B:311:ASP:OD1	1.95	0.67
1:B:160:GLN:H	1:B:281:ASN:HD21	1.42	0.67
1:C:267:ARG:HG3	1:C:267:ARG:HH11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:HD11	1:B:365:PHE:HZ	1.59	0.67
1:B:308:HIS:HB2	1:B:382:PRO:HA	1.76	0.67
1:A:316:LEU:HG	1:A:356:PHE:CD2	2.29	0.67
1:B:84:VAL:HG22	1:B:223:ARG:HD2	1.77	0.67
1:B:61:LYS:HB3	1:B:101:THR:CG2	2.26	0.66
1:C:5:THR:HG22	1:C:6:VAL:N	2.07	0.66
1:C:160:GLN:H	1:C:281:ASN:HD21	1.41	0.66
1:B:126:THR:HB	1:C:170:TRP:CH2	2.31	0.66
1:C:89:TRP:HE1	1:C:100:ASN:ND2	1.94	0.66
1:A:88:MET:CG	1:A:92:ALA:HA	2.25	0.66
1:A:267:ARG:HD3	1:A:267:ARG:N	2.09	0.66
1:C:267:ARG:HD3	1:C:267:ARG:N	2.10	0.66
1:C:84:VAL:C	1:C:86:PRO:HD3	2.16	0.66
1:A:384:LYS:HZ2	1:A:385:ASP:H	1.41	0.66
1:B:267:ARG:HD3	1:B:267:ARG:N	2.10	0.65
1:C:89:TRP:HE1	1:C:100:ASN:HD21	1.44	0.65
1:B:148:VAL:HG13	1:B:166:LEU:HB2	1.78	0.65
1:A:73:LYS:HB2	1:A:76:TYR:HB2	1.77	0.65
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.61	0.65
1:B:267:ARG:HG3	1:B:267:ARG:HH11	1.61	0.65
1:B:81:TYR:HB3	1:B:84:VAL:HG21	1.78	0.65
1:A:110:ARG:HB2	1:A:114:CYS:SG	2.37	0.65
1:A:222:ALA:O	1:A:232:PRO:HG2	1.97	0.65
1:B:5:THR:HG22	1:B:6:VAL:N	2.09	0.65
1:B:222:ALA:O	1:B:232:PRO:HG2	1.97	0.65
1:C:1:TYR:O	1:C:281:ASN:HA	1.97	0.65
1:C:148:VAL:HG13	1:C:166:LEU:HB2	1.77	0.65
1:A:83:GLY:HA2	1:A:98:SER:O	1.96	0.64
1:B:202:ASP:HB2	8:B:506:HOH:O	1.96	0.64
1:A:160:GLN:H	1:A:281:ASN:HD21	1.44	0.64
1:C:56:PRO:HD2	1:C:105:GLU:O	1.97	0.64
1:C:222:ALA:O	1:C:232:PRO:HG2	1.98	0.64
1:C:264:ASN:HB3	1:C:265:PRO:HD3	1.80	0.64
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.63	0.64
1:A:311:ASP:OD1	1:C:43:ASN:HB2	1.97	0.64
1:A:5:THR:HG22	1:A:6:VAL:N	2.08	0.63
1:C:104:SER:HB2	1:C:231:VAL:CG1	2.27	0.63
1:A:1:TYR:O	1:A:281:ASN:HA	1.98	0.63
1:B:100:ASN:N	1:B:100:ASN:ND2	2.46	0.63
1:C:86:PRO:CG	1:C:227:GLY:H	2.11	0.63
1:B:73:LYS:HB2	1:B:76:TYR:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HB3	1:B:265:PRO:HD3	1.80	0.63
1:C:74:PRO:O	1:C:75:ASP:OD2	2.17	0.63
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.63	0.63
1:A:2:GLU:HA	1:A:280:MET:O	1.99	0.63
1:B:29:LEU:HD12	1:B:30:GLN:H	1.62	0.63
1:C:85:TYR:N	1:C:86:PRO:HD3	2.14	0.63
1:B:67:GLU:HA	1:B:80:VAL:HG11	1.81	0.62
1:A:59:TYR:CB	1:A:103:LEU:HD23	2.28	0.62
1:B:59:TYR:CB	1:B:103:LEU:HD23	2.29	0.62
1:C:196:GLN:HE21	1:C:196:GLN:HA	1.64	0.62
1:A:148:VAL:HG13	1:A:166:LEU:HB2	1.80	0.62
1:B:36:THR:HB	1:B:270:ASN:HA	1.81	0.62
1:A:325:ASN:OD1	1:A:348:THR:N	2.32	0.62
1:C:2:GLU:HA	1:C:280:MET:O	2.00	0.62
1:C:85:TYR:O	8:C:501:HOH:O	2.16	0.62
1:C:325:ASN:OD1	1:C:348:THR:N	2.33	0.62
1:A:367:VAL:HG12	1:A:368:SER:N	2.14	0.62
1:B:81:TYR:HB3	1:B:84:VAL:CG2	2.29	0.62
1:C:36:THR:HB	1:C:270:ASN:HA	1.81	0.62
1:B:1:TYR:O	1:B:281:ASN:HA	2.00	0.62
1:B:2:GLU:HA	1:B:280:MET:O	1.99	0.62
1:B:61:LYS:HE3	1:B:64:GLY:CA	2.30	0.62
1:A:61:LYS:HE3	1:A:64:GLY:CA	2.29	0.61
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.65	0.61
1:B:94:CYS:SG	1:B:100:ASN:OD1	2.58	0.61
1:B:325:ASN:OD1	1:B:348:THR:N	2.33	0.61
1:C:29:LEU:HD12	1:C:30:GLN:H	1.65	0.61
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.63	0.61
1:A:191:PRO:HA	5:A:401:BR:BR	2.56	0.61
1:A:264:ASN:HB3	1:A:265:PRO:HD3	1.82	0.61
1:B:24:TYR:HD1	8:B:509:HOH:O	1.83	0.61
1:B:316:LEU:HD11	1:B:365:PHE:HE1	1.64	0.61
1:A:36:THR:HB	1:A:270:ASN:HA	1.83	0.61
1:A:85:TYR:CE2	1:A:87:PHE:HB3	2.36	0.61
1:A:71:LYS:H	1:A:76:TYR:HE2	1.48	0.61
1:C:367:VAL:HG12	1:C:368:SER:N	2.16	0.61
1:B:196:GLN:HE21	1:B:196:GLN:HA	1.66	0.61
1:A:94:CYS:O	1:A:95:PHE:HB2	2.00	0.61
1:A:316:LEU:HD11	1:A:365:PHE:HZ	1.58	0.60
1:C:247:LYS:HG3	1:C:247:LYS:O	2.01	0.60
1:A:316:LEU:HD11	1:A:365:PHE:HE1	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:CD1	1:C:365:PHE:CE1	2.83	0.60
1:A:316:LEU:CD1	1:A:365:PHE:CE1	2.83	0.60
1:B:71:LYS:H	1:B:76:TYR:HE2	1.47	0.60
1:C:384:LYS:HZ2	1:C:385:ASP:H	1.49	0.60
1:A:247:LYS:O	1:A:247:LYS:HG3	2.01	0.60
1:B:61:LYS:HD3	1:B:62:CYS:N	2.17	0.60
1:A:67:GLU:HA	1:A:80:VAL:HG11	1.81	0.60
1:B:247:LYS:O	1:B:247:LYS:HG3	2.01	0.60
1:B:367:VAL:HG12	1:B:368:SER:N	2.17	0.60
1:B:187:GLN:NE2	1:B:243:TRP:HE1	2.00	0.60
1:C:187:GLN:NE2	1:C:243:TRP:HE1	1.97	0.60
1:B:43:ASN:HB2	1:C:311:ASP:OD1	2.02	0.60
1:B:29:LEU:HD12	1:B:30:GLN:N	2.16	0.59
1:B:61:LYS:NZ	1:B:62:CYS:HB2	2.16	0.59
1:B:126:THR:HB	1:C:170:TRP:CZ3	2.36	0.59
1:B:84:VAL:HG11	1:B:223:ARG:HG3	1.84	0.59
1:A:312:PHE:HA	1:A:357:SER:HB2	1.84	0.59
1:B:264:ASN:HB3	1:B:265:PRO:CD	2.33	0.59
1:B:312:PHE:HA	1:B:357:SER:HB2	1.84	0.59
1:C:54:VAL:HG21	1:C:107:TYR:CZ	2.36	0.59
1:A:29:LEU:HD12	1:A:30:GLN:H	1.67	0.59
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.66	0.59
1:B:294:PRO:HG2	1:B:328:CYS:SG	2.43	0.59
1:C:294:PRO:HG2	1:C:328:CYS:SG	2.43	0.59
1:A:294:PRO:HG2	1:A:328:CYS:SG	2.43	0.59
1:A:187:GLN:NE2	1:A:243:TRP:HE1	1.99	0.59
1:B:58:PRO:HG3	1:B:231:VAL:HG22	1.85	0.58
1:C:21:ARG:CZ	1:C:24:TYR:CE2	2.84	0.58
1:B:373:ARG:HG3	1:B:373:ARG:HH11	1.68	0.58
1:A:320:TYR:CE1	1:A:346:VAL:HG13	2.38	0.58
1:A:61:LYS:HD3	1:A:62:CYS:N	2.18	0.58
1:B:316:LEU:CD1	1:B:365:PHE:CE1	2.85	0.58
1:C:29:LEU:HD12	1:C:30:GLN:N	2.18	0.58
1:A:61:LYS:NZ	1:A:62:CYS:HB2	2.18	0.58
1:B:320:TYR:CE1	1:B:346:VAL:HG13	2.39	0.58
1:C:312:PHE:HA	1:C:357:SER:HB2	1.85	0.58
1:A:88:MET:HG3	1:A:89:TRP:N	2.18	0.58
1:C:320:TYR:CE1	1:C:346:VAL:HG13	2.37	0.58
1:A:42:LEU:HD23	1:A:124:ALA:HB2	1.86	0.57
1:C:264:ASN:HB3	1:C:265:PRO:CD	2.33	0.57
1:A:167:SER:HB3	1:A:275:ASN:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HD23	1:C:124:ALA:HB2	1.85	0.57
1:A:80:VAL:HG12	1:A:103:LEU:HD12	1.85	0.57
1:B:84:VAL:O	1:B:86:PRO:CD	2.52	0.57
1:A:264:ASN:HB3	1:A:265:PRO:CD	2.35	0.57
1:B:80:VAL:HG12	1:B:103:LEU:HD12	1.85	0.57
1:A:29:LEU:HD12	1:A:30:GLN:N	2.20	0.57
1:A:5:THR:CG2	1:A:6:VAL:H	2.13	0.57
1:B:98:SER:C	1:B:99:GLU:HG3	2.25	0.56
1:C:21:ARG:CZ	1:C:24:TYR:HE2	2.17	0.56
1:C:36:THR:O	1:C:269:MET:HA	2.05	0.56
1:C:316:LEU:HD11	1:C:365:PHE:HE1	1.64	0.56
1:B:86:PRO:HB3	8:B:521:HOH:O	2.05	0.56
1:B:203:ILE:O	1:B:204:GLN:HG3	2.06	0.56
1:C:308:HIS:CB	1:C:382:PRO:HA	2.36	0.56
1:B:207:THR:HG22	1:B:210:SER:HB2	1.86	0.56
1:C:167:SER:HB3	1:C:275:ASN:OD1	2.06	0.56
1:A:207:THR:HG22	1:A:210:SER:HB2	1.87	0.56
1:B:10:VAL:HG23	1:B:10:VAL:O	2.04	0.56
1:C:68:CYS:HB3	1:C:103:LEU:HD21	1.86	0.56
1:B:308:HIS:CB	1:B:382:PRO:HA	2.36	0.56
1:A:341:GLU:HG3	1:A:354:LEU:HD22	1.88	0.56
1:A:207:THR:O	1:A:210:SER:HB3	2.06	0.55
1:B:65:ALA:HA	1:B:101:THR:CG2	2.26	0.55
1:B:167:SER:HB3	1:B:275:ASN:OD1	2.06	0.55
1:B:353:THR:O	1:B:354:LEU:HD23	2.06	0.55
1:C:373:ARG:HH11	1:C:373:ARG:HG3	1.71	0.55
1:C:193:GLY:N	8:C:502:HOH:O	2.36	0.55
1:C:341:GLU:HG3	1:C:354:LEU:HD22	1.88	0.55
1:A:284:ASP:CG	1:C:284:ASP:OD1	2.44	0.55
1:B:42:LEU:HD23	1:B:124:ALA:HB2	1.87	0.55
1:B:341:GLU:HG3	1:B:354:LEU:HD22	1.88	0.55
1:A:308:HIS:CB	1:A:382:PRO:HA	2.36	0.55
1:C:203:ILE:O	1:C:204:GLN:HG3	2.07	0.55
1:A:63:CYS:C	1:A:65:ALA:H	2.10	0.55
1:B:202:ASP:CB	8:B:506:HOH:O	2.55	0.55
1:B:46:TYR:CD1	1:B:46:TYR:C	2.81	0.54
1:A:36:THR:O	1:A:269:MET:HA	2.07	0.54
1:C:294:PRO:CA	1:C:324:LYS:HE2	2.37	0.54
1:A:63:CYS:SG	1:A:94:CYS:O	2.65	0.54
1:A:203:ILE:O	1:A:204:GLN:HG3	2.08	0.54
1:B:36:THR:O	1:B:269:MET:HA	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:O	1:C:21:ARG:CG	2.55	0.54
1:A:212:ASP:OD2	1:B:386:HIS:HB2	2.08	0.54
1:B:61:LYS:HZ2	1:B:62:CYS:N	1.87	0.54
1:C:108:VAL:HG12	1:C:109:ASP:N	2.23	0.54
1:A:353:THR:O	1:A:354:LEU:HD23	2.07	0.54
1:B:207:THR:O	1:B:210:SER:HB3	2.08	0.54
1:A:63:CYS:SG	1:A:94:CYS:C	2.87	0.54
1:A:139:ASN:HD22	1:A:139:ASN:C	2.12	0.54
1:C:207:THR:HG22	1:C:210:SER:HB2	1.89	0.53
1:C:104:SER:CB	1:C:231:VAL:HG13	2.37	0.53
1:B:21:ARG:NH2	8:B:503:HOH:O	2.38	0.53
1:B:108:VAL:HG12	1:B:109:ASP:N	2.24	0.53
1:C:332:SER:HB2	1:C:339:LEU:CD1	2.35	0.53
1:A:85:TYR:HD1	1:A:226:PRO:HB3	1.74	0.53
1:A:41:THR:OG1	1:A:127:ALA:HB2	2.08	0.53
1:A:283:PRO:C	1:A:285:SER:H	2.12	0.53
1:A:10:VAL:HG23	1:A:10:VAL:O	2.09	0.53
1:B:21:ARG:O	1:B:21:ARG:CG	2.57	0.52
1:A:85:TYR:CD1	1:A:226:PRO:HB3	2.45	0.52
1:B:387:ILE:N	1:B:387:ILE:HD12	2.25	0.52
1:C:78:CYS:SG	1:C:78:CYS:O	2.67	0.52
1:C:207:THR:O	1:C:210:SER:HB3	2.08	0.52
1:B:63:CYS:C	1:B:65:ALA:H	2.11	0.52
1:C:46:TYR:CD1	1:C:46:TYR:C	2.82	0.52
1:C:353:THR:O	1:C:354:LEU:HD23	2.09	0.52
1:A:46:TYR:CD1	1:A:46:TYR:C	2.82	0.52
1:A:63:CYS:HB2	1:A:96:CYS:O	2.09	0.52
1:B:86:PRO:HG2	1:B:229:VAL:HG12	1.92	0.52
1:C:41:THR:OG1	1:C:127:ALA:HB2	2.08	0.52
1:B:365:PHE:H	1:B:365:PHE:HD2	1.56	0.52
1:A:51:TYR:CD1	1:A:51:TYR:C	2.83	0.52
1:A:108:VAL:HG12	1:A:109:ASP:N	2.23	0.52
1:A:387:ILE:HD12	1:A:387:ILE:N	2.25	0.52
1:B:41:THR:OG1	1:B:127:ALA:HB2	2.09	0.52
1:A:365:PHE:H	1:A:365:PHE:HD2	1.57	0.52
1:C:387:ILE:HD12	1:C:387:ILE:N	2.25	0.52
1:A:88:MET:HG2	1:A:92:ALA:CA	2.40	0.51
1:A:311:ASP:H	1:C:43:ASN:HD22	1.58	0.51
1:C:10:VAL:HG23	1:C:10:VAL:O	2.09	0.51
1:C:31:MET:HE2	1:C:278:VAL:HG11	1.92	0.51
1:C:71:LYS:HD3	1:C:76:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TYR:O	1:A:101:THR:HA	2.11	0.51
1:B:332:SER:HB2	1:B:339:LEU:CD1	2.36	0.51
1:A:31:MET:HE2	1:A:278:VAL:HG11	1.92	0.51
1:A:207:THR:H	1:A:210:SER:HB2	1.75	0.51
1:B:88:MET:O	1:B:89:TRP:HB3	2.11	0.51
1:B:100:ASN:O	1:B:101:THR:HB	2.10	0.51
1:C:54:VAL:CG2	1:C:107:TYR:O	2.58	0.51
1:C:93:TYR:N	1:C:93:TYR:CD1	2.79	0.51
1:C:207:THR:H	1:C:210:SER:HB2	1.74	0.51
2:D:3:BMA:H5	2:D:5:NAG:HN2	1.76	0.51
1:B:51:TYR:CD1	1:B:51:TYR:C	2.84	0.50
1:B:25:SER:HB3	8:B:509:HOH:O	2.11	0.50
1:A:116:HIS:HB3	8:A:501:HOH:O	2.12	0.50
1:A:367:VAL:CG1	1:A:368:SER:N	2.73	0.50
1:B:84:VAL:O	1:B:86:PRO:N	2.44	0.50
1:C:220:LYS:HB3	1:C:234:THR:OG1	2.12	0.50
1:B:267:ARG:HG3	1:B:267:ARG:NH1	2.27	0.50
1:B:220:LYS:HB3	1:B:234:THR:OG1	2.12	0.50
1:C:283:PRO:C	1:C:285:SER:H	2.14	0.50
1:C:365:PHE:H	1:C:365:PHE:HD2	1.56	0.50
1:A:40:PRO:HB2	1:A:124:ALA:HB1	1.94	0.49
1:A:109:ASP:HA	1:A:213:LEU:CD2	2.42	0.49
1:B:43:ASN:HD22	1:C:311:ASP:H	1.58	0.49
1:C:40:PRO:HB2	1:C:124:ALA:HB1	1.93	0.49
1:A:62:CYS:O	1:A:101:THR:HG22	2.11	0.49
1:A:84:VAL:HG21	1:A:224:PRO:HB2	1.94	0.49
1:B:40:PRO:HB2	1:B:124:ALA:HB1	1.95	0.49
1:C:51:TYR:CD1	1:C:51:TYR:C	2.86	0.49
1:A:61:LYS:HE3	1:A:64:GLY:HA3	1.94	0.49
1:B:207:THR:H	1:B:210:SER:HB2	1.77	0.49
1:C:316:LEU:CD1	1:C:365:PHE:HE1	2.24	0.49
1:B:31:MET:HE2	1:B:278:VAL:HG11	1.95	0.49
1:C:217:THR:O	1:C:218:ALA:HB3	2.13	0.49
1:C:267:ARG:HG3	1:C:267:ARG:NH1	2.26	0.49
4:F:1:NAG:H62	4:F:2:NAG:C7	2.42	0.49
1:A:217:THR:O	1:A:218:ALA:HB3	2.13	0.49
1:B:283:PRO:C	1:B:285:SER:H	2.14	0.49
1:A:316:LEU:CD1	1:A:365:PHE:HE1	2.23	0.49
1:A:362:SER:HA	1:A:378:ALA:O	2.13	0.48
1:B:362:SER:HA	1:B:378:ALA:O	2.13	0.48
1:C:67:GLU:OE1	1:C:80:VAL:HG11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:SER:HA	1:C:378:ALA:O	2.12	0.48
1:C:20:GLU:O	1:C:22:PRO:HD3	2.13	0.48
1:A:316:LEU:HD21	1:A:365:PHE:HZ	1.78	0.48
1:B:24:TYR:N	1:B:24:TYR:CD2	2.81	0.48
1:B:182:ASP:C	1:B:263:THR:HG21	2.34	0.48
1:C:160:GLN:HB3	1:C:281:ASN:HD21	1.78	0.48
1:C:365:PHE:CD2	1:C:365:PHE:N	2.81	0.48
1:B:296:ILE:HD11	1:B:369:LEU:HB3	1.95	0.48
1:A:267:ARG:NH1	1:B:335:ASN:HD22	2.10	0.48
1:B:95:PHE:N	1:B:95:PHE:CD2	2.79	0.48
1:C:367:VAL:CG1	1:C:368:SER:N	2.76	0.48
1:A:160:GLN:HB3	1:A:281:ASN:HD21	1.78	0.48
1:B:136:MET:HG2	1:B:141:ASN:ND2	2.29	0.48
1:B:81:TYR:O	1:B:101:THR:HA	2.13	0.48
1:B:109:ASP:HA	1:B:213:LEU:CD2	2.44	0.48
1:A:296:ILE:HD11	1:A:369:LEU:HB3	1.96	0.48
1:B:62:CYS:O	1:B:101:THR:HG22	2.14	0.48
1:B:160:GLN:HB3	1:B:281:ASN:HD21	1.77	0.48
1:A:332:SER:HB2	1:A:339:LEU:CD1	2.38	0.48
1:C:109:ASP:HA	1:C:213:LEU:CD2	2.43	0.48
1:B:84:VAL:CG2	1:B:223:ARG:HD2	2.44	0.47
1:B:367:VAL:CG1	1:B:368:SER:N	2.77	0.47
1:B:85:TYR:HB3	1:B:100:ASN:HB2	1.95	0.47
1:B:281:ASN:C	1:B:282:LEU:HG	2.35	0.47
1:B:1:TYR:CD1	1:B:283:PRO:HB3	2.49	0.47
1:A:189:PHE:O	1:A:189:PHE:CD1	2.67	0.47
1:B:61:LYS:HE3	1:B:64:GLY:HA3	1.96	0.47
1:B:316:LEU:HD21	1:B:365:PHE:HZ	1.78	0.47
1:C:384:LYS:HZ2	1:C:384:LYS:HA	1.79	0.47
1:A:93:TYR:O	1:A:94:CYS:C	2.53	0.47
1:A:147:TYR:O	1:A:166:LEU:HG	2.15	0.47
1:A:220:LYS:HB3	1:A:234:THR:OG1	2.14	0.47
1:C:189:PHE:O	1:C:189:PHE:CD1	2.67	0.47
1:C:316:LEU:HD21	1:C:365:PHE:HZ	1.80	0.47
1:A:88:MET:CE	1:A:92:ALA:HA	2.44	0.47
1:B:95:PHE:HD2	1:B:96:CYS:N	2.13	0.47
1:A:243:TRP:HE3	1:A:244:LEU:HD12	1.80	0.47
1:B:80:VAL:HG23	1:B:80:VAL:O	2.15	0.47
1:B:85:TYR:CD2	1:B:85:TYR:O	2.67	0.47
1:C:1:TYR:CD1	1:C:283:PRO:HB3	2.49	0.47
1:A:63:CYS:SG	1:A:96:CYS:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PHE:CD2	1:A:365:PHE:N	2.82	0.47
1:B:85:TYR:O	1:B:85:TYR:CG	2.68	0.47
1:B:239:GLY:N	8:B:506:HOH:O	2.48	0.47
1:B:110:ARG:HG2	1:B:110:ARG:NH1	2.30	0.46
1:C:93:TYR:N	1:C:93:TYR:HD1	2.13	0.46
1:A:314:GLY:HA3	1:A:356:PHE:CE2	2.50	0.46
1:A:203:ILE:C	1:A:204:GLN:HG3	2.36	0.46
1:A:243:TRP:CE3	1:A:244:LEU:HD12	2.50	0.46
1:B:243:TRP:CE3	1:B:244:LEU:HD12	2.51	0.46
1:C:87:PHE:O	1:C:89:TRP:CD1	2.69	0.46
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.27	0.46
1:B:75:ASP:O	1:B:77:GLN:HG2	2.15	0.46
1:B:141:ASN:CG	3:E:1:NDG:N2	2.61	0.46
1:C:243:TRP:CE3	1:C:244:LEU:HD12	2.50	0.46
1:A:80:VAL:O	1:A:80:VAL:HG23	2.16	0.46
1:B:63:CYS:CA	1:B:100:ASN:HA	2.45	0.46
1:B:189:PHE:O	1:B:189:PHE:CD1	2.69	0.46
1:C:243:TRP:HE3	1:C:244:LEU:HD12	1.81	0.46
1:A:1:TYR:CD1	1:A:283:PRO:HB3	2.51	0.46
1:A:103:LEU:H	1:A:103:LEU:HD22	1.81	0.46
1:C:361:ALA:O	1:C:362:SER:HB2	2.16	0.46
1:A:65:ALA:HA	1:A:101:THR:CG2	2.29	0.46
1:A:281:ASN:C	1:A:282:LEU:HG	2.35	0.46
1:B:84:VAL:CG1	1:B:223:ARG:CG	2.94	0.46
1:C:85:TYR:C	8:C:501:HOH:O	2.53	0.46
1:C:203:ILE:C	1:C:204:GLN:HG3	2.36	0.46
1:A:110:ARG:HG2	1:A:110:ARG:NH1	2.30	0.46
1:B:314:GLY:HA3	1:B:356:PHE:CE2	2.51	0.46
1:C:147:TYR:O	1:C:166:LEU:HG	2.15	0.46
1:B:81:TYR:HB3	1:B:84:VAL:CB	2.46	0.46
1:B:217:THR:O	1:B:218:ALA:HB3	2.16	0.46
1:A:120:SER:O	1:A:178:VAL:HA	2.16	0.46
1:B:55:VAL:HG23	1:B:105:GLU:O	2.15	0.46
1:B:61:LYS:HD3	1:B:62:CYS:O	2.16	0.46
1:C:281:ASN:C	1:C:282:LEU:HG	2.36	0.46
1:A:8:PRO:HG3	1:A:13:PHE:CD2	2.51	0.45
1:A:336:VAL:HG22	1:A:336:VAL:O	2.16	0.45
1:C:55:VAL:HG21	1:C:231:VAL:HG21	1.97	0.45
1:C:182:ASP:C	1:C:263:THR:HG21	2.36	0.45
1:C:341:GLU:CG	1:C:354:LEU:HD22	2.45	0.45
1:A:61:LYS:HE3	1:A:64:GLY:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:CYS:SG	1:A:268:ALA:HB1	2.57	0.45
1:A:262:LYS:HA	1:A:262:LYS:HD3	1.76	0.45
1:A:320:TYR:HE1	1:A:346:VAL:HG13	1.82	0.45
1:C:57:SER:HA	1:C:58:PRO:HD3	1.76	0.45
1:B:84:VAL:HG13	1:B:223:ARG:HG2	1.98	0.45
1:B:96:CYS:C	1:B:98:SER:H	2.19	0.45
1:A:36:THR:O	1:A:36:THR:HG22	2.17	0.45
1:B:243:TRP:HE3	1:B:244:LEU:HD12	1.81	0.45
1:A:85:TYR:HA	1:A:86:PRO:HD3	1.62	0.45
1:A:136:MET:HG2	1:A:141:ASN:ND2	2.32	0.45
1:A:361:ALA:O	1:A:362:SER:HB2	2.16	0.45
1:C:55:VAL:CG2	1:C:231:VAL:HG21	2.47	0.45
1:C:61:LYS:HB2	1:C:101:THR:C	2.36	0.45
1:C:68:CYS:SG	1:C:103:LEU:HD11	2.56	0.45
1:A:182:ASP:C	1:A:263:THR:HG21	2.36	0.45
1:A:284:ASP:OD2	1:C:284:ASP:OD1	2.35	0.45
1:B:203:ILE:C	1:B:204:GLN:HG3	2.36	0.45
1:C:136:MET:HG2	1:C:141:ASN:ND2	2.32	0.45
1:A:81:TYR:CD2	1:A:223:ARG:HG3	2.50	0.45
1:A:230:HIS:N	1:A:230:HIS:CD2	2.85	0.45
1:B:5:THR:CG2	1:B:6:VAL:H	2.15	0.45
1:B:212:ASP:OD2	1:C:386:HIS:HB2	2.17	0.45
1:B:341:GLU:CG	1:B:354:LEU:HD22	2.46	0.45
1:A:103:LEU:HD22	1:A:103:LEU:N	2.32	0.45
1:A:283:PRO:C	1:A:285:SER:N	2.70	0.45
1:B:230:HIS:CD2	1:B:230:HIS:N	2.85	0.45
1:B:365:PHE:CD2	1:B:365:PHE:N	2.81	0.45
1:C:314:GLY:HA3	1:C:356:PHE:CE2	2.52	0.45
1:B:61:LYS:HE3	1:B:64:GLY:C	2.37	0.45
1:B:10:VAL:O	1:B:10:VAL:CG2	2.64	0.44
1:C:296:ILE:HD11	1:C:369:LEU:HB3	1.98	0.44
1:B:58:PRO:HG3	1:B:231:VAL:CG2	2.46	0.44
1:B:84:VAL:HG13	1:B:223:ARG:CG	2.48	0.44
1:C:67:GLU:OE2	1:C:80:VAL:HG11	2.16	0.44
1:B:120:SER:O	1:B:178:VAL:HA	2.16	0.44
1:C:8:PRO:HG3	1:C:13:PHE:CD2	2.53	0.44
1:C:369:LEU:O	1:C:370:CYS:HB2	2.17	0.44
1:B:316:LEU:CD1	1:B:365:PHE:HE1	2.25	0.44
1:C:230:HIS:CD2	1:C:230:HIS:N	2.85	0.44
1:B:103:LEU:HD22	1:B:103:LEU:H	1.83	0.44
1:C:68:CYS:SG	1:C:103:LEU:CD1	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:CYS:SG	1:C:268:ALA:HB1	2.57	0.44
1:C:336:VAL:HG22	1:C:336:VAL:O	2.17	0.44
1:A:55:VAL:HG23	1:A:105:GLU:O	2.18	0.44
1:C:120:SER:O	1:C:178:VAL:HA	2.18	0.44
1:B:283:PRO:C	1:B:285:SER:N	2.71	0.44
1:C:114:CYS:O	1:C:115:ARG:C	2.56	0.44
1:A:197:PRO:O	1:A:199:ARG:HG2	2.18	0.43
1:C:199:ARG:HG3	1:C:199:ARG:HH11	1.83	0.43
1:C:283:PRO:C	1:C:285:SER:N	2.71	0.43
1:A:284:ASP:OD1	1:B:284:ASP:CG	2.57	0.43
1:A:341:GLU:CG	1:A:354:LEU:HD22	2.47	0.43
1:B:199:ARG:HG3	1:B:199:ARG:HH11	1.83	0.43
1:A:69:SER:O	1:A:70:THR:HG23	2.18	0.43
3:E:4:MAN:C1	3:E:5:NAG:H2	2.48	0.43
1:B:147:TYR:O	1:B:166:LEU:HG	2.19	0.43
1:B:361:ALA:O	1:B:362:SER:HB2	2.18	0.43
1:C:63:CYS:SG	1:C:94:CYS:HB3	2.59	0.43
1:A:77:GLN:NE2	1:A:219:LEU:O	2.51	0.43
1:A:243:TRP:CH2	1:A:247:LYS:HD3	2.54	0.43
1:B:369:LEU:O	1:B:370:CYS:HB2	2.17	0.43
1:C:36:THR:O	1:C:36:THR:HG22	2.18	0.43
1:C:54:VAL:HG21	1:C:107:TYR:CD1	2.53	0.43
1:C:247:LYS:O	1:C:248:GLY:O	2.36	0.43
1:A:370:CYS:HB3	1:A:371:SER:H	1.59	0.43
1:B:8:PRO:HG3	1:B:13:PHE:CD2	2.53	0.43
1:C:243:TRP:CH2	1:C:247:LYS:HD3	2.54	0.43
1:A:247:LYS:O	1:A:248:GLY:O	2.36	0.43
1:A:369:LEU:O	1:A:370:CYS:HB2	2.18	0.43
1:B:259:CYS:SG	1:B:268:ALA:HB1	2.59	0.43
1:B:370:CYS:HB3	1:B:371:SER:H	1.60	0.43
1:A:251:LEU:O	1:A:253:THR:N	2.52	0.43
1:C:85:TYR:N	1:C:86:PRO:CD	2.81	0.43
1:B:267:ARG:NH1	1:C:335:ASN:HD22	2.16	0.42
1:C:71:LYS:HD3	1:C:76:TYR:CZ	2.54	0.42
1:A:139:ASN:C	1:A:139:ASN:ND2	2.72	0.42
1:C:68:CYS:HB3	1:C:103:LEU:CD2	2.49	0.42
1:A:6:VAL:CG2	1:A:275:ASN:HB2	2.49	0.42
1:B:6:VAL:CG2	1:B:275:ASN:HB2	2.49	0.42
1:B:115:ARG:HH12	1:B:209:GLU:HG3	1.83	0.42
1:C:190:PRO:HA	1:C:191:PRO:HD3	1.93	0.42
1:A:84:VAL:HG22	1:A:85:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:HA	1:A:256:PRO:HD3	1.88	0.42
1:B:99:GLU:OE1	1:B:99:GLU:N	2.52	0.42
1:B:262:LYS:HD3	1:B:262:LYS:HA	1.77	0.42
1:C:197:PRO:O	1:C:199:ARG:HG2	2.19	0.42
1:A:84:VAL:HG13	1:A:84:VAL:O	2.19	0.42
1:B:74:PRO:HB2	1:B:108:VAL:O	2.20	0.42
1:B:84:VAL:CG1	1:B:223:ARG:HG3	2.49	0.42
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.76	0.42
3:E:4:MAN:H4	3:E:5:NAG:O6	2.19	0.42
1:B:207:THR:HG23	1:B:210:SER:N	2.34	0.42
1:A:88:MET:HG2	1:A:92:ALA:N	2.34	0.42
1:A:75:ASP:O	1:A:77:GLN:HG2	2.19	0.42
1:A:235:GLN:HG2	1:A:236:THR:H	1.84	0.42
1:B:243:TRP:CH2	1:B:247:LYS:HD3	2.55	0.42
1:B:210:SER:OG	1:B:211:ASN:N	2.52	0.42
1:C:74:PRO:HG2	1:C:108:VAL:O	2.18	0.42
1:C:115:ARG:HH12	1:C:209:GLU:HG3	1.85	0.42
1:A:207:THR:HG23	1:A:210:SER:N	2.34	0.42
1:B:38:LEU:O	1:B:38:LEU:HD23	2.20	0.42
1:B:69:SER:O	1:B:70:THR:HG23	2.20	0.42
1:B:202:ASP:OD1	1:B:217:THR:HG22	2.20	0.42
1:C:141:ASN:CG	4:F:1:NAG:N2	2.73	0.42
1:C:210:SER:OG	1:C:211:ASN:N	2.53	0.42
1:B:114:CYS:O	1:B:115:ARG:C	2.57	0.41
1:B:320:TYR:HE1	1:B:346:VAL:HG13	1.82	0.41
1:B:360:SER:O	1:B:363:PRO:HD3	2.19	0.41
1:C:360:SER:O	1:C:363:PRO:HD3	2.19	0.41
1:A:312:PHE:CD2	1:A:340:GLN:HB2	2.55	0.41
1:B:59:TYR:O	1:B:103:LEU:CD2	2.68	0.41
1:C:110:ARG:HG2	1:C:110:ARG:NH1	2.31	0.41
1:C:192:TYR:HB3	8:C:502:HOH:O	2.21	0.41
1:C:255:ALA:HA	1:C:256:PRO:HD3	1.89	0.41
1:C:10:VAL:O	1:C:10:VAL:CG2	2.68	0.41
1:C:86:PRO:CG	1:C:227:GLY:N	2.82	0.41
1:A:170:TRP:CD1	1:A:170:TRP:C	2.92	0.41
1:B:251:LEU:O	1:B:253:THR:N	2.53	0.41
1:B:312:PHE:CA	1:B:357:SER:HB2	2.50	0.41
1:C:6:VAL:CG2	1:C:275:ASN:HB2	2.50	0.41
1:B:316:LEU:HD13	1:B:367:VAL:HG21	2.03	0.41
1:C:91:GLY:O	1:C:95:PHE:HD1	2.03	0.41
1:C:362:SER:N	1:C:363:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:O	1:A:103:LEU:CD2	2.69	0.41
1:B:246:GLU:O	1:B:247:LYS:C	2.59	0.41
1:C:77:GLN:NE2	8:C:504:HOH:O	2.53	0.41
1:A:316:LEU:HD13	1:A:367:VAL:HG21	2.01	0.41
1:C:320:TYR:HE1	1:C:346:VAL:HG13	1.81	0.41
1:A:38:LEU:HD13	1:A:170:TRP:O	2.21	0.41
1:A:43:ASN:HD22	1:B:311:ASP:H	1.68	0.41
1:A:67:GLU:OE1	1:A:80:VAL:HG21	2.21	0.41
1:A:88:MET:HG2	1:A:92:ALA:H	1.85	0.41
1:A:312:PHE:CA	1:A:357:SER:HB2	2.50	0.41
1:B:36:THR:O	1:B:36:THR:HG22	2.20	0.41
1:B:38:LEU:HD13	1:B:170:TRP:O	2.21	0.41
1:B:67:GLU:OE1	1:B:80:VAL:HG21	2.20	0.41
1:B:81:TYR:HB3	1:B:84:VAL:HB	2.01	0.41
1:B:84:VAL:O	1:B:85:TYR:C	2.59	0.41
1:B:108:VAL:CG1	1:B:109:ASP:N	2.84	0.41
1:B:336:VAL:HG22	1:B:336:VAL:O	2.20	0.41
1:C:38:LEU:HD13	1:C:170:TRP:O	2.21	0.41
1:C:316:LEU:HD13	1:C:367:VAL:HG21	2.03	0.41
1:A:10:VAL:O	1:A:10:VAL:CG2	2.69	0.41
1:A:114:CYS:O	1:A:115:ARG:C	2.59	0.41
1:A:115:ARG:HH12	1:A:209:GLU:HG3	1.85	0.41
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.86	0.41
1:B:103:LEU:HD22	1:B:103:LEU:N	2.36	0.41
1:B:116:HIS:O	1:B:117:ASP:HB2	2.20	0.41
1:B:161:PHE:HB3	1:B:163:PHE:CE1	2.56	0.41
1:B:192:TYR:CG	1:B:193:GLY:N	2.88	0.41
1:B:207:THR:HG23	1:B:210:SER:H	1.86	0.41
1:C:55:VAL:HG21	1:C:231:VAL:CG2	2.51	0.41
1:C:108:VAL:CG1	1:C:109:ASP:N	2.84	0.41
1:C:170:TRP:CD1	1:C:170:TRP:C	2.93	0.41
1:A:108:VAL:CG1	1:A:109:ASP:N	2.84	0.40
2:D:3:BMA:H3	2:D:5:NAG:N2	2.36	0.40
1:B:362:SER:N	1:B:363:PRO:CD	2.84	0.40
1:C:207:THR:HG23	1:C:210:SER:N	2.37	0.40
1:C:267:ARG:CD	1:C:267:ARG:N	2.83	0.40
1:A:31:MET:CE	1:A:278:VAL:HG11	2.51	0.40
7:B:401:PO4:O1	1:C:168:SER:HB2	2.22	0.40
1:C:24:TYR:CG	1:C:25:SER:N	2.89	0.40
1:A:360:SER:O	1:A:363:PRO:HD3	2.21	0.40
1:A:362:SER:N	1:A:363:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLN:CB	1:B:281:ASN:HD21	2.34	0.40
1:B:170:TRP:CD1	1:B:170:TRP:C	2.93	0.40
4:F:1:NAG:H62	4:F:2:NAG:HN2	1.82	0.40
1:B:95:PHE:CD2	1:B:96:CYS:N	2.89	0.40
1:B:197:PRO:O	1:B:199:ARG:HG2	2.20	0.40
1:C:31:MET:CE	1:C:278:VAL:HG11	2.51	0.40
1:C:261:ILE:HG22	1:C:262:LYS:N	2.36	0.40
2:D:3:BMA:H5	2:D:5:NAG:C7	2.51	0.40
2:D:3:BMA:H5	2:D:5:NAG:N2	2.35	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	389/391 (100%)	315 (81%)	50 (13%)	24 (6%)	1	13
1	B	389/391 (100%)	320 (82%)	46 (12%)	23 (6%)	1	13
1	C	389/391 (100%)	320 (82%)	49 (13%)	20 (5%)	1	15
All	All	1167/1173 (100%)	955 (82%)	145 (12%)	67 (6%)	2	14

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	96	CYS
1	A	97	ASP
1	A	192	TYR
1	A	308	HIS
1	B	69	SER
1	B	89	TRP
1	B	192	TYR

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Mol	Chain	Res	Type
1	B	308	HIS
1	C	87	PHE
1	C	192	TYR
1	C	308	HIS
1	A	65	ALA
1	A	69	SER
1	A	94	CYS
1	A	95	PHE
1	A	117	ASP
1	A	248	GLY
1	A	252	ASN
1	B	65	ALA
1	B	117	ASP
1	B	248	GLY
1	B	252	ASN
1	C	24	TYR
1	C	88	MET
1	C	89	TRP
1	C	117	ASP
1	C	248	GLY
1	A	24	TYR
1	B	24	TYR
1	B	101	THR
1	C	62	CYS
1	C	252	ASN
1	A	23	GLY
1	A	247	LYS
1	A	311	ASP
1	A	390	TYR
1	B	87	PHE
1	B	97	ASP
1	B	247	LYS
1	B	311	ASP
1	B	390	TYR
1	C	23	GLY
1	C	247	LYS
1	C	311	ASP
1	C	390	TYR
1	A	99	GLU
1	A	164	GLY
1	A	270	ASN
1	A	304	ALA

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Mol	Chain	Res	Type
1	B	23	GLY
1	B	270	ASN
1	B	304	ALA
1	C	304	ALA
1	A	22	PRO
1	A	266	VAL
1	B	22	PRO
1	B	91	GLY
1	B	164	GLY
1	B	266	VAL
1	C	85	TYR
1	C	266	VAL
1	B	191	PRO
1	C	22	PRO
1	C	164	GLY
1	A	191	PRO
1	C	191	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/336 (100%)	299 (89%)	37 (11%)	5	18
1	B	336/336 (100%)	294 (88%)	42 (12%)	3	15
1	C	336/336 (100%)	296 (88%)	40 (12%)	4	16
All	All	1008/1008 (100%)	889 (88%)	119 (12%)	7	16

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TYR
1	A	28	THR
1	A	31	MET
1	A	36	THR
1	A	47	ILE

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Mol	Chain	Res	Type
1	A	61	LYS
1	A	62	CYS
1	A	70	THR
1	A	75	ASP
1	A	88	MET
1	A	89	TRP
1	A	93	TYR
1	A	102	GLN
1	A	103	LEU
1	A	139	ASN
1	A	148	VAL
1	A	196	GLN
1	A	230	HIS
1	A	251	LEU
1	A	263	THR
1	A	267	ARG
1	A	271	CYS
1	A	280	MET
1	A	284	ASP
1	A	287	PHE
1	A	305	THR
1	A	308	HIS
1	A	322	THR
1	A	338	THR
1	A	365	PHE
1	A	370	CYS
1	A	377	SER
1	A	381	GLU
1	A	384	LYS
1	A	386	HIS
1	A	388	VAL
1	A	390	TYR
1	B	24	TYR
1	B	28	THR
1	B	31	MET
1	B	36	THR
1	B	47	ILE
1	B	61	LYS
1	B	62	CYS
1	B	70	THR
1	B	75	ASP
1	B	85	TYR

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Mol	Chain	Res	Type
1	B	87	PHE
1	B	88	MET
1	B	95	PHE
1	B	96	CYS
1	B	99	GLU
1	B	100	ASN
1	B	102	GLN
1	B	103	LEU
1	B	148	VAL
1	B	159	THR
1	B	196	GLN
1	B	230	HIS
1	B	251	LEU
1	B	263	THR
1	B	267	ARG
1	B	271	CYS
1	B	280	MET
1	B	284	ASP
1	B	287	PHE
1	B	305	THR
1	B	308	HIS
1	B	322	THR
1	B	338	THR
1	B	363	PRO
1	B	365	PHE
1	B	370	CYS
1	B	377	SER
1	B	381	GLU
1	B	384	LYS
1	B	386	HIS
1	B	388	VAL
1	B	390	TYR
1	C	24	TYR
1	C	28	THR
1	C	31	MET
1	C	36	THR
1	C	47	ILE
1	C	54	VAL
1	C	62	CYS
1	C	70	THR
1	C	78	CYS
1	C	82	THR

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Mol	Chain	Res	Type
1	C	85	TYR
1	C	93	TYR
1	C	95	PHE
1	C	96	CYS
1	C	148	VAL
1	C	155	THR
1	C	159	THR
1	C	196	GLN
1	C	230	HIS
1	C	251	LEU
1	C	263	THR
1	C	267	ARG
1	C	271	CYS
1	C	280	MET
1	C	284	ASP
1	C	287	PHE
1	C	305	THR
1	C	308	HIS
1	C	322	THR
1	C	338	THR
1	C	363	PRO
1	C	365	PHE
1	C	370	CYS
1	C	377	SER
1	C	381	GLU
1	C	384	LYS
1	C	385	ASP
1	C	386	HIS
1	C	388	VAL
1	C	390	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	43	ASN
1	A	102	GLN
1	A	125	HIS
1	A	142	GLN
1	A	152	HIS
1	A	187	GLN
1	A	196	GLN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	216	ASN
1	A	230	HIS
1	A	235	GLN
1	A	281	ASN
1	A	308	HIS
1	A	340	GLN
1	A	386	HIS
1	B	30	GLN
1	B	43	ASN
1	B	100	ASN
1	B	102	GLN
1	B	142	GLN
1	B	187	GLN
1	B	196	GLN
1	B	211	ASN
1	B	216	ASN
1	B	230	HIS
1	B	235	GLN
1	B	281	ASN
1	B	308	HIS
1	B	340	GLN
1	B	386	HIS
1	C	30	GLN
1	C	43	ASN
1	C	77	GLN
1	C	100	ASN
1	C	125	HIS
1	C	142	GLN
1	C	187	GLN
1	C	196	GLN
1	C	211	ASN
1	C	216	ASN
1	C	230	HIS
1	C	281	ASN
1	C	308	HIS
1	C	340	GLN
1	C	386	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

15 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
2	NAG	D	1	2,1	14,14,15	0.69	0	17,19,21	1.24	1 (5%)
2	NAG	D	2	2	14,14,15	0.76	0	17,19,21	1.04	2 (11%)
2	BMA	D	3	2	11,11,12	1.34	2 (18%)	15,15,17	0.64	0
2	BMA	D	4	2	11,11,12	1.37	2 (18%)	15,15,17	1.09	2 (13%)
2	NAG	D	5	2	14,14,15	1.21	0	17,19,21	0.77	0
2	FUL	D	6	2	10,10,11	0.92	1 (10%)	14,14,16	0.65	0
3	NDG	E	1	3	14,14,15	0.96	0	17,19,21	1.24	1 (5%)
3	NAG	E	2	3	14,14,15	0.85	0	17,19,21	0.93	1 (5%)
3	BMA	E	3	3	11,11,12	1.34	1 (9%)	15,15,17	1.58	3 (20%)
3	MAN	E	4	3	11,11,12	1.64	2 (18%)	15,15,17	1.41	2 (13%)
3	NAG	E	5	3	14,14,15	1.57	3 (21%)	17,19,21	0.99	1 (5%)
3	MAN	E	6	3	11,11,12	1.37	1 (9%)	15,15,17	1.21	3 (20%)
3	FUC	E	7	3	10,10,11	1.37	2 (20%)	14,14,16	0.90	1 (7%)
4	NAG	F	1	1,4	14,14,15	1.26	2 (14%)	17,19,21	0.67	0
4	NAG	F	2	4	14,14,15	1.34	3 (21%)	17,19,21	1.02	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
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	BMA	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	3/6/23/26	0/1/1/1
2	FUL	D	6	2	-	-	0/1/1/1
3	NDG	E	1	3	-	5/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	E	5	3	-	4/6/23/26	0/1/1/1
3	MAN	E	6	3	-	1/2/19/22	0/1/1/1
3	FUC	E	7	3	1/1/4/5	-	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	NAG	C1-C2	3.57	1.57	1.52
4	F	1	NAG	C1-C2	3.24	1.56	1.52
3	E	4	MAN	O2-C2	3.09	1.49	1.43
3	E	4	MAN	C2-C3	2.96	1.57	1.52
3	E	3	BMA	C2-C3	2.82	1.56	1.52
3	E	6	MAN	C2-C3	2.72	1.56	1.52
3	E	5	NAG	C3-C2	2.67	1.58	1.52
4	F	2	NAG	C3-C2	2.42	1.57	1.52
4	F	2	NAG	C4-C5	2.40	1.58	1.53
2	D	3	BMA	C2-C3	2.39	1.56	1.52
3	E	7	FUC	C4-C3	2.37	1.58	1.52
2	D	4	BMA	C2-C3	2.36	1.56	1.52
3	E	5	NAG	C8-C7	2.34	1.55	1.50
2	D	4	BMA	O2-C2	2.33	1.48	1.43
2	D	3	BMA	C4-C5	2.28	1.57	1.53
3	E	7	FUC	C2-C3	2.10	1.55	1.52
4	F	1	NAG	C8-C7	2.08	1.54	1.50
2	D	6	FUL	C2-C3	2.06	1.55	1.52
4	F	2	NAG	C4-C3	2.02	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	-4.26	117.19	122.90
3	E	3	BMA	C3-C4-C5	3.84	117.19	110.23
3	E	3	BMA	C2-C3-C4	3.64	117.25	110.86
3	E	4	MAN	O2-C2-C1	3.11	116.35	109.22
3	E	1	NDG	C3-C4-C5	-2.97	104.84	110.23
3	E	4	MAN	C2-C3-C4	2.76	115.72	110.86
3	E	6	MAN	C1-C2-C3	2.61	113.45	109.64
3	E	6	MAN	C1-O5-C5	2.49	115.52	112.19
3	E	2	NAG	C2-N2-C7	-2.48	119.58	122.90
4	F	2	NAG	C2-N2-C7	-2.35	119.75	122.90
3	E	3	BMA	C1-C2-C3	2.25	112.92	109.64
2	D	2	NAG	C3-C4-C5	2.25	114.31	110.23
2	D	4	BMA	C3-C4-C5	-2.25	106.16	110.23
2	D	4	BMA	C6-C5-C4	2.20	118.41	113.02
2	D	2	NAG	C2-N2-C7	-2.14	120.04	122.90
3	E	6	MAN	C3-C4-C5	2.13	114.09	110.23
3	E	5	NAG	C4-C3-C2	2.11	114.12	111.02
3	E	7	FUC	C1-C2-C3	2.09	112.69	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	7	FUC	C1

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
3	E	1	NDG	C8-C7-N2-C2
3	E	1	NDG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	5	NAG	C8-C7-N2-C2
3	E	5	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	D	4	BMA	C4-C5-C6-O6
3	E	5	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
2	D	4	BMA	O5-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6
3	E	1	NDG	O5-C5-C6-O6
3	E	1	NDG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	E	1	NDG	C3-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	5	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

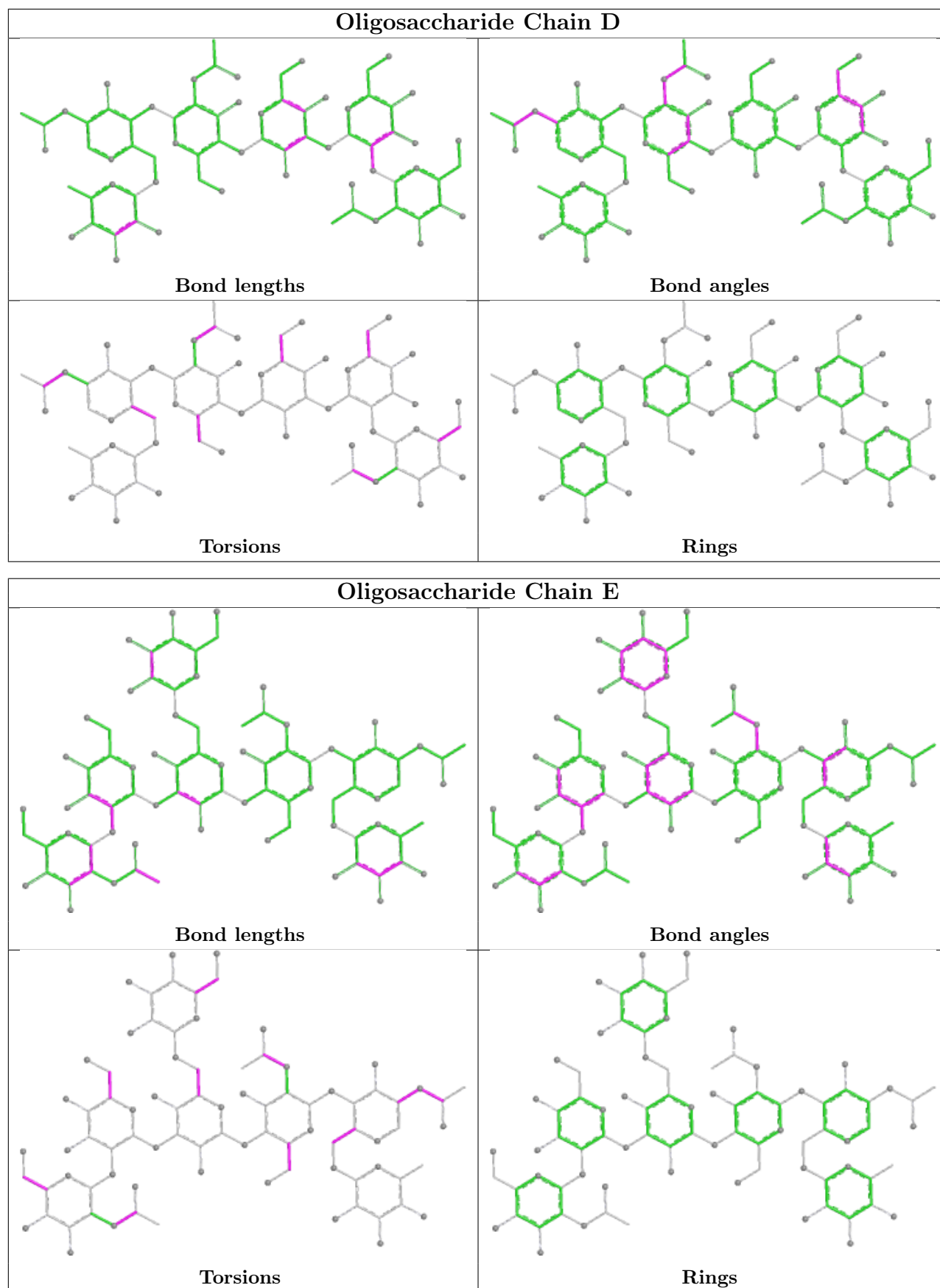
There are no ring outliers.

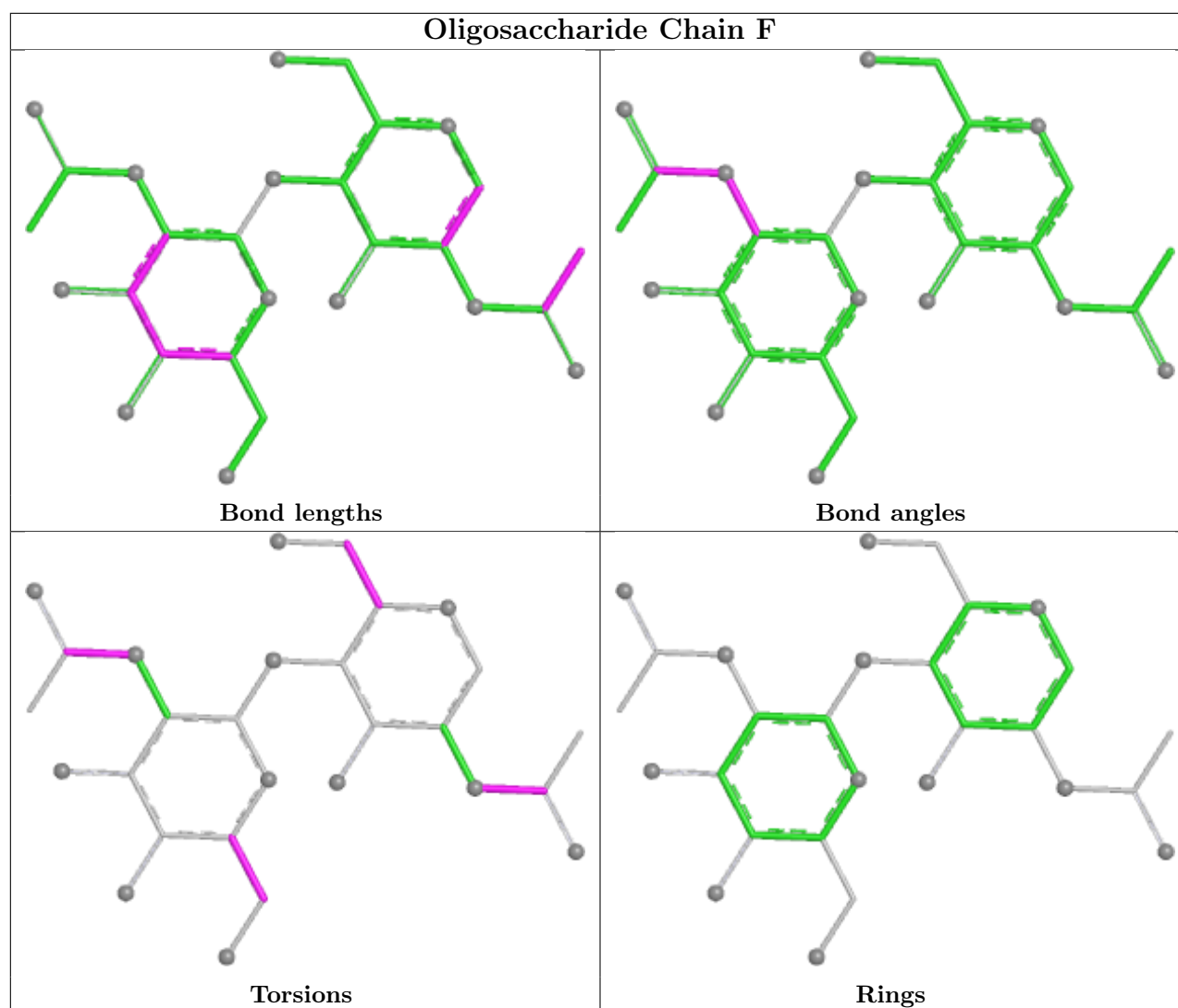
11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7	FUC	1	0
3	E	4	MAN	2	0
2	D	2	NAG	2	0
2	D	3	BMA	4	0
3	E	1	NDG	2	0
3	E	2	NAG	1	0
3	E	5	NAG	2	0
4	F	1	NAG	5	0
4	F	2	NAG	3	0
2	D	1	NAG	2	0
2	D	5	NAG	4	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](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PO4	B	401	-	4,4,4	0.75	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	401	PO4	1	0

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.

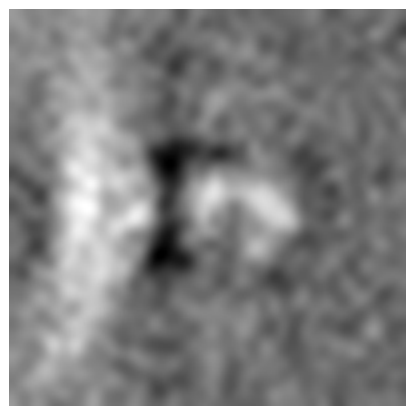
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27248. These allow visual inspection of the internal detail of the map and identification of artifacts.

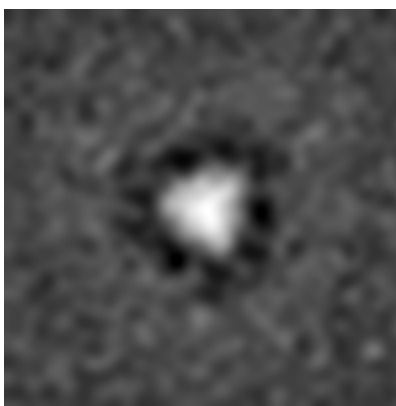
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

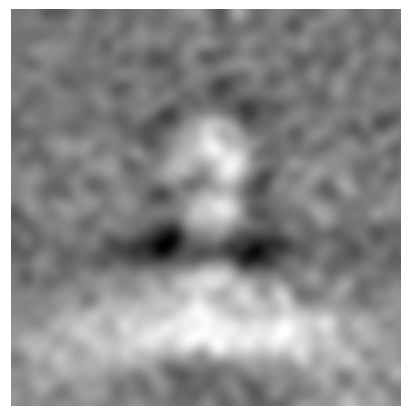
6.1.1 Primary map



X

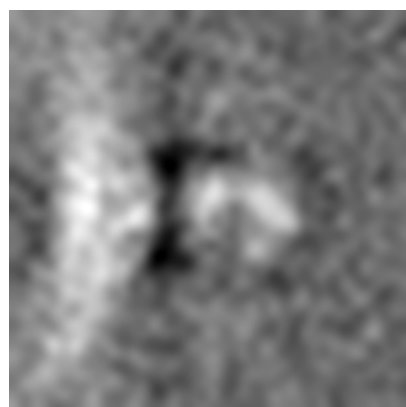


Y

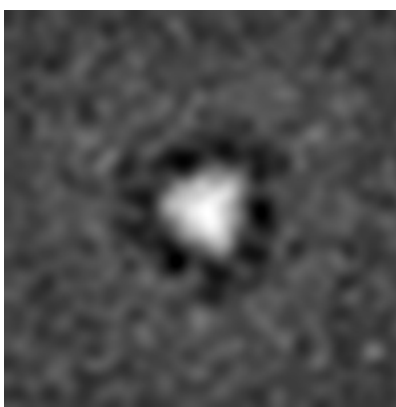


Z

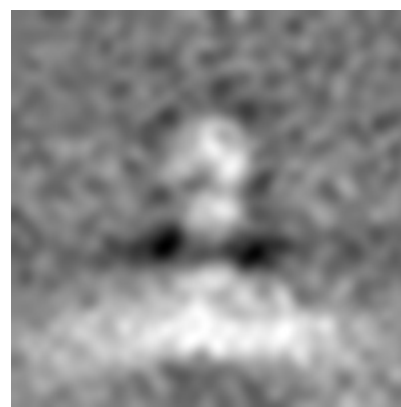
6.1.2 Raw map



X



Y

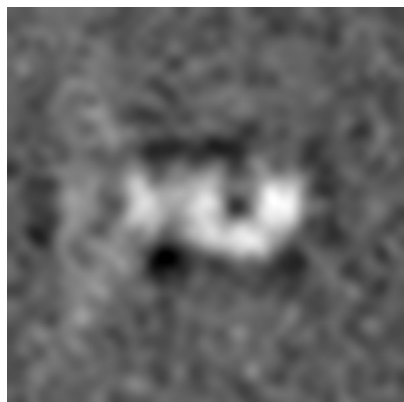


Z

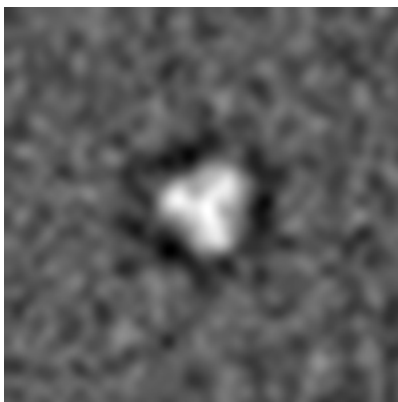
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

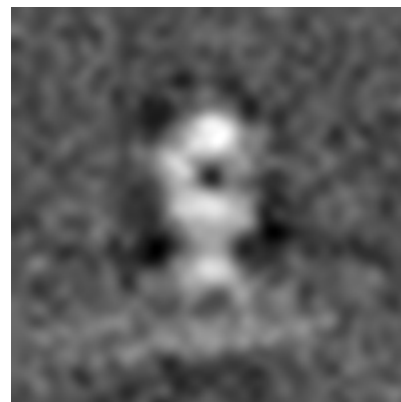
6.2.1 Primary map



X Index: 20

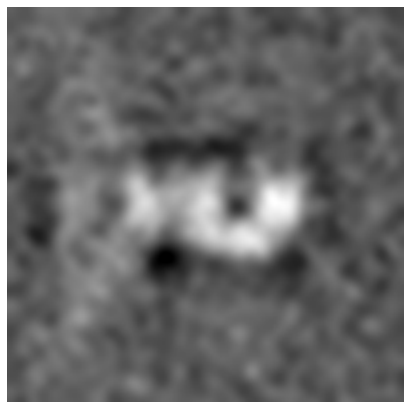


Y Index: 20

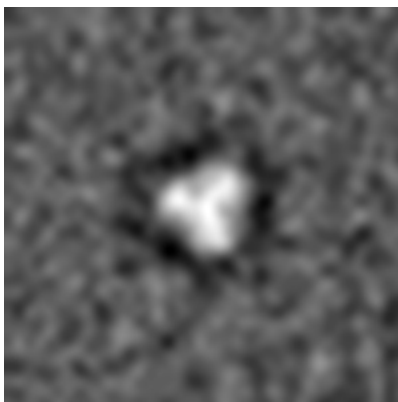


Z Index: 20

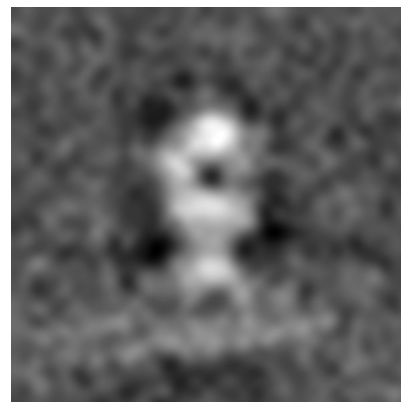
6.2.2 Raw map



X Index: 20



Y Index: 20

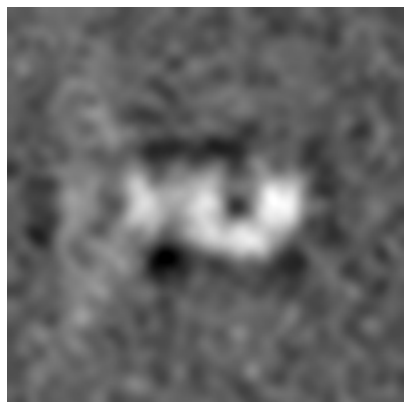


Z Index: 20

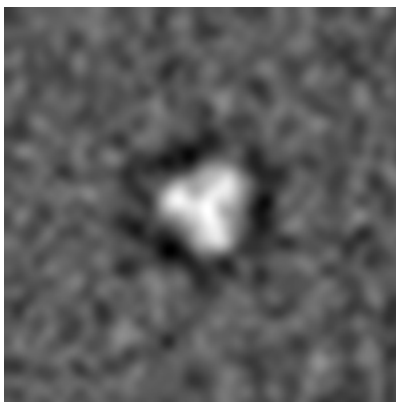
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 20

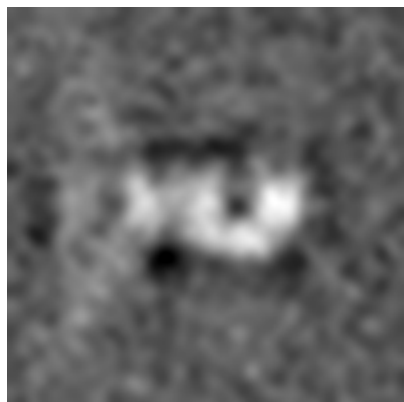


Y Index: 20

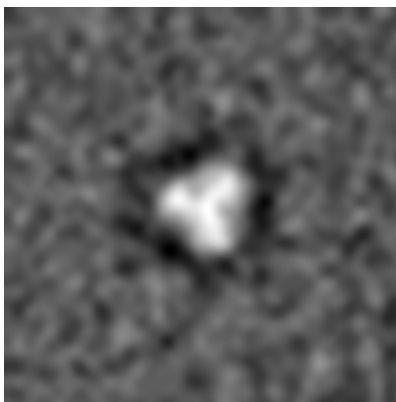


Z Index: 20

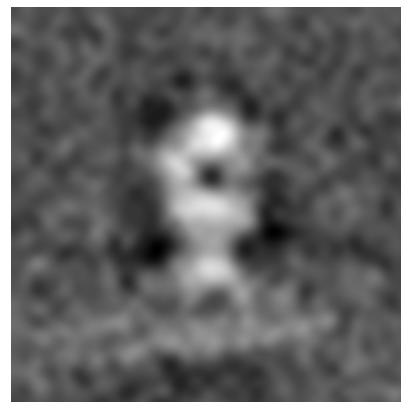
6.3.2 Raw map



X Index: 20



Y Index: 20

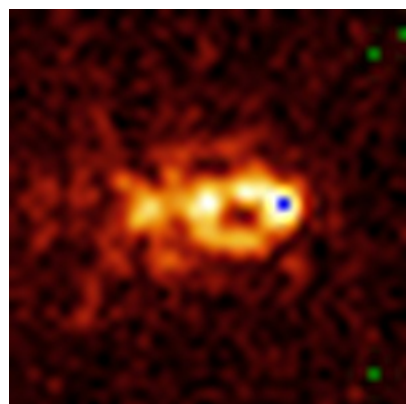


Z Index: 20

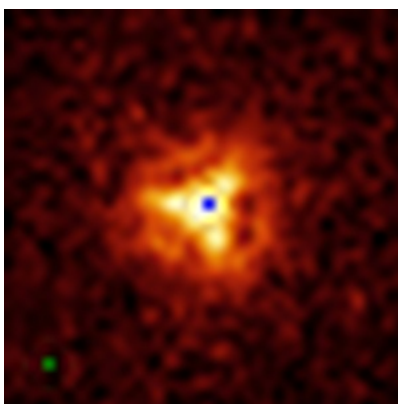
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

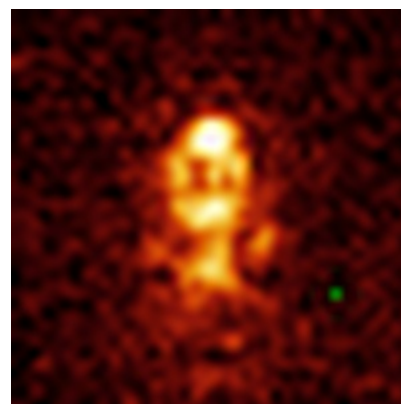
6.4.1 Primary map



X

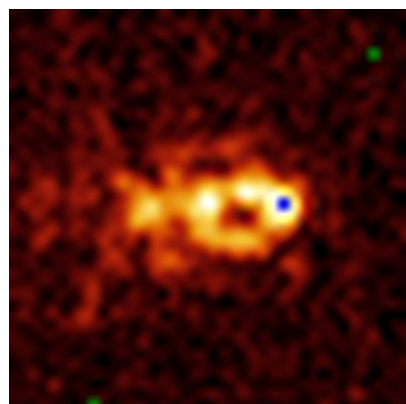


Y

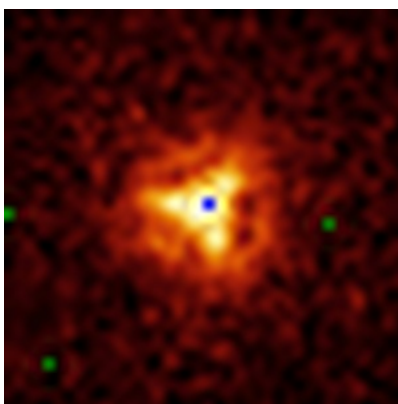


Z

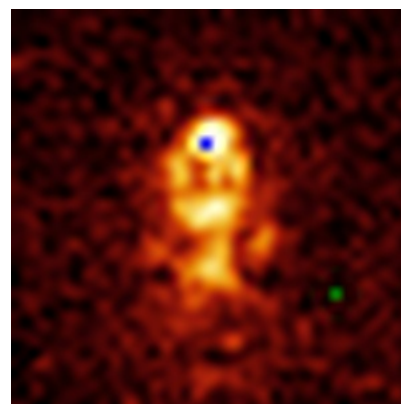
6.4.2 Raw map



X



Y

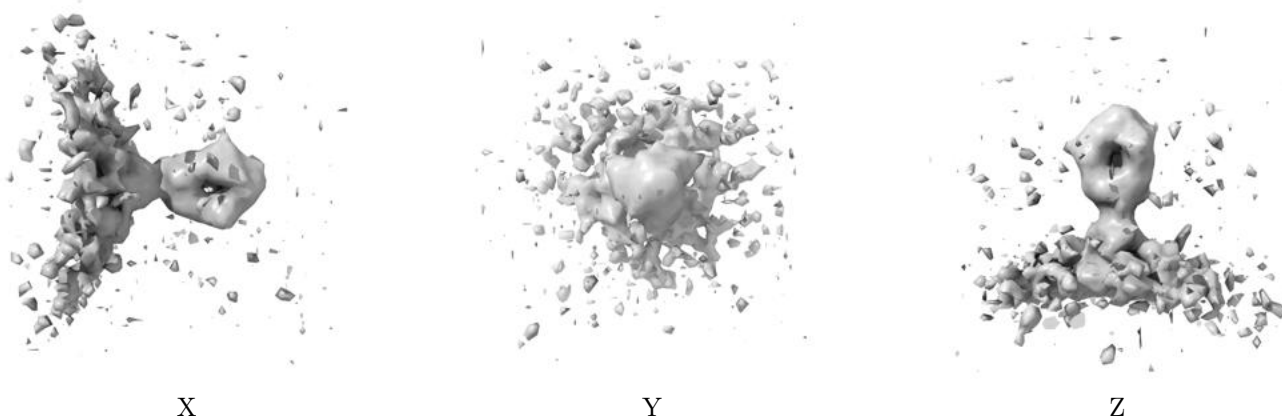


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

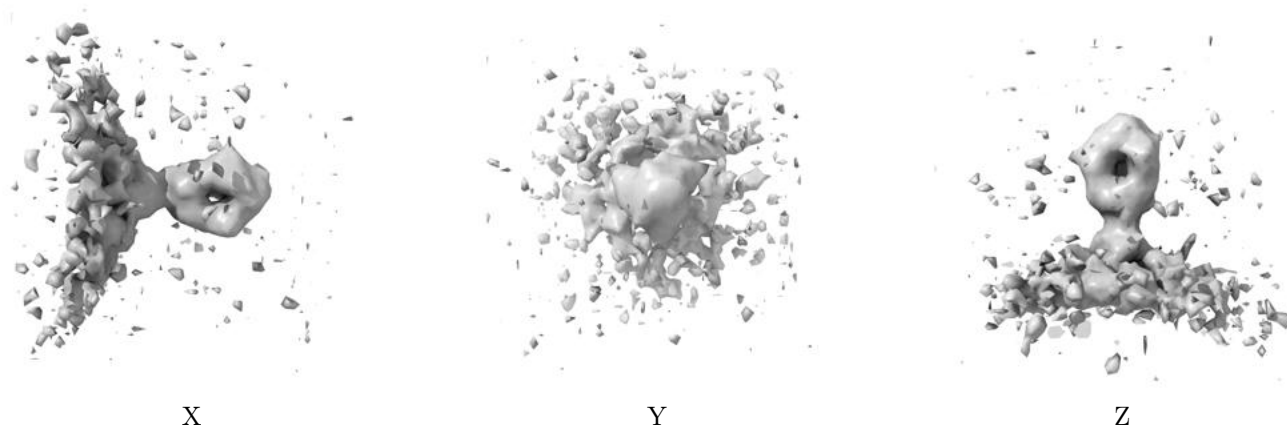
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.55. 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.

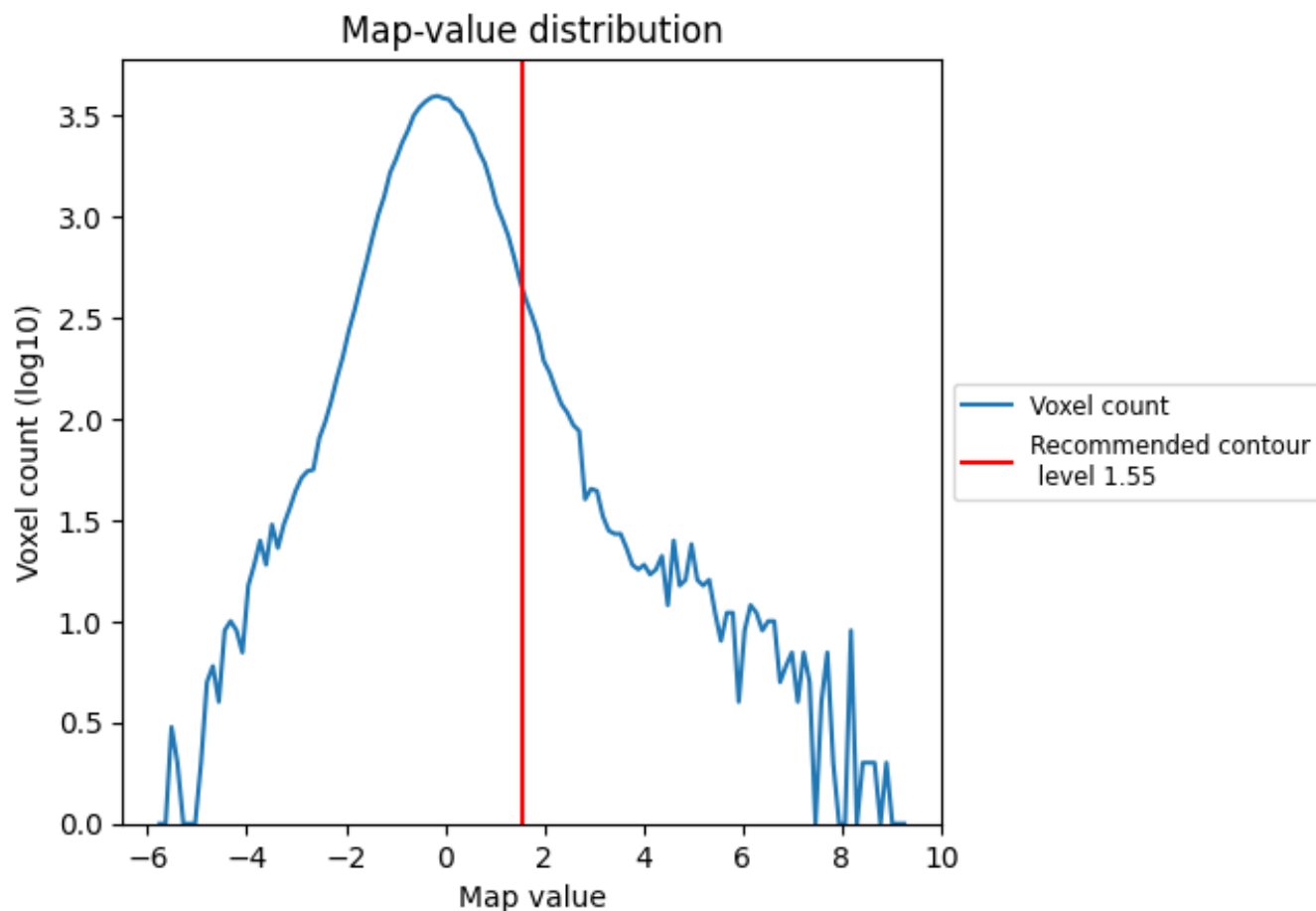
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

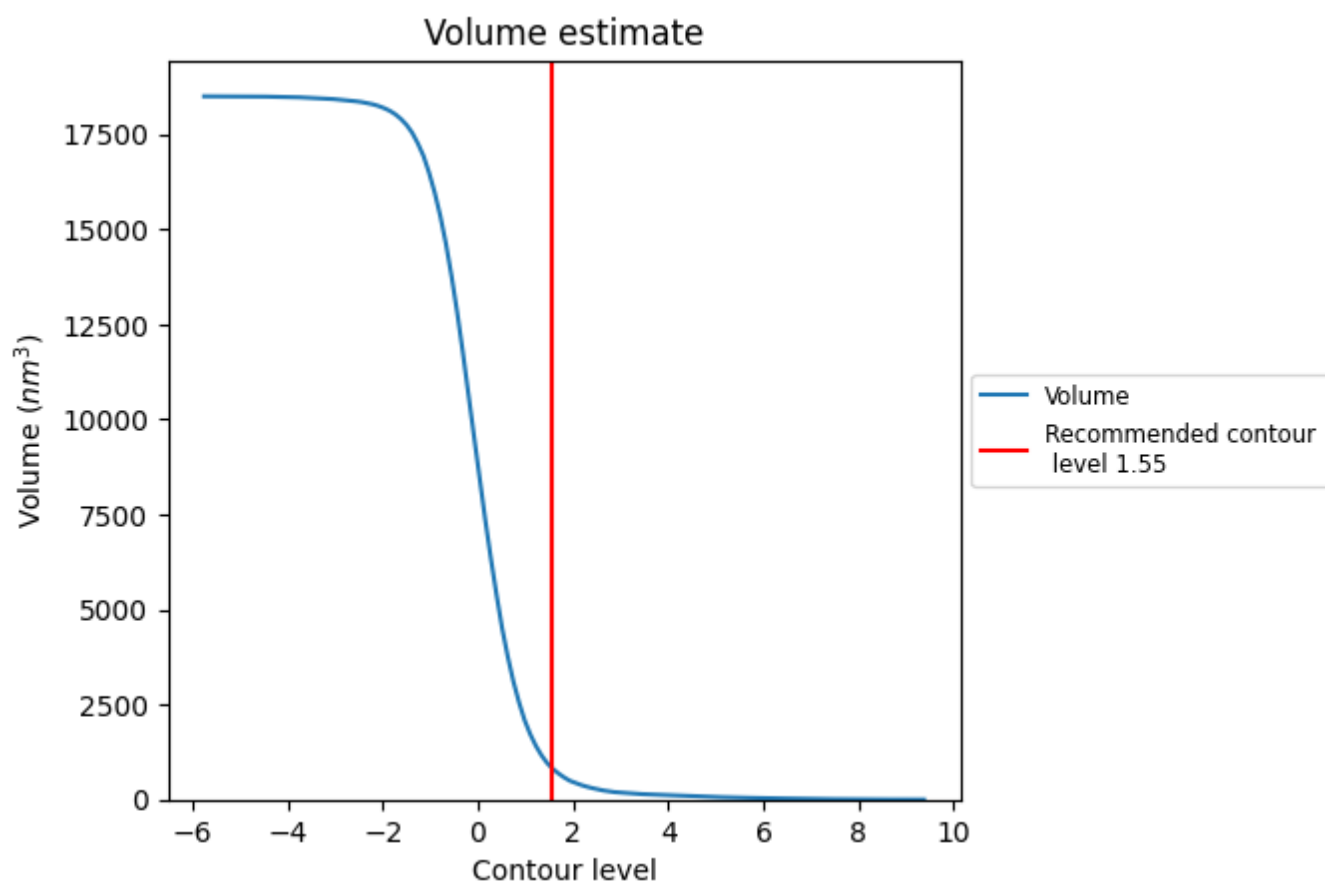
This section contains the results of statistical analysis of the map.

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.

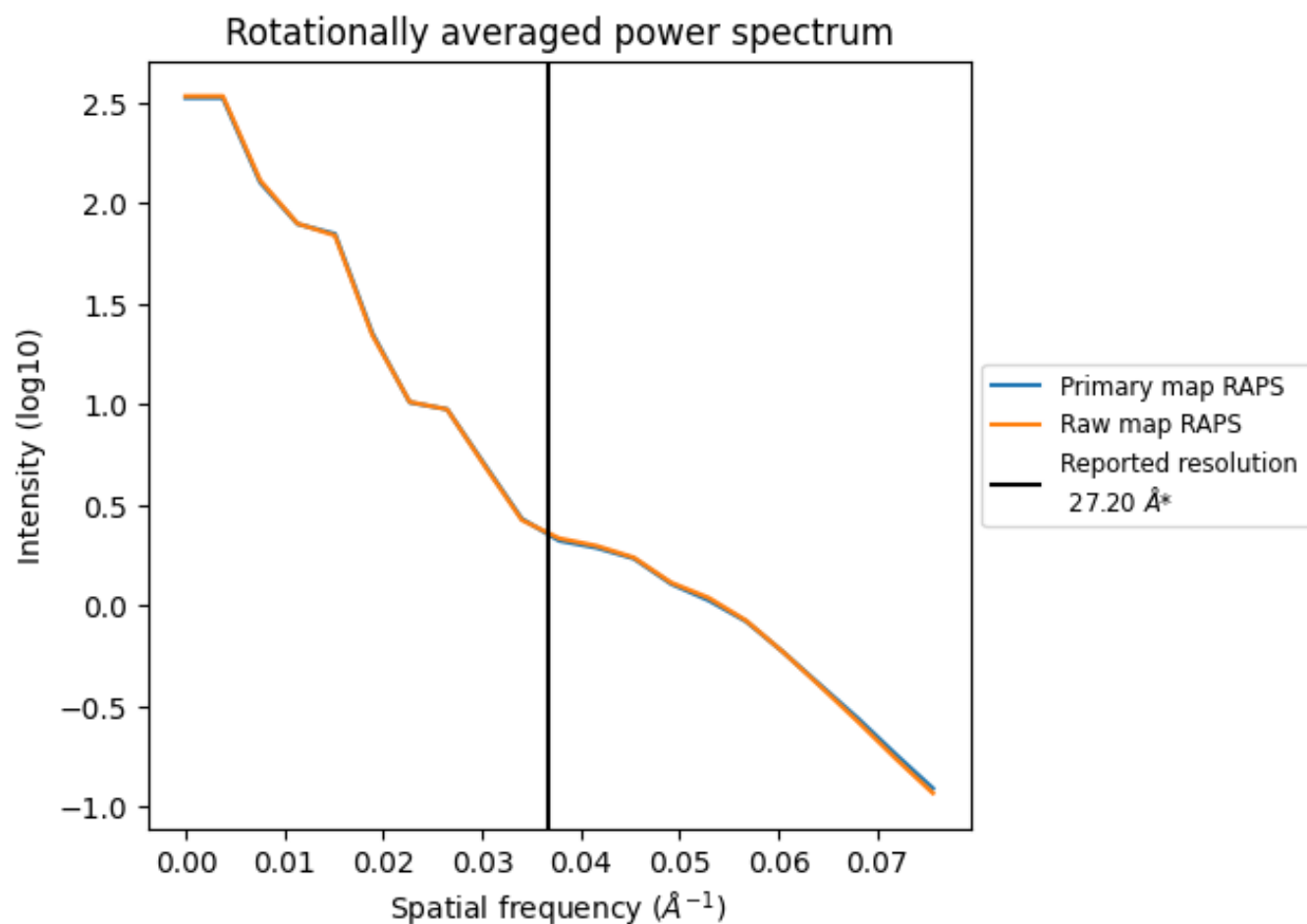
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 842 nm³; this corresponds to an approximate mass of 760 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 ⓘ

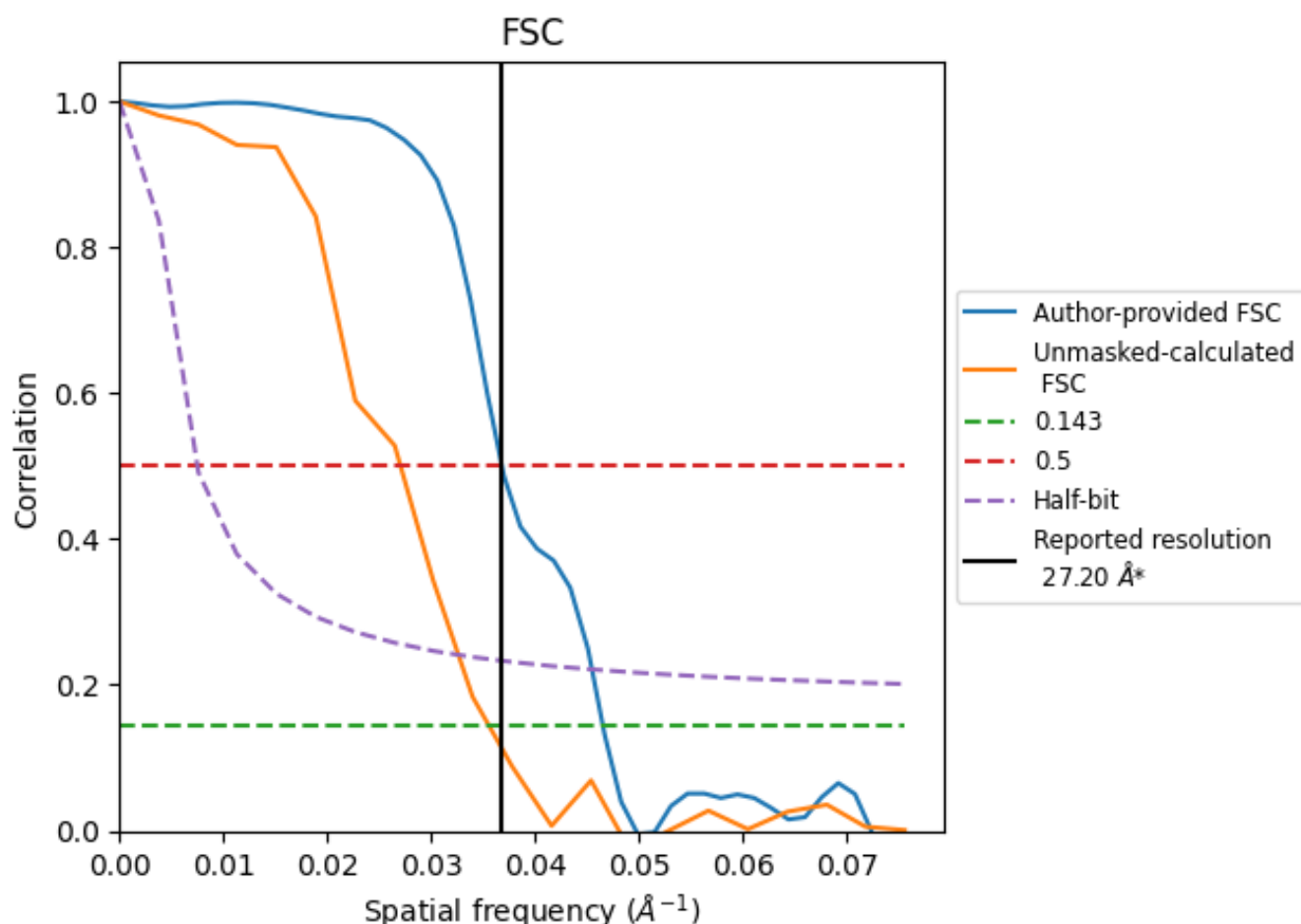


*Reported resolution corresponds to spatial frequency of 0.037 \AA^{-1}

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 0.037 Å⁻¹

8.2 Resolution estimates [i](#)

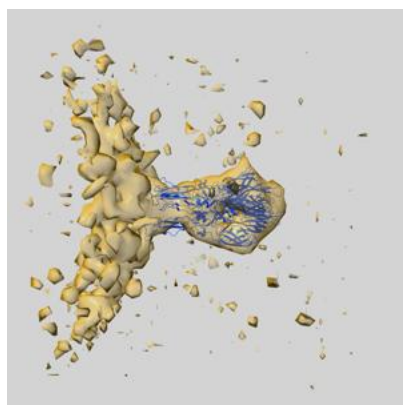
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	27.20	-
Author-provided FSC curve	21.51	27.17	21.83
Unmasked-calculated*	28.09	37.04	30.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 37.04 differs from the reported value 27.2 by more than 10 %

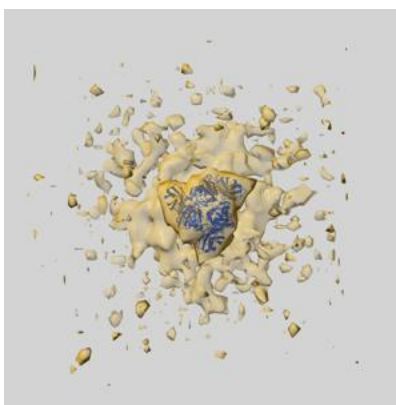
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27248 and PDB model 8D87. Per-residue inclusion information can be found in section [3](#) on page [7](#).

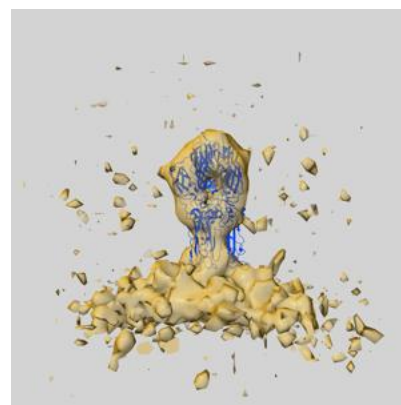
9.1 Map-model overlay [i](#)



X



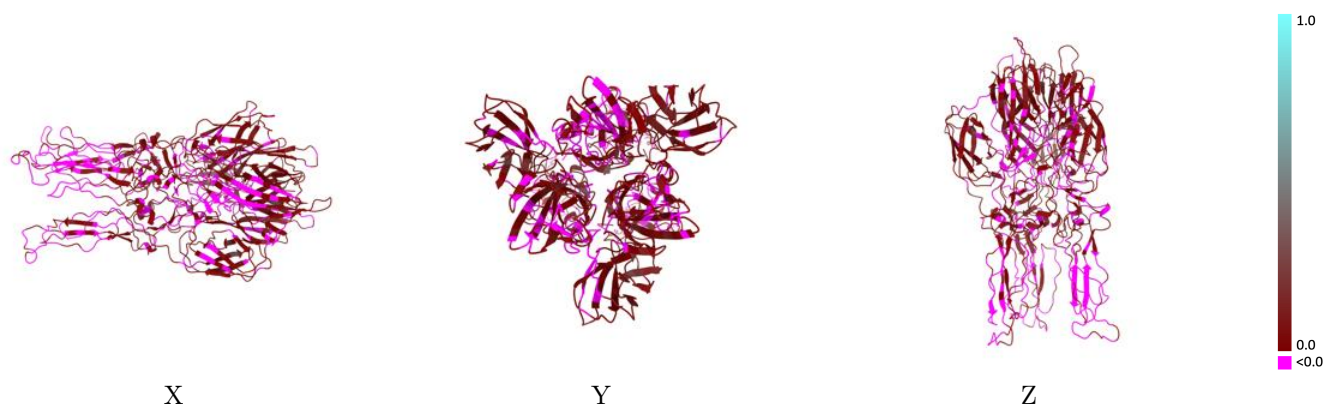
Y



Z

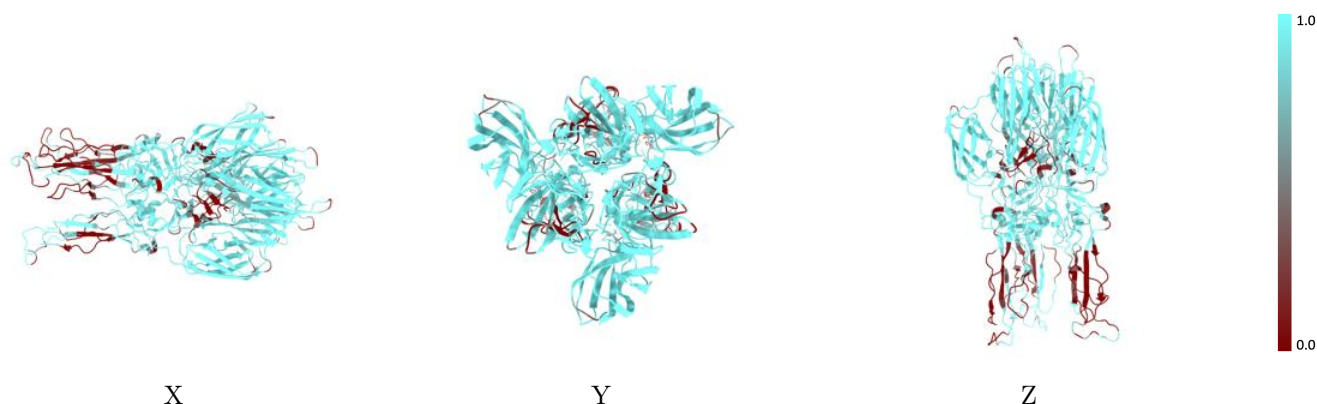
The images above show the 3D surface view of the map at the recommended contour level 1.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



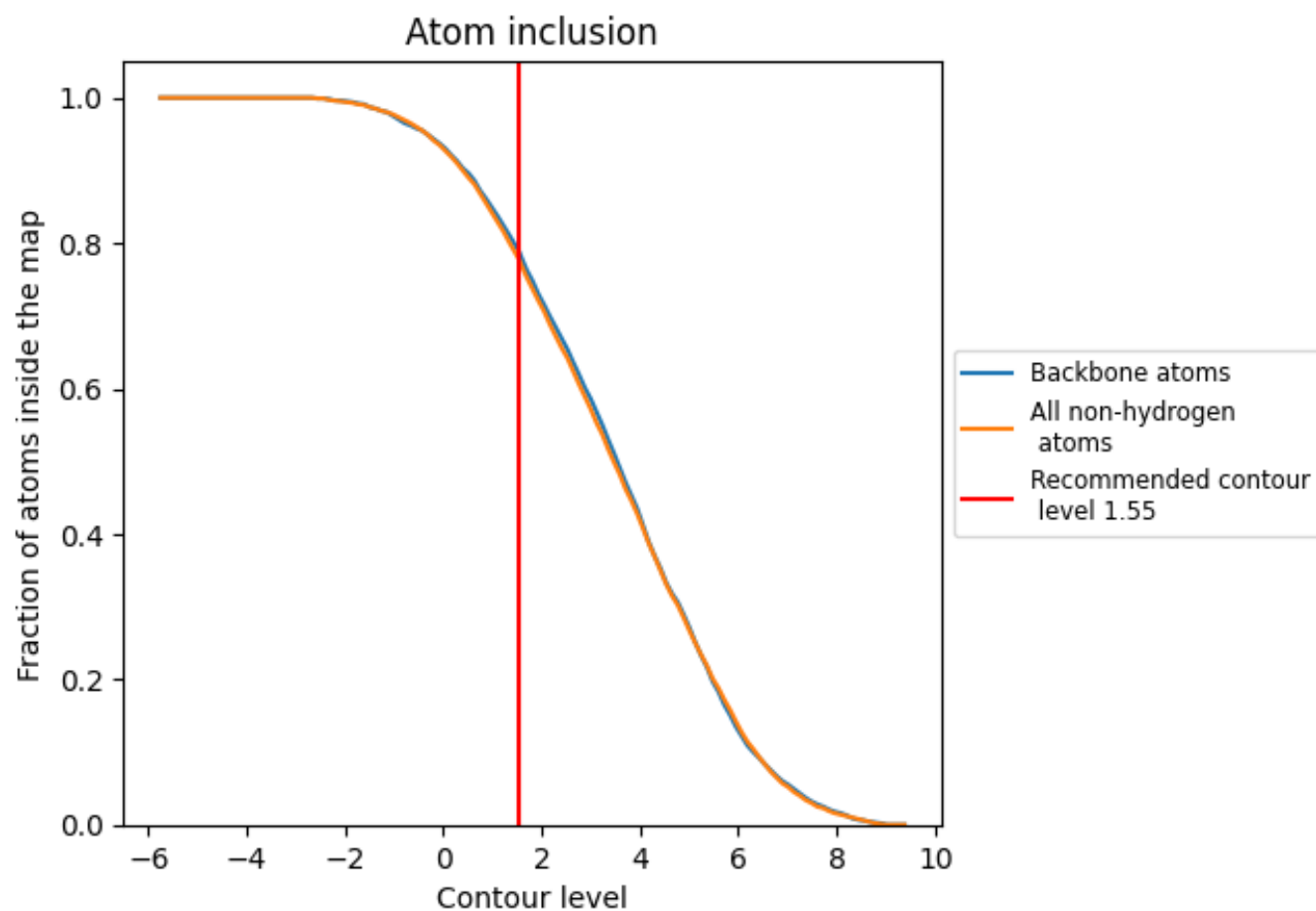
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7760	<div></div> 0.0290
A	<div></div> 0.7520	<div></div> 0.0210
B	<div></div> 0.7900	<div></div> 0.0370
C	<div></div> 0.8280	<div></div> 0.0310
D	<div></div> 0.1620	<div></div> -0.0280
E	<div></div> 0.0710	<div></div> 0.0090
F	<div></div> 0.5000	<div></div> 0.0540

