Full wwPDB EM Validation Report ⓘ

Sep 5, 2023 – 12:44 PM EDT

PDB ID	:	8TY1
EMDB ID	:	EMD-41710
Title	:	Cryo-EM structure of coagulation factor VIII bound to NB2E9
Authors	:	Childers, K.C.; Spiegel, P.C.
Deposited on	:	2023-08-24
Resolution	:	3.46 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:

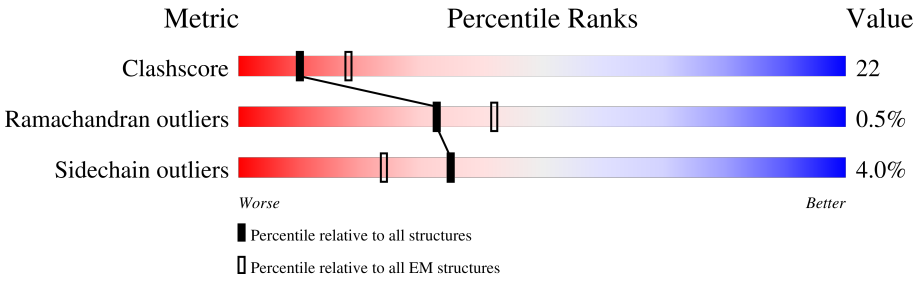
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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 <=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	1467	5% 46% 37% · 16%
2	B	216	· 57% 36% · 6%
3	C	235	· 55% 42% ·
4	D	4	25% 50% 25%
4	E	4	50% 50% 50%
4	F	4	25% 75%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13508 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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1236	Total	C	N	O	S	0	0
			10004	6426	1714	1812	52		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1627	ALA	SER	conflict	UNP P00451
A	1632	PRO	HIS	conflict	UNP P00451
A	1635	ALA	THR	conflict	UNP P00451
A	1636	SER	ARG	conflict	UNP P00451

- Molecule 2 is a protein called NB2E9 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	204	Total	C	N	O	S	0	0
			1570	988	267	311	4		

- Molecule 3 is a protein called NB2E9 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1784	1120	303	352	9		

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

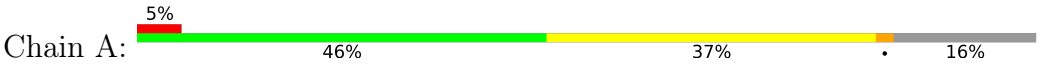
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	4	Total	C	N	O	0	0
			50	28	2	20		
4	E	4	Total	C	N	O	0	0
			50	28	2	20		
4	F	4	Total	C	N	O	0	0
			50	28	2	20		

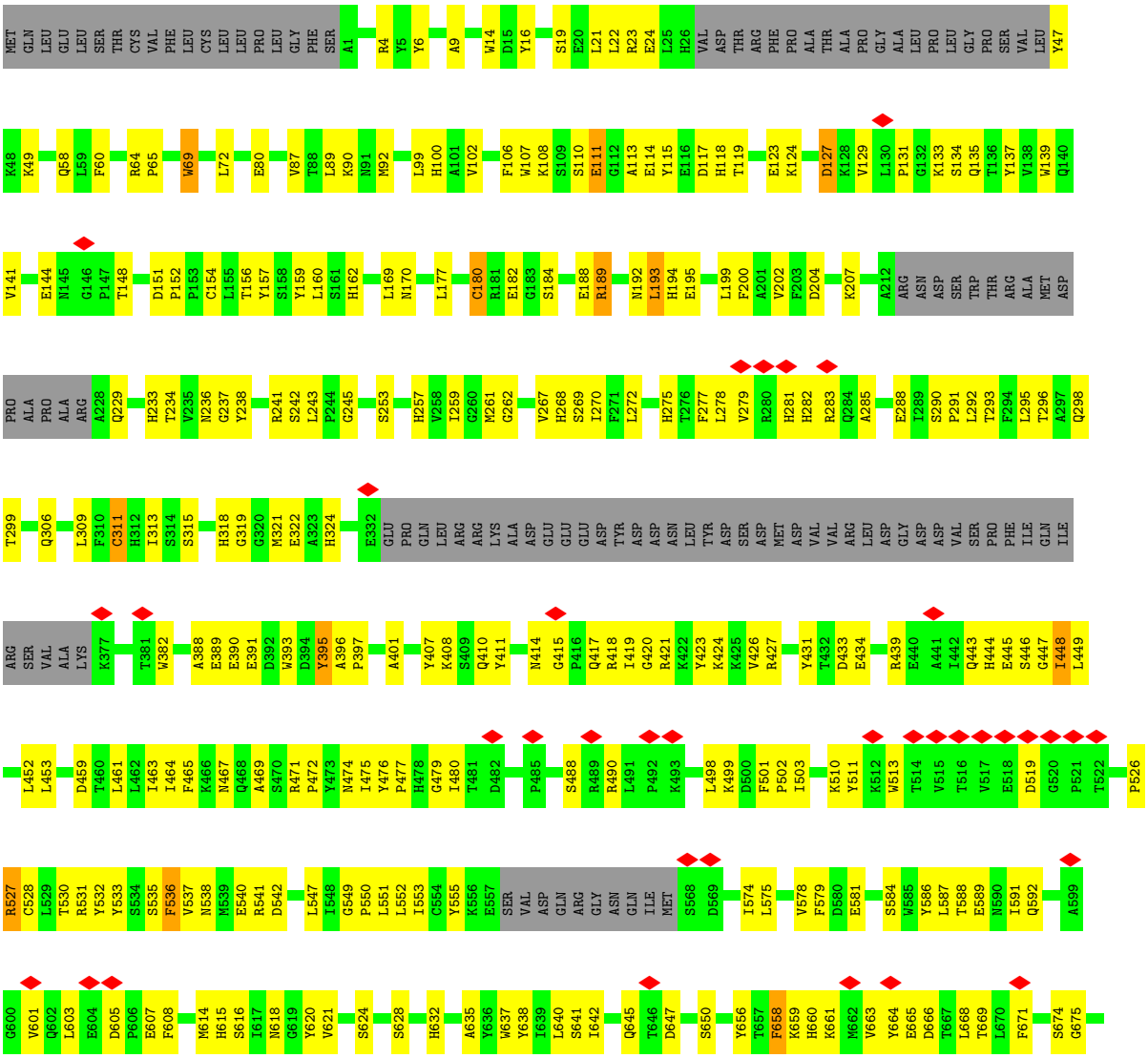
3 Residue-property plots (i)

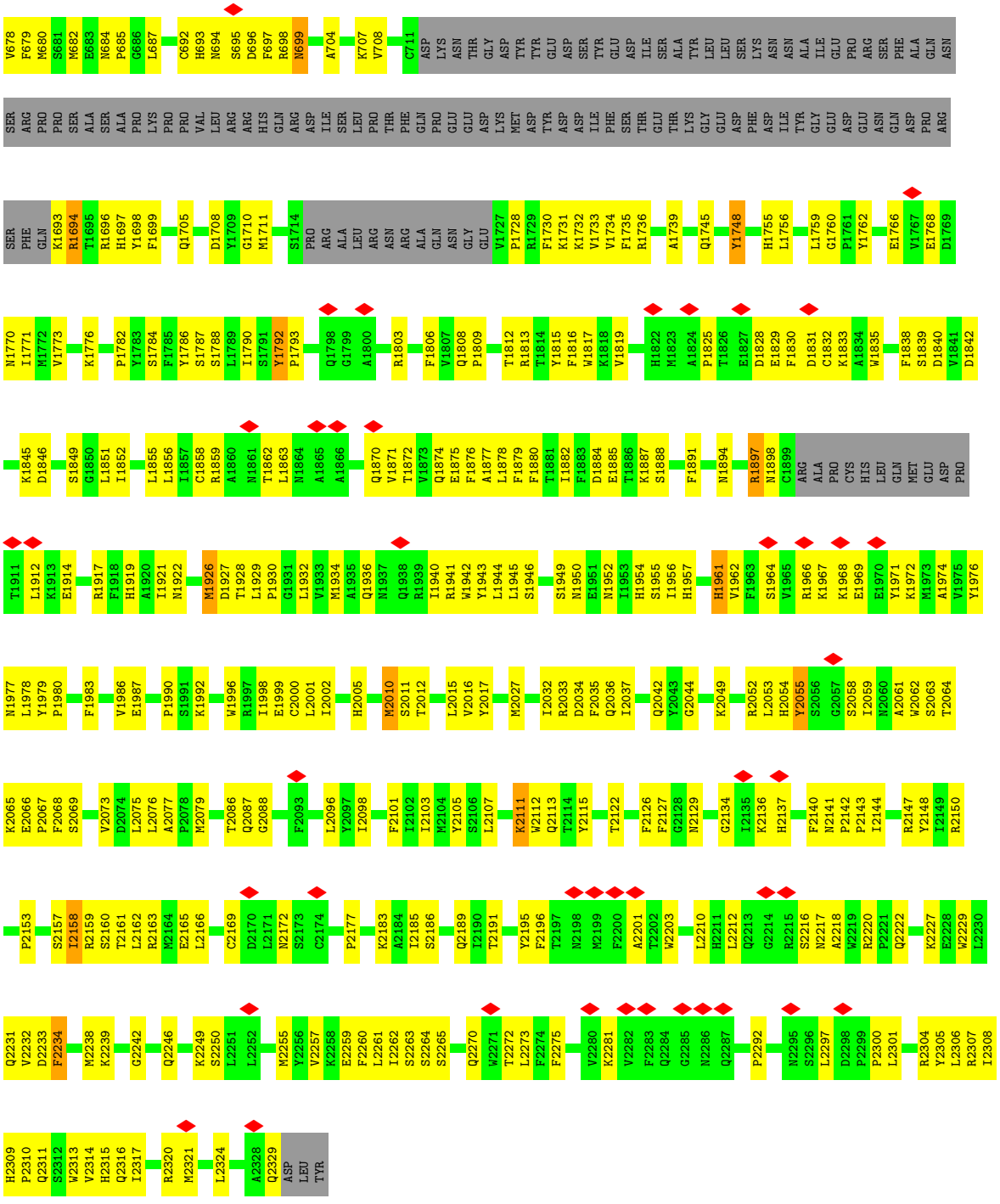
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Coagulation factor VIII

Chain A:

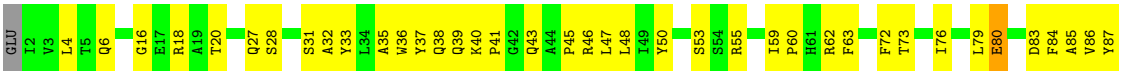


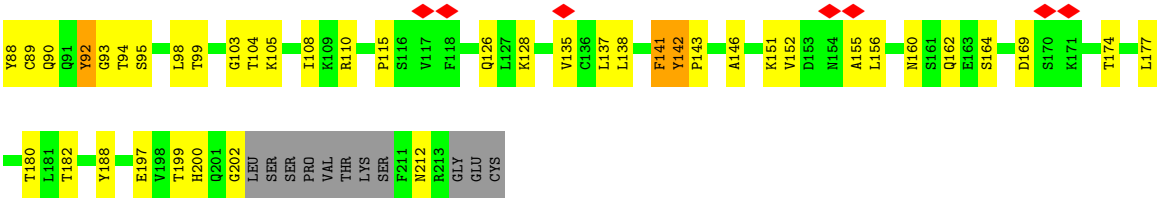




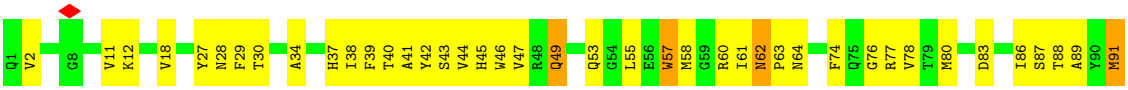
• Molecule 2: NB2E9 light chain

Chain B:

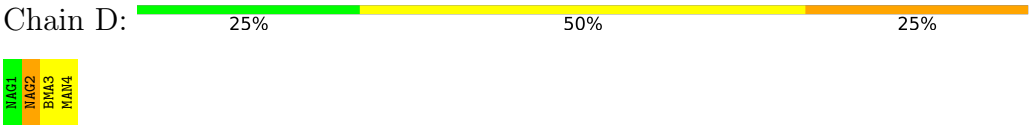




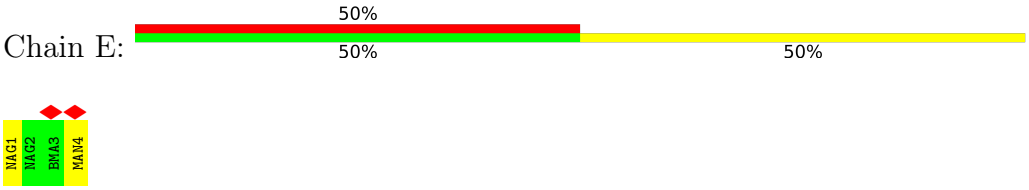
• Molecule 3: NB2E9 heavy chain



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



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



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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94935	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.692	Depositor
Minimum map value	-0.392	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0443	Depositor
Map size (Å)	425.52, 425.52, 425.52	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.788, 0.788, 0.788	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/10285	0.58	1/13941 (0.0%)
2	B	0.31	0/1604	0.58	0/2177
3	C	0.30	0/1830	0.55	1/2492 (0.0%)
All	All	0.32	0/13719	0.58	2/18610 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	209	PRO	CA-N-CD	-6.79	101.99	111.50
1	A	193	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	CYS	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	10004	0	9751	427	0
2	B	1570	0	1526	68	0
3	C	1784	0	1717	97	0
4	D	50	0	43	1	0
4	E	50	0	43	0	0
4	F	50	0	43	3	0
All	All	13508	0	13123	576	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 22.

All (576) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:SER:HA	1:A:2160:SER:O	1.65	0.96
1:A:110:SER:HG	1:A:139:TRP:HE1	1.15	0.94
3:C:107:ALA:HB2	3:C:127:TRP:HE1	1.38	0.89
2:B:18:ARG:HA	2:B:76:ILE:O	1.75	0.85
3:C:46:TRP:NE1	3:C:80:MET:SD	2.50	0.84
1:A:154:CYS:HA	1:A:180:CYS:HB3	1.60	0.84
1:A:427:ARG:HD3	1:A:448:ILE:HA	1.57	0.84
1:A:581:GLU:HB3	1:A:587:LEU:HD13	1.61	0.82
1:A:1877:ALA:O	1:A:1922:ASN:ND2	2.12	0.82
1:A:389:GLU:OE2	1:A:439:ARG:NH2	2.14	0.81
1:A:2068:PHE:HE2	3:C:120:THR:HG21	1.45	0.81
2:B:59:ILE:HD12	2:B:60:PRO:HD2	1.62	0.80
1:A:2150:ARG:HH12	3:C:116:VAL:HG21	1.46	0.80
1:A:22:LEU:HG	1:A:23:ARG:HH21	1.45	0.80
1:A:111:GLU:OE2	1:A:115:TYR:OH	2.01	0.78
3:C:101:THR:HA	3:C:133:VAL:O	1.84	0.77
1:A:1946:SER:OG	1:A:1952:ASN:ND2	2.20	0.75
1:A:99:LEU:HD21	1:A:139:TRP:HZ2	1.50	0.75
2:B:151:LYS:HE3	2:B:151:LYS:HA	1.67	0.75
1:A:156:THR:HG21	1:A:257:HIS:HB3	1.68	0.74
1:A:2315:HIS:O	1:A:2316:GLN:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:TRP:CZ3	1:A:2307:ARG:HG2	2.24	0.72
1:A:2265:SER:O	1:A:2305:TYR:HB2	1.90	0.72
1:A:531:ARG:HE	1:A:553:ILE:HD11	1.53	0.71
1:A:1693:LYS:N	1:A:1768:GLU:O	2.23	0.71
1:A:661:LYS:HG2	1:A:1968:LYS:HD3	1.74	0.70
1:A:1878:LEU:HD22	1:A:1921:ILE:HD11	1.74	0.70
1:A:2141:ASN:HB2	1:A:2142:PRO:HD3	1.72	0.69
1:A:1880:PHE:HD2	1:A:2010:MET:HG3	1.57	0.69
1:A:2062:TRP:O	1:A:2161:THR:HA	1.93	0.69
2:B:152:VAL:O	2:B:155:ALA:HB3	1.91	0.69
1:A:1957:HIS:HB3	1:A:1999:GLU:HB3	1.74	0.69
1:A:1870:GLN:O	1:A:1872:THR:N	2.23	0.69
1:A:1825:PRO:HB3	1:A:1829:GLU:HG2	1.76	0.68
1:A:694:ASN:HB2	1:A:697:PHE:HB2	1.75	0.68
1:A:89:LEU:HD13	1:A:99:LEU:HB2	1.75	0.68
2:B:92:TYR:HA	2:B:98:LEU:HG	1.74	0.68
1:A:2260:PHE:HB2	1:A:2308:ILE:HD11	1.76	0.67
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.30	0.67
1:A:2034:ASP:HB2	1:A:2049:LYS:HB2	1.77	0.67
1:A:669:THR:HG21	1:A:1979:TYR:HB3	1.76	0.66
3:C:41:ALA:HB2	3:C:110:ASP:HB2	1.77	0.66
1:A:620:TYR:HB3	1:A:624:SER:HB2	1.76	0.66
1:A:2203:TRP:HB3	1:A:2220:ARG:H	1.60	0.66
1:A:156:THR:HG22	1:A:259:ILE:HD11	1.78	0.65
1:A:1894:ASN:O	1:A:1897:ARG:NH1	2.29	0.65
3:C:115:ILE:HG13	3:C:116:VAL:H	1.62	0.65
1:A:1952:ASN:OD1	1:A:1954:HIS:NE2	2.29	0.65
1:A:415:GLY:HA3	1:A:418:ARG:NH1	2.12	0.65
3:C:145:VAL:O	3:C:233:LYS:NZ	2.29	0.65
1:A:2098:ILE:HD13	1:A:2153:PRO:HB3	1.78	0.65
1:A:1990:PRO:HB2	1:A:2016:VAL:HG11	1.80	0.64
1:A:69:TRP:HD1	1:A:243:LEU:HD11	1.60	0.64
3:C:159:THR:HG23	3:C:209:PRO:HD3	1.79	0.64
1:A:2255:MET:HA	1:A:2314:VAL:O	1.97	0.64
1:A:1838:PHE:HB3	1:A:1852:ILE:HD12	1.79	0.63
1:A:530:THR:OG1	1:A:640:LEU:HD11	1.98	0.63
1:A:6:TYR:HB3	1:A:60:PHE:CZ	2.34	0.63
1:A:414:ASN:ND2	1:A:419:ILE:O	2.32	0.63
3:C:149:ALA:HB2	3:C:235:VAL:HG12	1.81	0.63
1:A:446:SER:HB3	1:A:449:LEU:HD11	1.81	0.63
1:A:1694:ARG:HH21	1:A:1696:ARG:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLN:HA	1:A:418:ARG:HD3	1.81	0.62
1:A:1992:LYS:HB3	1:A:1996:TRP:HZ2	1.64	0.62
1:A:2088:GLY:O	1:A:2163:ARG:NH2	2.30	0.62
1:A:87:VAL:HG11	1:A:99:LEU:HD13	1.82	0.62
1:A:531:ARG:HE	1:A:553:ILE:CD1	2.13	0.62
1:A:2189:GLN:NE2	1:A:2233:ASP:O	2.32	0.62
1:A:528:CYS:HA	1:A:553:ILE:O	1.99	0.62
1:A:4:ARG:HH11	1:A:6:TYR:HE2	1.47	0.62
1:A:2201:ALA:HB1	1:A:2203:TRP:HD1	1.64	0.61
3:C:47:VAL:HG21	3:C:55:LEU:HD12	1.82	0.61
1:A:135:GLN:OE1	1:A:137:TYR:OH	2.14	0.61
1:A:291:PRO:HB2	1:A:2002:ILE:HD12	1.81	0.61
2:B:16:GLY:N	2:B:79:LEU:O	2.30	0.61
1:A:2234:PHE:HD2	1:A:2238:MET:HG2	1.65	0.61
1:A:1875:GLU:HA	1:A:1941:ARG:O	2.00	0.61
3:C:37:HIS:HB3	3:C:120:THR:HB	1.83	0.61
1:A:267:VAL:HG12	1:A:290:SER:HA	1.82	0.61
1:A:2033:ARG:NH1	1:A:2035:PHE:HB3	2.16	0.61
1:A:2229:TRP:CZ3	1:A:2231:GLN:HB2	2.36	0.61
1:A:2265:SER:HA	1:A:2270:GLN:HE21	1.65	0.61
4:F:1:NAG:O3	4:F:2:NAG:N2	2.28	0.61
1:A:658:PHE:HE1	1:A:668:LEU:HB2	1.65	0.60
1:A:1943:TYR:HB3	1:A:1983:PHE:HE2	1.65	0.60
1:A:6:TYR:OH	1:A:58:GLN:NE2	2.34	0.60
1:A:19:SER:OG	1:A:242:SER:OG	2.19	0.60
3:C:107:ALA:HB2	3:C:127:TRP:NE1	2.14	0.60
3:C:145:VAL:HG22	3:C:166:VAL:HG13	1.83	0.60
2:B:38:GLN:O	2:B:46:ARG:N	2.35	0.60
1:A:1949:SER:OG	1:A:1950:ASN:N	2.35	0.60
1:A:474:ASN:ND2	1:A:501:PHE:O	2.25	0.60
1:A:1870:GLN:C	1:A:1872:THR:H	2.05	0.60
1:A:390:GLU:HB3	1:A:424:LYS:HE3	1.83	0.59
1:A:477:PRO:HD3	1:A:513:TRP:CZ2	2.37	0.59
1:A:2066:GLU:HA	2:B:95:SER:H	1.67	0.59
2:B:110:ARG:O	2:B:142:TYR:OH	2.15	0.59
1:A:396:ALA:HB3	1:A:421:ARG:HE	1.66	0.59
1:A:1914:GLU:HA	1:A:1917:ARG:HD3	1.83	0.59
3:C:76:GLY:O	3:C:95:ARG:NH1	2.35	0.59
1:A:1825:PRO:HG3	1:A:1833:LYS:HB2	1.85	0.59
2:B:151:LYS:NZ	2:B:156:LEU:HD13	2.17	0.59
1:A:108:LYS:HG3	1:A:123:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1739:ALA:H	1:A:1745:GLN:HE21	1.51	0.59
1:A:1944:LEU:HD12	1:A:1986:VAL:HG11	1.84	0.59
1:A:395:TYR:HB2	1:A:621:VAL:HG12	1.84	0.59
1:A:2063:SER:HB2	1:A:2161:THR:HG23	1.85	0.59
1:A:531:ARG:HH21	1:A:553:ILE:HG12	1.67	0.59
1:A:269:SER:O	1:A:270:ILE:HD13	2.04	0.58
1:A:1955:SER:O	1:A:2000:CYS:HA	2.03	0.58
1:A:574:ILE:HD11	1:A:637:TRP:HZ3	1.67	0.58
1:A:1770:ASN:HB3	1:A:1816:PHE:HE1	1.68	0.58
3:C:221:ASN:HD21	3:C:230:LYS:HE3	1.68	0.58
1:A:1943:TYR:HB3	1:A:1983:PHE:CE2	2.38	0.58
2:B:128:LYS:N	2:B:128:LYS:HD3	2.18	0.58
3:C:111:ASN:OD1	3:C:121:SER:OG	2.19	0.58
1:A:1711:MET:SD	1:A:1711:MET:N	2.76	0.58
2:B:93:GLY:H	2:B:98:LEU:HD12	1.68	0.58
2:B:40:LYS:HD3	2:B:41:PRO:HD2	1.84	0.58
1:A:281:HIS:HA	1:A:526:PRO:HD3	1.86	0.58
1:A:159:TYR:HB3	1:A:177:LEU:HD12	1.85	0.57
1:A:2027:MET:HB2	1:A:2165:GLU:OE1	2.03	0.57
1:A:635:ALA:HB1	1:A:637:TRP:HE1	1.68	0.57
1:A:2068:PHE:CE2	3:C:120:THR:HG21	2.34	0.57
1:A:49:LYS:HD2	1:A:72:LEU:HD21	1.85	0.57
1:A:117:ASP:OD2	1:A:119:THR:OG1	2.21	0.57
1:A:295:LEU:HD12	1:A:296:THR:H	1.68	0.57
1:A:1929:LEU:HD23	1:A:1932:LEU:HD11	1.87	0.57
2:B:36:TRP:CZ3	2:B:89:CYS:HB3	2.39	0.57
1:A:1745:GLN:N	1:A:1745:GLN:OE1	2.37	0.57
1:A:2017:TYR:CE2	1:A:2143:PRO:HG2	2.39	0.57
1:A:2203:TRP:CG	1:A:2220:ARG:HB2	2.40	0.57
2:B:160:ASN:ND2	2:B:182:THR:O	2.32	0.57
3:C:83:ASP:OD2	3:C:86:ILE:N	2.38	0.57
1:A:668:LEU:HD12	1:A:669:THR:H	1.69	0.57
1:A:2201:ALA:HB1	1:A:2203:TRP:CD1	2.40	0.57
1:A:1998:ILE:O	1:A:2011:SER:OG	2.14	0.56
1:A:2073:VAL:HG11	1:A:2166:LEU:HD11	1.87	0.56
1:A:124:LYS:O	1:A:124:LYS:NZ	2.28	0.56
1:A:1710:GLY:HA2	1:A:1928:THR:HG21	1.88	0.56
1:A:1941:ARG:NH2	1:A:1943:TYR:OH	2.38	0.56
3:C:96:LEU:HD22	3:C:135:VAL:HG21	1.88	0.56
1:A:1926:MET:HA	1:A:2012:THR:HB	1.88	0.56
1:A:279:VAL:HG23	1:A:282:HIS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LEU:HA	1:A:707:LYS:HZ2	1.70	0.56
1:A:2068:PHE:O	2:B:33:TYR:OH	2.23	0.56
1:A:498:LEU:HD21	1:A:511:TYR:HD2	1.71	0.56
1:A:2185:ILE:HD11	1:A:2234:PHE:CE1	2.41	0.56
3:C:234:ARG:NH1	3:C:235:VAL:O	2.38	0.56
1:A:658:PHE:CE1	1:A:668:LEU:HB2	2.41	0.56
1:A:2107:LEU:HD12	1:A:2111:LYS:HZ1	1.71	0.56
1:A:532:TYR:CZ	1:A:642:ILE:HG21	2.41	0.55
1:A:453:LEU:HD12	1:A:551:LEU:HG	1.87	0.55
1:A:1941:ARG:HG2	1:A:1987:GLU:HG2	1.89	0.55
2:B:60:PRO:HG2	2:B:62:ARG:HH11	1.71	0.55
2:B:98:LEU:HB3	3:C:57:TRP:CG	2.42	0.55
1:A:641:SER:O	1:A:645:GLN:NE2	2.39	0.55
1:A:148:THR:N	1:A:151:ASP:OD2	2.38	0.55
1:A:2191:THR:HG22	1:A:2231:GLN:HB3	1.89	0.55
2:B:88:TYR:HD2	2:B:103:GLY:HA2	1.72	0.55
3:C:86:ILE:HD12	3:C:86:ILE:H	1.72	0.55
1:A:1730:PHE:HB3	1:A:1894:ASN:ND2	2.22	0.54
1:A:461:LEU:HD23	1:A:461:LEU:H	1.72	0.54
1:A:2129:ASN:HD21	1:A:2162:LEU:HD11	1.71	0.54
1:A:527:ARG:HB2	1:A:555:TYR:HB3	1.88	0.54
1:A:241:ARG:HB3	1:A:324:HIS:CD2	2.42	0.54
1:A:535:SER:HB3	1:A:542:ASP:CG	2.28	0.54
1:A:579:PHE:HB2	1:A:614:MET:SD	2.47	0.54
1:A:1977:ASN:O	1:A:1978:LEU:HD23	2.08	0.54
1:A:2067:PRO:HD3	2:B:95:SER:H	1.73	0.54
2:B:88:TYR:CD2	2:B:103:GLY:HA2	2.43	0.54
1:A:1735:PHE:HB2	1:A:1760:GLY:HA3	1.89	0.54
1:A:111:GLU:O	1:A:113:ALA:N	2.40	0.54
1:A:114:GLU:HG2	1:A:127:ASP:OD2	2.07	0.54
1:A:275:HIS:HE1	1:A:299:THR:HB	1.73	0.54
1:A:693:HIS:HA	1:A:698:ARG:HD2	1.90	0.54
1:A:407:TYR:CE2	1:A:699:ASN:ND2	2.76	0.54
1:A:1766:GLU:OE1	1:A:1858:CYS:HB2	2.08	0.54
1:A:1862:THR:HG23	1:A:1863:LEU:HD12	1.90	0.53
1:A:1879:PHE:CD1	1:A:1945:LEU:HD23	2.43	0.53
1:A:2066:GLU:HB3	2:B:94:THR:HB	1.89	0.53
2:B:115:PRO:HB3	2:B:141:PHE:HA	1.89	0.53
1:A:541:ARG:NH2	1:A:584:SER:O	2.37	0.53
1:A:1786:TYR:CZ	1:A:1788:SER:HA	2.43	0.53
1:A:1756:LEU:HD21	1:A:1762:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:PRO:HD2	2:B:146:ALA:HB2	1.89	0.53
3:C:102:ALA:HB3	3:C:104:TYR:HE1	1.73	0.53
1:A:19:SER:HG	1:A:242:SER:HG	1.54	0.53
1:A:124:LYS:NZ	1:A:127:ASP:HB2	2.24	0.53
1:A:1874:GLN:HG3	1:A:1876:PHE:CE1	2.44	0.53
1:A:2087:GLN:NE2	1:A:2134:GLY:O	2.38	0.53
1:A:80:GLU:OE2	1:A:184:SER:N	2.42	0.53
1:A:474:ASN:OD1	1:A:475:ILE:N	2.41	0.53
1:A:107:TRP:CD1	1:A:1992:LYS:HG3	2.44	0.53
1:A:395:TYR:HB3	1:A:620:TYR:HA	1.91	0.53
1:A:397:PRO:HD2	1:A:624:SER:HB3	1.89	0.53
1:A:532:TYR:CE1	1:A:642:ILE:HG12	2.44	0.53
1:A:1831:ASP:HA	1:A:1859:ARG:CZ	2.38	0.53
2:B:33:TYR:CE1	2:B:94:THR:HG21	2.43	0.53
1:A:144:GLU:O	1:A:1972:LYS:NZ	2.42	0.52
1:A:2002:ILE:HB	1:A:2005:HIS:HD2	1.74	0.52
1:A:2033:ARG:HH12	1:A:2035:PHE:HB3	1.73	0.52
2:B:39:GLN:O	2:B:85:ALA:HB1	2.09	0.52
1:A:532:TYR:CE2	1:A:642:ILE:HG21	2.43	0.52
1:A:1829:GLU:HG3	1:A:1830:PHE:N	2.24	0.52
1:A:110:SER:CB	1:A:139:TRP:HE1	2.21	0.52
1:A:2086:THR:H	1:A:2136:LYS:HZ1	1.58	0.52
1:A:2065:LYS:HG2	1:A:2159:ARG:HG2	1.90	0.52
4:D:2:NAG:H3	4:D:2:NAG:H83	1.90	0.52
1:A:2027:MET:SD	1:A:2037:ILE:HD11	2.49	0.52
1:A:479:GLY:O	1:A:531:ARG:NH1	2.43	0.52
1:A:1912:LEU:HG	1:A:1914:GLU:H	1.73	0.52
1:A:1955:SER:O	1:A:1956:ILE:HD13	2.10	0.52
2:B:197:GLU:OE1	2:B:199:THR:OG1	2.17	0.52
3:C:147:PRO:HB2	3:C:235:VAL:HG13	1.91	0.52
3:C:157:GLU:HG3	3:C:159:THR:H	1.75	0.52
1:A:275:HIS:CE1	1:A:299:THR:HB	2.45	0.52
1:A:1756:LEU:HD21	1:A:1762:TYR:HE1	1.74	0.52
3:C:18:VAL:HG12	3:C:96:LEU:HD21	1.92	0.52
1:A:2077:ALA:O	1:A:2079:MET:HG3	2.09	0.52
3:C:11:VAL:HG22	3:C:134:THR:HB	1.91	0.52
2:B:39:GLN:HB2	2:B:45:PRO:HB3	1.92	0.52
1:A:2105:TYR:HA	1:A:2148:TYR:O	2.10	0.51
2:B:4:LEU:HD13	2:B:90:GLN:HA	1.92	0.51
1:A:14:TRP:HD1	1:A:16:TYR:H	1.57	0.51
1:A:2262:ILE:HG21	1:A:2301:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:O	1:A:2172:ASN:ND2	2.38	0.51
1:A:1885:GLU:O	1:A:1891:PHE:HB2	2.11	0.51
3:C:224:HIS:HB3	3:C:229:THR:HG22	1.93	0.51
1:A:685:PRO:HA	1:A:708:VAL:HG11	1.92	0.51
1:A:131:PRO:O	1:A:133:LYS:HE2	2.11	0.51
1:A:467:ASN:ND2	1:A:471:ARG:O	2.40	0.51
1:A:253:SER:HB2	1:A:298:GLN:HE21	1.75	0.51
1:A:2263:SER:OG	1:A:2307:ARG:NE	2.44	0.51
1:A:476:TYR:HB3	1:A:536:PHE:CE2	2.45	0.51
1:A:1940:ILE:HD11	1:A:1942:TRP:HE1	1.75	0.51
1:A:1999:GLU:OE1	1:A:2000:CYS:N	2.44	0.51
1:A:47:TYR:HE1	1:A:229:GLN:HG2	1.76	0.51
1:A:2061:ALA:HB3	1:A:2161:THR:HG22	1.93	0.51
2:B:135:VAL:HG23	2:B:180:THR:HG22	1.93	0.51
3:C:208:VAL:O	3:C:210:SER:N	2.44	0.51
3:C:110:ASP:HB3	3:C:126:TYR:HE1	1.76	0.50
1:A:535:SER:HB2	1:A:547:LEU:HD12	1.93	0.50
1:A:575:LEU:N	1:A:618:ASN:OD1	2.44	0.50
1:A:2027:MET:O	1:A:2052:ARG:NH1	2.35	0.50
2:B:126:GLN:NE2	3:C:147:PRO:O	2.44	0.50
1:A:2076:LEU:HA	1:A:2147:ARG:HH21	1.76	0.50
1:A:464:ILE:HG23	1:A:510:LYS:HG3	1.92	0.50
1:A:1782:PRO:HB3	1:A:1808:GLN:HA	1.93	0.50
1:A:306:GLN:OE1	1:A:324:HIS:ND1	2.44	0.50
1:A:642:ILE:HD12	1:A:642:ILE:H	1.77	0.50
1:A:2076:LEU:HD23	1:A:2147:ARG:HH21	1.77	0.50
1:A:2177:PRO:HD3	1:A:2324:LEU:HD22	1.93	0.50
1:A:14:TRP:O	1:A:47:TYR:HB2	2.12	0.50
1:A:388:ALA:HA	1:A:427:ARG:O	2.12	0.50
1:A:393:TRP:HB2	1:A:427:ARG:HH22	1.76	0.50
1:A:2086:THR:H	1:A:2136:LYS:NZ	2.09	0.50
1:A:1945:LEU:HD22	1:A:1983:PHE:CE1	2.47	0.50
1:A:1733:VAL:HG13	1:A:1851:LEU:HG	1.93	0.50
1:A:2203:TRP:HB3	1:A:2220:ARG:N	2.27	0.50
2:B:53:SER:OG	3:C:114:ASP:OD2	2.28	0.49
3:C:143:PRO:HD3	3:C:229:THR:HG21	1.94	0.49
2:B:162:GLN:NE2	2:B:180:THR:OG1	2.34	0.49
1:A:99:LEU:HD21	1:A:139:TRP:CZ2	2.39	0.49
2:B:38:GLN:NE2	2:B:83:ASP:OD1	2.44	0.49
1:A:2150:ARG:NH1	3:C:116:VAL:HG21	2.20	0.49
1:A:243:LEU:O	1:A:245:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:PHE:CZ	1:A:1921:ILE:HD12	2.48	0.49
1:A:2055:TYR:O	1:A:2163:ARG:NH1	2.44	0.49
1:A:538:ASN:O	1:A:542:ASP:N	2.39	0.49
1:A:1708:ASP:OD1	1:A:1728:PRO:HG2	2.13	0.49
1:A:471:ARG:HE	1:A:472:PRO:HD2	1.77	0.48
1:A:659:LYS:HB3	1:A:679:PHE:HB2	1.95	0.48
3:C:30:THR:OG1	4:F:1:NAG:H4	2.13	0.48
1:A:9:ALA:O	1:A:92:MET:HB3	2.13	0.48
1:A:660:HIS:N	1:A:663:VAL:O	2.44	0.48
1:A:200:PHE:CZ	1:A:270:ILE:HG13	2.47	0.48
1:A:1803:ARG:HE	1:A:1813:ARG:HH22	1.60	0.48
1:A:2079:MET:HB3	1:A:2169:CYS:O	2.13	0.48
1:A:2113:GLN:OE1	1:A:2113:GLN:N	2.46	0.48
1:A:472:PRO:HB2	1:A:502:PRO:HB2	1.96	0.48
1:A:1829:GLU:HG3	1:A:1830:PHE:H	1.78	0.48
3:C:57:TRP:CH2	3:C:60:ARG:HB2	2.48	0.48
3:C:136:SER:HB3	3:C:170:PHE:CZ	2.49	0.48
1:A:1748:TYR:HE2	1:A:2122:THR:HG1	1.61	0.48
3:C:108:ARG:O	3:C:124:PHE:HA	2.14	0.48
1:A:1828:ASP:O	1:A:1966:ARG:HB3	2.14	0.48
1:A:1849:SER:HG	1:A:1888:SER:HG	1.61	0.48
1:A:1964:SER:HA	1:A:1972:LYS:HA	1.95	0.48
2:B:151:LYS:HZ2	2:B:156:LEU:HD13	1.77	0.48
1:A:290:SER:HB2	1:A:293:THR:OG1	2.14	0.48
1:A:2220:ARG:HG2	1:A:2317:ILE:O	2.13	0.48
1:A:1708:ASP:HA	1:A:1728:PRO:O	2.13	0.48
1:A:1792:TYR:HD1	1:A:1793:PRO:HD2	1.79	0.48
3:C:49:GLN:O	3:C:102:ALA:HB1	2.14	0.48
1:A:1787:SER:O	1:A:1787:SER:OG	2.20	0.47
1:A:1919:HIS:HB3	1:A:2010:MET:CE	2.44	0.47
2:B:48:LEU:HD21	2:B:63:PHE:CD2	2.50	0.47
3:C:113:PHE:HB2	3:C:120:THR:O	2.14	0.47
1:A:390:GLU:HA	1:A:426:VAL:HA	1.96	0.47
1:A:650:SER:OG	1:A:692:CYS:O	2.19	0.47
3:C:38:ILE:HG13	3:C:39:PHE:H	1.79	0.47
1:A:283:ARG:NH2	1:A:526:PRO:HA	2.30	0.47
1:A:393:TRP:HB2	1:A:427:ARG:NH2	2.30	0.47
1:A:2257:VAL:HG11	1:A:2310:PRO:HB3	1.94	0.47
1:A:1945:LEU:HD22	1:A:1983:PHE:CD1	2.50	0.47
1:A:2183:LYS:HA	1:A:2183:LYS:HD3	1.75	0.47
2:B:37:TYR:CE1	2:B:47:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HB3	1:A:24:GLU:HG2	1.96	0.47
1:A:200:PHE:HB3	1:A:321:MET:HE1	1.96	0.47
1:A:647:ASP:HB2	1:A:1950:ASN:HD21	1.79	0.47
1:A:1784:SER:O	1:A:1839:SER:OG	2.22	0.47
2:B:55:ARG:HB3	2:B:59:ILE:HG23	1.96	0.47
2:B:98:LEU:HD23	2:B:99:THR:N	2.29	0.47
3:C:12:LYS:O	3:C:135:VAL:HA	2.15	0.47
3:C:80:MET:HE2	3:C:89:ALA:HB1	1.96	0.47
1:A:129:VAL:HG11	1:A:135:GLN:HE22	1.79	0.47
1:A:397:PRO:HG3	1:A:444:HIS:CE1	2.49	0.47
1:A:1790:ILE:HG22	1:A:1817:TRP:CZ3	2.49	0.47
1:A:434:GLU:N	1:A:434:GLU:OE1	2.48	0.47
1:A:453:LEU:HD11	1:A:533:TYR:CE2	2.49	0.47
1:A:1696:ARG:HG2	1:A:1698:TYR:CE2	2.50	0.47
1:A:1862:THR:OG1	1:A:1870:GLN:OE1	2.26	0.47
1:A:199:LEU:N	1:A:236:ASN:OD1	2.42	0.47
3:C:83:ASP:OD1	3:C:88:THR:N	2.39	0.47
3:C:108:ARG:HG2	3:C:126:TYR:HB2	1.97	0.47
1:A:480:ILE:HA	1:A:531:ARG:NH1	2.31	0.46
1:A:614:MET:HE2	1:A:616:SER:HB2	1.97	0.46
1:A:2313:TRP:CG	1:A:2317:ILE:HG12	2.50	0.46
2:B:50:TYR:CZ	3:C:112:TYR:HB2	2.50	0.46
3:C:80:MET:CE	3:C:89:ALA:HB1	2.45	0.46
3:C:168:ASP:HA	3:C:199:LEU:HB2	1.96	0.46
1:A:1879:PHE:HD1	1:A:1945:LEU:HD23	1.79	0.46
1:A:261:MET:SD	1:A:262:GLY:N	2.88	0.46
1:A:1874:GLN:NE2	1:A:1875:GLU:O	2.49	0.46
1:A:2242:GLY:O	1:A:2324:LEU:N	2.43	0.46
2:B:83:ASP:O	2:B:87:TYR:OH	2.19	0.46
1:A:47:TYR:CE1	1:A:229:GLN:HG2	2.51	0.46
1:A:69:TRP:HA	1:A:238:TYR:HE2	1.80	0.46
1:A:1731:LYS:O	1:A:1732:LYS:HD2	2.16	0.46
2:B:39:GLN:HA	2:B:45:PRO:HA	1.96	0.46
2:B:98:LEU:HD13	3:C:57:TRP:NE1	2.30	0.46
2:B:212:ASN:OD1	2:B:212:ASN:N	2.48	0.46
3:C:12:LYS:HG3	3:C:18:VAL:HB	1.97	0.46
1:A:472:PRO:O	1:A:537:VAL:HG11	2.15	0.46
1:A:1696:ARG:HD3	1:A:1698:TYR:OH	2.15	0.46
1:A:2034:ASP:OD1	1:A:2034:ASP:N	2.48	0.46
1:A:2103:ILE:HD12	1:A:2103:ILE:HA	1.85	0.46
1:A:2239:LYS:HG3	1:A:2300:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:HD3	1:A:1971:TYR:HB3	1.97	0.46
1:A:426:VAL:HG21	1:A:469:ALA:HB2	1.97	0.46
1:A:574:ILE:HD11	1:A:637:TRP:CZ3	2.49	0.46
1:A:1961:HIS:CD2	1:A:1990:PRO:HA	2.51	0.46
3:C:78:VAL:HG22	3:C:93:LEU:HD13	1.97	0.46
3:C:110:ASP:HB3	3:C:126:TYR:CE1	2.50	0.46
3:C:111:ASN:OD1	3:C:123:TYR:HB2	2.16	0.46
1:A:202:VAL:H	1:A:261:MET:HE3	1.81	0.46
1:A:433:ASP:OD1	1:A:433:ASP:N	2.48	0.46
1:A:2058:SER:OG	1:A:2059:ILE:N	2.47	0.46
3:C:29:PHE:CE1	3:C:87:SER:HA	2.50	0.46
1:A:605:ASP:N	1:A:605:ASP:OD1	2.48	0.46
1:A:2053:LEU:HD23	1:A:2054:HIS:N	2.31	0.46
2:B:45:PRO:HB2	3:C:127:TRP:HZ3	1.80	0.46
1:A:169:LEU:HD12	1:A:261:MET:SD	2.55	0.45
1:A:188:GLU:HG2	1:A:189:ARG:HG3	1.97	0.45
1:A:607:GLU:HG2	1:A:608:PHE:N	2.30	0.45
1:A:635:ALA:HB1	1:A:637:TRP:NE1	2.30	0.45
1:A:1927:ASP:N	1:A:2012:THR:OG1	2.48	0.45
2:B:92:TYR:O	2:B:94:THR:N	2.45	0.45
1:A:193:LEU:HD12	1:A:195:GLU:H	1.81	0.45
2:B:47:LEU:HD12	2:B:48:LEU:N	2.31	0.45
1:A:1782:PRO:HB3	1:A:1809:PRO:HD3	1.96	0.45
1:A:2261:LEU:O	1:A:2308:ILE:HD12	2.16	0.45
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.72	0.45
1:A:389:GLU:OE2	1:A:431:TYR:OH	2.34	0.45
1:A:2234:PHE:HD2	1:A:2238:MET:CG	2.30	0.45
1:A:100:HIS:ND1	1:A:162:HIS:HB2	2.31	0.45
1:A:311:CYS:SG	1:A:319:GLY:HA2	2.57	0.45
1:A:1832:CYS:HB2	1:A:1858:CYS:HB3	1.81	0.45
1:A:1884:ASP:HB3	1:A:1887:LYS:HB2	1.98	0.45
1:A:2263:SER:OG	1:A:2307:ARG:HB2	2.16	0.45
2:B:35:ALA:HB2	3:C:123:TYR:HE2	1.82	0.45
2:B:62:ARG:NH2	2:B:80:GLU:OE2	2.47	0.45
3:C:44:VAL:HA	3:C:107:ALA:O	2.16	0.45
1:A:290:SER:O	1:A:292:LEU:N	2.49	0.45
1:A:696:ASP:OD1	1:A:696:ASP:N	2.49	0.45
1:A:1773:VAL:HG13	1:A:1815:TYR:HB2	1.98	0.45
1:A:1855:LEU:C	1:A:1856:LEU:HD12	2.36	0.45
1:A:2075:LEU:HB2	1:A:2147:ARG:O	2.15	0.45
1:A:2212:LEU:O	1:A:2217:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TYR:HA	2:B:92:TYR:CE1	2.51	0.45
2:B:164:SER:OG	3:C:191:PRO:O	2.35	0.45
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.87	0.45
1:A:2263:SER:HB2	1:A:2273:LEU:HA	1.99	0.45
3:C:221:ASN:HB2	3:C:232:ASP:OD1	2.17	0.45
1:A:519:ASP:OD1	1:A:519:ASP:N	2.43	0.45
1:A:581:GLU:O	1:A:587:LEU:HB2	2.17	0.45
1:A:658:PHE:HB2	1:A:678:VAL:HG13	1.99	0.45
1:A:2105:TYR:HB3	1:A:2144:ILE:HD13	1.97	0.45
1:A:277:PHE:HB2	1:A:285:ALA:HA	1.99	0.45
2:B:20:THR:HG23	2:B:73:THR:HG23	1.99	0.45
3:C:46:TRP:HB2	3:C:58:MET:HB3	1.98	0.45
1:A:1739:ALA:H	1:A:1745:GLN:NE2	2.14	0.44
1:A:2015:LEU:HD12	1:A:2016:VAL:N	2.32	0.44
1:A:2246:GLN:HB2	1:A:2292:PRO:HB3	1.99	0.44
3:C:45:HIS:CD2	3:C:60:ARG:HG3	2.51	0.44
3:C:178:TRP:HE1	3:C:204:SER:C	2.19	0.44
3:C:233:LYS:HB3	3:C:233:LYS:HE2	1.82	0.44
1:A:2232:VAL:HG13	1:A:2306:LEU:HB2	1.99	0.44
2:B:164:SER:O	2:B:177:LEU:HD12	2.18	0.44
3:C:42:TYR:HB2	3:C:63:PRO:HD2	1.98	0.44
3:C:62:ASN:HD21	3:C:64:ASN:HB2	1.82	0.44
1:A:16:TYR:OH	1:A:234:THR:HG21	2.17	0.44
1:A:530:THR:HG22	1:A:638:TYR:HD1	1.82	0.44
2:B:200:HIS:CD2	2:B:202:GLY:H	2.35	0.44
3:C:126:TYR:O	3:C:127:TRP:CD1	2.71	0.44
1:A:1955:SER:HB2	1:A:2001:LEU:HB2	1.98	0.44
2:B:41:PRO:O	2:B:43:GLN:NE2	2.47	0.44
3:C:162:LEU:HD22	3:C:235:VAL:HG11	1.99	0.44
1:A:315:SER:HB3	1:A:318:HIS:HB2	2.00	0.44
3:C:41:ALA:O	3:C:108:ARG:HB2	2.17	0.44
1:A:108:LYS:HE3	1:A:123:GLU:O	2.17	0.44
1:A:443:GLN:NE2	1:A:444:HIS:O	2.37	0.44
1:A:1919:HIS:HB3	1:A:2010:MET:HE2	1.99	0.44
3:C:145:VAL:HG21	3:C:222:VAL:HG21	2.00	0.44
1:A:391:GLU:OE1	1:A:427:ARG:NH2	2.47	0.44
1:A:1812:THR:O	1:A:1813:ARG:HG2	2.18	0.44
1:A:1882:ILE:HD11	1:A:1917:ARG:HG2	1.98	0.44
1:A:601:VAL:HG23	1:A:603:LEU:H	1.82	0.44
1:A:2115:TYR:HE1	1:A:2142:PRO:HD2	1.82	0.44
1:A:69:TRP:CD1	1:A:243:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:TRP:HB2	1:A:427:ARG:HH12	1.82	0.44
1:A:2203:TRP:CD2	1:A:2216:SER:HB2	2.52	0.44
2:B:6:GLN:NE2	2:B:104:THR:H	2.16	0.44
3:C:162:LEU:HD23	3:C:162:LEU:HA	1.88	0.44
1:A:659:LYS:HB2	1:A:664:TYR:CZ	2.52	0.43
1:A:1940:ILE:HD11	1:A:1942:TRP:NE1	2.32	0.43
2:B:137:LEU:HD23	2:B:138:LEU:N	2.33	0.43
1:A:267:VAL:HG21	1:A:671:PHE:CE1	2.53	0.43
1:A:588:THR:HA	1:A:591:ILE:HG12	2.00	0.43
1:A:660:HIS:HB2	1:A:665:GLU:OE1	2.18	0.43
2:B:39:GLN:HG3	2:B:45:PRO:HG3	2.00	0.43
1:A:108:LYS:CG	1:A:123:GLU:HB3	2.48	0.43
1:A:133:LYS:O	1:A:135:GLN:NE2	2.26	0.43
1:A:1879:PHE:N	1:A:1922:ASN:OD1	2.48	0.43
1:A:2096:LEU:HD23	1:A:2159:ARG:HB2	2.00	0.43
1:A:1870:GLN:HG2	1:A:1872:THR:HB	2.00	0.43
1:A:2261:LEU:HG	1:A:2309:HIS:HB2	2.00	0.43
1:A:99:LEU:CD2	1:A:139:TRP:HZ2	2.25	0.43
1:A:552:LEU:HD11	1:A:638:TYR:CD1	2.53	0.43
3:C:40:THR:HG22	3:C:42:TYR:OH	2.18	0.43
1:A:272:LEU:H	1:A:277:PHE:HZ	1.65	0.43
1:A:445:GLU:HA	1:A:620:TYR:CE2	2.53	0.43
1:A:447:GLY:O	1:A:449:LEU:N	2.42	0.43
1:A:1756:LEU:O	1:A:1759:LEU:HB2	2.19	0.43
2:B:182:THR:HG23	3:C:167:LYS:HZ1	1.84	0.43
3:C:42:TYR:CD1	3:C:43:SER:N	2.87	0.43
1:A:415:GLY:HA3	1:A:418:ARG:HH11	1.81	0.43
1:A:2064:THR:HG21	1:A:2069:SER:HB3	2.01	0.43
3:C:97:THR:OG1	3:C:99:ASP:OD1	2.25	0.43
1:A:463:ILE:HD13	1:A:513:TRP:CD2	2.53	0.43
1:A:1928:THR:O	1:A:1930:PRO:HD3	2.18	0.43
1:A:2140:PHE:HE2	1:A:2144:ILE:HD12	1.83	0.43
2:B:27:GLN:OE1	2:B:28:SER:N	2.52	0.43
3:C:74:PHE:HB3	3:C:78:VAL:HG23	1.99	0.43
2:B:152:VAL:O	2:B:155:ALA:CB	2.64	0.43
3:C:144:SER:HB2	3:C:167:LYS:O	2.19	0.43
3:C:216:LYS:O	3:C:234:ARG:NH2	2.52	0.43
1:A:390:GLU:N	1:A:426:VAL:HG23	2.34	0.42
1:A:1697:HIS:HB3	1:A:1699:PHE:CE1	2.54	0.42
1:A:2103:ILE:HB	1:A:2126:PHE:CE1	2.54	0.42
1:A:2259:GLU:HB2	1:A:2311:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ASP:HB3	2:B:174:THR:H	1.84	0.42
1:A:401:ALA:HA	1:A:408:LYS:HE2	1.99	0.42
1:A:671:PHE:O	1:A:674:SER:OG	2.31	0.42
2:B:31:SER:HA	2:B:72:PHE:HE2	1.85	0.42
1:A:90:LYS:HA	1:A:134:SER:HA	2.01	0.42
1:A:102:VAL:HG12	1:A:157:TYR:HB3	2.01	0.42
1:A:309:LEU:O	1:A:322:GLU:HA	2.20	0.42
1:A:446:SER:CB	1:A:449:LEU:HD11	2.48	0.42
1:A:1835:TRP:HB2	1:A:1855:LEU:HB3	2.01	0.42
1:A:2264:SER:O	1:A:2272:THR:OG1	2.37	0.42
3:C:77:ARG:HG3	3:C:94:SER:O	2.20	0.42
1:A:426:VAL:CG1	1:A:547:LEU:HD21	2.49	0.42
1:A:2034:ASP:HA	1:A:2052:ARG:HH21	1.85	0.42
3:C:46:TRP:CZ2	3:C:91:MET:HB3	2.54	0.42
1:A:407:TYR:HE2	1:A:699:ASN:ND2	2.15	0.42
1:A:111:GLU:HG2	1:A:115:TYR:HE1	1.85	0.42
1:A:452:LEU:HA	1:A:550:PRO:HG2	2.02	0.42
1:A:589:GLU:O	1:A:592:GLN:HG3	2.19	0.42
1:A:656:TYR:CE2	1:A:684:ASN:HB2	2.55	0.42
1:A:1755:HIS:CD2	1:A:1756:LEU:HD22	2.54	0.42
2:B:32:ALA:O	3:C:123:TYR:OH	2.36	0.42
2:B:84:PHE:CE2	2:B:108:ILE:HG13	2.55	0.42
1:A:6:TYR:HB3	1:A:60:PHE:CE1	2.54	0.42
1:A:233:HIS:NE2	1:A:268:HIS:HD2	2.18	0.42
1:A:1954:HIS:CE1	1:A:2005:HIS:CE1	3.07	0.42
1:A:2107:LEU:HD12	1:A:2111:LYS:NZ	2.33	0.42
3:C:39:PHE:CZ	3:C:41:ALA:HB3	2.54	0.42
3:C:57:TRP:HH2	3:C:60:ARG:HB2	1.84	0.42
1:A:2042:GLN:O	1:A:2044:GLY:N	2.53	0.42
1:A:2195:TYR:O	1:A:2222:GLN:HG3	2.20	0.42
1:A:233:HIS:CE1	1:A:318:HIS:ND1	2.87	0.42
1:A:288:GLU:OE1	1:A:288:GLU:N	2.53	0.42
1:A:2227:LYS:H	1:A:2227:LYS:HG2	1.57	0.42
3:C:102:ALA:HB3	3:C:104:TYR:CE1	2.54	0.42
1:A:1842:ASP:OD1	1:A:1845:LYS:HB2	2.20	0.42
3:C:28:ASN:HB2	4:F:1:NAG:O5	2.20	0.42
3:C:178:TRP:HE3	3:C:179:ASN:H	1.66	0.42
1:A:16:TYR:HE1	1:A:237:GLY:O	2.03	0.41
1:A:382:TRP:O	1:A:461:LEU:HA	2.20	0.41
1:A:471:ARG:NE	1:A:472:PRO:HD2	2.35	0.41
1:A:1782:PRO:HG2	1:A:1806:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2203:TRP:HZ3	1:A:2218:ALA:HB3	1.84	0.41
1:A:2242:GLY:HA3	1:A:2324:LEU:HD12	2.01	0.41
1:A:170:ASN:OD1	1:A:204:ASP:HB3	2.20	0.41
2:B:110:ARG:NH1	2:B:174:THR:HA	2.35	0.41
3:C:145:VAL:HA	3:C:165:LEU:O	2.20	0.41
1:A:393:TRP:HB2	1:A:427:ARG:NH1	2.34	0.41
1:A:642:ILE:HD12	1:A:642:ILE:N	2.36	0.41
1:A:1705:GLN:CD	1:A:1734:VAL:HG21	2.40	0.41
1:A:2304:ARG:HG3	1:A:2305:TYR:CD1	2.55	0.41
1:A:1894:ASN:HB3	1:A:1897:ARG:HH12	1.86	0.41
1:A:2157:SER:C	1:A:2158:ILE:HD12	2.40	0.41
1:A:578:VAL:HG22	1:A:615:HIS:CG	2.56	0.41
2:B:62:ARG:HH12	2:B:63:PHE:HE1	1.68	0.41
1:A:459:ASP:OD1	1:A:459:ASP:N	2.53	0.41
1:A:1786:TYR:OH	1:A:1788:SER:HA	2.21	0.41
1:A:1846:ASP:HA	1:A:1849:SER:HB2	2.03	0.41
1:A:2210:LEU:HA	1:A:2320:ARG:HB3	2.02	0.41
3:C:34:ALA:HB2	3:C:42:TYR:OH	2.20	0.41
1:A:268:HIS:ND1	1:A:313:ILE:HD13	2.36	0.41
1:A:472:PRO:HA	1:A:503:ILE:O	2.21	0.41
1:A:1736:ARG:HA	1:A:1736:ARG:HD3	1.80	0.41
1:A:1967:LYS:O	1:A:1969:GLU:N	2.53	0.41
1:A:2186:SER:OG	1:A:2189:GLN:HG3	2.21	0.41
2:B:86:VAL:HG22	2:B:105:LYS:HD3	2.03	0.41
3:C:28:ASN:ND2	3:C:30:THR:O	2.53	0.41
1:A:192:ASN:C	1:A:194:HIS:H	2.23	0.41
1:A:488:SER:OG	1:A:490:ARG:O	2.35	0.41
1:A:1932:LEU:HD22	1:A:1942:TRP:CZ3	2.56	0.41
1:A:2064:THR:HG22	1:A:2160:SER:OG	2.20	0.41
1:A:129:VAL:HG11	1:A:135:GLN:NE2	2.36	0.41
1:A:407:TYR:HD1	1:A:411:TYR:CE1	2.38	0.41
1:A:417:GLN:OE1	1:A:417:GLN:N	2.53	0.41
1:A:420:GLY:O	1:A:423:TYR:OH	2.21	0.41
1:A:628:SER:OG	1:A:707:LYS:O	2.14	0.41
1:A:650:SER:HB2	1:A:693:HIS:HD2	1.86	0.41
1:A:682:MET:O	1:A:682:MET:HG3	2.21	0.41
1:A:1870:GLN:C	1:A:1872:THR:N	2.71	0.41
1:A:1962:VAL:HG23	1:A:1974:ALA:HB2	2.02	0.41
3:C:46:TRP:CE2	3:C:91:MET:HB3	2.55	0.41
3:C:109:ALA:HA	3:C:123:TYR:O	2.20	0.41
3:C:230:LYS:HE2	3:C:230:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:PHE:HB3	1:A:511:TYR:HE1	1.86	0.40
1:A:1771:ILE:HD13	1:A:1819:VAL:HG13	2.03	0.40
1:A:1840:ASP:N	1:A:1840:ASP:OD1	2.54	0.40
3:C:168:ASP:H	3:C:195:GLN:HE22	1.69	0.40
3:C:171:PRO:HD2	3:C:224:HIS:HE1	1.85	0.40
1:A:106:PHE:HB3	1:A:139:TRP:HD1	1.86	0.40
1:A:1934:MET:HG3	1:A:1990:PRO:HG3	2.03	0.40
1:A:2032:ILE:HG23	1:A:2036:GLN:NE2	2.36	0.40
1:A:2063:SER:OG	1:A:2159:ARG:NH2	2.54	0.40
1:A:408:LYS:HE3	1:A:408:LYS:HB3	1.91	0.40
1:A:542:ASP:O	1:A:547:LEU:HB2	2.21	0.40
1:A:2101:PHE:O	1:A:2126:PHE:N	2.51	0.40
1:A:527:ARG:HG3	1:A:555:TYR:H	1.85	0.40
1:A:1944:LEU:HD22	1:A:1956:ILE:HG13	2.04	0.40
1:A:2002:ILE:H	1:A:2002:ILE:HG12	1.64	0.40
1:A:2263:SER:CB	1:A:2273:LEU:HA	2.51	0.40
3:C:2:VAL:HG11	3:C:108:ARG:NH2	2.35	0.40
3:C:44:VAL:HB	3:C:61:ILE:HG23	2.03	0.40
3:C:170:PHE:CE2	3:C:171:PRO:HB3	2.56	0.40
1:A:64:ARG:HG3	1:A:65:PRO:HD2	2.02	0.40
1:A:640:LEU:HD12	1:A:675:GLY:HA3	2.04	0.40
1:A:2107:LEU:O	1:A:2147:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1220/1467 (83%)	1068 (88%)	146 (12%)	6 (0%)	29 66
2	B	200/216 (93%)	186 (93%)	14 (7%)	0	100 100
3	C	233/235 (99%)	217 (93%)	14 (6%)	2 (1%)	17 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1653/1918 (86%)	1471 (89%)	174 (10%)	8 (0%)	32 66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1871	VAL
1	A	1926	MET
1	A	704	ALA
1	A	2158	ILE
3	C	111	ASN
1	A	448	ILE
3	C	209	PRO
1	A	141	VAL

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	1094/1301 (84%)	1050 (96%)	44 (4%)	31 63
2	B	173/184 (94%)	168 (97%)	5 (3%)	42 71
3	C	199/199 (100%)	190 (96%)	9 (4%)	27 60
All	All	1466/1684 (87%)	1408 (96%)	58 (4%)	35 63

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	TRP
1	A	111	GLU
1	A	127	ASP
1	A	160	LEU
1	A	182	GLU
1	A	189	ARG
1	A	311	CYS
1	A	395	TYR

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Mol	Chain	Res	Type
1	A	499	LYS
1	A	527	ARG
1	A	536	PHE
1	A	540	GLU
1	A	586	TYR
1	A	632	HIS
1	A	658	PHE
1	A	666	ASP
1	A	680	MET
1	A	695	SER
1	A	699	ASN
1	A	1694	ARG
1	A	1748	TYR
1	A	1776	LYS
1	A	1792	TYR
1	A	1897	ARG
1	A	1898	ASN
1	A	1936	GLN
1	A	1961	HIS
1	A	1976	TYR
1	A	1980	PRO
1	A	2010	MET
1	A	2055	TYR
1	A	2111	LYS
1	A	2112	TRP
1	A	2127	PHE
1	A	2137	HIS
1	A	2196	PHE
1	A	2234	PHE
1	A	2249	LYS
1	A	2250	SER
1	A	2275	PHE
1	A	2281	LYS
1	A	2297	LEU
1	A	2321	MET
1	A	2329	GLN
2	B	80	GLU
2	B	92	TYR
2	B	141	PHE
2	B	142	TYR
2	B	188	TYR
3	C	27	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	49	GLN
3	C	53	GLN
3	C	57	TRP
3	C	62	ASN
3	C	91	MET
3	C	113	PHE
3	C	164	CYS
3	C	228	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	ASN
1	A	1919	HIS
1	A	2005	HIS
1	A	2231	GLN
3	C	1	GLN
3	C	45	HIS
3	C	64	ASN
3	C	221	ASN

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)

12 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	0.25	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.43	0	17,19,21	1.27	1 (5%)
4	BMA	D	3	4	11,11,12	0.91	1 (9%)	15,15,17	1.26	1 (6%)
4	MAN	D	4	4	11,11,12	0.79	0	15,15,17	1.24	2 (13%)
4	NAG	E	1	4,1	14,14,15	0.73	1 (7%)	17,19,21	1.49	1 (5%)
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.43	0
4	BMA	E	3	4	11,11,12	0.68	0	15,15,17	0.96	0
4	MAN	E	4	4	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
4	NAG	F	1	4,3	14,14,15	0.21	0	17,19,21	0.69	0
4	NAG	F	2	4	14,14,15	0.26	0	17,19,21	0.52	0
4	BMA	F	3	4	11,11,12	0.57	0	15,15,17	0.81	0
4	MAN	F	4	4	11,11,12	0.87	1 (9%)	15,15,17	1.24	2 (13%)

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	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	1/1/1/1
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	O5-C1	2.62	1.47	1.43
4	F	4	MAN	C1-C2	2.49	1.57	1.52
4	D	3	BMA	C1-C2	2.20	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	C1-O5-C5	5.66	119.86	112.19
4	D	2	NAG	C2-N2-C7	4.31	129.04	122.90
4	D	3	BMA	C1-O5-C5	3.49	116.93	112.19
4	D	4	MAN	C1-O5-C5	3.29	116.65	112.19
4	F	4	MAN	C1-O5-C5	2.81	116.00	112.19
4	D	4	MAN	O2-C2-C3	-2.26	105.61	110.14
4	E	4	MAN	C1-O5-C5	2.21	115.19	112.19
4	F	4	MAN	O2-C2-C3	-2.12	105.88	110.14
4	E	4	MAN	O2-C2-C3	-2.10	105.92	110.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7
4	D	2	NAG	C3-C2-N2-C7
4	F	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

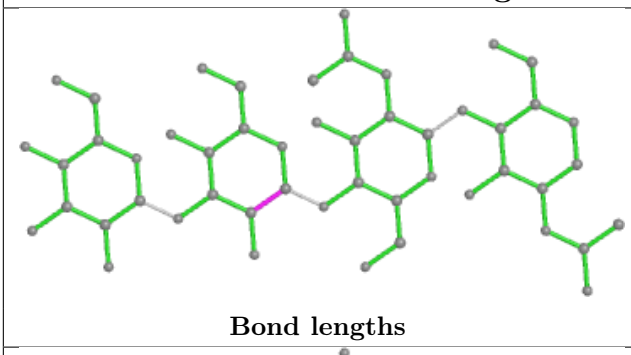
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 4 short contacts:

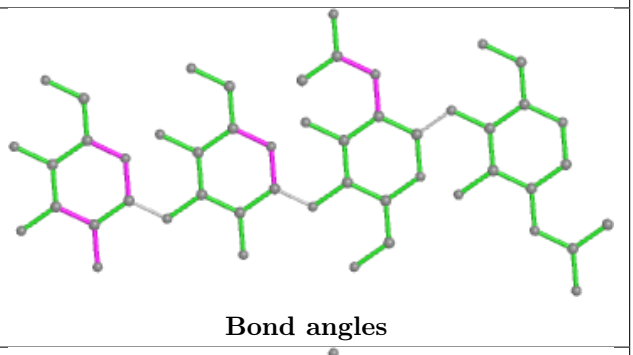
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	3	0
4	F	2	NAG	1	0
4	D	2	NAG	1	0

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

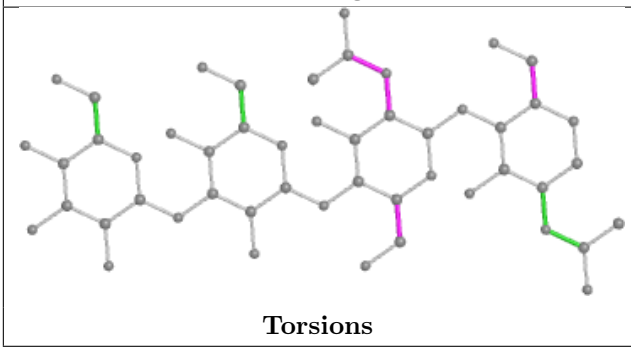
Oligosaccharide Chain D



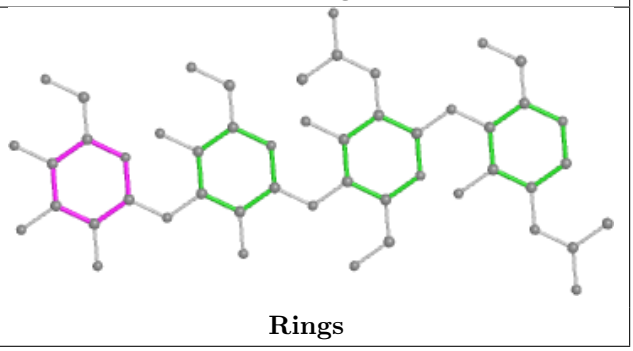
Bond lengths



Bond angles

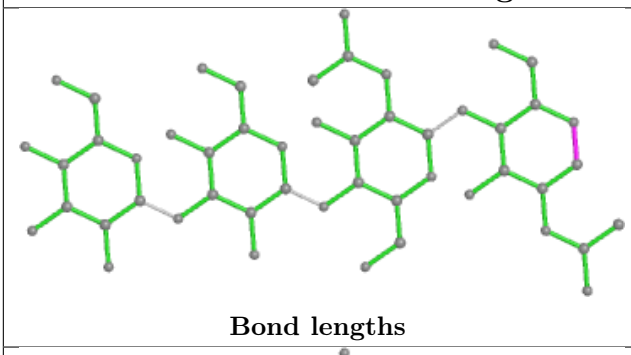


Torsions

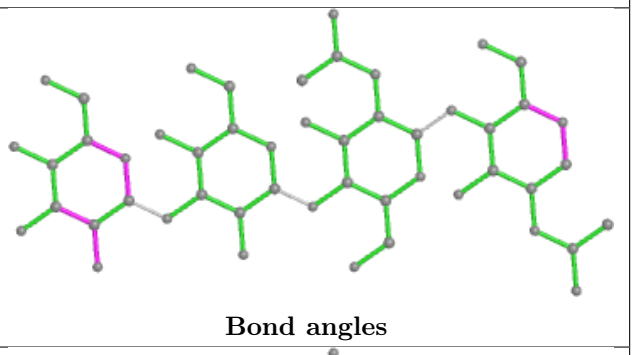


Rings

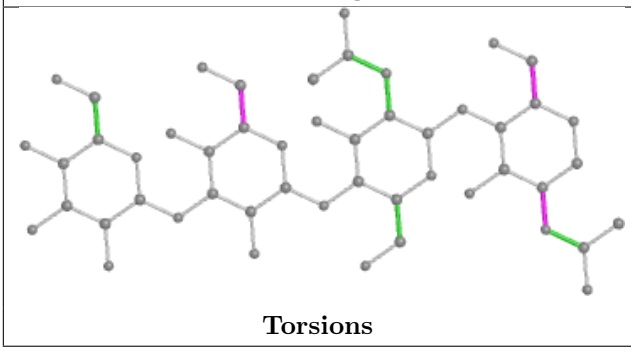
Oligosaccharide Chain E



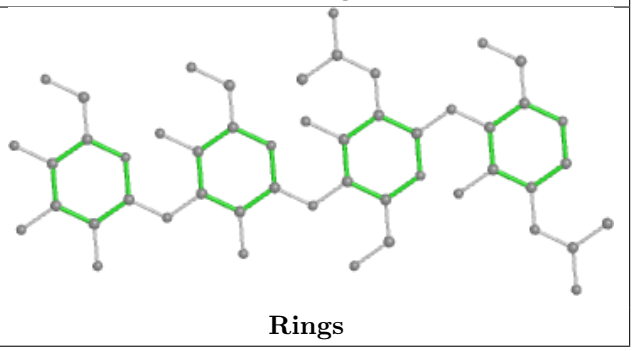
Bond lengths



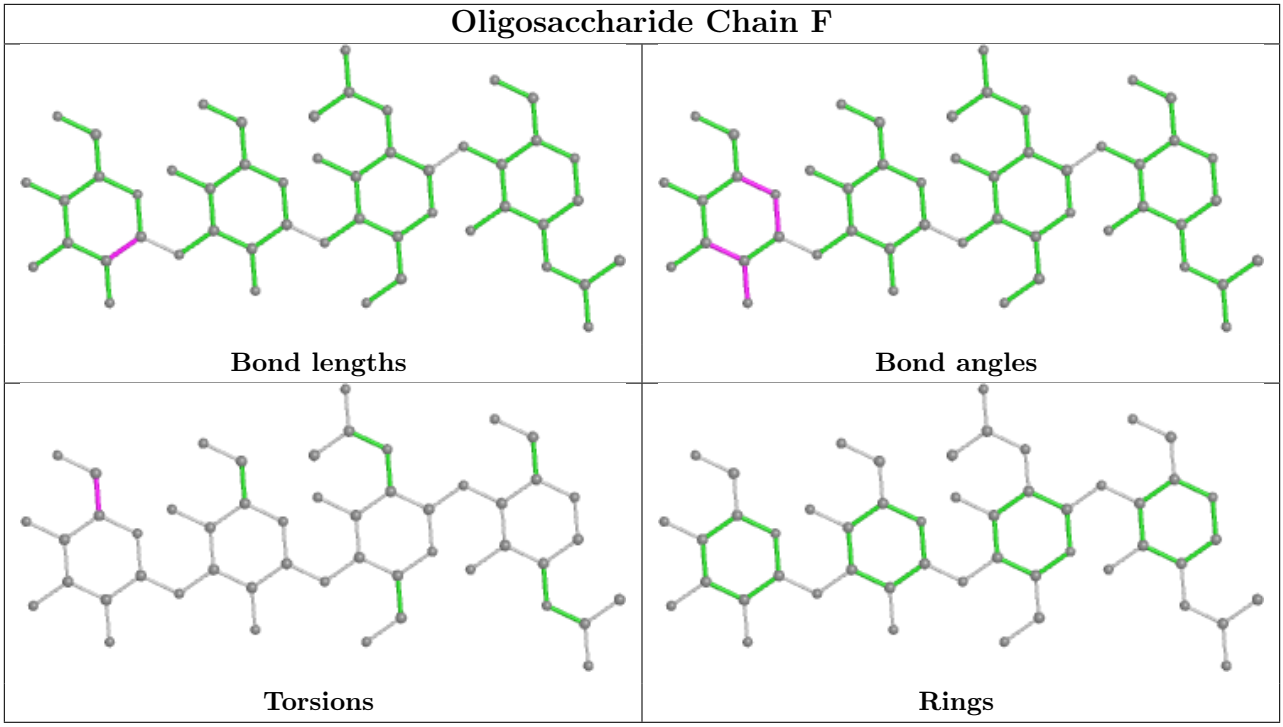
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

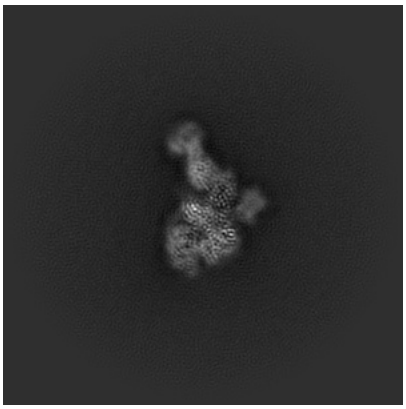
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41710. These allow visual inspection of the internal detail of the map and identification of artifacts.

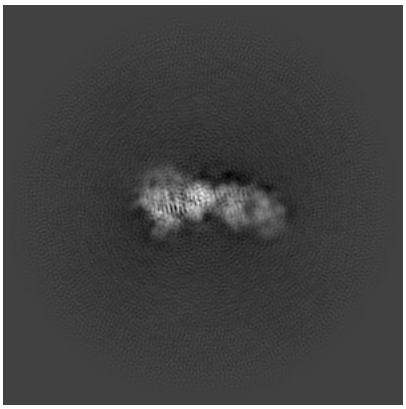
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

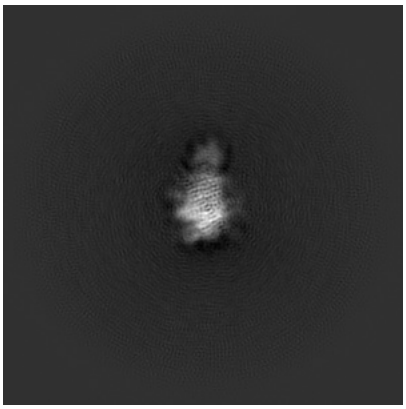
6.1.1 Primary map



X

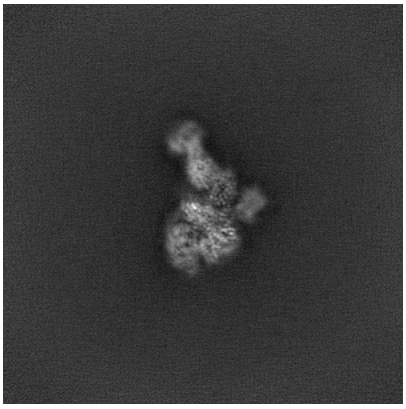


Y

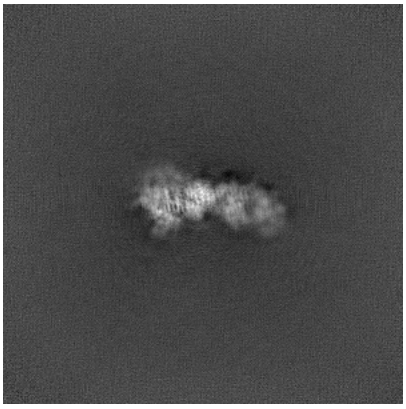


Z

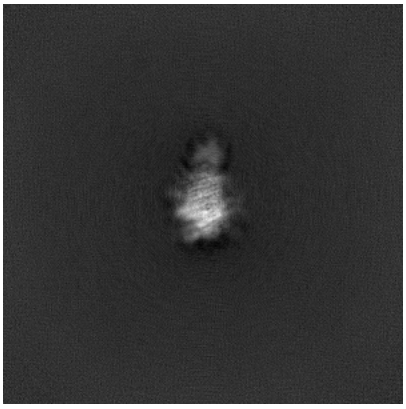
6.1.2 Raw map



X



Y

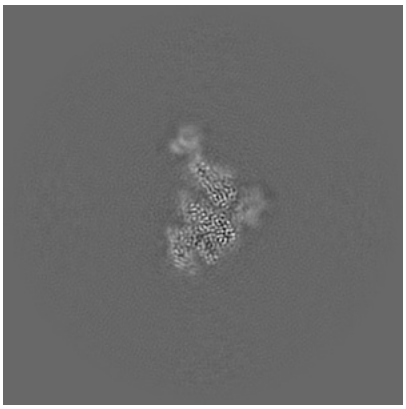


Z

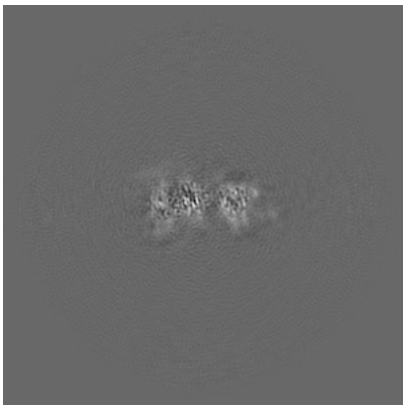
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

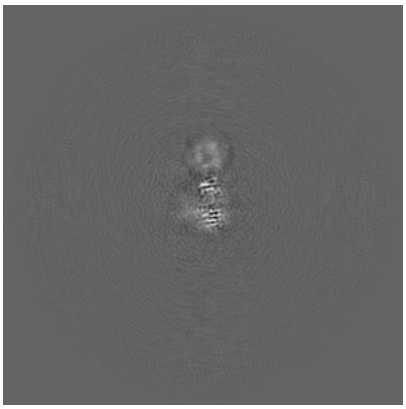
6.2.1 Primary map



X Index: 270

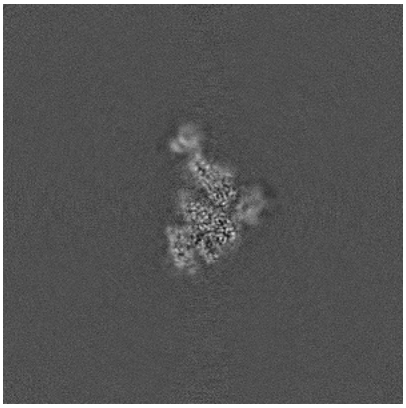


Y Index: 270

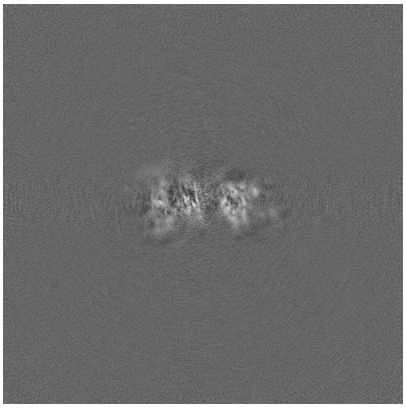


Z Index: 270

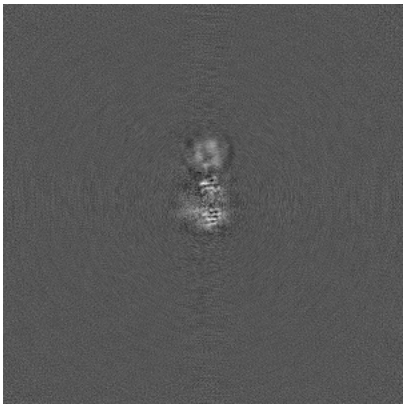
6.2.2 Raw map



X Index: 270



Y Index: 270

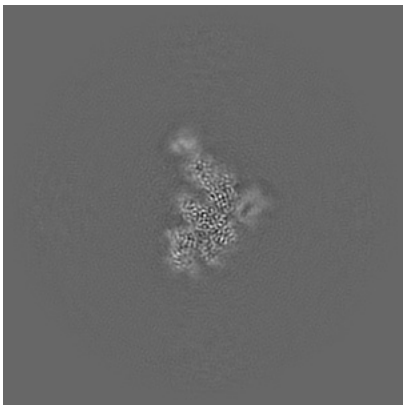


Z Index: 270

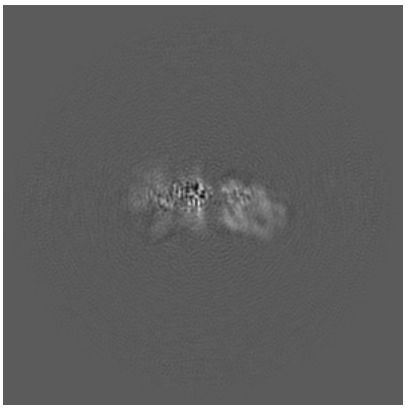
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

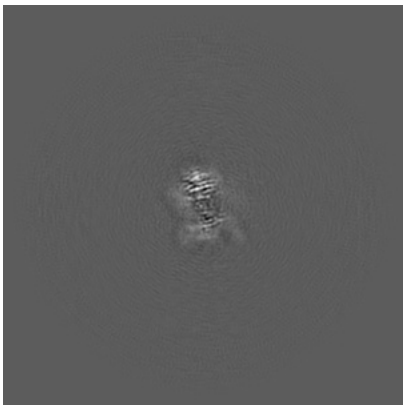
6.3.1 Primary map



X Index: 274

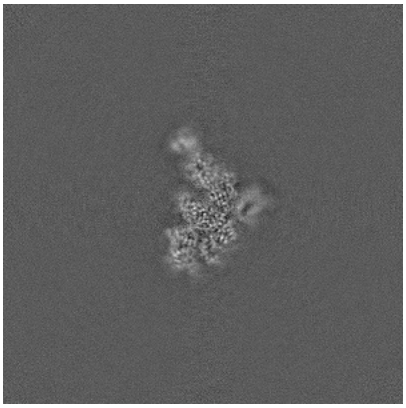


Y Index: 258

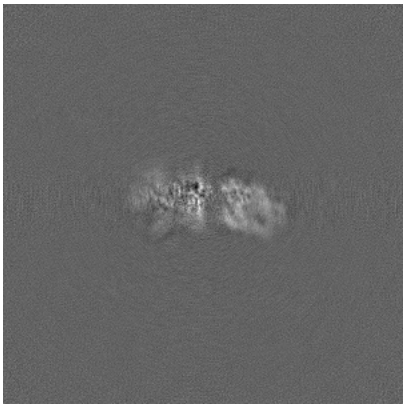


Z Index: 224

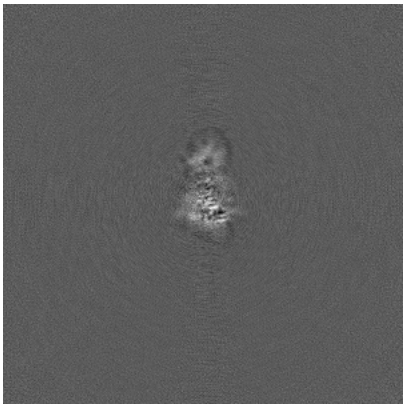
6.3.2 Raw map



X Index: 274



Y Index: 258

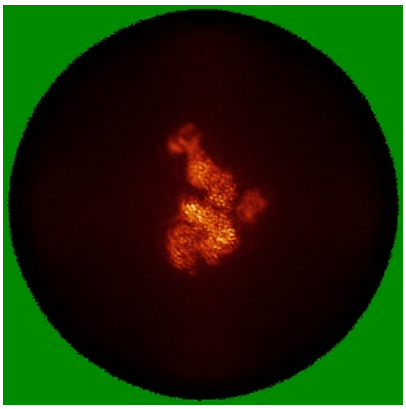


Z Index: 261

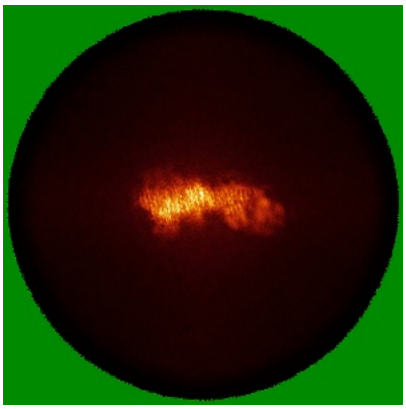
The images above show the largest variance slices of the map in three orthogonal directions.

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

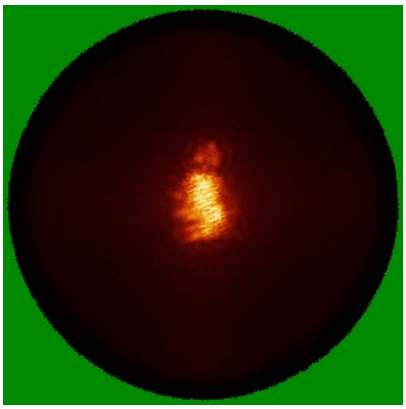
6.4.1 Primary map



X

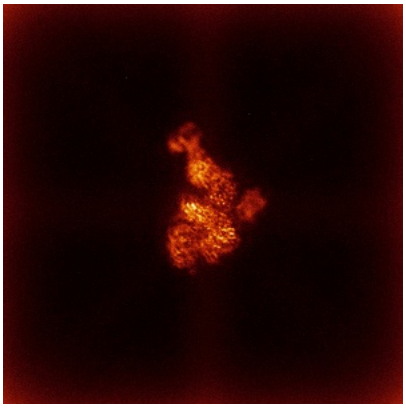


Y

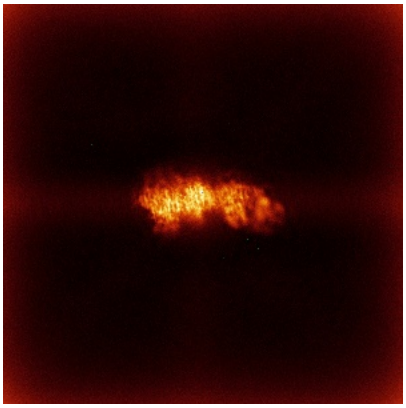


Z

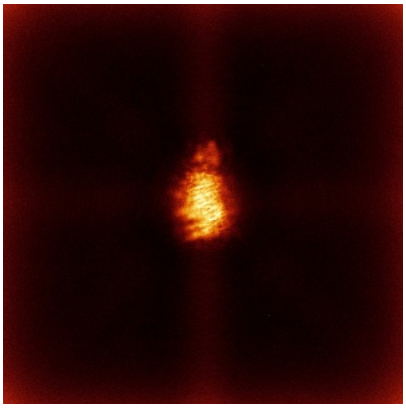
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0443. 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

X Y Z

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.

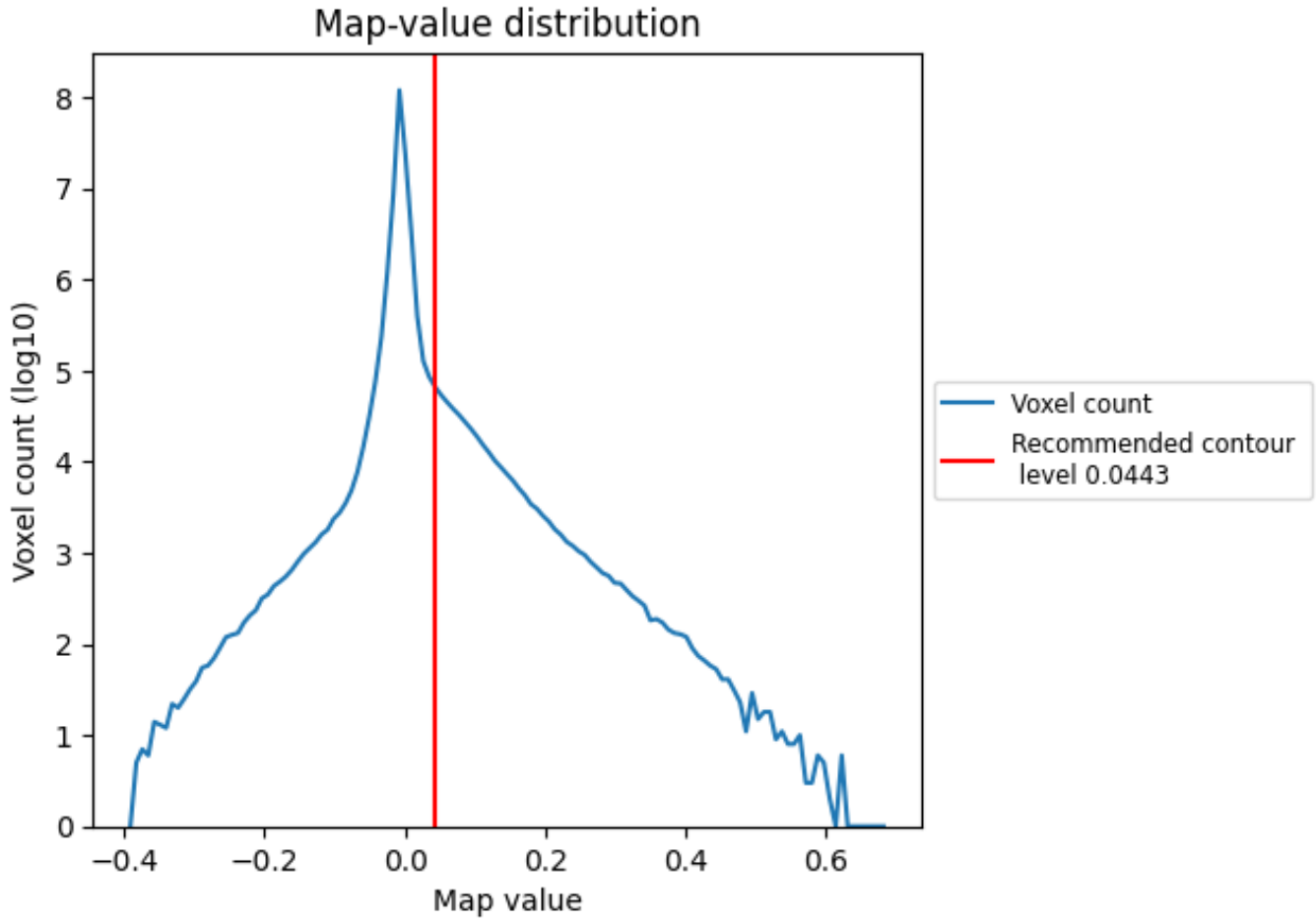
6.6 Mask visualisation (i)

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

7 Map analysis

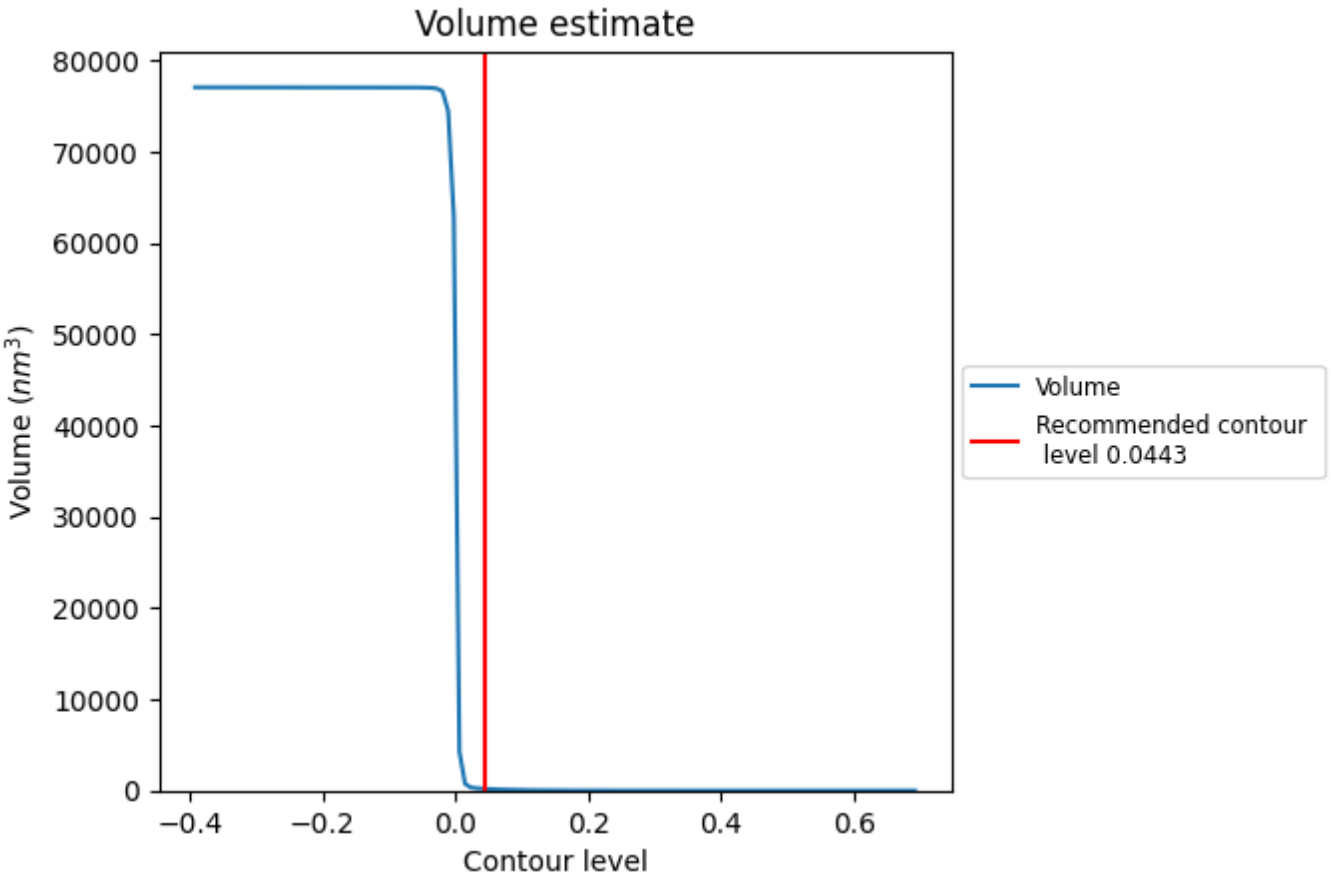
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

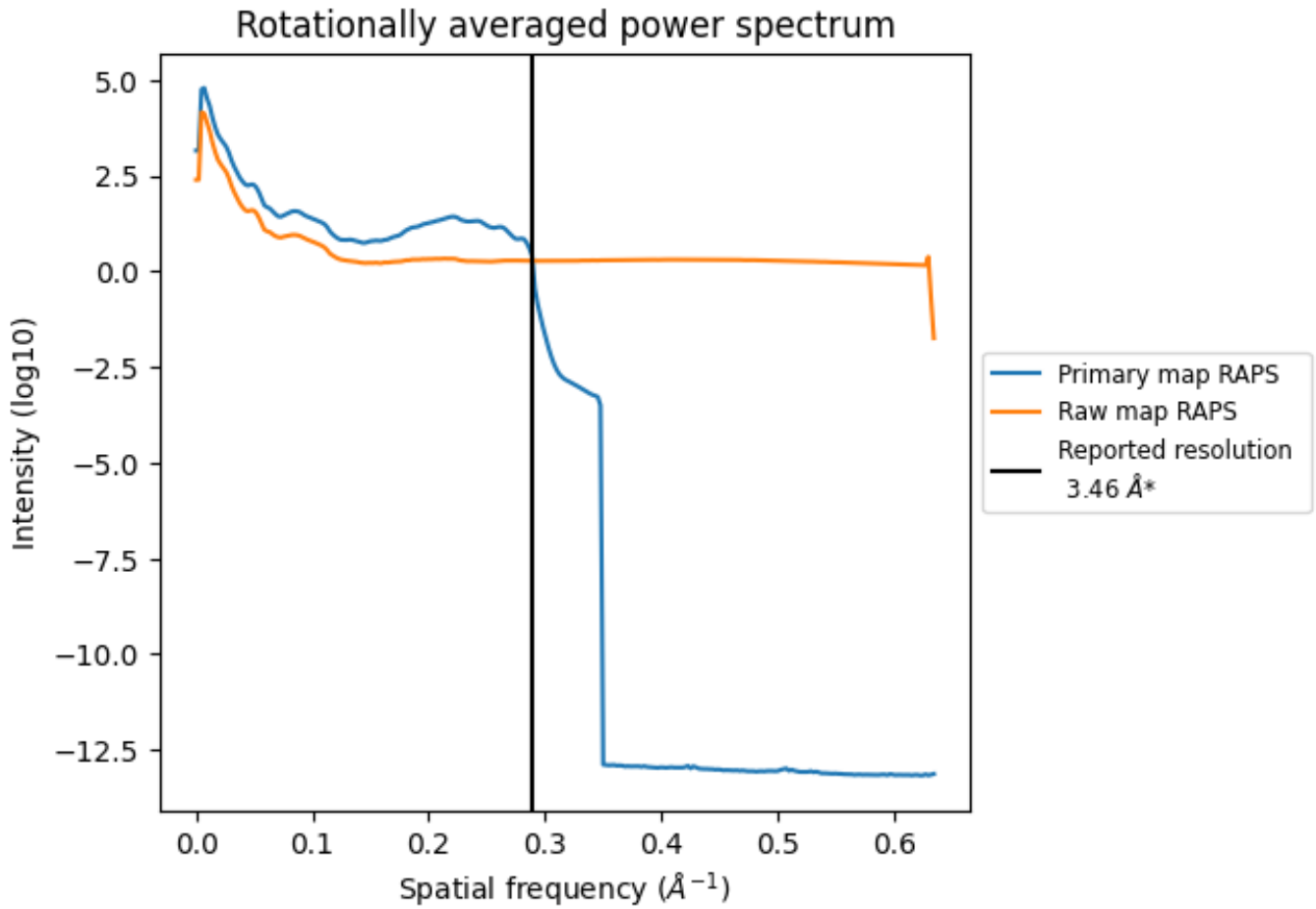
7.2 Volume estimate



The volume at the recommended contour level is 194 nm^3; this corresponds to an approximate mass of 175 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)

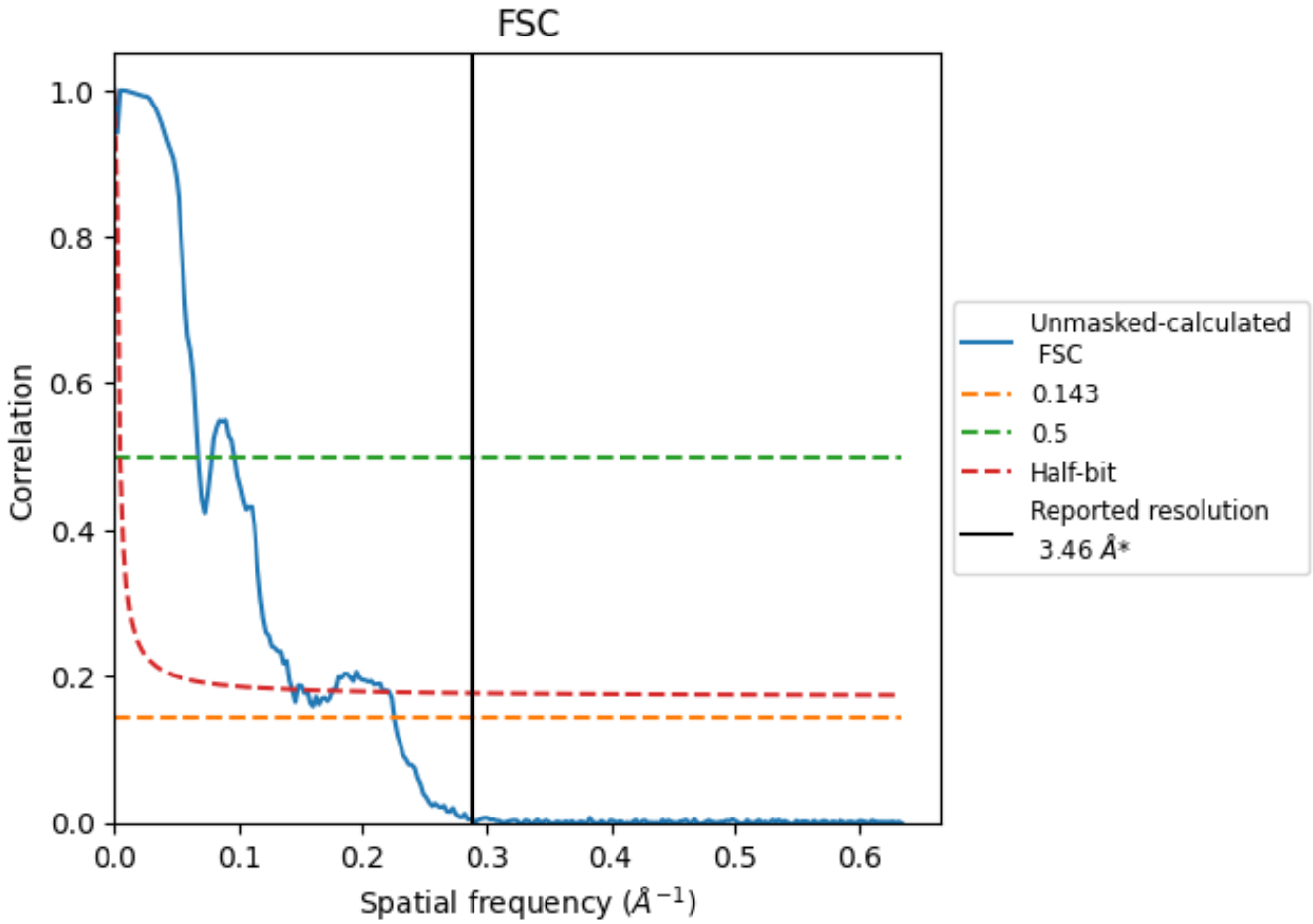


*Reported resolution corresponds to spatial frequency of 0.289 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.289 Å^{-1}

8.2 Resolution estimates (i)

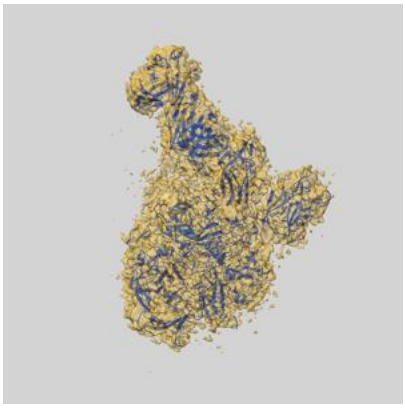
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	14.79	6.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.46 by more than 10 %

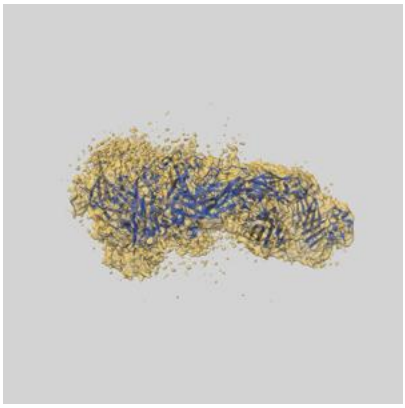
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41710 and PDB model 8TY1. Per-residue inclusion information can be found in section 3 on page 5.

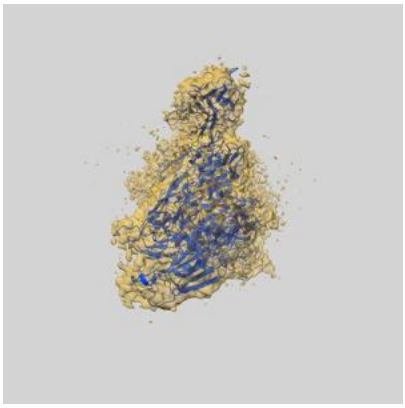
9.1 Map-model overlay



X



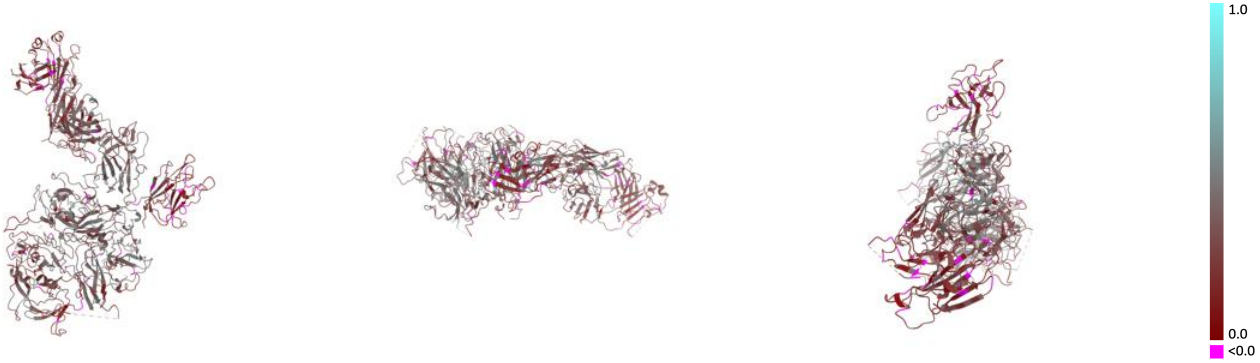
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0443 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)



X Y Z

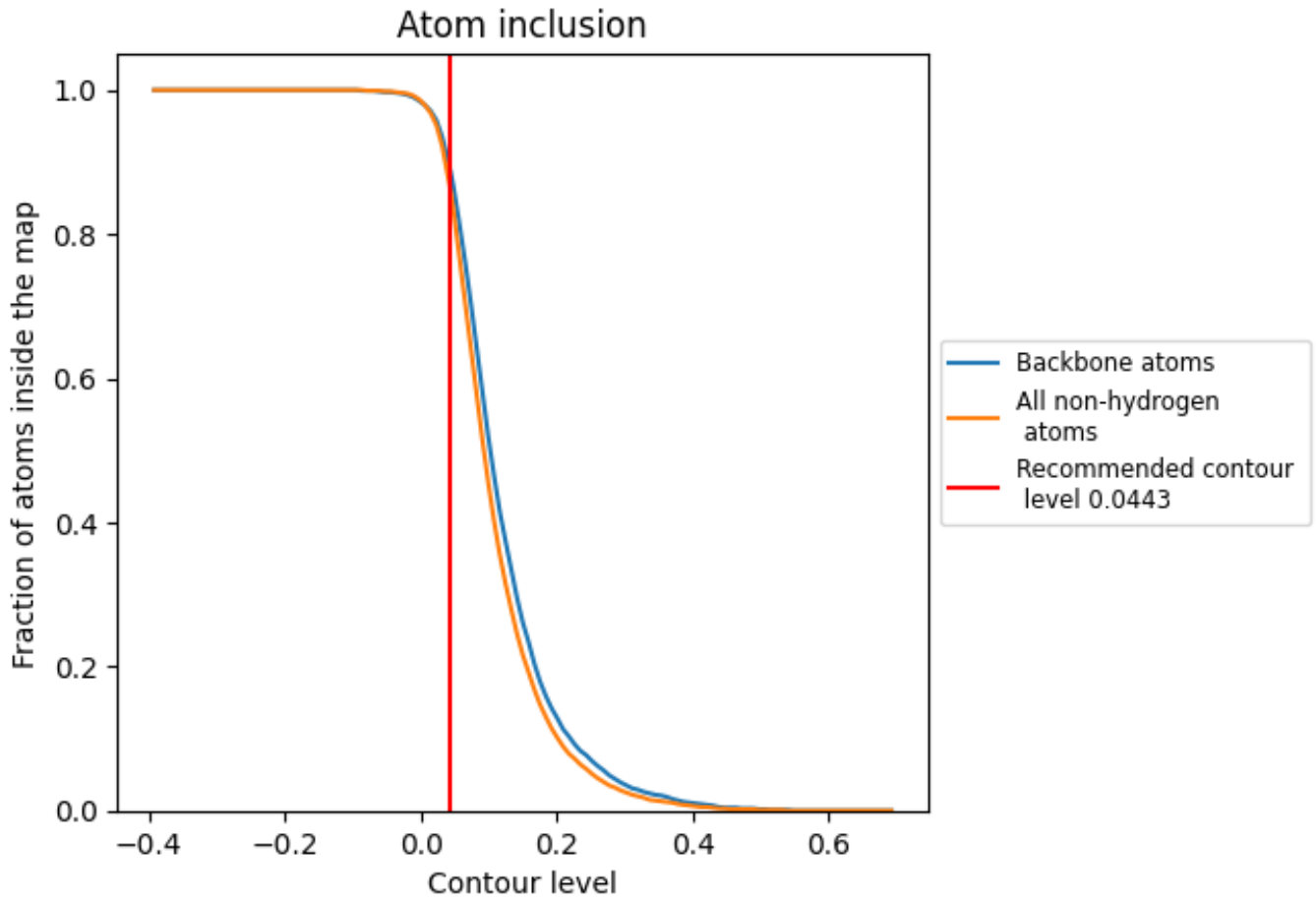
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

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 (0.0443).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.0443) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.3120
A	0.8450	0.3310
B	0.9100	0.2550
C	0.9160	0.2640
D	0.7200	0.1720
E	0.5000	0.1050
F	0.6800	0.3110