



Full wwPDB EM Validation Report ⓘ

Oct 7, 2025 – 12:11 PM EDT

PDB ID : 9E8C / pdb_00009e8c
EMDB ID : EMD-47716
Title : Integrin αIIbβ3 dimer conformation from human platelet membrane crude preparation
Authors : Han, X.; Nieman, M.T.
Deposited on : 2024-11-05
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

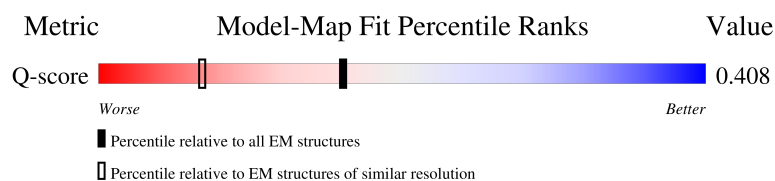
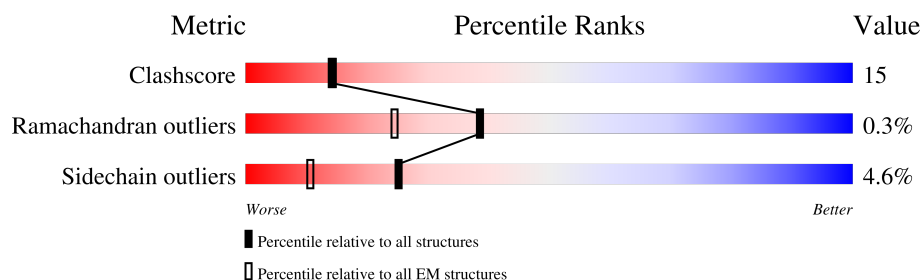
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

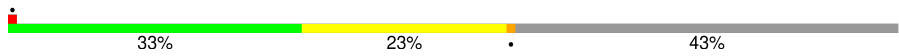
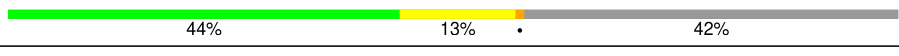
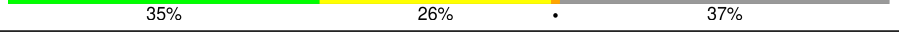
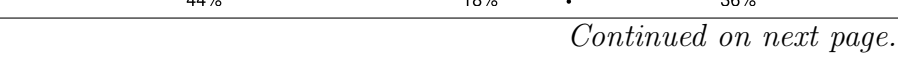
The reported resolution of this entry is 3.00 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1039	
1	C	1039	
2	B	788	
2	D	788	

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Mol	Chain	Length	Quality of chain
3	E	3	 100%
3	K	3	 67% 33%
4	G	2	 50% 50%
4	M	2	 50% 50%
5	H	3	 33% 67%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17076 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.

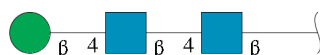
- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4525	2866	785	859	15		
1	C	602	Total	C	N	O	S	0	0
			4599	2908	803	872	16		

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	493	Total	C	N	O	S	0	0
			3762	2333	637	752	40		
2	D	506	Total	C	N	O	S	0	0
			3891	2407	668	776	40		

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



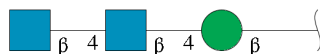
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

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



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	Ca	0
			4	4	
6	B	2	Total	Ca	0
			2	2	
6	C	4	Total	Ca	0
			4	4	
6	D	2	Total	Ca	0
			2	2	

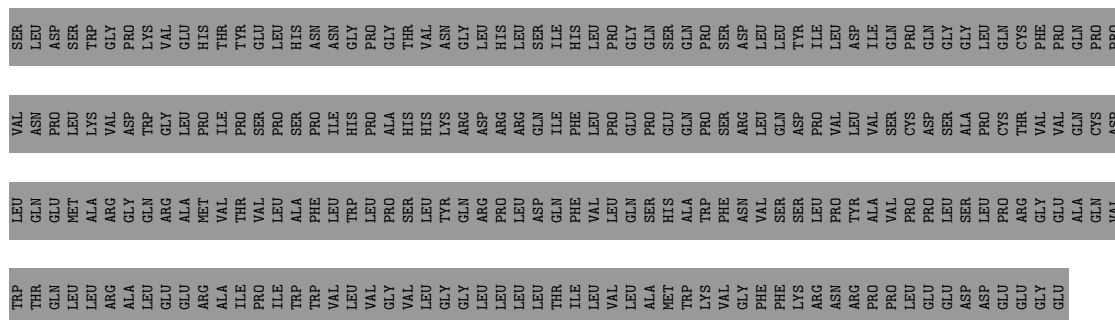
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



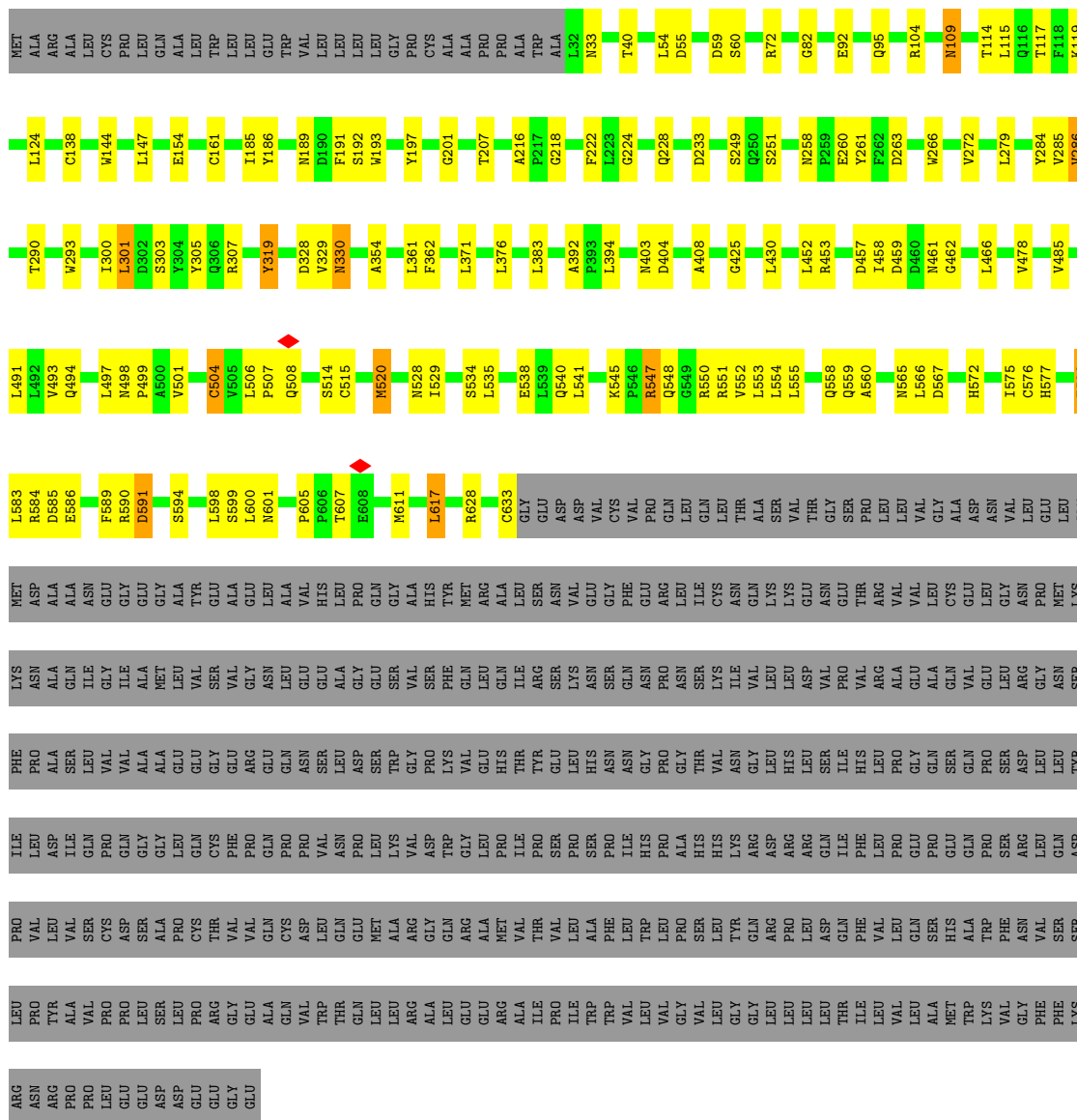
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

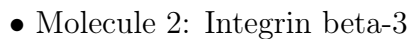
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	D	1	Total	Mg	0
			1	1	

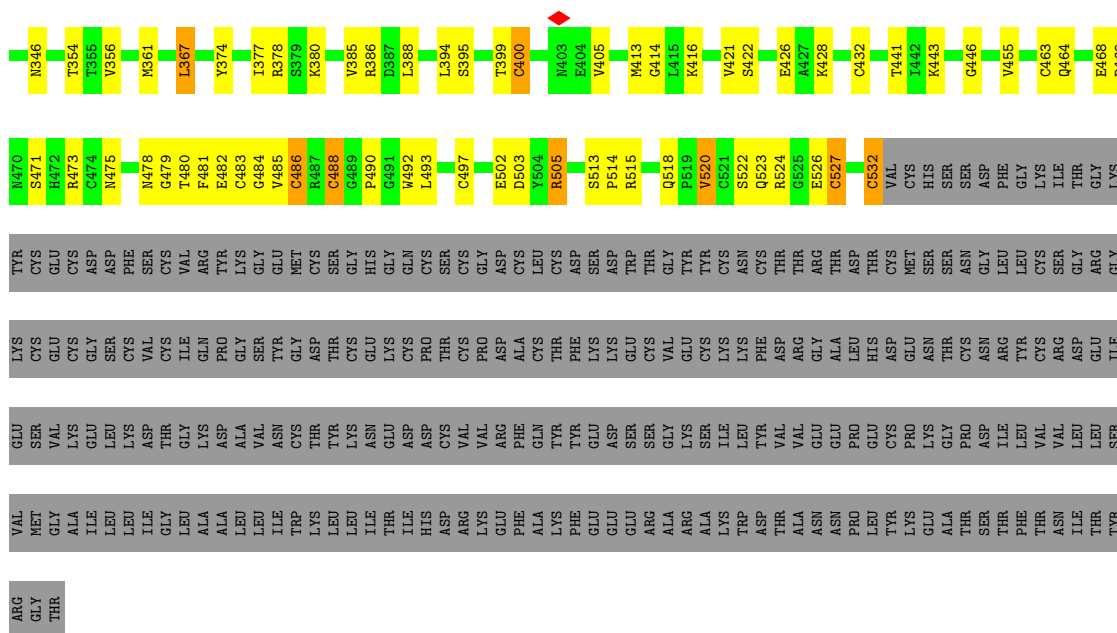


- Molecule 1: Integrin alpha-IIb

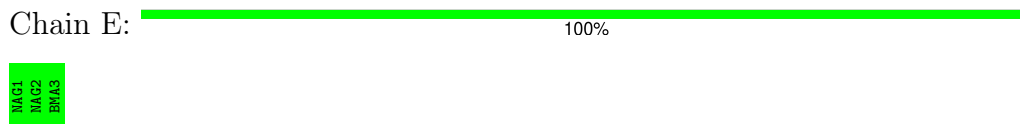


- Molecule 2: Integrin beta-3

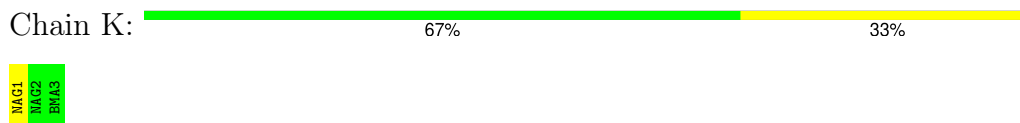




- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose

Chain H:  33% 67%

 MAG1
MAG2
MAG3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	274866	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 ($e^-/\text{\AA}^2$)	36.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.800	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/4637	0.39	0/6321
1	C	0.21	0/4713	0.36	0/6420
2	B	0.21	0/3825	0.41	1/5180 (0.0%)
2	D	0.25	0/3962	0.44	0/5369
All	All	0.22	0/17137	0.40	1/23290 (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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	512	CYS	N-CA-C	-5.35	105.85	112.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	515	ARG	Sidechain
2	D	473	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4525	0	4367	174	0
1	C	4599	0	4462	96	0
2	B	3762	0	3611	163	0
2	D	3891	0	3768	103	0
3	E	39	0	34	0	0
3	K	39	0	34	1	0
4	G	28	0	25	1	0
4	M	28	0	25	1	0
5	H	39	0	34	1	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
7	A	42	0	39	2	0
7	B	14	0	13	1	0
7	C	42	0	39	0	0
7	D	14	0	13	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
All	All	17076	0	16464	514	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 15.

All (514) 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)
2:D:469:PRO:HA	2:D:480:THR:HA	1.42	1.02
2:B:522:SER:HB3	2:B:527:CYS:HA	1.57	0.85
1:A:220:TYR:CE1	1:A:255:ASP:HB2	2.17	0.78
2:D:167:GLN:HG3	2:D:367:LEU:HD11	1.65	0.78
1:A:73:THR:HG22	1:A:74:LEU:N	1.97	0.78
2:B:131:ARG:HG3	2:B:133:VAL:H	1.50	0.75
1:A:73:THR:HG22	1:A:74:LEU:H	1.50	0.75
1:C:362:PHE:HB3	1:C:371:LEU:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:493:LEU:HD21	2:D:503:ASP:H	1.53	0.73
2:B:167:GLN:HG3	2:B:367:LEU:HD11	1.71	0.72
1:A:470:ALA:HB3	1:A:473:ALA:HB2	1.70	0.71
2:B:37:SER:HB3	2:B:41:GLN:HG3	1.72	0.71
2:B:504:TYR:HD2	2:B:524:ARG:HD2	1.55	0.71
1:A:273:GLY:HA3	1:A:326:VAL:HG11	1.72	0.71
1:C:285:VAL:HG22	1:C:300:ILE:HG12	1.73	0.71
2:B:512:CYS:HB3	2:B:521:CYS:H	1.56	0.70
2:D:469:PRO:HA	2:D:480:THR:CA	2.20	0.70
1:A:457:ASP:HA	1:A:464:PRO:HA	1.73	0.70
1:A:80:GLU:HB3	1:A:121:ARG:HE	1.54	0.70
2:D:471:SER:HB2	2:D:481:PHE:HB2	1.72	0.70
2:B:439:SER:HA	2:B:453:VAL:O	1.92	0.69
2:D:469:PRO:CA	2:D:480:THR:HA	2.21	0.69
1:A:220:TYR:CE2	1:A:255:ASP:HA	2.28	0.69
1:A:270:VAL:HG12	1:A:286:VAL:HG12	1.74	0.69
2:B:510:ASP:HA	2:B:514:PRO:HA	1.75	0.68
1:A:80:GLU:O	1:A:121:ARG:N	2.25	0.68
2:B:388:LEU:HD12	2:B:389:PRO:HD2	1.74	0.68
2:D:35:GLY:O	2:D:41:GLN:NE2	2.27	0.67
1:A:363:LEU:HD11	1:A:429:GLY:HA2	1.76	0.67
1:C:520:MET:SD	1:C:520:MET:N	2.68	0.67
1:A:189:ASN:ND2	1:A:190:ASP:OD1	2.25	0.66
1:A:66:ILE:HG23	1:A:87:CYS:HB2	1.77	0.66
1:A:220:TYR:CZ	1:A:255:ASP:HB2	2.30	0.66
2:D:83:PRO:O	2:D:119:ARG:NH1	2.28	0.66
1:C:109:ASN:OD1	1:C:109:ASN:N	2.26	0.66
1:A:197:TYR:HE1	1:A:221:TYR:HA	1.59	0.66
1:C:547:ARG:O	2:D:505:ARG:NH1	2.29	0.65
2:B:58:PRO:HD3	2:B:473:ARG:HH12	1.62	0.65
2:D:394:LEU:HA	2:D:426:GLU:O	1.96	0.65
1:A:398:ASP:HB2	1:A:484:VAL:HG21	1.78	0.65
1:A:571:LYS:HD3	1:A:575:ILE:HD11	1.78	0.65
2:B:259:ASP:HA	2:B:264:TRP:HD1	1.62	0.65
1:C:461:ASN:O	1:C:528:ASN:ND2	2.29	0.65
2:D:157:ILE:HG22	2:D:233:VAL:HG11	1.79	0.65
2:D:265:ARG:O	2:D:270:HIS:NE2	2.25	0.65
2:B:136:TYR:HD1	2:B:137:PRO:HD2	1.63	0.64
2:B:205:ASP:OD1	2:B:205:ASP:N	2.29	0.64
1:A:81:THR:HB	1:A:122:GLN:HE21	1.62	0.64
1:A:392:ALA:HB2	1:A:452:LEU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HB2	1:A:424:LEU:HD11	1.80	0.63
1:A:73:THR:CG2	1:A:74:LEU:H	2.10	0.63
1:A:218:GLY:HA2	1:A:222:PHE:HA	1.79	0.63
2:B:89:VAL:HA	2:B:114:ILE:HA	1.80	0.63
2:B:134:GLU:HA	2:B:417:ILE:HG13	1.80	0.63
1:A:45:PRO:HD2	1:A:50:PHE:HB2	1.80	0.63
2:B:318:LEU:HD22	2:B:351:ILE:HD11	1.79	0.63
1:A:115:LEU:HB3	1:A:146:VAL:HG22	1.79	0.63
1:A:554:LEU:HD23	1:A:581:ALA:HB2	1.80	0.62
2:B:463:CYS:O	2:B:467:ALA:N	2.30	0.62
2:D:165:ALA:HB2	2:D:226:VAL:HG11	1.80	0.62
1:A:164:ALA:HB1	1:A:171:ARG:HH11	1.64	0.62
1:A:495:ASP:OD2	1:A:628:ARG:NH1	2.32	0.62
2:D:361:MET:SD	2:D:361:MET:N	2.71	0.62
2:B:84:VAL:HG12	2:B:86:GLU:HG3	1.82	0.62
1:A:482:GLN:HE21	1:A:616:VAL:HG23	1.63	0.62
2:B:111:PRO:HD2	2:B:128:ILE:HG22	1.81	0.62
1:C:485:VAL:HG22	1:C:529:ILE:HD12	1.81	0.61
1:A:453:ARG:HB3	1:A:467:ILE:HD11	1.83	0.61
2:B:333:ILE:HG12	2:B:373:ALA:HB1	1.82	0.61
2:D:39:CYS:HB2	2:D:464:GLN:HB2	1.81	0.61
1:A:327:THR:HB	1:A:393:PRO:HB3	1.81	0.61
1:C:293:TRP:HB3	2:D:343:LEU:HD13	1.81	0.61
1:A:202:PHE:HZ	2:B:287:ARG:HB3	1.64	0.61
2:B:134:GLU:HG2	2:B:417:ILE:HG23	1.81	0.61
1:C:552:VAL:HG22	1:C:583:LEU:HD13	1.82	0.61
1:A:492:LEU:HB2	1:A:519:GLN:HB3	1.83	0.61
2:B:58:PRO:HD3	2:B:473:ARG:NH1	2.16	0.61
2:D:488:CYS:HB2	2:D:492:TRP:HB2	1.83	0.61
2:B:170:LYS:HG3	2:B:171:LEU:HG	1.83	0.60
2:B:245:PRO:HB2	2:B:281:HIS:CE1	2.36	0.60
2:D:329:ASN:OD1	2:D:443:LYS:NZ	2.34	0.60
2:D:160:LEU:HB3	2:D:229:PHE:HE2	1.66	0.60
2:D:483:CYS:O	2:D:485:VAL:N	2.33	0.60
2:B:37:SER:OG	2:B:487:ARG:NH1	2.34	0.60
1:A:602:VAL:O	1:A:621:THR:OG1	2.20	0.60
1:A:258:ASN:ND2	1:A:260:GLU:OE1	2.35	0.60
2:B:85:SER:HA	2:B:118:LEU:HA	1.83	0.60
1:C:218:GLY:HA2	1:C:222:PHE:HA	1.83	0.60
1:C:498:ASN:ND2	1:C:633:CYS:O	2.35	0.59
2:D:479:GLY:HA3	2:D:497:CYS:SG	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLU:HG3	1:A:563:THR:HB	1.85	0.59
1:C:504:CYS:N	1:C:515:CYS:SG	2.75	0.59
2:D:332:LEU:HB3	2:D:354:THR:HG22	1.85	0.59
1:A:533:LEU:HD23	1:A:568:LEU:HB2	1.84	0.58
2:B:134:GLU:HG3	2:B:418:GLY:HA3	1.84	0.58
2:D:29:ASN:OD1	2:D:69:ASN:ND2	2.36	0.58
1:A:55:ASP:OD1	1:A:56:PHE:N	2.34	0.58
1:A:624:GLN:O	1:A:626:GLN:NE2	2.36	0.58
1:C:540:GLN:HB2	1:C:599:SER:HB3	1.85	0.58
2:B:51:TRP:NE1	2:B:483:CYS:O	2.36	0.58
1:A:192:SER:HG	1:A:193:TRP:CD1	2.21	0.58
1:A:544:GLN:HE22	1:A:545:LYS:HD3	1.69	0.58
2:B:169:ARG:NH2	2:B:172:THR:O	2.36	0.58
2:B:245:PRO:O	2:B:281:HIS:NE2	2.37	0.58
1:C:185:ILE:O	1:C:189:ASN:ND2	2.37	0.58
1:C:547:ARG:NH2	1:C:559:GLN:OE1	2.37	0.58
2:D:90:LEU:HD12	2:D:113:ARG:HD2	1.86	0.58
2:B:28:PRO:O	2:B:32:THR:OG1	2.22	0.57
2:B:332:LEU:HB3	2:B:354:THR:HG22	1.86	0.57
1:A:146:VAL:HG21	1:A:180:ASN:HA	1.86	0.57
1:A:365:PRO:HG2	1:A:370:ALA:HB1	1.86	0.57
2:B:118:LEU:HD21	2:B:124:LYS:HB2	1.86	0.57
2:B:172:THR:HG21	2:B:175:LEU:HB2	1.87	0.57
2:D:400:CYS:HA	2:D:421:VAL:HG23	1.85	0.57
2:B:168:MET:HE3	2:B:371:VAL:HG22	1.86	0.57
1:C:207:THR:HG22	1:C:272:VAL:HG11	1.85	0.57
2:D:63:ARG:HD2	2:D:485:VAL:HG13	1.85	0.57
1:A:57:HIS:ND1	1:A:130:SER:OG	2.25	0.57
1:A:121:ARG:O	1:A:141:TRP:HB2	2.04	0.57
1:A:457:ASP:OD2	1:A:462:GLY:N	2.38	0.56
1:C:192:SER:HG	1:C:193:TRP:CD1	2.23	0.56
1:A:82:GLY:HA3	1:A:124:LEU:N	2.20	0.56
1:A:73:THR:CG2	1:A:74:LEU:N	2.63	0.56
1:A:40:THR:HB	1:A:478:VAL:HB	1.87	0.56
1:A:182:LEU:HD23	1:A:182:LEU:H	1.70	0.56
2:B:153:ASP:HB3	2:B:363:SER:HB3	1.88	0.56
1:C:258:ASN:ND2	1:C:260:GLU:OE1	2.34	0.56
2:D:277:ASP:OD1	2:D:277:ASP:N	2.39	0.56
2:B:70:LEU:HB3	2:B:75:CYS:HB2	1.87	0.56
1:C:501:VAL:H	1:C:514:SER:HB2	1.72	0.56
2:B:499:CYS:SG	2:B:500:SER:N	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HD13	1:A:580:MET:HG3	1.87	0.55
2:D:65:ASP:OD1	2:D:66:LEU:N	2.37	0.55
1:A:174:TYR:CZ	1:A:176:PRO:HG3	2.42	0.55
2:B:512:CYS:SG	2:B:522:SER:HB2	2.46	0.55
2:D:503:ASP:OD2	2:D:505:ARG:NH1	2.40	0.55
2:D:502:GLU:HB3	2:D:505:ARG:HH21	1.72	0.55
2:B:492:TRP:CE3	2:B:498:GLU:HA	2.42	0.55
1:A:198:CYS:HA	1:A:218:GLY:C	2.32	0.55
1:A:118:PHE:HB2	1:A:143:HIS:HB2	1.89	0.55
1:A:220:TYR:CD2	1:A:255:ASP:HA	2.42	0.55
1:A:402:TYR:CZ	1:A:427:SER:HB2	2.43	0.55
2:B:406:ILE:HG22	2:B:409:LEU:H	1.71	0.55
2:D:486:CYS:HB3	2:D:497:CYS:SG	2.48	0.54
1:C:548:GLN:O	2:D:505:ARG:NH1	2.39	0.54
2:B:230:ASN:HA	2:B:233:VAL:HG12	1.89	0.54
1:A:72:ARG:NH2	2:B:290:GLY:O	2.41	0.54
1:A:144:TRP:NE1	1:A:179:GLY:O	2.34	0.54
1:A:329:VAL:HA	1:A:403:ASN:HB2	1.88	0.54
2:B:271:LEU:HD22	2:B:333:ILE:HD11	1.89	0.54
2:B:469:PRO:HA	2:B:480:THR:HA	1.89	0.54
2:B:109:VAL:HG22	2:B:130:VAL:HG12	1.89	0.54
2:B:130:VAL:O	2:B:420:THR:HA	2.08	0.54
2:B:331:ASN:OD1	2:B:378:ARG:NH1	2.40	0.54
2:B:522:SER:N	2:B:526:GLU:O	2.39	0.54
1:A:95:GLN:N	1:A:95:GLN:OE1	2.41	0.54
2:D:124:LYS:HG3	4:G:1:NAG:HN2	1.72	0.54
1:A:331:GLY:HA3	1:A:402:TYR:HD1	1.73	0.54
1:A:589:PHE:HE1	1:A:592:LYS:HB3	1.72	0.54
1:C:491:LEU:HD13	1:C:520:MET:HB3	1.90	0.54
1:C:40:THR:HB	1:C:478:VAL:HB	1.90	0.53
1:A:136:VAL:HG13	1:A:163:LEU:HG	1.90	0.53
1:A:138:CYS:HA	1:A:161:CYS:HA	1.88	0.53
1:A:190:ASP:OD1	1:A:190:ASP:N	2.38	0.53
2:B:113:ARG:HH11	2:B:454:GLN:HE22	1.55	0.53
1:C:263:ASP:O	1:C:290:THR:OG1	2.26	0.53
2:D:513:SER:HB3	2:D:518:GLN:HB2	1.90	0.53
2:B:47:PRO:HA	2:B:119:ARG:HH11	1.74	0.53
1:C:330:ASN:HD22	1:C:330:ASN:H	1.56	0.53
1:C:494:GLN:HE22	1:C:497:LEU:HD11	1.73	0.53
1:C:541:LEU:HA	1:C:598:LEU:HD12	1.91	0.53
1:A:394:LEU:HA	1:A:455:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:468:GLU:HB3	2:D:481:PHE:HB3	1.91	0.53
1:A:104:ARG:H	1:A:119:LYS:HE2	1.73	0.53
2:B:83:PRO:HB3	2:B:458:ASP:HB3	1.89	0.53
1:C:319:TYR:OH	2:D:285:ASP:OD1	2.23	0.53
2:D:378:ARG:HA	2:D:378:ARG:HH11	1.74	0.53
2:B:130:VAL:HG21	2:B:381:VAL:HG11	1.90	0.53
1:C:82:GLY:HA3	1:C:124:LEU:HB3	1.89	0.53
2:B:259:ASP:HA	2:B:264:TRP:CD1	2.44	0.53
2:B:275:THR:HG22	2:B:335:ALA:HB3	1.90	0.53
1:C:584:ARG:HH21	1:C:589:PHE:HA	1.74	0.52
1:A:48:SER:HB3	1:A:472:GLY:HA2	1.91	0.52
1:A:54:LEU:HB3	1:A:68:VAL:HG22	1.91	0.52
1:A:170:ARG:HE	1:A:235:PHE:HD1	1.57	0.52
1:A:390:ALA:HB1	1:A:452:LEU:HB2	1.91	0.52
2:B:443:LYS:NZ	2:B:444:PRO:O	2.42	0.52
2:D:57:LEU:O	2:D:61:SER:N	2.42	0.52
1:C:408:ALA:HB2	1:C:452:LEU:HD11	1.91	0.52
1:A:394:LEU:HD23	1:A:454:GLY:HA3	1.92	0.52
2:B:151:LYS:HB2	2:B:238:VAL:HG21	1.91	0.52
1:A:202:PHE:CD2	1:A:217:PRO:HG3	2.44	0.52
1:A:52:PHE:HE2	2:B:292:VAL:HG11	1.74	0.52
2:D:89:VAL:HA	2:D:114:ILE:HG22	1.92	0.52
2:D:520:VAL:HG23	2:D:523:GLN:HA	1.92	0.52
1:A:220:TYR:CE2	1:A:255:ASP:CA	2.93	0.52
2:B:511:GLU:HB2	2:B:521:CYS:SG	2.49	0.52
1:A:136:VAL:HG12	1:A:161:CYS:SG	2.49	0.51
2:B:163:LYS:HG3	2:B:367:LEU:HG	1.90	0.51
2:D:475:ASN:ND2	4:M:2:NAG:O7	2.43	0.51
1:A:467:ILE:HG22	1:A:478:VAL:HG22	1.92	0.51
2:B:139:ASP:OD1	2:B:265:ARG:NH2	2.42	0.51
1:C:361:LEU:HB3	1:C:376:LEU:HB3	1.92	0.51
1:C:545:LYS:HB3	1:C:550:ARG:HD3	1.92	0.51
2:B:51:TRP:HE1	2:B:483:CYS:C	2.18	0.51
1:C:228:GLN:OE1	1:C:251:SER:OG	2.25	0.51
1:C:491:LEU:HD22	1:C:600:LEU:HB2	1.92	0.51
2:D:395:SER:O	7:D:804:NAG:O6	2.28	0.51
1:A:108:ARG:CZ	1:A:242:ILE:HG13	2.40	0.51
1:A:202:PHE:CZ	2:B:287:ARG:HB3	2.44	0.51
1:A:319:TYR:CE2	2:B:284:LEU:HB2	2.46	0.51
2:B:254:GLN:HA	2:B:257:VAL:HG22	1.93	0.51
1:C:301:LEU:HB3	1:C:307:ARG:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:LEU:HB2	2:D:131:ARG:HH21	1.76	0.51
2:D:211:LEU:HD21	2:D:214:PHE:HE1	1.76	0.51
1:C:394:LEU:HD21	1:C:466:LEU:HD13	1.91	0.51
2:B:61:SER:HB2	2:B:62:PRO:HD2	1.93	0.51
1:C:117:THR:HG22	1:C:144:TRP:HE3	1.76	0.50
1:C:501:VAL:HG12	1:C:514:SER:HA	1.93	0.50
1:A:134:VAL:HG11	1:A:231:VAL:HG11	1.93	0.50
1:C:554:LEU:O	1:C:558:GLN:NE2	2.44	0.50
2:B:43:LEU:HD21	2:B:80:ILE:HD11	1.92	0.50
2:B:394:LEU:HG	2:B:427:ALA:HA	1.93	0.50
1:C:425:GLY:HA2	1:C:430:LEU:HB2	1.93	0.50
1:A:146:VAL:H	1:A:153:ALA:HB3	1.75	0.50
1:A:345:MET:HE3	1:A:353:LEU:HD12	1.92	0.50
1:A:516:PHE:HZ	1:A:552:VAL:HG11	1.77	0.50
1:C:548:GLN:HB2	2:D:505:ARG:CZ	2.40	0.50
2:D:137:PRO:HB3	2:D:174:ASN:HB3	1.92	0.50
1:A:449:GLY:HA2	1:A:468:VAL:HG13	1.94	0.50
1:C:361:LEU:HD22	1:C:430:LEU:HD22	1.92	0.50
1:A:203:SER:HB2	1:A:270:VAL:HG22	1.93	0.49
2:B:169:ARG:O	2:B:169:ARG:NE	2.41	0.49
2:D:514:PRO:O	2:D:515:ARG:HG2	2.12	0.49
2:D:123:SER:HB3	2:D:428:LYS:HG3	1.93	0.49
1:A:131:TRP:O	1:A:134:VAL:HG12	2.12	0.49
2:B:119:ARG:HG2	2:B:122:ASP:HB2	1.95	0.49
1:A:589:PHE:O	1:A:592:LYS:NZ	2.45	0.49
2:D:334:PHE:HB2	2:D:356:VAL:HG22	1.95	0.49
1:C:534:SER:HA	1:C:567:ASP:HA	1.95	0.49
1:C:541:LEU:O	1:C:550:ARG:NH1	2.43	0.49
1:A:293:TRP:CD1	2:B:343:LEU:HD12	2.48	0.49
1:C:538:GLU:HB3	1:C:601:ASN:HB3	1.95	0.49
2:B:66:LEU:O	2:B:70:LEU:HG	2.13	0.49
2:B:523:GLN:O	2:B:524:ARG:NH1	2.36	0.49
1:C:216:ALA:O	1:C:224:GLY:HA2	2.13	0.49
1:C:329:VAL:HA	1:C:403:ASN:HB2	1.94	0.49
1:C:457:ASP:OD2	1:C:462:GLY:N	2.43	0.49
2:D:224:ASP:OD1	2:D:224:ASP:N	2.36	0.49
1:A:117:THR:HG22	1:A:144:TRP:CE3	2.47	0.49
2:D:116:LEU:HD23	2:D:455:VAL:HG22	1.95	0.49
1:A:394:LEU:HD21	1:A:466:LEU:HD13	1.95	0.48
1:C:233:ASP:OD2	1:C:249:SER:OG	2.27	0.48
2:D:480:THR:C	2:D:482:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:CYS:HB3	2:B:497:CYS:SG	2.52	0.48
2:B:125:ASN:HA	2:B:426:GLU:HA	1.93	0.48
1:C:506:LEU:HG	1:C:507:PRO:HD2	1.94	0.48
2:D:490:PRO:HA	2:D:493:LEU:HD23	1.95	0.48
1:A:353:LEU:HD11	2:B:350:LEU:HD22	1.95	0.48
1:A:555:LEU:HG	1:A:582:PHE:HD2	1.77	0.48
2:D:40:GLN:HB2	2:D:464:GLN:HE22	1.79	0.48
2:D:93:ARG:N	2:D:112:GLN:OE1	2.47	0.48
2:B:155:TRP:HA	2:B:158:GLN:HG2	1.95	0.48
2:B:158:GLN:HB3	2:B:234:LYS:HE2	1.96	0.48
1:C:535:LEU:HD22	1:C:617:LEU:HD11	1.96	0.48
2:D:152:ASP:N	2:D:152:ASP:OD1	2.46	0.48
2:D:271:LEU:HD11	2:D:374:TYR:HD1	1.79	0.48
2:D:492:TRP:O	2:D:497:CYS:HA	2.13	0.48
1:A:486:LYS:HE2	1:A:619:GLY:HA3	1.94	0.48
1:C:95:GLN:OE1	1:C:95:GLN:N	2.46	0.48
1:A:122:GLN:HB2	1:A:139:ALA:HB1	1.95	0.48
1:A:508:GLN:H	1:A:508:GLN:CD	2.22	0.47
1:A:547:ARG:HH11	1:A:548:GLN:H	1.61	0.47
2:B:506:PRO:HA	2:B:515:ARG:HD3	1.95	0.47
1:A:33:ASN:HB2	1:A:482:GLN:HG2	1.96	0.47
1:A:397:LEU:HA	1:A:464:PRO:HD2	1.96	0.47
2:B:62:PRO:O	2:B:64:CYS:N	2.47	0.47
2:B:392:LEU:HD11	2:B:457:PHE:HZ	1.79	0.47
1:A:460:ASP:OD1	1:C:572:HIS:N	2.46	0.47
2:D:91:GLU:OE2	2:D:93:ARG:NH2	2.48	0.47
2:D:140:ILE:HD11	2:D:168:MET:HE2	1.96	0.47
2:D:256:THR:HG23	2:D:330:ILE:HD12	1.96	0.47
2:D:414:GLY:O	2:D:416:LYS:NZ	2.47	0.47
2:B:321:MET:HE2	2:B:321:MET:HA	1.96	0.47
1:C:591:ASP:OD1	1:C:591:ASP:N	2.32	0.47
2:D:109:VAL:O	2:D:112:GLN:NE2	2.34	0.47
1:A:539:LEU:HD23	1:A:562:THR:O	2.15	0.47
2:B:286:GLY:O	2:B:290:GLY:N	2.47	0.47
2:B:314:ASP:OD1	2:B:315:TYR:N	2.48	0.47
1:C:59:ASP:OD1	1:C:60:SER:N	2.47	0.47
2:D:527:CYS:HB2	2:D:532:CYS:HB3	1.36	0.47
2:B:482:GLU:N	2:B:485:VAL:O	2.47	0.47
1:C:138:CYS:HB3	1:C:201:GLY:HA3	1.96	0.47
1:A:438:LEU:HB3	1:A:479:TYR:CZ	2.49	0.47
2:B:267:ASP:OD1	2:B:448:LYS:NZ	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:ARG:NH1	1:C:591:ASP:O	2.43	0.47
2:D:522:SER:OG	2:D:524:ARG:NE	2.47	0.47
2:B:88:ARG:NH1	2:B:89:VAL:O	2.47	0.47
2:B:218:HIS:O	2:B:305:ASN:ND2	2.48	0.47
2:B:512:CYS:HB3	2:B:520:VAL:HB	1.95	0.47
1:A:342:PRO:O	1:A:386:ARG:HA	2.15	0.47
2:B:98:LYS:HG2	2:B:135:ASP:HB3	1.97	0.47
2:B:401:LEU:O	2:B:421:VAL:HA	2.14	0.47
2:B:513:SER:N	2:B:521:CYS:O	2.47	0.47
2:D:43:LEU:HD22	2:D:119:ARG:NH2	2.30	0.47
1:A:280:ASN:HB3	7:A:1105:NAG:H83	1.97	0.47
2:B:342:ASN:HA	2:B:345:GLN:HG2	1.97	0.47
2:B:449:ASP:N	2:B:449:ASP:OD1	2.48	0.47
1:C:104:ARG:H	1:C:119:LYS:HD2	1.80	0.47
1:A:215:GLY:HA2	1:A:226:LEU:HD12	1.98	0.46
2:D:37:SER:N	2:D:41:GLN:OE1	2.36	0.46
2:B:522:SER:OG	2:B:523:GLN:N	2.40	0.46
1:C:258:ASN:HB3	1:C:261:TYR:HD1	1.80	0.46
1:C:284:TYR:CE2	1:C:303:SER:HA	2.49	0.46
1:A:104:ARG:HE	1:A:106:GLU:HG3	1.80	0.46
1:A:237:SER:HB2	1:A:247:VAL:HG13	1.98	0.46
2:B:211:LEU:HB2	2:B:237:SER:HB2	1.96	0.46
2:D:120:PRO:HG3	2:D:432:CYS:HB2	1.97	0.46
2:D:475:ASN:ND2	2:D:478:ASN:HD21	2.14	0.46
2:B:259:ASP:OD1	2:B:259:ASP:N	2.49	0.46
1:C:138:CYS:HA	1:C:161:CYS:HA	1.97	0.46
2:D:331:ASN:HB3	2:D:377:ILE:HD13	1.97	0.46
1:A:290:THR:HA	1:A:294:THR:HA	1.98	0.46
1:A:463:TYR:CE2	1:A:483:PRO:HA	2.51	0.46
1:A:486:LYS:HG2	1:A:619:GLY:HA3	1.98	0.46
2:B:439:SER:HB3	2:B:454:GLN:HG3	1.98	0.46
2:D:475:ASN:HB3	2:D:478:ASN:HD21	1.81	0.46
2:D:314:ASP:OD1	2:D:315:TYR:N	2.48	0.46
1:A:198:CYS:HA	1:A:219:GLY:N	2.31	0.46
2:B:294:PRO:HA	2:B:314:ASP:HB3	1.98	0.46
1:A:53:SER:OG	1:A:125:GLY:O	2.33	0.45
1:A:543:ARG:HE	1:A:599:SER:HB2	1.81	0.45
2:B:98:LYS:HA	2:B:134:GLU:HB2	1.96	0.45
2:B:131:ARG:NE	2:B:420:THR:OG1	2.50	0.45
1:C:590:ARG:H	1:C:590:ARG:HE	1.65	0.45
2:D:98:LYS:NZ	2:D:135:ASP:OD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:SER:O	1:C:628:ARG:NH1	2.49	0.45
1:A:599:SER:HA	1:A:624:GLN:HA	1.97	0.45
2:B:127:SER:HA	2:B:424:SER:HA	1.97	0.45
1:A:534:SER:HB2	1:A:605:PRO:HG3	1.98	0.45
2:B:125:ASN:HD21	7:B:804:NAG:HN2	1.63	0.45
2:B:500:SER:HB3	2:B:502:GLU:HG2	1.98	0.45
2:D:51:TRP:HA	2:D:63:ARG:O	2.16	0.45
2:D:245:PRO:HB2	2:D:281:HIS:NE2	2.32	0.45
2:B:108:GLN:HG2	2:B:133:VAL:HB	1.97	0.45
2:B:52:CYS:SG	2:B:70:LEU:HD13	2.57	0.45
2:B:70:LEU:O	2:B:75:CYS:N	2.45	0.45
2:B:220:LEU:HD22	2:B:229:PHE:HA	1.98	0.45
2:D:29:ASN:O	2:D:32:THR:N	2.48	0.45
2:D:339:ASN:ND2	2:D:340:VAL:HG13	2.30	0.45
1:A:315:GLN:OE1	1:A:345:MET:N	2.38	0.45
1:A:419:GLN:HG2	1:A:439:ASP:HA	1.98	0.45
2:B:95:LEU:HD13	2:B:131:ARG:HB2	1.98	0.45
2:B:108:GLN:O	2:B:131:ARG:N	2.50	0.45
1:A:329:VAL:HG11	1:A:405:ILE:HG23	1.98	0.45
1:A:395:GLY:C	1:A:403:ASN:HA	2.41	0.45
1:A:498:ASN:HB3	1:A:501:VAL:HG23	1.99	0.45
1:A:542:ASP:N	1:A:597:VAL:O	2.44	0.45
2:B:49:CYS:HA	2:B:66:LEU:HA	1.99	0.45
1:C:114:THR:HB	1:C:147:LEU:HB2	1.98	0.45
1:C:553:LEU:HB2	1:C:582:PHE:HD2	1.82	0.45
1:A:33:ASN:ND2	1:A:481:ALA:HB1	2.32	0.45
1:A:34:LEU:HD12	1:A:422:VAL:HG21	1.98	0.45
1:A:82:GLY:HA3	1:A:124:LEU:H	1.79	0.45
2:B:334:PHE:O	2:B:357:GLY:N	2.46	0.45
1:A:205:VAL:HB	1:A:270:VAL:HG23	1.98	0.44
1:A:343:LEU:HD11	2:B:283:ALA:HB3	1.99	0.44
2:B:524:ARG:HD3	2:B:524:ARG:HA	1.84	0.44
2:B:528:LEU:HB3	2:B:531:GLN:HG3	1.99	0.44
1:C:301:LEU:HD13	1:C:305:TYR:HA	2.00	0.44
1:A:138:CYS:SG	1:A:204:SER:HB3	2.57	0.44
1:A:151:GLU:OE1	1:A:182:LEU:HB2	2.17	0.44
1:A:316:MET:HB2	1:A:316:MET:HE3	1.66	0.44
2:B:158:GLN:NE2	2:B:234:LYS:HA	2.32	0.44
1:C:328:ASP:O	1:C:403:ASN:ND2	2.45	0.44
1:A:450:PHE:CG	1:A:471:TYR:HD2	2.36	0.44
2:B:61:SER:O	2:B:63:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:O	2:B:115:ALA:N	2.44	0.44
1:A:142:GLN:HE21	1:A:142:GLN:HB3	1.65	0.44
1:A:485:VAL:HG22	1:A:529:ILE:HG23	1.99	0.44
2:B:414:GLY:O	2:B:416:LYS:NZ	2.39	0.44
1:C:186:TYR:HB3	1:C:191:PHE:HA	1.99	0.44
1:C:547:ARG:NH1	1:C:560:ALA:H	2.16	0.44
2:D:176:ARG:NH1	2:D:265:ARG:HD3	2.33	0.44
2:D:184:ASP:HB3	2:D:213:MET:HE3	2.00	0.44
1:A:197:TYR:CE2	2:B:242:ARG:HD3	2.53	0.44
2:B:276:THR:O	2:B:336:VAL:HA	2.18	0.44
2:D:187:VAL:HG22	2:D:188:SER:H	1.82	0.44
2:D:151:LYS:HA	2:D:238:VAL:HG11	1.99	0.44
2:B:382:GLU:HB2	2:B:445:VAL:HB	1.99	0.43
1:A:289:PRO:HB2	1:A:319:TYR:CD1	2.52	0.43
1:C:258:ASN:HB3	1:C:261:TYR:CD1	2.54	0.43
1:A:265:TYR:CZ	2:B:288:LEU:HG	2.53	0.43
2:B:362:ASP:OD1	2:B:362:ASP:N	2.43	0.43
2:B:461:CYS:HB2	2:B:464:GLN:H	1.84	0.43
2:B:132:GLN:HB2	2:B:418:GLY:H	1.82	0.43
1:C:330:ASN:HD22	1:C:330:ASN:N	2.16	0.43
1:C:354:ALA:HB1	1:C:383:LEU:HD21	2.00	0.43
2:D:57:LEU:HD12	2:D:58:PRO:HD2	2.00	0.43
1:A:54:LEU:HB2	1:A:66:ILE:HD11	2.01	0.43
1:A:338:LEU:HD21	1:A:405:ILE:HG21	2.00	0.43
2:B:454:GLN:N	2:B:454:GLN:OE1	2.51	0.43
1:A:285:VAL:HG13	1:A:300:ILE:HD13	2.01	0.43
1:A:544:GLN:H	1:A:544:GLN:HG3	1.66	0.43
2:B:93:ARG:N	2:B:112:GLN:HE22	2.16	0.43
2:D:91:GLU:HB3	2:D:113:ARG:HB3	2.00	0.43
2:D:324:LYS:O	2:D:328:LYS:HG2	2.18	0.43
1:A:117:THR:HG22	1:A:144:TRP:HE3	1.83	0.43
1:A:508:GLN:HG2	1:A:509:THR:H	1.83	0.43
2:B:241:ASN:ND2	2:B:243:ASP:O	2.52	0.43
1:A:551:ARG:NE	1:A:592:LYS:HA	2.33	0.43
2:B:219:VAL:HG12	2:B:232:GLU:HG3	2.01	0.43
2:B:271:LEU:HD23	2:B:331:ASN:HB2	2.01	0.43
2:D:86:GLU:O	2:D:117:ARG:N	2.42	0.43
1:A:599:SER:HB3	1:A:622:HIS:NE2	2.34	0.42
1:A:90:ARG:HH21	1:A:92:GLU:HG3	1.84	0.42
1:A:554:LEU:HA	1:A:581:ALA:HA	2.01	0.42
1:C:55:ASP:HA	1:C:453:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:380:LYS:HG3	2:D:413:MET:HG3	1.99	0.42
1:A:194:ASP:OD1	1:A:195:LYS:N	2.52	0.42
2:B:444:PRO:HG2	2:B:447:PHE:HB2	2.02	0.42
1:C:92:GLU:H	1:C:92:GLU:CD	2.28	0.42
1:C:553:LEU:HB2	1:C:582:PHE:CD2	2.55	0.42
2:D:329:ASN:HB3	2:D:446:GLY:O	2.19	0.42
5:H:2:NAG:H3	5:H:3:NAG:H2	2.00	0.42
1:A:525:THR:C	1:A:529:ILE:HD11	2.44	0.42
2:B:51:TRP:O	2:B:80:ILE:HB	2.19	0.42
2:B:96:SER:O	2:B:131:ARG:NH1	2.53	0.42
1:A:54:LEU:O	1:A:453:ARG:NH2	2.39	0.42
2:B:119:ARG:HE	2:B:119:ARG:HB2	1.65	0.42
2:B:284:LEU:H	2:B:314:ASP:CG	2.23	0.42
1:A:405:ILE:HD11	1:A:430:LEU:HD21	2.02	0.42
2:B:46:SER:HB3	2:B:49:CYS:SG	2.60	0.42
1:C:72:ARG:NH2	2:D:290:GLY:O	2.53	0.42
1:C:272:VAL:HG12	1:C:284:TYR:HD1	1.84	0.42
1:C:545:LYS:O	1:C:550:ARG:NE	2.52	0.42
1:C:491:LEU:HB2	1:C:600:LEU:HD22	2.02	0.42
1:C:628:ARG:NH1	1:C:628:ARG:HA	2.34	0.42
2:D:385:VAL:HG12	2:D:388:LEU:HB2	2.02	0.42
2:B:275:THR:HA	2:B:335:ALA:O	2.20	0.42
1:A:285:VAL:HG11	1:A:337:LEU:HD11	2.02	0.42
1:A:618:HIS:CG	1:A:619:GLY:H	2.38	0.42
1:C:266:TRP:CZ2	1:C:286:VAL:HG11	2.55	0.42
2:D:185:LYS:HA	2:D:186:PRO:HD3	1.89	0.42
2:D:399:THR:HB	2:D:422:SER:OG	2.20	0.42
1:A:410:PRO:HA	1:A:448:PHE:O	2.19	0.41
1:A:541:LEU:HD12	1:A:552:VAL:HG23	2.01	0.41
1:A:547:ARG:C	1:A:549:GLY:H	2.28	0.41
2:B:125:ASN:OD1	2:B:125:ASN:N	2.50	0.41
2:D:135:ASP:OD1	2:D:135:ASP:N	2.52	0.41
1:A:34:LEU:O	1:A:436:GLN:NE2	2.45	0.41
1:A:502:LYS:NZ	1:A:512:PRO:O	2.35	0.41
2:B:97:ASP:OD1	2:B:97:ASP:N	2.44	0.41
2:B:197:GLU:O	2:B:201:ASN:N	2.46	0.41
2:B:216:TYR:O	2:B:307:TYR:N	2.50	0.41
2:D:325:LEU:HD11	2:D:332:LEU:HD22	2.01	0.41
2:B:83:PRO:HG2	2:B:119:ARG:HB2	2.02	0.41
2:B:498:GLU:N	2:B:498:GLU:OE1	2.54	0.41
1:A:266:TRP:HD1	1:A:288:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HB3	1:C:144:TRP:CH2	2.56	0.41
1:C:547:ARG:NH2	1:C:548:GLN:HG3	2.34	0.41
2:D:318:LEU:HD23	2:D:318:LEU:HA	1.91	0.41
1:A:61:HIS:ND1	1:C:577:HIS:HA	2.35	0.41
2:B:185:LYS:HB2	2:B:185:LYS:HE3	1.87	0.41
2:B:513:SER:OG	2:B:522:SER:HA	2.20	0.41
1:C:376:LEU:HD23	1:C:430:LEU:HD23	2.01	0.41
1:A:151:GLU:OE1	1:A:152:GLU:N	2.53	0.41
2:B:220:LEU:HB2	2:B:232:GLU:HG2	2.01	0.41
2:B:276:THR:HG22	2:B:336:VAL:HG12	2.03	0.41
1:C:33:ASN:OD1	1:C:33:ASN:N	2.54	0.41
1:C:565:ASN:OD1	1:C:565:ASN:N	2.54	0.41
2:D:136:TYR:CD1	2:D:137:PRO:HD2	2.56	0.41
1:A:211:GLU:H	1:A:211:GLU:HG3	1.72	0.41
1:A:385:GLY:HA2	1:A:411:TYR:C	2.46	0.41
1:C:548:GLN:O	2:D:505:ARG:HD3	2.21	0.41
2:B:248:GLY:HA3	2:B:274:PHE:HZ	1.86	0.41
2:B:277:ASP:OD1	2:B:277:ASP:N	2.54	0.41
2:B:474:CYS:SG	2:B:479:GLY:HA3	2.61	0.41
1:A:52:PHE:CE2	2:B:292:VAL:HG11	2.54	0.41
1:A:67:VAL:HG22	1:A:128:VAL:HG11	2.02	0.41
1:A:216:ALA:O	1:A:224:GLY:HA2	2.21	0.41
1:A:355:GLU:HB3	1:A:384:TYR:CD1	2.55	0.41
1:A:398:ASP:CB	1:A:484:VAL:HG21	2.49	0.41
2:B:176:ARG:HH11	2:B:265:ARG:HD3	1.86	0.41
2:B:307:TYR:CG	2:B:310:SER:HB2	2.56	0.41
1:C:392:ALA:HB2	1:C:452:LEU:HB3	2.02	0.41
1:C:499:PRO:HB3	1:C:589:PHE:HE1	1.85	0.41
2:D:52:CYS:H	2:D:63:ARG:HA	1.85	0.41
2:D:346:ASN:HD22	3:K:1:NAG:H83	1.86	0.41
2:D:386:ARG:HB3	2:D:441:THR:HB	2.03	0.41
1:A:571:LYS:HE2	1:A:573:SER:HB3	2.03	0.41
1:C:590:ARG:NH1	2:D:526:GLU:HG2	2.35	0.41
1:C:605:PRO:O	1:C:607:THR:N	2.53	0.41
1:A:537:ALA:HB1	1:A:600:LEU:HD21	2.02	0.40
1:A:553:LEU:HB3	1:A:582:PHE:CE1	2.56	0.40
1:A:622:HIS:ND1	7:A:1106:NAG:O6	2.45	0.40
2:B:324:LYS:HD3	2:B:324:LYS:HA	1.79	0.40
2:B:520:VAL:N	2:B:526:GLU:HB3	2.36	0.40
1:C:459:ASP:OD1	1:C:459:ASP:N	2.42	0.40
2:D:158:GLN:H	2:D:158:GLN:HG2	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TYR:HB2	1:A:223:LEU:HB3	2.03	0.40
2:B:217:LYS:HA	2:B:306:HIS:HA	2.02	0.40
2:B:249:PHE:HB3	2:B:316:PRO:HG2	2.03	0.40
1:A:233:ASP:OD2	1:A:247:VAL:HG12	2.20	0.40
1:A:576:CYS:HB2	1:C:60:SER:O	2.20	0.40
2:B:50:ALA:HB1	2:B:80:ILE:HG21	2.02	0.40
1:A:493:VAL:HG21	1:A:598:LEU:HG	2.02	0.40
1:A:541:LEU:HB2	1:A:552:VAL:HG23	2.04	0.40
2:B:248:GLY:HA3	2:B:274:PHE:CZ	2.57	0.40
1:C:585:ASP:OD1	1:C:586:GLU:N	2.55	0.40
2:D:164:LEU:HD23	2:D:177:ILE:HD13	2.02	0.40
2:B:391:GLU:HG3	2:B:433:PRO:HG3	2.03	0.40
2:B:486:CYS:HB3	2:B:488:CYS:SG	2.62	0.40
1:C:293:TRP:CD1	2:D:279:LYS:HE2	2.57	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	589/1039 (57%)	549 (93%)	39 (7%)	1 (0%)	44	77
1	C	600/1039 (58%)	569 (95%)	30 (5%)	1 (0%)	44	77
2	B	477/788 (60%)	430 (90%)	44 (9%)	3 (1%)	22	57
2	D	504/788 (64%)	459 (91%)	43 (8%)	2 (0%)	30	66
All	All	2170/3654 (59%)	2007 (92%)	156 (7%)	7 (0%)	38	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	63	ARG

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Mol	Chain	Res	Type
2	D	484	GLY
2	D	520	VAL
1	A	154	GLU
1	C	154	GLU
2	B	133	VAL
2	B	62	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	482/864 (56%)	456 (95%)	26 (5%)	18	50
1	C	491/864 (57%)	468 (95%)	23 (5%)	22	56
2	B	431/690 (62%)	412 (96%)	19 (4%)	24	58
2	D	448/690 (65%)	431 (96%)	17 (4%)	28	62
All	All	1852/3108 (60%)	1767 (95%)	85 (5%)	25	56

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	54	LEU
1	A	66	ILE
1	A	115	LEU
1	A	134	VAL
1	A	191	PHE
1	A	197	TYR
1	A	198	CYS
1	A	202	PHE
1	A	213	VAL
1	A	251	SER
1	A	261	TYR
1	A	266	TRP
1	A	308	LEU
1	A	319	TYR

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Mol	Chain	Res	Type
1	A	339	VAL
1	A	361	LEU
1	A	371	LEU
1	A	405	ILE
1	A	489	VAL
1	A	504	CYS
1	A	505	VAL
1	A	516	PHE
1	A	541	LEU
1	A	553	LEU
1	A	566	LEU
2	B	42	CYS
2	B	69	ASN
2	B	82	PHE
2	B	119	ARG
2	B	146	LEU
2	B	157	ILE
2	B	177	ILE
2	B	188	SER
2	B	205	ASP
2	B	233	VAL
2	B	295	ASN
2	B	367	LEU
2	B	396	PHE
2	B	426	GLU
2	B	449	ASP
2	B	455	VAL
2	B	488	CYS
2	B	493	LEU
2	B	512	CYS
1	C	54	LEU
1	C	109	ASN
1	C	197	TYR
1	C	279	LEU
1	C	286	VAL
1	C	301	LEU
1	C	319	TYR
1	C	330	ASN
1	C	404	ASP
1	C	458	ILE
1	C	493	VAL
1	C	504	CYS

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Mol	Chain	Res	Type
1	C	508	GLN
1	C	520	MET
1	C	547	ARG
1	C	555	LEU
1	C	566	LEU
1	C	575	ILE
1	C	576	CYS
1	C	582	PHE
1	C	591	ASP
1	C	611	MET
1	C	617	LEU
2	D	39	CYS
2	D	52	CYS
2	D	64	CYS
2	D	133	VAL
2	D	157	ILE
2	D	197	GLU
2	D	208	THR
2	D	213	MET
2	D	367	LEU
2	D	400	CYS
2	D	405	VAL
2	D	463	CYS
2	D	486	CYS
2	D	488	CYS
2	D	505	ARG
2	D	527	CYS
2	D	532	CYS

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

Mol	Chain	Res	Type
1	A	116	GLN
1	A	122	GLN
1	A	482	GLN
1	A	531	GLN
1	A	577	HIS
2	B	29	ASN
2	B	108	GLN
2	B	270	HIS
2	B	434	GLN
2	B	531	GLN

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Mol	Chain	Res	Type
1	C	78	GLN
1	C	116	GLN
1	C	189	ASN
1	C	475	GLN
1	C	527	HIS
2	D	129	GLN
2	D	236	GLN
2	D	368	GLN
2	D	402	ASN
2	D	464	GLN
2	D	478	ASN
2	D	523	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	2,3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.39	0
3	BMA	E	3	3	11,11,12	0.61	0	15,15,17	0.69	0
4	NAG	G	1	4	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.45	0
5	BMA	H	1	5	11,11,12	0.61	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	H	2	5	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
5	NAG	H	3	5	14,14,15	0.76	1 (7%)	17,19,21	0.39	0
3	NAG	K	1	2,3	14,14,15	0.28	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	BMA	K	3	3	11,11,12	0.58	0	15,15,17	0.69	0
4	NAG	M	1	4	14,14,15	0.23	0	17,19,21	0.56	0
4	NAG	M	2	4	14,14,15	0.21	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	NAG	O5-C1	2.19	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	O4-C4-C3	2.32	115.84	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

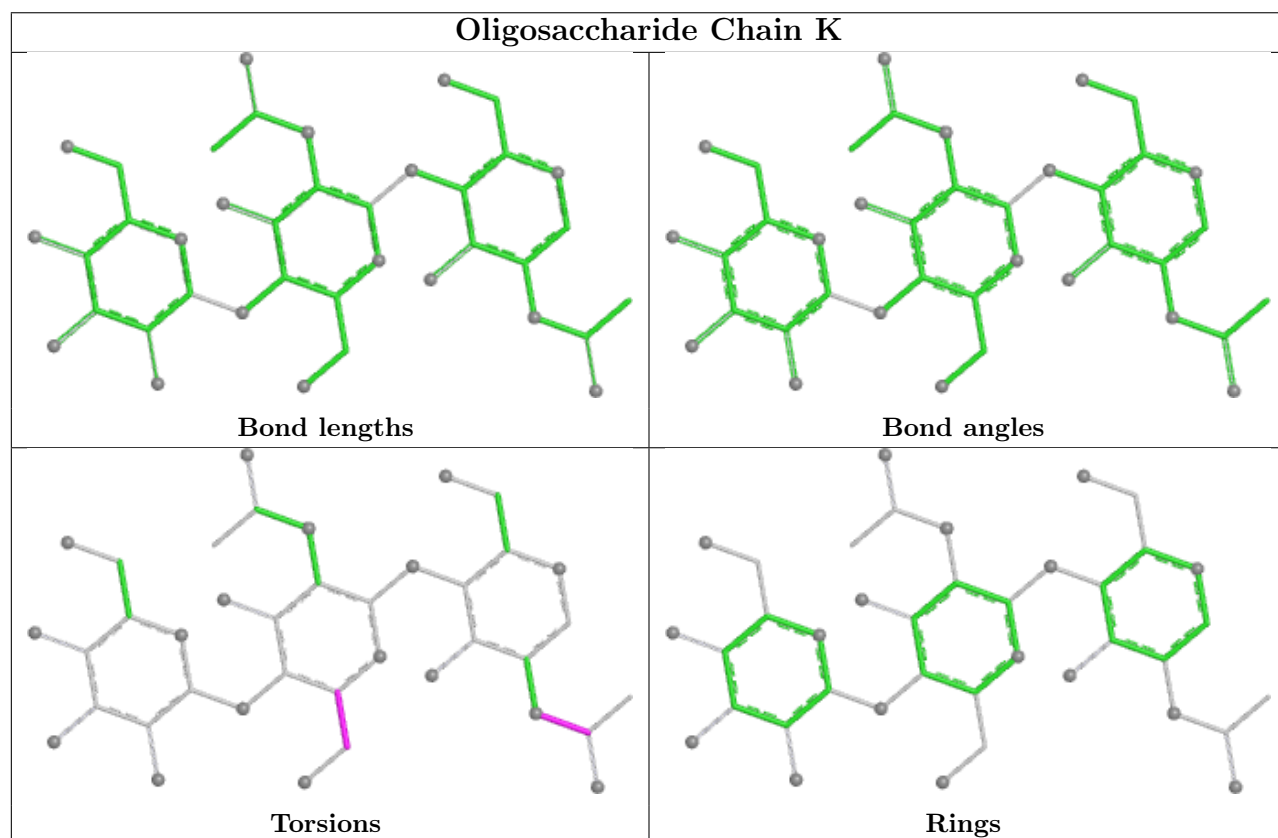
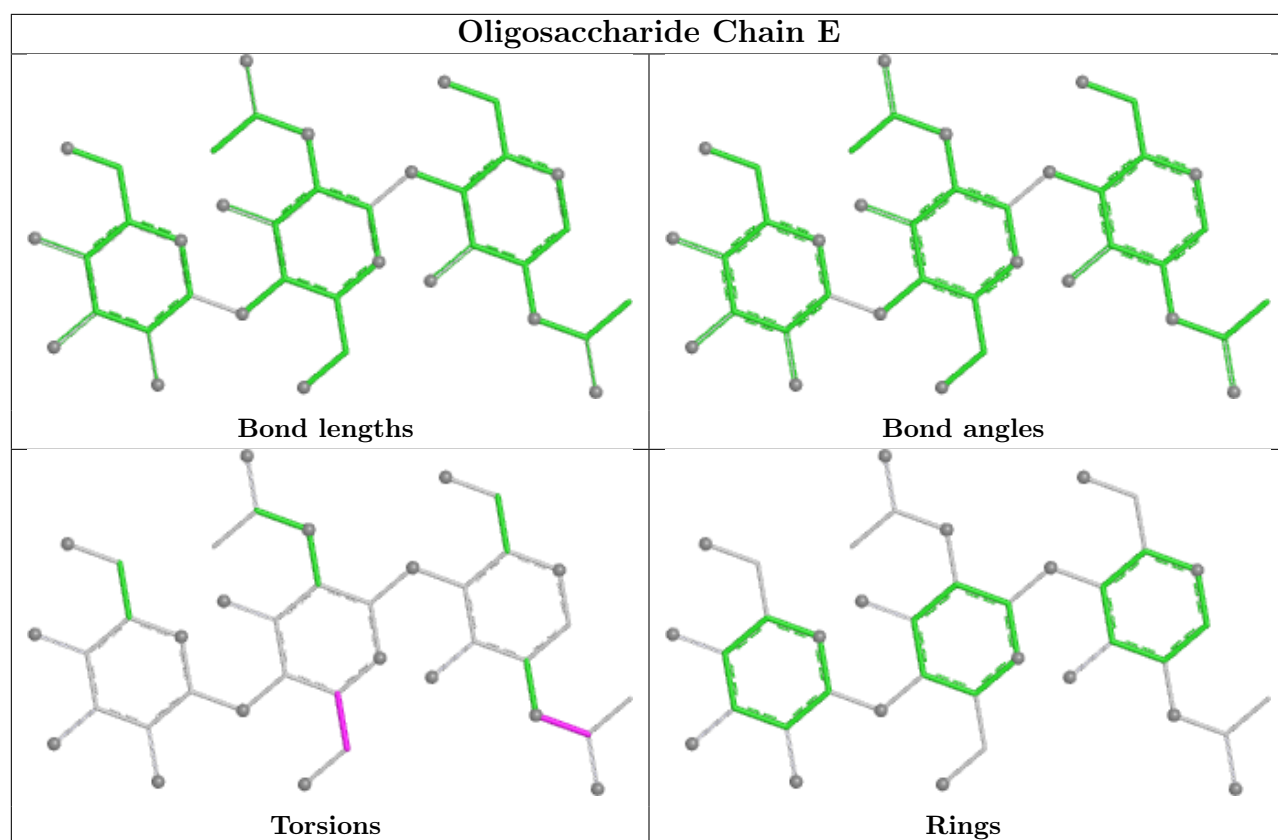
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
5	H	1	BMA	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
5	H	3	NAG	O5-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7
4	M	1	NAG	C1-C2-N2-C7

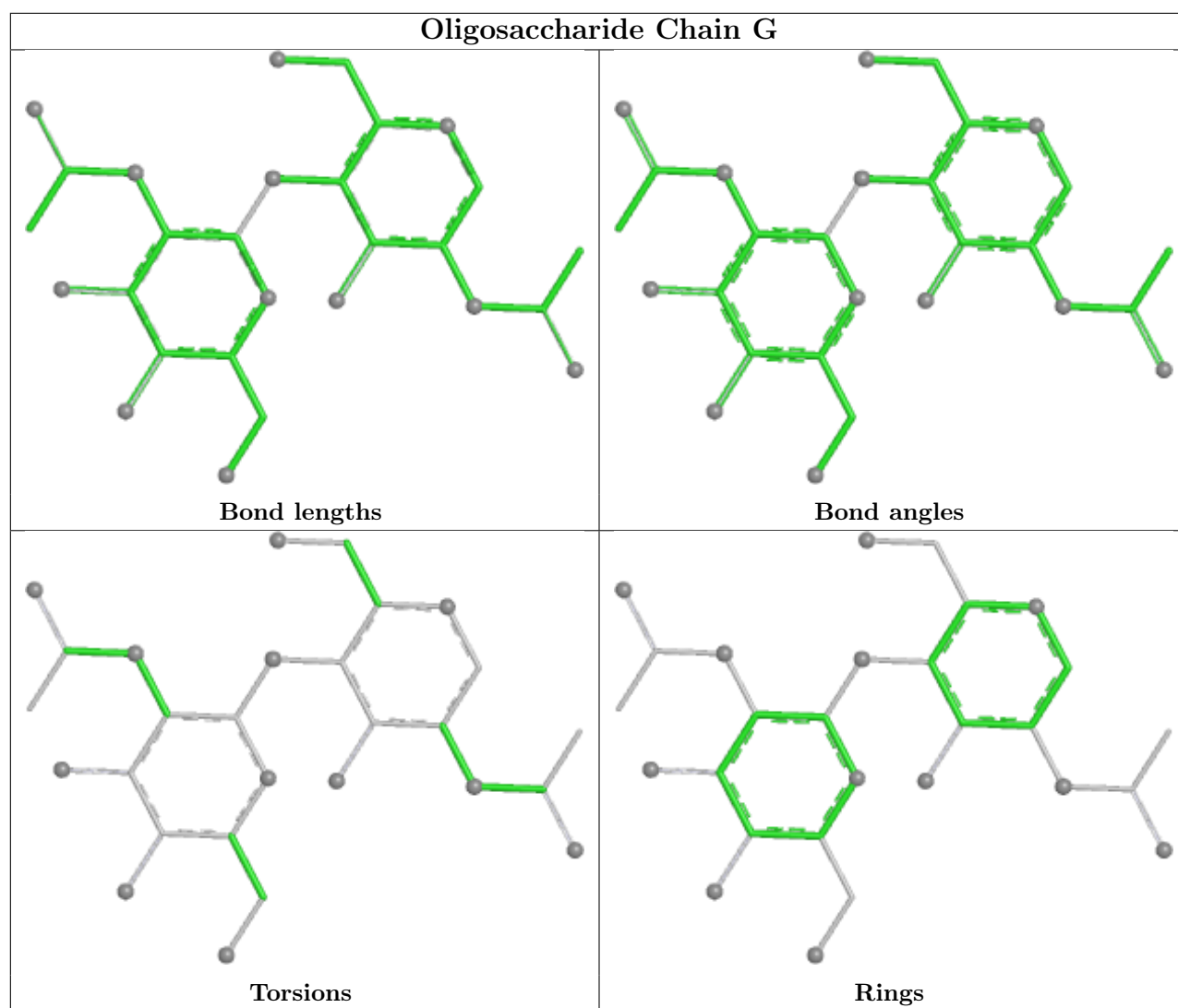
There are no ring outliers.

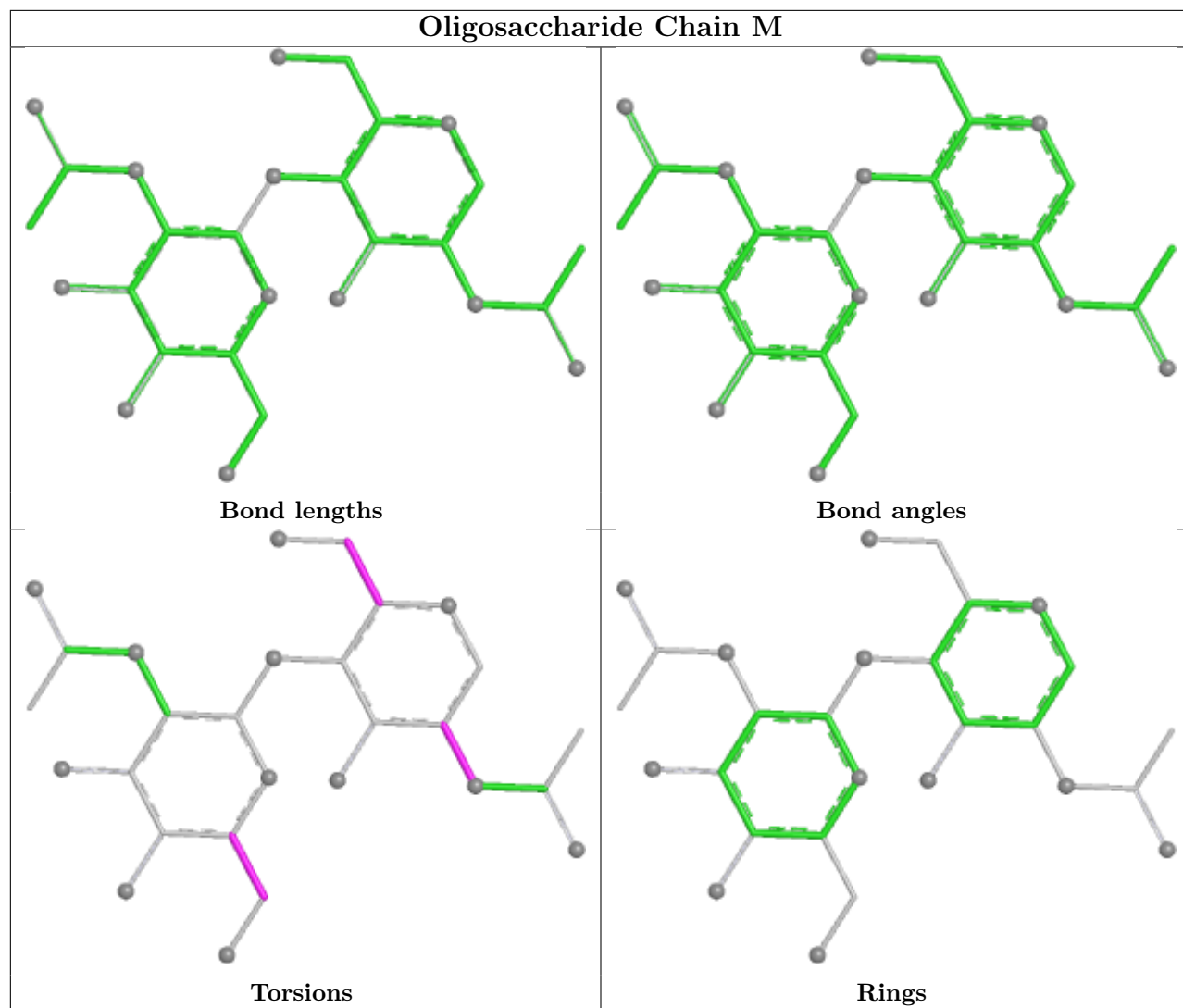
5 monomers are involved in 4 short contacts:

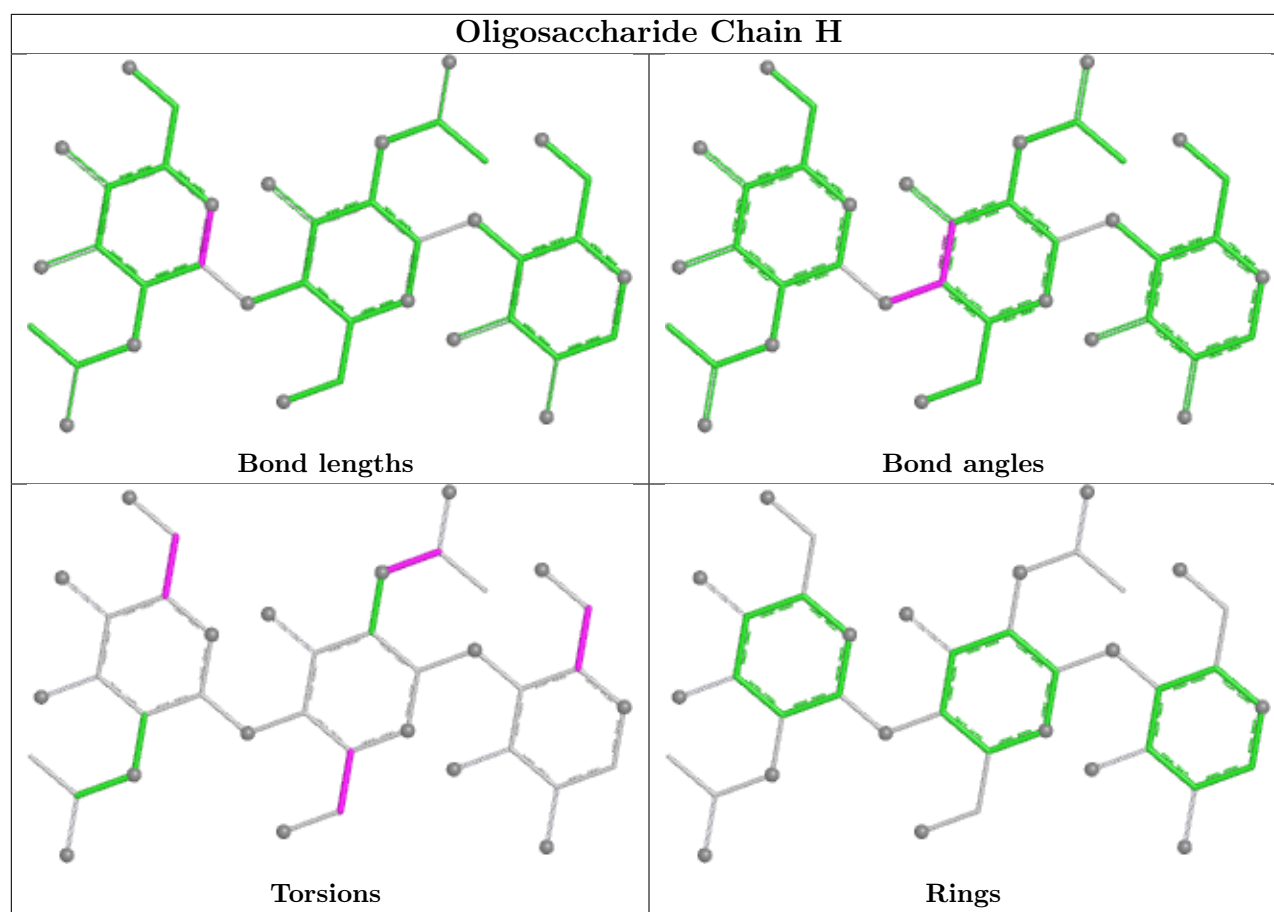
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	2	NAG	1	0
5	H	3	NAG	1	0
3	K	1	NAG	1	0
5	H	2	NAG	1	0
4	G	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	NAG	A	1107	-	14,14,15	0.18	0	17,19,21	0.46	0
7	NAG	A	1106	-	14,14,15	0.20	0	17,19,21	0.42	0
7	NAG	C	1107	-	14,14,15	0.20	0	17,19,21	0.44	0
7	NAG	C	1105	1	14,14,15	0.24	0	17,19,21	0.48	0
7	NAG	B	804	-	14,14,15	0.22	0	17,19,21	0.43	0
7	NAG	D	804	-	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
7	NAG	A	1105	1	14,14,15	0.84	1 (7%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	1106	-	14,14,15	0.57	0	17,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1107	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1106	-	-	0/6/23/26	0/1/1/1
7	NAG	C	1107	-	-	2/6/23/26	0/1/1/1
7	NAG	C	1105	1	-	4/6/23/26	0/1/1/1
7	NAG	B	804	-	-	2/6/23/26	0/1/1/1
7	NAG	D	804	-	-	2/6/23/26	0/1/1/1
7	NAG	A	1105	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1106	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1105	NAG	O5-C1	2.58	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1105	NAG	C1-O5-C5	3.71	117.16	112.19
7	D	804	NAG	C1-O5-C5	2.50	115.54	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	804	NAG	O5-C5-C6-O6
7	C	1107	NAG	O5-C5-C6-O6
7	C	1107	NAG	C4-C5-C6-O6
7	B	804	NAG	C4-C5-C6-O6
7	C	1105	NAG	O5-C5-C6-O6
7	A	1105	NAG	C8-C7-N2-C2
7	A	1105	NAG	O7-C7-N2-C2
7	C	1105	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	C	1105	NAG	O7-C7-N2-C2
7	D	804	NAG	C8-C7-N2-C2
7	D	804	NAG	O7-C7-N2-C2
7	C	1105	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1106	NAG	1	0
7	B	804	NAG	1	0
7	D	804	NAG	1	0
7	A	1105	NAG	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.

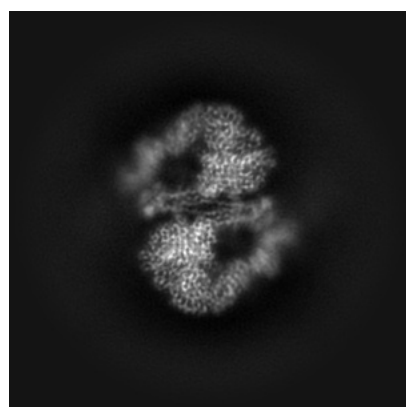
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47716. These allow visual inspection of the internal detail of the map and identification of artifacts.

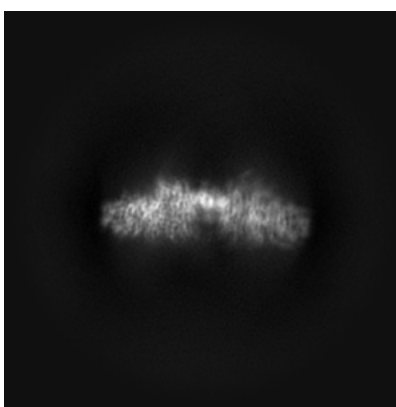
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

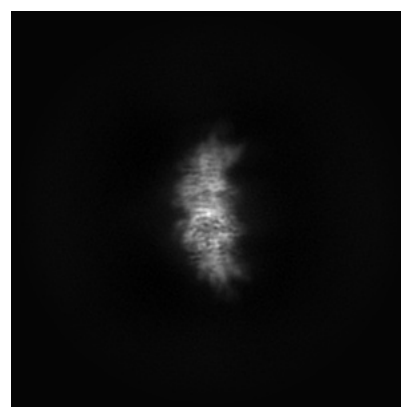
6.1.1 Primary map



X



Y

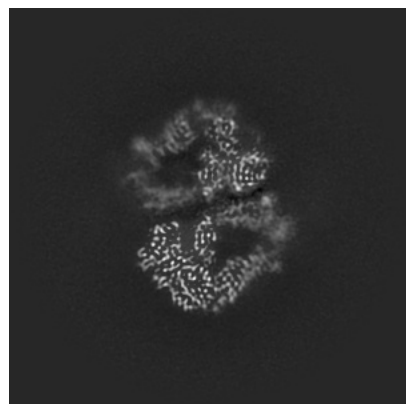


Z

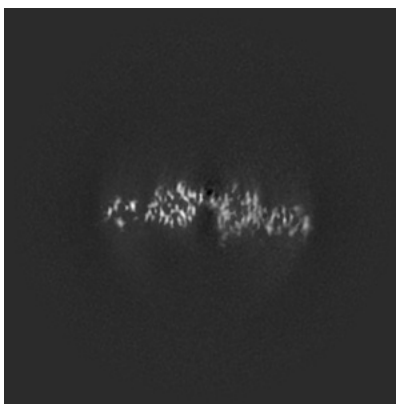
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

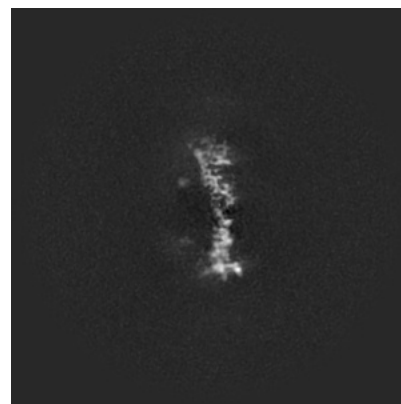
6.2.1 Primary map



X Index: 150



Y Index: 150

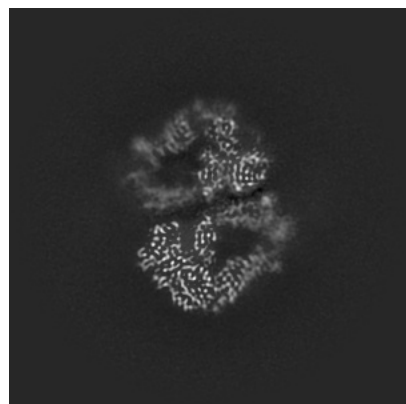


Z Index: 150

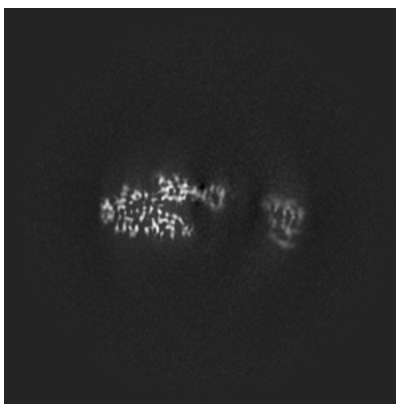
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

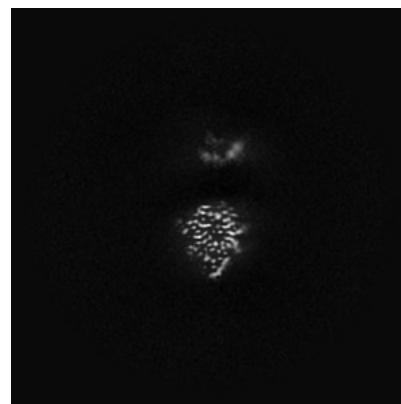
6.3.1 Primary map



X Index: 150



Y Index: 132

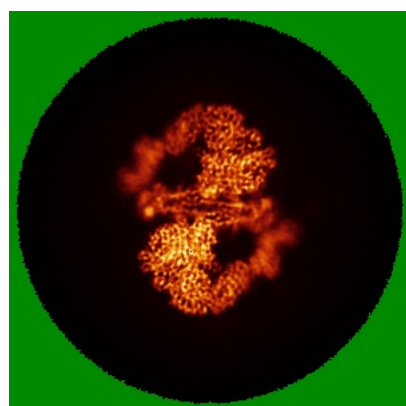


Z Index: 118

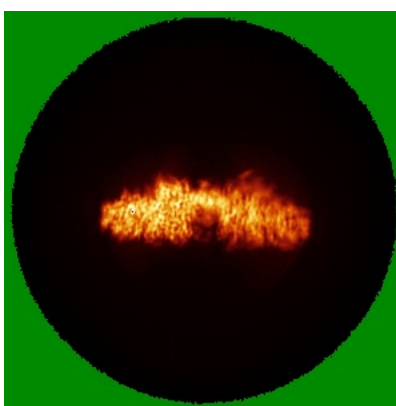
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

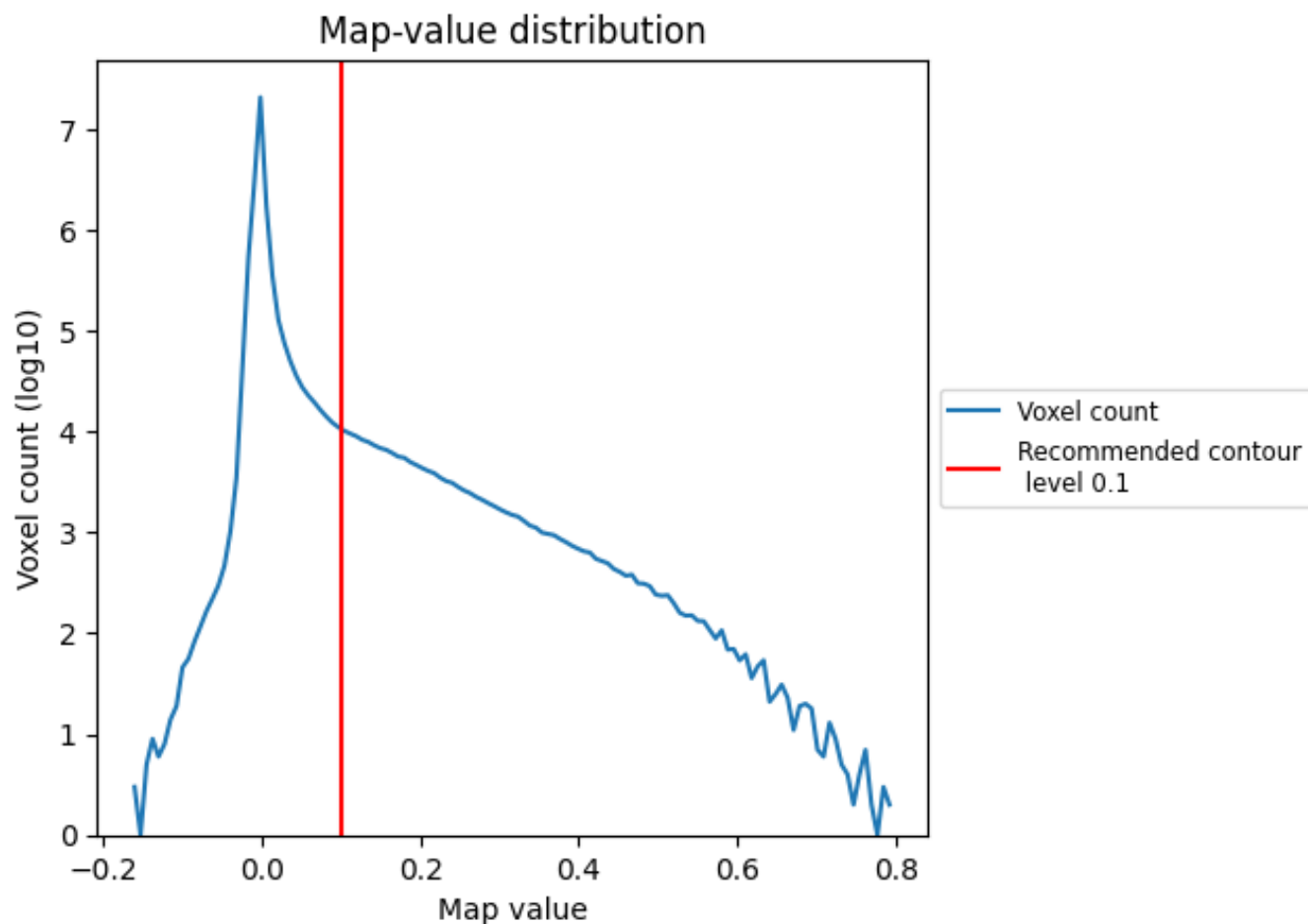
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

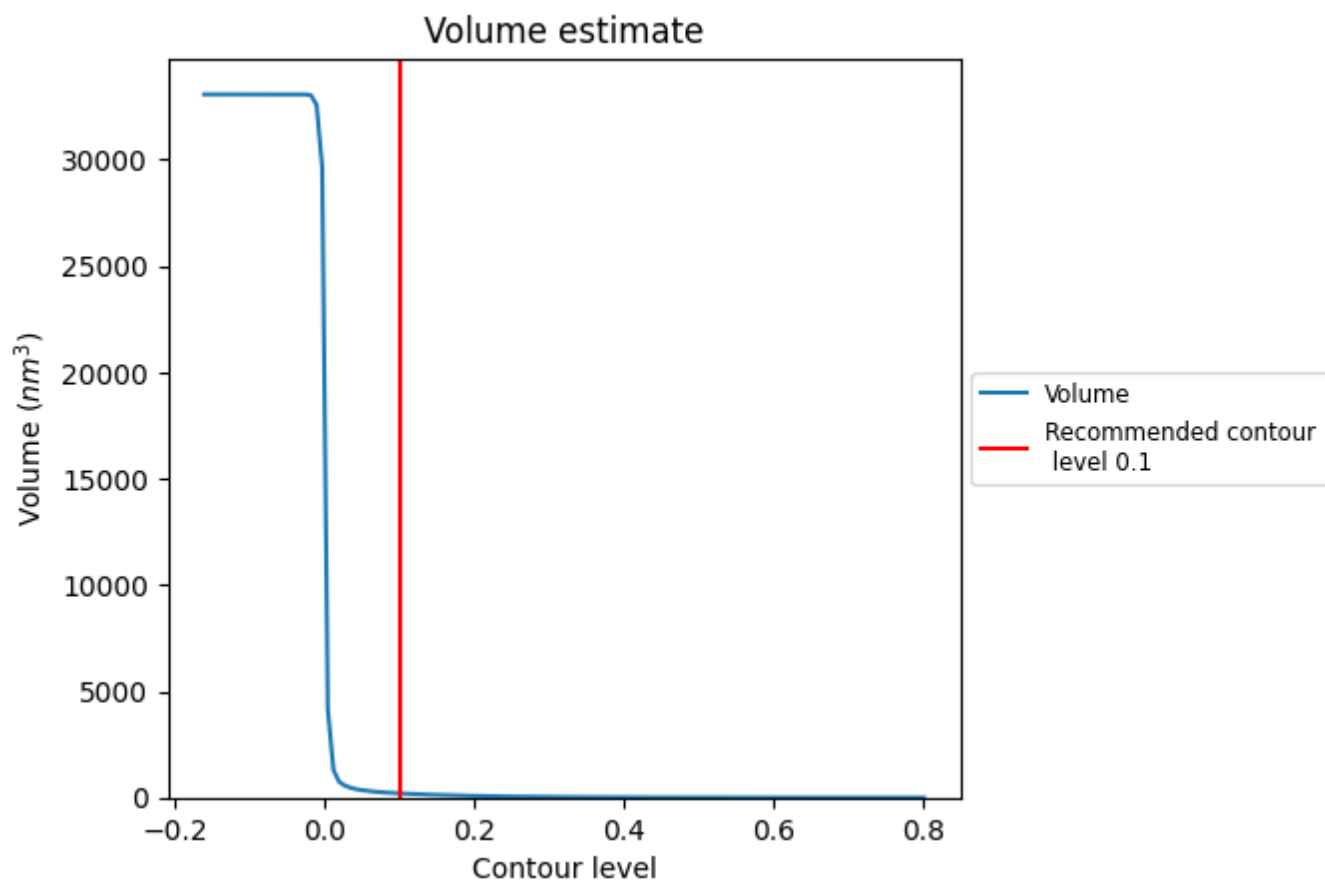
This section contains the results of statistical analysis of the map.

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.

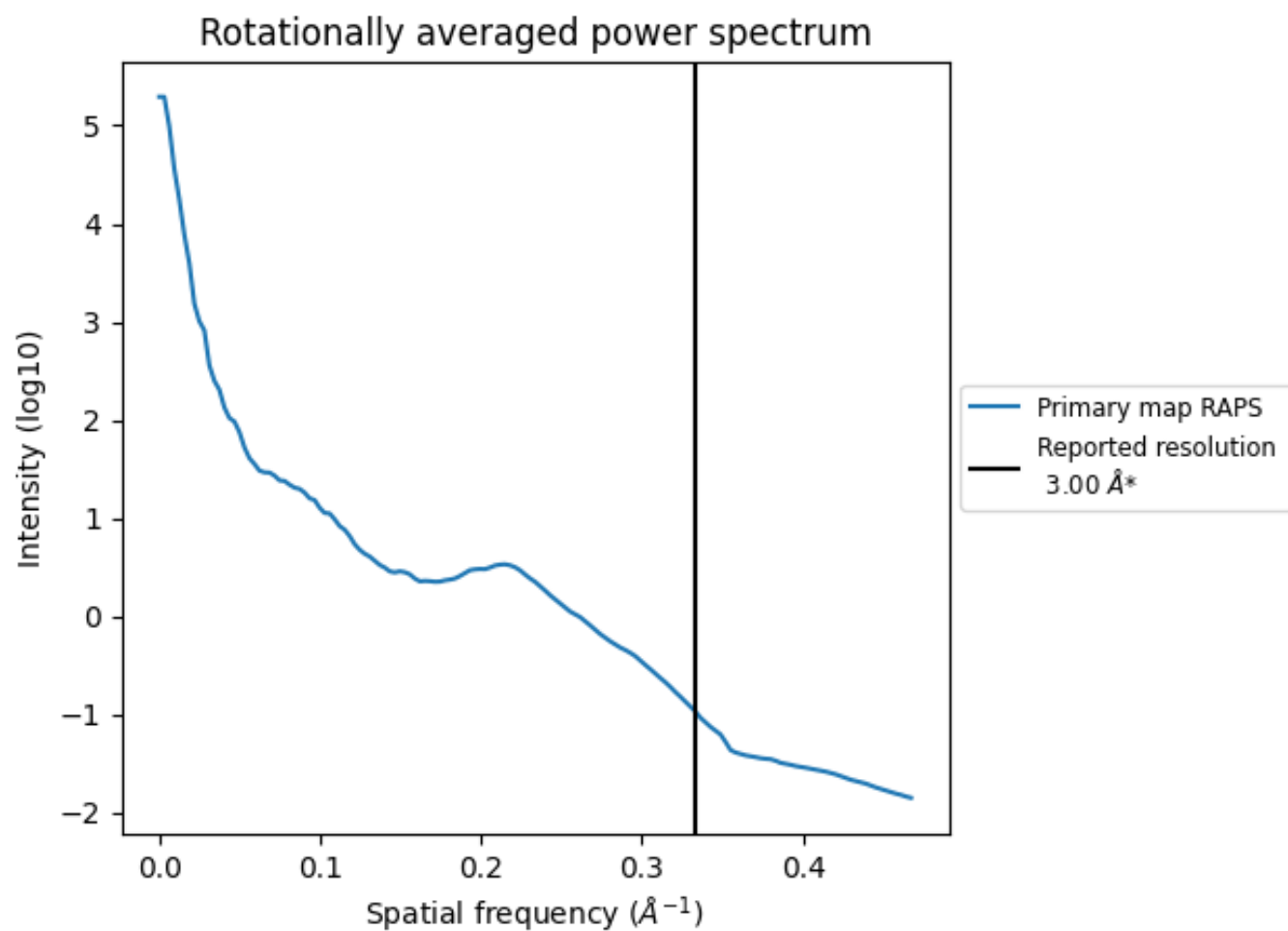
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm^3 ; this corresponds to an approximate mass of 178 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 0.333 Å⁻¹

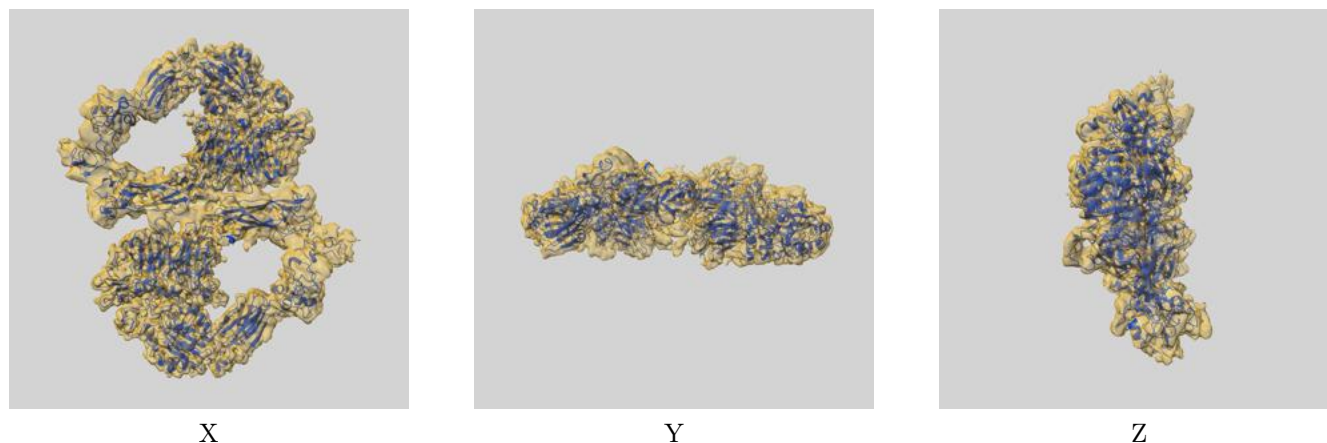
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

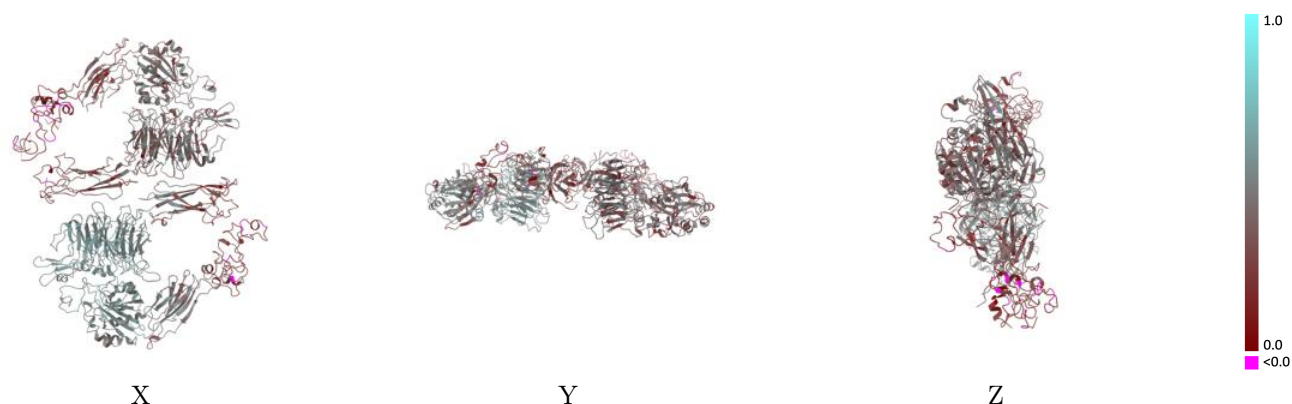
This section contains information regarding the fit between EMDB map EMD-47716 and PDB model 9E8C. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



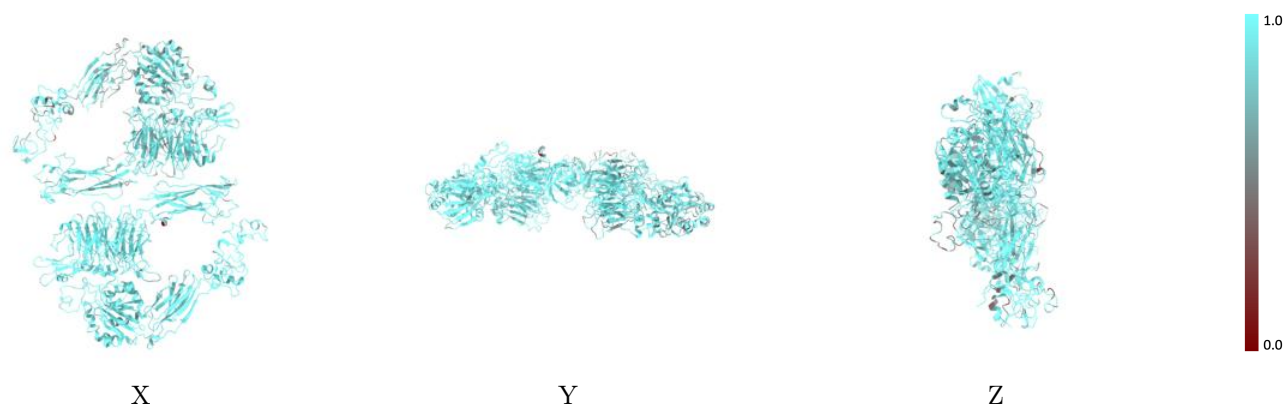
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



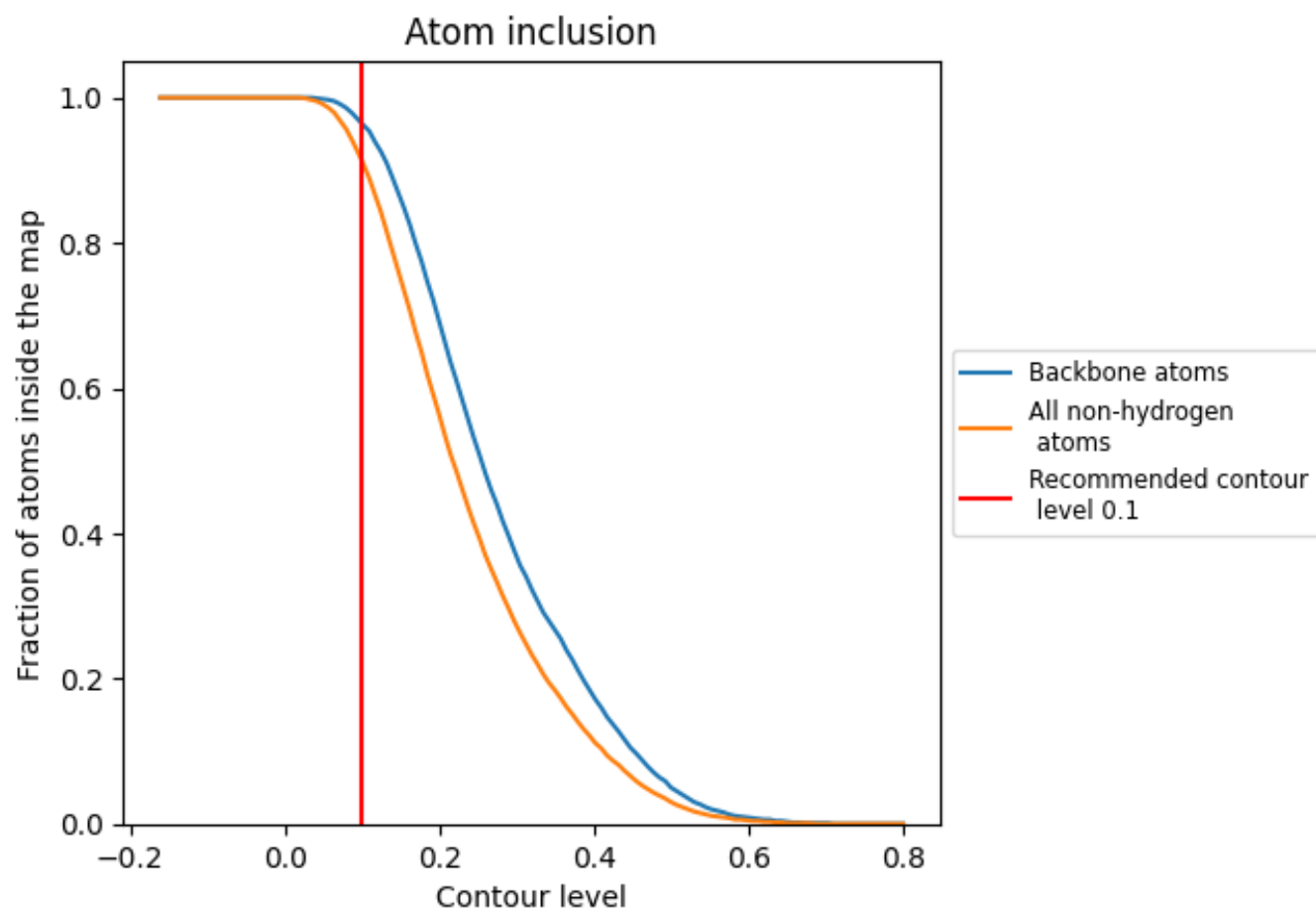
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9130</div>	<div><div></div>0.4080</div>
A	<div><div></div>0.8990</div>	<div><div></div>0.3840</div>
B	<div><div></div>0.8320</div>	<div><div></div>0.3200</div>
C	<div><div></div>0.9640</div>	<div><div></div>0.4870</div>
D	<div><div></div>0.9460</div>	<div><div></div>0.4320</div>
E	<div><div></div>0.8460</div>	<div><div></div>0.3540</div>
G	<div><div></div>0.9290</div>	<div><div></div>0.2940</div>
H	<div><div></div>0.9740</div>	<div><div></div>0.3550</div>
K	<div><div></div>0.9230</div>	<div><div></div>0.4620</div>
M	<div><div></div>0.8930</div>	<div><div></div>0.2320</div>

1.0

0.0

<0.0