Full wwPDB EM Validation Report ⓘ

May 27, 2024 – 03:15 PM JST

PDB ID	:	8JIZ
EMDB ID	:	EMD-36335
Title	:	Cryo-EM structure of GluN1-2A NMDAR in complex with human Fab5F6 in two fab bind conformation
Authors	:	Wang, H.; Zhu, S.
Deposited on	:	2023-05-29
Resolution	:	3.80 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:

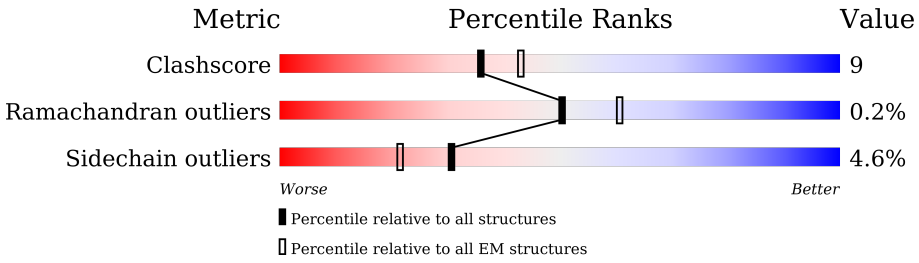
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.80 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	841	66% 22% • 10%
1	C	841	71% 18% • 10%
2	B	847	5% 66% 25% • 8%
2	D	847	69% 21% • 8%
3	E	259	39% 71% 16% 12%
3	G	259	10% 69% 16% 15%
4	F	236	37% 75% 15% • 9%
4	H	236	9% 70% 20% 9%

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Mol	Chain	Length	Quality of chain
5	I	2	100%
5	J	2	100%
5	K	2	100%
5	L	2	100%
5	M	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31002 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 Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5950	3847	967	1099	37		
1	C	756	Total	C	N	O	S	0	0
			5940	3836	972	1094	38		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	782	Total	C	N	O	S	0	0
			6120	3905	1063	1118	34		
2	D	776	Total	C	N	O	S	0	0
			6094	3883	1055	1122	34		

- Molecule 3 is a protein called Fab5F6 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	228	Total	C	N	O	S	0	0
			1708	1080	280	340	8		
3	G	219	Total	C	N	O	S	0	0
			1650	1049	270	324	7		

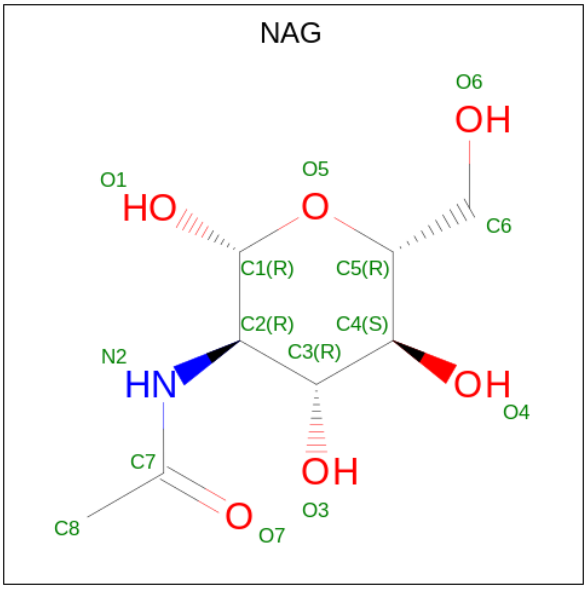
- Molecule 4 is a protein called Fab5F6 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	214	Total	C	N	O	S	0	0
			1644	1028	276	334	6		
4	H	214	Total	C	N	O	S	0	0
			1644	1028	276	334	6		

- Molecule 5 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
5	I	2	Total C N O 28 16 2 10	0	0
5	J	2	Total C N O 28 16 2 10	0	0
5	K	2	Total C N O 28 16 2 10	0	0
5	L	2	Total C N O 28 16 2 10	0	0
5	M	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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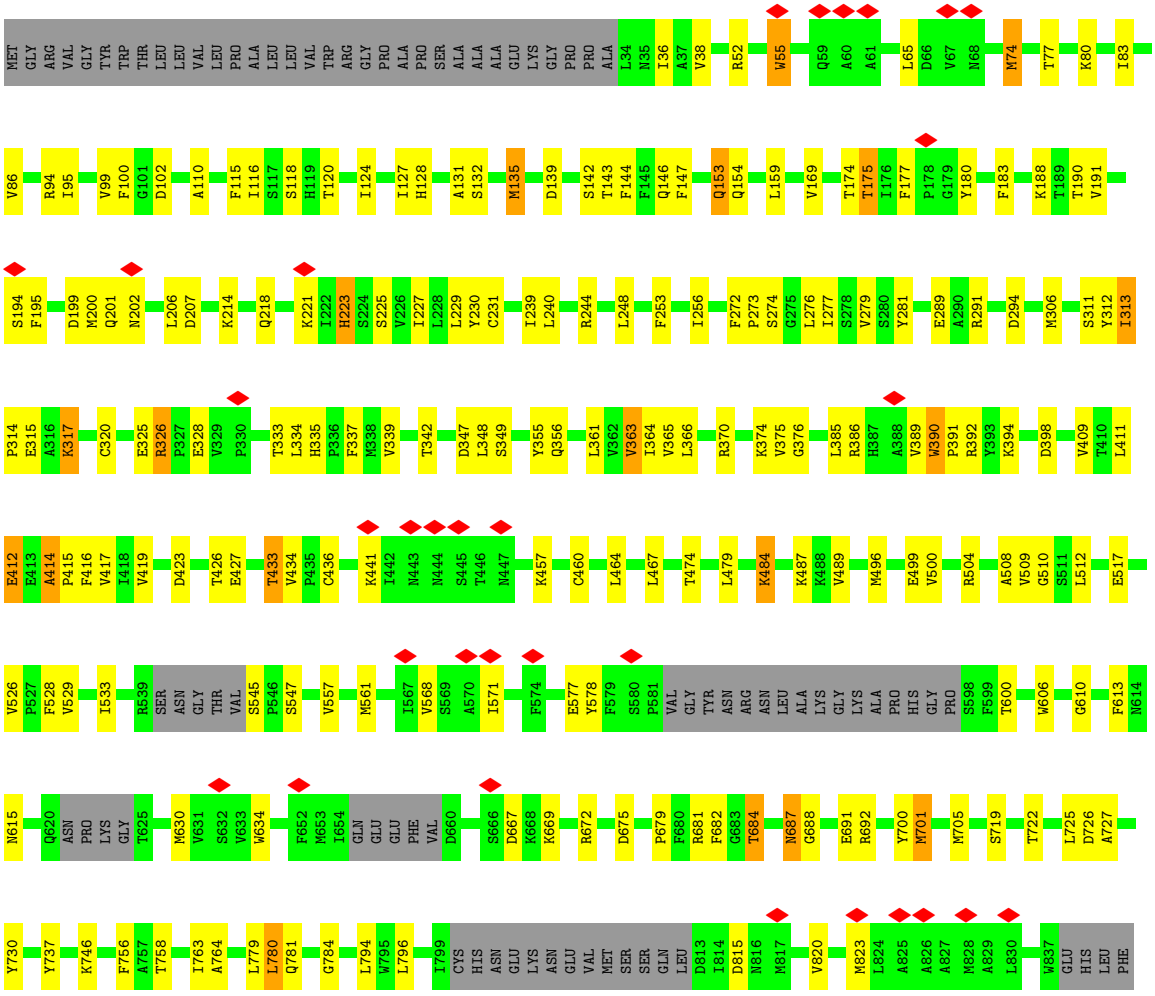
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

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.

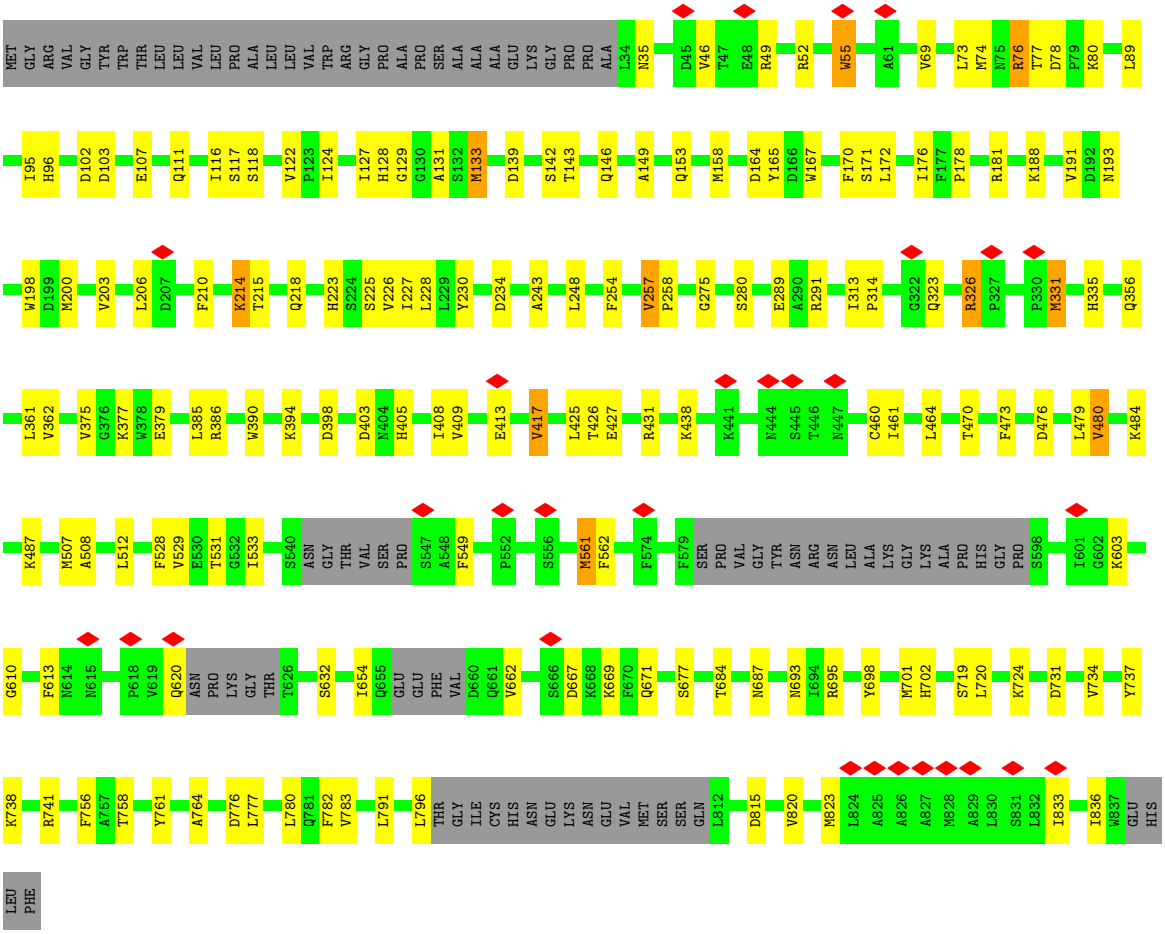
• Molecule 1: Glutamate receptor ionotropic, NMDA 2A

Chain A:



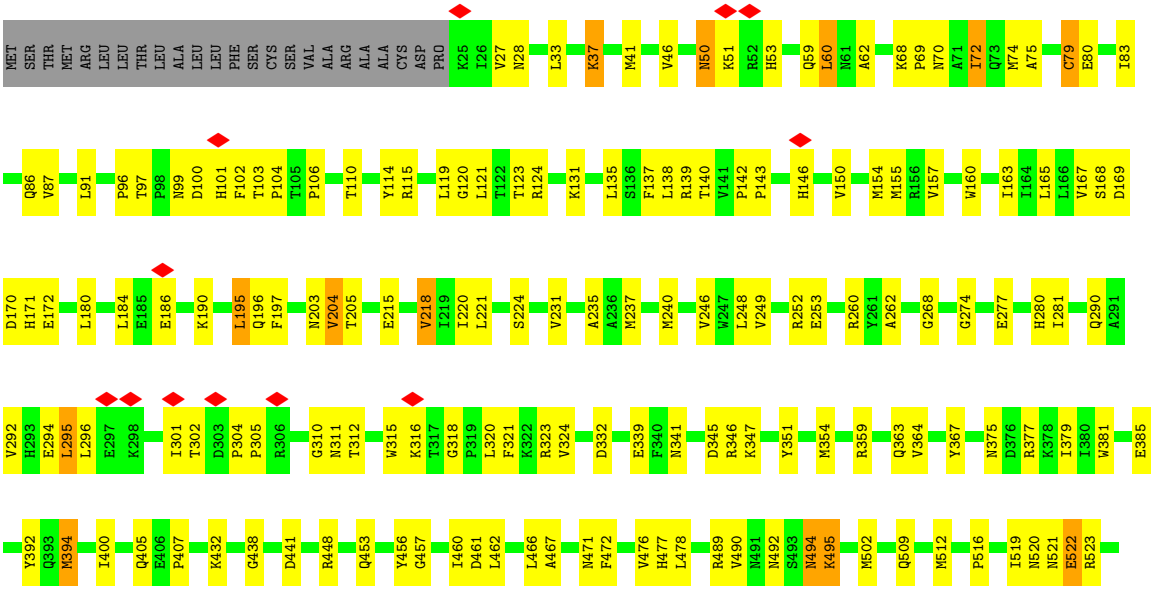
• Molecule 1: Glutamate receptor ionotropic, NMDA 2A

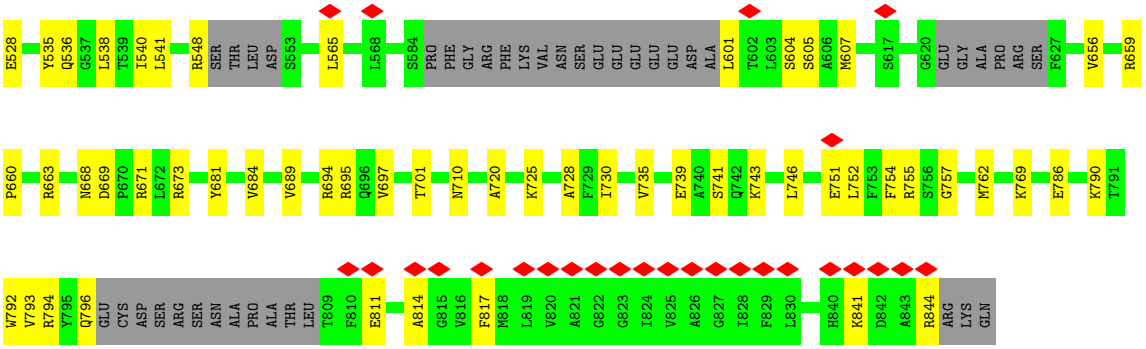
Chain C:



• Molecule 2: Glutamate receptor ionotropic, NMDA 1

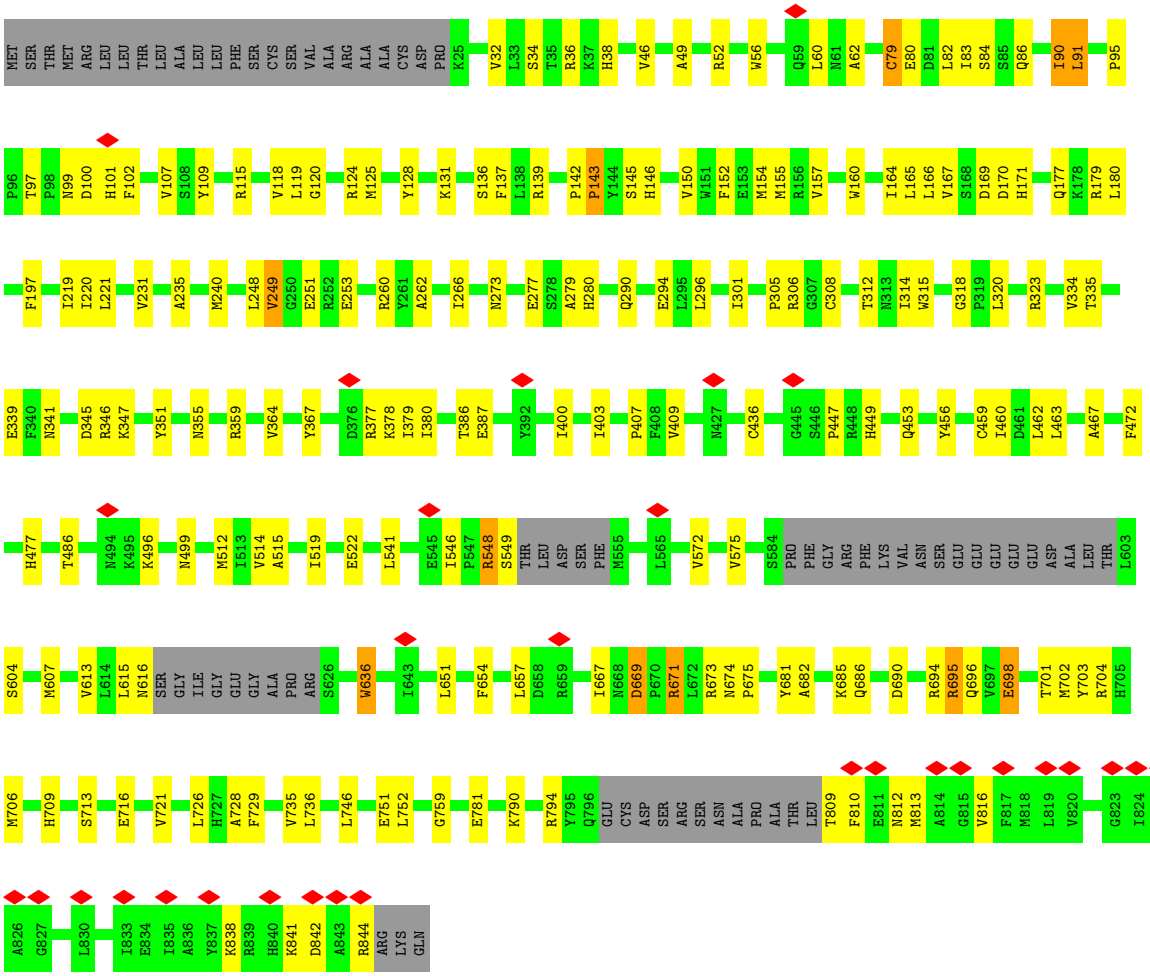
Chain B:





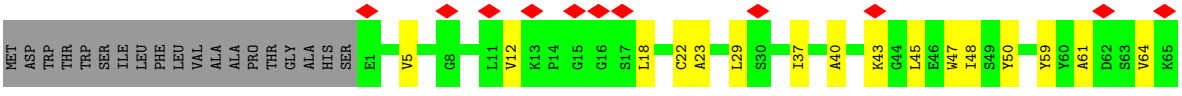
• Molecule 2: Glutamate receptor ionotropic, NMDA 1

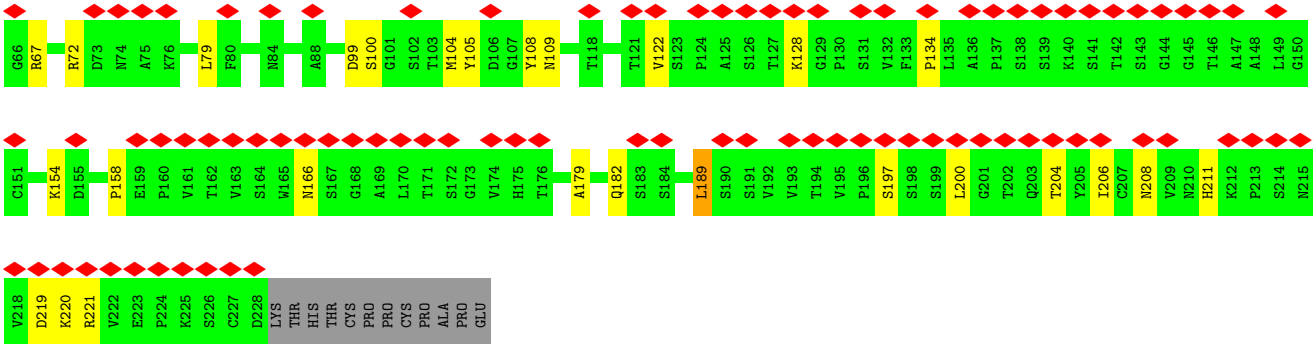
Chain D:



• Molecule 3: Fab5F6 Heavy Chain

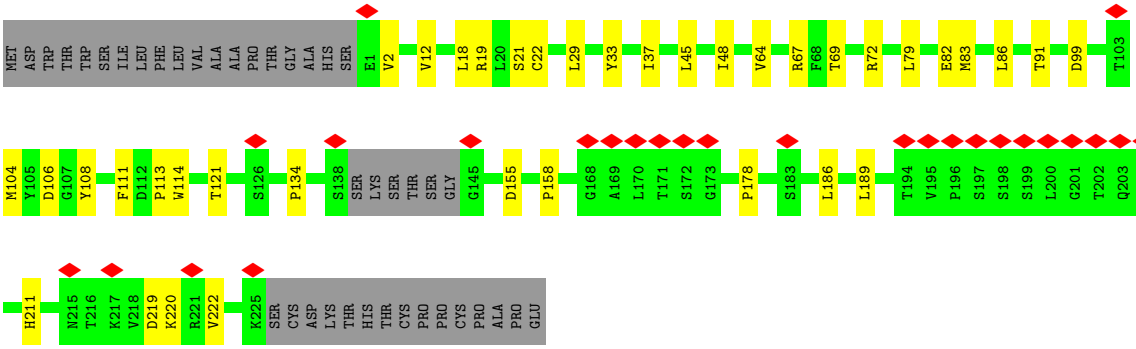
Chain E:





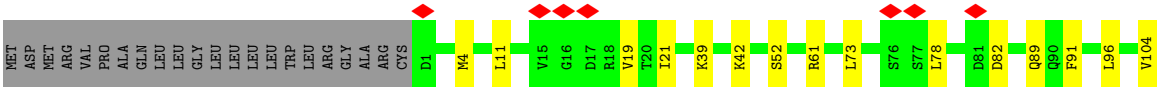
• Molecule 3: Fab5F6 Heavy Chain

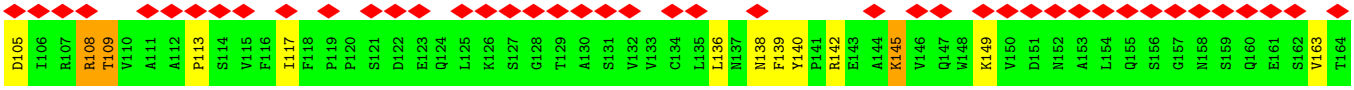
Chain G:

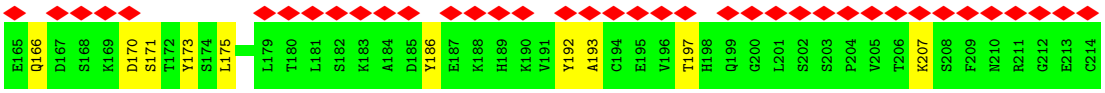


• Molecule 4: Fab5F6 Light Chain

Chain F:

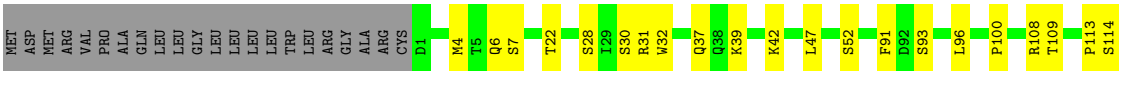


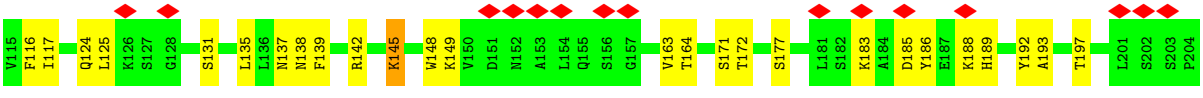


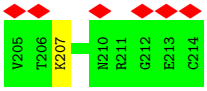


• Molecule 4: Fab5F6 Light Chain

Chain H:







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

Chain I: 100%

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

Chain J: 100%

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

Chain K: 100%

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

Chain L: 100%

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

Chain M: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	295623	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	410.40002, 410.40002, 410.40002	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/6092	0.45	0/8276
1	C	0.24	0/6080	0.44	0/8253
2	B	0.24	0/6253	0.46	0/8472
2	D	0.24	0/6226	0.45	0/8434
3	E	0.24	0/1751	0.46	0/2386
3	G	0.24	0/1692	0.46	0/2306
4	F	0.24	0/1680	0.46	0/2285
4	H	0.24	0/1680	0.46	0/2285
All	All	0.24	0/31454	0.45	0/42697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5950	0	5826	118	0
1	C	5940	0	5838	96	0
2	B	6120	0	6066	124	0
2	D	6094	0	6042	115	0
3	E	1708	0	1661	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1650	0	1608	22	0
4	F	1644	0	1597	22	0
4	H	1644	0	1597	29	0
5	I	28	0	25	1	0
5	J	28	0	25	0	0
5	K	28	0	25	2	0
5	L	28	0	25	0	0
5	M	28	0	25	0	0
6	A	14	0	13	1	0
6	B	28	0	26	0	0
6	C	14	0	13	0	0
6	D	56	0	52	0	0
All	All	31002	0	30464	524	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 9.

All (524) 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:279:ALA:HB1	2:D:334:VAL:HG21	1.65	0.79
2:B:601:LEU:N	2:B:605:SER:HG	1.80	0.78
1:A:508:ALA:HB3	1:A:764:ALA:HB3	1.69	0.74
2:B:142:PRO:HD3	2:B:346:ARG:HB3	1.69	0.73
2:B:155:MET:HG3	2:B:160:TRP:HB2	1.69	0.73
3:G:206:ILE:HD11	3:G:219:ASP:HB3	1.71	0.71
2:B:172:GLU:HG3	2:B:252:ARG:HH22	1.56	0.71
3:G:37:ILE:HD11	3:G:45:LEU:HB3	1.75	0.69
4:F:108:ARG:NH1	4:F:170:ASP:O	2.26	0.68
1:A:244:ARG:HH22	1:A:398:ASP:HB2	1.58	0.68
1:A:195:PHE:HB3	2:D:496:LYS:HG3	1.74	0.68
2:B:441:ASP:HB2	2:B:448:ARG:HD2	1.77	0.67
2:B:351:TYR:HB2	2:B:367:TYR:HB3	1.77	0.67
3:G:22:CYS:HB3	3:G:79:LEU:HB3	1.76	0.66
2:B:220:ILE:HG12	2:B:248:LEU:HB2	1.78	0.66
1:C:377:LYS:HB3	1:C:385:LEU:HB3	1.76	0.66
2:B:221:LEU:HB3	2:B:249:VAL:HG13	1.76	0.66
2:D:809:THR:N	2:D:813:MET:SD	2.69	0.66
1:C:52:ARG:HA	1:C:55:TRP:HD1	1.62	0.65
1:C:667:ASP:O	1:C:671:GLN:NE2	2.29	0.65
1:A:780:LEU:HD11	2:B:519:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:ILE:HD11	3:E:45:LEU:HB3	1.79	0.65
1:C:171:SER:HB2	1:C:227:ILE:HA	1.79	0.64
2:B:339:GLU:HG2	2:B:347:LYS:HB3	1.78	0.64
2:B:218:VAL:HG12	2:B:246:VAL:HB	1.80	0.64
2:D:115:ARG:HB3	2:D:318:GLY:HA3	1.79	0.64
2:D:696:GLN:NE2	2:D:698:GLU:OE2	2.30	0.64
2:D:131:LYS:NZ	2:D:137:PHE:O	2.30	0.64
2:D:167:VAL:HG21	2:D:177:GLN:HB2	1.78	0.64
1:A:412:GLU:HG3	1:A:419:VAL:HG12	1.81	0.63
2:D:467:ALA:HA	2:D:472:PHE:HB2	1.81	0.63
1:A:159:LEU:HD13	1:A:190:THR:HG21	1.82	0.62
1:C:693:ASN:ND2	2:D:781:GLU:OE1	2.32	0.62
2:B:131:LYS:HB2	1:C:178:PRO:HG2	1.81	0.62
4:F:117:ILE:HG22	4:F:207:LYS:HE2	1.81	0.62
2:B:405:GLN:HG3	2:B:516:PRO:HG3	1.82	0.62
3:G:64:VAL:HG12	3:G:67:ARG:HH21	1.65	0.62
1:A:781:GLN:OE1	2:B:695:ARG:NH1	2.32	0.62
2:B:204:VAL:HG11	2:B:231:VAL:HG12	1.81	0.62
2:D:667:ILE:O	2:D:673:ARG:NH2	2.32	0.62
1:A:83:ILE:HG12	1:A:116:ILE:HD11	1.80	0.62
1:A:433:THR:HB	1:A:457:LYS:HB2	1.81	0.62
1:A:433:THR:OG1	1:A:434:VAL:N	2.33	0.62
2:B:565:LEU:HD13	1:C:820:VAL:HG11	1.82	0.62
1:A:229:LEU:HD21	1:A:239:ILE:HG21	1.81	0.61
2:B:541:LEU:HD11	2:B:746:LEU:HB3	1.82	0.61
3:E:40:ALA:HB3	3:E:43:LYS:HB2	1.83	0.61
1:A:688:GLY:N	1:A:691:GLU:OE2	2.30	0.61
1:A:147:PHE:O	1:A:356:GLN:NE2	2.33	0.61
3:E:208:ASN:ND2	3:E:219:ASP:OD2	2.31	0.61
3:E:64:VAL:HG12	3:E:67:ARG:HH21	1.66	0.61
1:A:313:ILE:HD12	1:A:314:PRO:HD2	1.82	0.61
2:D:155:MET:HB2	2:D:160:TRP:HB2	1.83	0.61
4:F:113:PRO:HB3	4:F:139:PHE:HB3	1.82	0.61
2:B:495:LYS:HA	1:C:193:ASN:HB3	1.83	0.60
2:B:381:TRP:HB2	2:B:385:GLU:HB2	1.84	0.60
2:D:351:TYR:HB2	2:D:367:TYR:HB3	1.84	0.60
1:A:194:SER:H	2:D:496:LYS:HD2	1.67	0.60
1:A:256:ILE:HG12	1:A:277:ILE:HB	1.84	0.60
2:D:790:LYS:HD3	2:D:794:ARG:HG3	1.83	0.59
1:C:408:ILE:HG12	1:C:507:MET:HB3	1.83	0.59
2:D:164:ILE:HB	2:D:219:ILE:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HA	1:A:200:MET:HG3	1.84	0.59
1:A:175:THR:OG1	1:A:231:CYS:SG	2.60	0.59
1:A:386:ARG:NH1	1:A:389:VAL:O	2.35	0.58
1:C:313:ILE:HD12	1:C:314:PRO:HD2	1.86	0.58
1:C:508:ALA:HB3	1:C:764:ALA:HB3	1.85	0.58
2:D:90:ILE:HG23	2:D:118:VAL:HG12	1.84	0.58
2:D:364:VAL:HG11	2:D:379:ILE:HG23	1.85	0.58
2:B:752:LEU:HD13	2:B:755:ARG:HD3	1.85	0.58
3:E:5:VAL:HB	3:E:23:ALA:HB3	1.86	0.58
1:A:135:MET:SD	1:A:135:MET:N	2.77	0.57
2:B:46:VAL:HG11	2:B:62:ALA:HB2	1.86	0.57
2:D:99:ASN:ND2	4:H:52:SER:OG	2.36	0.57
2:D:155:MET:HA	2:D:160:TRP:HD1	1.69	0.57
1:A:86:VAL:HG11	1:A:116:ILE:HG21	1.86	0.57
1:C:228:LEU:HB3	1:C:230:TYR:HE2	1.69	0.57
2:D:142:PRO:HD3	2:D:346:ARG:HB3	1.85	0.57
2:B:96:PRO:HG3	3:E:104:MET:HG2	1.84	0.57
2:D:290:GLN:NE2	2:D:294:GLU:OE2	2.37	0.57
1:C:133:MET:SD	1:C:133:MET:N	2.78	0.57
2:B:461:ASP:OD2	2:B:792:TRP:NE1	2.37	0.57
4:H:145:LYS:HB3	4:H:197:THR:HB	1.86	0.57
1:A:127:ILE:HG22	1:A:128:HIS:H	1.70	0.57
3:G:111:PHE:O	3:G:114:TRP:NE1	2.35	0.57
1:C:127:ILE:HG22	1:C:128:HIS:H	1.68	0.57
2:D:220:ILE:HG12	2:D:248:LEU:HB2	1.87	0.57
2:B:790:LYS:HD3	2:B:794:ARG:HG3	1.86	0.57
1:C:143:THR:HG22	1:C:335:HIS:HE1	1.70	0.57
3:G:208:ASN:ND2	3:G:219:ASP:OD2	2.37	0.57
1:A:615:ASN:OD1	2:D:616:ASN:ND2	2.33	0.56
1:A:339:VAL:O	1:A:349:SER:OG	2.22	0.56
2:D:694:ARG:HH21	2:D:703:TYR:HB3	1.70	0.56
1:A:147:PHE:HE2	1:A:348:LEU:HD22	1.70	0.56
1:A:487:LYS:HE3	1:A:687:ASN:HA	1.86	0.56
2:B:221:LEU:HD11	2:B:231:VAL:HG21	1.87	0.56
2:B:364:VAL:HG11	2:B:379:ILE:HG23	1.88	0.56
2:B:492:ASN:OD1	2:B:494:ASN:ND2	2.38	0.56
1:A:517:GLU:OE2	1:A:692:ARG:NH1	2.38	0.56
2:B:438:GLY:HA3	2:B:478:LEU:HB3	1.88	0.56
2:D:690:ASP:OD1	2:D:694:ARG:NH1	2.38	0.56
2:B:70:ASN:OD1	1:C:323:GLN:NE2	2.38	0.56
2:D:100:ASP:OD1	2:D:101:HIS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:OD1	1:A:139:ASP:N	2.39	0.56
1:C:531:THR:OG1	1:C:731:ASP:OD1	2.23	0.56
2:D:463:LEU:HD13	2:D:514:VAL:HG21	1.87	0.56
2:B:115:ARG:HB3	2:B:318:GLY:HA3	1.88	0.56
4:F:142:ARG:HD2	4:F:163:VAL:HG21	1.88	0.55
2:D:613:VAL:HG11	2:D:636:TRP:HE1	1.71	0.55
2:B:131:LYS:NZ	2:B:137:PHE:O	2.39	0.55
2:B:394:MET:SD	2:B:394:MET:N	2.78	0.55
2:D:407:PRO:HG2	2:D:735:VAL:HA	1.88	0.55
2:B:512:MET:HG2	2:B:762:MET:HG2	1.89	0.55
3:E:22:CYS:HB3	3:E:79:LEU:HB3	1.88	0.55
1:C:96:HIS:NE2	1:C:314:PRO:O	2.39	0.55
2:D:79:CYS:HA	2:D:83:ILE:HD13	1.87	0.55
2:D:277:GLU:N	3:G:106:ASP:OD2	2.35	0.55
2:B:33:LEU:HD11	2:B:281:ILE:HD12	1.89	0.55
2:B:262:ALA:O	2:B:359:ARG:NH1	2.39	0.55
2:D:36:ARG:NH1	4:H:28:SER:O	2.40	0.55
1:C:719:SER:HB2	1:C:724:LYS:HB2	1.89	0.54
2:D:262:ALA:HB1	2:D:266:ILE:HD12	1.88	0.54
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.90	0.54
2:B:290:GLN:NE2	2:B:294:GLU:OE2	2.40	0.54
1:C:331:MET:SD	1:C:331:MET:N	2.79	0.54
3:E:29:LEU:O	3:E:72:ARG:NH2	2.40	0.54
2:D:145:SER:HB2	2:D:179:ARG:HD2	1.89	0.54
2:B:786:GLU:OE1	2:B:786:GLU:N	2.38	0.54
1:C:102:ASP:OD1	1:C:103:ASP:N	2.40	0.54
2:B:69:PRO:HA	2:B:102:PHE:HE1	1.73	0.54
2:D:260:ARG:O	2:D:359:ARG:NH2	2.41	0.53
1:A:326:ARG:H	1:A:326:ARG:HD3	1.72	0.53
2:B:50:ASN:HA	2:B:59:GLN:HG2	1.91	0.53
4:F:61:ARG:NH2	4:F:82:ASP:OD1	2.40	0.53
4:F:149:LYS:HB2	4:F:193:ALA:HB3	1.91	0.53
3:G:158:PRO:O	3:G:211:HIS:NE2	2.38	0.53
1:A:684:THR:HG23	1:A:705:MET:HE1	1.89	0.53
2:B:535:TYR:HA	2:B:757:GLY:HA2	1.90	0.53
2:D:169:ASP:N	2:D:197:PHE:O	2.41	0.53
2:D:499:ASN:HD21	2:D:686:GLN:HE21	1.56	0.53
3:G:69:THR:HB	3:G:82:GLU:HB2	1.91	0.53
2:B:522:GLU:OE1	2:B:523:ARG:N	2.41	0.53
1:C:46:VAL:HG13	1:C:73:LEU:HD13	1.90	0.53
2:D:681:TYR:HB3	2:D:728:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:91:PHE:HA	4:H:96:LEU:HD22	1.90	0.53
2:B:260:ARG:O	2:B:359:ARG:NH2	2.42	0.53
3:E:48:ILE:HG23	3:E:64:VAL:HG21	1.90	0.53
1:C:409:VAL:HG21	1:C:480:VAL:HG13	1.91	0.52
2:D:221:LEU:HD11	2:D:231:VAL:HG21	1.91	0.52
4:F:4:MET:SD	4:F:4:MET:N	2.82	0.52
4:H:142:ARG:HD2	4:H:163:VAL:HG21	1.90	0.52
2:B:163:ILE:HD11	2:B:220:ILE:HG13	1.90	0.52
2:B:694:ARG:O	1:C:431:ARG:NH1	2.43	0.52
2:D:262:ALA:O	2:D:359:ARG:NH1	2.42	0.52
2:D:378:LYS:HZ2	2:D:380:ILE:HG22	1.74	0.52
2:D:436:CYS:O	2:D:453:GLN:N	2.36	0.52
2:D:721:VAL:HG21	2:D:729:PHE:HB2	1.91	0.52
4:H:138:ASN:HA	4:H:172:THR:HB	1.91	0.52
1:A:174:THR:HG23	1:A:207:ASP:HB3	1.91	0.52
2:B:195:LEU:H	2:B:195:LEU:HD23	1.74	0.52
1:C:74:MET:SD	1:C:74:MET:N	2.82	0.52
1:A:464:LEU:HB2	1:A:509:VAL:HG21	1.91	0.52
1:A:533:ILE:HB	1:A:756:PHE:HB3	1.91	0.52
2:B:407:PRO:HG2	2:B:735:VAL:HA	1.92	0.52
2:D:91:LEU:HD12	2:D:119:LEU:HB2	1.91	0.52
4:F:136:LEU:HB2	4:F:175:LEU:HB3	1.92	0.52
1:A:52:ARG:HA	1:A:55:TRP:HD1	1.74	0.52
2:B:59:GLN:HG3	2:B:60:LEU:H	1.74	0.52
2:B:535:TYR:O	2:B:536:GLN:NE2	2.40	0.52
2:B:697:VAL:HG21	1:C:431:ARG:HB2	1.92	0.52
2:B:341:ASN:ND2	2:B:345:ASP:O	2.42	0.52
2:B:467:ALA:HA	2:B:472:PHE:HB2	1.91	0.52
4:F:108:ARG:HH21	4:F:140:TYR:HB2	1.74	0.52
3:G:91:THR:HG23	3:G:121:THR:HA	1.91	0.52
4:H:39:LYS:HB2	4:H:42:LYS:HB3	1.91	0.52
2:D:221:LEU:HB3	2:D:249:VAL:HG13	1.90	0.52
1:A:412:GLU:HA	1:A:417:VAL:HB	1.91	0.52
1:A:672:ARG:HB3	1:A:675:ASP:HB3	1.92	0.52
1:A:679:PRO:HG2	1:A:681:ARG:HH12	1.75	0.52
1:C:375:VAL:O	1:C:386:ARG:NH1	2.42	0.52
2:B:305:PRO:HB3	2:B:311:ASN:HD22	1.74	0.51
2:D:456:TYR:HA	2:D:460:ILE:HG12	1.91	0.51
2:D:548:ARG:H	2:D:548:ARG:NE	2.07	0.51
2:B:302:THR:HG21	2:B:316:LYS:HB2	1.92	0.51
1:C:122:VAL:O	1:C:143:THR:OG1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:GLN:OE1	2:B:375:ASN:ND2	2.43	0.51
1:A:116:ILE:O	1:A:120:THR:HG22	2.11	0.51
1:A:154:GLN:HG2	1:A:361:LEU:HD11	1.91	0.51
2:B:438:GLY:O	2:B:453:GLN:NE2	2.42	0.51
2:D:355:ASN:HD22	2:D:379:ILE:HG22	1.76	0.51
1:C:776:ASP:OD1	1:C:777:LEU:N	2.44	0.51
2:D:669:ASP:OD2	2:D:671:ARG:NE	2.43	0.51
4:H:37:GLN:HB2	4:H:47:LEU:HD11	1.91	0.51
1:C:167:TRP:HB3	1:C:226:VAL:HG21	1.92	0.51
1:A:169:VAL:O	1:A:225:SER:HB2	2.10	0.51
1:A:681:ARG:NH2	1:A:726:ASP:OD1	2.43	0.51
4:F:39:LYS:HB2	4:F:42:LYS:HB3	1.93	0.51
1:A:143:THR:HG22	1:A:335:HIS:HE1	1.75	0.50
1:A:207:ASP:N	1:A:207:ASP:OD1	2.43	0.50
1:A:333:THR:HG1	1:A:335:HIS:HD1	1.58	0.50
1:C:533:ILE:HB	1:C:756:PHE:HB3	1.93	0.50
1:A:52:ARG:HD2	1:A:289:GLU:HB3	1.94	0.50
2:B:86:GLN:NE2	2:B:304:PRO:O	2.44	0.50
1:A:499:GLU:HG3	1:A:504:ARG:HB3	1.92	0.50
2:B:215:GLU:HB3	2:B:392:TYR:HE1	1.76	0.50
1:C:280:SER:O	1:C:362:VAL:N	2.43	0.50
3:E:197:SER:HA	3:E:200:LEU:HD13	1.93	0.50
2:B:68:LYS:HB2	2:B:74:MET:HB2	1.93	0.50
3:E:61:ALA:HB3	3:E:64:VAL:HG22	1.93	0.50
1:A:100:PHE:HE1	1:A:102:ASP:HB2	1.76	0.50
1:C:153:GLN:NE2	1:C:356:GLN:O	2.43	0.50
1:A:386:ARG:HH22	1:A:391:PRO:HD3	1.75	0.50
1:A:528:PHE:HD1	1:A:529:VAL:HG23	1.77	0.50
2:B:310:GLY:N	1:C:78:ASP:OD2	2.34	0.50
1:C:549:PHE:HD1	1:C:815:ASP:HB3	1.76	0.50
1:A:202:ASN:OD1	1:A:202:ASN:N	2.45	0.50
2:B:101:HIS:HB3	2:B:103:THR:HG23	1.94	0.50
1:C:46:VAL:HA	1:C:73:LEU:HD22	1.94	0.49
2:D:34:SER:HB2	2:D:38:HIS:ND1	2.26	0.49
1:A:131:ALA:O	1:A:146:GLN:NE2	2.45	0.49
2:B:274:GLY:O	2:B:280:HIS:NE2	2.45	0.49
1:A:100:PHE:CE1	1:A:102:ASP:HB2	2.47	0.49
2:D:296:LEU:HD23	2:D:301:ILE:HD13	1.94	0.49
1:C:76:ARG:H	1:C:76:ARG:HD3	1.76	0.49
1:A:682:PHE:HA	1:A:727:ALA:HB3	1.94	0.49
3:G:134:PRO:HD3	3:G:220:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:HB3	1:A:361:LEU:H	1.76	0.49
1:A:561:MET:SD	1:A:561:MET:N	2.79	0.49
2:B:811:GLU:HA	2:B:814:ALA:HB3	1.95	0.49
2:D:86:GLN:NE2	2:D:305:PRO:O	2.43	0.49
1:A:342:THR:HA	1:A:347:ASP:HB3	1.95	0.49
1:A:74:MET:SD	1:A:74:MET:N	2.86	0.49
1:A:701:MET:N	1:A:701:MET:SD	2.86	0.49
2:B:135:LEU:HG	1:C:111:GLN:HE22	1.77	0.49
1:C:257:VAL:HG22	1:C:258:PRO:HD2	1.95	0.49
5:K:1:NAG:H61	5:K:2:NAG:O5	2.13	0.49
1:A:376:GLY:HA2	1:A:385:LEU:HB3	1.95	0.48
2:B:119:LEU:HD13	2:B:138:LEU:HB2	1.95	0.48
2:B:540:ILE:HG12	2:B:730:ILE:HG12	1.95	0.48
1:C:632:SER:OG	2:D:615:LEU:O	2.31	0.48
1:A:496:MET:HE1	1:A:510:GLY:HA3	1.95	0.48
2:B:663:ARG:O	2:B:671:ARG:NH1	2.44	0.48
2:B:28:ASN:HD22	2:B:87:VAL:HG12	1.79	0.48
2:D:46:VAL:HG11	2:D:62:ALA:HB2	1.95	0.48
4:H:113:PRO:HB3	4:H:139:PHE:HB3	1.95	0.48
1:C:398:ASP:OD1	1:C:398:ASP:N	2.45	0.48
1:C:102:ASP:HB3	1:C:129:GLY:HA3	1.95	0.48
1:A:577:GLU:HB2	1:A:600:THR:HG23	1.96	0.48
2:B:75:ALA:HB2	2:B:106:PRO:HB2	1.94	0.48
1:C:128:HIS:HB2	1:C:291:ARG:NH1	2.27	0.48
1:C:131:ALA:O	1:C:146:GLN:NE2	2.46	0.48
2:D:519:ILE:HD11	2:D:759:GLY:HA3	1.96	0.48
4:F:186:TYR:O	4:F:192:TYR:OH	2.31	0.48
1:C:225:SER:O	1:C:254:PHE:N	2.46	0.48
1:C:403:ASP:OD1	1:C:403:ASP:N	2.46	0.48
1:A:423:ASP:OD1	1:A:423:ASP:N	2.46	0.48
2:D:166:LEU:HD12	2:D:221:LEU:HD12	1.95	0.48
3:E:12:VAL:HG21	3:E:18:LEU:HB2	1.94	0.48
2:D:751:GLU:HG2	2:D:752:LEU:H	1.79	0.48
1:A:206:LEU:HD21	1:A:218:GLN:HG3	1.95	0.48
1:A:128:HIS:HA	1:A:132:SER:HB3	1.95	0.47
2:D:400:ILE:HG22	2:D:512:MET:HB3	1.94	0.47
3:G:48:ILE:HG23	3:G:64:VAL:HG21	1.95	0.47
1:A:334:LEU:HA	1:A:337:PHE:HD2	1.78	0.47
4:H:148:TRP:HE1	4:H:177:SER:HG	1.60	0.47
1:A:199:ASP:N	1:A:199:ASP:OD1	2.48	0.47
2:D:339:GLU:HG2	2:D:347:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:H	2:D:312:THR:HG21	1.79	0.47
1:C:89:LEU:HB3	1:C:95:ILE:HD13	1.96	0.47
2:D:165:LEU:HD22	2:D:180:LEU:HD23	1.95	0.47
2:B:72:ILE:HD13	2:B:72:ILE:H	1.79	0.47
2:B:124:ARG:HE	2:B:143:PRO:HA	1.80	0.47
1:C:561:MET:SD	1:C:561:MET:N	2.80	0.47
2:B:538:LEU:HD22	2:B:689:VAL:HG22	1.96	0.47
1:C:52:ARG:NH1	1:C:289:GLU:OE2	2.47	0.47
1:C:228:LEU:HB3	1:C:230:TYR:CE2	2.49	0.47
2:D:82:LEU:HD22	2:D:90:ILE:HD12	1.96	0.47
2:D:463:LEU:HB2	2:D:514:VAL:HG11	1.97	0.47
3:G:104:MET:HB3	3:G:108:TYR:HD2	1.79	0.47
1:A:279:VAL:HB	1:A:363:VAL:HG12	1.96	0.47
2:B:99:ASN:ND2	4:F:52:SER:OG	2.48	0.47
2:B:751:GLU:HG2	2:B:752:LEU:H	1.80	0.47
3:E:154:LYS:NZ	3:E:182:GLN:OE1	2.46	0.47
1:C:379:GLU:OE1	1:C:379:GLU:N	2.48	0.47
2:B:681:TYR:HB3	2:B:728:ALA:HB3	1.97	0.47
4:H:30:SER:OG	4:H:31:ARG:N	2.47	0.47
1:A:128:HIS:HB2	1:A:291:ARG:NH1	2.30	0.46
2:B:235:ALA:HB1	2:B:240:MET:HB2	1.97	0.46
2:B:296:LEU:HA	2:B:301:ILE:HD11	1.97	0.46
4:F:145:LYS:HB3	4:F:197:THR:HB	1.97	0.46
1:A:177:PHE:HB3	1:A:180:TYR:HD2	1.79	0.46
2:D:49:ALA:HA	2:D:52:ARG:HG2	1.96	0.46
2:D:541:LEU:HD22	2:D:736:LEU:HD22	1.97	0.46
4:H:4:MET:SD	4:H:4:MET:N	2.89	0.46
2:B:528:GLU:OE1	2:B:769:LYS:NZ	2.48	0.46
2:D:613:VAL:HG11	2:D:636:TRP:NE1	2.30	0.46
3:G:83:MET:HB3	3:G:86:LEU:HD21	1.98	0.46
4:H:108:ARG:HE	4:H:171:SER:HB2	1.80	0.46
2:D:709:HIS:CD2	2:D:726:LEU:HD11	2.51	0.46
1:A:118:SER:HB3	1:A:142:SER:HB3	1.98	0.46
2:B:203:ASN:C	2:B:205:THR:H	2.19	0.46
2:B:456:TYR:HA	2:B:460:ILE:HG12	1.97	0.46
2:D:170:ASP:OD1	2:D:171:HIS:N	2.45	0.46
3:G:205:TYR:HB2	3:G:222:VAL:HB	1.98	0.46
4:H:149:LYS:HB2	4:H:193:ALA:HB3	1.96	0.46
1:C:139:ASP:HB3	1:C:142:SER:HB3	1.98	0.46
1:C:176:ILE:HA	1:C:181:ARG:HH22	1.80	0.46
3:E:99:ASP:N	3:E:99:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ASP:OD1	1:A:667:ASP:N	2.49	0.46
2:B:100:ASP:OD1	2:B:101:HIS:N	2.44	0.46
2:B:720:ALA:HB1	2:B:725:LYS:HB2	1.98	0.46
3:G:2:VAL:HG12	3:G:113:PRO:HG3	1.97	0.46
1:A:687:ASN:N	1:A:687:ASN:OD1	2.49	0.46
3:E:100:SER:OG	3:E:108:TYR:O	2.32	0.46
3:E:206:ILE:HD11	3:E:219:ASP:HB3	1.98	0.46
3:G:155:ASP:HA	3:G:186:LEU:HB3	1.97	0.46
1:A:110:ALA:HB2	1:A:131:ALA:HA	1.97	0.46
2:B:91:LEU:HB3	2:B:121:LEU:HD21	1.98	0.46
1:A:311:SER:HB2	1:A:312:TYR:HD1	1.81	0.45
2:B:224:SER:HA	2:B:252:ARG:HD2	1.98	0.45
2:B:277:GLU:HB2	3:E:105:TYR:CG	2.51	0.45
2:B:400:ILE:O	2:B:477:HIS:N	2.43	0.45
2:D:486:THR:OG1	2:D:686:GLN:O	2.20	0.45
1:A:390:TRP:CD1	1:A:391:PRO:HD2	2.51	0.45
1:C:52:ARG:HA	1:C:55:TRP:CD1	2.47	0.45
1:C:243:ALA:HB1	1:C:248:LEU:HB2	1.98	0.45
1:C:610:GLY:HA2	1:C:613:PHE:CE2	2.51	0.45
1:C:820:VAL:O	1:C:823:MET:HG3	2.15	0.45
2:D:838:LYS:NZ	2:D:842:ASP:OD2	2.38	0.45
3:G:33:TYR:HB2	3:G:99:ASP:HB2	1.97	0.45
4:H:186:TYR:O	4:H:192:TYR:OH	2.33	0.45
1:A:128:HIS:HB2	1:A:291:ARG:HH11	1.81	0.45
1:A:500:VAL:HG21	1:A:508:ALA:HB2	1.99	0.45
2:B:135:LEU:HD11	1:C:107:GLU:HG2	1.99	0.45
2:D:152:PHE:O	2:D:155:MET:HG2	2.16	0.45
2:D:675:PRO:HG3	2:D:702:MET:HA	1.99	0.45
5:K:1:NAG:H4	5:K:2:NAG:H2	1.70	0.45
2:B:268:GLY:N	2:B:354:MET:O	2.50	0.45
2:D:403:ILE:HG22	2:D:515:ALA:HB1	1.99	0.45
4:F:91:PHE:HA	4:F:96:LEU:HD22	1.98	0.45
4:H:114:SER:HB2	4:H:137:ASN:HB3	1.98	0.45
1:A:390:TRP:O	1:A:392:ARG:N	2.46	0.45
2:B:140:THR:HB	2:B:346:ARG:HH21	1.80	0.45
1:C:49:ARG:HA	1:C:52:ARG:HE	1.81	0.45
2:D:95:PRO:HG2	2:D:102:PHE:HB3	1.98	0.45
2:B:741:SER:OG	2:B:796:GLN:O	2.30	0.45
1:C:734:VAL:O	1:C:738:LYS:HG2	2.17	0.45
4:F:108:ARG:HD2	4:F:109:THR:N	2.32	0.45
2:B:155:MET:HA	2:B:160:TRP:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HB3	1:C:203:VAL:HG22	1.99	0.45
1:C:417:VAL:HG12	1:C:461:ILE:HG12	1.99	0.45
2:D:253:GLU:N	2:D:253:GLU:OE1	2.50	0.45
3:E:158:PRO:O	3:E:211:HIS:NE2	2.46	0.45
4:H:114:SER:HB3	4:H:116:PHE:HE2	1.81	0.45
1:A:115:PHE:HB2	2:D:109:TYR:HD2	1.82	0.45
2:D:541:LEU:HD11	2:D:746:LEU:HB3	1.99	0.45
3:E:179:ALA:HB2	3:E:189:LEU:HD23	1.97	0.45
2:B:332:ASP:OD1	2:B:332:ASP:N	2.50	0.45
4:H:125:LEU:HB3	4:H:183:LYS:HZ3	1.83	0.45
2:D:548:ARG:H	2:D:548:ARG:HE	1.65	0.44
4:H:7:SER:O	4:H:22:THR:OG1	2.34	0.44
1:A:272:PHE:O	1:A:370:ARG:NH1	2.45	0.44
1:A:411:LEU:HG	1:A:484:LYS:HA	1.99	0.44
2:B:203:ASN:O	2:B:205:THR:N	2.51	0.44
1:C:386:ARG:NH1	1:C:386:ARG:HA	2.31	0.44
2:B:548:ARG:HA	2:B:548:ARG:HH11	1.83	0.44
2:D:36:ARG:HB2	4:H:93:SER:HB3	1.98	0.44
2:D:549:SER:HA	2:D:812:ASN:HB2	2.00	0.44
4:F:105:ASP:OD2	4:F:173:TYR:OH	2.35	0.44
3:G:19:ARG:HH11	3:G:21:SER:HB3	1.83	0.44
2:B:165:LEU:HD22	2:B:180:LEU:HD23	1.99	0.44
1:C:476:ASP:OD1	1:C:476:ASP:N	2.51	0.44
1:A:409:VAL:HG11	1:A:499:GLU:HG2	1.99	0.44
2:B:155:MET:HA	2:B:160:TRP:CD1	2.52	0.44
2:B:169:ASP:HA	2:B:196:GLN:HE21	1.83	0.44
1:C:35:ASN:HB2	1:C:95:ILE:HA	1.98	0.44
1:C:118:SER:HB3	1:C:142:SER:HB3	2.00	0.44
1:C:695:ARG:HE	1:C:702:HIS:CE1	2.36	0.44
1:A:467:LEU:HD21	1:A:779:LEU:HD22	1.99	0.44
1:C:149:ALA:HB3	1:C:361:LEU:HD21	2.00	0.44
1:C:487:LYS:NZ	1:C:687:ASN:OD1	2.44	0.44
4:F:21:ILE:HB	4:F:73:LEU:HB3	1.99	0.44
1:A:115:PHE:HB2	2:D:109:TYR:CD2	2.53	0.44
1:A:240:LEU:HD13	1:A:273:PRO:HD2	2.00	0.44
2:B:739:GLU:OE1	2:B:743:LYS:NZ	2.47	0.44
1:C:170:PHE:HB2	1:C:200:MET:HA	1.98	0.44
2:D:341:ASN:ND2	2:D:345:ASP:O	2.46	0.44
1:A:691:GLU:HG2	1:A:692:ARG:HD3	1.99	0.43
2:B:75:ALA:HB1	2:B:110:THR:HG21	1.99	0.43
1:C:117:SER:HB2	1:C:124:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:VAL:HG12	1:C:669:LYS:HD2	2.00	0.43
3:E:50:TYR:HE1	3:E:59:TYR:HB2	1.82	0.43
5:I:1:NAG:H4	5:I:2:NAG:H2	1.72	0.43
1:A:180:TYR:CD1	1:A:230:TYR:HB3	2.54	0.43
1:C:326:ARG:H	1:C:326:ARG:HD3	1.83	0.43
2:D:541:LEU:HB2	2:D:736:LEU:HD13	2.00	0.43
2:D:674:ASN:OD1	2:D:674:ASN:N	2.51	0.43
2:D:142:PRO:HB2	2:D:146:HIS:HB2	2.01	0.43
2:D:522:GLU:OE2	2:D:695:ARG:NH1	2.51	0.43
1:A:248:LEU:HA	1:A:253:PHE:HE1	1.83	0.43
1:A:784:GLY:HA2	2:B:754:PHE:HE1	1.84	0.43
1:C:603:LYS:NZ	1:C:620:GLN:O	2.39	0.43
2:D:115:ARG:HD3	2:D:136:SER:HB2	1.99	0.43
2:D:409:VAL:HG22	2:D:459:CYS:SG	2.58	0.43
4:H:124:GLN:HE22	4:H:131:SER:HB2	1.82	0.43
4:H:188:LYS:HG3	4:H:189:HIS:CD2	2.53	0.43
1:C:165:TYR:HH	1:C:386:ARG:HH21	1.58	0.43
4:F:19:VAL:HG21	4:F:78:LEU:HD13	2.00	0.43
1:A:38:VAL:HG23	1:A:99:VAL:HB	2.01	0.43
1:A:223:HIS:HB2	1:A:227:ILE:HD11	1.99	0.43
2:B:170:ASP:OD1	2:B:171:HIS:N	2.43	0.43
1:C:188:LYS:HA	1:C:191:VAL:HG12	2.01	0.43
2:D:378:LYS:HE3	2:D:386:THR:HG23	1.99	0.43
2:D:813:MET:HA	2:D:816:VAL:HG12	2.01	0.43
3:E:104:MET:HG3	3:E:105:TYR:H	1.84	0.43
1:A:610:GLY:HA2	1:A:613:PHE:CE1	2.54	0.43
2:B:253:GLU:N	2:B:253:GLU:OE1	2.51	0.43
1:C:470:THR:HG1	1:C:782:PHE:HZ	1.63	0.43
2:D:235:ALA:HB1	2:D:240:MET:HB2	2.01	0.43
2:D:273:ASN:O	2:D:280:HIS:NE2	2.48	0.43
4:H:138:ASN:ND2	4:H:138:ASN:O	2.52	0.43
2:B:79:CYS:SG	2:B:80:GLU:N	2.92	0.43
2:D:154:MET:HA	2:D:157:VAL:HG22	2.01	0.43
2:D:447:PRO:O	2:D:449:HIS:ND1	2.46	0.43
3:E:166:ASN:HA	3:E:206:ILE:HG23	2.01	0.43
3:G:29:LEU:O	3:G:72:ARG:NH2	2.52	0.43
4:H:32:TRP:HB3	4:H:91:PHE:CE2	2.54	0.43
2:B:684:VAL:O	2:B:710:ASN:HB3	2.19	0.42
2:D:146:HIS:O	2:D:150:VAL:HG23	2.19	0.42
3:E:99:ASP:HB3	3:E:109:ASN:HD22	1.84	0.42
1:A:426:THR:OG1	1:A:427:GLU:OE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:PHE:CD2	1:C:529:VAL:HG23	2.54	0.42
2:D:604:SER:O	2:D:607:MET:HG3	2.20	0.42
4:H:117:ILE:HG22	4:H:207:LYS:HE2	2.00	0.42
1:A:489:VAL:HG21	6:A:900:NAG:H81	2.01	0.42
1:A:568:VAL:HA	1:A:571:ILE:HG22	2.01	0.42
2:B:668:ASN:HA	2:B:673:ARG:HH12	1.85	0.42
1:C:438:LYS:HE2	1:C:479:LEU:HD22	2.01	0.42
2:D:685:LYS:HD3	2:D:685:LYS:HA	1.90	0.42
2:D:713:SER:HB3	2:D:716:GLU:HG3	2.00	0.42
1:C:223:HIS:O	1:C:223:HIS:ND1	2.47	0.42
2:D:139:ARG:NH2	2:D:143:PRO:HG3	2.35	0.42
2:B:37:LYS:HD2	2:B:37:LYS:H	1.85	0.42
2:B:155:MET:HE1	2:B:184:LEU:HD21	2.02	0.42
1:C:158:MET:SD	1:C:230:TYR:OH	2.58	0.42
3:E:134:PRO:HD3	3:E:220:LYS:HG2	2.01	0.42
1:A:36:ILE:H	1:A:36:ILE:HG12	1.67	0.42
2:B:79:CYS:O	2:B:83:ILE:HB	2.19	0.42
2:B:656:VAL:HG21	1:C:654:ILE:HG22	2.01	0.42
3:G:178:PRO:HD3	4:H:164:THR:HG22	2.00	0.42
1:A:688:GLY:O	1:A:692:ARG:NE	2.53	0.42
2:B:295:LEU:HD23	2:B:324:VAL:HG21	2.01	0.42
2:B:604:SER:O	2:B:607:MET:HG3	2.20	0.42
2:D:84:SER:HA	2:D:306:ARG:O	2.19	0.42
4:H:6:GLN:HG3	4:H:100:PRO:HD2	2.02	0.42
4:H:116:PHE:HB2	4:H:135:LEU:HB3	2.02	0.42
1:A:277:ILE:HG12	1:A:365:VAL:HG22	2.01	0.42
2:B:168:SER:HA	2:B:197:PHE:HB3	2.01	0.42
4:H:185:ASP:HA	4:H:188:LYS:HG2	2.02	0.42
1:A:820:VAL:O	1:A:823:MET:HG3	2.20	0.42
2:D:306:ARG:HH11	2:D:306:ARG:HA	1.85	0.42
1:A:496:MET:SD	1:A:508:ALA:HB1	2.60	0.41
2:B:163:ILE:HA	2:B:218:VAL:HG23	2.02	0.41
2:B:520:ASN:OD1	2:B:521:ASN:N	2.51	0.41
1:C:234:ASP:OD1	1:C:234:ASP:N	2.53	0.41
4:F:138:ASN:O	4:F:138:ASN:ND2	2.53	0.41
2:B:146:HIS:O	2:B:150:VAL:HG23	2.20	0.41
2:B:312:THR:HG21	1:C:77:THR:H	1.85	0.41
2:B:441:ASP:O	2:B:448:ARG:NE	2.53	0.41
1:C:417:VAL:HG13	1:C:460:CYS:HB2	2.03	0.41
2:B:104:PRO:HG3	2:B:123:THR:HG22	2.00	0.41
2:D:32:VAL:N	2:D:91:LEU:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:541:LEU:O	2:D:729:PHE:N	2.49	0.41
4:F:11:LEU:HD11	4:F:104:VAL:HG22	2.02	0.41
2:B:115:ARG:HB2	2:B:315:TRP:HB3	2.01	0.41
1:C:484:LYS:HE2	1:C:484:LYS:HB2	1.92	0.41
2:D:541:LEU:HB3	2:D:729:PHE:HB3	2.02	0.41
3:G:12:VAL:HG21	3:G:18:LEU:HB2	2.01	0.41
1:A:701:MET:O	1:A:705:MET:HG3	2.21	0.41
2:B:841:LYS:HG3	2:B:844:ARG:NH1	2.35	0.41
1:C:210:PHE:HA	1:C:215:THR:HG21	2.03	0.41
1:C:780:LEU:HA	1:C:783:VAL:HG22	2.02	0.41
2:D:124:ARG:NH1	2:D:251:GLU:OE1	2.48	0.41
2:D:125:MET:HB2	2:D:128:TYR:HE2	1.86	0.41
2:D:682:ALA:HA	2:D:706:MET:SD	2.61	0.41
1:A:124:ILE:HB	1:A:144:PHE:HD1	1.85	0.41
1:A:317:LYS:HE3	1:A:317:LYS:HB2	1.95	0.41
1:C:698:TYR:HB3	1:C:701:MET:HB3	2.00	0.41
3:E:47:TRP:HZ2	3:E:50:TYR:HD1	1.67	0.41
1:A:274:SER:HA	1:A:366:LEU:HD23	2.01	0.41
2:B:120:GLY:H	2:B:139:ARG:HA	1.86	0.41
2:B:154:MET:HA	2:B:157:VAL:HG22	2.03	0.41
1:A:415:PRO:HG2	1:A:416:PHE:CD2	2.56	0.41
2:B:27:VAL:HG11	2:B:292:VAL:HG11	2.03	0.41
2:B:457:GLY:H	2:B:460:ILE:HG12	1.86	0.41
2:B:462:LEU:O	2:B:466:LEU:HG	2.21	0.41
1:C:116:ILE:HD13	1:C:116:ILE:HA	1.94	0.41
2:D:120:GLY:H	2:D:139:ARG:HA	1.84	0.41
2:D:334:VAL:HG23	2:D:335:THR:HG23	2.02	0.41
4:F:89:GLN:HE21	4:F:96:LEU:HB3	1.85	0.41
1:A:80:LYS:NZ	2:D:80:GLU:OE2	2.40	0.41
1:A:780:LEU:HD13	1:A:780:LEU:HA	1.81	0.41
1:C:737:TYR:CZ	1:C:741:ARG:HD2	2.56	0.41
1:C:833:ILE:O	1:C:836:ILE:HG22	2.21	0.41
1:C:206:LEU:HD22	1:C:215:THR:HG22	2.02	0.40
1:C:275:GLY:HA2	1:C:394:LYS:HD2	2.03	0.40
2:D:841:LYS:HG3	2:D:844:ARG:NH1	2.36	0.40
3:E:204:THR:OG1	3:E:221:ARG:NH2	2.47	0.40
1:A:364:ILE:HG22	1:A:374:LYS:HA	2.02	0.40
1:A:719:SER:HB2	1:A:725:LEU:HD23	2.04	0.40
1:A:737:TYR:HD1	1:A:796:LEU:HA	1.86	0.40
1:C:214:LYS:O	1:C:218:GLN:HG2	2.22	0.40
1:C:425:LEU:HG	1:C:426:THR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:ARG:HB2	2:D:314:ILE:HD11	2.03	0.40
2:D:447:PRO:HB2	2:D:449:HIS:HE1	1.85	0.40
2:D:572:VAL:HA	2:D:575:VAL:HG22	2.03	0.40
4:F:166:GLN:HB3	4:F:171:SER:HA	2.03	0.40
1:A:390:TRP:CG	1:A:391:PRO:HD2	2.57	0.40
1:A:291:ARG:HA	1:A:294:ASP:OD2	2.21	0.40
1:A:526:VAL:HG21	1:A:780:LEU:HD22	2.02	0.40
2:D:694:ARG:NH2	2:D:703:TYR:O	2.54	0.40
1:A:153:GLN:H	1:A:153:GLN:HG2	1.59	0.40
1:A:169:VAL:HA	1:A:201:GLN:HB2	2.04	0.40
1:A:547:SER:HA	1:A:815:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	749/841 (89%)	693 (92%)	54 (7%)	2 (0%)	41 74
1	C	744/841 (88%)	716 (96%)	28 (4%)	0	100 100
2	B	772/847 (91%)	718 (93%)	49 (6%)	5 (1%)	25 62
2	D	766/847 (90%)	737 (96%)	28 (4%)	1 (0%)	51 83
3	E	226/259 (87%)	217 (96%)	9 (4%)	0	100 100
3	G	215/259 (83%)	209 (97%)	6 (3%)	0	100 100
4	F	212/236 (90%)	208 (98%)	4 (2%)	0	100 100
4	H	212/236 (90%)	208 (98%)	4 (2%)	0	100 100
All	All	3896/4366 (89%)	3706 (95%)	182 (5%)	8 (0%)	50 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	ALA
2	B	204	VAL
2	B	659	ARG
2	B	660	PRO
1	A	95	ILE
2	B	509	GLN
2	D	143	PRO
2	B	476	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	645/729 (88%)	592 (92%)	53 (8%)	11	40
1	C	647/729 (89%)	618 (96%)	29 (4%)	27	57
2	B	656/730 (90%)	622 (95%)	34 (5%)	23	54
2	D	659/730 (90%)	630 (96%)	29 (4%)	28	57
3	E	192/218 (88%)	189 (98%)	3 (2%)	62	79
3	G	184/218 (84%)	183 (100%)	1 (0%)	88	94
4	F	189/207 (91%)	186 (98%)	3 (2%)	62	79
4	H	189/207 (91%)	187 (99%)	2 (1%)	73	85
All	All	3361/3768 (89%)	3207 (95%)	154 (5%)	31	56

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	TRP
1	A	65	LEU
1	A	74	MET
1	A	94	ARG
1	A	135	MET
1	A	153	GLN
1	A	175	THR
1	A	183	PHE

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Mol	Chain	Res	Type
1	A	188	LYS
1	A	214	LYS
1	A	221	LYS
1	A	223	HIS
1	A	276	LEU
1	A	306	MET
1	A	313	ILE
1	A	315	GLU
1	A	317	LYS
1	A	320	CYS
1	A	325	GLU
1	A	326	ARG
1	A	328	GLU
1	A	355	TYR
1	A	363	VAL
1	A	375	VAL
1	A	390	TRP
1	A	394	LYS
1	A	412	GLU
1	A	433	THR
1	A	436	CYS
1	A	441	LYS
1	A	460	CYS
1	A	474	THR
1	A	479	LEU
1	A	484	LYS
1	A	512	LEU
1	A	545	SER
1	A	557	VAL
1	A	578	TYR
1	A	606	TRP
1	A	630	MET
1	A	634	TRP
1	A	669	LYS
1	A	684	THR
1	A	687	ASN
1	A	700	TYR
1	A	701	MET
1	A	722	THR
1	A	730	TYR
1	A	746	LYS
1	A	758	THR

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Mol	Chain	Res	Type
1	A	763	ILE
1	A	780	LEU
1	A	794	LEU
2	B	37	LYS
2	B	41	MET
2	B	50	ASN
2	B	51	LYS
2	B	53	HIS
2	B	60	LEU
2	B	72	ILE
2	B	79	CYS
2	B	97	THR
2	B	114	TYR
2	B	167	VAL
2	B	186	GLU
2	B	190	LYS
2	B	195	LEU
2	B	218	VAL
2	B	237	MET
2	B	295	LEU
2	B	320	LEU
2	B	321	PHE
2	B	323	ARG
2	B	377	ARG
2	B	394	MET
2	B	432	LYS
2	B	471	ASN
2	B	489	ARG
2	B	490	VAL
2	B	494	ASN
2	B	495	LYS
2	B	502	MET
2	B	522	GLU
2	B	669	ASP
2	B	701	THR
2	B	793	VAL
2	B	817	PHE
1	C	55	TRP
1	C	69	VAL
1	C	76	ARG
1	C	80	LYS
1	C	133	MET

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Mol	Chain	Res	Type
1	C	164	ASP
1	C	198	TRP
1	C	214	LYS
1	C	257	VAL
1	C	326	ARG
1	C	331	MET
1	C	390	TRP
1	C	405	HIS
1	C	413	GLU
1	C	417	VAL
1	C	427	GLU
1	C	464	LEU
1	C	473	PHE
1	C	480	VAL
1	C	512	LEU
1	C	561	MET
1	C	562	PHE
1	C	677	SER
1	C	684	THR
1	C	720	LEU
1	C	758	THR
1	C	761	TYR
1	C	791	LEU
1	C	796	LEU
2	D	56	TRP
2	D	60	LEU
2	D	79	CYS
2	D	90	ILE
2	D	91	LEU
2	D	97	THR
2	D	107	VAL
2	D	249	VAL
2	D	308	CYS
2	D	315	TRP
2	D	320	LEU
2	D	323	ARG
2	D	377	ARG
2	D	387	GLU
2	D	462	LEU
2	D	477	HIS
2	D	546	ILE
2	D	548	ARG

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Mol	Chain	Res	Type
2	D	636	TRP
2	D	651	LEU
2	D	654	PHE
2	D	657	LEU
2	D	669	ASP
2	D	671	ARG
2	D	695	ARG
2	D	698	GLU
2	D	701	THR
2	D	704	ARG
2	D	810	PHE
3	E	122	VAL
3	E	128	LYS
3	E	189	LEU
4	F	108	ARG
4	F	109	THR
4	F	145	LYS
3	G	189	LEU
4	H	109	THR
4	H	145	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	163	GLN
1	A	193	ASN
1	A	216	GLN
1	A	356	GLN
1	A	404	ASN
1	A	693	ASN
1	A	766	GLN
2	B	196	GLN
2	B	363	GLN
2	B	375	ASN
2	B	494	ASN
2	B	696	GLN
2	B	705	HIS
1	C	35	ASN
1	C	85	HIS
1	C	111	GLN
1	C	146	GLN

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Mol	Chain	Res	Type
1	C	356	GLN
1	C	671	GLN
1	C	693	ASN
2	D	696	GLN
3	E	39	GLN
3	E	109	ASN
4	F	38	GLN
4	F	89	GLN
3	G	182	GLN
4	H	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

10 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	$\#\|Z\| > 2$
5	NAG	I	1	2,5	14,14,15	0.17	0	17,19,21	0.48	0
5	NAG	I	2	5	14,14,15	0.55	0	17,19,21	0.45	0
5	NAG	J	1	2,5	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	J	2	5	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	K	1	2,5	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	K	2	5	14,14,15	0.52	0	17,19,21	0.49	0
5	NAG	L	1	2,5	14,14,15	0.19	0	17,19,21	0.48	0
5	NAG	L	2	5	14,14,15	0.53	0	17,19,21	0.46	0
5	NAG	M	1	2,5	14,14,15	0.27	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	NAG	L	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	1/6/23/26	0/1/1/1
5	NAG	M	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C1-C2-N2-C7

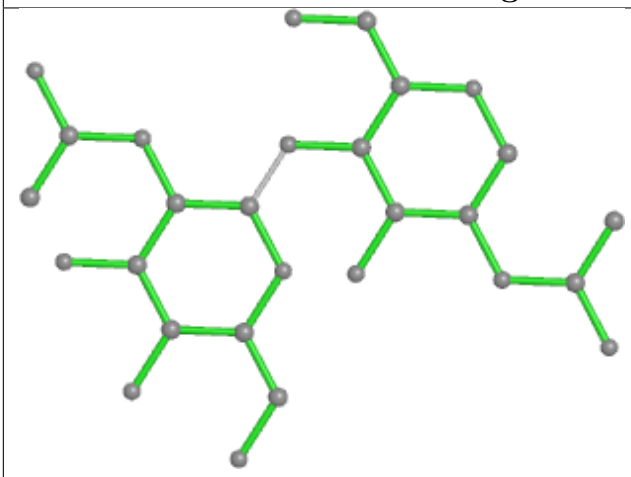
There are no ring outliers.

4 monomers are involved in 3 short contacts:

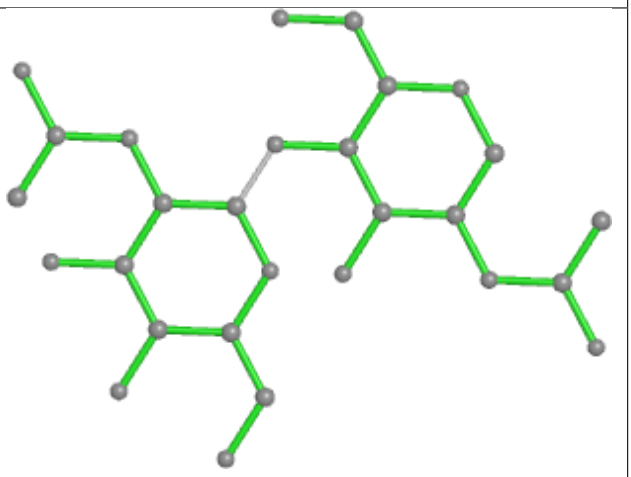
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	1	0
5	K	2	NAG	2	0
5	K	1	NAG	2	0
5	I	2	NAG	1	0

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

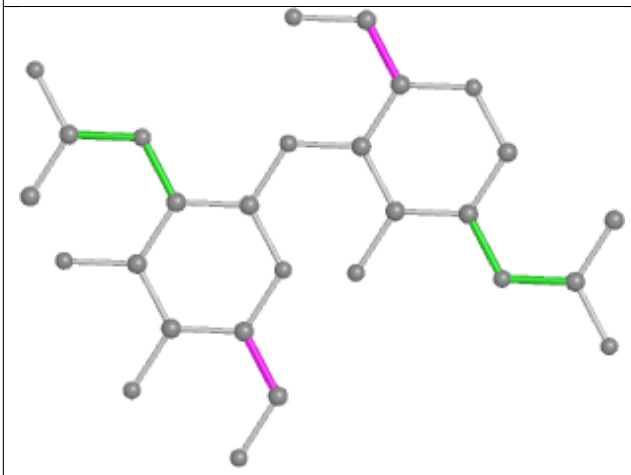
Oligosaccharide Chain I



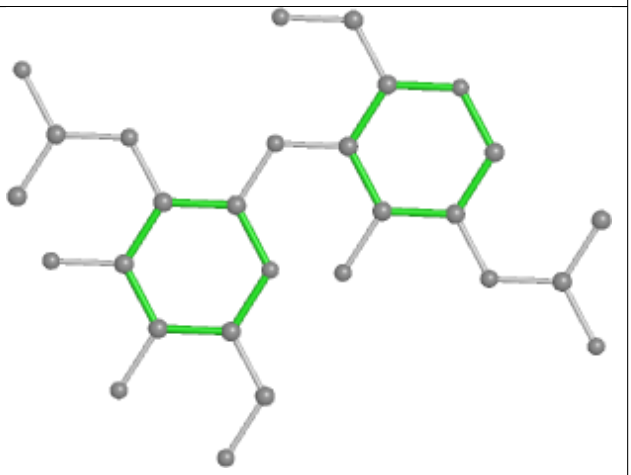
Bond lengths



Bond angles

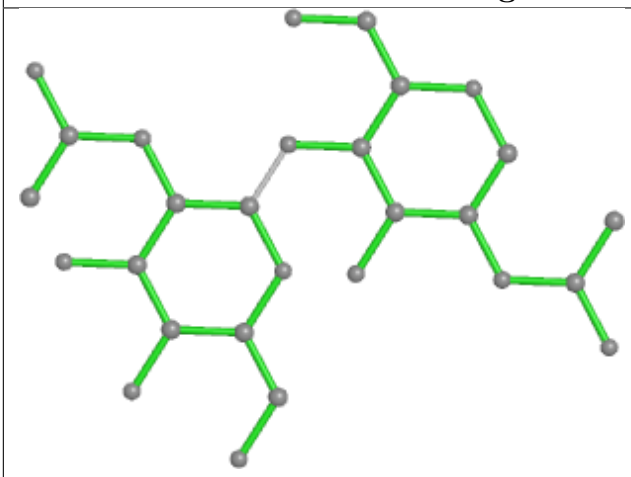


Torsions

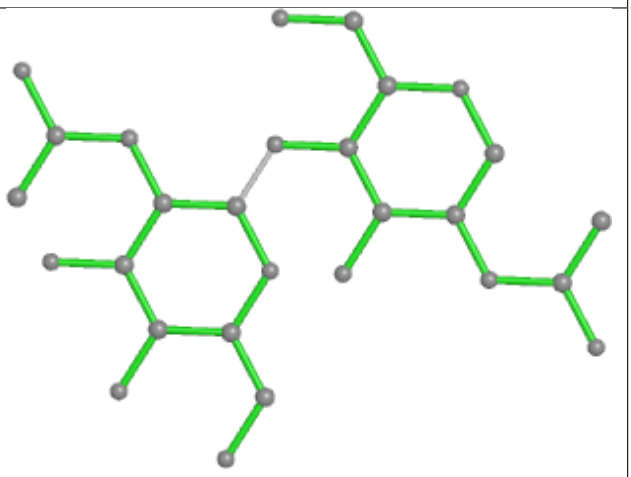


Rings

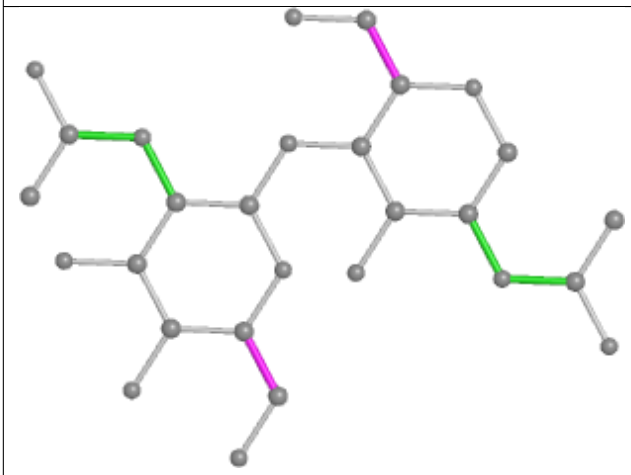
Oligosaccharide Chain J



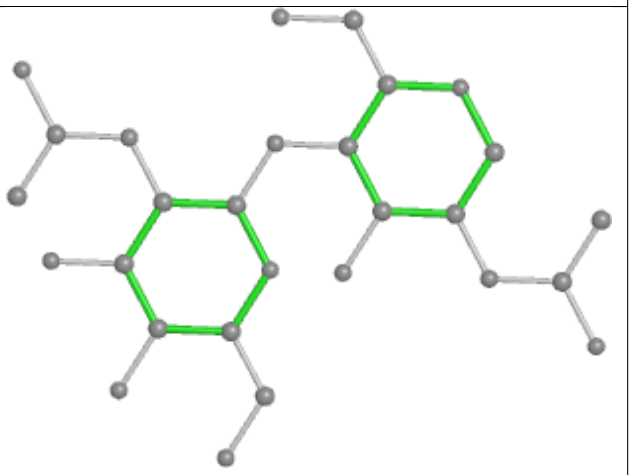
Bond lengths



Bond angles

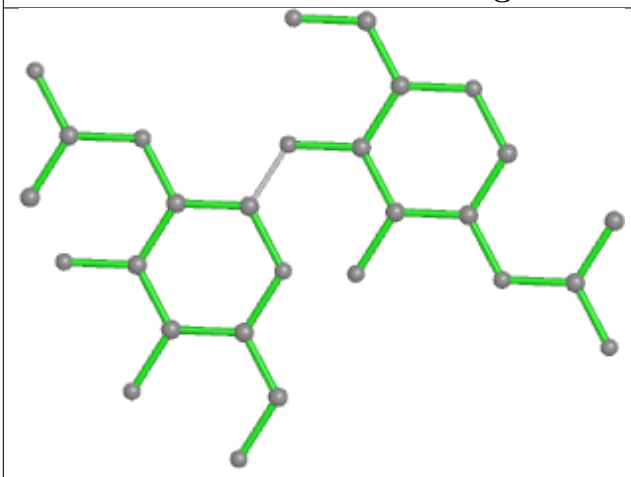


Torsions

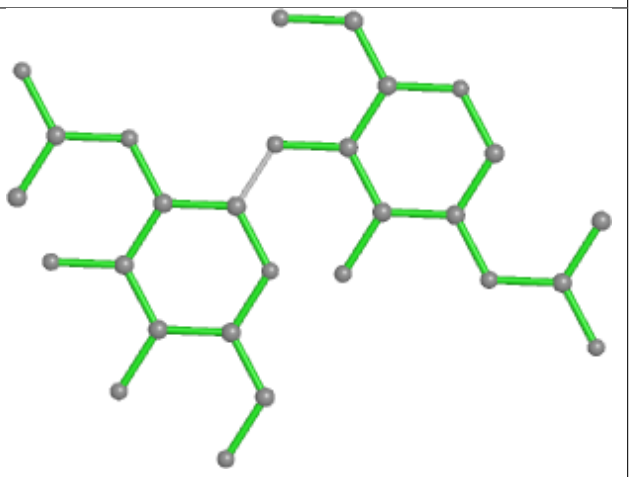


Rings

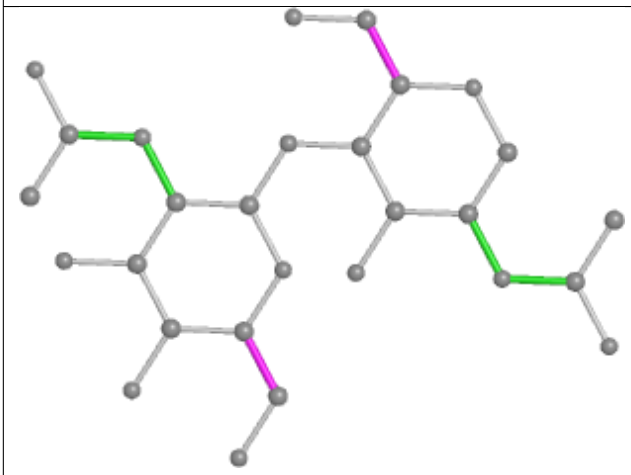
Oligosaccharide Chain K



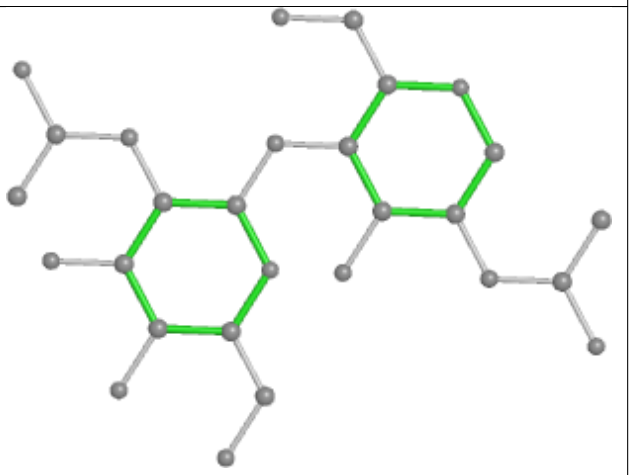
Bond lengths



Bond angles

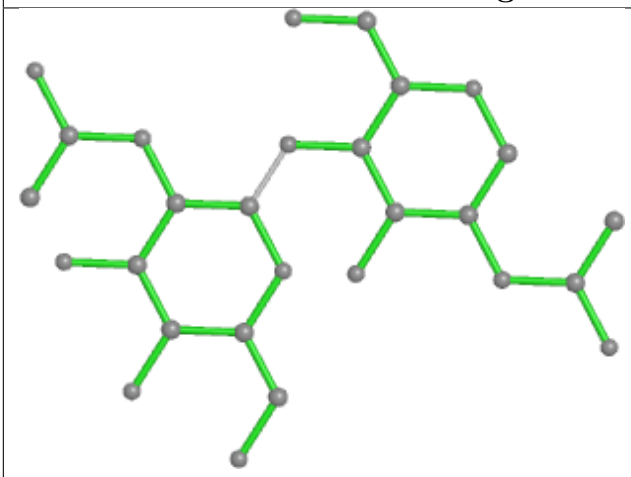


Torsions

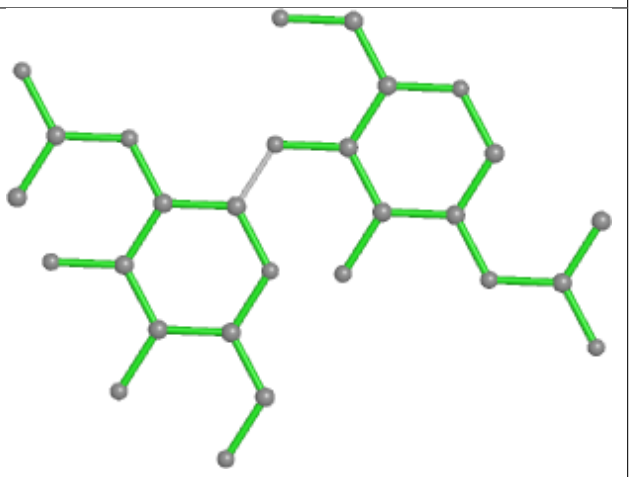


Rings

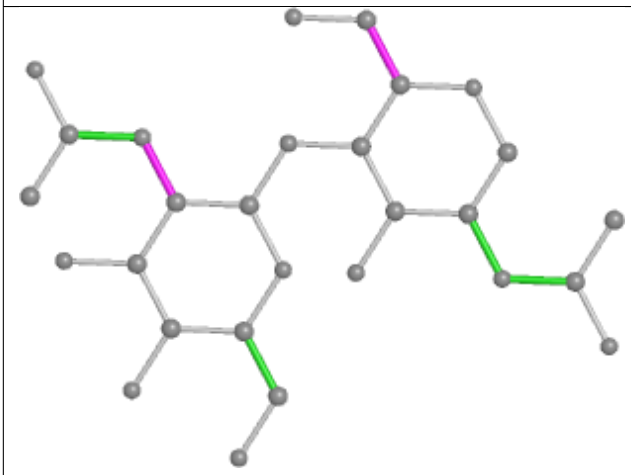
Oligosaccharide Chain L



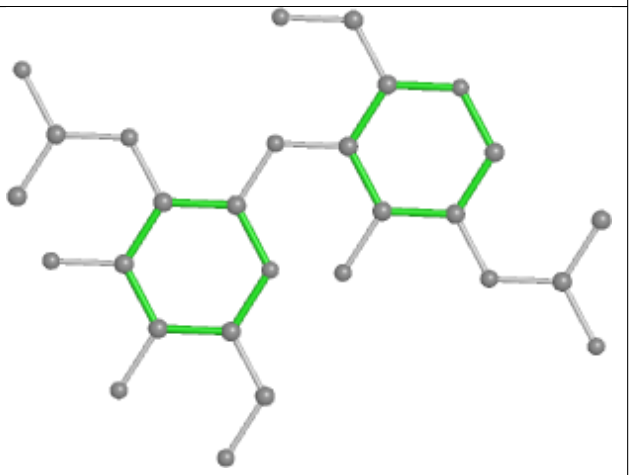
Bond lengths



Bond angles

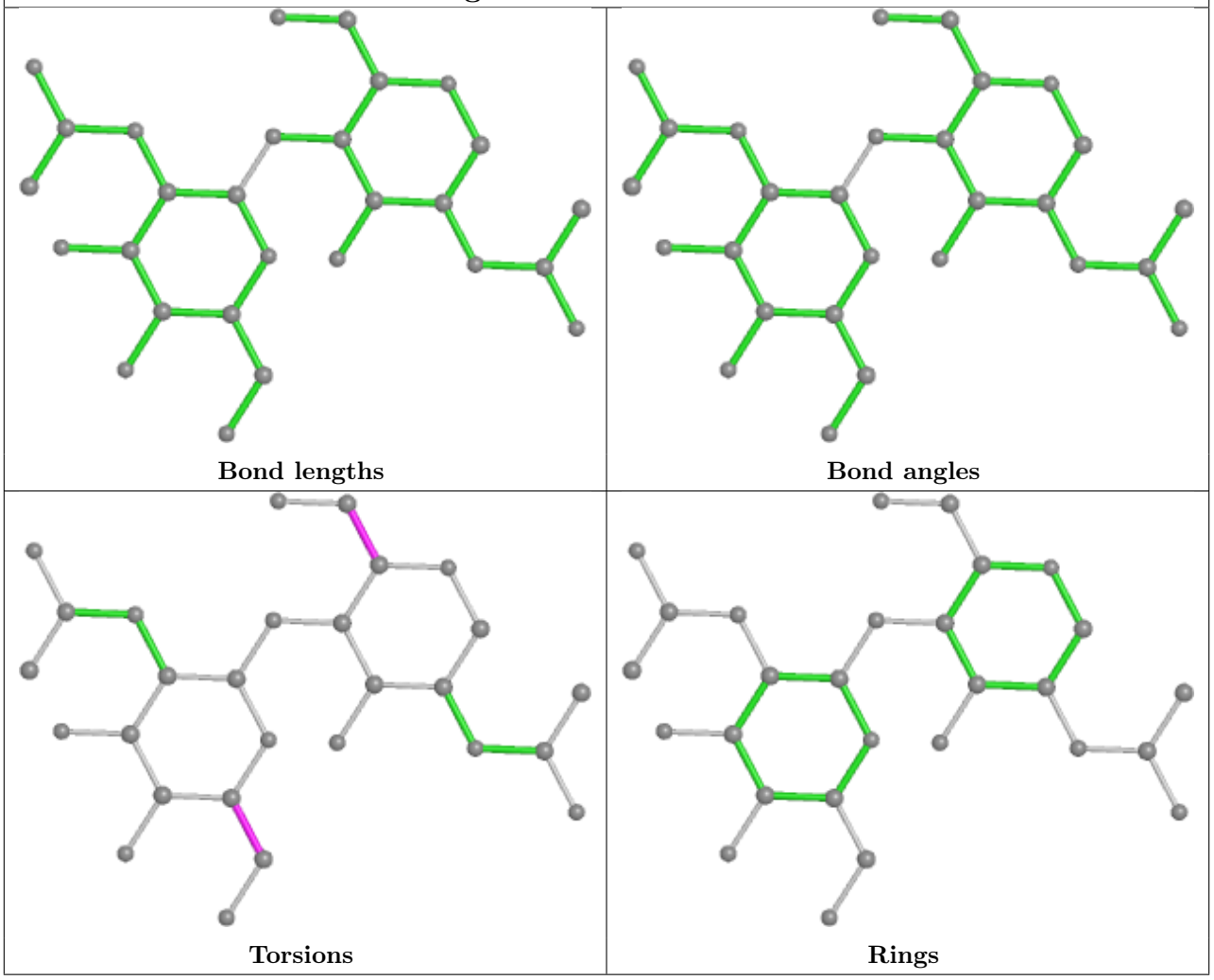


Torsions



Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	C	900	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	D	901	2	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	D	902	2	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	A	900	1	14,14,15	0.26	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	D	903	2	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	D	904	2	14,14,15	0.86	1 (7%)	17,19,21	0.97	1 (5%)
6	NAG	B	902	2	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	B	901	2	14,14,15	0.21	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	900	1	-	2/6/23/26	0/1/1/1
6	NAG	D	901	2	-	2/6/23/26	0/1/1/1
6	NAG	D	902	2	-	2/6/23/26	0/1/1/1
6	NAG	A	900	1	-	2/6/23/26	0/1/1/1
6	NAG	D	903	2	-	0/6/23/26	0/1/1/1
6	NAG	D	904	2	-	2/6/23/26	0/1/1/1
6	NAG	B	902	2	-	2/6/23/26	0/1/1/1
6	NAG	B	901	2	-	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)
6	D	904	NAG	O5-C1	2.81	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	904	NAG	C1-O5-C5	3.78	117.31	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	901	NAG	O5-C5-C6-O6
6	B	902	NAG	O5-C5-C6-O6
6	A	900	NAG	O5-C5-C6-O6
6	B	901	NAG	C4-C5-C6-O6
6	D	902	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	902	NAG	C4-C5-C6-O6
6	D	902	NAG	C4-C5-C6-O6
6	A	900	NAG	C4-C5-C6-O6
6	C	900	NAG	O5-C5-C6-O6
6	D	904	NAG	O5-C5-C6-O6
6	D	904	NAG	C4-C5-C6-O6
6	C	900	NAG	C4-C5-C6-O6
6	D	901	NAG	C4-C5-C6-O6
6	D	901	NAG	O5-C5-C6-O6

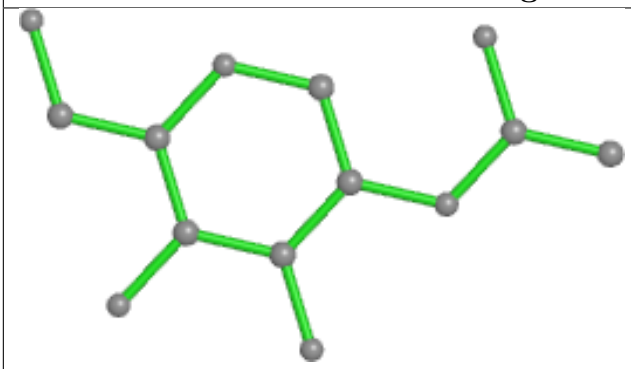
There are no ring outliers.

1 monomer is involved in 1 short contact:

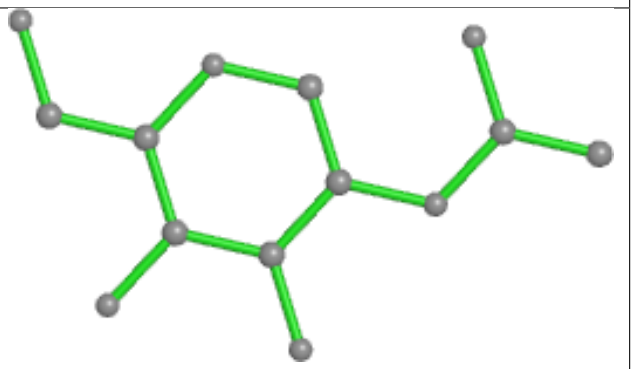
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	NAG	1	0

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

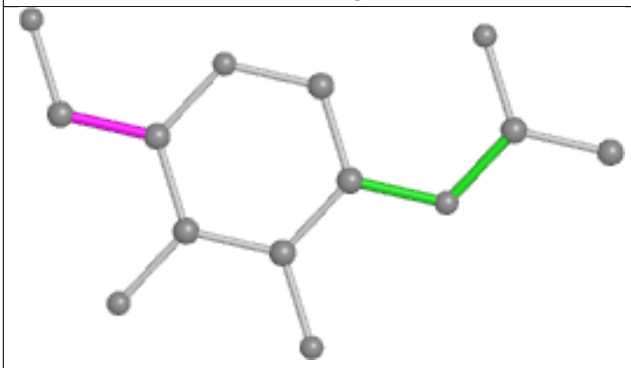
Ligand NAG C 900



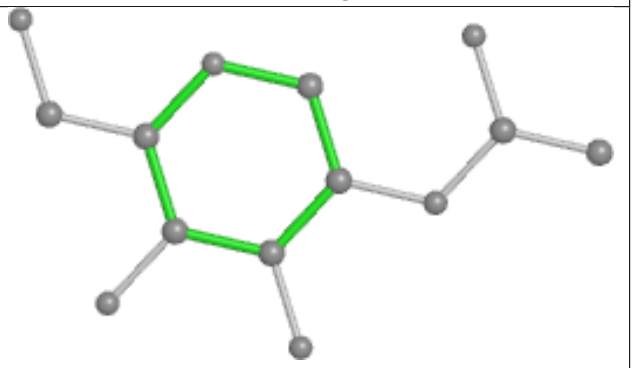
Bond lengths



Bond angles

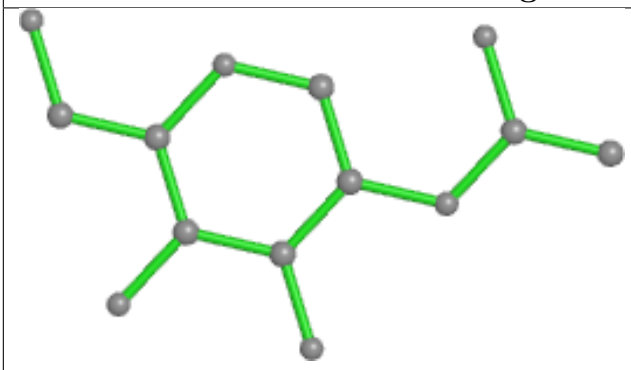


Torsions

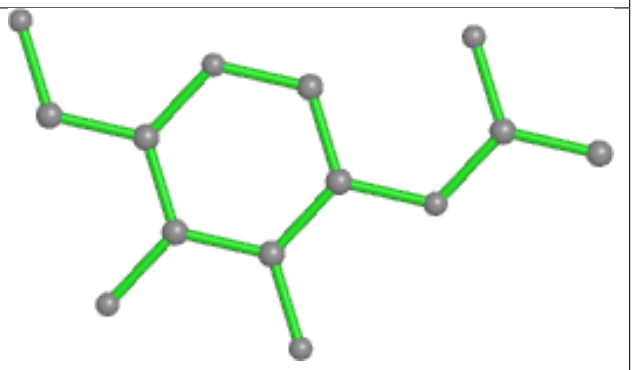


Rings

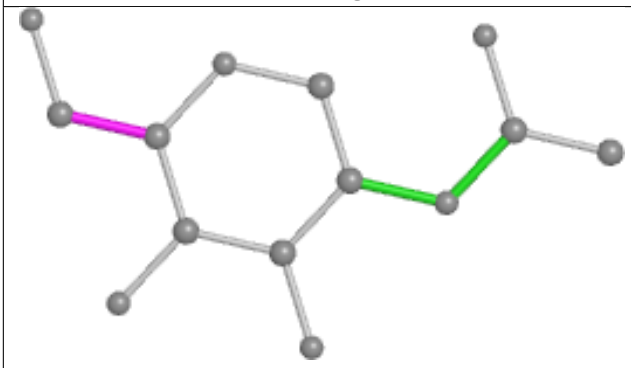
Ligand NAG D 901



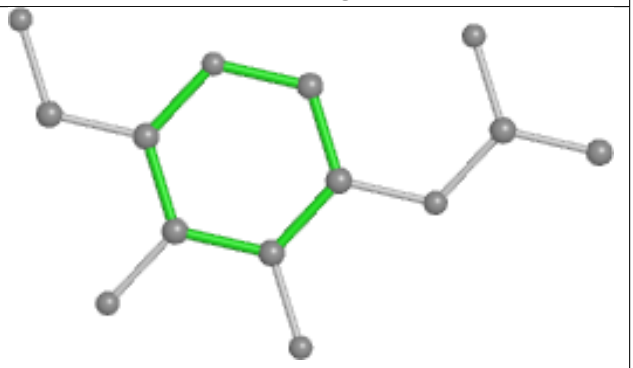
Bond lengths



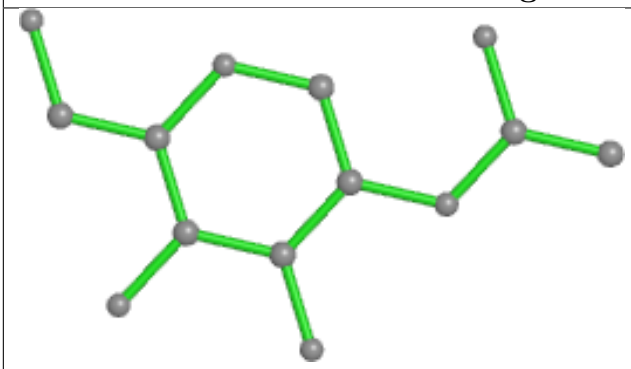
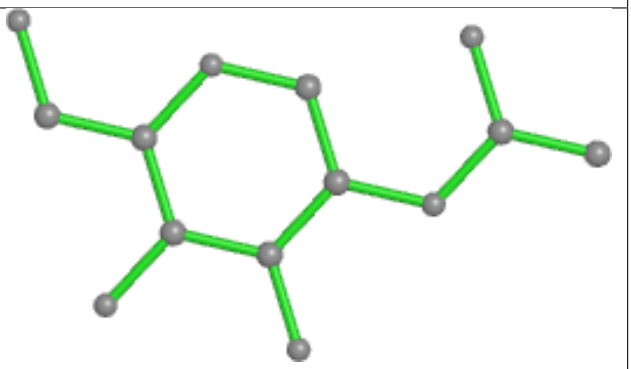
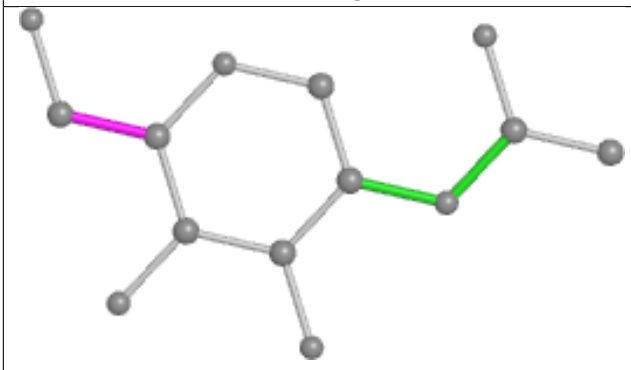
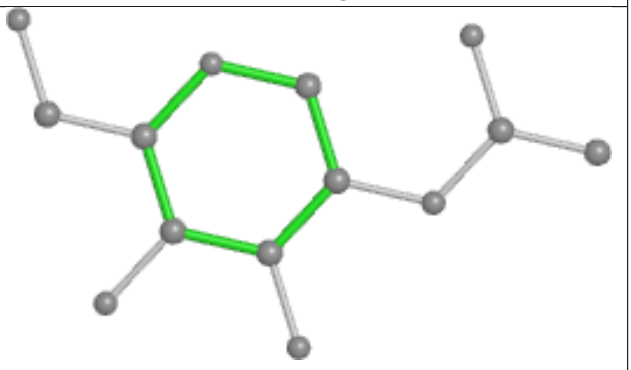
Bond angles

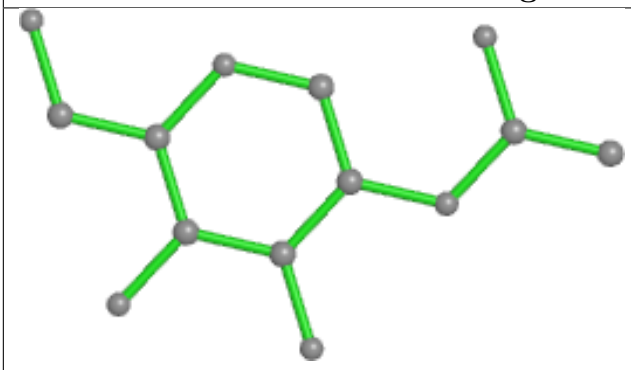
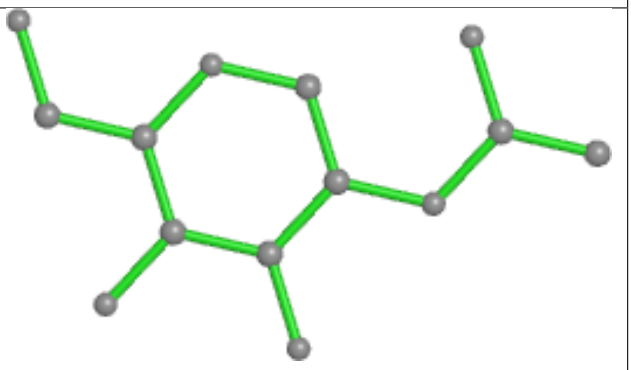
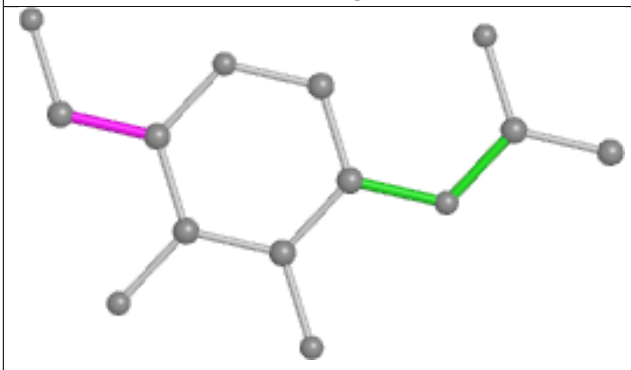
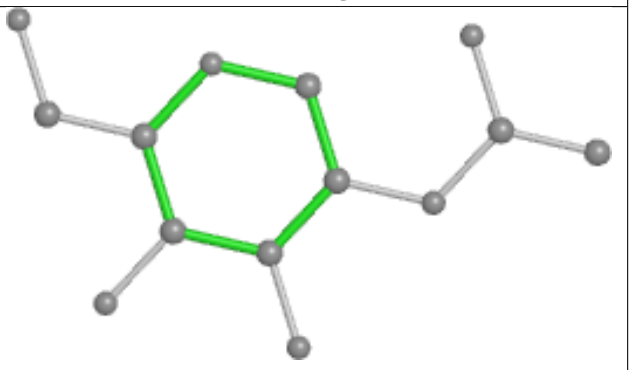


Torsions

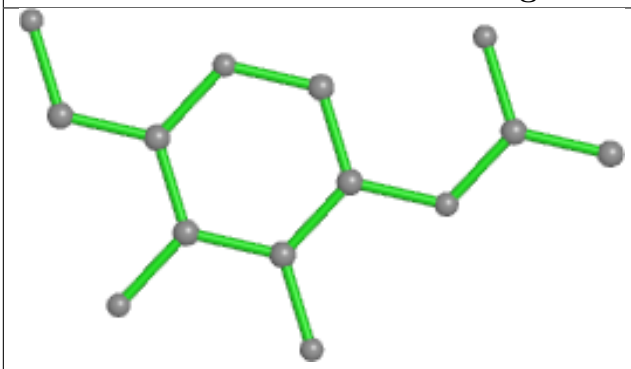


Rings

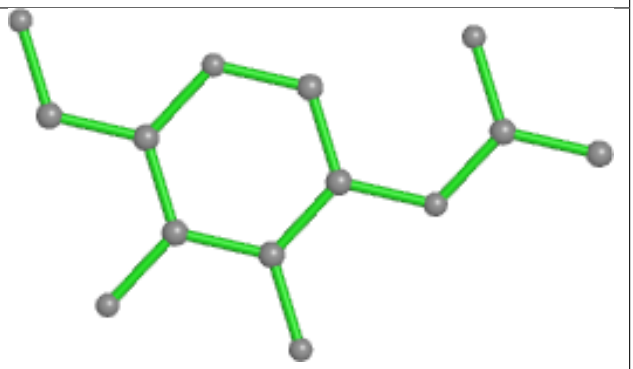
Ligand NAG D 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

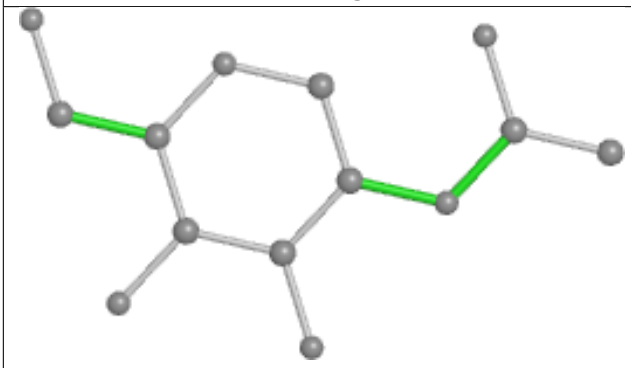
Ligand NAG D 903



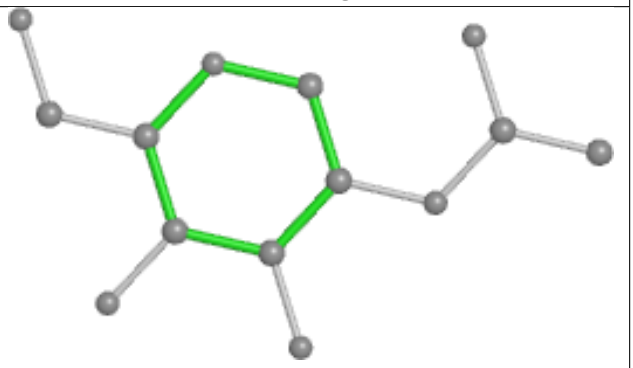
Bond lengths



Bond angles

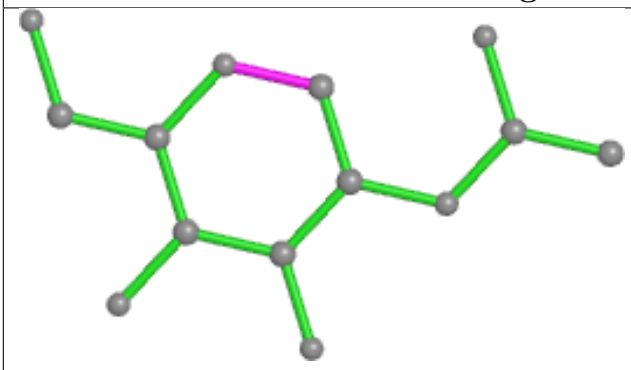


Torsions

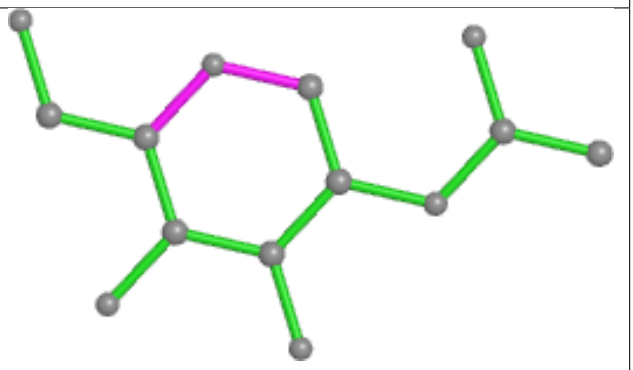


Rings

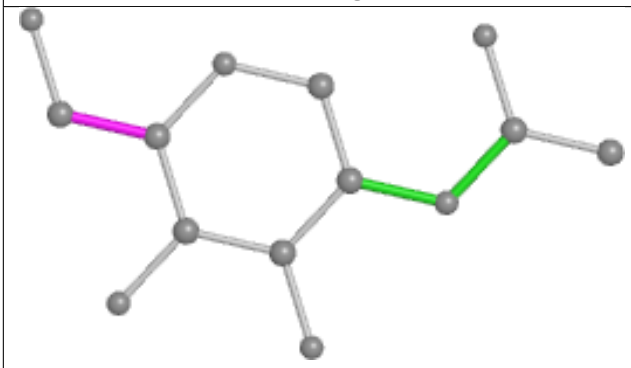
Ligand NAG D 904



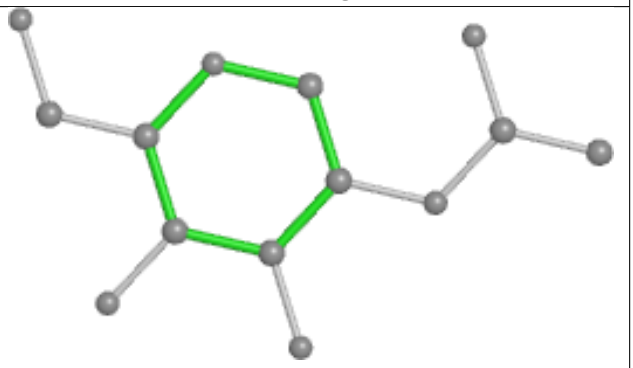
Bond lengths



Bond angles

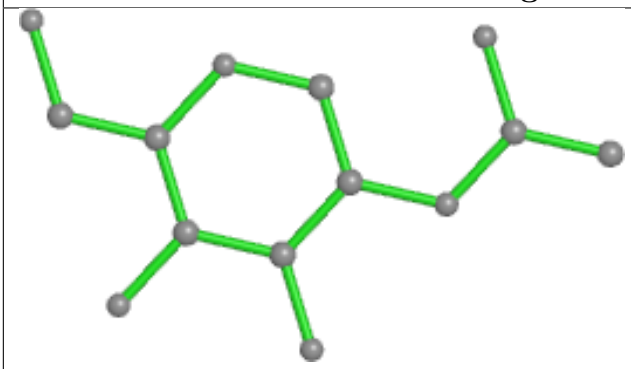


Torsions

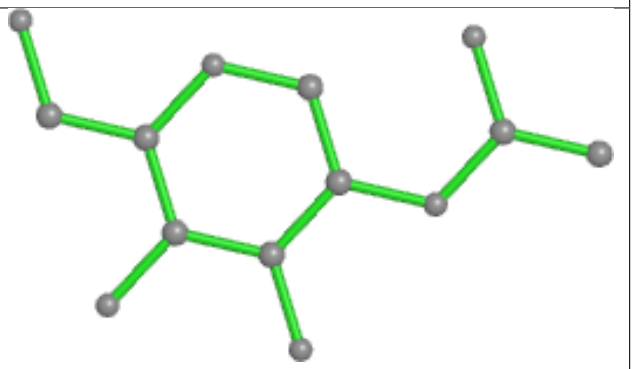


Rings

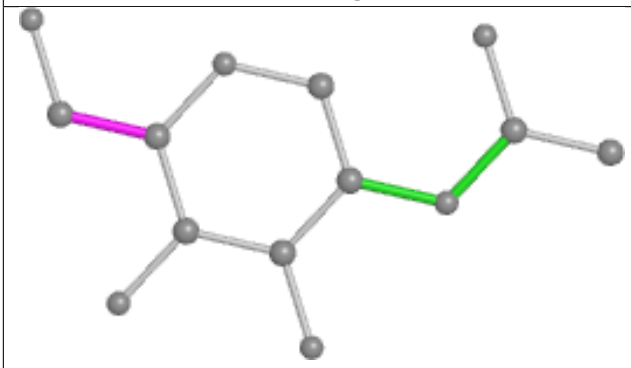
Ligand NAG B 902



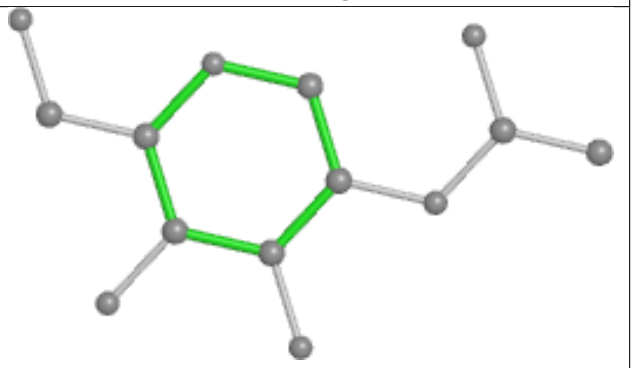
Bond lengths



Bond angles

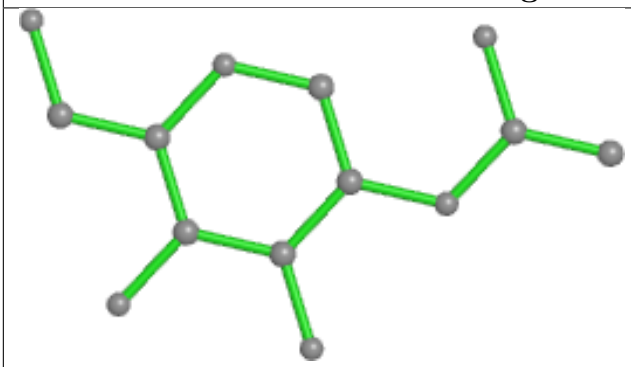


Torsions

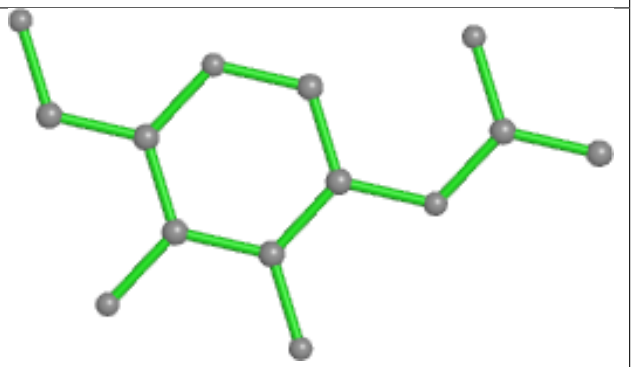


Rings

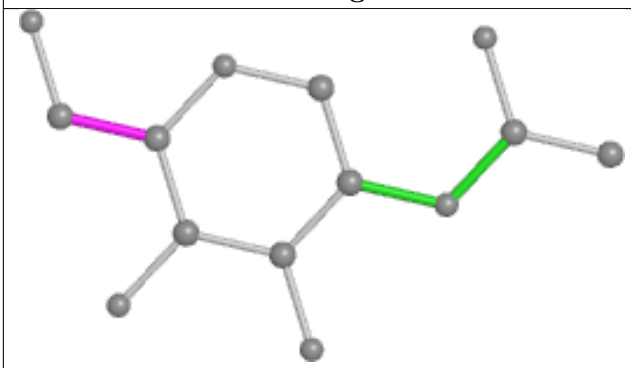
Ligand NAG B 901



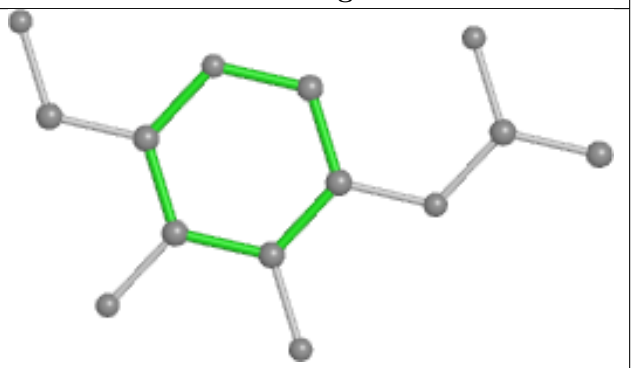
Bond lengths



Bond angles



Torsions



Rings

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.

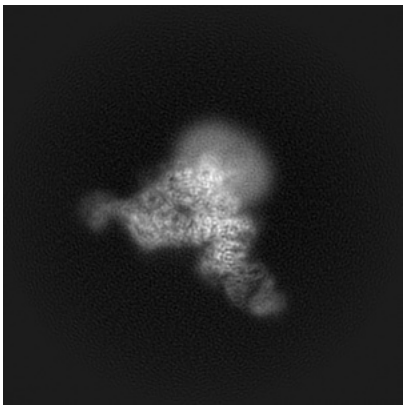
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36335. These allow visual inspection of the internal detail of the map and identification of artifacts.

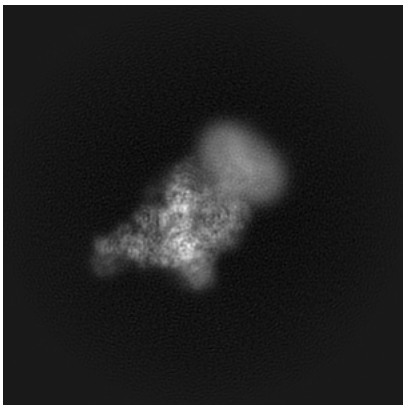
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

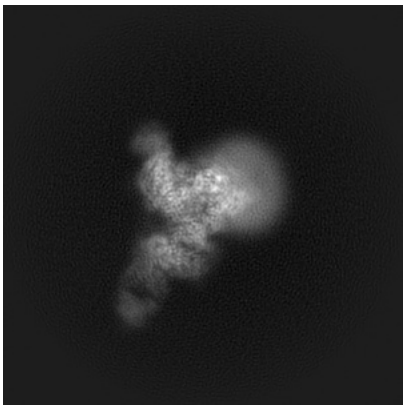
6.1.1 Primary map



X

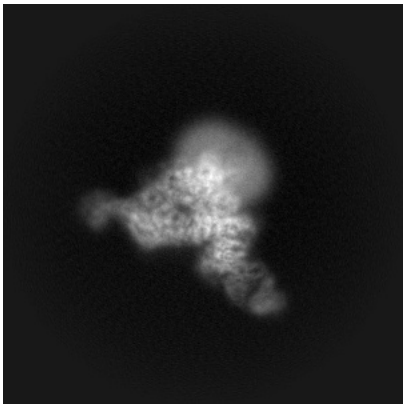


Y

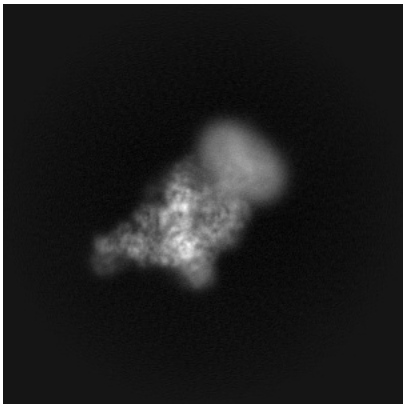


Z

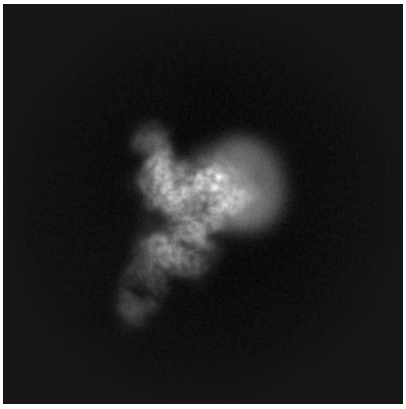
6.1.2 Raw map



X



Y

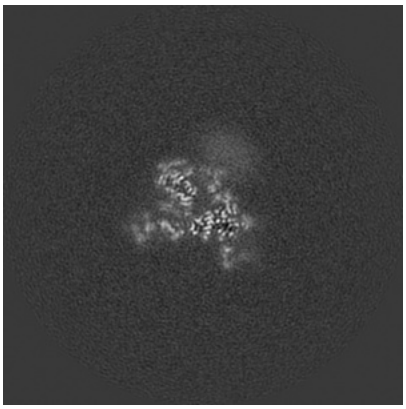


Z

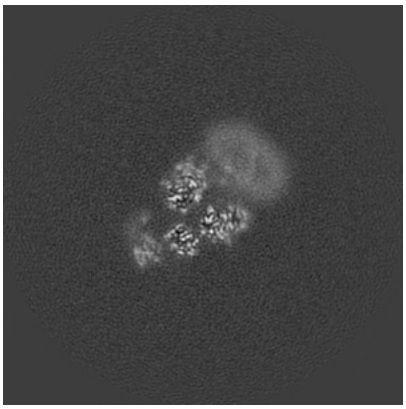
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

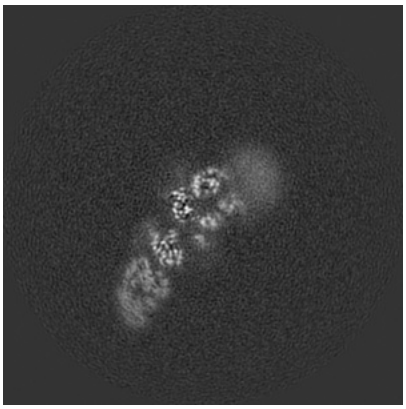
6.2.1 Primary map



X Index: 190

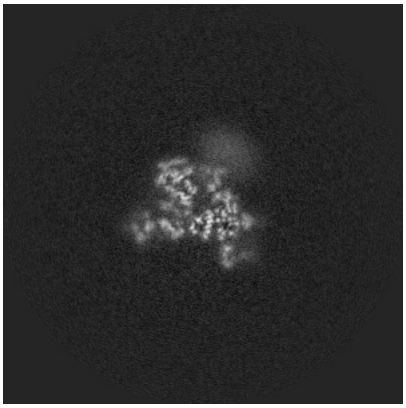


Y Index: 190

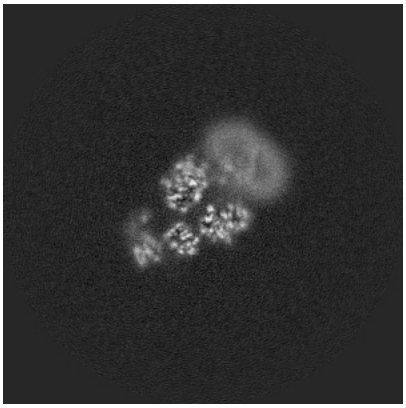


Z Index: 190

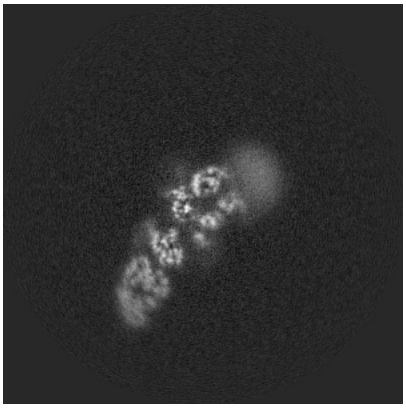
6.2.2 Raw map



X Index: 190



Y Index: 190

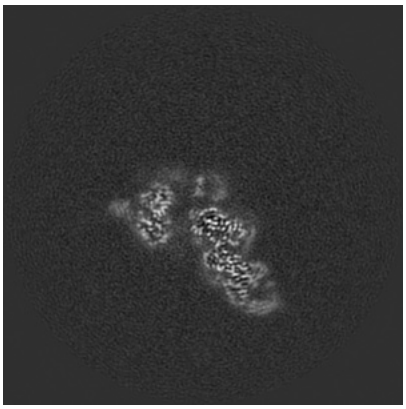


Z Index: 190

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

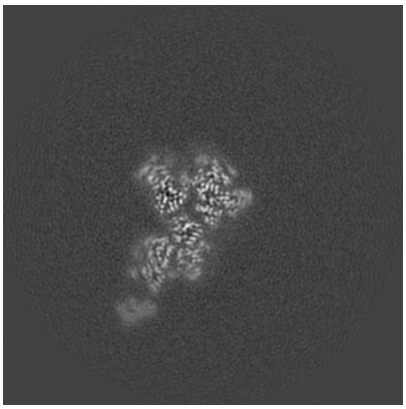
6.3 Largest variance slices (i)

6.3.1 Primary map



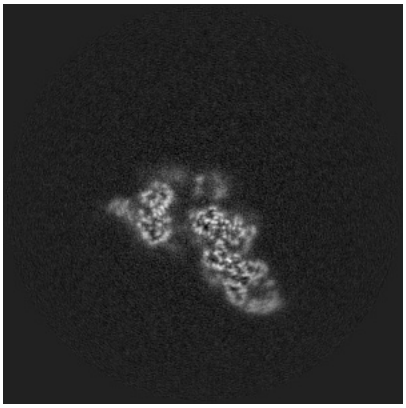
X Index: 154

Y Index: 205

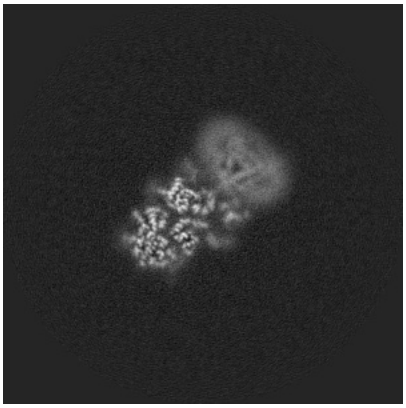


Z Index: 174

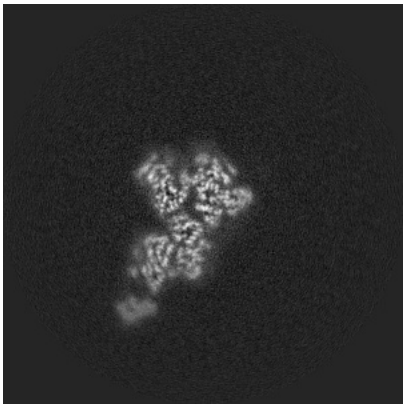
6.3.2 Raw map



X Index: 153



Y Index: 205

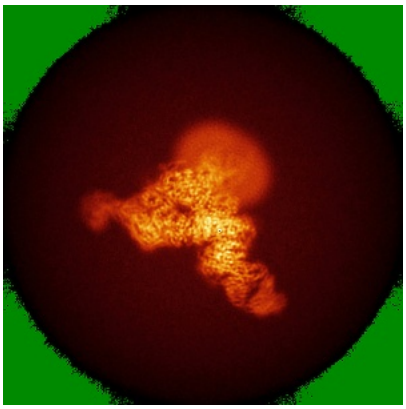


Z Index: 174

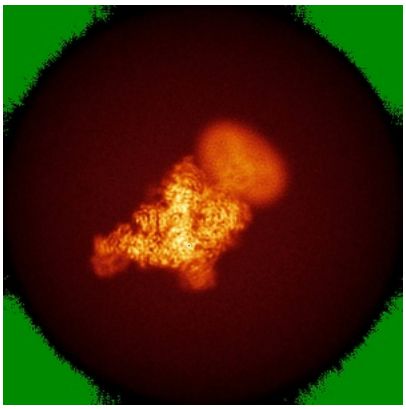
The images above show the largest variance slices of the map in three orthogonal directions.

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

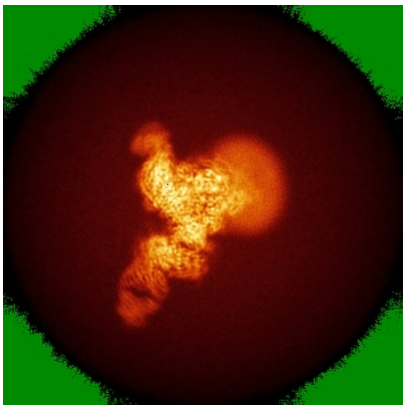
6.4.1 Primary map



X

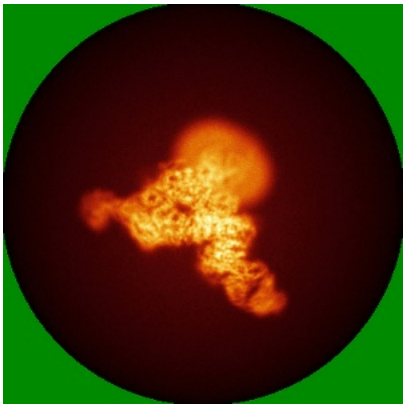


Y

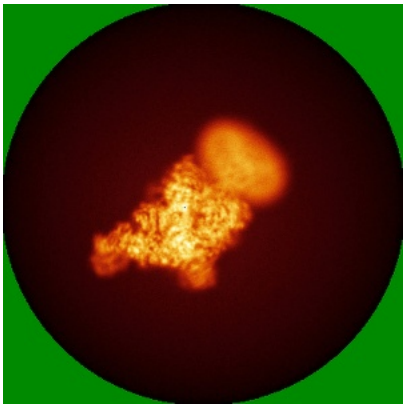


Z

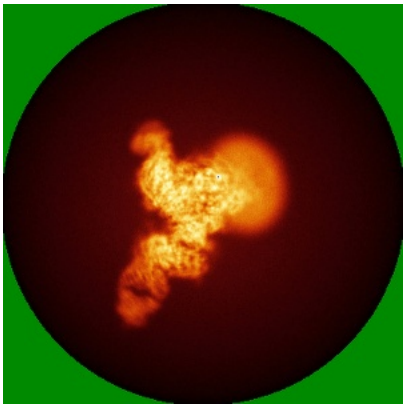
6.4.2 Raw map



X



Y

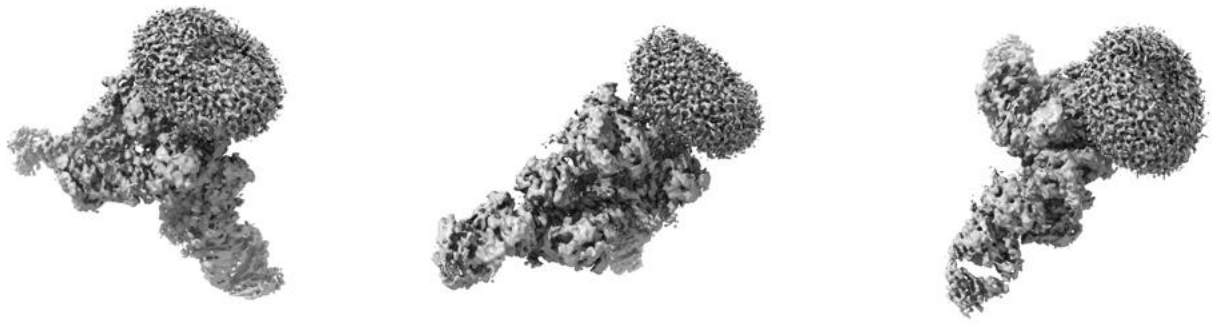


Z

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)

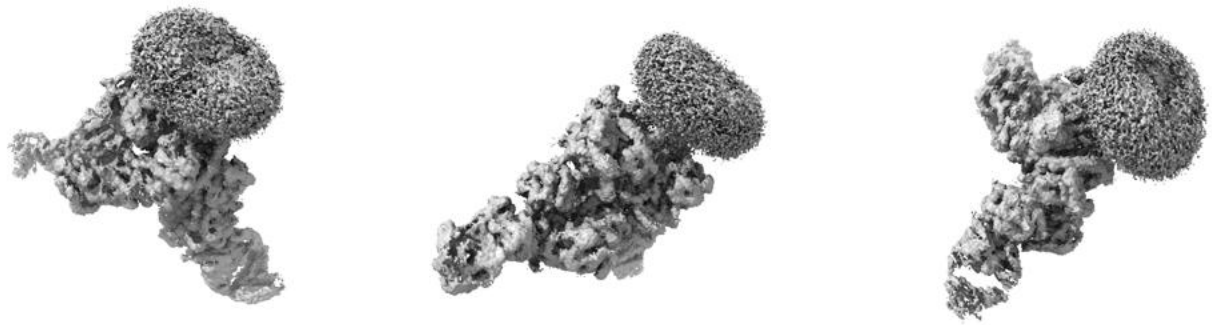
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

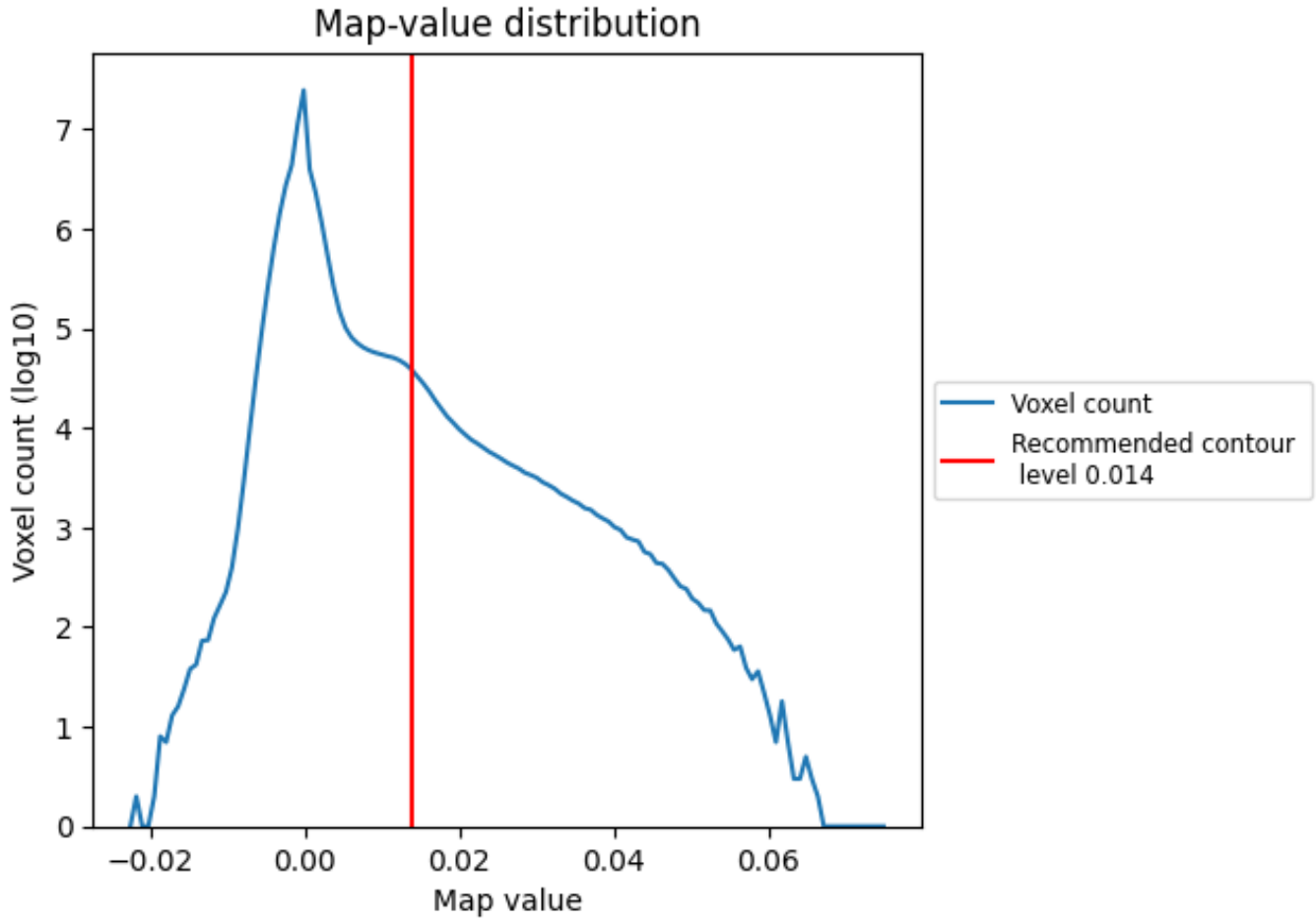
6.6 Mask visualisation (i)

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

7 Map analysis

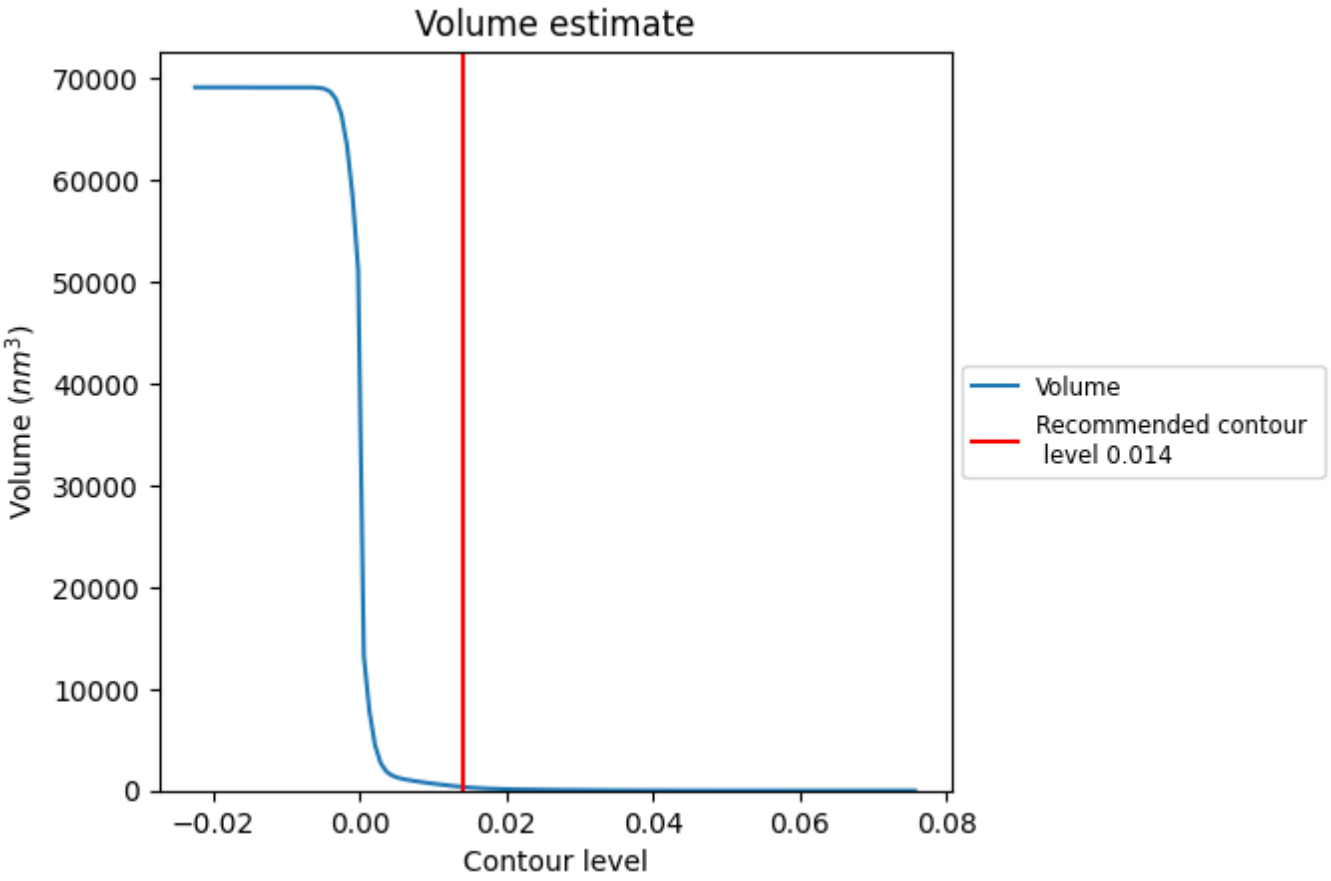
This section contains the results of statistical analysis of the map.

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.

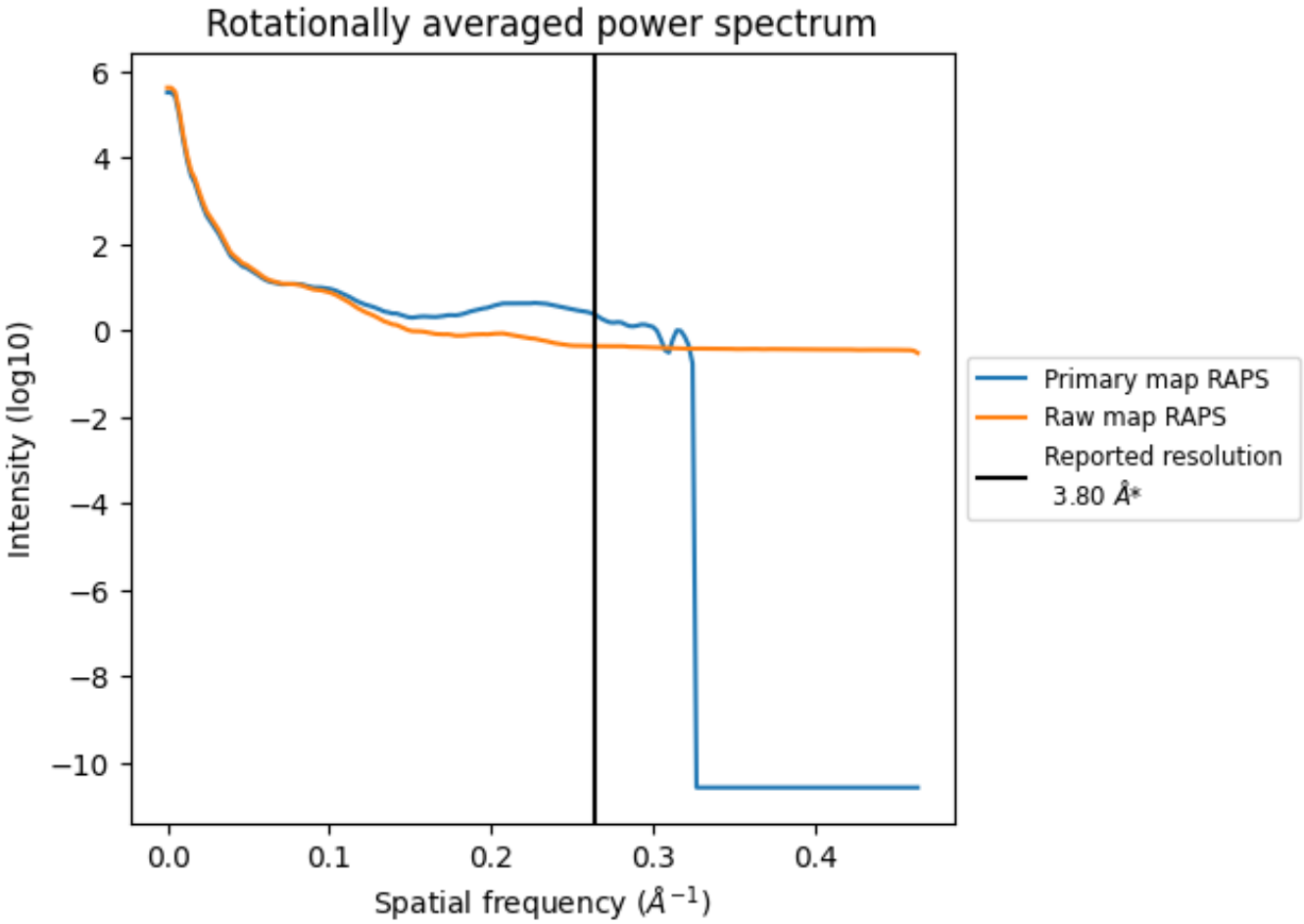
7.2 Volume estimate



The volume at the recommended contour level is 357 nm^3; this corresponds to an approximate mass of 323 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)

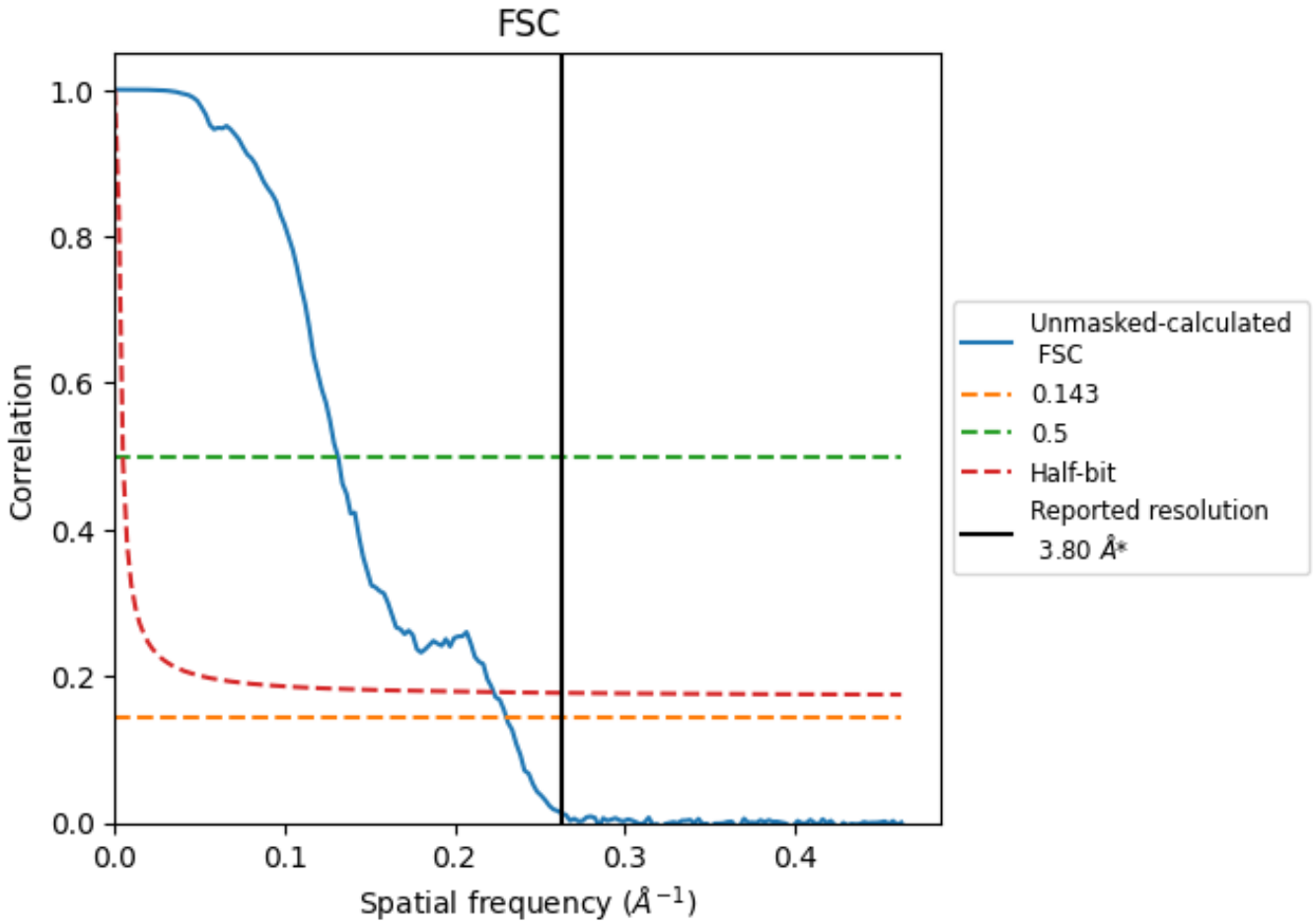


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

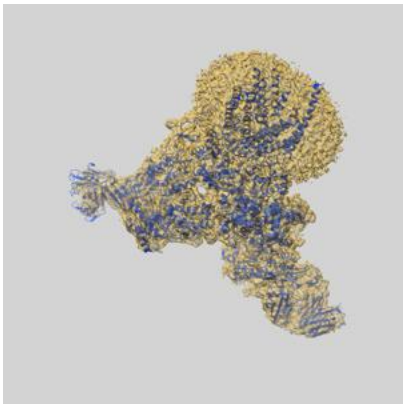
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	7.62	4.48

*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 4.34 differs from the reported value 3.8 by more than 10 %

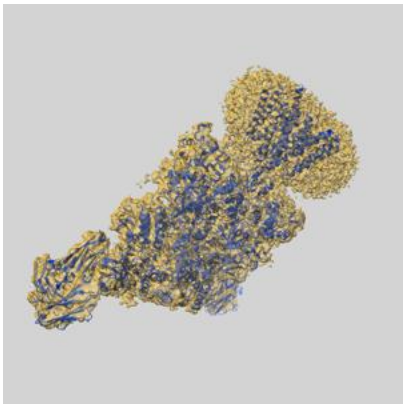
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36335 and PDB model 8JIZ. Per-residue inclusion information can be found in section 3 on page 7.

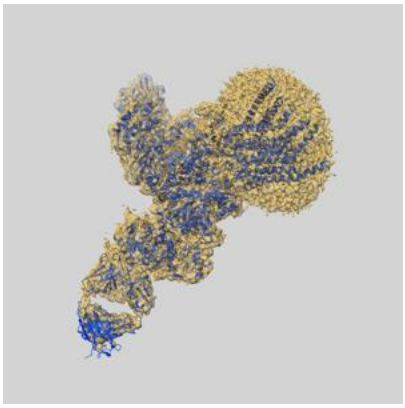
9.1 Map-model overlay



X



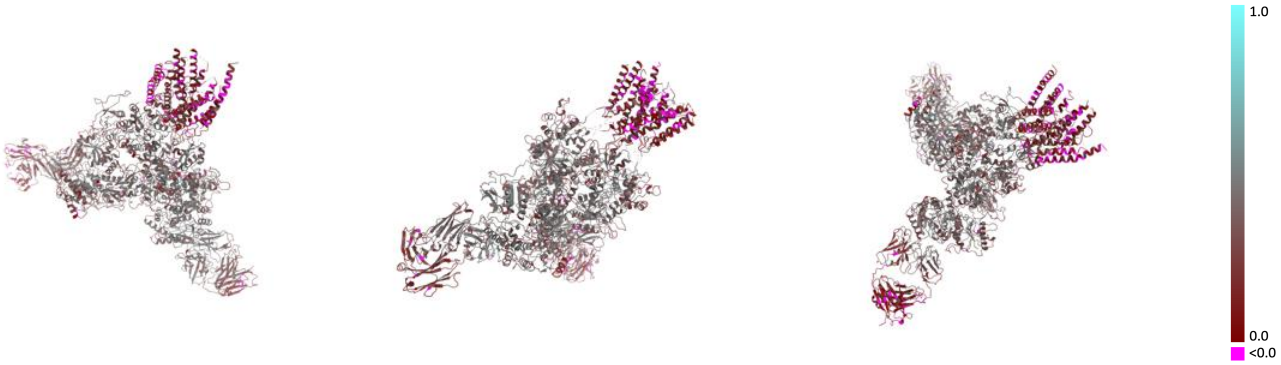
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

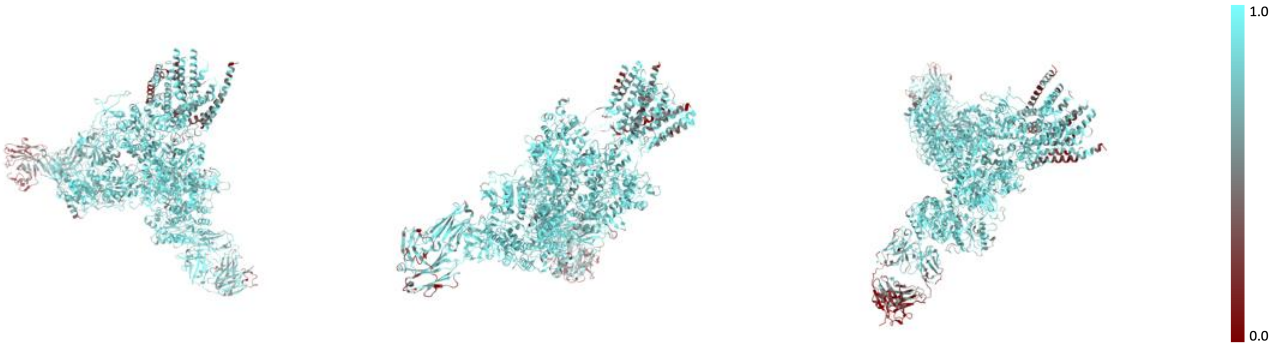
9.2 Q-score mapped to coordinate model (i)



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.

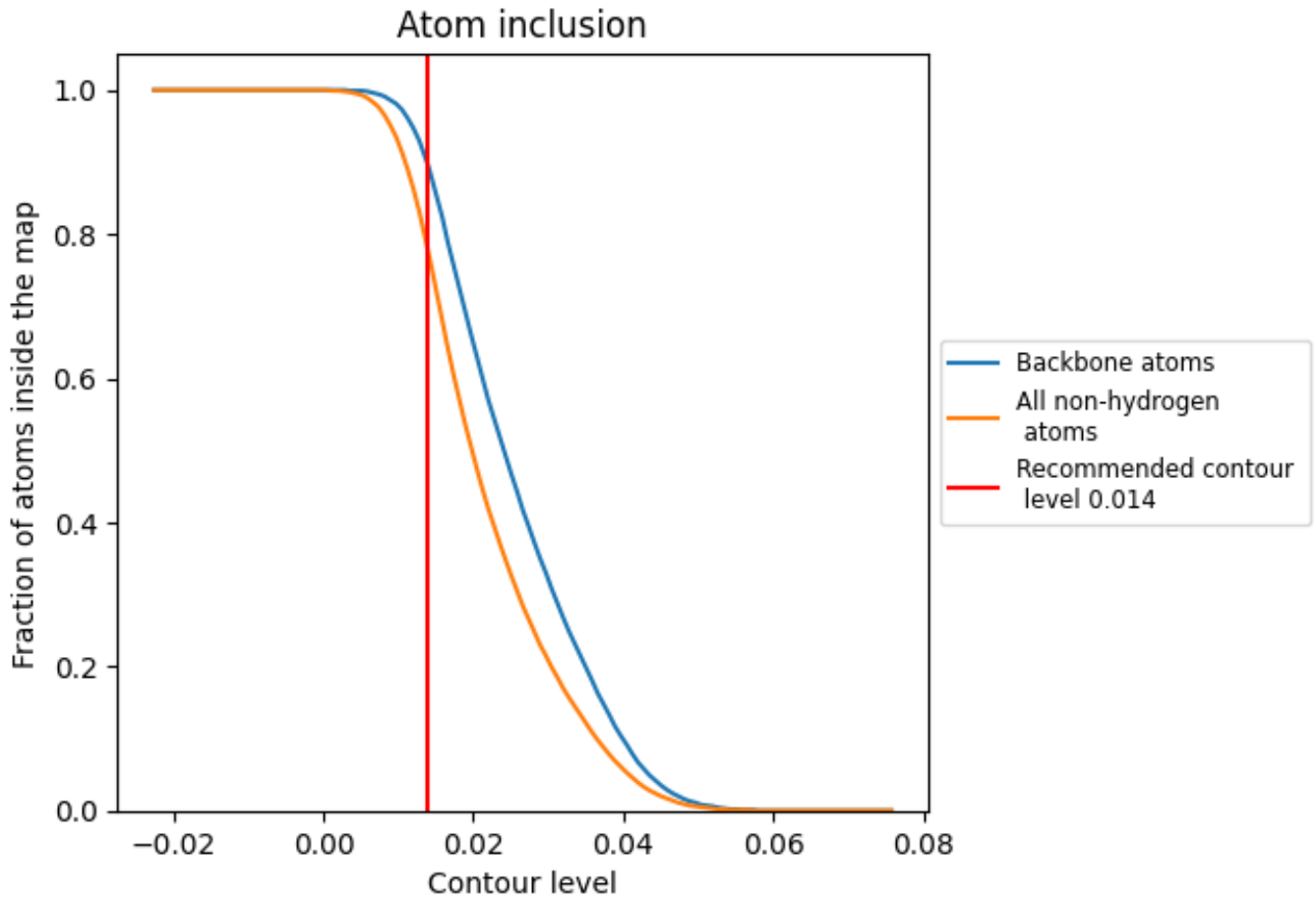
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.3350
A	0.8160	0.3450
B	0.8200	0.3370
C	0.8120	0.3410
D	0.8330	0.3640
E	0.4630	0.2160
F	0.4870	0.2580
G	0.7610	0.3500
H	0.7460	0.3370
I	0.7500	0.3440
J	0.6790	0.3690
K	0.7140	0.3530
L	0.8570	0.4100
M	0.7860	0.2950