



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 11:41 PM JST

PDB ID : 8JX9
EMDB ID : EMD-36693
Title : rat megalin bodyA
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-30
Resolution : 3.80 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

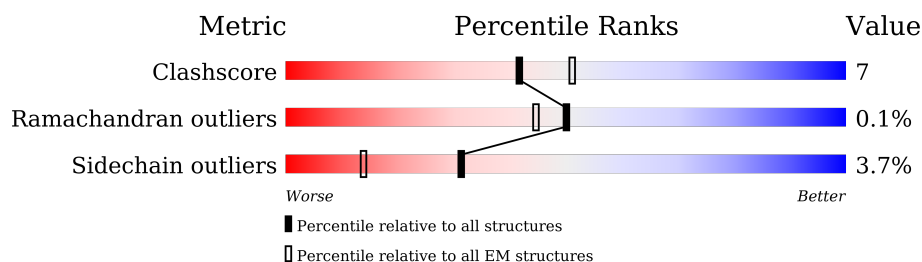
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



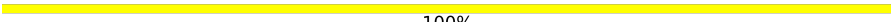
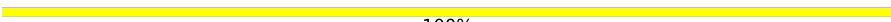
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4660	 7% 7% 92%
1	B	4660	 19% 77%
2	O	5	 80% 20%
3	C	3	 33% 67% 67%
3	D	3	 67% 33%
4	E	5	 40% 40% 60%
4	H	5	 20% 60% 20% 20%
4	I	5	 20% 60% 20%

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Mol	Chain	Length	Quality of chain
5	F	2	 100%
5	G	2	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11822 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 LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2904	1844	493	549	18		
1	B	1077	Total	C	N	O	S	0	0
			8455	5100	1537	1687	131		

- Molecule 2 is a protein called ligand.

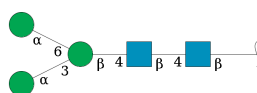
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	5	Total	C	N	O	0	0
			28	16	6	6		

- 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	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

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



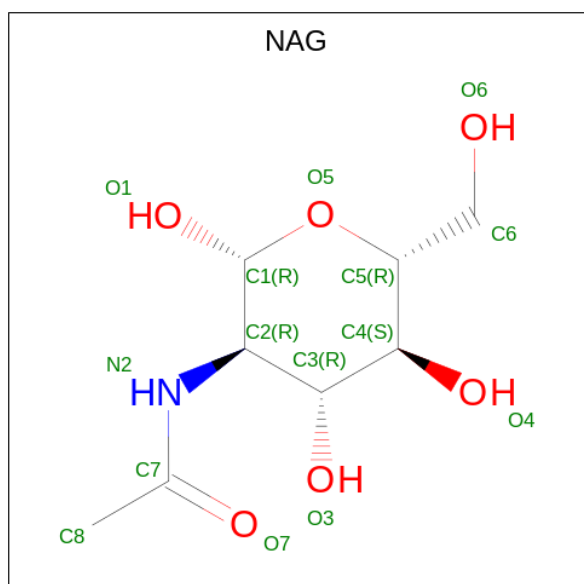
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	5	Total	C	N	O	0	0
			61	34	2	25		
4	H	5	Total	C	N	O	0	0
			61	34	2	25		
4	I	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



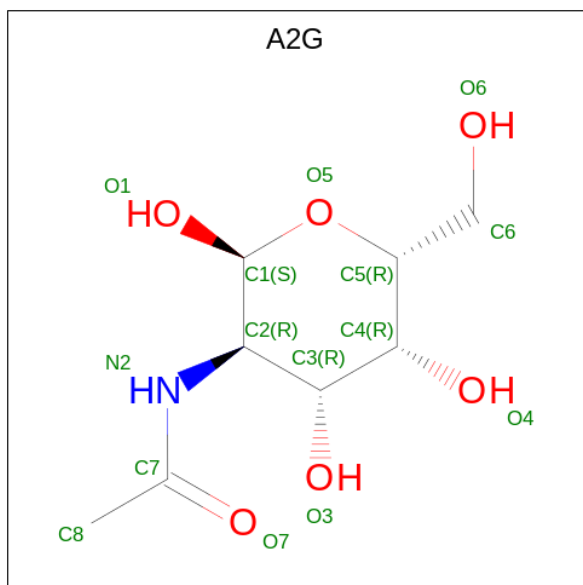
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 7 is 2-acetamido-2-deoxy- α -D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	B	20	Total	Ca	0
			20	20	





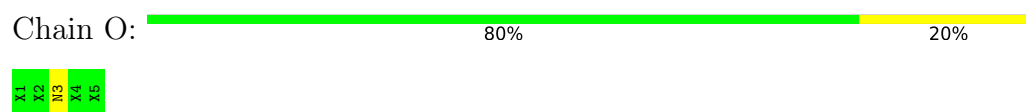
L4279	D4280	F4282	E4283	D4284	L4286	Y4287	W4288	Y4289	A4290	E4292	E4293	G4294	E4295	W4296	W4297	E4298	Y4299	N4300	K4301	F4302	G4303	K4304	E4305	K4306	K4307	E4308	K4309	V4310	L4311	V4312	V4313	K4314	P4315	W4316	L4317	T4318	Q4319	V4320	K4321	T4322	F4323	H4324	Q4325	L4326	L4327	Y4328	N4329	Q4330	S4331	V4332	S4333	M4334	P4335	C4336	S4337	K4338	
G4219	E4220	H4221	R4222	S4223	V4224	L4225	W4226	S4227	E4228	N4229	L4230	G4231	W4232	P4233	M4234	L4236	S4237	I4238	D4239	Y4240	L4241	M4242	D4243	D4244	R4245	W4246	Y4247	W4248	S4249	D4250	S4251	K4252	E4253	D4254	V4255	L4256	E4257	A4258	Y4259	K4260	Y4261	D4262	G4263	T4264	K4265	R4266	R4267	L4268	K4269	I4270	N4271	E4272	A4273	M4274	K4275	P4276	F4277
A4150	V4151	D4152	W4153	S4154	G4155	R4156	H4157	L4158	Y4159	D4162	S4165	A4171	T4172	L4173	D4174	G4175	R4176	Y4177	R4178	K4179	W4180	L4181	Q4185	L4186	D4187	A4190	K4191	T4192	A4193	W4194	N4195	P4196	K4197	L4198	G4199	L4200	W4201	F4202	W4203	T4204	D4205	Q4206	G4207	K4208	Q4209	P4210	K4211	I4212	E4213	S4214	A4215	W4216	N4217	K4218			
E4081	E4082	E4083	E4084	H4085	I4086	Q4087	T4088	I4089	D4090	Y4091	D4092	W4093	D4094	P4095	H4097	I4098	G4099	L4100	S4101	V4102	W4103	Y4104	Y4105	T4106	L4108	A4116	I4117	K4118	R4119	A4120	Y4121	I4122	P4123	M4124	F4125	E4126	S4127	G4128	S4129	M4130	N4131	P4132	I4133	E4074	R4134	E4135	V4136	D4137	L4138	Y4142	L4143	P4146	D4147	G4148	L4149		
G4219	E4220	H4221	R4222	S4223	V4224	L4225	W4226	S4227	E4228	N4229	L4230	G4231	W4232	P4233	M4234	L4236	S4237	I4238	D4239	Y4240	L4241	M4242	D4243	D4244	R4245	W4246	Y4247	W4248	S4249	D4250	S4251	K4252	E4253	D4254	V4255	L4256	E4257	A4258	Y4259	K4260	Y4261	D4262	G4263	T4264	K4265	R4266	R4267	L4268	K4269	I4270	N4271	E4272	A4273	M4274	K4275	P4276	F4277
A4150	V4151	D4152	W4153	S4154	G4155	R4156	H4157	L4158	Y4159	D4162	S4165	A4171	T4172	L4173	D4174	G4175	R4176	Y4177	R4178	K4179	W4180	L4181	Q4185	L4186	D4187	A4190	K4191	T4192	A4193	W4194	N4195	P4196	K4197	L4198	G4199	L4200	W4201	F4202	W4203	T4204	D4205	Q4206	G4207	K4208	Q4209	P4210	K4211	I4212	E4213	S4214	A4215	W4216	N4217	K4218			
E4081	E4082	E4083	E4084	H4085	I4086	Q4087	T4088	I4089	D4090	Y4091	D4092	W4093	D4094	P4095	H4097	I4098	G4099	L4100	S4101	V4102	W4103	Y4104	Y4105	T4106	L4108	A4116	I4117	K4118	R4119	A4120	Y4121	I4122	P4123	M4124	F4125	E4126	S4127	G4128	S4129	M4130	N4131	P4132	I4133	E4074	R4134	E4135	V4136	D4137	L4138	Y4142	L4143	P4146	D4147	G4148	L4149		
G4219	E4220	H4221	R4222	S4223	V4224	L4225	W4226	S4227	E4228	N4229	L4230	G4231	W4232	P4233	M4234	L4236	S4237	I4238	D4239	Y4240	L4241	M4242	D4243	D4244	R4245	W4246	Y4247	W4248	S4249	D4250	S4251	K4252	E4253	D4254	V4255	L4256	E4257	A4258	Y4259	K4260	Y4261	D4262	G4263	T4264	K4265	R4266	R4267	L4268	K4269	I4270	N4271	E4272	A4273	M4274	K4275	P4276	F4277
A4150	V4151	D4152	W4153	S4154	G4155	R4156	H4157	L4158	Y4159	D4162	S4165	A4171	T4172	L4173	D4174	G4175	R4176	Y4177	R4178	K4179	W4180	L4181	Q4185	L4186	D4187	A4190	K4191	T4192	A4193	W4194	N4195	P4196	K4197	L4198	G4199	L4200	W4201	F4202	W4203	T4204	D4205	Q4206	G4207	K4208	Q4209	P4210	K4211	I4212	E4213	S4214	A4215	W4216	N4217	K4218			
E4081	E4082	E4083	E4084	H4085	I4086	Q4087	T4088	I4089	D4090	Y4091	D4092	W4093	D4094	P4095	H4097	I4098	G4099	L4100	S4101	V4102	W4103	Y4104	Y4105	T4106	L4108	A4116	I4117	K4118	R4119	A4120	Y4121	I4122	P4123	M4124	F4125	E4126	S4127	G4128	S4129	M4130	N4131	P4132	I4133	E4074	R4134	E4135	V4136	D4137	L4138	Y4142	L4143	P4146	D4147	G4148	L4149		
G4219	E4220	H4221	R4222	S4223	V4224	L4225	W4226	S4227	E4228	N4229	L4230	G4231	W4232	P4233	M4234	L4236	S4237	I4238	D4239	Y4240	L4241	M4242	D4243	D4244	R4245	W4246	Y4247	W4248	S4249	D4250	S4251	K4252	E4253	D4254	V4255	L4256	E4257	A4258	Y4259	K4260	Y4261	D4262	G4263	T4264	K4265	R4266	R4267	L4268	K4269	I4270	N4271	E4272	A4273	M4274	K4275	P4276	F4277
A4150	V4151	D4152	W4153	S4154	G4155	R4156	H4157	L4158	Y4159	D4162	S4165	A4171	T4172	L4173	D4174	G4175	R4176	Y4177	R4178	K4179	W4180	L4181	Q4185	L4186	D4187	A4190	K4191	T4192	A4193	W4194	N4195	P4196	K4197	L4198	G4199	L4200	W4201	F4202	W4203	T4204	D4205	Q4206	G4207	K4208	Q4209	P4210	K4211	I4212	E4213	S4214	A4215	W4216	N4217	K4218			
E4081	E4082	E4083	E4084	H4085	I4086	Q4087	T4088	I4089	D4090	Y4091	D4092	W4093	D4094	P4095	H4097	I4098	G4099	L4100	S4101	V4102	W4103	Y4104	Y4105	T4106	L4108	A4116	I4117	K4118	R4119	A4120	Y4121	I4122	P4123	M4124	F4125	E4126	S4127	G4128	S4129	M4130	N4131	P4132	I4133	E4074	R4134	E4135	V4136	D4137	L4138	Y4142	L4143	P4146	D4147	G4148	L4149		



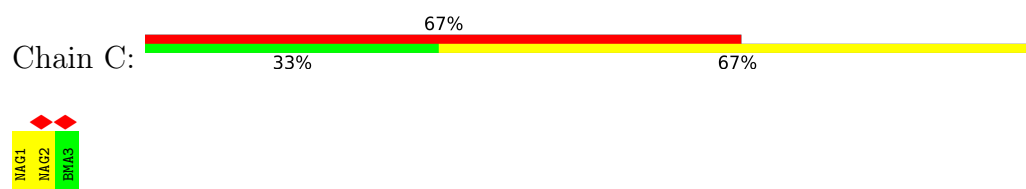




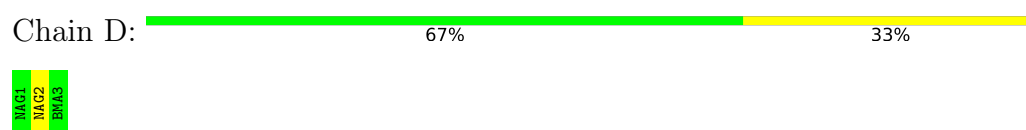
- Molecule 2: ligand



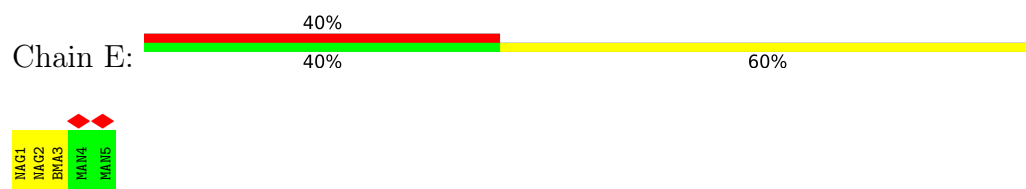
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



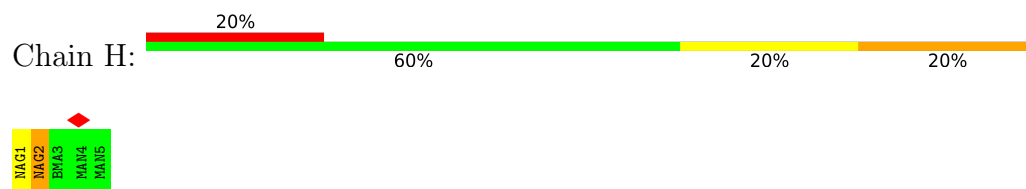
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



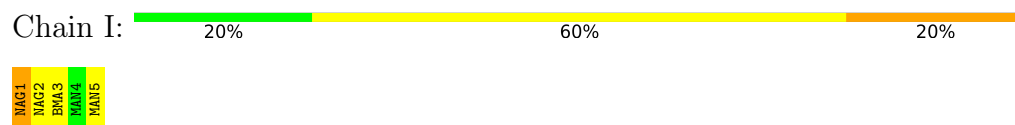
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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

Chain F:  100%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.411, 1.411, 1.411	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, MAN, A2G, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2981	0.49	0/4047
1	B	0.26	0/8659	0.53	0/11737
2	O	0.20	0/7	0.51	0/8
All	All	0.25	0/11647	0.52	0/15792

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2904	0	2797	27	0
1	B	8455	0	7529	120	0
2	O	28	0	12	1	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
4	E	61	0	52	1	0
4	H	61	0	52	1	0
4	I	61	0	52	1	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	26	1	0
7	B	70	0	60	11	0
8	B	20	0	0	0	0
All	All	11822	0	10698	149	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 7.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:THR:OG1	7:B:4703:A2G:C1	1.90	1.19
1:B:3799:THR:OG1	7:B:4706:A2G:C1	1.92	1.18
1:B:1225:THR:CB	7:B:4703:A2G:C1	2.26	1.12
1:B:1225:THR:HB	7:B:4703:A2G:C1	1.83	1.08
1:B:3799:THR:CB	7:B:4706:A2G:C1	2.36	1.03
1:B:3799:THR:HB	7:B:4706:A2G:C1	2.02	0.89
1:B:1225:THR:HB	7:B:4703:A2G:O5	1.83	0.79
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.46	0.78
1:B:3146:MET:SD	1:B:3151:SER:HB3	2.27	0.74
1:B:3009:ARG:HG2	1:B:3011:SER:H	1.56	0.70
1:B:3082:PHE:N	1:B:3090:ILE:O	2.24	0.70
1:B:3123:ARG:HG2	1:B:3150:ARG:HH11	1.58	0.69
1:B:3790:SER:OG	1:B:3793:ARG:NH2	2.26	0.68
1:B:3082:PHE:HB2	1:B:3092:MET:HG3	1.75	0.66
1:B:3799:THR:HB	7:B:4706:A2G:O5	1.95	0.66
1:A:4129:SER:O	1:A:4130:ASN:ND2	2.30	0.64
1:B:3425:THR:HG22	1:B:3432:VAL:HG22	1.80	0.64
1:B:3270:ARG:HH12	1:B:3597:GLU:HG2	1.63	0.63
1:B:3366:ILE:HD11	1:B:3369:PRO:HB3	1.80	0.62
1:B:3799:THR:HB	7:B:4706:A2G:C5	2.30	0.62
1:B:3867:ASN:ND2	1:B:3869:CYS:O	2.33	0.61
1:A:4310:VAL:HG12	1:A:4311:LEU:HG	1.80	0.61
1:A:4179:LYS:HA	1:A:4357:GLN:HB2	1.83	0.59
1:B:3123:ARG:HG2	1:B:3150:ARG:NH1	2.16	0.59
1:B:1225:THR:HG1	7:B:4703:A2G:C1	2.14	0.59
1:B:3210:TYR:OH	1:B:3764:SER:N	2.33	0.59
1:B:3283:SER:HB3	1:B:3484:ILE:HD11	1.84	0.58
1:B:3146:MET:O	1:B:3149:LYS:NZ	2.37	0.58
1:B:3605:ASN:ND2	1:B:3623:ASP:OD2	2.36	0.58
1:B:3025:ASP:OD1	1:B:3025:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3805:PHE:N	1:B:3813:VAL:O	2.37	0.57
1:A:4289:VAL:HG11	1:A:4317:LEU:HD22	1.88	0.56
1:B:3096:CYS:HA	1:B:3108:GLU:HG3	1.87	0.56
1:B:3849:PHE:O	1:B:3856:CYS:HB2	2.06	0.56
1:B:3074:GLU:OE1	1:B:3083:ARG:NH2	2.39	0.55
1:B:1254:HIS:N	1:B:1263:GLU:OE2	2.40	0.54
1:B:3122:SER:O	1:B:3123:ARG:C	2.46	0.54
1:B:3289:LEU:HD21	1:B:3339:TRP:HB2	1.88	0.54
1:A:4093:TRP:CE2	1:A:4325:GLN:HB3	2.43	0.53
1:B:3600:GLU:HB2	1:B:3609:ILE:O	2.09	0.53
1:B:3862:ILE:HG22	1:B:3863:CYS:SG	2.49	0.53
1:B:3038:GLN:HG2	1:B:3046:CYS:HB3	1.91	0.52
1:B:3083:ARG:HA	1:B:3089:CYS:HB3	1.92	0.52
4:I:1:NAG:H62	4:I:2:NAG:C7	2.40	0.52
1:B:1225:THR:CB	7:B:4703:A2G:O5	2.51	0.52
1:B:3238:ARG:NH1	1:B:3464:GLN:O	2.42	0.52
1:B:3671:ASP:N	1:B:3671:ASP:OD1	2.43	0.51
1:B:3805:PHE:HE2	1:B:3830:ASP:HA	1.75	0.51
1:B:3150:ARG:O	1:B:3151:SER:HB2	2.10	0.51
1:B:3015:ASP:N	1:B:3026:GLU:OE1	2.42	0.51
1:B:3039:PHE:HD2	1:B:3047:ILE:HD11	1.76	0.51
1:B:3123:ARG:CG	1:B:3150:ARG:HH11	2.24	0.51
1:B:3791:ASP:OD1	1:B:3791:ASP:N	2.37	0.51
1:B:3901:GLY:O	1:B:3904:LEU:HD22	2.10	0.51
1:B:3344:VAL:HG11	1:B:3653:SER:HB2	1.92	0.51
1:B:3016:ARG:NH2	1:B:3044:GLY:O	2.44	0.50
1:B:2965:ARG:HH12	1:B:2966:ARG:NH2	2.09	0.50
1:B:3870:VAL:O	1:B:3871:ASP:C	2.48	0.50
1:A:4085:HIS:O	1:A:4108:LEU:N	2.38	0.50
1:B:3203:LEU:HD22	1:B:3456:ILE:HD11	1.94	0.50
1:B:3662:CYS:SG	1:B:3667:ASP:HB3	2.52	0.50
1:B:3842:THR:OG1	1:B:3843:TYR:N	2.46	0.49
1:B:3079:LEU:HD22	1:B:3080:HIS:H	1.77	0.48
1:B:3505:ARG:HH11	1:B:3506:ASP:H	1.59	0.48
1:A:4148:GLY:HA3	1:A:4191:ALA:HA	1.95	0.48
1:B:3448:ASN:OD1	6:B:4701:NAG:N2	2.47	0.48
1:A:4384:ARG:HB3	1:A:4411:TYR:CD1	2.49	0.48
1:B:3000:PHE:N	1:B:3008:VAL:O	2.47	0.48
1:B:3207:ASN:HB2	1:B:3210:TYR:HB2	1.94	0.48
1:A:4087:GLN:HB2	1:A:4108:LEU:HD13	1.95	0.48
1:A:4162:ASP:HB3	1:A:4165:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3016:ARG:N	1:B:3026:GLU:OE1	2.42	0.47
1:B:3326:ARG:HH12	2:O:3:ASN:HB3	1.77	0.47
1:B:3621:CYS:SG	1:B:3626:ASP:HB3	2.55	0.47
1:B:3658:VAL:HG23	1:B:3693:ARG:HB3	1.96	0.47
1:B:3135:PHE:HZ	1:B:3150:ARG:NH2	2.12	0.47
1:B:2936:MET:SD	1:B:2940:ASP:HB3	2.55	0.47
1:B:3736:PRO:HD2	1:B:3739:TRP:CE3	2.49	0.47
1:B:3416:THR:HG21	1:B:3457:HIS:HA	1.96	0.46
1:B:3258:LEU:HA	1:B:3258:LEU:HD23	1.67	0.46
1:B:3083:ARG:HG2	1:B:3083:ARG:HH11	1.81	0.46
1:B:1247:ASN:O	1:B:1250:GLU:HG3	2.16	0.46
1:B:2969:PRO:HD2	1:B:2972:TRP:HE1	1.80	0.46
1:B:3291:ALA:HA	1:B:3325:PRO:HD2	1.97	0.46
1:A:4061:PRO:HG3	1:A:4089:ILE:HG12	1.98	0.46
1:B:3009:ARG:HE	1:B:3009:ARG:H	1.64	0.46
1:B:3720:PRO:HA	1:B:3728:ARG:HH12	1.79	0.46
1:B:3131:THR:N	1:B:3134:SER:O	2.40	0.46
1:A:4086:ILE:HG22	1:A:4107:VAL:HG12	1.98	0.46
1:B:2993:ARG:HG3	1:B:2995:CYS:H	1.80	0.46
1:B:3296:LEU:HD22	1:B:3309:ILE:HD11	1.97	0.46
1:B:3840:ASN:OD1	1:B:3842:THR:HG22	2.17	0.45
1:B:3659:ASP:OD2	1:B:3708:ARG:NE	2.50	0.45
1:B:3170:GLU:HB3	1:B:3177:ILE:HG23	1.98	0.45
1:B:3670:ILE:HA	1:B:3673:CYS:HB2	1.99	0.45
1:B:3123:ARG:HG3	1:B:3123:ARG:O	2.17	0.44
1:B:3885:CYS:HB3	1:B:3898:CYS:HB3	1.81	0.44
1:B:2917:ASN:N	1:B:2935:ASP:OD2	2.40	0.44
1:B:3112:GLY:O	1:B:3114:ASN:N	2.44	0.44
1:A:4218:ASN:ND2	1:A:4220:GLU:OE2	2.36	0.44
1:A:4108:LEU:HD12	1:A:4146:PRO:HD2	1.98	0.44
1:B:3351:ILE:HD12	1:B:3358:LYS:HB3	1.99	0.44
1:A:4102:VAL:HG22	1:A:4121:TYR:CE1	2.52	0.44
1:B:3081:GLN:N	1:B:3092:MET:SD	2.92	0.43
1:B:3799:THR:HG22	1:B:3800:CYS:N	2.33	0.43
1:A:4121:TYR:OH	1:A:4379:MET:SD	2.76	0.43
1:B:3421:THR:HG21	1:B:3434:LYS:HD2	2.00	0.43
1:B:3891:PHE:HE1	1:B:3921:HIS:HD1	1.67	0.43
1:B:2988:GLN:NE2	1:B:2989:ASN:OD1	2.46	0.43
1:A:4213:GLU:HG2	1:A:4224:VAL:HG22	2.01	0.43
1:B:3049:ARG:HD3	1:B:3049:ARG:O	2.19	0.43
1:B:3013:ARG:HG2	1:B:3014:CYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3417:ILE:HD12	1:B:3417:ILE:N	2.34	0.43
1:A:4123:PRO:HB3	1:A:4125:PHE:CZ	2.54	0.43
1:B:3091:GLU:OE1	1:B:3093:GLY:N	2.47	0.43
4:H:1:NAG:O6	4:H:2:NAG:N2	2.52	0.43
1:B:3126:HIS:ND1	1:B:3152:CYS:HB2	2.34	0.42
1:B:1248:THR:HG23	1:B:1249:TRP:HD1	1.83	0.42
1:B:3149:LYS:HA	1:B:3149:LYS:HD3	1.94	0.42
1:B:3556:ARG:CG	1:B:3822:ARG:HH12	2.32	0.42
1:B:3269:HIS:CE1	1:B:3270:ARG:HG3	2.54	0.42
1:B:3918:LYS:HG2	1:B:3919:GLU:H	1.85	0.42
1:B:3013:ARG:HG2	1:B:3014:CYS:SG	2.60	0.42
1:B:3245:TRP:CE2	1:B:3254:GLU:HB2	2.55	0.42
1:B:3744:THR:OG1	1:B:3746:ASP:OD1	2.36	0.42
1:B:3805:PHE:CE2	1:B:3830:ASP:HA	2.55	0.42
1:A:4084:GLU:OE2	1:A:4085:HIS:HB2	2.20	0.41
1:A:4096:GLU:OE2	1:A:4121:TYR:OH	2.26	0.41
1:A:4299:GLN:NE2	1:A:4305:GLU:O	2.38	0.41
1:B:3556:ARG:HE	1:B:3822:ARG:HH12	1.68	0.41
1:A:4116:ALA:HA	1:A:4143:LEU:HD12	2.02	0.41
1:B:3213:ASN:HB2	1:B:3224:ILE:HG13	2.02	0.41
1:A:4259:ILE:HD12	1:A:4266:ARG:HB2	2.02	0.41
1:B:2958:VAL:HA	1:B:2966:ARG:HD2	2.01	0.41
1:B:3132:ILE:HG23	1:B:3133:THR:HG23	2.01	0.41
1:B:3392:GLU:OE1	1:B:3401:ARG:NH2	2.49	0.41
1:A:4142:TYR:HB3	1:B:3793:ARG:HG2	2.02	0.41
1:A:4375:LEU:H	1:A:4375:LEU:HD23	1.85	0.41
1:B:3618:VAL:N	1:B:3627:GLU:OE2	2.54	0.41
1:B:3861:TRP:HB3	1:B:3868:ASP:OD2	2.20	0.41
1:B:3083:ARG:HG2	1:B:3083:ARG:NH1	2.36	0.41
1:A:4238:ILE:HG12	1:A:4246:VAL:HG23	2.03	0.40
1:B:3122:SER:HA	1:B:3150:ARG:CZ	2.50	0.40
1:A:4215:ALA:HB2	1:A:4222:ARG:HA	2.03	0.40
1:B:3000:PHE:HD2	1:B:3013:ARG:NH2	2.19	0.40
1:B:3139:CYS:SG	1:B:3145:LEU:HD22	2.61	0.40
1:B:3505:ARG:H	1:B:3505:ARG:HD3	1.86	0.40
1:B:3761:CYS:HB3	1:B:3765:GLU:HB2	2.04	0.40
1:B:3887:SER:OG	1:B:3888:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	359/4660 (8%)	334 (93%)	25 (7%)	0	100	100
1	B	1073/4660 (23%)	985 (92%)	87 (8%)	1 (0%)	48	79
2	O	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1433/9325 (15%)	1320 (92%)	112 (8%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3123	ARG

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	320/4089 (8%)	309 (97%)	11 (3%)	32	55
1	B	965/4089 (24%)	928 (96%)	37 (4%)	28	52
2	O	1/1 (100%)	1 (100%)	0	100	100
All	All	1286/8179 (16%)	1238 (96%)	48 (4%)	31	53

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4062	GLU
1	A	4075	LYS

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Mol	Chain	Res	Type
1	A	4083	GLU
1	A	4085	HIS
1	A	4090	ASP
1	A	4147	ASP
1	A	4194	VAL
1	A	4217	MET
1	A	4359	SER
1	A	4375	LEU
1	A	4387	HIS
1	B	1233	LEU
1	B	1270	LYS
1	B	1271	THR
1	B	2938	ASP
1	B	2959	ASN
1	B	2972	TRP
1	B	3006	ARG
1	B	3009	ARG
1	B	3017	ARG
1	B	3031	TYR
1	B	3035	HIS
1	B	3038	GLN
1	B	3092	MET
1	B	3107	ASP
1	B	3118	ASP
1	B	3146	MET
1	B	3168	LYS
1	B	3235	ASP
1	B	3290	ASP
1	B	3315	ASP
1	B	3317	ASN
1	B	3373	THR
1	B	3426	ASP
1	B	3467	MET
1	B	3505	ARG
1	B	3515	SER
1	B	3534	CYS
1	B	3693	ARG
1	B	3708	ARG
1	B	3791	ASP
1	B	3797	MET
1	B	3822	ARG
1	B	3844	CYS

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Mol	Chain	Res	Type
1	B	3852	LYS
1	B	3894	ASP
1	B	3897	ARG
1	B	3904	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3057	ASN
1	B	3066	GLN
1	B	3602	GLN
1	B	3733	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

25 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	C	1	1,3	14,14,15	0.44	0	17,19,21	2.39	3 (17%)
3	NAG	C	2	3	14,14,15	0.52	0	17,19,21	1.15	1 (5%)
3	BMA	C	3	3	11,11,12	0.24	0	15,15,17	0.82	0
3	NAG	D	1	1,3	14,14,15	0.37	0	17,19,21	0.87	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	3	3	11,11,12	0.25	0	15,15,17	0.83	0
4	NAG	E	1	4,1	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.79	0
4	BMA	E	3	4	11,11,12	0.26	0	15,15,17	1.15	2 (13%)
4	MAN	E	4	4	11,11,12	0.22	0	15,15,17	0.62	0
4	MAN	E	5	4	11,11,12	0.25	0	15,15,17	0.64	0
5	NAG	F	1	1,5	14,14,15	0.36	0	17,19,21	1.12	1 (5%)
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	1.16	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	1.42	1 (5%)
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.34	0	17,19,21	0.65	0
4	NAG	H	2	4	14,14,15	0.31	0	17,19,21	0.98	1 (5%)
4	BMA	H	3	4	11,11,12	0.29	0	15,15,17	0.82	0
4	MAN	H	4	4	11,11,12	0.25	0	15,15,17	0.70	0
4	MAN	H	5	4	11,11,12	0.23	0	15,15,17	0.67	0
4	NAG	I	1	4,1	14,14,15	0.35	0	17,19,21	1.10	2 (11%)
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.59	0
4	BMA	I	3	4	11,11,12	0.26	0	15,15,17	1.08	2 (13%)
4	MAN	I	4	4	11,11,12	0.23	0	15,15,17	0.65	0
4	MAN	I	5	4	11,11,12	0.41	0	15,15,17	1.18	2 (13%)

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

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

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	8.04	123.08	112.19
5	G	1	NAG	C1-O5-C5	5.08	119.08	112.19
3	C	1	NAG	O4-C4-C5	-4.15	98.99	109.30
4	I	1	NAG	C1-O5-C5	3.53	116.98	112.19
3	C	2	NAG	C1-O5-C5	3.07	116.35	112.19
3	D	2	NAG	O5-C1-C2	-2.96	106.61	111.29
4	I	5	MAN	C1-C2-C3	2.85	113.16	109.67
5	F	2	NAG	O5-C1-C2	-2.72	107.00	111.29
4	E	3	BMA	C1-C2-C3	2.65	112.93	109.67
5	G	2	NAG	C1-O5-C5	2.61	115.73	112.19
5	F	1	NAG	C1-O5-C5	-2.55	108.74	112.19
3	C	1	NAG	C6-C5-C4	-2.41	107.35	113.00
4	I	3	BMA	C1-C2-C3	2.29	112.48	109.67
4	E	3	BMA	C1-O5-C5	2.26	115.25	112.19
4	I	3	BMA	O5-C5-C6	2.15	110.58	107.20
4	I	1	NAG	C1-C2-N2	-2.04	107.00	110.49
4	H	2	NAG	O5-C1-C2	-2.04	108.07	111.29
4	I	5	MAN	O5-C5-C6	2.02	110.36	107.20

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	I	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
4	I	1	NAG	C1-C2-N2-C7
3	C	1	NAG	O7-C7-N2-C2
4	I	3	BMA	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C1-C2-N2-C7
4	E	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C1-C2-N2-C7
5	F	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
4	H	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7
5	F	2	NAG	C8-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
4	I	2	NAG	O7-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
4	H	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 3 short contacts:

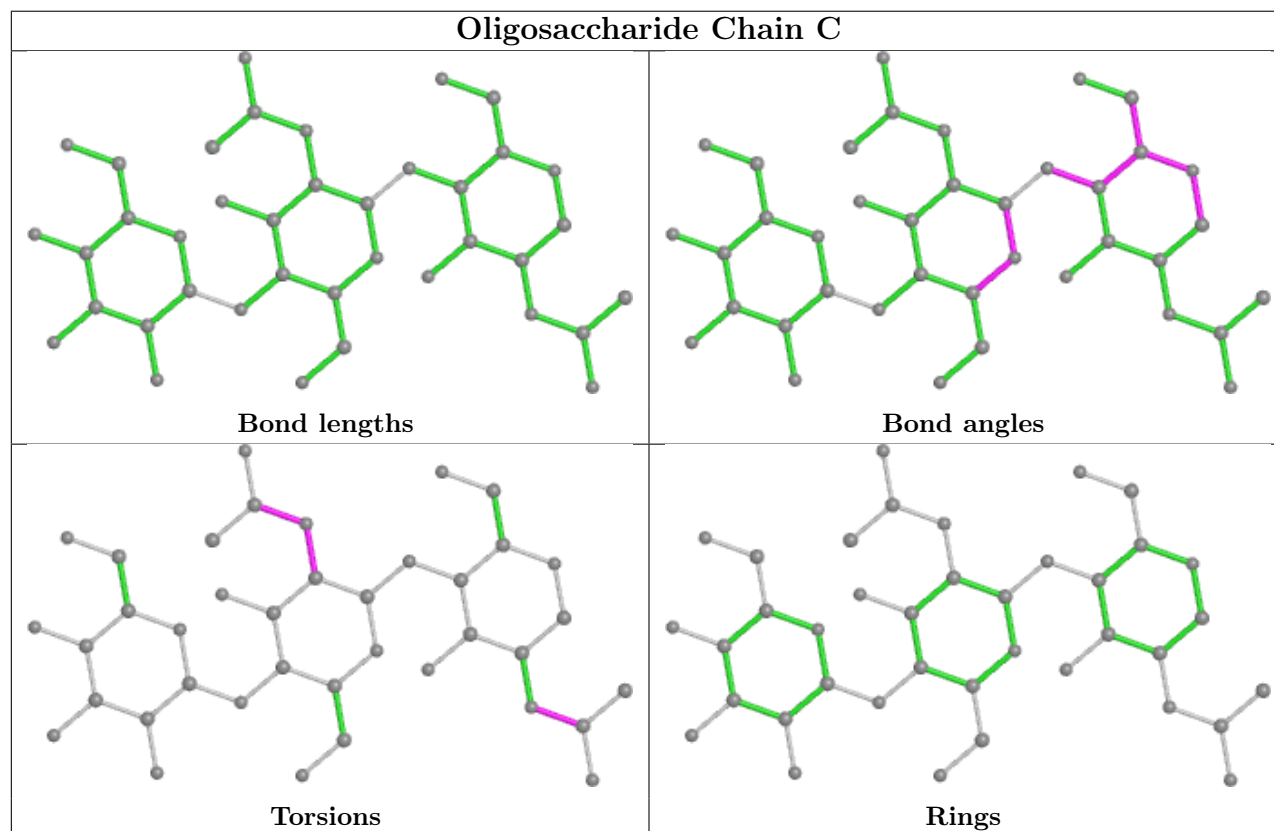
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	E	1	NAG	1	0

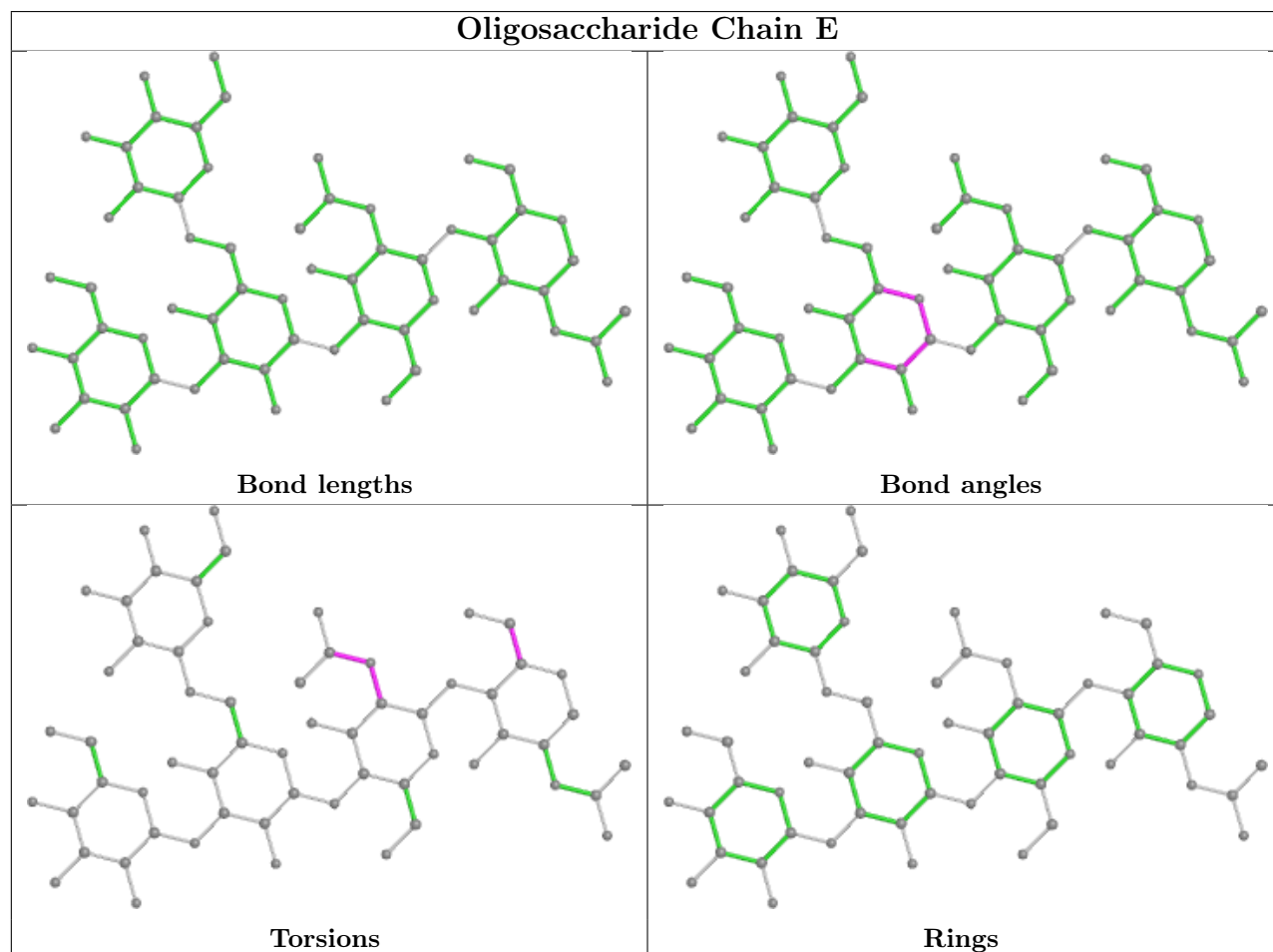
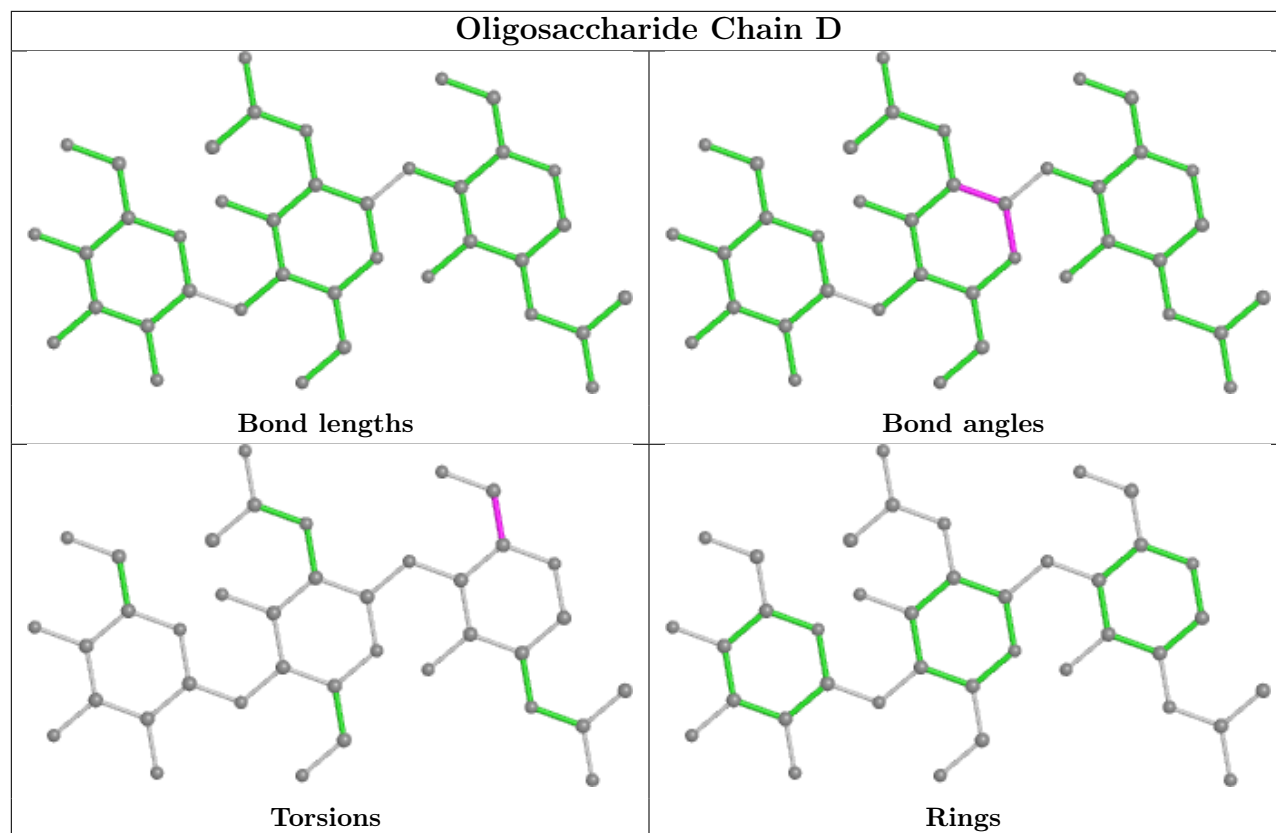
Continued on next page...

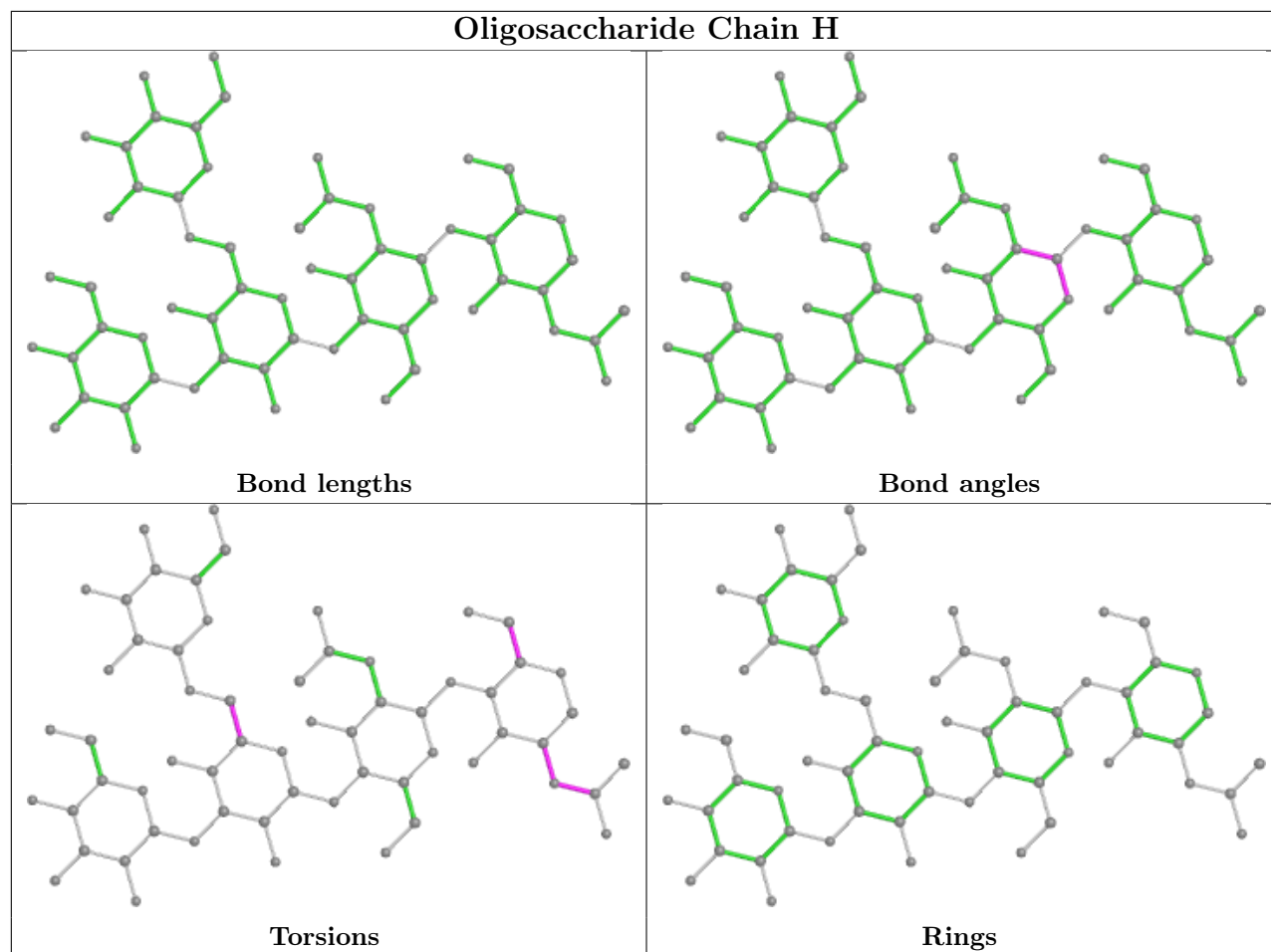
Continued from previous page...

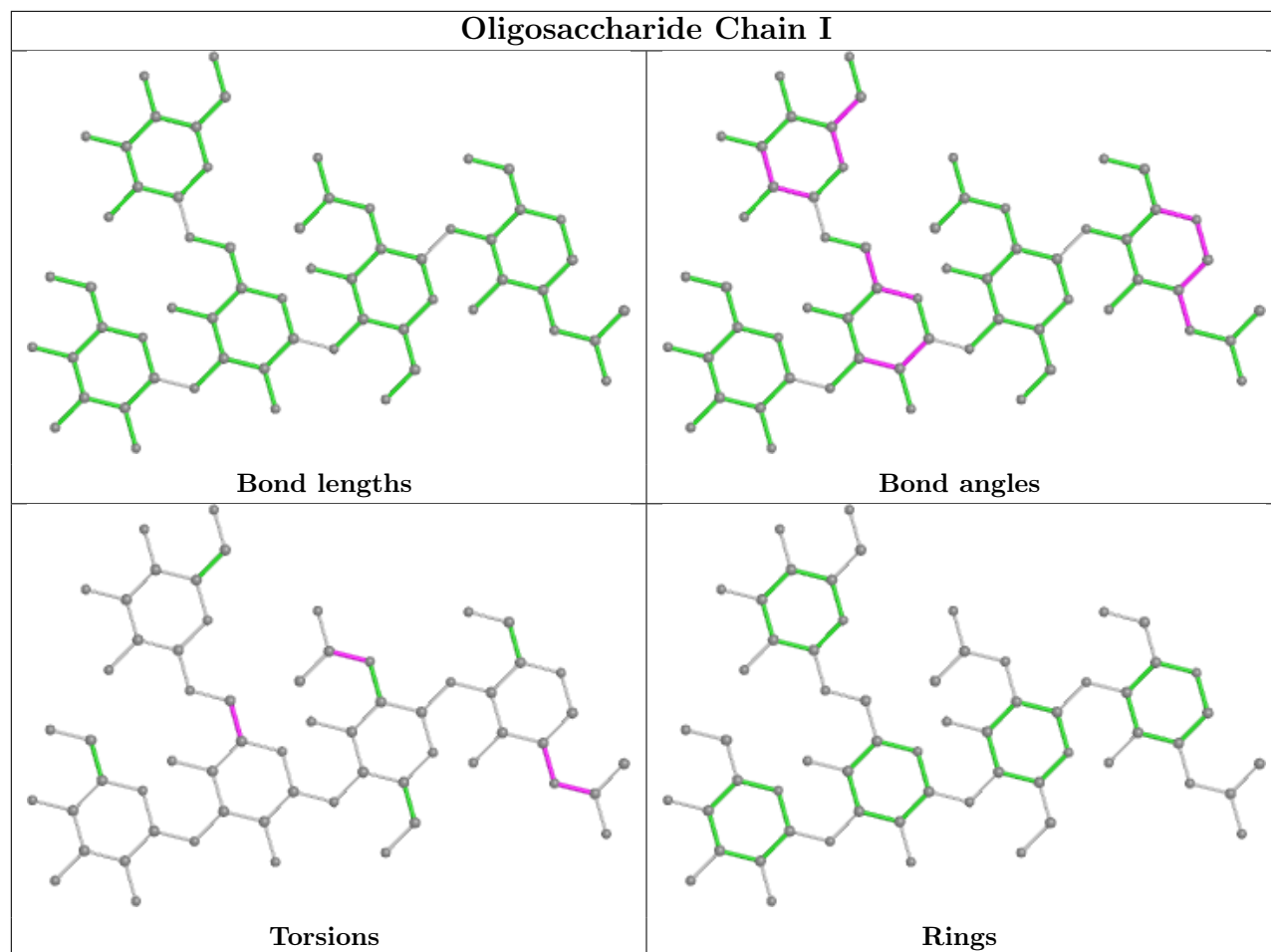
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
4	E	2	NAG	1	0
4	H	2	NAG	1	0
4	I	2	NAG	1	0

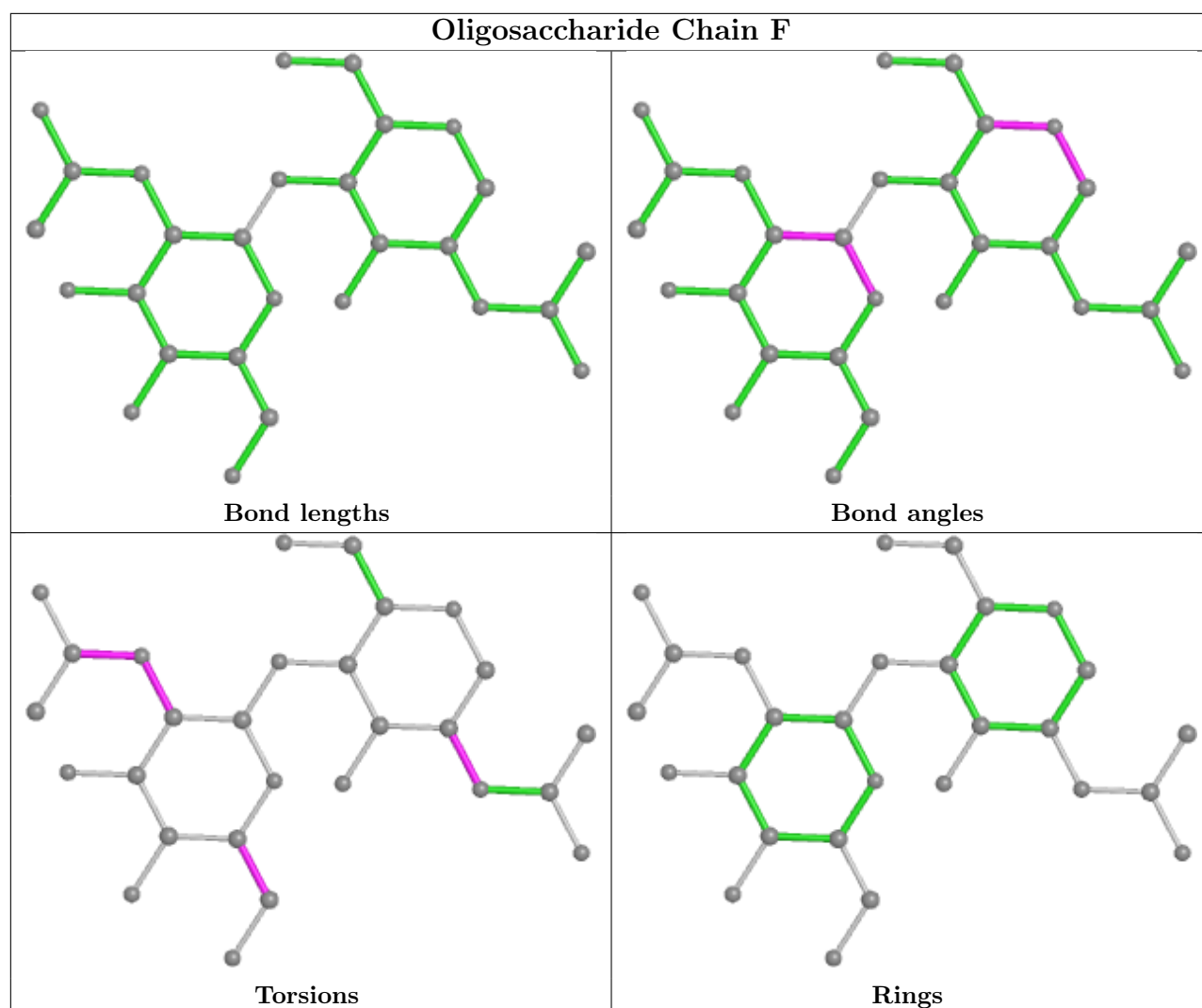
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

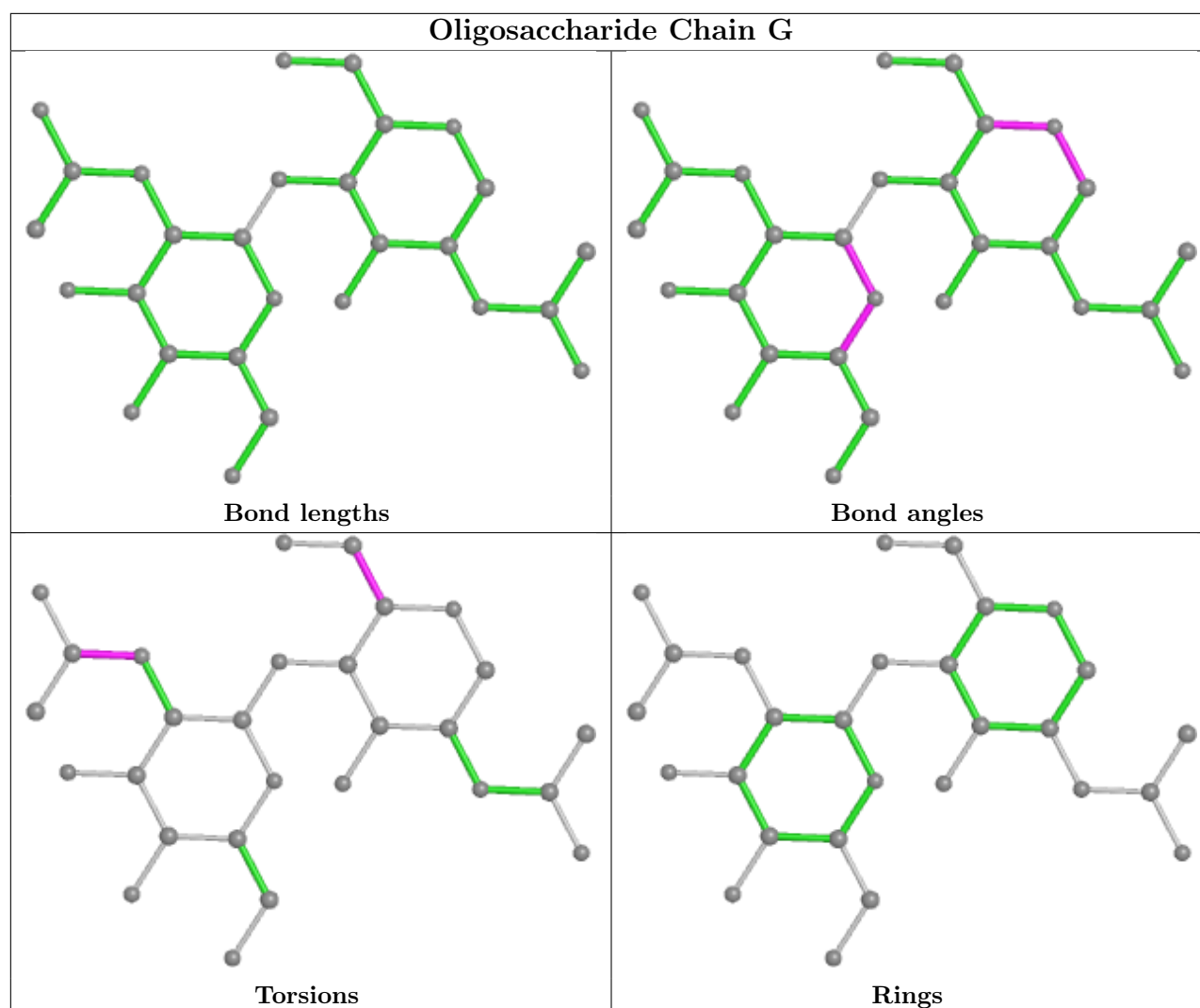












5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 20 are monoatomic - leaving 7 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	$\# Z > 2$
6	NAG	B	4702	1	14,14,15	0.33	0	17,19,21	0.74	1 (5%)
7	A2G	B	4705	1	14,14,15	0.42	0	17,19,21	0.67	1 (5%)
7	A2G	B	4707	1	14,14,15	0.40	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	4701	1	14,14,15	0.39	0	17,19,21	1.18	1 (5%)
7	A2G	B	4704	1	14,14,15	0.41	0	17,19,21	0.62	1 (5%)
7	A2G	B	4706	-	14,14,15	0.40	0	17,19,21	2.18	3 (17%)
7	A2G	B	4703	-	14,14,15	0.42	0	17,19,21	1.50	3 (17%)

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	B	4702	1	-	1/6/23/26	0/1/1/1
7	A2G	B	4705	1	-	0/6/23/26	0/1/1/1
7	A2G	B	4707	1	-	0/6/23/26	0/1/1/1
6	NAG	B	4701	1	-	4/6/23/26	0/1/1/1
7	A2G	B	4704	1	-	1/6/23/26	0/1/1/1
7	A2G	B	4706	-	-	0/6/23/26	0/1/1/1
7	A2G	B	4703	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4706	A2G	O5-C1-C2	7.90	123.76	111.29
7	B	4703	A2G	C1-C2-N2	4.68	118.48	110.49
6	B	4701	NAG	C1-O5-C5	3.70	117.20	112.19
7	B	4706	A2G	C1-O5-C5	3.50	116.93	112.19
7	B	4703	A2G	O5-C1-C2	2.88	115.83	111.29
7	B	4705	A2G	O5-C1-C2	-2.37	107.54	111.29
7	B	4703	A2G	C1-O5-C5	2.27	115.27	112.19
7	B	4704	A2G	O5-C1-C2	-2.22	107.79	111.29
7	B	4706	A2G	C1-C2-N2	2.11	114.10	110.49
6	B	4702	NAG	O5-C5-C6	2.07	110.44	107.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	4701	NAG	C3-C2-N2-C7
6	B	4701	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	B	4701	NAG	C8-C7-N2-C2
6	B	4702	NAG	O5-C5-C6-O6
7	B	4704	A2G	O5-C5-C6-O6
6	B	4701	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	4701	NAG	1	0
7	B	4706	A2G	5	0
7	B	4703	A2G	6	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.

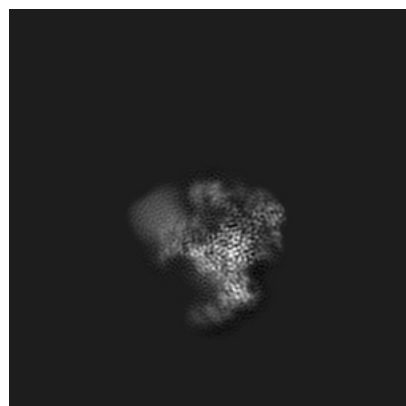
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36693. These allow visual inspection of the internal detail of the map and identification of artifacts.

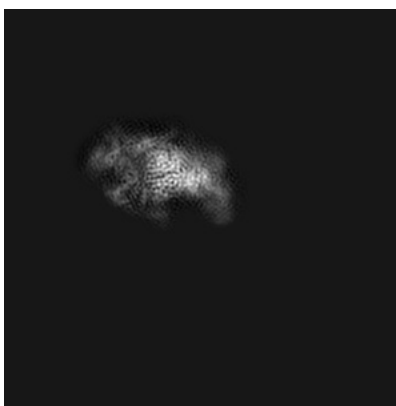
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

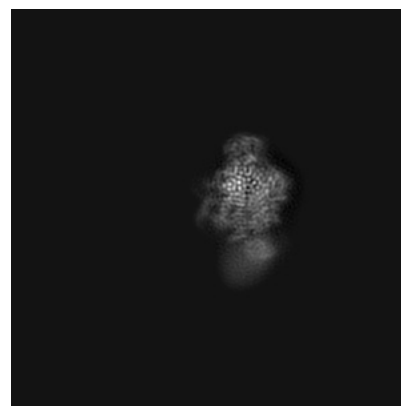
6.1.1 Primary map



X

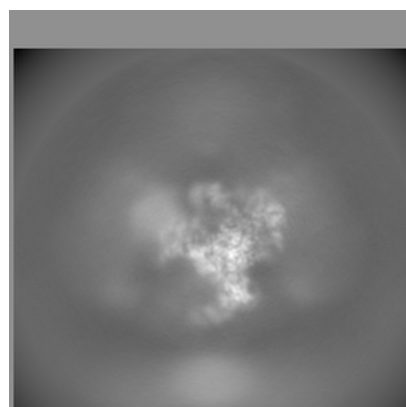


Y

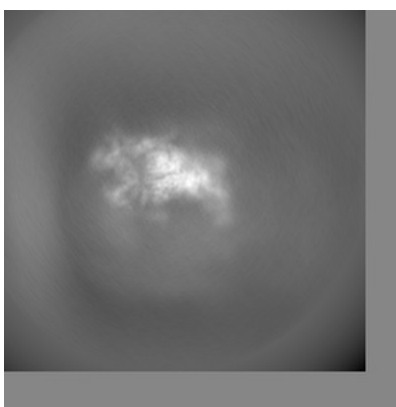


Z

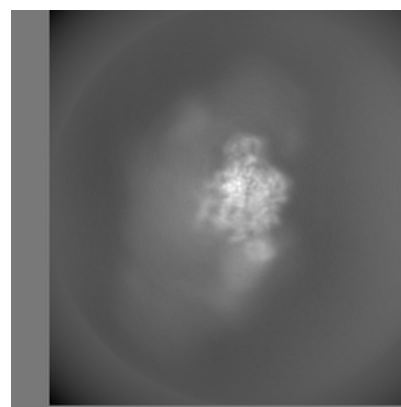
6.1.2 Raw map



X



Y

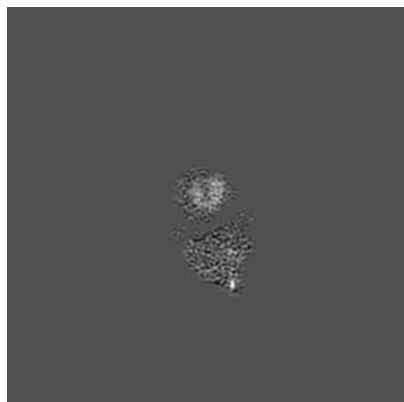


Z

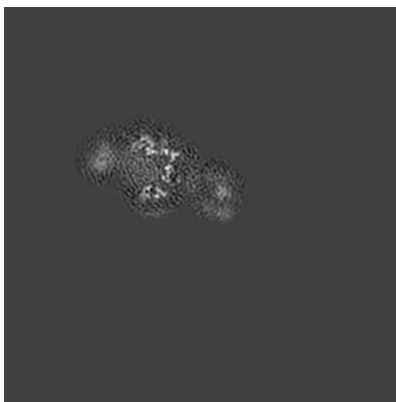
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 130

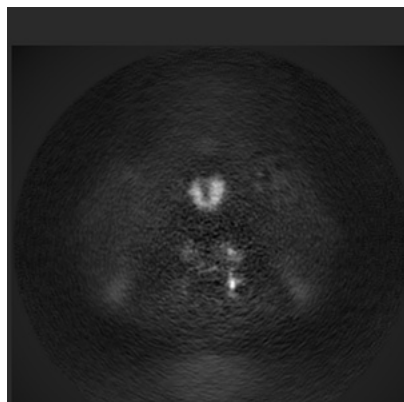


Y Index: 130

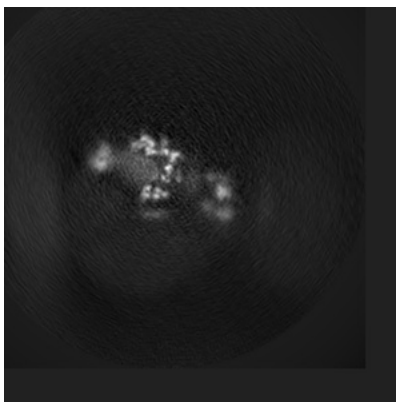


Z Index: 130

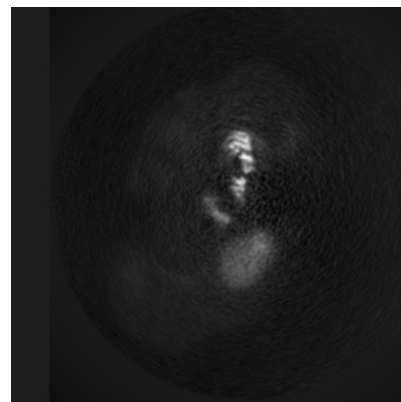
6.2.2 Raw map



X Index: 130



Y Index: 130

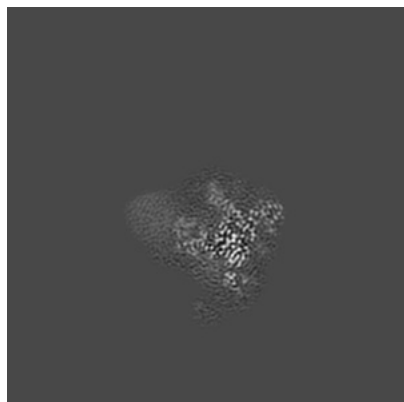


Z Index: 130

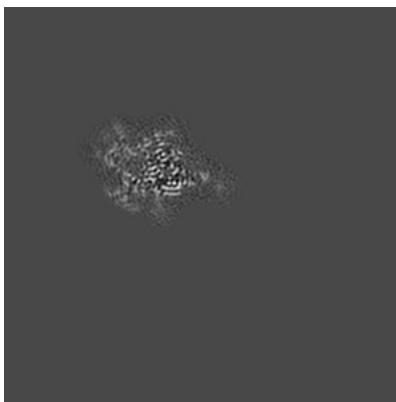
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

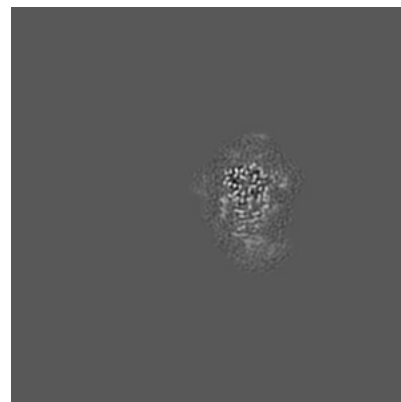
6.3.1 Primary map



X Index: 148

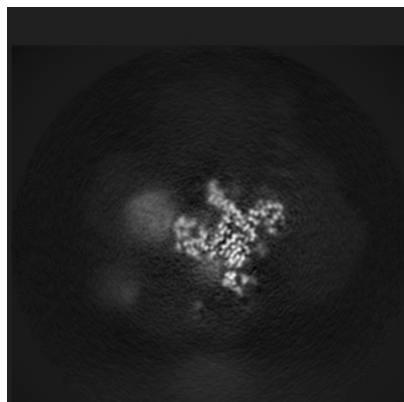


Y Index: 145

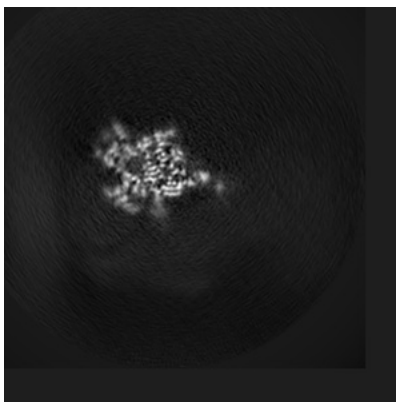


Z Index: 105

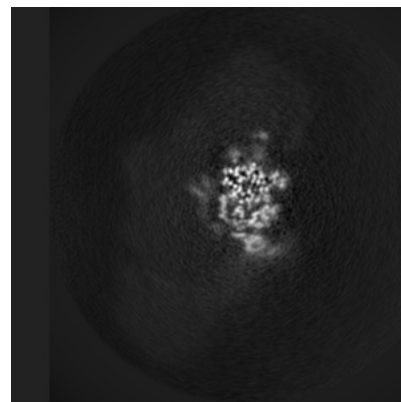
6.3.2 Raw map



X Index: 148



Y Index: 145

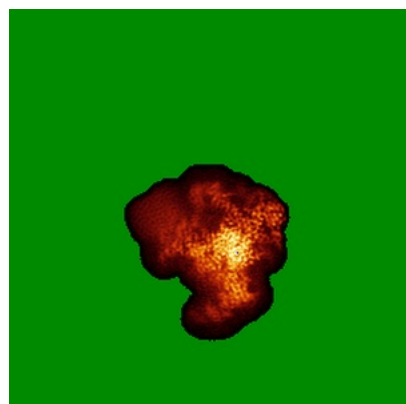


Z Index: 104

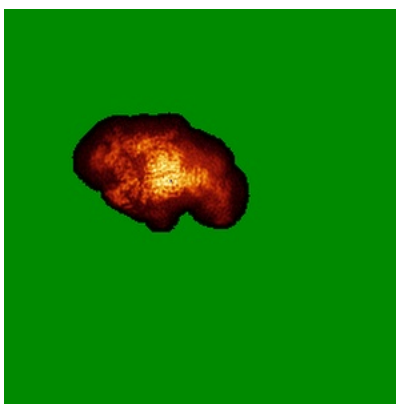
The images above show the largest variance slices of the map in three orthogonal directions.

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

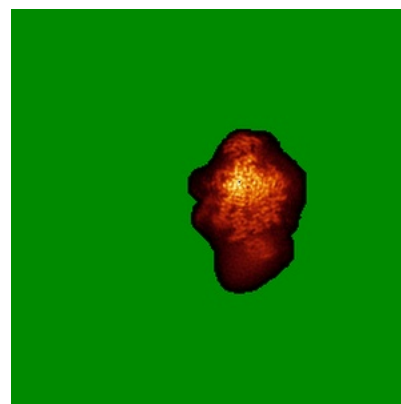
6.4.1 Primary map



X

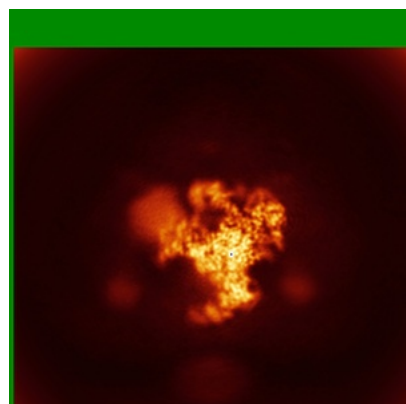


Y

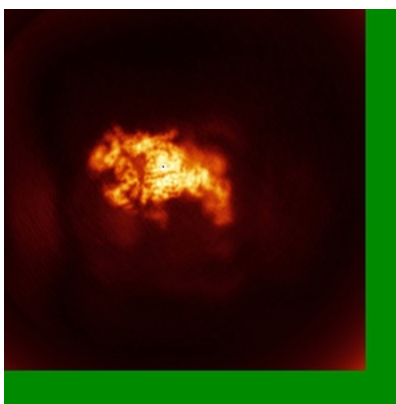


Z

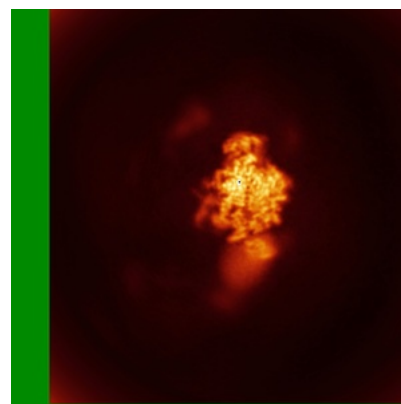
6.4.2 Raw map



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.

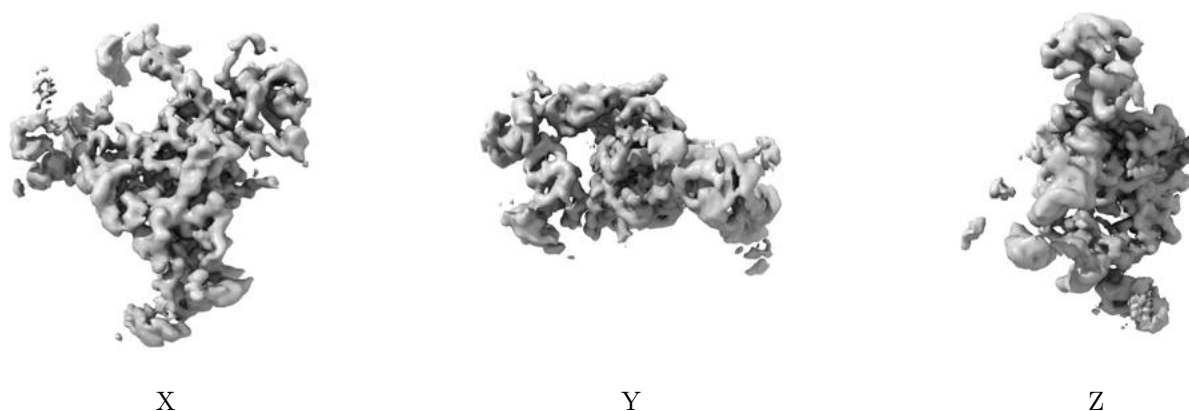
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

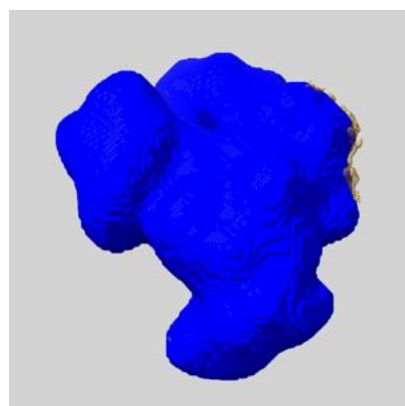
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

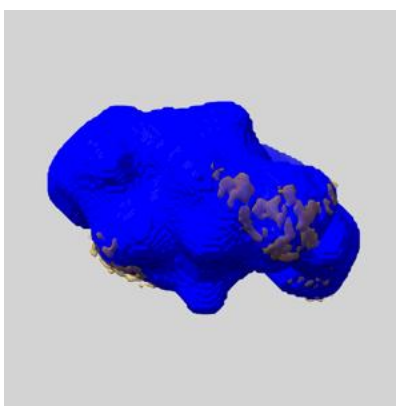
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

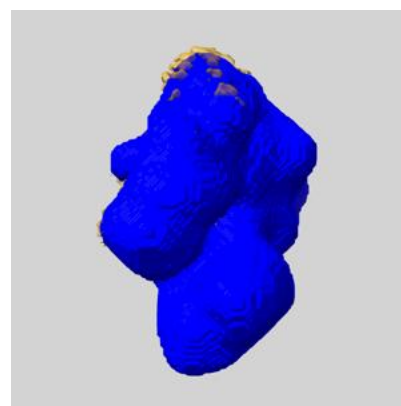
6.6.1 emd_36693_msk_1.map [i](#)



X



Y

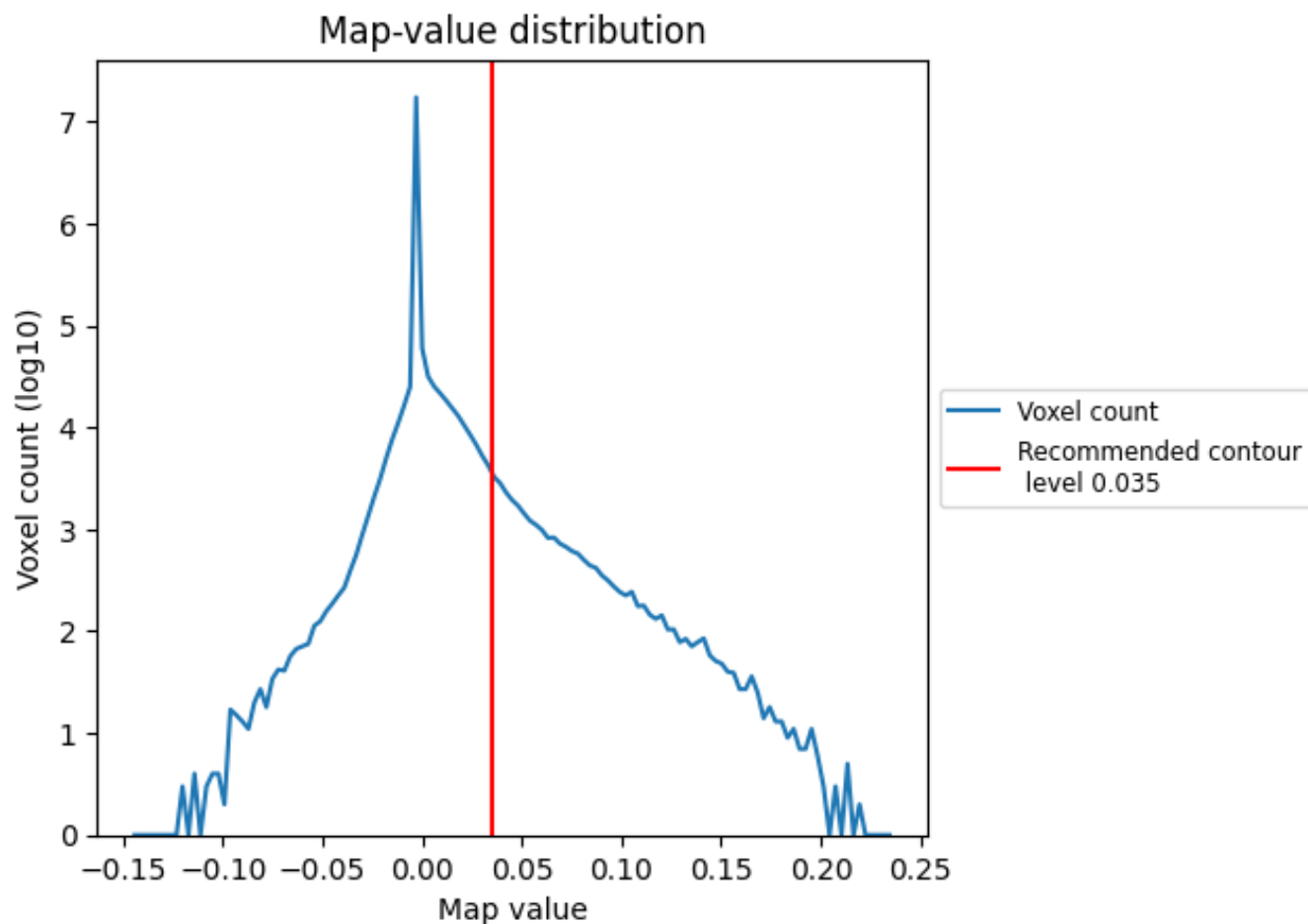


Z

7 Map analysis [i](#)

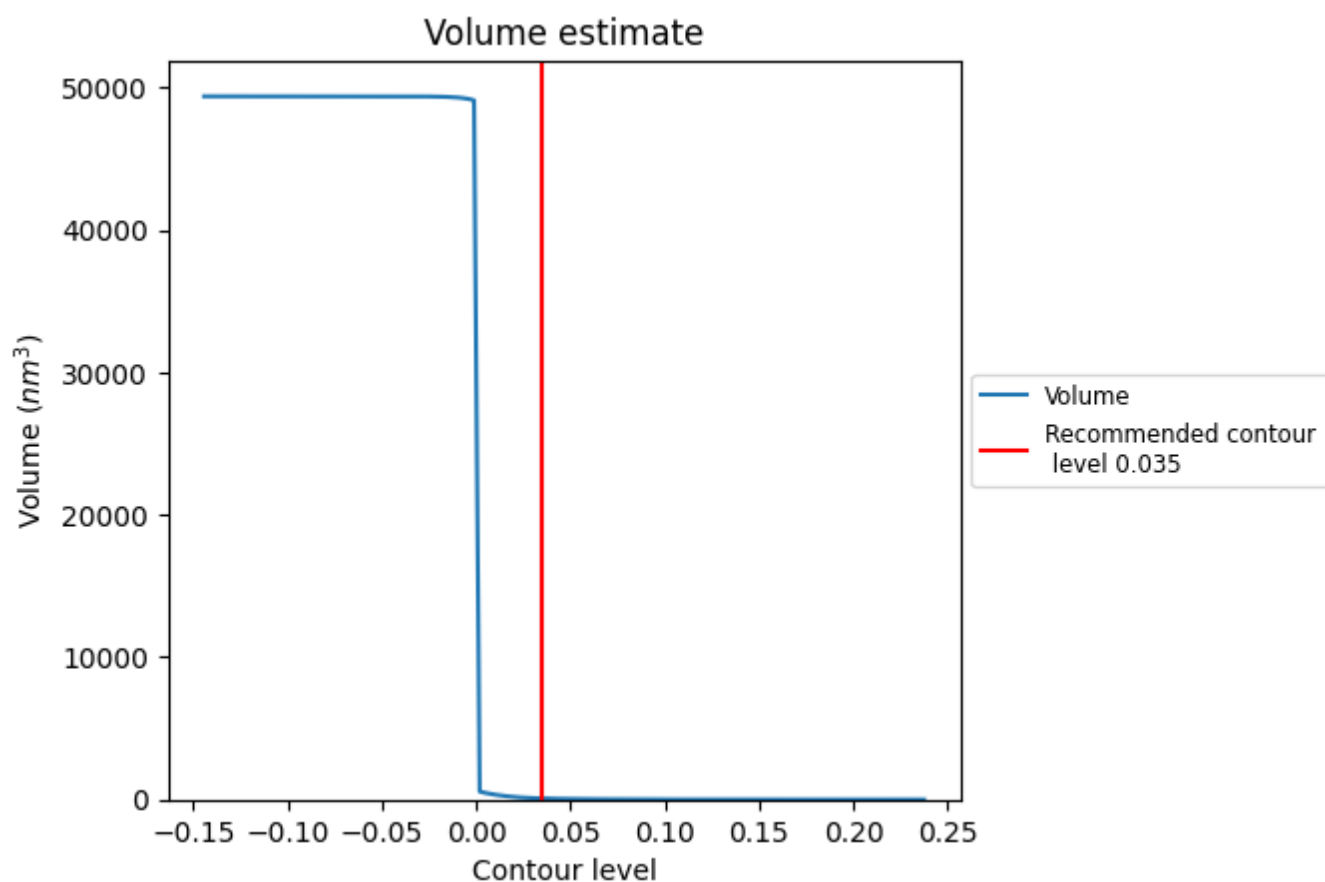
This section contains the results of statistical analysis of the map.

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.

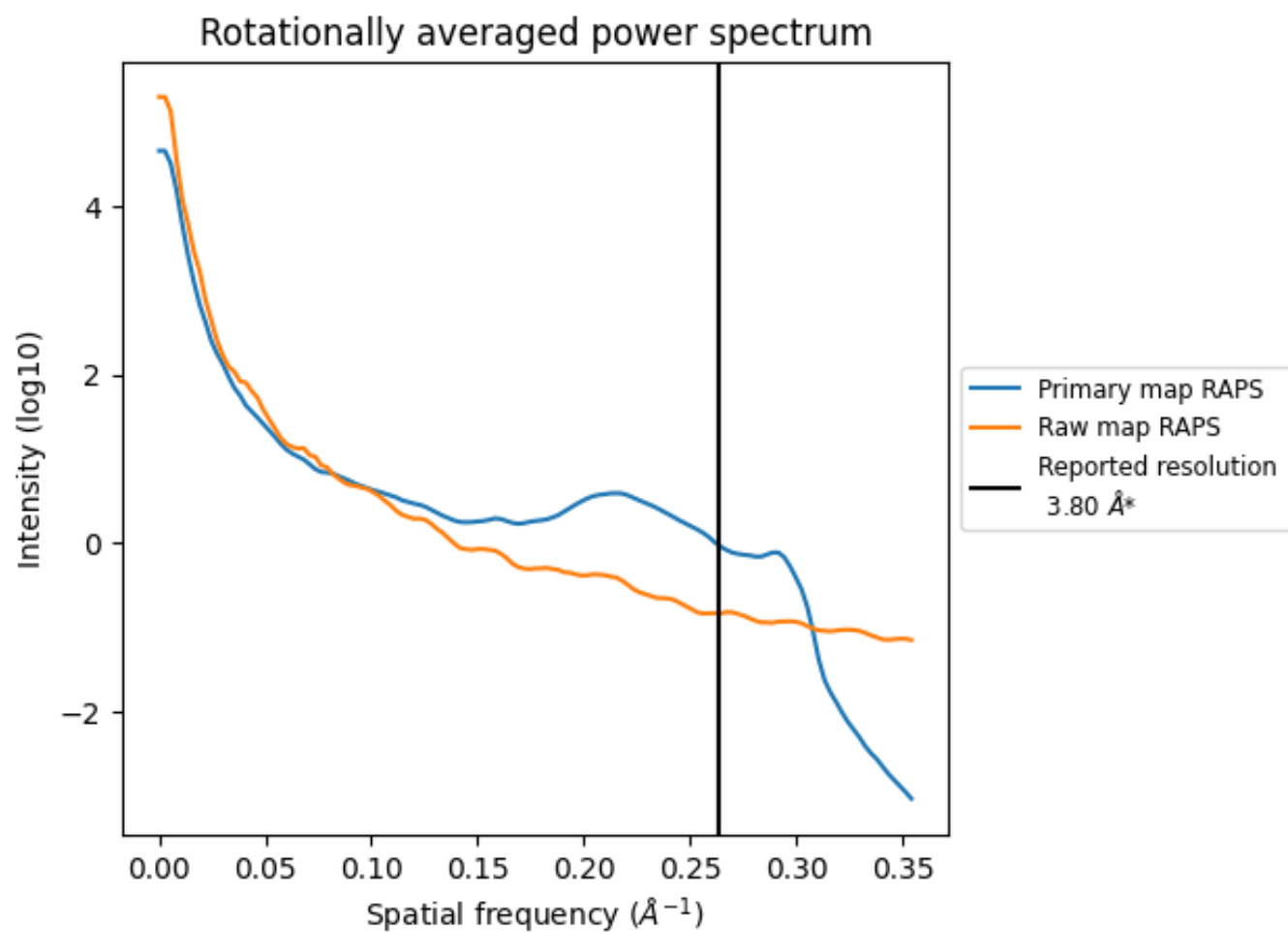
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 70 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 ⓘ

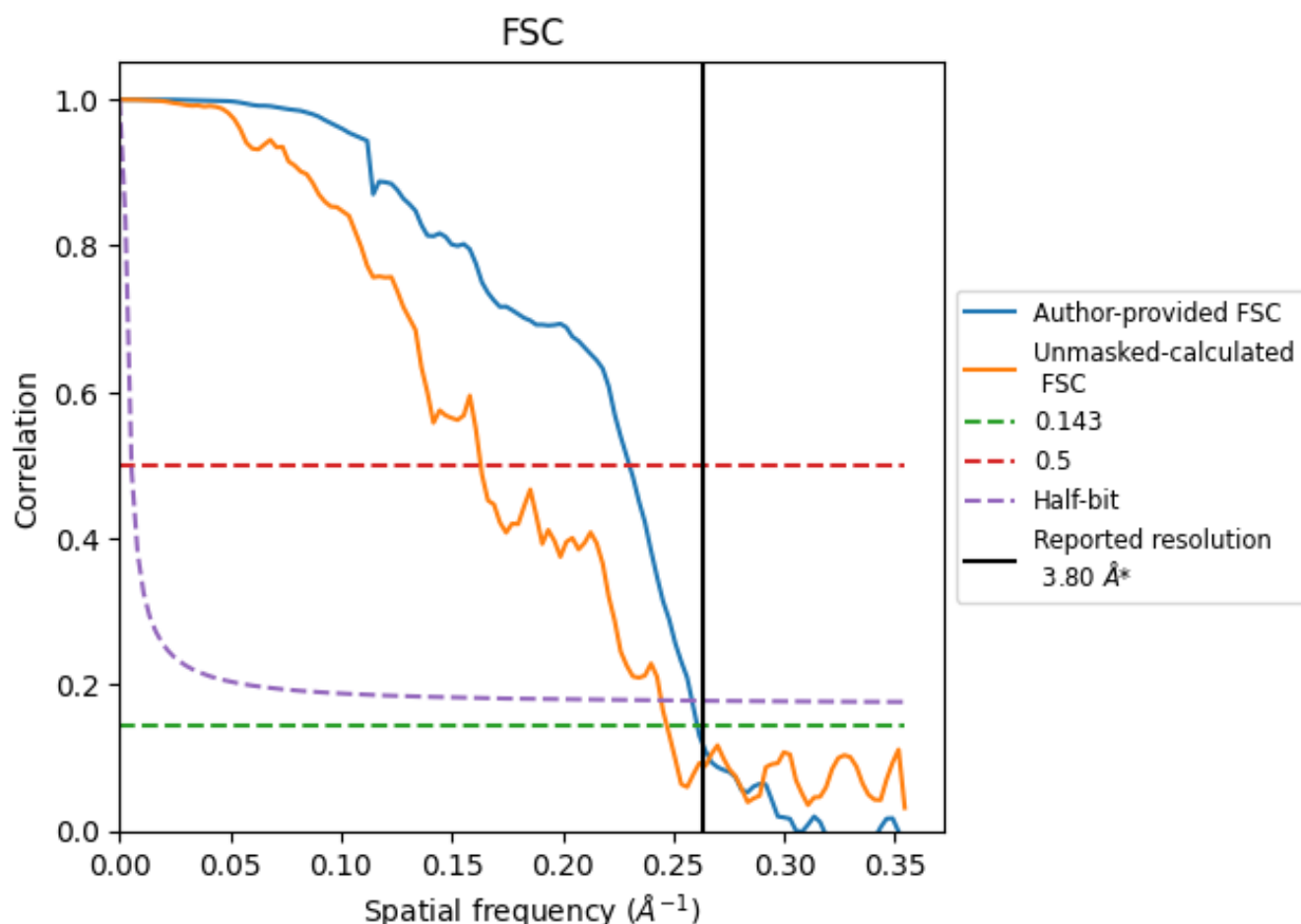


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

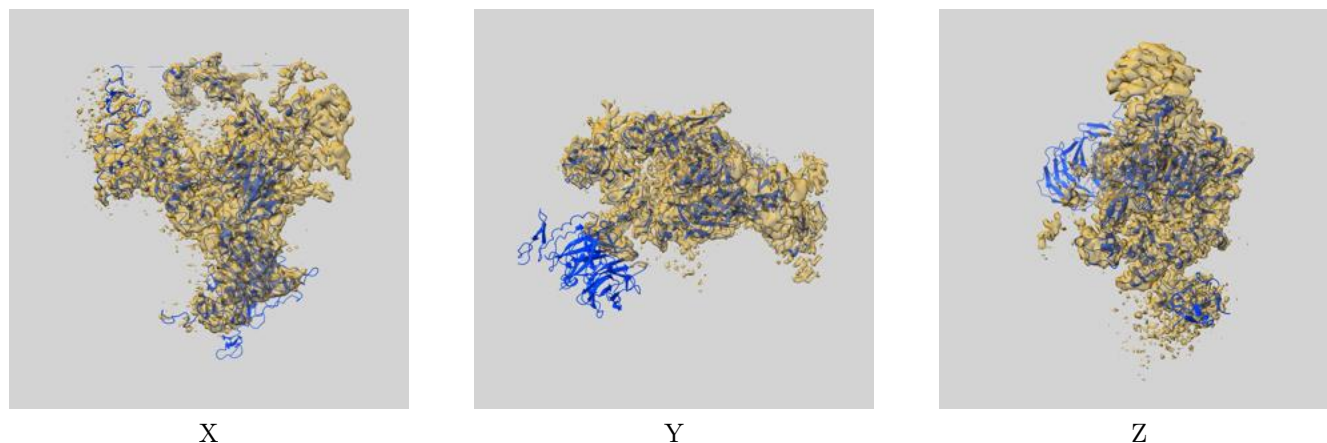
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.35	3.87
Unmasked-calculated*	4.05	6.13	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

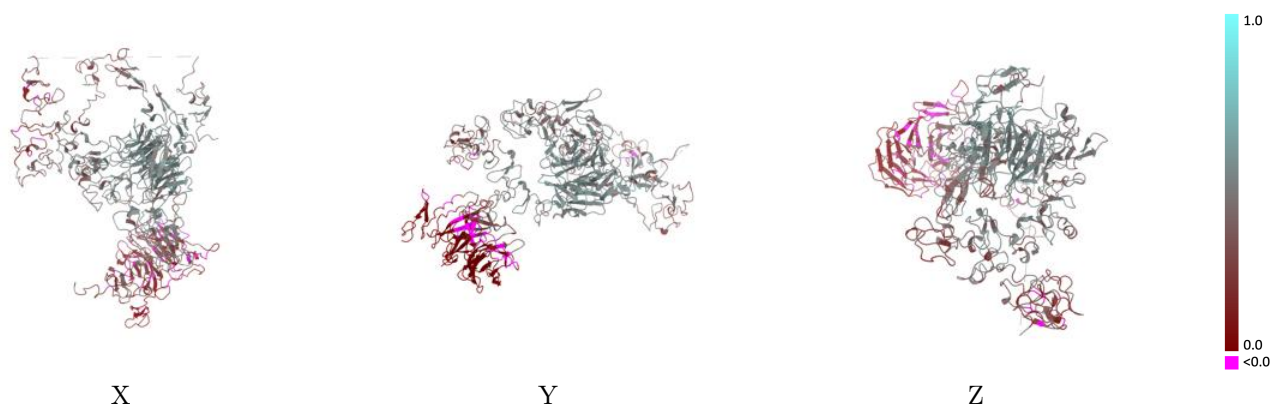
This section contains information regarding the fit between EMDB map EMD-36693 and PDB model 8JX9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



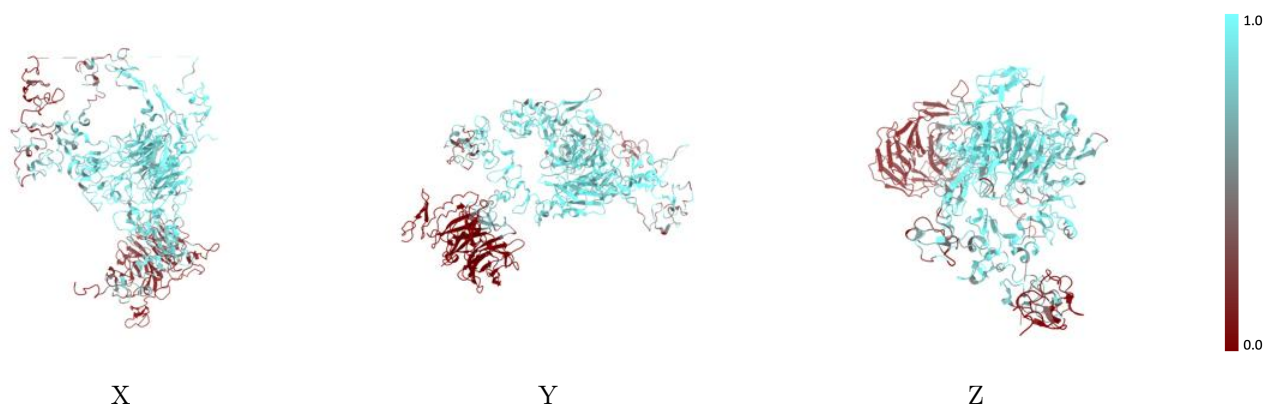
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



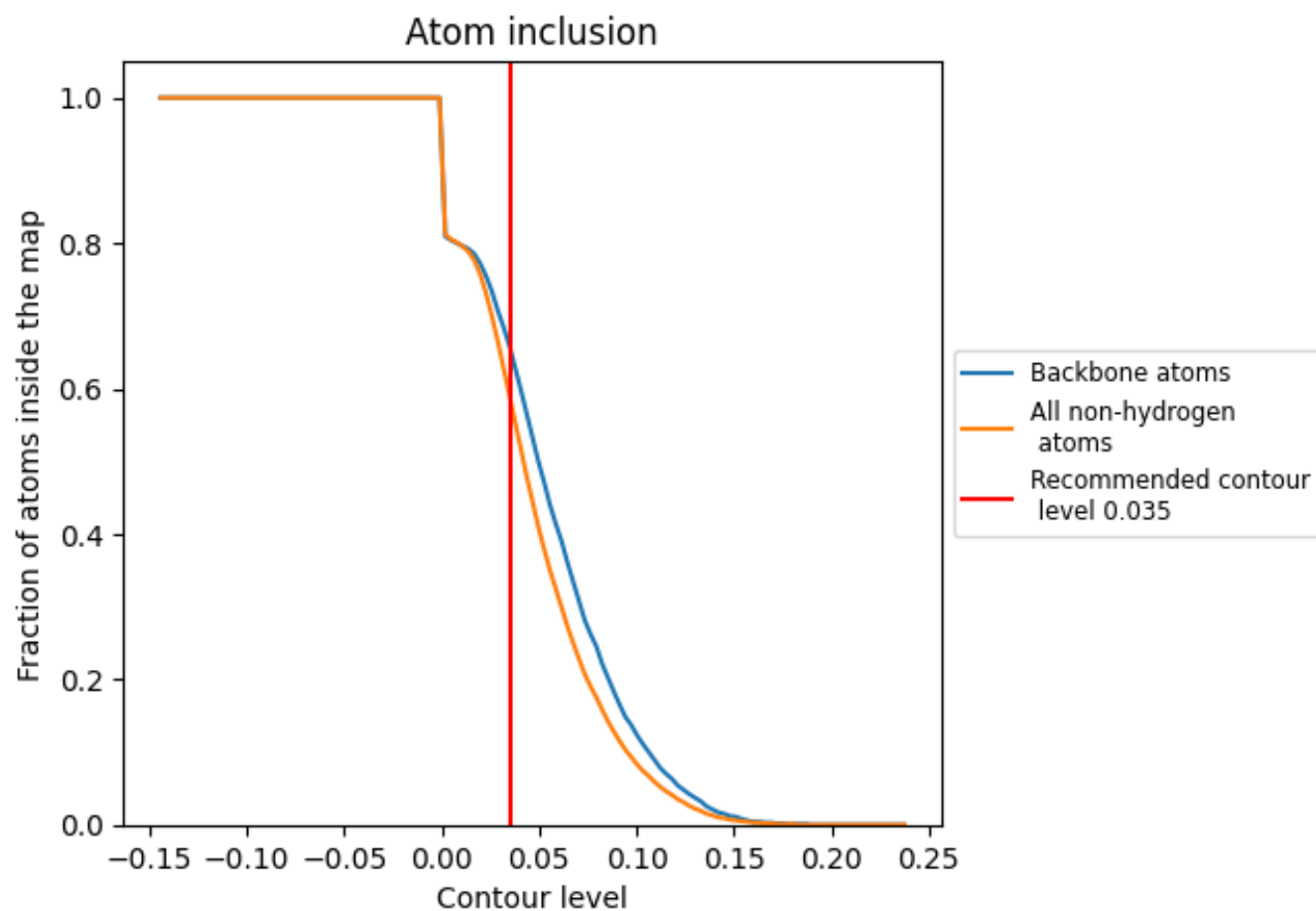
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).























9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5900	 0.3480
A	 0.0930	 0.0690
B	 0.7560	 0.4390
C	 0.3330	 0.3370
D	 0.7950	 0.5070
E	 0.6890	 0.4650
F	 0.5360	 0.4360
G	 0.5710	 0.4210
H	 0.5250	 0.3520
I	 0.7380	 0.4320
O	 1.0000	 0.5960

