



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 06:13 PM EDT

PDB ID : 8E59
EMDB ID : EMD-27907
Title : Human L-type voltage-gated calcium channel Cav1.3 in the presence of Amiodarone at 3.1 Angstrom resolution
Authors : Gao, S.; Yao, X.; Yan, N.
Deposited on : 2022-08-20
Resolution : 3.10 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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

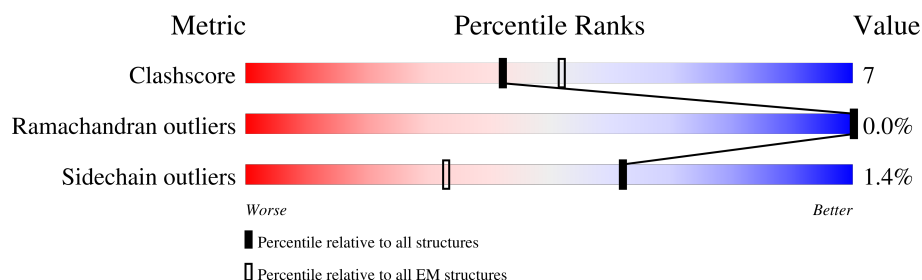
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	2161	<div> <div>18%</div> <div>47%</div> <div>9%</div> <div>43%</div> </div>
2	D	1103	<div> <div>6%</div> <div>70%</div> <div>16%</div> <div>14%</div> </div>
3	C	484	<div> <div>67%</div> <div>55%</div> <div>12%</div> <div>33%</div> </div>
4	B	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
5	E	2	<div> <div>50%</div> <div>100%</div> </div>
5	G	2	<div> <div>50%</div> <div>100%</div> </div>
5	H	2	<div> <div>50%</div> <div>50%</div> </div>
6	F	4	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 20309 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 Voltage-dependent L-type calcium channel subunit alpha-1D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1230	Total	C	N	O	S	0	0
			9900	6517	1597	1715	71		

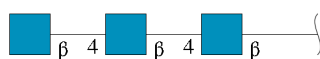
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	948	Total	C	N	O	S	0	0
			7570	4803	1269	1467	31		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2575	1619	467	479	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	B	3	Total	C	N	O	0	0
			42	24	3	15		

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



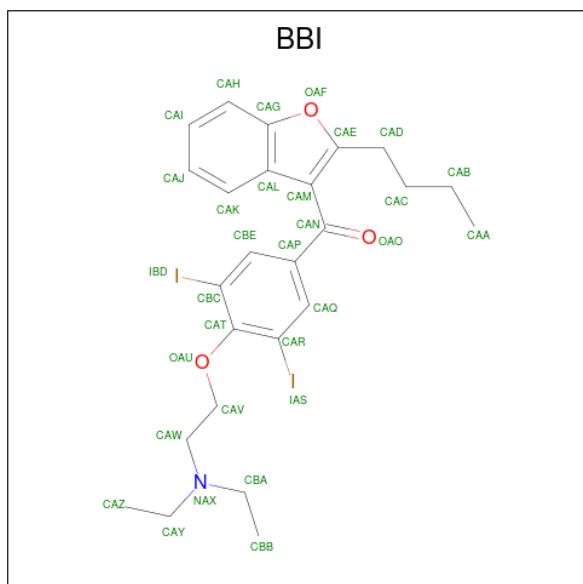
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 7 is (2-butyl-1-benzofuran-3-yl){4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl}methanone (three-letter code: BBI) (formula: C₂₅H₂₉I₂NO₃) (labeled as "Ligand of Interest" by depositor).

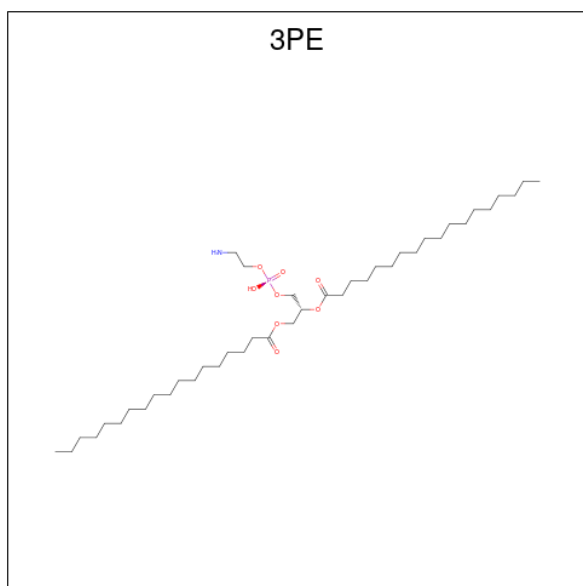


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	I	N	O	0
			31	25	2	1	3	

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

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Ca	0
			1	1	
8	D	1	Total	Ca	0
			1	1	

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			21	13	1	6	1	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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



LYS	PHE	VAL	SER	ALA	THR	LYS	HIS	GLU	ILE	ALA	ASP	ASP	CYS	ASP	LEU	THR	ILE	ASP	GLU	MET	SER	ALA	ALA	SER	THR	LEU	LEU	ASN	ASN	VAL	ARG	ARG	ALA	ASN	GLY	ASP	ASP	VAL	GLY	PRO	LEU	SER	HIS	ARG	GLN	ASP	TYR	GLU	LEU	GLN	ASP	PHE	GLY	PRO	GLY	TYR	SER	
ASP	GLU	GLU	PRO	ASP	PRO	GLY	ARG	ASP	GLU	GLU	ASP	LEU	ALA	ASP	GLN	SER	LEU	MET	ILE	CYS	ILE	THR	THR	LEU	LEU	LEU	LEU	GLY	ASN	ASN	VAL	ARG	PRO	ARG	ALA	ASN	GLY	ASP	VAL	GLY	PRO	LEU	SER	HIS	ARG	GLN	ASP	TYR	GLU	LEU	GLN	ASP	PHE	GLY	PRO	GLY	TYR	SER

● Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D: 

MET	ALA	ALA	GLY	CYS	LEU	LEU	ALA	LEU	THR	LEU	THR	LEU	PHE	GLN	SER	LEU	LEU	ASN	ASP	GLY	PRO	SER	SER	GLU	GLU	PRO	F27	T32	S35	Q41	E42	D43	L44	A48	K49	T50	A51	S52	D59	I60	Y61	Y68	N73	N74	A75	V79	E105	K106	V107	Q108	A109																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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● Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3

Chain C: 

MET	TYR	ASP	SER	VAL	PRO	GLY	PHE	GLU	ASP	SER	GLU	ALA	GLY	SER	ALA	ALA	THR	SER	TYR	THR	THR	ARG	PRO	SER	SER	ASP	SER	VAL	SER	LEU	GLU	GLU	ASP	ARG	E38	S39	A40	R41	R42	E43	V44	E45	S46	Q47	A48	Q49	Q50	Q51	L52	E53	R54	A55	K56	H57	K58	P59	V60
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LYS	ASP	SER	TYR	H361	Q301	S241	V181	P121	A61
SER	SER	ARG	PRO	HIS	R302	S242	L182	Q122	F62
ASP	ARG	PRO	ALA	ALA	L303	A243	V183	R123	A63
SER	LEU	PRO	GLY	GLY	I304	R244	G184	L124	V64
TYR	GLU	PRO	GLY	S306	R305	S245	P185	E125	R65
ASP	GLY	ASP	GLY	R307	S306	S246	S186	S126	T66
TYR	TYR	TYR	LEU	LEU	G308	I247	L187	I127	N67
ALA	ALA	ALA	LEU	LEU	K309	A248	K188	R128	V68
ASP	ASP	ASP	GLY	GLY	K309	E249	G189	L129	S69
ALA	ALA	ALA	PRO	PRO	S310	V250	Y190	K130	Y70
GLN	GLN	SER	SER	SER	Q311	Q251	E191	Q131	C71
ASP	ASP	ALA	ALA	ALA	M312	S252	V192	E132	G72
LEU	LEU	ILE	LEU	LEU	K313	E253	T193	Q133	V73
TYR	TYR	TYR	PRO	PRO	H314	I254	D194	K134	L74
GLN	GLN	GLY	GLY	GLY	L315	E255	M195	A135	D75
PRO	PRO	LEU	LEU	LEU	T316	R256	M196	R136	E76
HIS	HIS	GLN	ASN	ASN	V317	I257	Q197	R137	E77
GLN	GLN	GLN	GLN	GLN	Q318	F258	K198	S138	C78
HIS	HIS	GLN	GLN	GLN	Q319	E259	A199	G139	P79
THR	THR	LEU	LEU	LEU	M320	L260	L200	N140	V80
SER	SER	GLY	GLY	GLY	A321	A261	F201	Q141	Q81
LEU	LEU	LEU	LEU	LEU	Y322	K262	D202	S142	G82
PRO	PRO	ARG	ARG	ARG	D323	S263	F203	S143	S83
SER	SER	GLY	GLY	GLY	K324	L264	L204	L144	G84
ASN	ASN	GLU	GLU	GLU	L325	Q265	K205	S145	V85
GLY	GLY	HIS	HIS	HIS	L326	L266	H206	D146	N86
HIS	HIS	SER	SER	SER	V326	L266	R207	I147	F87
ASP	ASP	PRO	PRO	PRO	Q327	V267	F208	G148	E88
PRO	PRO	LEU	LEU	LEU	C328	V268	D209	N149	A89
GLN	GLN	GLU	GLU	GLU	P329	L269	G210	R150	K90
ASP	ASP	ARG	ARG	ARG	P330	D270	R211	R151	D91
ARG	ARG	LEU	LEU	LEU	E331	A271	I212	S152	F92
LEU	LEU	LEU	LEU	LEU	S332	D272	S213	P153	L93
ALA	ALA	MET	ALA	ALA	F333	T273	S213	S152	F92
GLN	GLN	ASP	ASP	ASP	D334	L274	I214	P154	H94
ASP	ASP	SER	SER	SER	V335	N275	T215	P155	I95
SER	SER	GLU	GLU	GLU	I336	H276	R216	S156	K96
GLU	GLU	SER	SER	SER	L337	P277	V217	L157	E97
ASP	ASP	GLU	GLU	GLU	D338	A278	T218	A158	K98
SER	SER	SER	SER	SER	E339	Q279	A219	K159	Y99
ASP	ASP	ARG	ARG	ARG	N340	L280	D220	Q160	S100
ARG	ARG	ASN	ASN	ASN	Q341	A281	L221	K161	N101
ASN	ASN	TRP	TRP	TRP	L342	K282	S222	Q162	D102
GLN	GLN	TRP	TRP	TRP	E343	T283	L223	K163	W103
ARG	ARG	THR	THR	THR	D344	S284	A224	Q164	W104
ASN	ASN	GLY	GLY	GLY	A345	L285	K225	A165	I105
ARG	ARG	SER	SER	SER	C346	A286	R226	E166	G106
PRO	PRO	SER	SER	SER	E347	E347	S227	H167	R107
TRP	TRP	GLN	GLN	GLN	H348	I288	V228	V168	L108
PRO	PRO	ARG	ARG	ARG	L349	I289	L229	P169	V109
TRP	TRP	ASN	ASN	ASN	A350	V290	N230	P170	K110
ARG	ARG	E351	E351	E351	F291	V291	N231	Y171	E111
ASN	ASN	V352	V352	V352	V292	K293	P232	D172	G112
ARG	ARG	L353	L353	L353	K293	K293	G233	V173	G113
PRO	PRO	E354	E354	E354	V294	V294	K234	V174	D114
TRP	TRP	V355	V355	V355	S295	S295	R235	P175	I115
PRO	PRO	Y356	Y356	Y356	S296	S296	T236	S176	A116
ARG	ARG	W357	W357	W357	F297	F297	I237	M177	F117
TRP	TRP	R358	R358	R358	K298	K298	I238	R178	I118
PRO	PRO	A359	A359	A359	V299	V299	E239	P119	P119
ASP	ASP	T360	T360	T360	L300	L300	R240	V180	S120

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



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

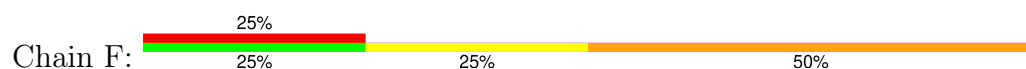




- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86836	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BBI, NAG, 3PE, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/10127	0.44	0/13716
2	D	0.25	0/7728	0.46	0/10477
3	C	0.23	0/2624	0.48	0/3544
All	All	0.25	0/20479	0.45	0/27737

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	9900	0	10071	125	0
2	D	7570	0	7367	108	0
3	C	2575	0	2619	33	0
4	B	42	0	37	3	0
5	E	28	0	25	0	0
5	G	28	0	25	1	0
5	H	28	0	25	1	0
6	F	56	0	49	3	0
7	A	31	0	29	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	1	0	0	0	0
9	A	21	0	23	1	0
10	D	28	0	25	0	0
All	All	20309	0	20295	265	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 (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ALA:HB3	3:C:195:MET:HB3	1.62	0.80
1:A:603:ILE:O	1:A:607:LEU:HB2	1.81	0.79
2:D:732:ARG:HG2	2:D:814:ILE:HG22	1.71	0.71
1:A:953:ASN:HD22	1:A:953:ASN:N	1.89	0.70
2:D:653:PHE:HB3	2:D:746:LYS:HD3	1.73	0.70
1:A:348:ASP:HB2	1:A:1227:TYR:HB2	1.73	0.69
2:D:802:ILE:HG22	2:D:803:GLN:HG2	1.76	0.67
1:A:263:SER:HA	1:A:266:LYS:HE3	1.76	0.67
2:D:848:MET:HA	2:D:1019:GLU:HA	1.77	0.67
2:D:313:ARG:HD2	2:D:534:VAL:HG12	1.76	0.67
2:D:313:ARG:HH21	2:D:1043:PRO:HG3	1.60	0.66
1:A:1481:HIS:HB3	1:A:1516:LEU:HD22	1.76	0.66
1:A:251:VAL:HG23	1:A:257:LEU:HB3	1.79	0.65
2:D:844:ASN:ND2	2:D:865:ASP:OD2	2.30	0.64
1:A:306:SER:O	1:A:334:ARG:NH2	2.32	0.63
1:A:1238:ASP:O	1:A:1242:MET:HG3	1.99	0.63
3:C:157:LEU:HD23	3:C:162:GLN:HG3	1.81	0.62
2:D:895:ASN:OD1	5:H:1:NAG:O3	2.10	0.62
3:C:304:ILE:HG21	3:C:315:LEU:HD13	1.81	0.62
1:A:149:PHE:HB3	1:A:153:ASP:HB3	1.82	0.61
1:A:542:SER:OG	1:A:555:GLN:NE2	2.34	0.61
2:D:185:TRP:HA	4:B:1:NAG:H82	1.81	0.61
2:D:204:LEU:HD11	2:D:493:SER:HB2	1.81	0.61
1:A:627:PHE:HA	1:A:630:THR:HG22	1.81	0.61
2:D:747:GLU:O	2:D:750:GLU:HG3	2.00	0.61
1:A:1278:ILE:HD12	1:A:1278:ILE:H	1.66	0.61
2:D:735:VAL:HG22	2:D:741:THR:HG23	1.83	0.61
1:A:953:ASN:N	1:A:953:ASN:ND2	2.47	0.60
1:A:145:ILE:HD11	1:A:161:LEU:HD21	1.84	0.60
1:A:445:ALA:HB2	3:C:199:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:TRP:O	1:A:554:ILE:HG13	2.03	0.59
2:D:994:LEU:N	2:D:1001:ARG:O	2.29	0.59
2:D:675:ASN:ND2	2:D:677:THR:OG1	2.34	0.59
2:D:659:THR:OG1	2:D:742:ARG:NH1	2.36	0.59
1:A:1326:LEU:O	1:A:1330:LEU:HB2	2.03	0.59
2:D:464:LEU:HD12	2:D:465:PRO:HD2	1.85	0.59
1:A:315:ALA:O	1:A:324:ARG:NH2	2.36	0.59
2:D:157:ARG:NH2	2:D:222:PRO:O	2.36	0.59
2:D:526:ASN:ND2	2:D:564:ALA:O	2.36	0.58
2:D:157:ARG:HH12	2:D:224:VAL:HG12	1.67	0.58
2:D:259:ASP:HB2	2:D:362:THR:HG22	1.84	0.58
2:D:109:ALA:HA	2:D:470:THR:HG22	1.86	0.58
2:D:994:LEU:HB3	2:D:1001:ARG:HB2	1.86	0.57
1:A:904:ALA:HB2	1:A:1362:PHE:HE1	1.68	0.57
1:A:169:LEU:O	1:A:173:THR:HG22	2.04	0.57
1:A:924:TYR:HE1	1:A:970:PHE:HB3	1.70	0.56
4:B:2:NAG:H83	4:B:2:NAG:H3	1.86	0.56
2:D:843:ARG:NH1	2:D:865:ASP:OD1	2.33	0.56
2:D:496:ASP:OD1	2:D:499:ARG:NH1	2.38	0.56
1:A:299:LYS:O	1:A:317:CYS:N	2.30	0.55
1:A:202:PHE:O	1:A:206:ILE:HG23	2.06	0.55
1:A:543:GLU:HG2	1:A:555:GLN:HE22	1.70	0.55
1:A:755:LEU:HD21	1:A:1150:PHE:HB2	1.88	0.55
2:D:676:ASN:O	2:D:676:ASN:ND2	2.38	0.55
6:F:4:NAG:H3	6:F:4:NAG:H83	1.87	0.55
1:A:1015:ILE:HA	1:A:1150:PHE:HE2	1.72	0.55
1:A:1452:ALA:O	1:A:1456:ILE:HG23	2.06	0.55
1:A:1070:PRO:HG2	2:D:233:ILE:HD11	1.88	0.55
1:A:1382:GLN:HG3	1:A:1410:GLU:HB3	1.88	0.55
1:A:413:ARG:NH1	1:A:757:ASP:OD1	2.40	0.54
1:A:1103:TRP:CD1	1:A:1104:PRO:HD3	2.42	0.54
1:A:417:LYS:HZ3	1:A:422:PHE:HD2	1.56	0.54
2:D:736:THR:HG23	2:D:810:ALA:HB2	1.89	0.54
2:D:864:HIS:O	2:D:866:ASP:N	2.41	0.54
2:D:312:VAL:HG21	2:D:532:ILE:HD11	1.90	0.54
1:A:1547:ASN:O	1:A:1587:LYS:NZ	2.39	0.54
3:C:179:PRO:HG2	3:C:287:PRO:HB3	1.90	0.54
1:A:1248:PHE:O	1:A:1251:GLU:HG3	2.08	0.53
1:A:1401:ARG:HH11	1:A:1411:ILE:HD11	1.73	0.53
2:D:855:ASP:HB2	2:D:1012:ASN:HB2	1.89	0.53
1:A:1180:LEU:HG	1:A:1587:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:ILE:H	1:A:1494:PRO:HB3	1.73	0.53
2:D:357:ILE:HG22	2:D:383:ARG:HB2	1.91	0.53
2:D:296:SER:HB3	2:D:330:ILE:HG12	1.89	0.53
1:A:653:LEU:HD12	1:A:746:VAL:HG12	1.91	0.53
1:A:953:ASN:N	1:A:956:ASN:OD1	2.42	0.53
3:C:357:TRP:O	3:C:361:HIS:ND1	2.32	0.53
1:A:610:MET:HG3	1:A:612:PRO:HD3	1.89	0.52
2:D:273:ARG:HD2	2:D:323:ASN:HA	1.92	0.52
2:D:594:SER:OG	2:D:596:ASP:O	2.27	0.52
3:C:64:VAL:HG22	3:C:95:ILE:HD11	1.92	0.52
1:A:933:GLU:OE2	1:A:997:ARG:NH2	2.43	0.52
1:A:301:CYS:HA	1:A:333:CYS:HB3	1.92	0.52
1:A:1034:VAL:O	1:A:1038:LYS:HB2	2.10	0.52
2:D:280:LEU:HA	2:D:283:LEU:HD12	1.90	0.52
1:A:927:THR:HG21	1:A:970:PHE:HE2	1.75	0.52
1:A:989:LEU:HG	1:A:992:LEU:HD12	1.92	0.52
1:A:1219:THR:OG1	1:A:1326:LEU:HD13	2.09	0.52
1:A:1573:LEU:HA	1:A:1577:ILE:HG12	1.91	0.52
1:A:695:LEU:HD23	9:A:2203:3PE:H252	1.91	0.51
1:A:1513:GLN:HB3	1:A:1515:PRO:HD2	1.92	0.51
1:A:626:ILE:HG21	1:A:1024:LEU:HD11	1.93	0.51
6:F:3:NAG:H83	6:F:3:NAG:H3	1.93	0.51
1:A:1049:LYS:HB3	1:A:1054:GLU:HG3	1.93	0.51
2:D:289:VAL:HG12	2:D:310:ALA:HB2	1.93	0.51
2:D:970:SER:OG	2:D:971:LYS:N	2.42	0.51
1:A:1193:PRO:HA	1:A:1196:TYR:HB3	1.93	0.51
2:D:528:GLN:O	2:D:901:GLN:NE2	2.44	0.50
2:D:515:ILE:HG22	2:D:618:SER:HB2	1.94	0.50
2:D:744:TYR:HB3	2:D:745:PRO:HD3	1.93	0.50
2:D:296:SER:HA	2:D:332:ASP:HB2	1.94	0.49
1:A:646:SER:OG	1:A:649:SER:OG	2.30	0.49
1:A:1278:ILE:HA	1:A:1281:ILE:HG12	1.94	0.49
2:D:653:PHE:CE1	2:D:659:THR:HB	2.46	0.49
1:A:367:THR:HG21	1:A:1401:ARG:HG3	1.94	0.49
1:A:583:PHE:O	1:A:589:ARG:NH2	2.30	0.49
2:D:421:ILE:HD12	2:D:424:GLN:HE21	1.77	0.49
2:D:1027:ASP:OD1	2:D:1027:ASP:N	2.44	0.49
2:D:595:GLN:HB3	2:D:762:SER:HB2	1.95	0.49
3:C:223:LEU:HA	3:C:225:LYS:HE2	1.93	0.49
1:A:636:LEU:HD12	1:A:1017:ASN:HB3	1.94	0.48
1:A:904:ALA:HB2	1:A:1362:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:GLU:HB2	1:A:1164:LYS:HE3	1.94	0.48
1:A:1169:ASP:N	1:A:1169:ASP:OD1	2.47	0.47
1:A:1185:LEU:HD13	1:A:1486:LYS:HB3	1.96	0.47
3:C:173:VAL:H	3:C:226:ARG:HH12	1.60	0.47
3:C:277:PRO:HB3	3:C:289:ILE:HG21	1.96	0.47
1:A:903:LEU:HB2	1:A:990:ARG:HH11	1.78	0.47
1:A:1015:ILE:HA	1:A:1150:PHE:CE2	2.48	0.47
2:D:50:THR:O	2:D:719:TYR:OH	2.31	0.47
2:D:240:ARG:NH2	2:D:278:GLU:O	2.47	0.47
3:C:107:ARG:HB3	3:C:115:ILE:HD13	1.97	0.47
3:C:63:ALA:HB2	3:C:94:HIS:HD2	1.79	0.47
1:A:287:ILE:O	1:A:291:GLU:HG3	2.15	0.47
2:D:1061:ASP:OD1	2:D:1061:ASP:N	2.46	0.47
1:A:274:ILE:HD11	1:A:404:VAL:HG21	1.96	0.47
1:A:876:ARG:HG2	1:A:940:THR:HA	1.96	0.47
2:D:399:ILE:HA	2:D:402:MET:HE2	1.96	0.47
2:D:485:LEU:HD22	6:F:1:NAG:H82	1.95	0.47
2:D:605:ARG:HD3	2:D:624:PRO:HB3	1.97	0.47
2:D:650:PRO:HA	2:D:653:PHE:CE1	2.50	0.47
2:D:204:LEU:HD22	2:D:456:LEU:HD21	1.96	0.47
2:D:669:ASP:N	2:D:669:ASP:OD1	2.48	0.47
3:C:307:ARG:HG2	3:C:311:GLN:HG3	1.97	0.47
3:C:321:ALA:HA	3:C:324:LYS:HG2	1.97	0.47
3:C:294:VAL:HG21	3:C:300:LEU:HD13	1.97	0.46
1:A:254:VAL:HG12	1:A:257:LEU:H	1.80	0.46
2:D:61:TYR:O	2:D:68:TYR:OH	2.28	0.46
3:C:92:PHE:HD2	3:C:109:VAL:HG11	1.80	0.46
2:D:880:PRO:HB3	2:D:1030:LEU:HA	1.97	0.46
2:D:48:ALA:O	2:D:52:SER:OG	2.28	0.46
2:D:254:MET:HE3	2:D:283:LEU:HD21	1.98	0.46
3:C:60:VAL:HA	3:C:96:LYS:HG2	1.97	0.46
3:C:290:VAL:HG13	3:C:335:VAL:HG13	1.97	0.46
1:A:540:ILE:HG21	1:A:623:LEU:HD13	1.96	0.46
2:D:634:LYS:HE2	2:D:634:LYS:HB3	1.74	0.46
2:D:32:THR:O	2:D:35:SER:OG	2.27	0.45
2:D:1039:ASP:OD2	2:D:1039:ASP:N	2.49	0.45
1:A:1509:LEU:HD12	1:A:1518:PHE:HE2	1.81	0.45
2:D:344:LEU:O	2:D:351:ARG:NH1	2.40	0.45
2:D:355:ASN:OD1	2:D:1061:ASP:HB3	2.16	0.45
1:A:211:SER:O	1:A:215:GLU:HG2	2.17	0.45
2:D:653:PHE:HZ	2:D:680:LEU:CD2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:HG23	1:A:257:LEU:CB	2.46	0.45
2:D:653:PHE:O	2:D:746:LYS:HG2	2.16	0.45
1:A:153:ASP:OD1	1:A:154:SER:N	2.48	0.45
1:A:528:LEU:O	1:A:531:VAL:HG12	2.17	0.45
1:A:244:VAL:O	1:A:247:PRO:HD2	2.17	0.45
1:A:1215:ILE:HD12	1:A:1329:LEU:HD23	1.98	0.45
1:A:1379:ASP:OD1	1:A:1385:ARG:NH1	2.50	0.45
1:A:925:ALA:O	1:A:929:ILE:HG13	2.17	0.45
2:D:254:MET:HG2	2:D:289:VAL:HG23	1.98	0.45
2:D:254:MET:SD	2:D:359:MET:HG3	2.57	0.45
2:D:462:GLY:O	2:D:489:GLY:HA2	2.17	0.45
3:C:136:ARG:O	3:C:137:ARG:NH1	2.50	0.45
2:D:73:ASN:N	2:D:628:PHE:O	2.39	0.44
1:A:278:VAL:HG22	1:A:397:VAL:HG21	1.99	0.44
3:C:214:ILE:HG22	3:C:268:VAL:HB	1.99	0.44
1:A:411:LYS:HG3	1:A:1471:THR:HG22	1.99	0.44
1:A:1087:VAL:O	1:A:1091:MET:HG3	2.17	0.44
1:A:1339:LEU:HD12	1:A:1469:TYR:HE2	1.82	0.44
1:A:214:LEU:O	1:A:218:THR:HB	2.18	0.44
2:D:409:TYR:HB2	2:D:429:VAL:HG21	1.99	0.44
1:A:646:SER:HG	1:A:649:SER:HG	1.66	0.43
3:C:52:LEU:HD22	3:C:115:ILE:HG21	2.00	0.43
1:A:210:PHE:HD1	1:A:210:PHE:O	2.01	0.43
1:A:1024:LEU:O	1:A:1028:MET:HG3	2.18	0.43
1:A:1272:PHE:HE1	1:A:1324:MET:HB3	1.83	0.43
2:D:44:LEU:HD11	2:D:821:TRP:CZ2	2.53	0.43
2:D:147:PRO:HB3	2:D:163:HIS:NE2	2.33	0.43
2:D:745:PRO:O	2:D:746:LYS:C	2.54	0.43
1:A:145:ILE:HG13	1:A:161:LEU:HD11	2.00	0.43
1:A:577:LEU:HD23	1:A:582:TYR:HE1	1.83	0.43
1:A:690:ASN:OD1	1:A:690:ASN:N	2.51	0.43
3:C:99:TYR:HB2	3:C:105:ILE:HD12	2.00	0.43
1:A:250:LEU:O	1:A:254:VAL:HG23	2.19	0.43
2:D:125:TYR:HH	2:D:149:PHE:HZ	1.67	0.43
2:D:568:ASN:OD1	2:D:569:ASP:N	2.50	0.43
3:C:180:VAL:HG22	3:C:288:ILE:HD12	2.00	0.43
1:A:251:VAL:O	1:A:258:GLN:HG3	2.18	0.43
1:A:301:CYS:HB2	1:A:311:GLU:OE1	2.19	0.43
1:A:285:TYR:O	1:A:385:TYR:OH	2.28	0.43
2:D:649:LYS:HB3	2:D:651:ASP:OD2	2.19	0.43
1:A:644:LEU:O	1:A:647:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:OH	1:A:216:GLN:OE1	2.37	0.43
1:A:274:ILE:O	1:A:278:VAL:HG23	2.19	0.43
1:A:1198:PHE:HD2	1:A:1258:ALA:HB2	1.84	0.43
2:D:107:VAL:HG11	2:D:188:ALA:HB3	2.01	0.43
2:D:667:CYS:HB3	2:D:697:CYS:HB2	1.84	0.43
3:C:181:VAL:HG12	3:C:269:LEU:HB2	2.01	0.43
1:A:1129:SER:O	1:A:1133:ILE:HG12	2.19	0.42
2:D:435:VAL:HG21	2:D:482:GLN:HA	2.01	0.42
2:D:693:ASN:OD1	2:D:694:ASN:N	2.52	0.42
1:A:154:SER:OG	1:A:155:ASN:N	2.53	0.42
2:D:276:VAL:HG11	2:D:322:VAL:HG21	2.01	0.42
3:C:223:LEU:HB2	3:C:250:VAL:HG11	2.01	0.42
3:C:121:PRO:HG3	3:C:171:TYR:HD2	1.84	0.42
1:A:533:VAL:HG11	1:A:629:VAL:HG11	2.01	0.42
1:A:1287:SER:OG	1:A:1288:GLU:OE1	2.34	0.42
2:D:757:GLU:HG2	2:D:760:GLU:HG2	2.02	0.42
1:A:984:ARG:O	1:A:987:ARG:HG2	2.20	0.42
1:A:1422:ASP:N	1:A:1422:ASP:OD1	2.51	0.42
2:D:147:PRO:HB3	2:D:163:HIS:CE1	2.55	0.42
1:A:1220:LEU:O	1:A:1224:MET:HG3	2.20	0.42
2:D:459:VAL:HG12	2:D:493:SER:HA	2.01	0.42
1:A:563:LEU:HD22	1:A:602:THR:HG21	2.01	0.41
1:A:1046:ASP:HB3	1:A:1059:PHE:CE2	2.54	0.41
1:A:1051:ASN:OD1	1:A:1051:ASN:N	2.52	0.41
2:D:615:THR:OG1	2:D:616:ASP:N	2.53	0.41
2:D:704:ARG:HA	2:D:704:ARG:HD2	1.88	0.41
3:C:182:LEU:HD23	3:C:290:VAL:HB	2.01	0.41
5:G:1:NAG:H61	5:G:2:NAG:H82	2.01	0.41
1:A:438:TYR:OH	3:C:339:GLU:O	2.33	0.41
1:A:441:TRP:CD1	3:C:342:LEU:HD13	2.55	0.41
1:A:649:SER:O	1:A:653:LEU:HD23	2.21	0.41
2:D:105:GLU:HG2	2:D:466:VAL:HG13	2.02	0.41
2:D:295:ASN:ND2	2:D:328:LYS:O	2.41	0.41
3:C:180:VAL:HB	3:C:268:VAL:HG22	2.00	0.41
1:A:685:ARG:NH2	1:A:1112:ASP:OD1	2.53	0.41
1:A:1512:ILE:HB	1:A:1517:GLY:HA3	2.02	0.41
2:D:182:GLU:OE1	2:D:185:TRP:NE1	2.48	0.41
2:D:373:PHE:CE2	2:D:402:MET:HG2	2.55	0.41
2:D:601:ASP:OD2	2:D:601:ASP:N	2.52	0.41
2:D:755:ASN:HD22	2:D:760:GLU:HB2	1.85	0.41
2:D:849:ASP:N	2:D:849:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:ARG:CZ	4:B:1:NAG:H62	2.50	0.41
2:D:463:THR:HG23	2:D:487:VAL:HG13	2.02	0.41
1:A:256:SER:O	1:A:259:VAL:HG22	2.21	0.41
1:A:1184:PRO:HG3	1:A:1546:PHE:CG	2.55	0.41
1:A:570:MET:SD	1:A:595:VAL:HG11	2.60	0.41
2:D:979:THR:HG23	2:D:1033:GLN:HG2	2.03	0.41
1:A:1418:GLY:O	1:A:1419:LYS:HD3	2.21	0.41
2:D:241:ARG:HA	2:D:241:ARG:HD2	1.85	0.41
2:D:1019:GLU:H	2:D:1019:GLU:CD	2.23	0.41
2:D:75:ALA:O	2:D:79:VAL:HG23	2.20	0.41
2:D:662:ALA:HA	2:D:663:PRO:HD3	1.91	0.41
3:C:153:PRO:HA	3:C:154:PRO:HD3	1.93	0.41
1:A:1364:TYR:CE2	1:A:1447:PHE:HB2	2.56	0.41
2:D:735:VAL:HG21	2:D:763:PHE:HZ	1.86	0.41
2:D:794:VAL:O	2:D:813:GLY:HA3	2.21	0.41
1:A:1584:THR:HA	1:A:1587:LYS:HD3	2.02	0.40
1:A:1584:THR:HG22	1:A:1587:LYS:HD3	2.02	0.40
2:D:596:ASP:O	2:D:598:ARG:N	2.52	0.40
2:D:653:PHE:HZ	2:D:680:LEU:HD21	1.85	0.40
1:A:1106:LEU:HD12	1:A:1106:LEU:HA	1.89	0.40
1:A:180:ILE:HG22	1:A:181:ILE:HG23	2.04	0.40
1:A:1340:LEU:O	1:A:1344:ILE:HG12	2.21	0.40
3:C:173:VAL:N	3:C:226:ARG:HH12	2.19	0.40
1:A:246:ARG:HB2	1:A:247:PRO:HD3	2.04	0.40
1:A:1408:TRP:HA	1:A:1411:ILE:HD12	2.04	0.40
2:D:750:GLU:C	2:D:752:TRP:H	2.25	0.40
2:D:744:TYR:O	2:D:746:LYS:N	2.55	0.40
2:D:747:GLU:O	2:D:748:ALA:C	2.58	0.40
2:D:875:PHE:HE2	2:D:882:LEU:HD23	1.86	0.40
3:C:296:SER:HB3	3:C:299:VAL:HG23	2.04	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	1214/2161 (56%)	1152 (95%)	61 (5%)	1 (0%)	48	79
2	D	936/1103 (85%)	879 (94%)	57 (6%)	0	100	100
3	C	322/484 (66%)	314 (98%)	8 (2%)	0	100	100
All	All	2472/3748 (66%)	2345 (95%)	126 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1260	LYS

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	1086/1902 (57%)	1073 (99%)	13 (1%)	67	83
2	D	837/971 (86%)	821 (98%)	16 (2%)	52	75
3	C	287/426 (67%)	284 (99%)	3 (1%)	73	86
All	All	2210/3299 (67%)	2178 (99%)	32 (1%)	62	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	CYS
1	A	166	TYR
1	A	210	PHE
1	A	256	SER
1	A	258	GLN
1	A	876	ARG
1	A	953	ASN
1	A	1068	ASP
1	A	1150	PHE

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Mol	Chain	Res	Type
1	A	1435	CYS
1	A	1499	ARG
1	A	1510	ARG
1	A	1534	MET
2	D	41	GLN
2	D	108	GLN
2	D	297	ASN
2	D	476	LYS
2	D	648	LEU
2	D	651	ASP
2	D	652	ASN
2	D	654	GLU
2	D	668	ASN
2	D	671	LYS
2	D	686	PHE
2	D	746	LYS
2	D	747	GLU
2	D	824	ASN
2	D	849	ASP
2	D	1029	ARG
3	C	195	MET
3	C	256	ARG
3	C	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	555	GLN
2	D	751	ASN
2	D	844	ASN

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 ⓘ

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1	2,4	14,14,15	0.41	0	17,19,21	0.56	0
4	NAG	B	2	4	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
4	NAG	B	3	4	14,14,15	0.35	0	17,19,21	0.39	0
5	NAG	E	1	2,5	14,14,15	0.39	0	17,19,21	0.54	0
5	NAG	E	2	5	14,14,15	0.44	0	17,19,21	0.78	0
6	NAG	F	1	2,6	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	F	3	6	14,14,15	0.96	1 (7%)	17,19,21	1.76	3 (17%)
6	NAG	F	4	6	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
5	NAG	G	1	2,5	14,14,15	0.39	0	17,19,21	0.47	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.47	0
5	NAG	H	1	2,5	14,14,15	0.77	1 (7%)	17,19,21	1.22	1 (5%)
5	NAG	H	2	5	14,14,15	0.23	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	5/6/23/26	0/1/1/1
4	NAG	B	3	4	-	4/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	NAG	F	3	6	-	6/6/23/26	0/1/1/1
6	NAG	F	4	6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.14	1.49	1.43
5	H	1	NAG	O5-C1	2.06	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	NAG	C1-O5-C5	4.79	118.61	112.19
5	H	1	NAG	C1-O5-C5	4.67	118.45	112.19
6	F	3	NAG	C2-N2-C7	4.62	129.09	122.90
6	F	4	NAG	C2-N2-C7	4.57	129.03	122.90
4	B	2	NAG	C2-N2-C7	4.55	129.00	122.90
6	F	4	NAG	C1-C2-N2	2.11	113.76	110.43
4	B	2	NAG	C1-C2-N2	2.10	113.74	110.43
6	F	3	NAG	C1-C2-N2	2.09	113.72	110.43

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3	NAG	C4-C5-C6-O6
6	F	3	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
6	F	3	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	B	3	NAG	O5-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	3	NAG	C8-C7-N2-C2
4	B	3	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2

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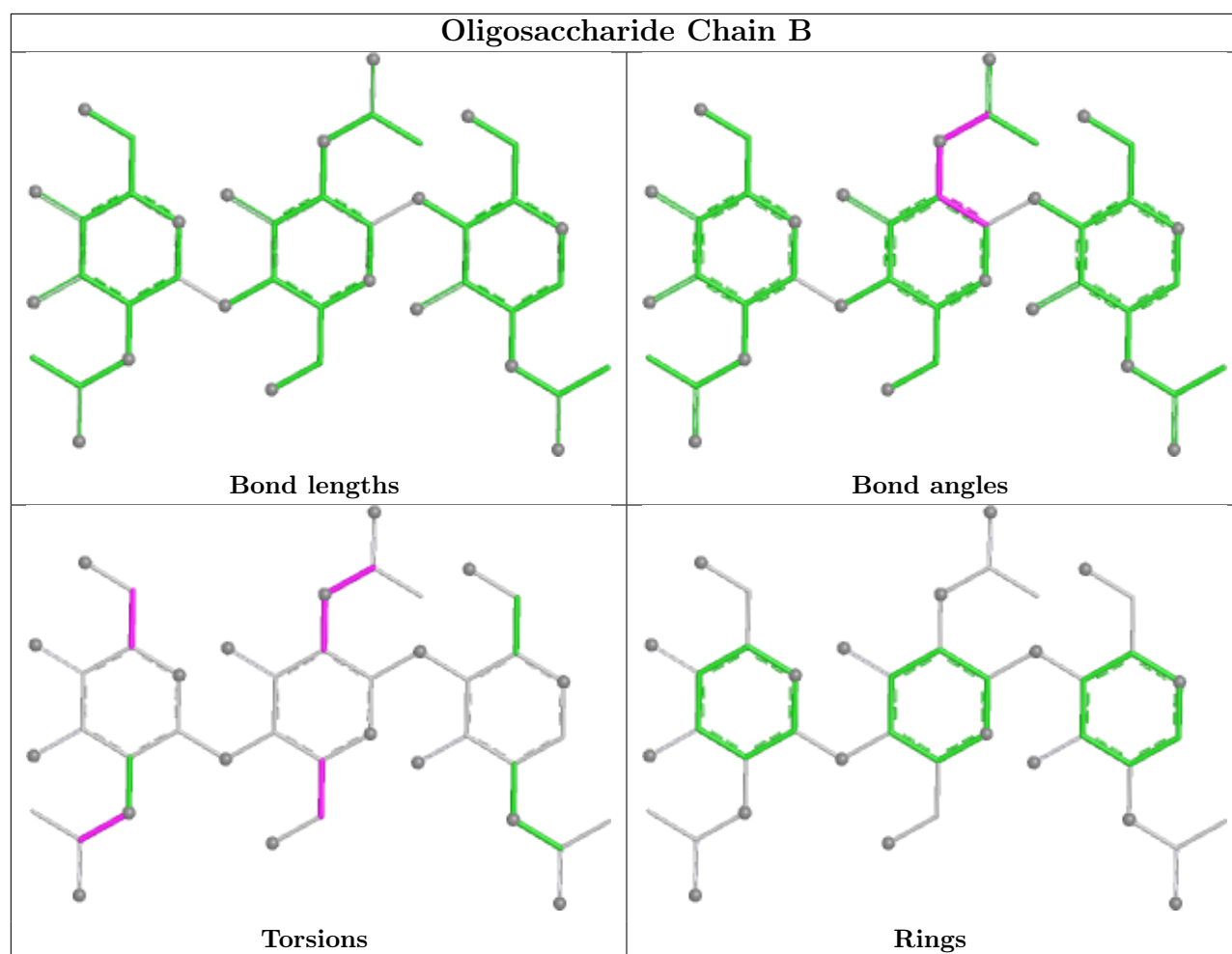
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O7-C7-N2-C2
6	F	3	NAG	C8-C7-N2-C2
6	F	3	NAG	O7-C7-N2-C2
6	F	4	NAG	C8-C7-N2-C2
6	F	4	NAG	O7-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
5	E	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7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

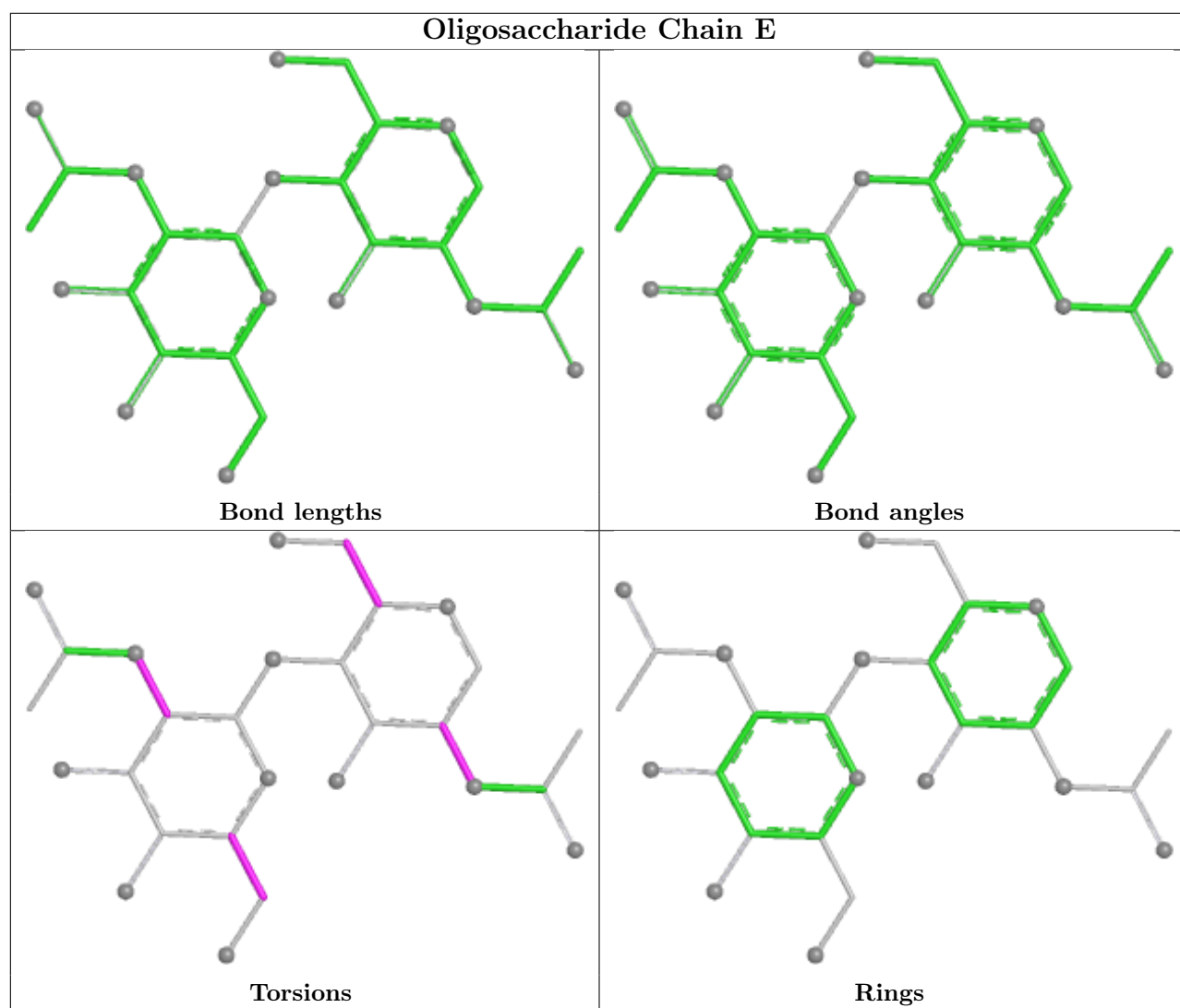
There are no ring outliers.

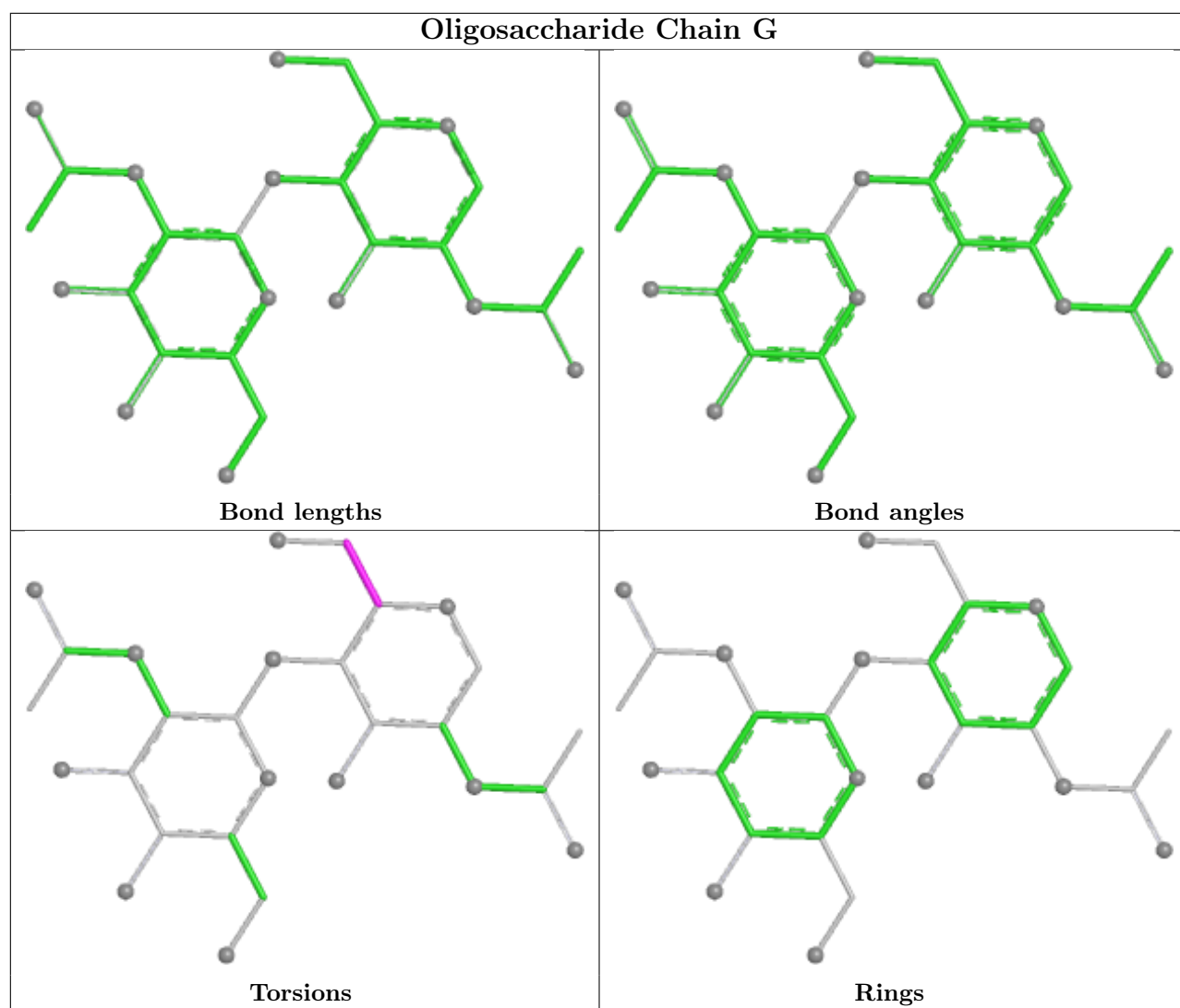
8 monomers are involved in 8 short contacts:

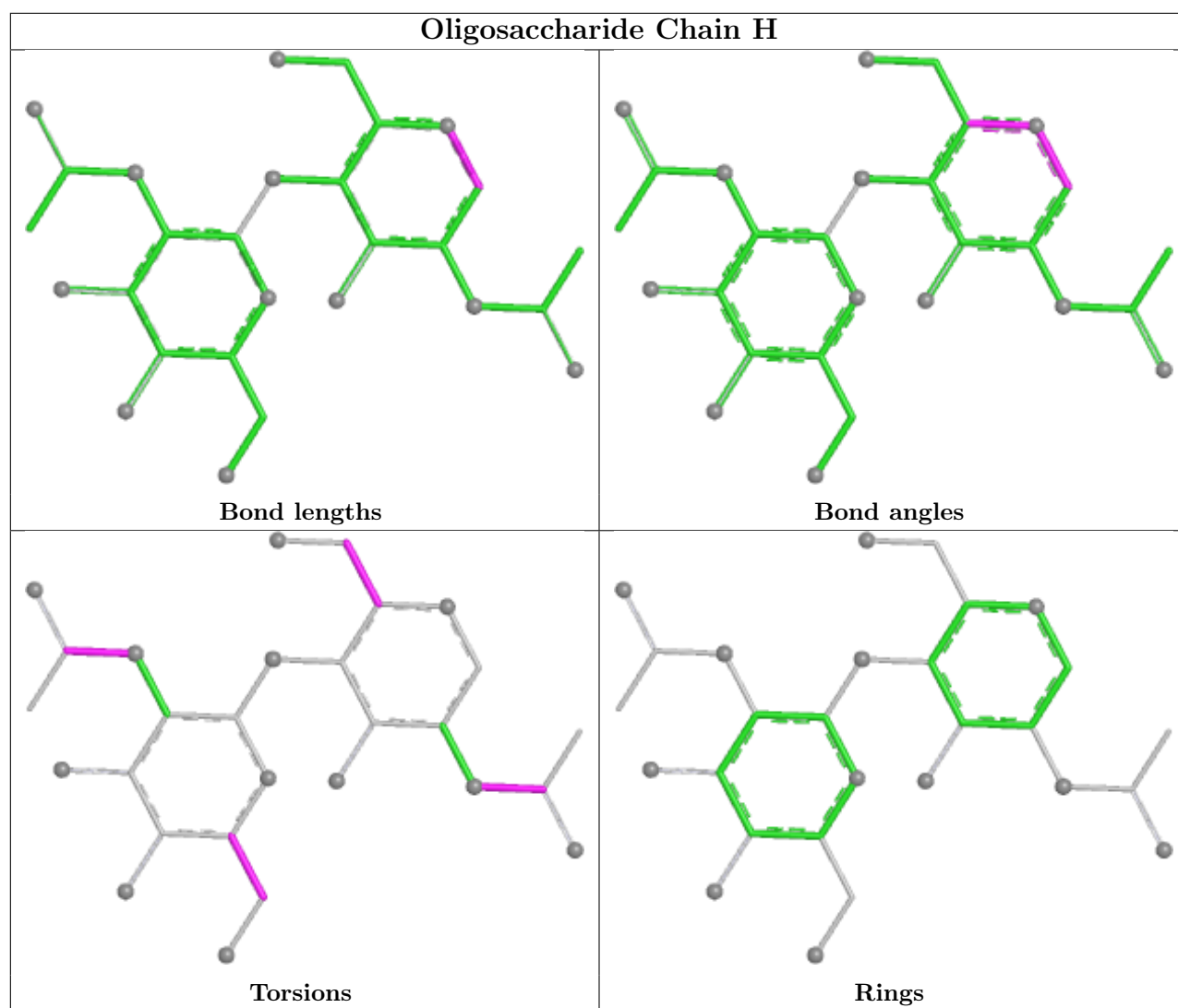
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
6	F	4	NAG	1	0
4	B	1	NAG	2	0
6	F	1	NAG	1	0
5	G	1	NAG	1	0
4	B	2	NAG	1	0
5	G	2	NAG	1	0
6	F	3	NAG	1	0

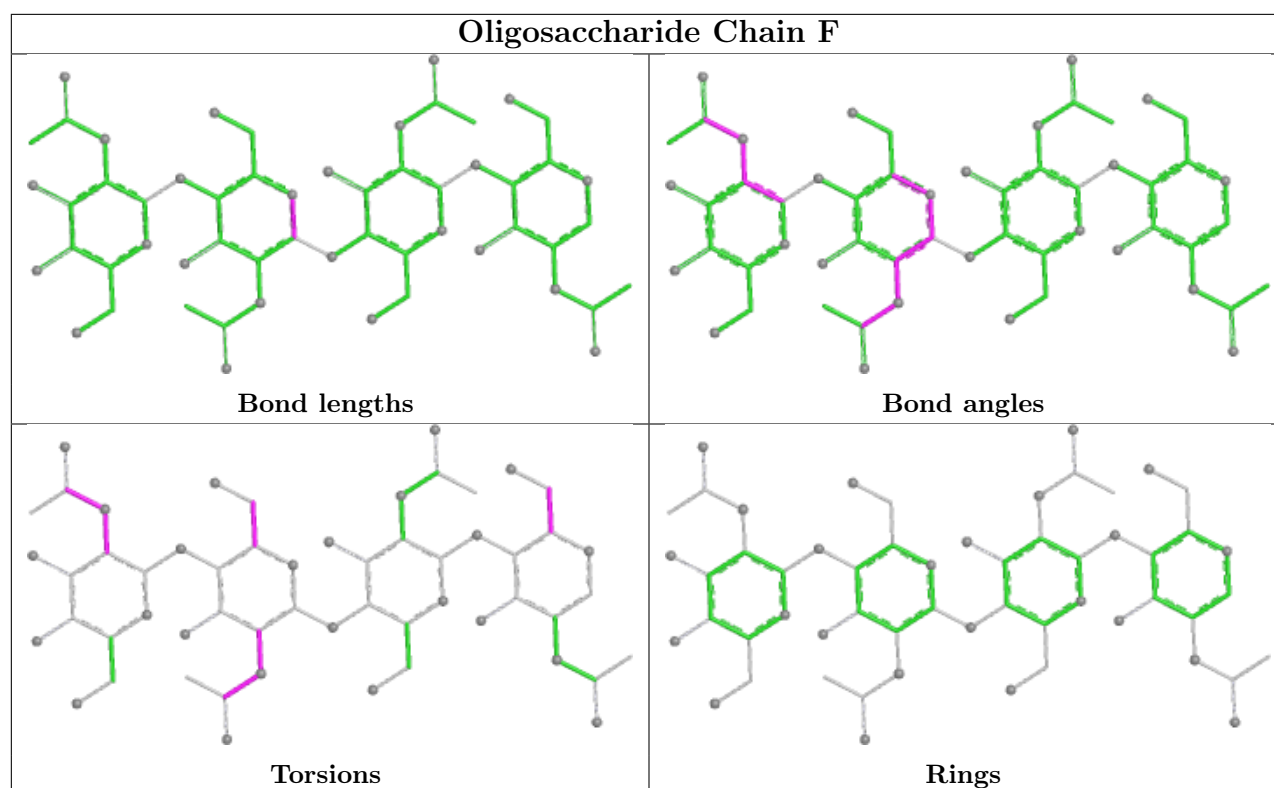
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
10	NAG	D	1201	2	14,14,15	0.43	0	17,19,21	0.65	0
10	NAG	D	1202	-	14,14,15	0.22	0	17,19,21	0.43	0
7	BB1	A	2201	-	28,33,33	1.89	5 (17%)	36,45,45	2.75	12 (33%)
9	3PE	A	2203	-	20,20,50	0.70	0	22,23,55	0.74	1 (4%)

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
10	NAG	D	1201	2	-	4/6/23/26	0/1/1/1
10	NAG	D	1202	-	-	0/6/23/26	0/1/1/1
7	BBi	A	2201	-	-	6/18/22/22	0/3/3/3
9	3PE	A	2203	-	-	8/21/21/54	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2201	BBi	CBC-IBD	-5.12	1.99	2.10
7	A	2201	BBi	CAR-IAS	-4.96	1.99	2.10
7	A	2201	BBi	CAW-CAV	3.64	1.61	1.50
7	A	2201	BBi	CAP-CAN	3.05	1.54	1.49
7	A	2201	BBi	CAW-NAX	2.82	1.53	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2201	BBi	CAM-CAN-CAP	8.74	131.40	119.45
7	A	2201	BBi	OAO-CAN-CAM	-5.86	112.00	119.41
7	A	2201	BBi	CAK-CAL-CAG	-5.67	116.80	120.38
7	A	2201	BBi	CAQ-CAP-CBE	-5.28	113.48	119.65
7	A	2201	BBi	CAC-CAD-CAE	4.52	123.57	112.85
7	A	2201	BBi	OAU-CAV-CAW	4.10	118.13	107.79
7	A	2201	BBi	CAR-CAT-CBC	-3.93	109.44	118.70
7	A	2201	BBi	CAQ-CAR-CAT	2.61	126.82	121.66
7	A	2201	BBi	OAU-CAT-CBC	2.53	126.61	120.81
9	A	2203	3PE	O12-P-O14	2.42	123.71	112.44
7	A	2201	BBi	CBE-CBC-CAT	2.36	126.31	121.66
7	A	2201	BBi	OAO-CAN-CAP	-2.22	116.60	120.15
7	A	2201	BBi	CAT-CAR-IAS	-2.01	116.02	119.32

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2201	BBi	CAC-CAD-CAE-CAM
9	A	2203	3PE	C1-O11-P-O12
9	A	2203	3PE	C1-O11-P-O13
9	A	2203	3PE	C11-O13-P-O14
9	A	2203	3PE	O13-C11-C12-N
9	A	2203	3PE	O11-C1-C2-O21

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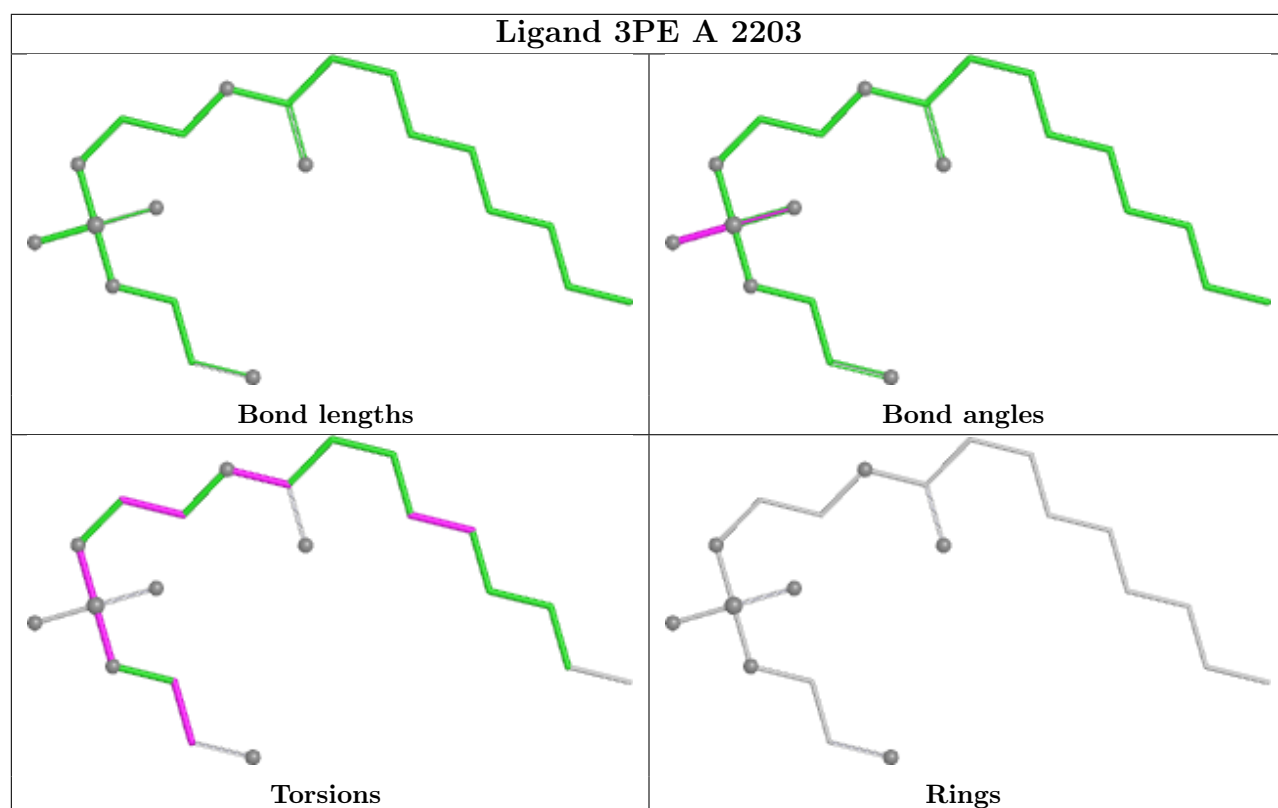
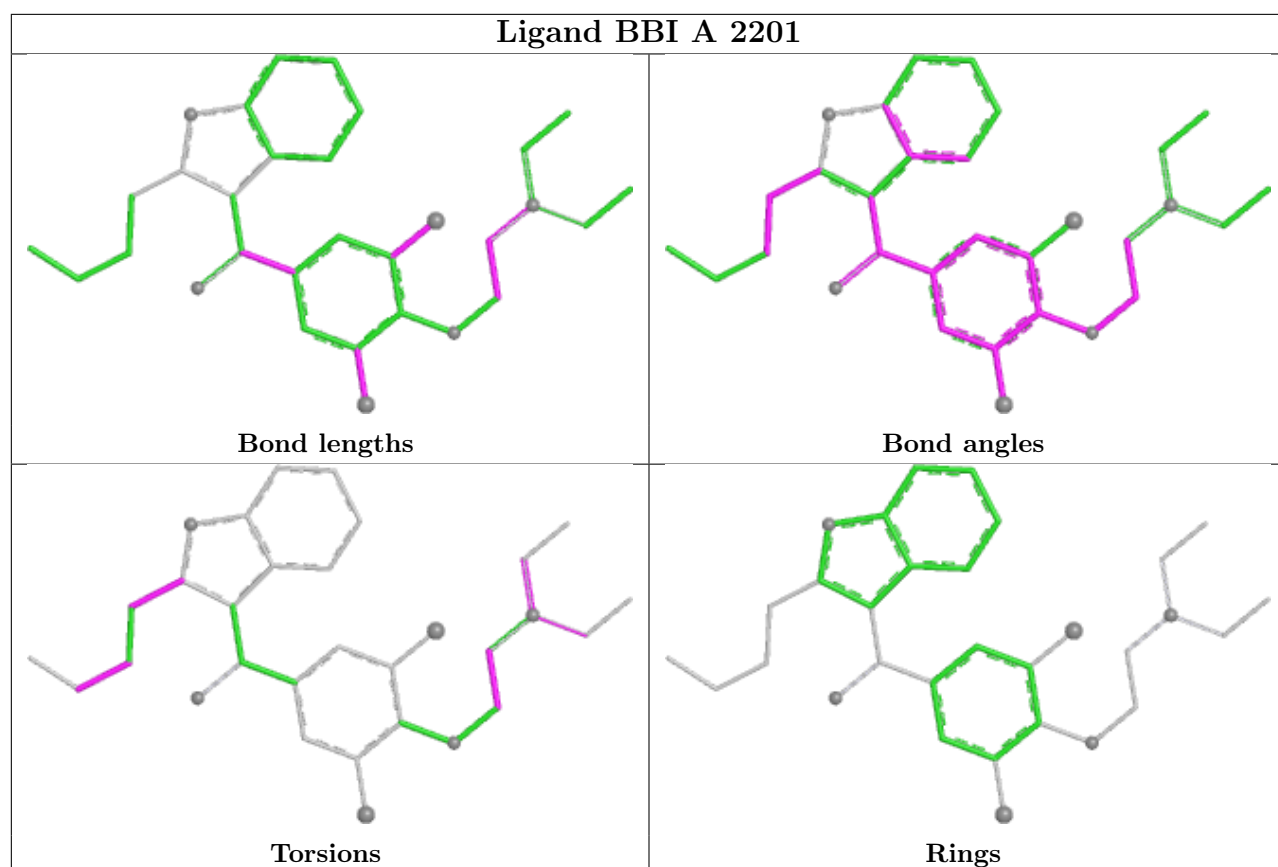
Mol	Chain	Res	Type	Atoms
10	D	1201	NAG	O5-C5-C6-O6
10	D	1201	NAG	C4-C5-C6-O6
7	A	2201	BBi	OAU-CAV-CAW-NAX
9	A	2203	3PE	C22-C21-O21-C2
9	A	2203	3PE	O22-C21-O21-C2
7	A	2201	BBi	CBB-CBA-NAX-CAW
7	A	2201	BBi	CBB-CBA-NAX-CAY
7	A	2201	BBi	CAZ-CAY-NAX-CAW
10	D	1201	NAG	C3-C2-N2-C7
10	D	1201	NAG	C1-C2-N2-C7
9	A	2203	3PE	C23-C24-C25-C26
7	A	2201	BBi	CAA-CAB-CAC-CAD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2203	3PE	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 than 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.



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.

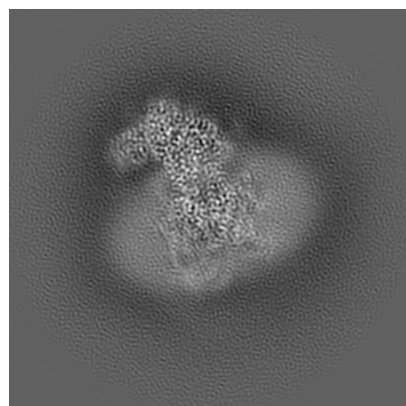
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27907. These allow visual inspection of the internal detail of the map and identification of artifacts.

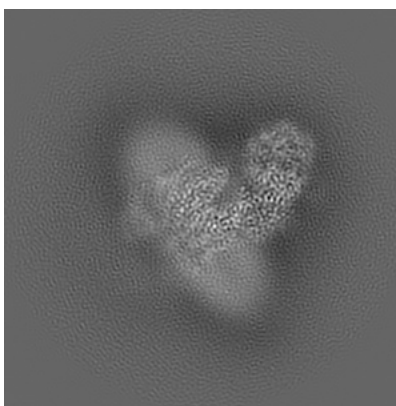
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

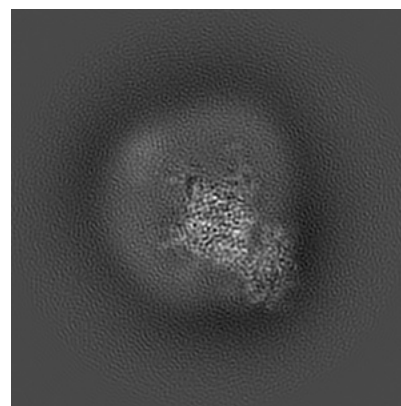
6.1.1 Primary map



X

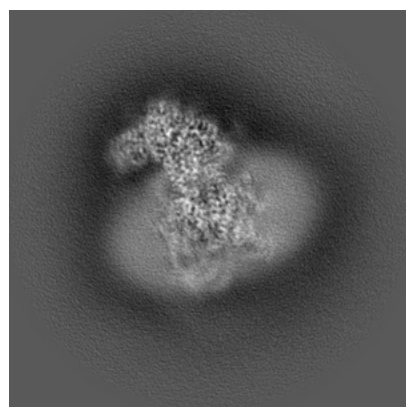


Y

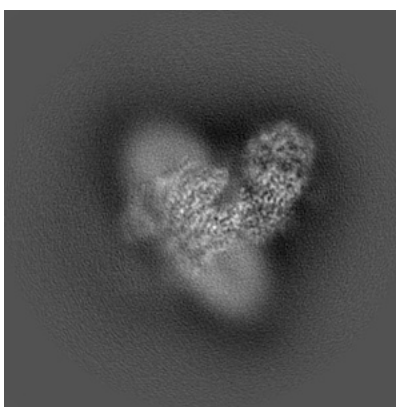


Z

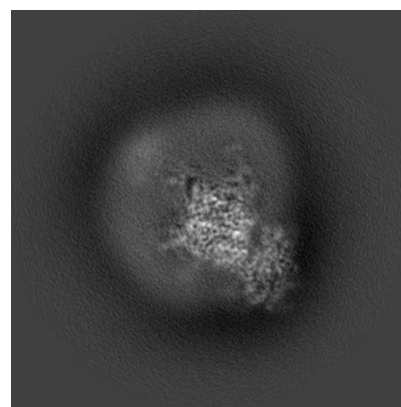
6.1.2 Raw map



X



Y

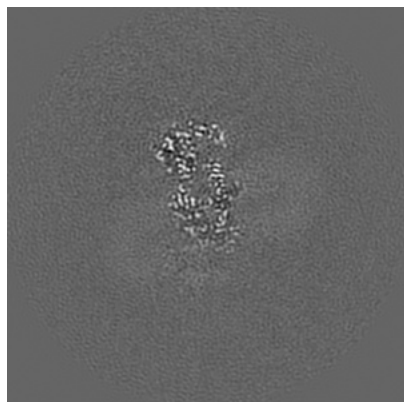


Z

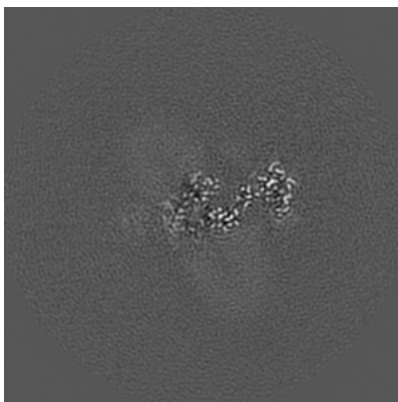
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

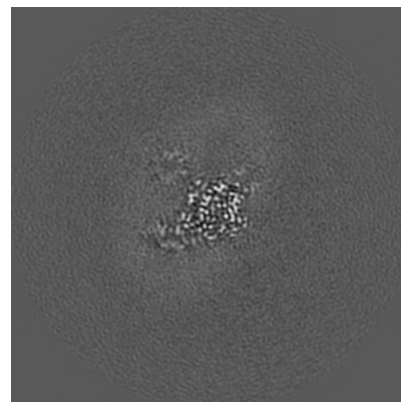
6.2.1 Primary map



X Index: 140

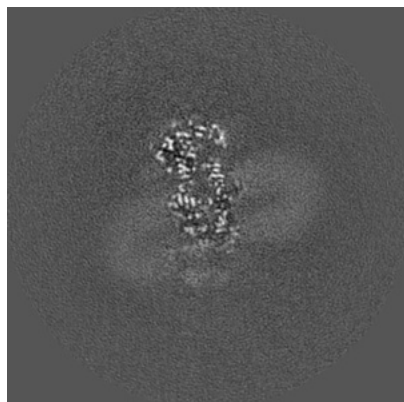


Y Index: 140

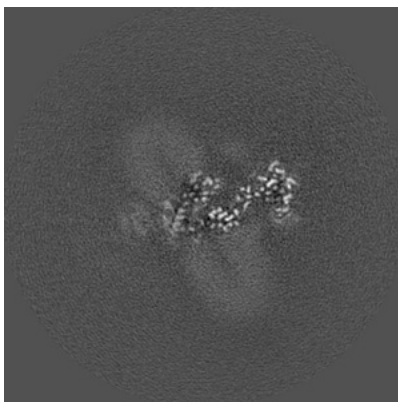


Z Index: 140

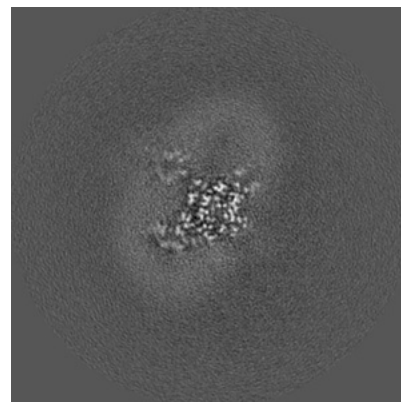
6.2.2 Raw map



X Index: 140



Y Index: 140

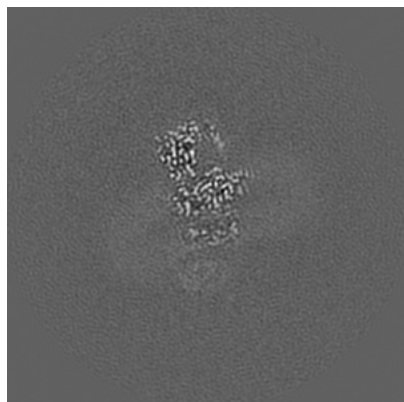


Z Index: 140

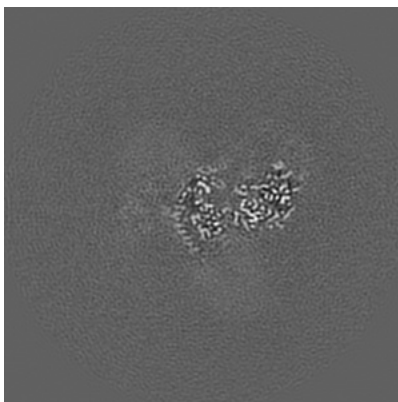
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

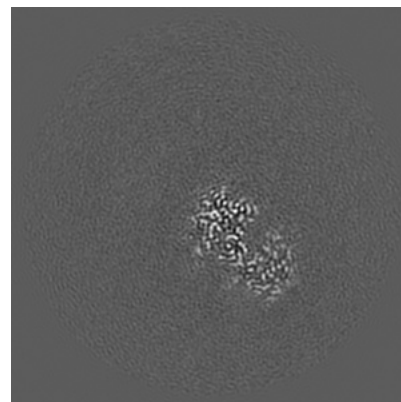
6.3.1 Primary map



X Index: 135

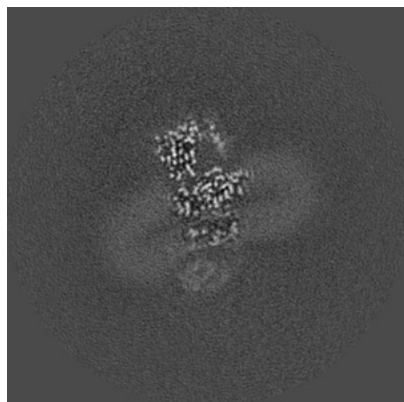


Y Index: 130

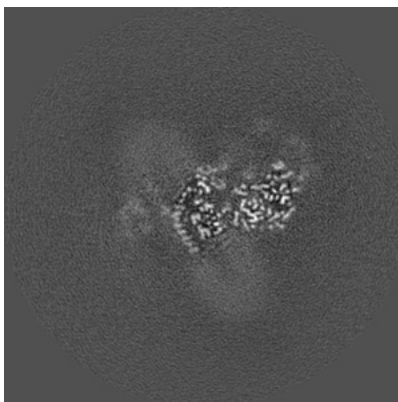


Z Index: 190

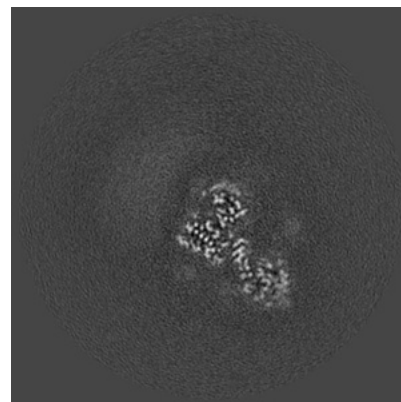
6.3.2 Raw map



X Index: 135



Y Index: 130

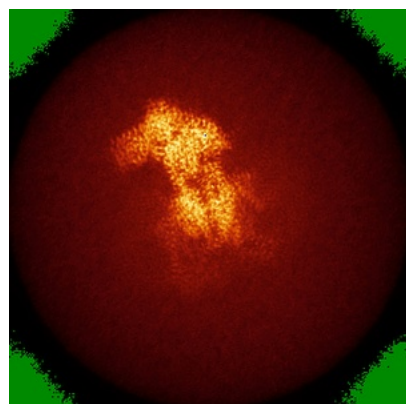


Z Index: 182

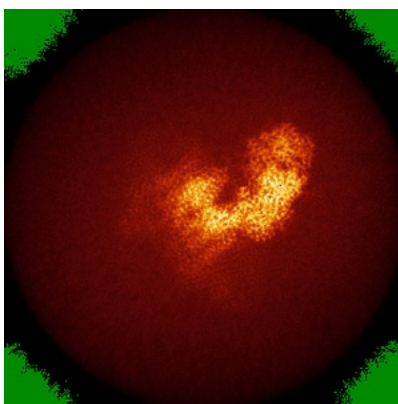
The images above show the largest variance slices of the map in three orthogonal directions.

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

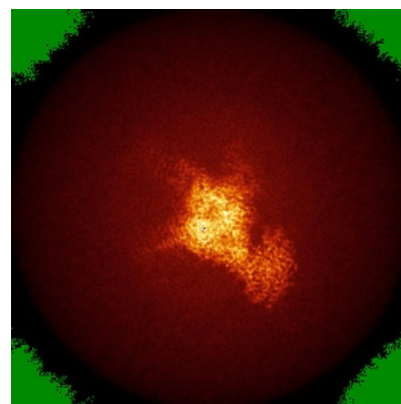
6.4.1 Primary map



X

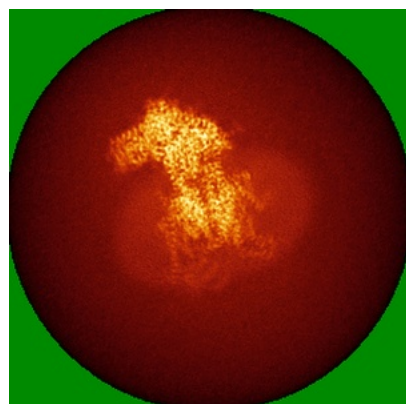


Y

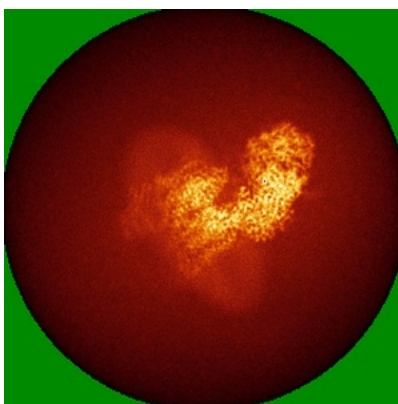


Z

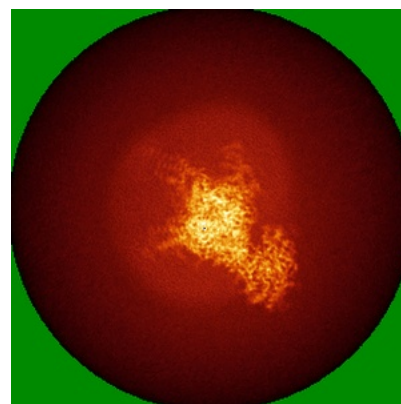
6.4.2 Raw map



X



Y

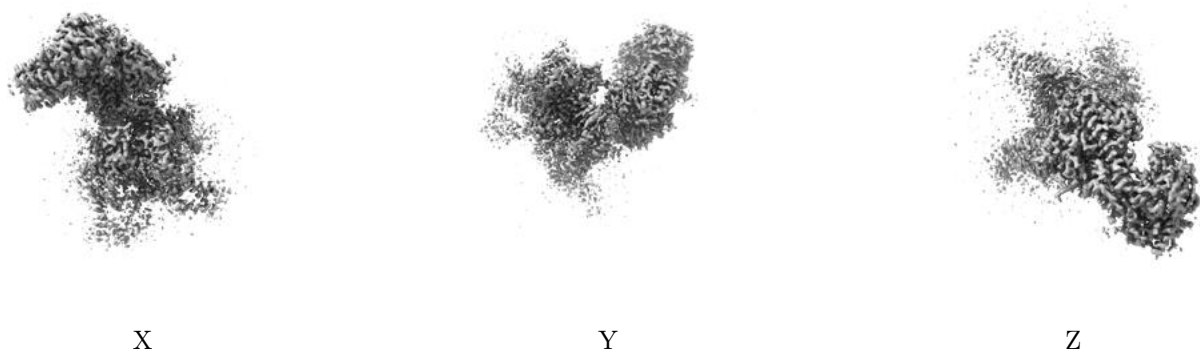


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

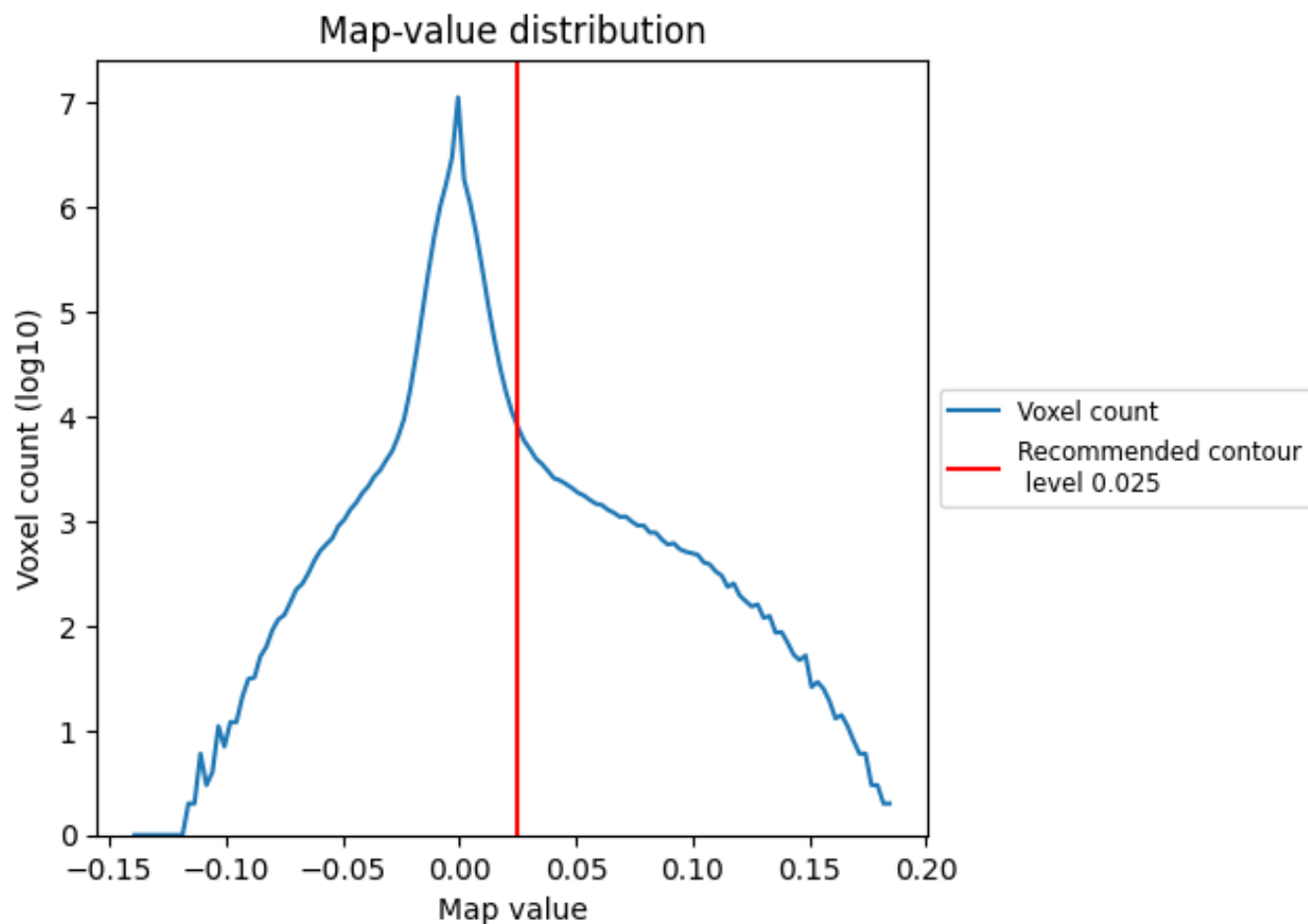
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

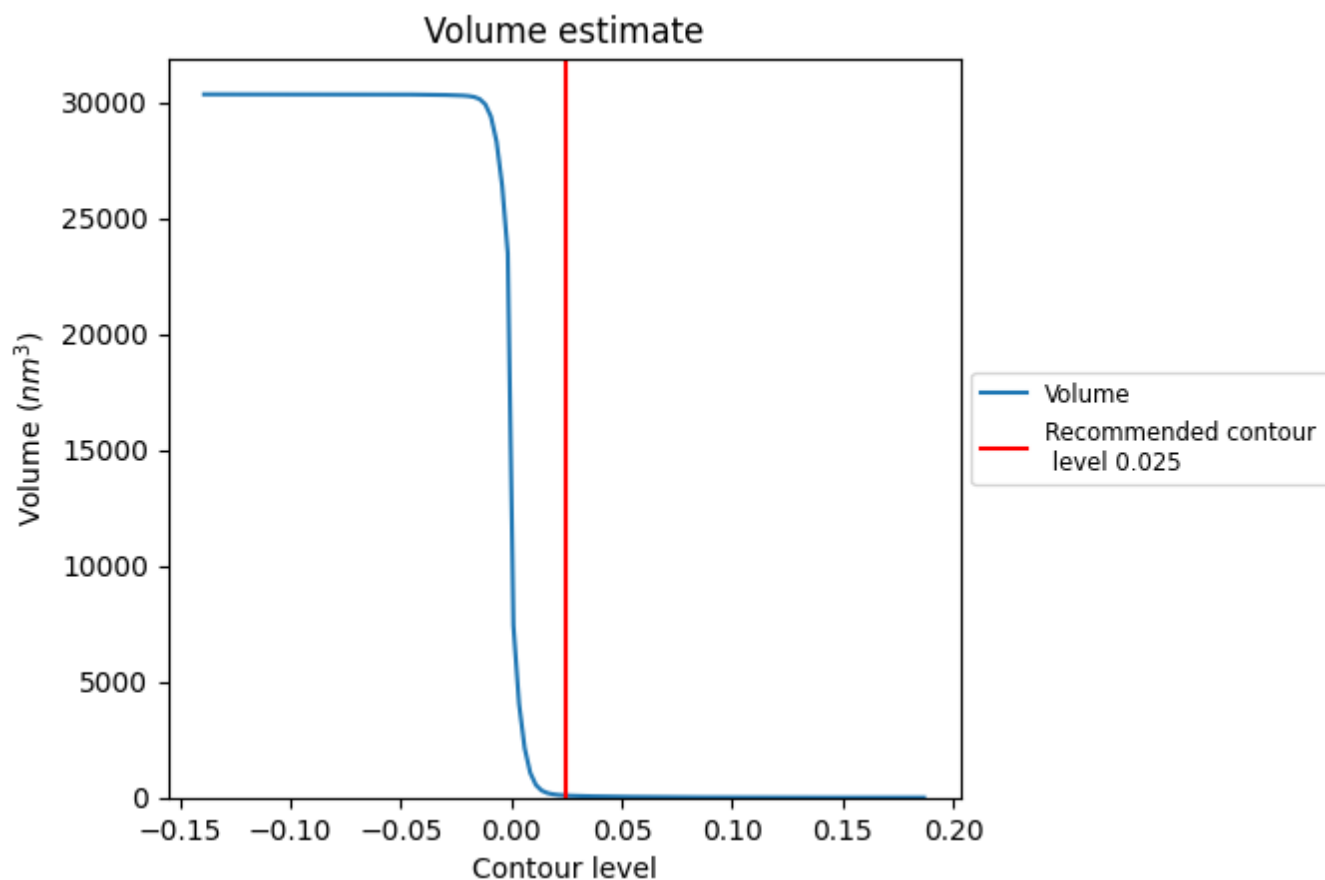
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

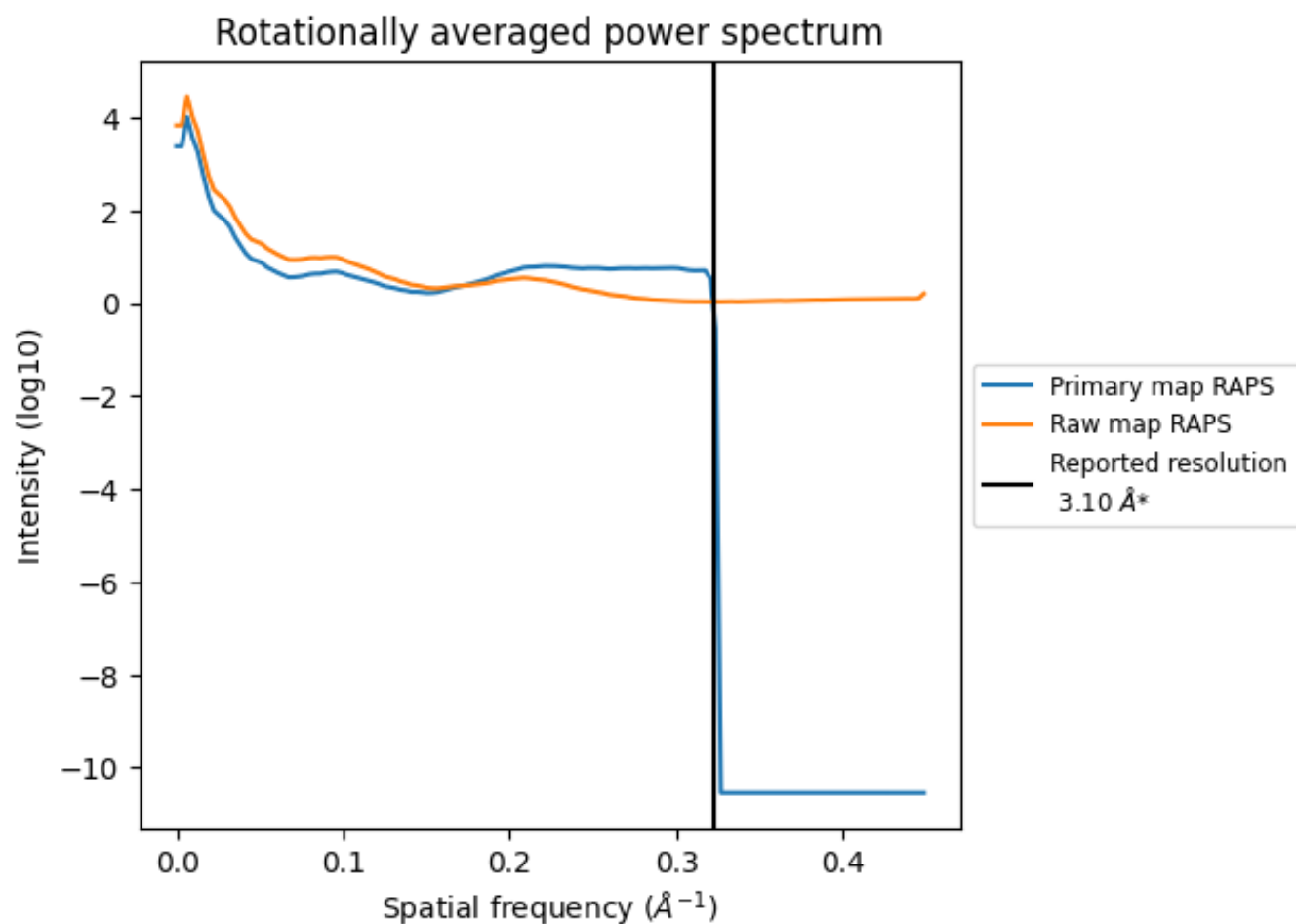
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 80 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 ⓘ

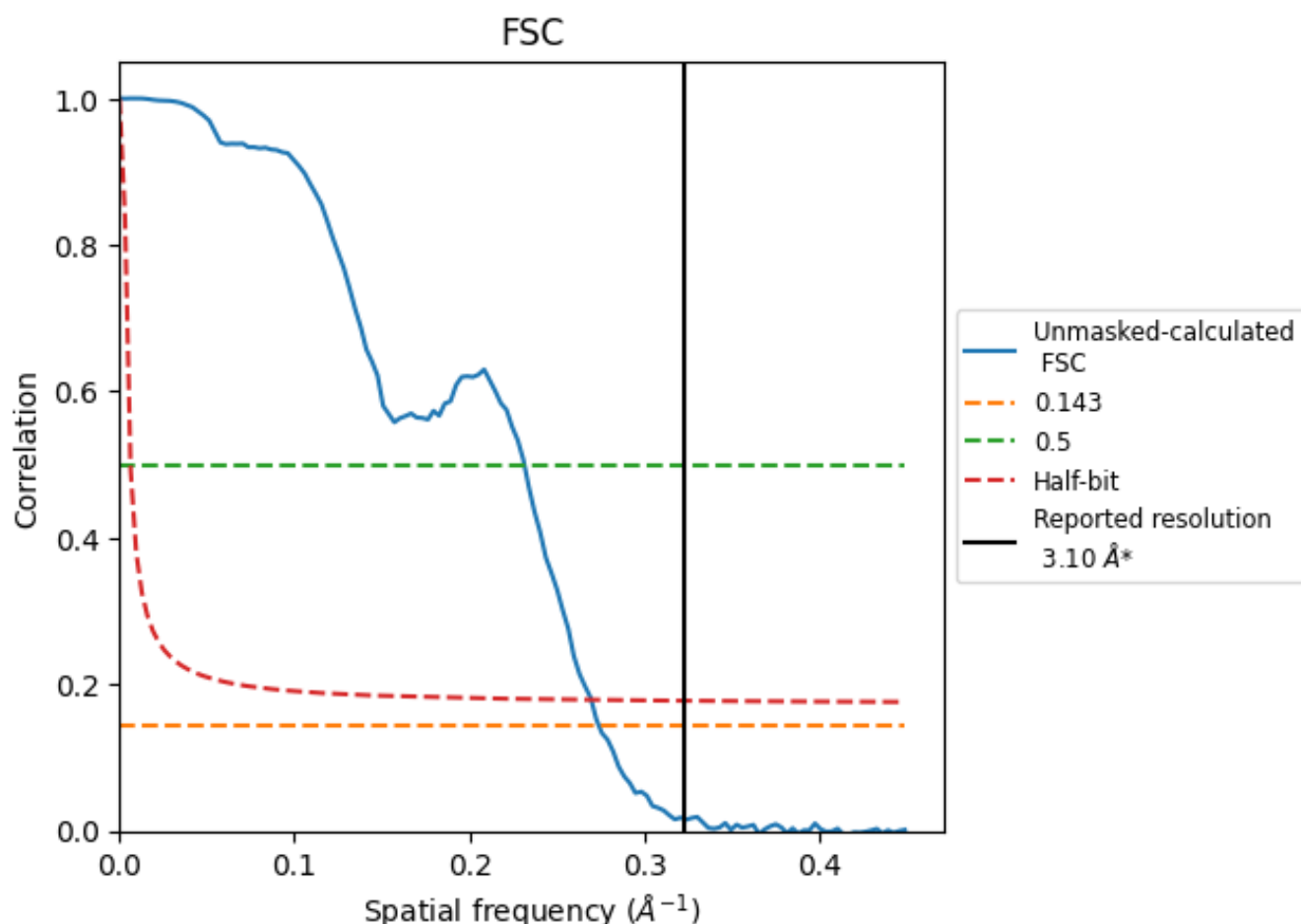


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

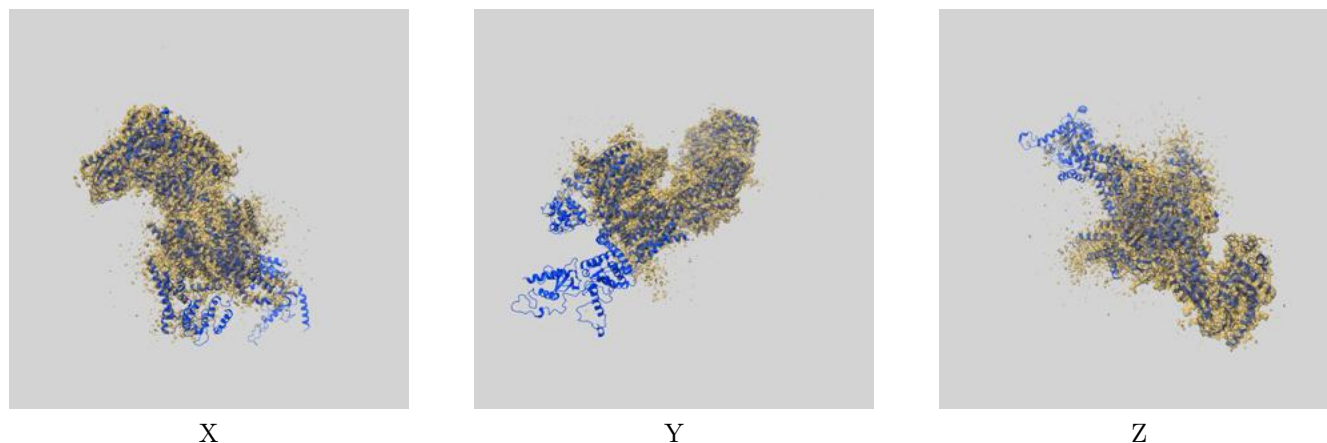
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.32	3.71

*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 3.65 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

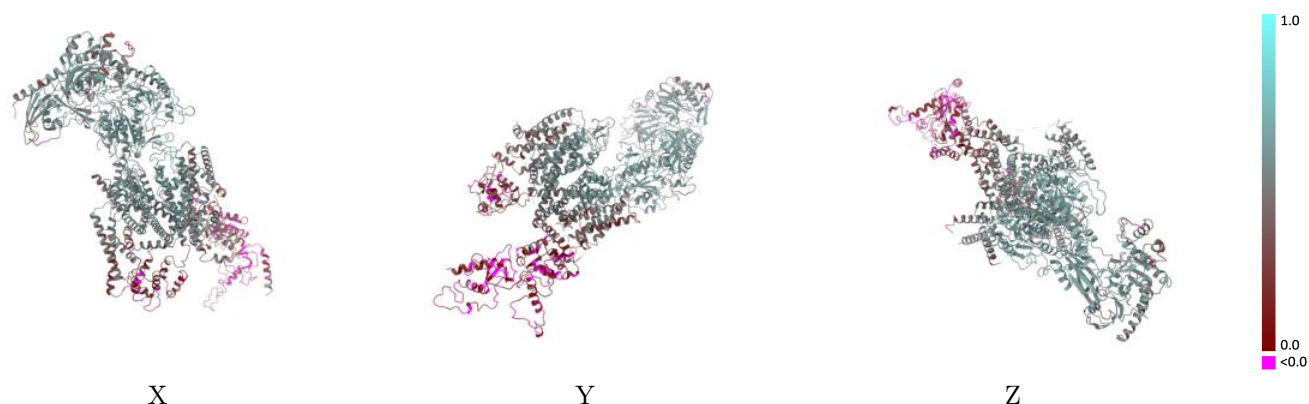
This section contains information regarding the fit between EMDB map EMD-27907 and PDB model 8E59. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



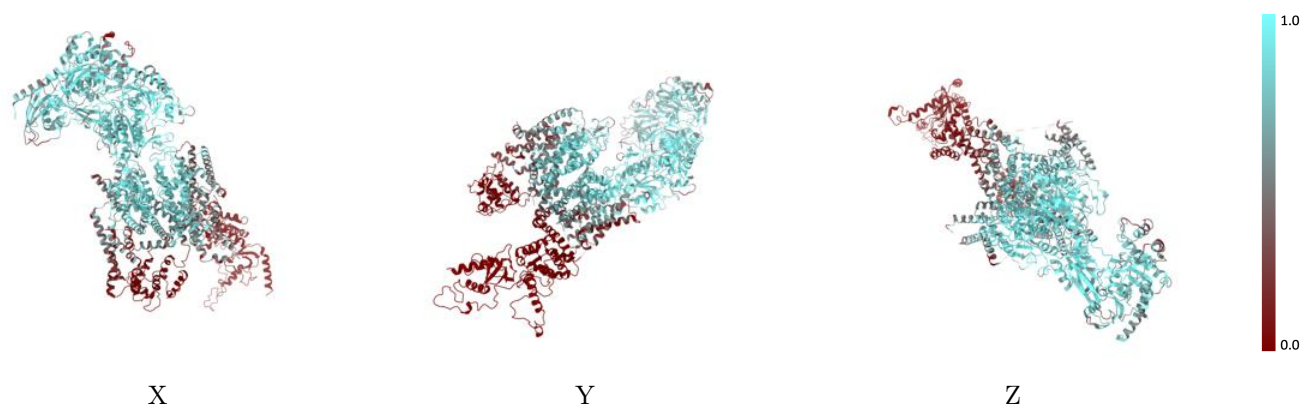
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



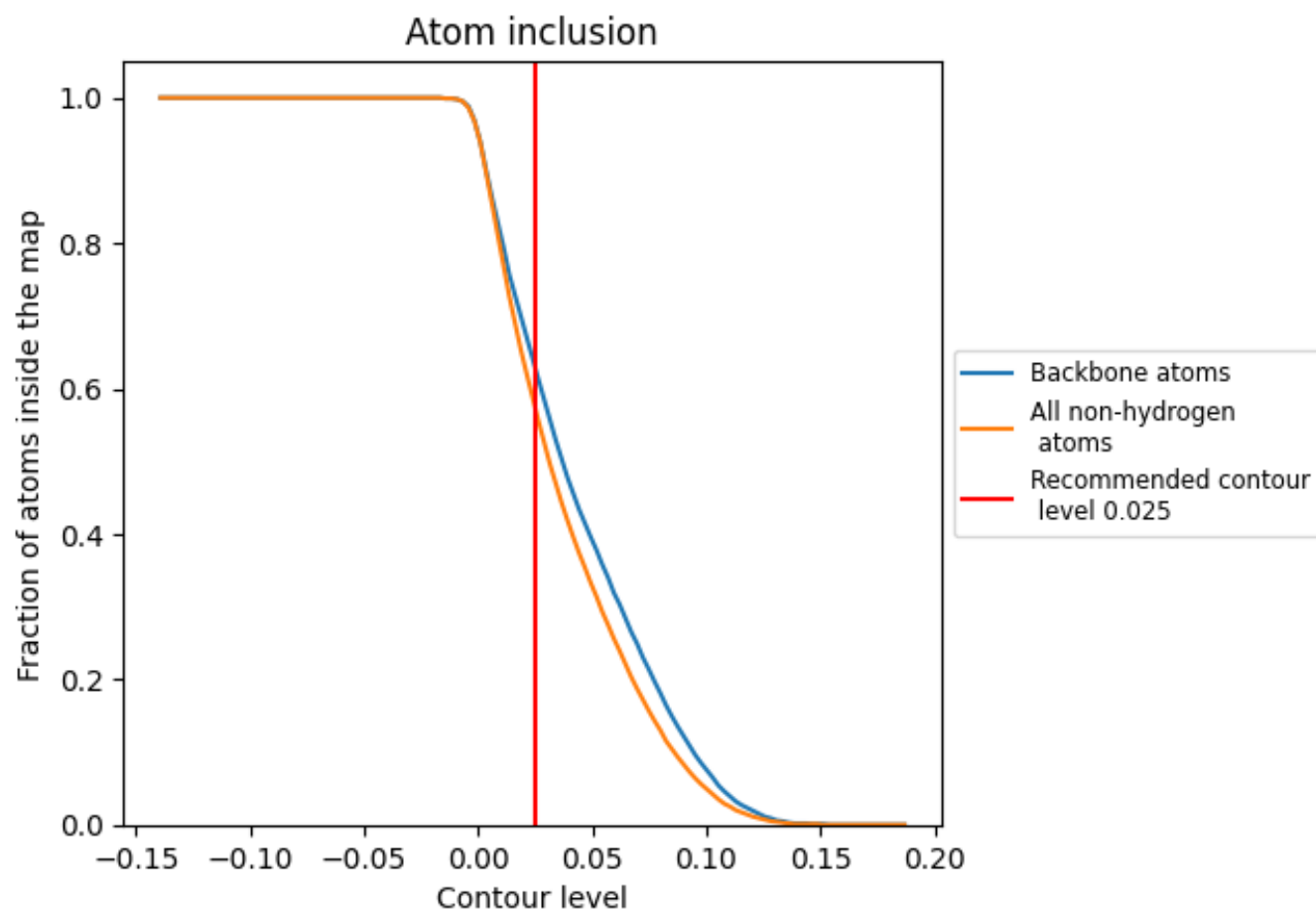
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 57% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5740	<div></div> 0.4460
A	<div></div> 0.5520	<div></div> 0.4570
B	<div></div> 0.4760	<div></div> 0.3740
C	<div></div> 0.0000	<div></div> 0.1040
D	<div></div> 0.7970	<div></div> 0.5490
E	<div></div> 0.2500	<div></div> 0.2890
F	<div></div> 0.6070	<div></div> 0.4050
G	<div></div> 0.4290	<div></div> 0.3650
H	<div></div> 0.5360	<div></div> 0.3400

1.0

0.0

<0.0