



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:38 PM UTC

PDB ID : 8EPL / pdb_00008epl
EMDB ID : EMD-28529
Title : Human R-type voltage-gated calcium channel Cav2.3 at 3.1 Angstrom resolution
Authors : Gao, S.; Yao, X.; Yan, N.
Deposited on : 2022-10-06
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary 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:

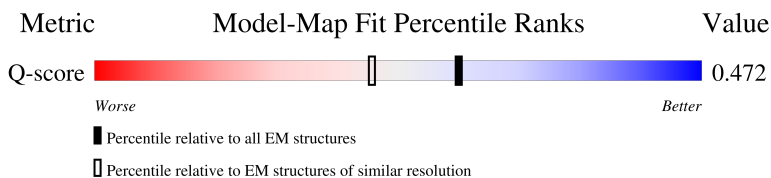
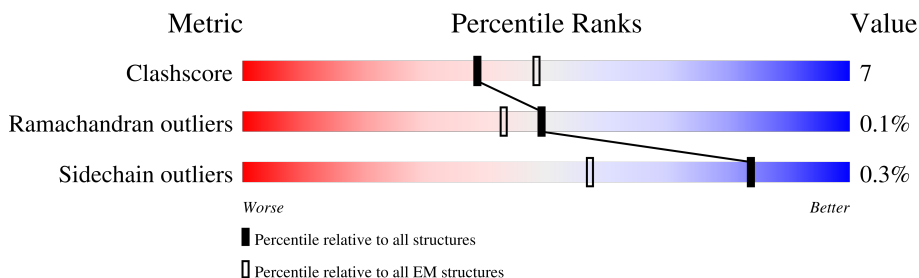
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	2313	15% 46% 9% 45%
2	B	484	66% 55% 12% 33%
3	C	1103	16% 70% 16% 14%
4	D	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
4	E	2	100%
			50%50%
4	G	2	50%
			50%50%
4	H	2	50%
			50%50%
5	F	4	50%
			50%50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20953 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 R-type calcium channel subunit alpha-1E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1274	Total	C	N	O	S	0	0
			10316	6777	1688	1775	76		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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

- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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

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



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

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

cetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

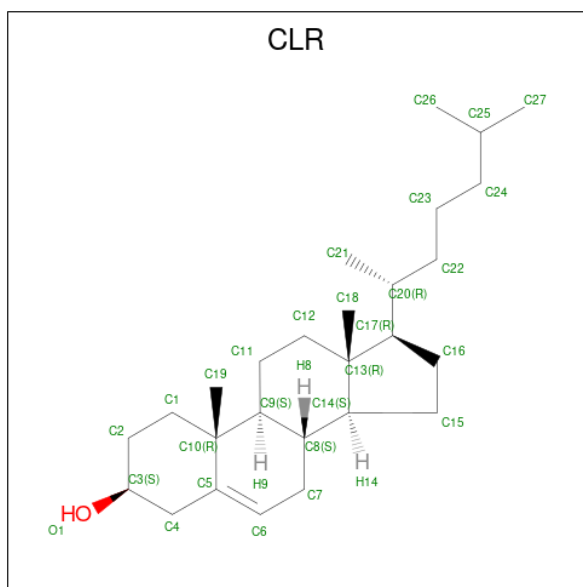


Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	4	Total	C	N	O	0	0
			56	32	4	20		

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

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



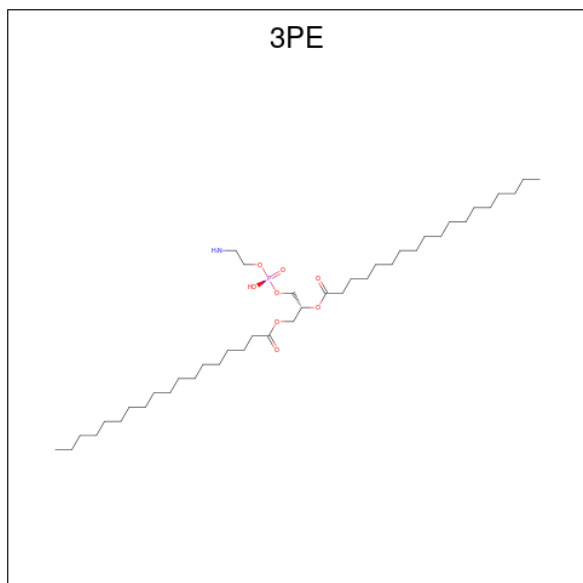
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	

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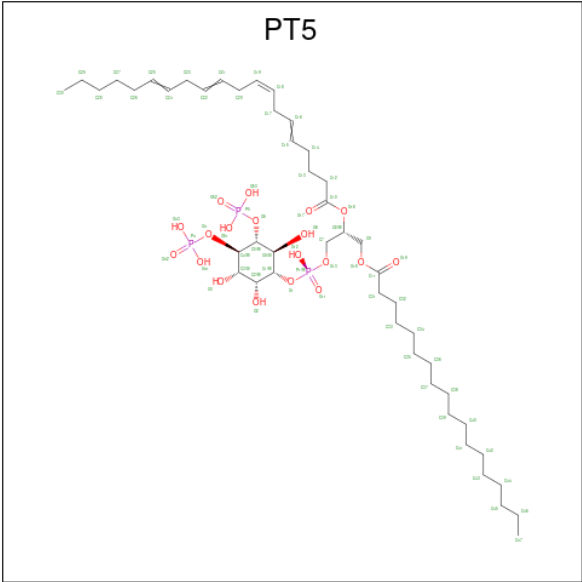
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	
7	A	1	Total	C	O	0
			28	27	1	

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



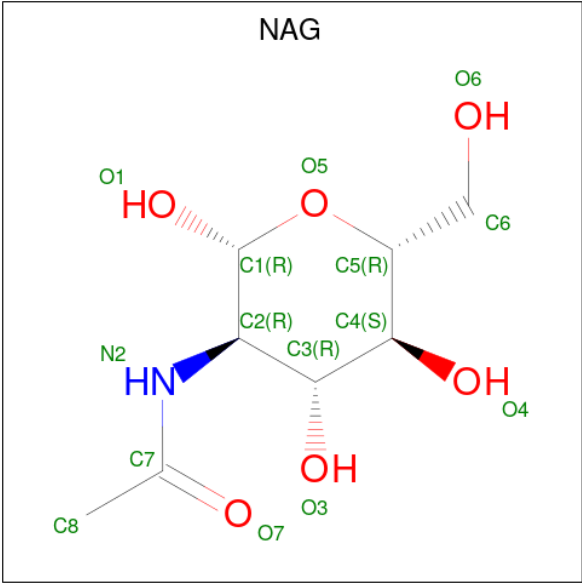
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
8	A	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 9 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	A	1	64	42	19	3	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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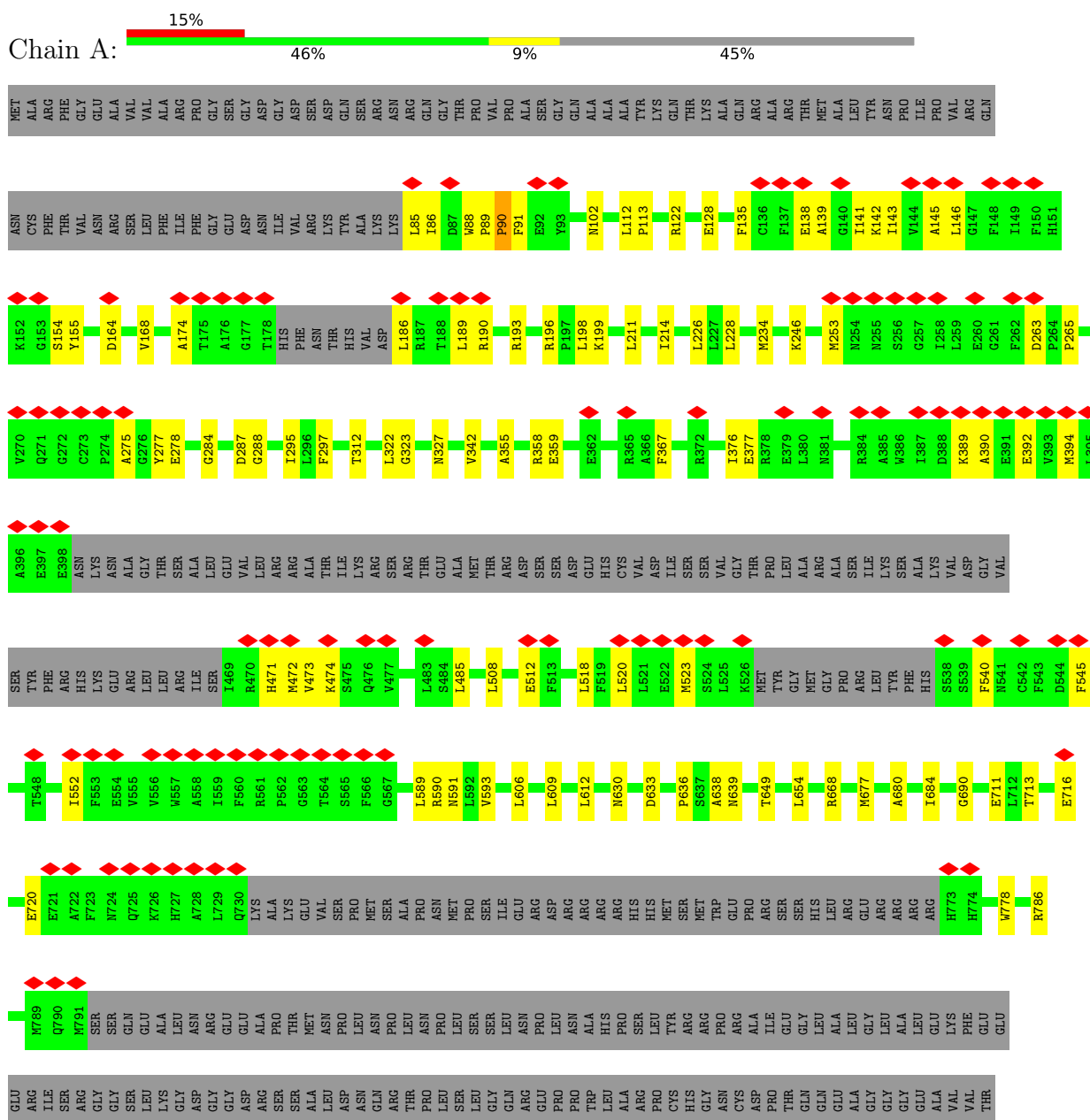
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	C	1	14	8	1	5	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

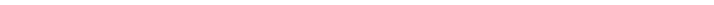
- Molecule 1: Voltage-dependent R-type calcium channel subunit alpha-1E





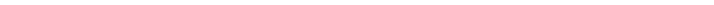
PRO	GLY	PRO	LEU	SER
MET	LEU	GLY	ALA	SER
MET	HIS	HIS	LEU	LEU
CYS	GLU	ASP	ASP	ILE
GLY	ASP	SER	ASP	HIS
ALA	HIS	SER	ASP	ALA
VAL	HIS	SER	HIS	GLY
ASN	ALA	ALA	ALA	GLY
ASN	SER	SER	SER	ILE
LEU	ASP	SER	ASP	SER
LEU	CYS	PRO	CYS	PRO
SER	GLY	PRO	GLY	PRO
ASP	GLU	GLU	GLU	ASP
THR	GLU	THR	GLU	ALA
GLU	GLU	THR	THR	GLY
ASP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

- Molecule 2: Voltage-dependent L-type calcium channel subunit beta-3

Chain B:  66% 55% 12% 33%

Lys	Ser	His61	Q301	S241	V181	P121	A61
Asp	Ser	His	R302	S242	L182	Q122	F62
Ser	Arg	Pro	R303	A243	V183	R123	A63
Tyr	His	Ala	I304	R244	G184	L124	V64
	Leu	Pro		S245	P185	E125	A65
Leu	Glu	Gly	R305	S246	S186	S126	T66
Pro	Glu	Gly	R307	I247	L187	I127	N67
Asp	Tyr	Leu	G308	A248	K188	R128	V68
Ala	Leu	Leu	K309	E249	G189	L129	S69
Asp	Gly	Gly	S310	V250	Y190	K130	Y70
Ala	Pro	Pro	S311	Q251	E191	Q131	C71
Tyr	Ser	Ser	Q311	S252	V192	E132	G72
Gln	Ala	Ala	M312	E253	T193	Q133	
Leu	Leu	Ile	K313	E254	D194	K134	V73
Tyr	Pro	Gly	H314	E255	M195	A135	L74
Gln	Pro	Gly	L315	E256	M196	R136	D75
Pro	His	Gln	T316	R256	M196	R137	E76
His	Gln	Asn	V317	I257	Q197	R137	E77
Gln	Gln	Gln	Q318	F258	K198	S138	C78
His	His	Gln	M319	E259	A199	G139	F79
Tyr	Ser	Leu	M320	L260	L200	N140	V80
Ser	Leu	Gly	A321	A261	F201	P141	Q81
Gly	Gly	Leu	Y322	K262	D202	S142	G82
Asp	Pro	Arg	D323	S263	F203	S143	S83
Pro	Arg	Gly	K324	L264	L204	L144	G84
Ser	Ala	Glu	L325	Q265	K205	S145	V85
Ala	Glu	His	L326	L266	H206	D146	N86
His	Ser	His	V326	V267	R207	I147	F87
Ser	Asp	Pro	Q327	V268	F208	G148	E88
Asp	Pro	Leu	C328	V269	D209	N149	A89
Pro	Gln	Glu	P329	L269	R150	R150	K90
Gln	Arg	Asp	P330	D270	R211	R151	D91
Leu	Leu	Ser	E331	A271	I211	S152	F92
Leu	Met	Ala	S332	D272	I212	P153	L93
Ala	Met	Ala	F333	T273	S213	P154	H94
Gln	Pro	Pro	D334	I274	I214	P154	V44
Asp	Ser	Ser	V335	N275	T215	P155	E45
Glu	Glu	Glu	I336	H276	R216	S156	K96
His	Ala	Ala	L337	P277	V217	L157	E97
Asn	Ser	Ser	D338	A278	T218	A158	K98
His	His	Ser	E339	Q279	A219	K159	Y99
Ser	Asp	Asp	N340	L280	D220	Q160	S100
Arg	Arg	Arg	Q341	A281	L221	K161	N101
Gln	Gln	Gln	L342	K282	S222	Q162	D102
Trp	Trp	Trp	E343	T283	L223	K163	V103
Arg	Thr	Thr	D344	S284	A224	Q164	V104
Gly	Gly	Gly		L285	K225	A165	I105
Asn	Ser	Ser	A345	A286	R226	E166	G106
Ser	Arg	Arg	C346	E287	S227	H167	R107
Pro	Gln	Gln	E347	I288	V228	V168	L108
Arg	Arg	Arg	H348	I289	L229	P169	V109
Trp	Trp	Trp	L349	V290	N230	P170	K110
Pro	Pro	Pro	A350	F291	N231	Y171	E111
			E351	V292	P232	D172	G112
			Y352	K293	G233	V173	G113
			L353	V294	K234	V174	D114
			E354	S295	R235	P175	I115
			V355	S296	T236	S176	A116
			Y356	P297	I237	M177	F117
			W357	K298	I238	R178	I118
			R358	V299	E239	P179	P119
			A359	L300	R240	V180	S120
			T360				

- Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain C:  16% 70% 16% 14%

[illegible]



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	118244	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	0.194	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: CA, PT5, 3PE, NAG, CLR

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	0.11	0/10565	0.27	0/14299
2	B	0.10	0/2624	0.28	0/3544
3	C	0.12	0/7728	0.28	0/10477
All	All	0.11	0/20917	0.28	0/28320

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	10316	0	10452	146	0
2	B	2575	0	2619	35	0
3	C	7570	0	7368	121	0
4	D	28	0	25	2	0
4	E	28	0	25	1	0
4	G	28	0	25	1	0
4	H	28	0	25	3	0
5	F	56	0	49	4	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	140	0	230	10	0
8	A	76	0	103	1	0
9	A	64	0	66	5	0
10	C	42	0	39	2	0
All	All	20953	0	21026	308	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.

The worst 5 of 308 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:113:PRO:HG3	1:A:630:ASN:HD21	1.38	0.87
3:C:895:ASN:HB3	4:H:1:NAG:H2	1.67	0.76
3:C:1001:ARG:HG2	3:C:1019:GLU:HB2	1.66	0.75
1:A:1401:ILE:HD11	7:A:2402:CLR:H181	1.70	0.74
1:A:89:PRO:HB2	1:A:90:PRO:HD3	1.69	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1258/2313 (54%)	1203 (96%)	54 (4%)	1 (0%)	48	78
2	B	322/484 (66%)	311 (97%)	10 (3%)	1 (0%)	36	67
3	C	936/1103 (85%)	885 (95%)	51 (5%)	0	100	100
All	All	2516/3900 (64%)	2399 (95%)	115 (5%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
2	B	287	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1123/2023 (56%)	1120 (100%)	3 (0%)	86	87
2	B	287/426 (67%)	285 (99%)	2 (1%)	76	82
3	C	837/971 (86%)	836 (100%)	1 (0%)	88	90
All	All	2247/3420 (66%)	2241 (100%)	6 (0%)	84	87

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	118	ILE
2	B	331	GLU
3	C	595	GLN
1	A	186	LEU
1	A	86	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	694	ASN
3	C	753	GLN
3	C	1042	ASN
3	C	885	HIS
3	C	723	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	D	1	4,3	14,14,15	0.35	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.44	0	17,19,21	1.34	2 (11%)
4	NAG	E	1	4,3	14,14,15	0.55	0	17,19,21	0.45	0
4	NAG	E	2	4	14,14,15	0.60	0	17,19,21	0.84	0
5	NAG	F	1	5,3	14,14,15	0.38	0	17,19,21	0.67	0
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	0.58	0
5	NAG	F	3	5	14,14,15	1.05	1 (7%)	17,19,21	1.25	1 (5%)
5	NAG	F	4	5	14,14,15	0.62	1 (7%)	17,19,21	1.33	2 (11%)
4	NAG	G	1	4,3	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	H	1	4,3	14,14,15	0.81	1 (7%)	17,19,21	0.64	0
4	NAG	H	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.22	1 (5%)

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

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	NAG	O5-C1	3.64	1.49	1.43
4	H	2	NAG	O5-C1	3.27	1.49	1.43
4	H	1	NAG	C1-C2	2.52	1.55	1.52
5	F	4	NAG	C1-C2	2.07	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	NAG	C1-O5-C5	4.94	118.81	112.19
4	H	2	NAG	C1-O5-C5	4.60	118.35	112.19
4	D	2	NAG	C2-N2-C7	4.55	129.00	122.90
5	F	4	NAG	C2-N2-C7	4.55	128.99	122.90
5	F	4	NAG	C1-C2-N2	2.17	113.85	110.43

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C1-C2-N2-C7
5	F	1	NAG	O5-C5-C6-O6
5	F	4	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 11 short contacts:

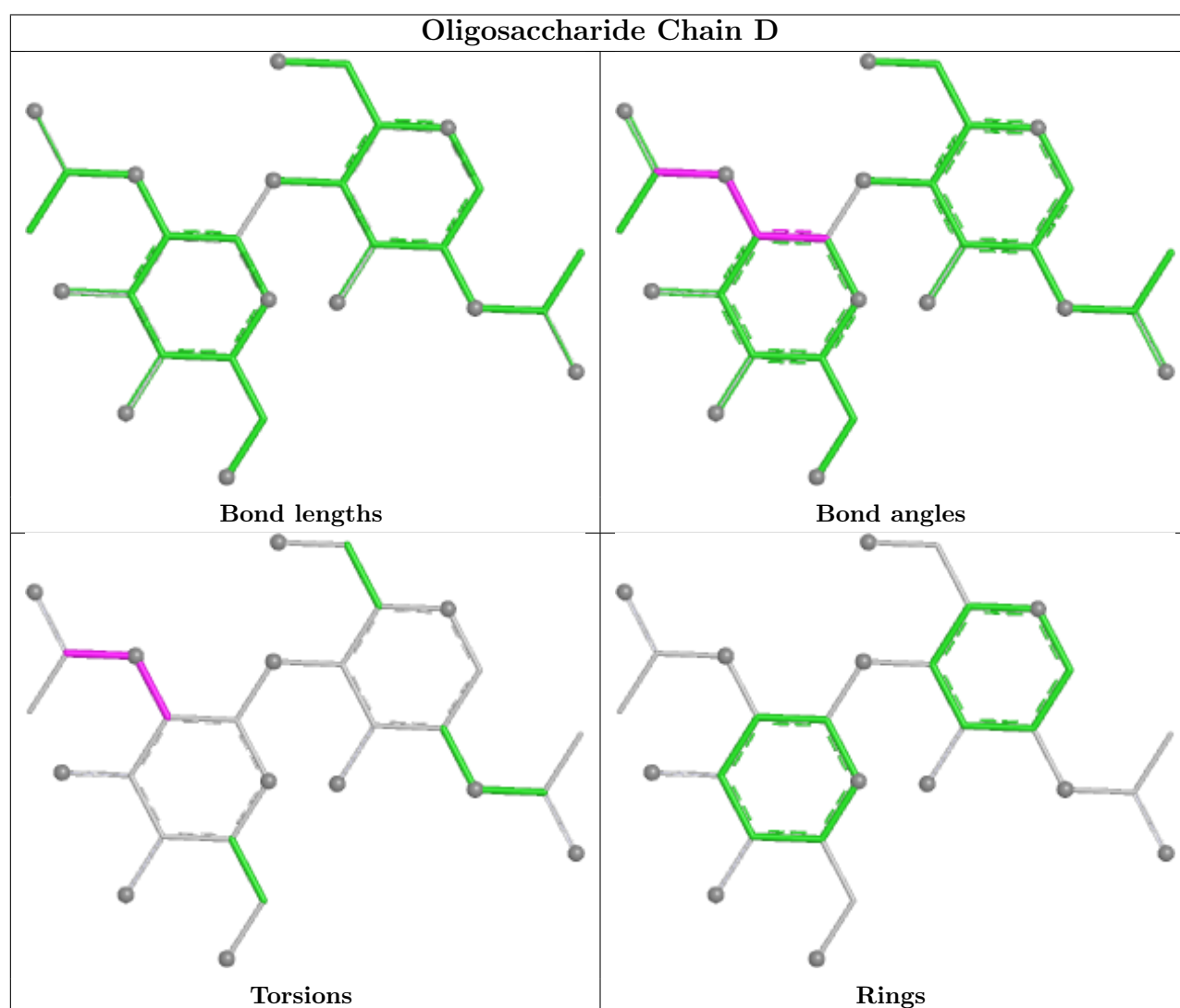
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2	NAG	1	0

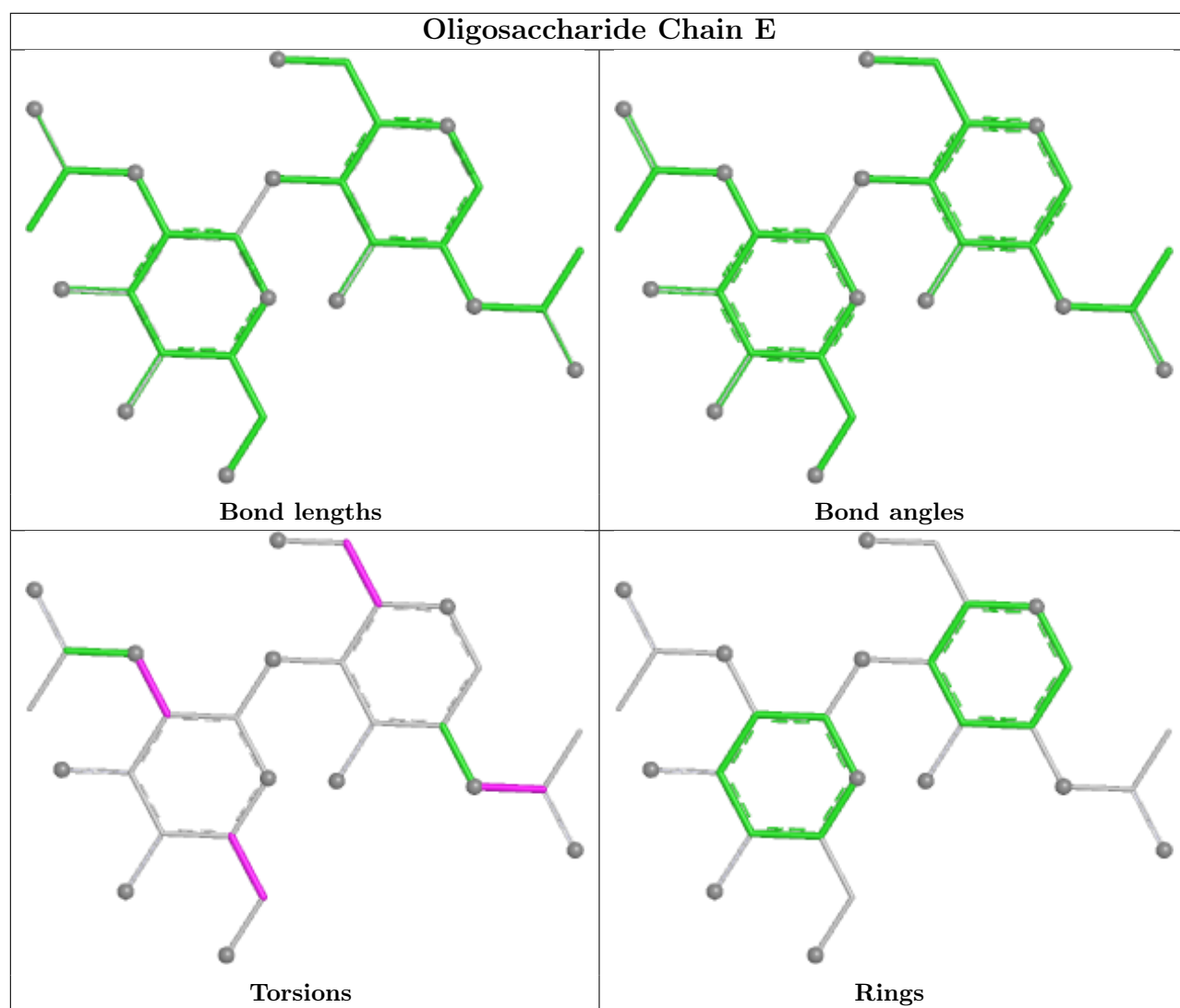
Continued on next page...

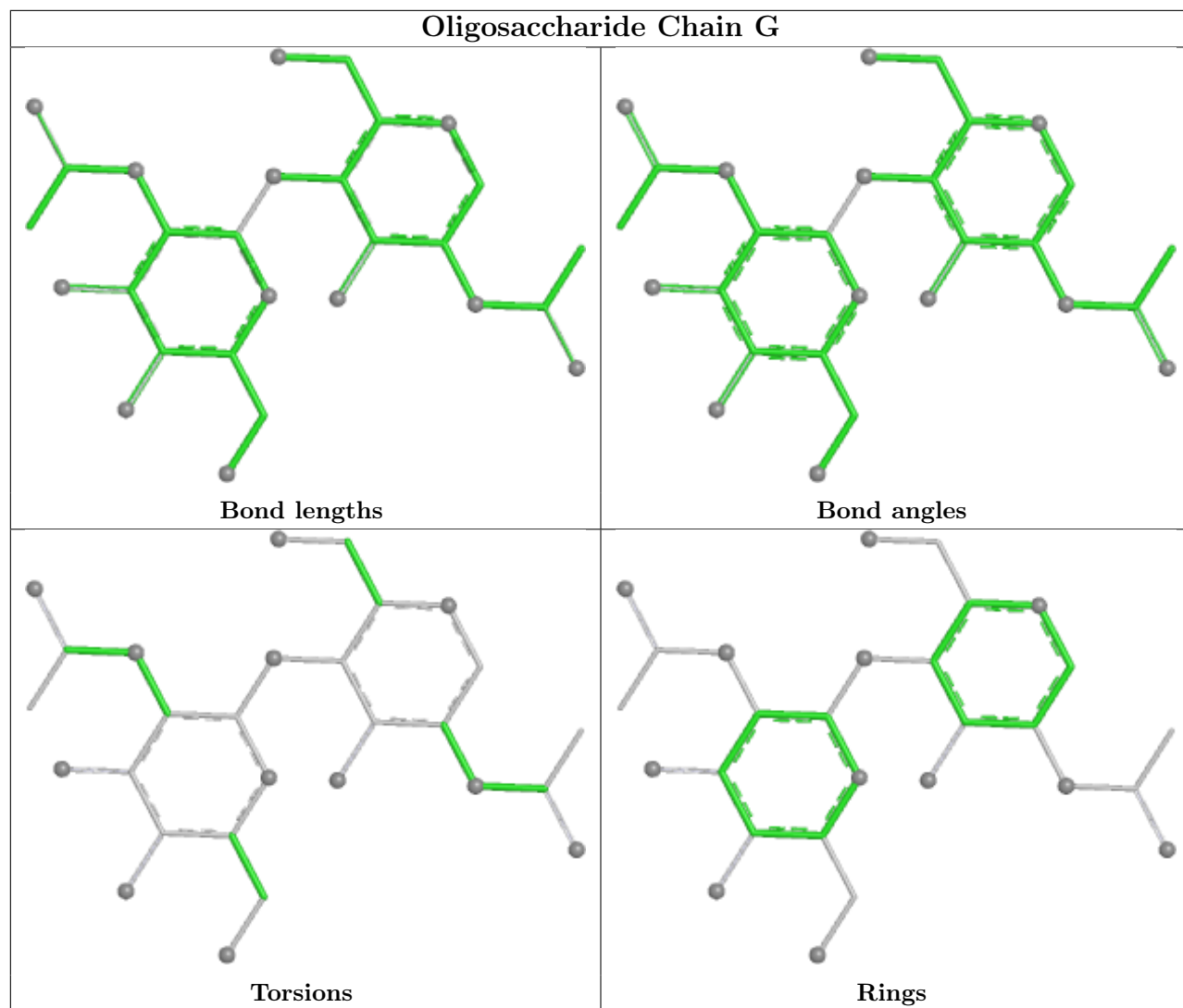
Continued from previous page...

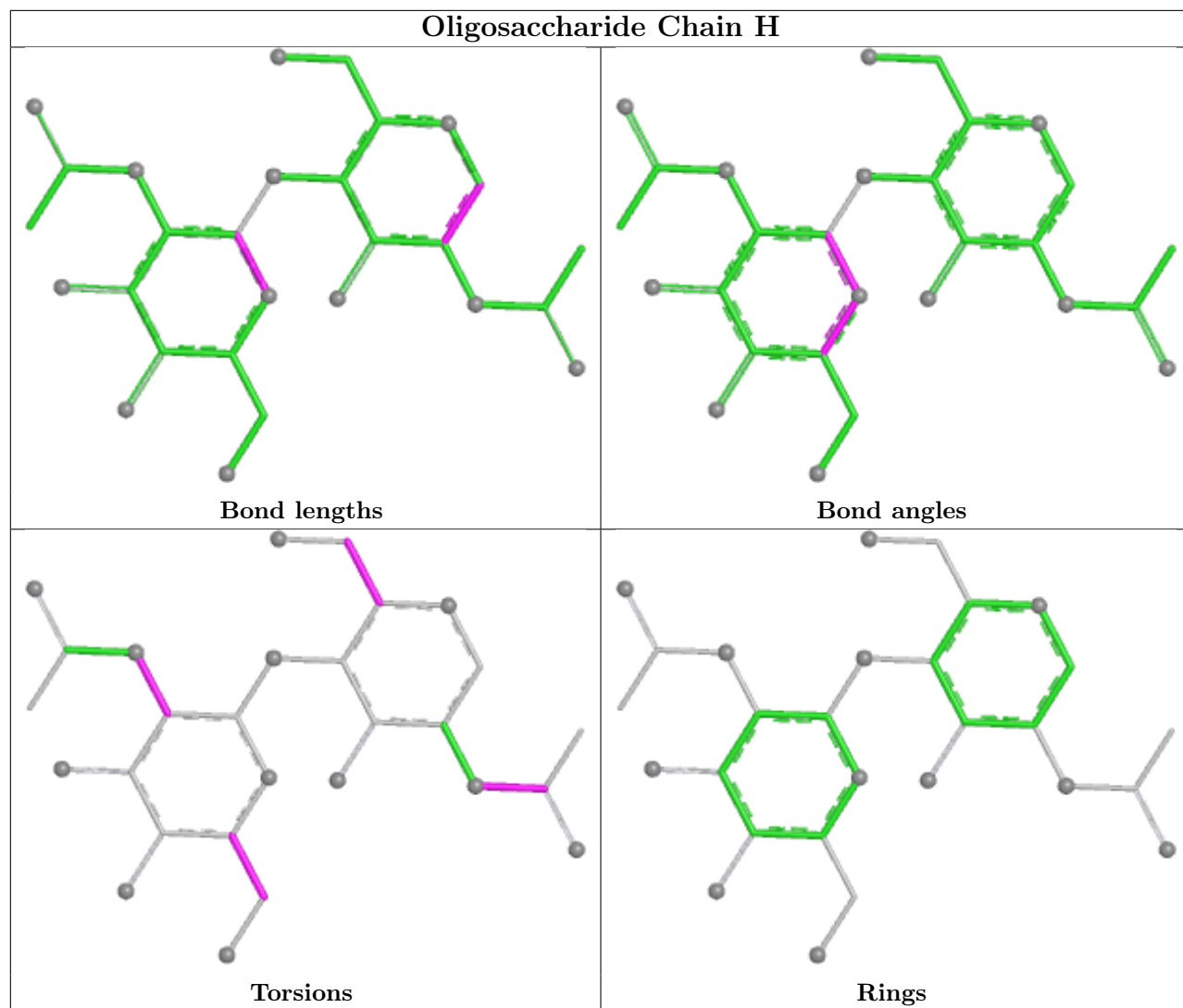
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	2	0
5	F	1	NAG	2	0
4	H	1	NAG	3	0
5	F	3	NAG	1	0
4	E	2	NAG	1	0
4	G	1	NAG	1	0
5	F	4	NAG	2	0

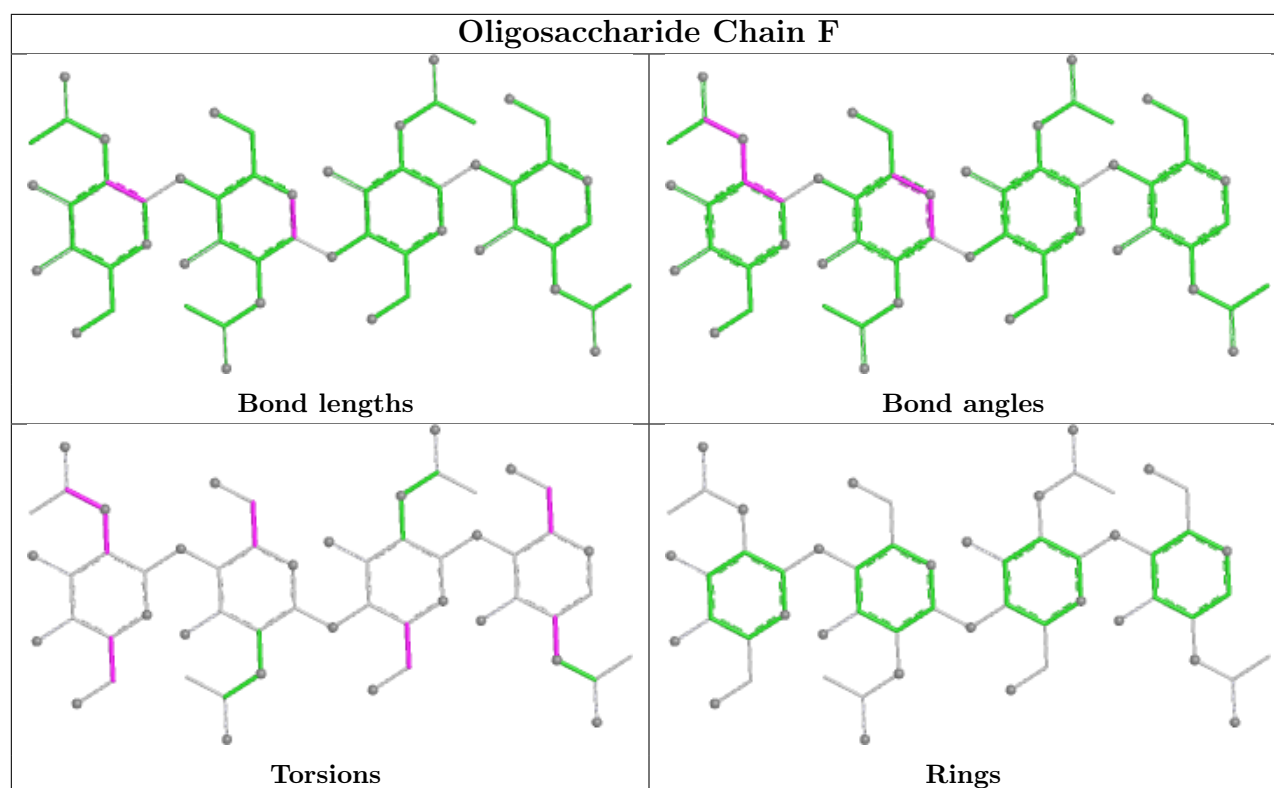
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z > 2$
8	3PE	A	2408	-	34,34,50	0.61	0	37,39,55	0.63	1 (2%)
10	NAG	C	1202	3	14,14,15	0.80	1 (7%)	17,19,21	0.98	1 (5%)
7	CLR	A	2407	-	31,31,31	0.37	0	48,48,48	0.68	1 (2%)
9	PT5	A	2409	-	64,64,69	1.38	7 (10%)	79,82,87	1.20	6 (7%)
10	NAG	C	1201	3	14,14,15	0.45	0	17,19,21	0.51	0
10	NAG	C	1203	-	14,14,15	0.18	0	17,19,21	0.48	0
7	CLR	A	2402	-	31,31,31	0.39	0	48,48,48	0.78	0
7	CLR	A	2403	-	31,31,31	0.38	0	48,48,48	0.56	0
7	CLR	A	2404	-	31,31,31	0.41	0	48,48,48	0.67	0
7	CLR	A	2405	-	31,31,31	0.37	0	48,48,48	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	3PE	A	2406	-	40,40,50	0.56	0	43,45,55	0.65	2 (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
8	3PE	A	2408	-	-	10/38/38/54	-
10	NAG	C	1202	3	-	2/6/23/26	0/1/1/1
7	CLR	A	2407	-	-	7/10/68/68	0/4/4/4
9	PT5	A	2409	-	-	33/61/85/90	0/1/1/1
10	NAG	C	1201	3	-	2/6/23/26	0/1/1/1
10	NAG	C	1203	-	-	4/6/23/26	0/1/1/1
7	CLR	A	2402	-	-	7/10/68/68	0/4/4/4
7	CLR	A	2403	-	-	1/10/68/68	0/4/4/4
7	CLR	A	2404	-	-	6/10/68/68	0/4/4/4
7	CLR	A	2405	-	-	8/10/68/68	0/4/4/4
8	3PE	A	2406	-	-	16/44/44/54	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2409	PT5	P4-O4	4.02	1.66	1.59
9	A	2409	PT5	P5-O5	3.78	1.66	1.59
9	A	2409	PT5	O18-C11	3.55	1.43	1.33
9	A	2409	PT5	P1-O1	2.95	1.68	1.59
9	A	2409	PT5	C31-C11	2.68	1.58	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2409	PT5	O16-C10-C12	3.92	119.97	111.48
10	C	1202	NAG	C1-O5-C5	3.82	117.30	112.19
9	A	2409	PT5	C23-C22-C21	3.50	153.07	123.57
9	A	2409	PT5	C17-C16-C15	3.44	152.59	123.57
9	A	2409	PT5	C20-C19-C18	3.36	151.89	123.57

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

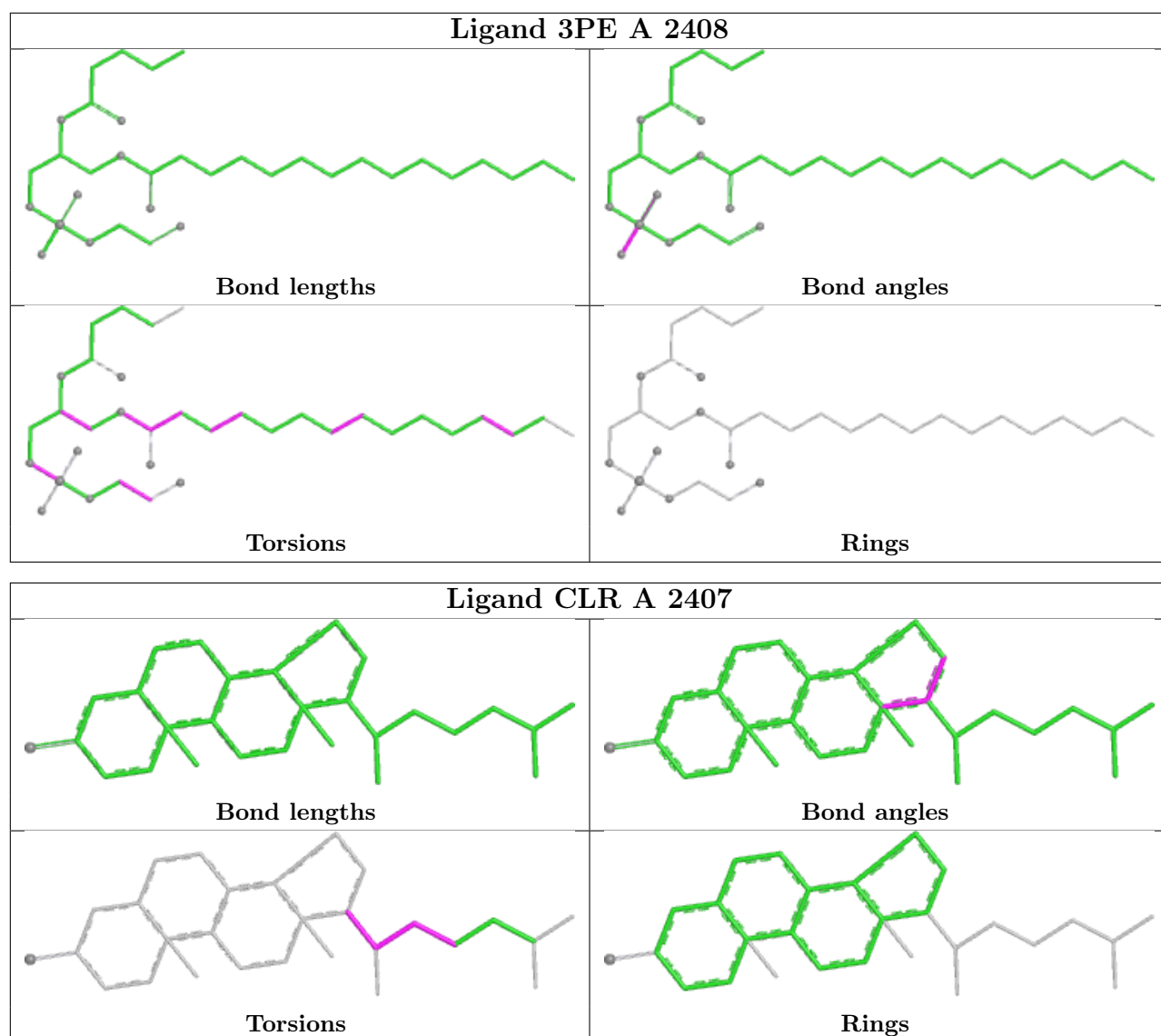
Mol	Chain	Res	Type	Atoms
8	A	2406	3PE	C11-O13-P-O12
8	A	2406	3PE	C11-O13-P-O14
8	A	2408	3PE	C1-O11-P-O14
8	A	2408	3PE	O13-C11-C12-N
9	A	2409	PT5	C3-C4-O4-P4

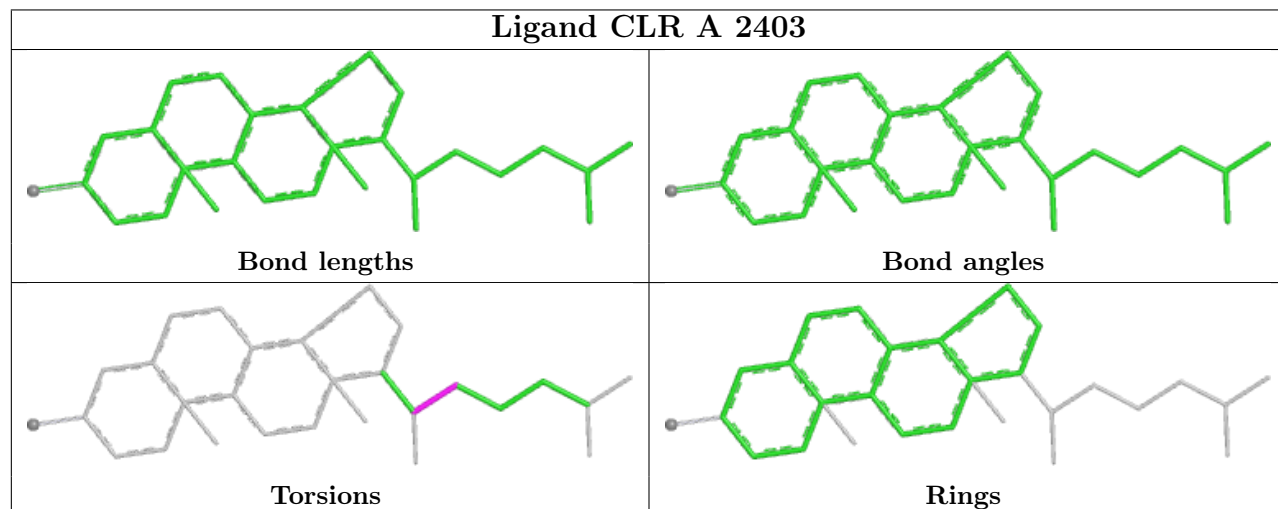
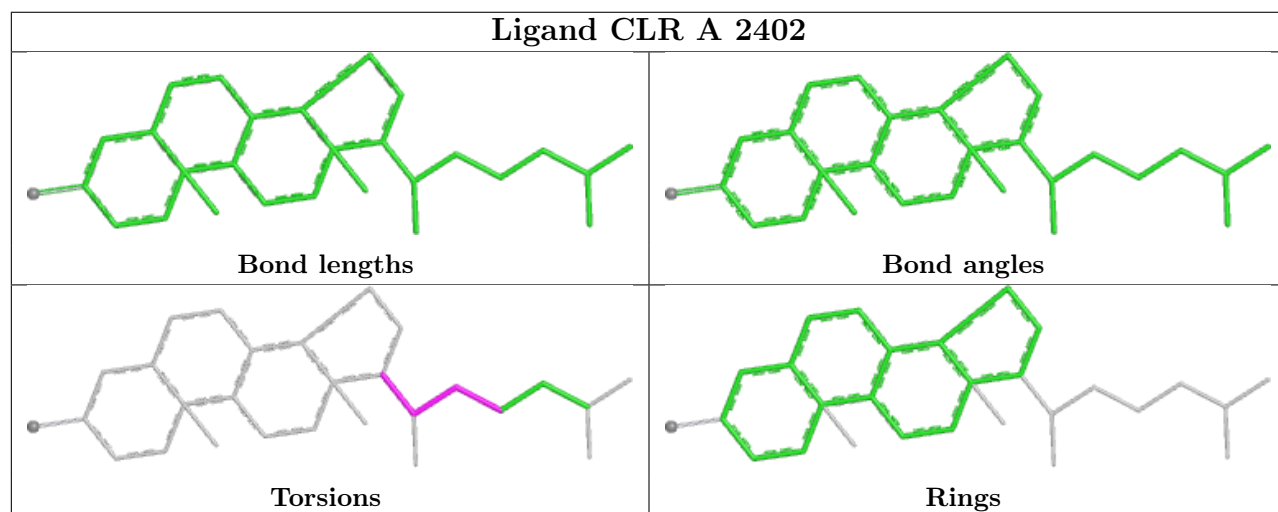
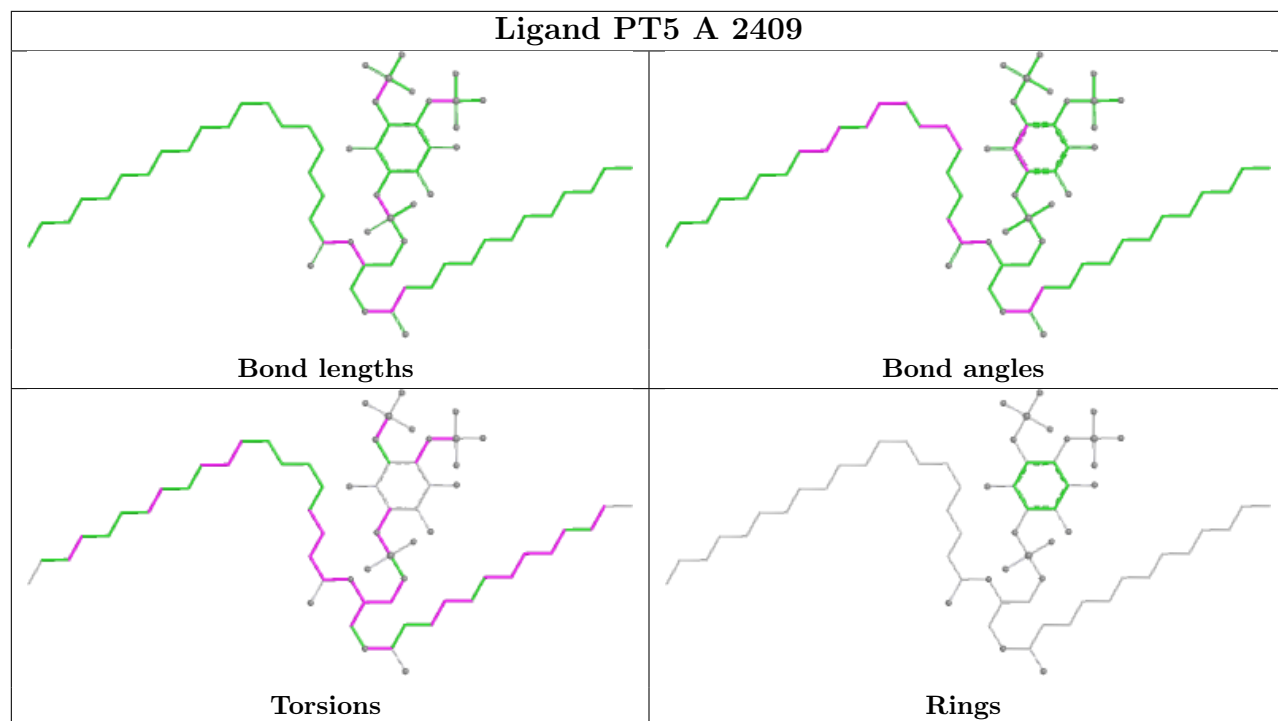
There are no ring outliers.

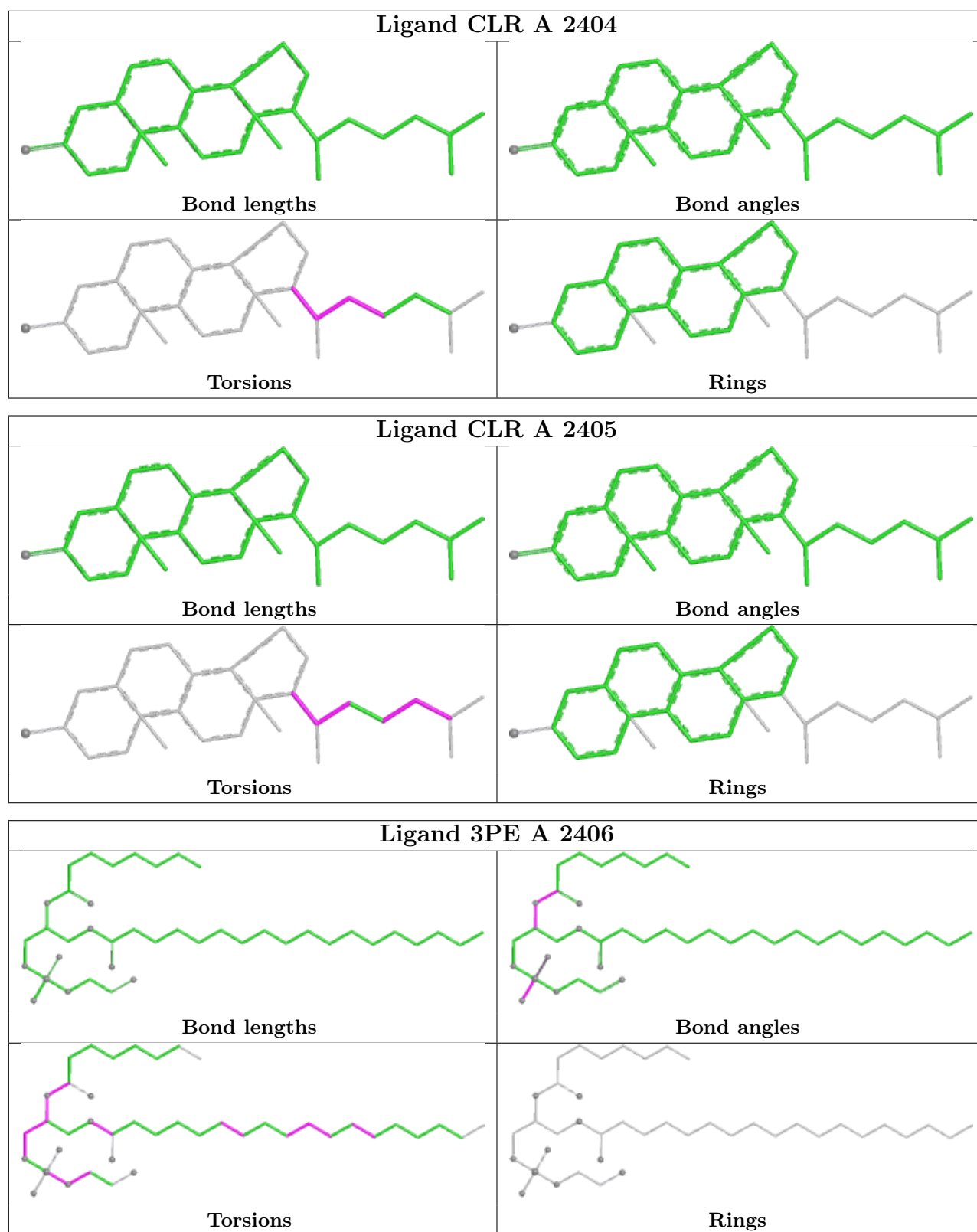
7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1202	NAG	2	0
7	A	2407	CLR	2	0
9	A	2409	PT5	5	0
7	A	2402	CLR	5	0
7	A	2404	CLR	2	0
7	A	2405	CLR	1	0
8	A	2406	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

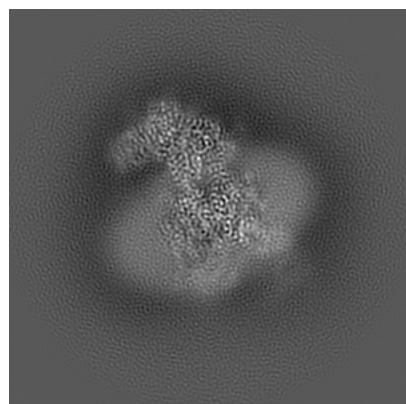
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28529. These allow visual inspection of the internal detail of the map and identification of artifacts.

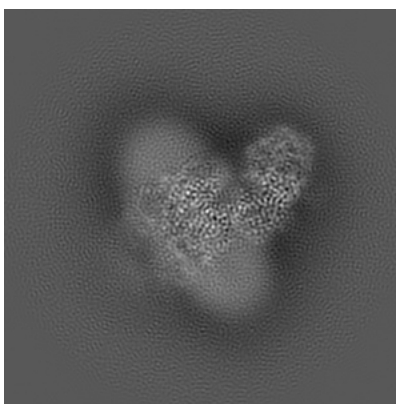
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

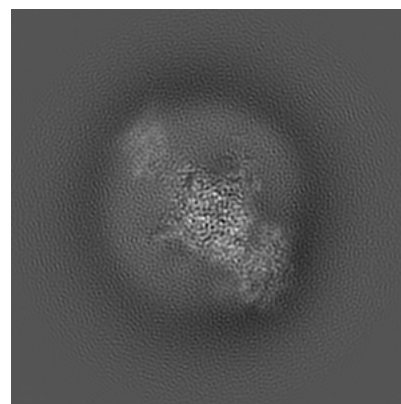
6.1.1 Primary map



X

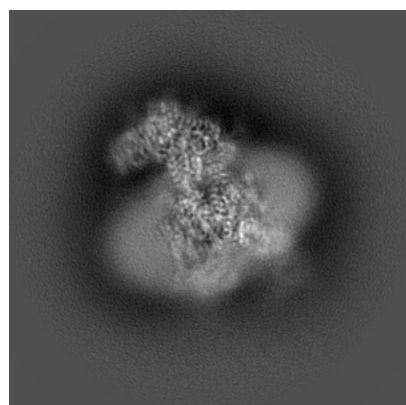


Y

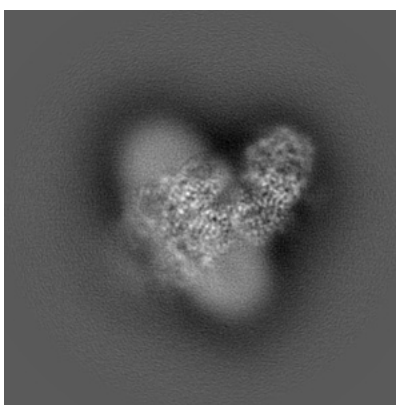


Z

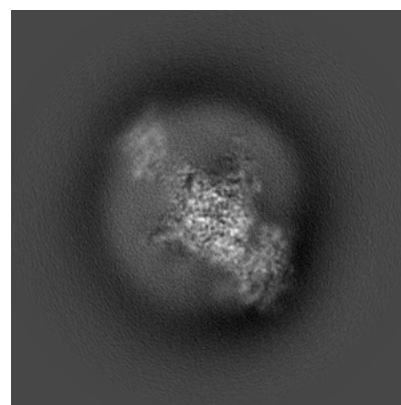
6.1.2 Raw map



X



Y

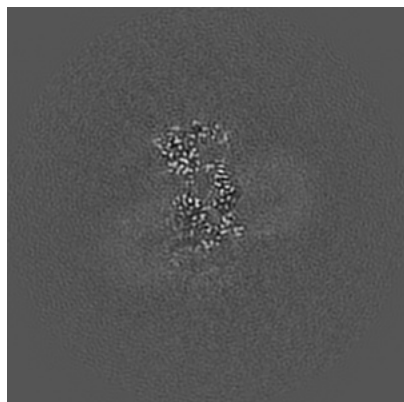


Z

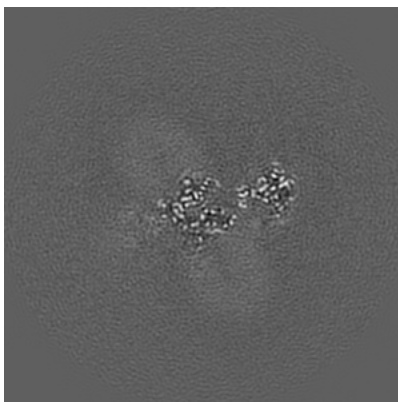
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

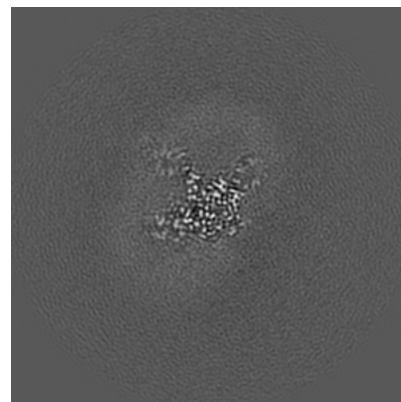
6.2.1 Primary map



X Index: 140

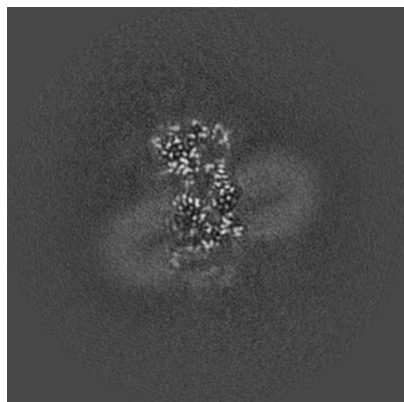


Y Index: 140

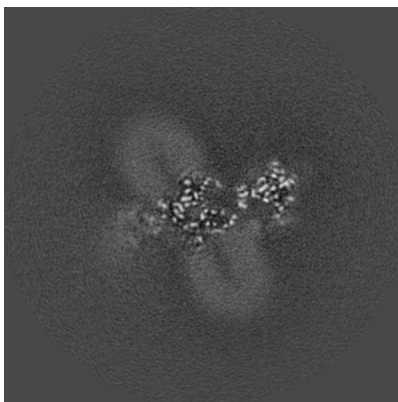


Z Index: 140

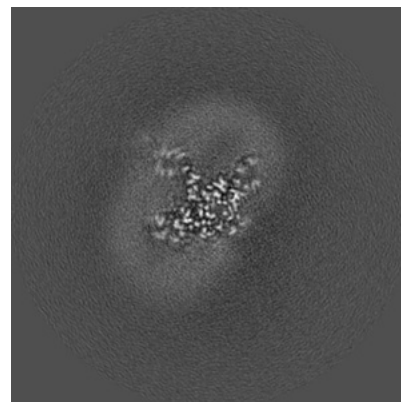
6.2.2 Raw map



X Index: 140



Y Index: 140

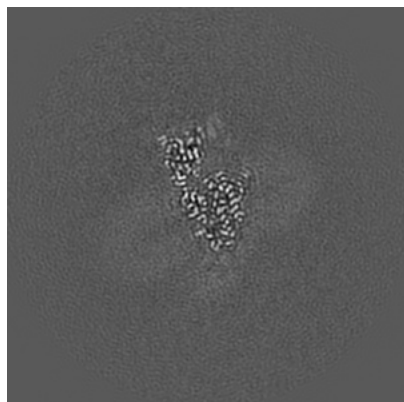


Z Index: 140

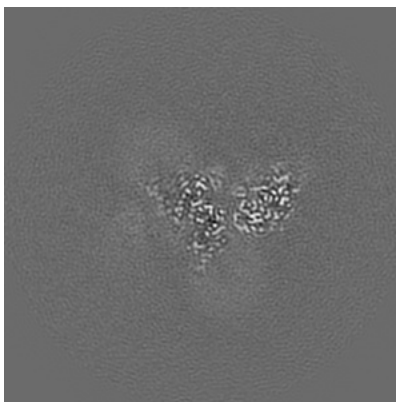
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

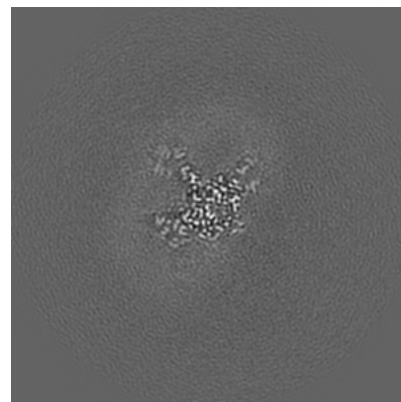
6.3.1 Primary map



X Index: 130

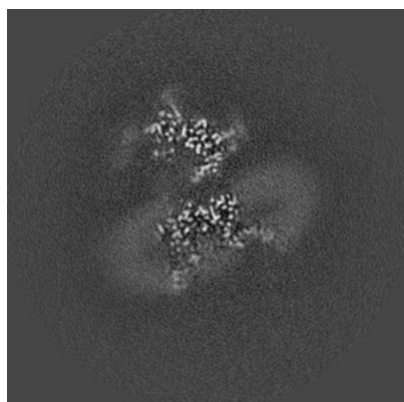


Y Index: 132

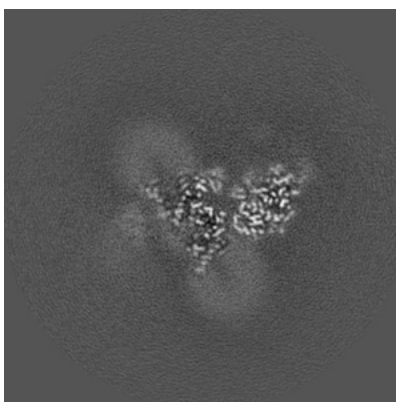


Z Index: 141

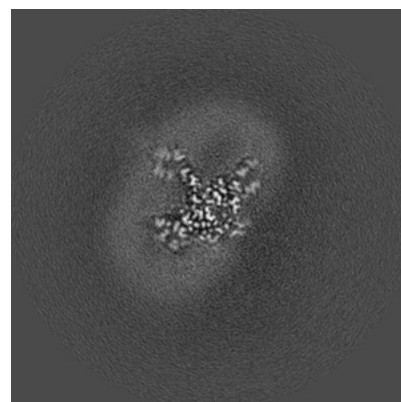
6.3.2 Raw map



X Index: 149



Y Index: 132

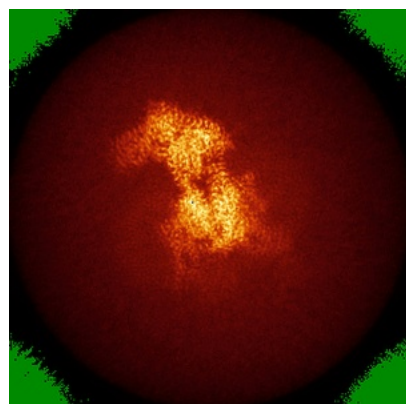


Z Index: 141

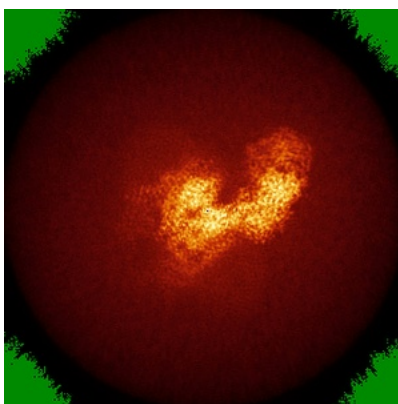
The images above show the largest variance slices of the map in three orthogonal directions.

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

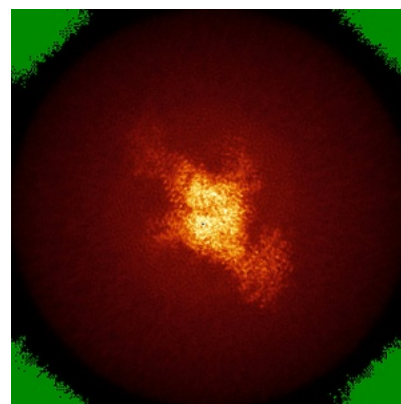
6.4.1 Primary map



X

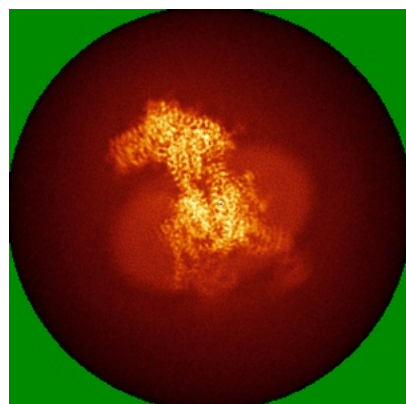


Y

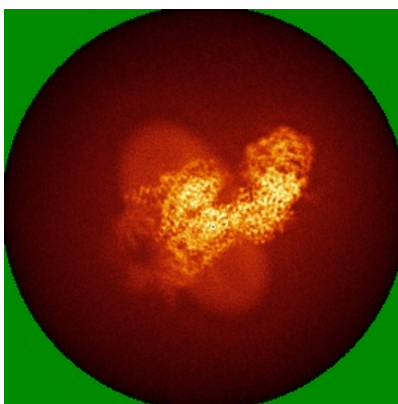


Z

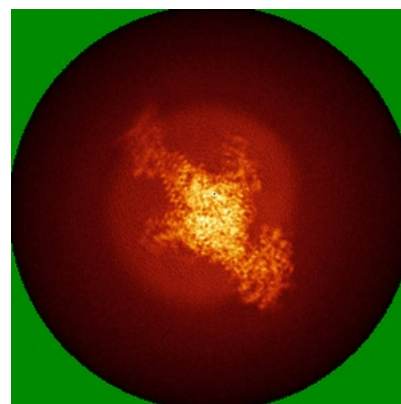
6.4.2 Raw map



X



Y

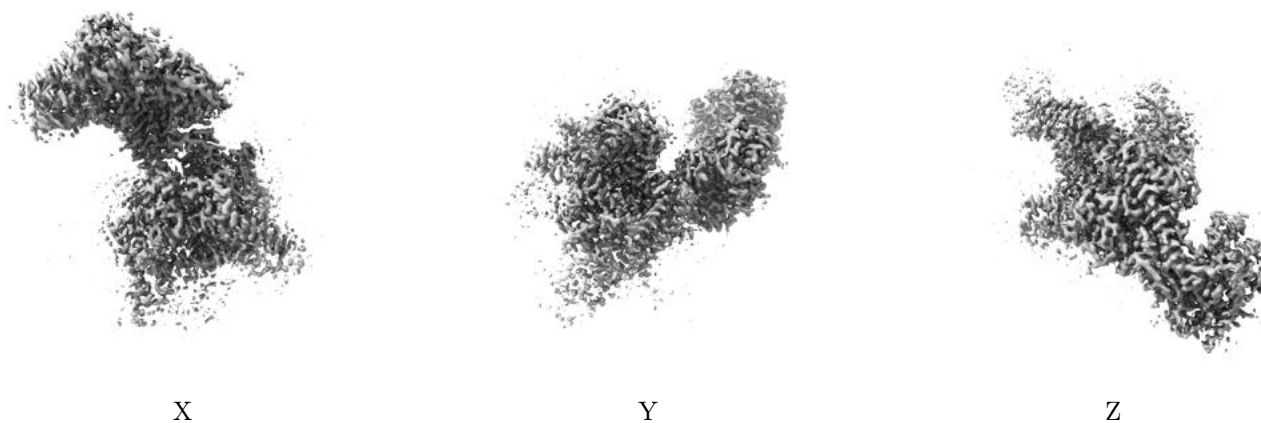


Z

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 0.03. 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.

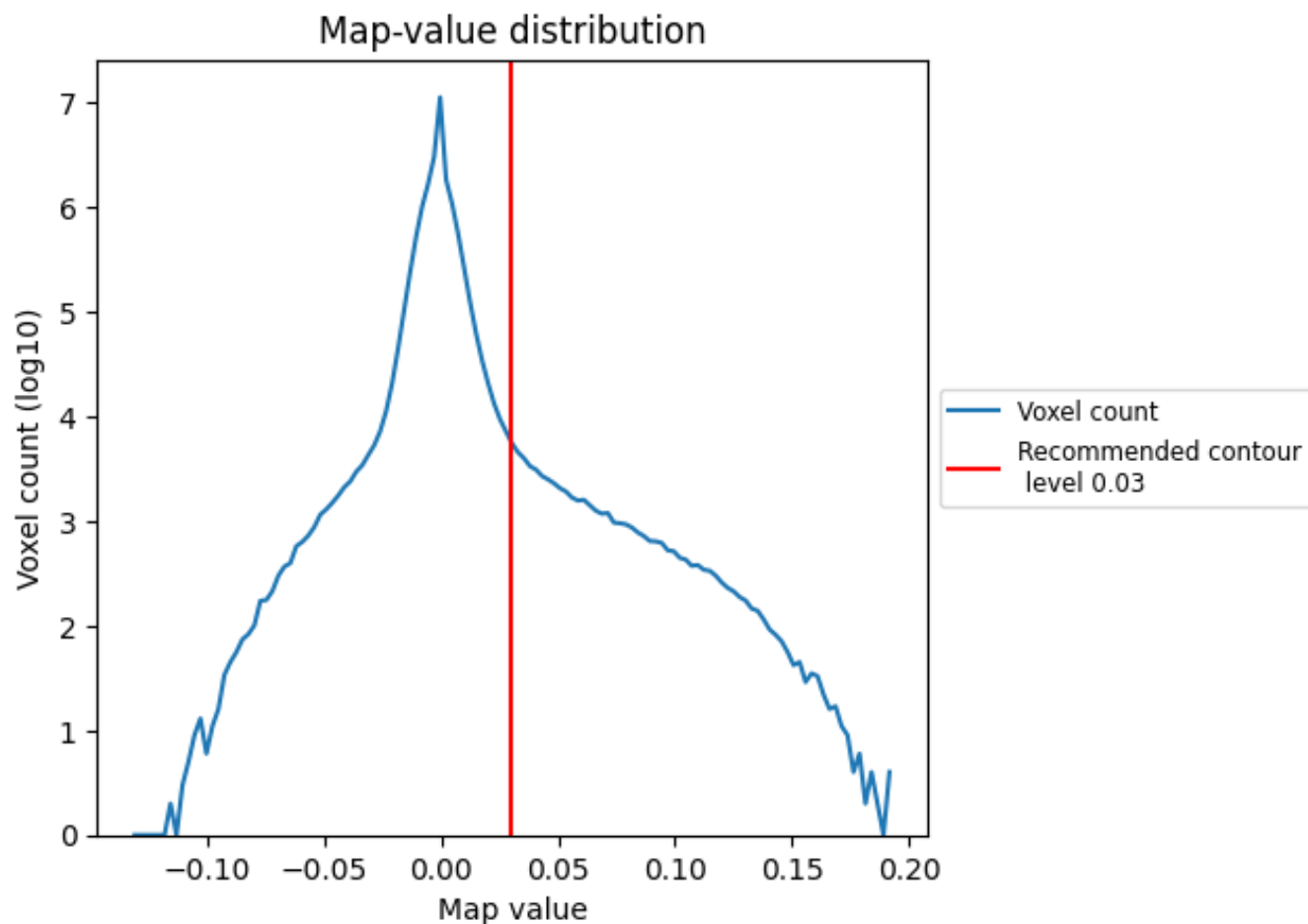
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

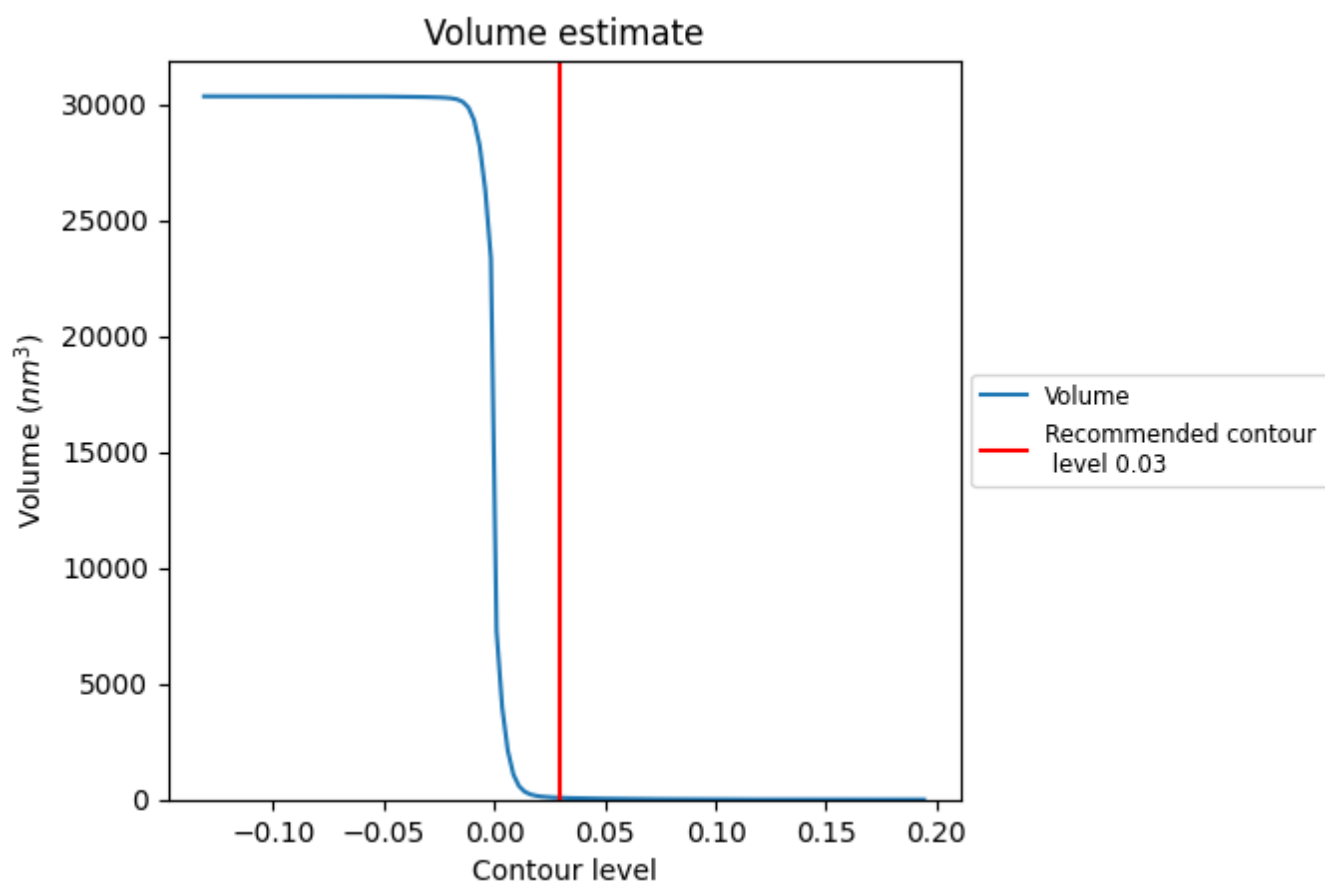
This section contains the results of statistical analysis of the map.

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.

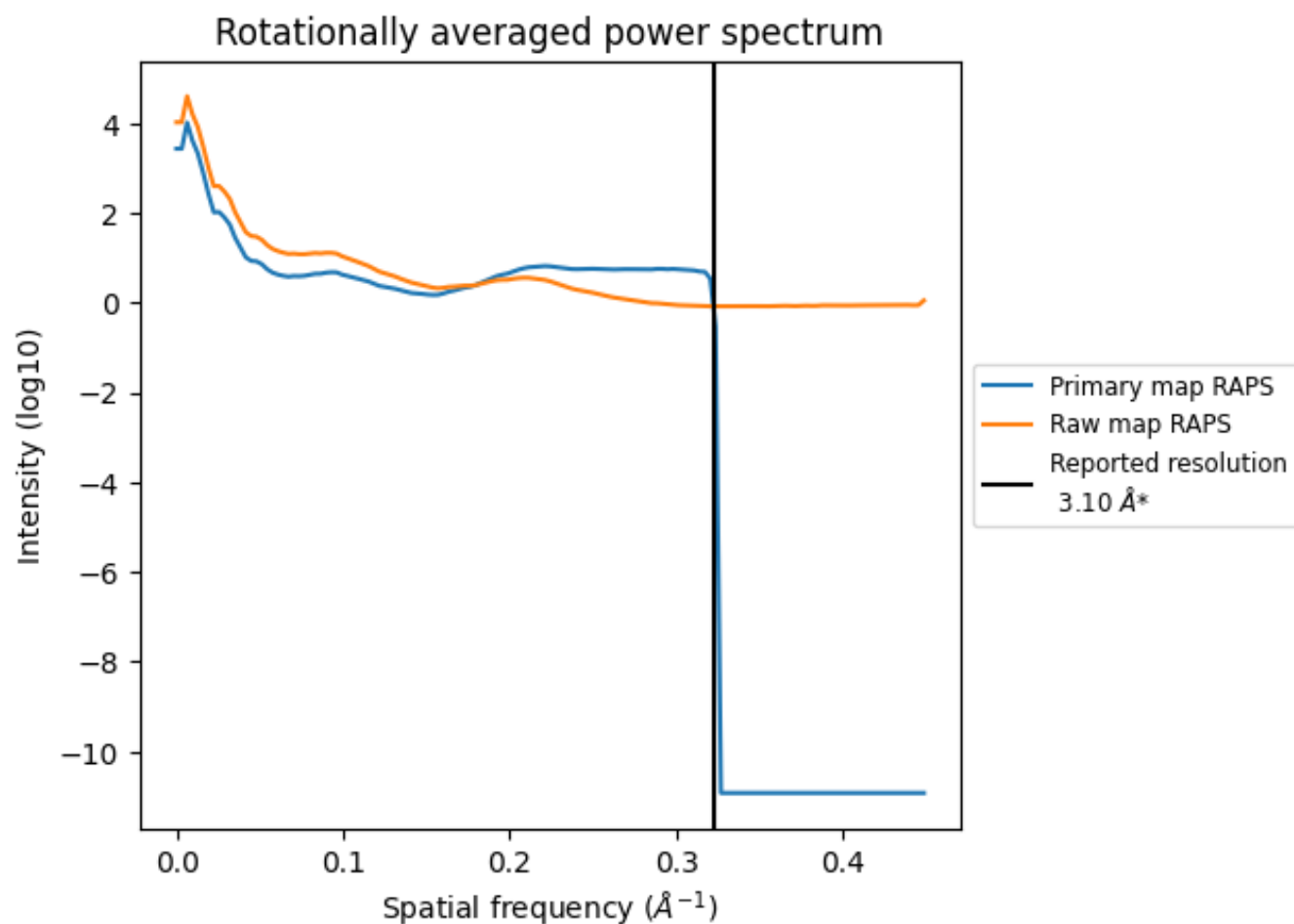
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 69 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 ⓘ

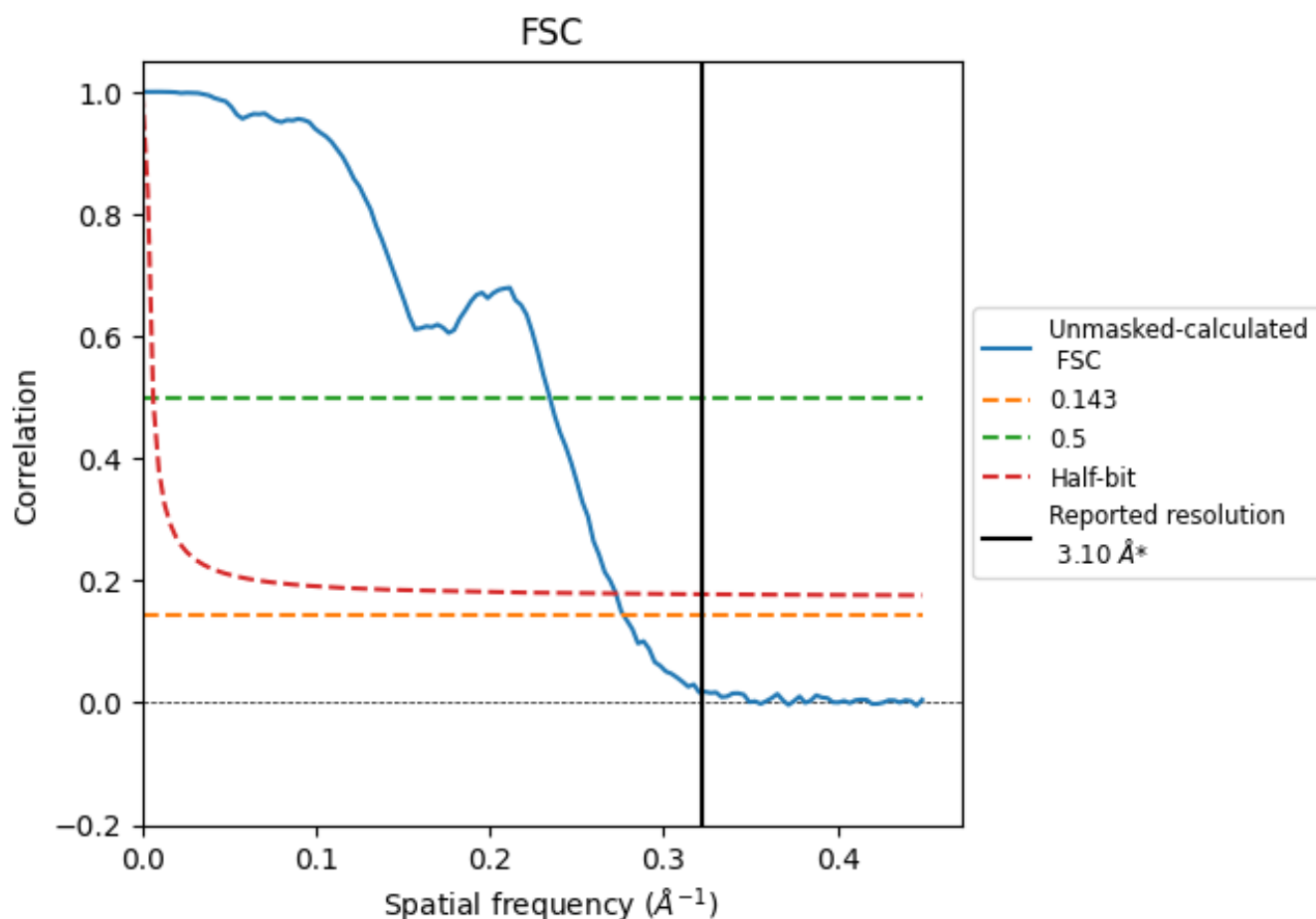


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

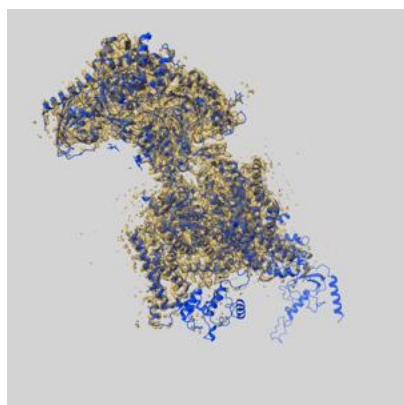
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.26	3.67

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

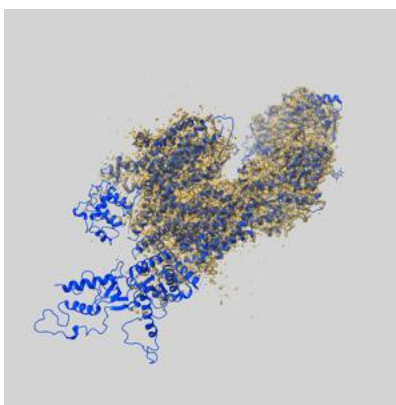
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28529 and PDB model 8EPL. Per-residue inclusion information can be found in section [3](#) on page [9](#).

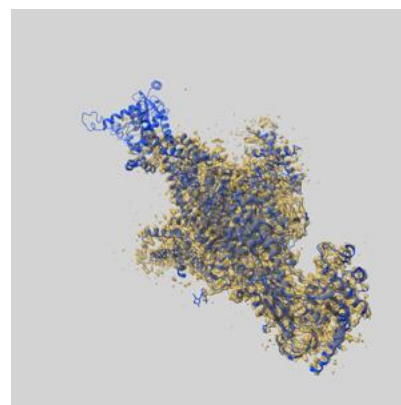
9.1 Map-model overlay [i](#)



X



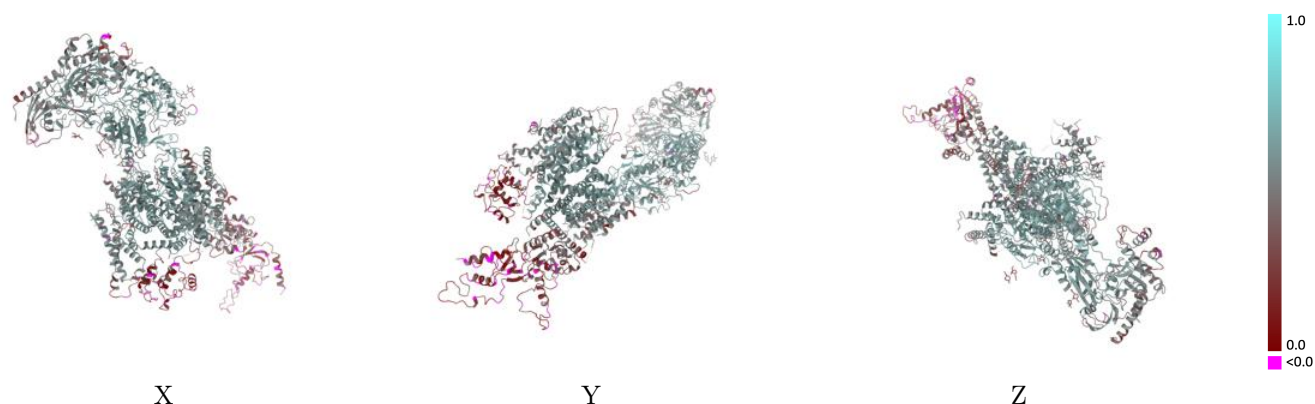
Y



Z

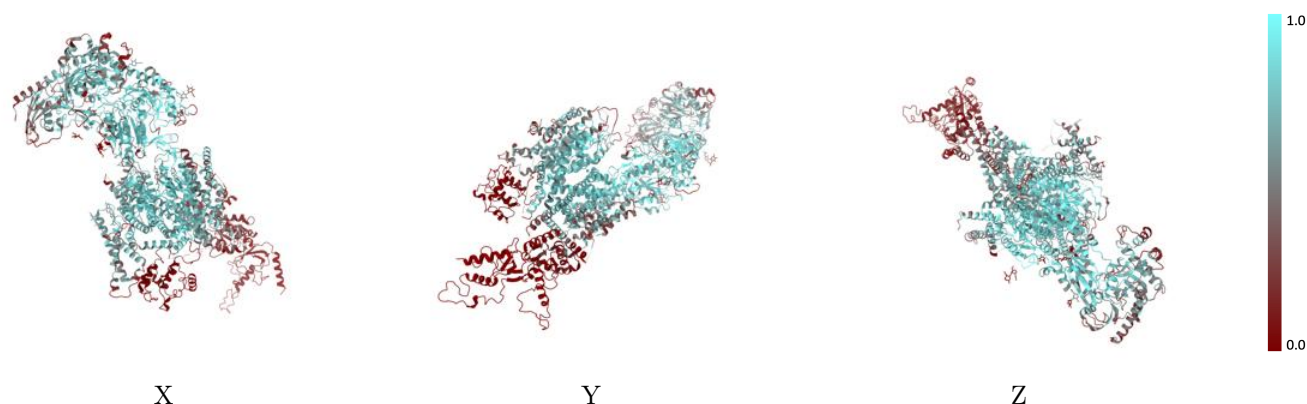
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



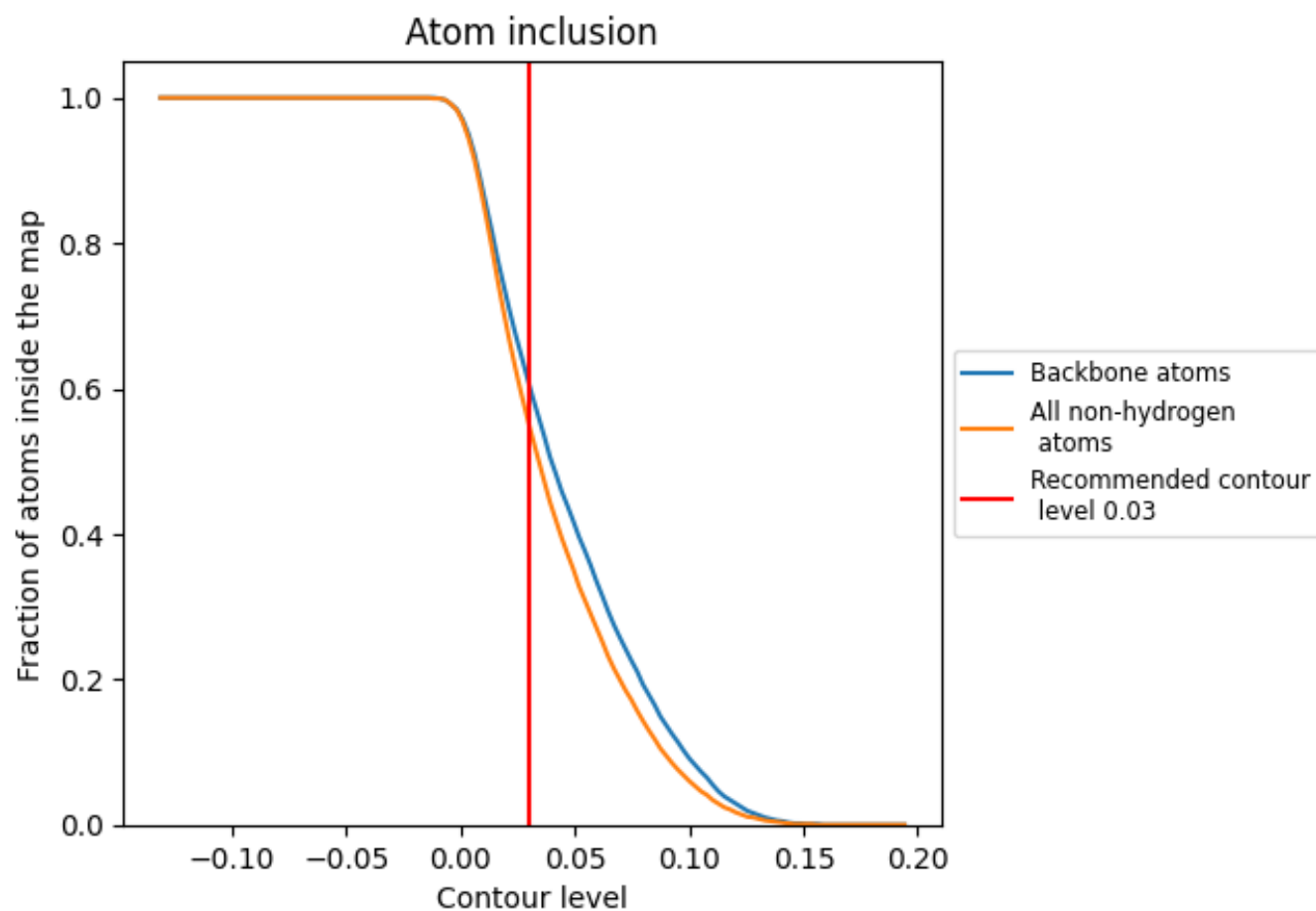
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 55% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5500	0.4720
A	0.5920	0.4900
B	0.0360	0.2270
C	0.6710	0.5310
D	0.3570	0.4250
E	0.0710	0.2490
F	0.4110	0.4220
G	0.2140	0.4810
H	0.2860	0.3200

1.0

0.0

<0.0