



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:01 AM UTC

PDB ID : 8XMN / pdb_00008xmn
EMDB ID : EMD-38483
Title : Voltage-gated sodium channel Nav1.7 variant M2
Authors : Yan, N.; Li, Z.; Wu, Q.; Huang, G.
Deposited on : 2023-12-27
Resolution : 3.37 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:

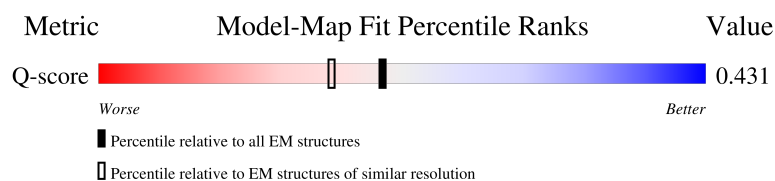
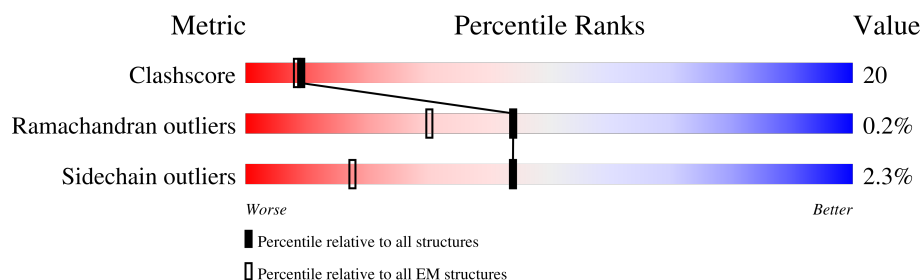
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.37 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	14287 (2.87 - 3.87)

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	2031	 5% 36% 26% 37%
2	B	230	 34% 41% 25%
3	C	227	 33% 26% 26% 48%
4	D	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	E	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13110 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 Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1277	Total	C	N	O	S	0	0
			10299	6825	1618	1778	78		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	866	PHE	LEU	variant	UNP Q15858
A	1454	CYS	GLY	variant	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	LEU	-	expression tag	UNP Q07699
B	220	GLU	-	expression tag	UNP Q07699
B	221	HIS	-	expression tag	UNP Q07699
B	222	HIS	-	expression tag	UNP Q07699
B	223	HIS	-	expression tag	UNP Q07699
B	224	HIS	-	expression tag	UNP Q07699
B	225	HIS	-	expression tag	UNP Q07699
B	226	HIS	-	expression tag	UNP Q07699
B	227	HIS	-	expression tag	UNP Q07699
B	228	HIS	-	expression tag	UNP Q07699
B	229	HIS	-	expression tag	UNP Q07699
B	230	HIS	-	expression tag	UNP Q07699

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	3	0
			980	615	172	183	10		

There are 12 discrepancies between the modelled and reference sequences:

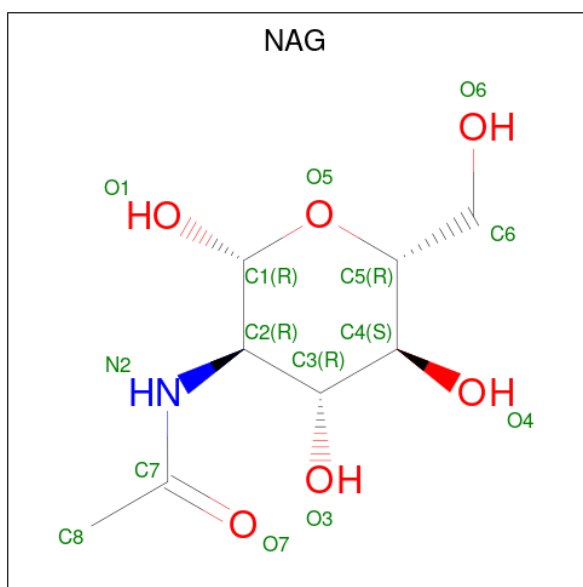
Chain	Residue	Modelled	Actual	Comment	Reference
C	216	LEU	-	expression tag	UNP O60939
C	217	GLU	-	expression tag	UNP O60939
C	218	HIS	-	expression tag	UNP O60939
C	219	HIS	-	expression tag	UNP O60939
C	220	HIS	-	expression tag	UNP O60939
C	221	HIS	-	expression tag	UNP O60939
C	222	HIS	-	expression tag	UNP O60939
C	223	HIS	-	expression tag	UNP O60939
C	224	HIS	-	expression tag	UNP O60939
C	225	HIS	-	expression tag	UNP O60939
C	226	HIS	-	expression tag	UNP O60939
C	227	HIS	-	expression tag	UNP O60939

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



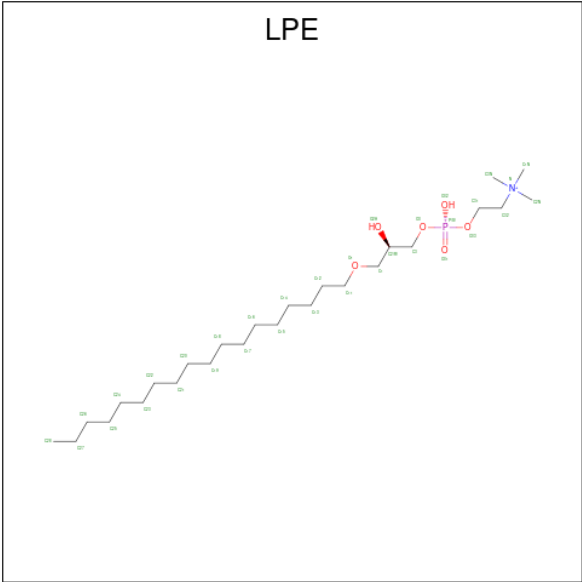
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



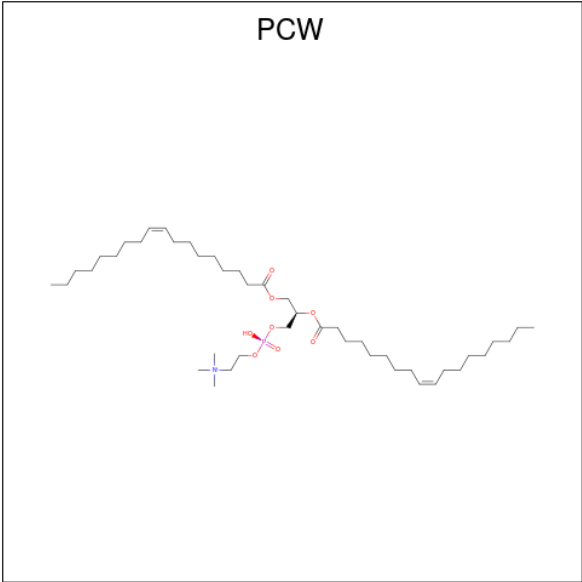
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
6	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).

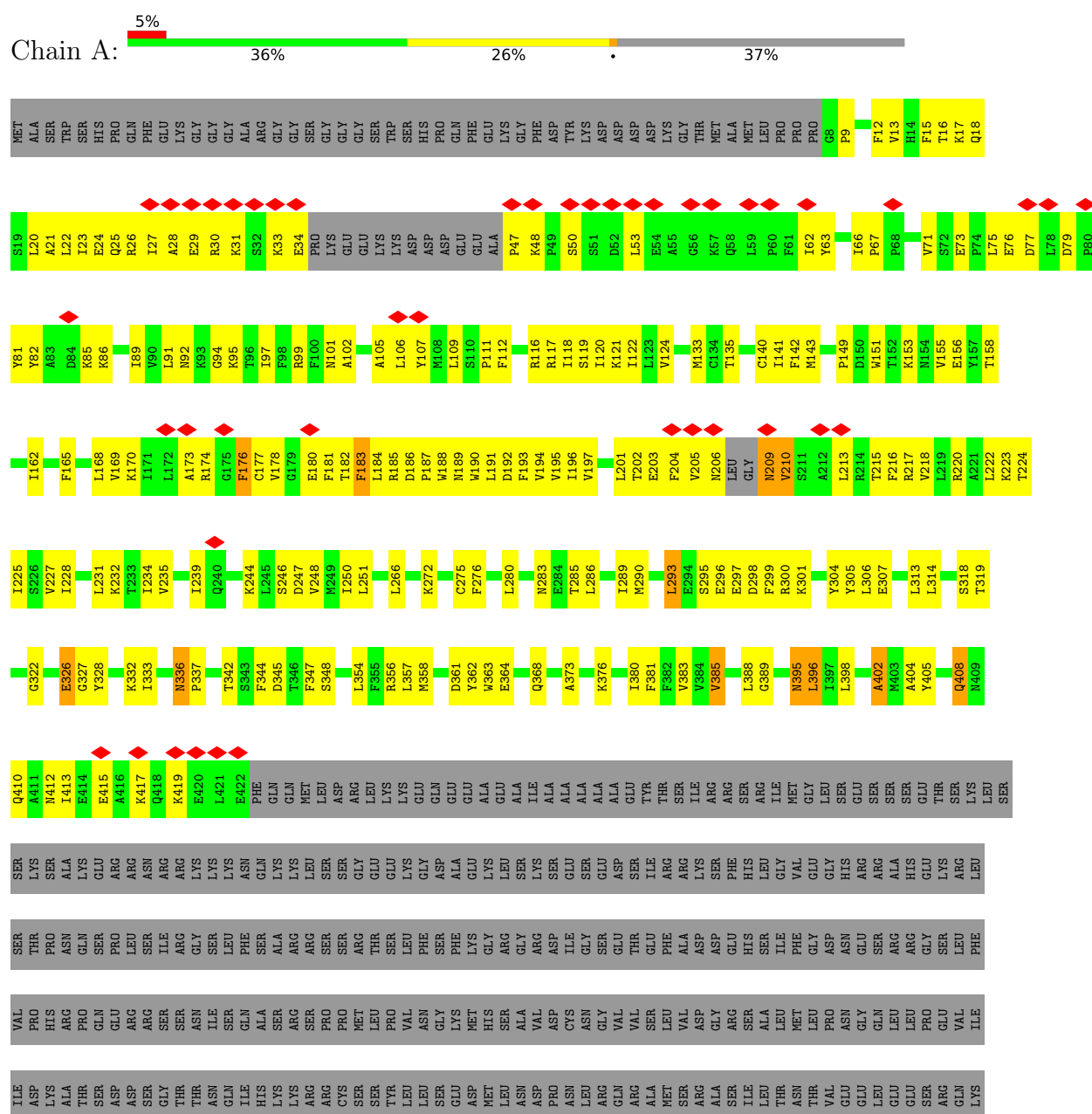


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
7	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
7	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

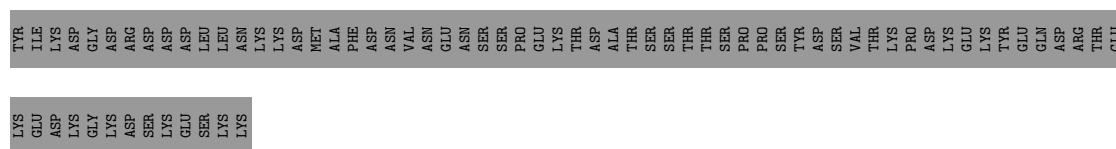
3 Residue-property plots

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.

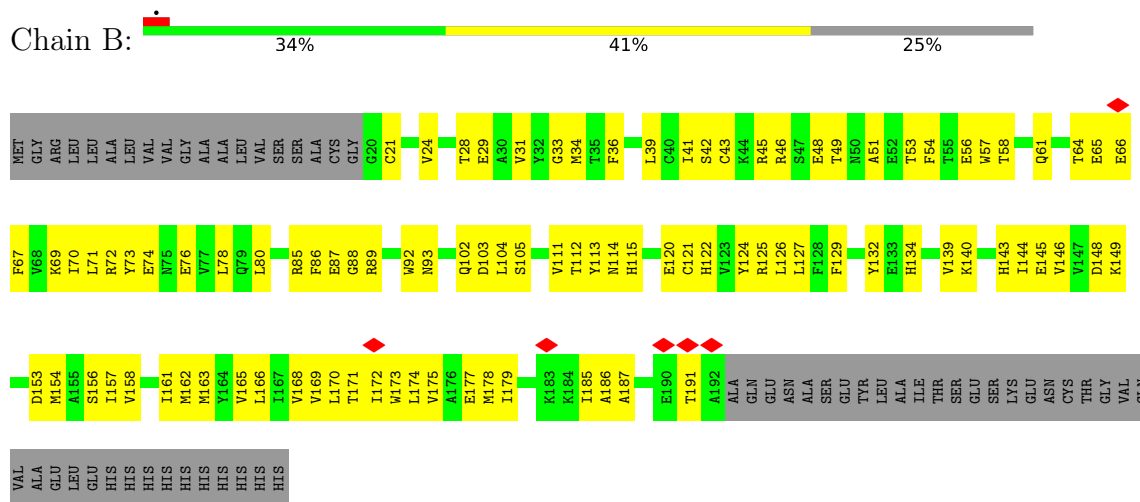
- Molecule 1: Sodium channel protein type 9 subunit alpha



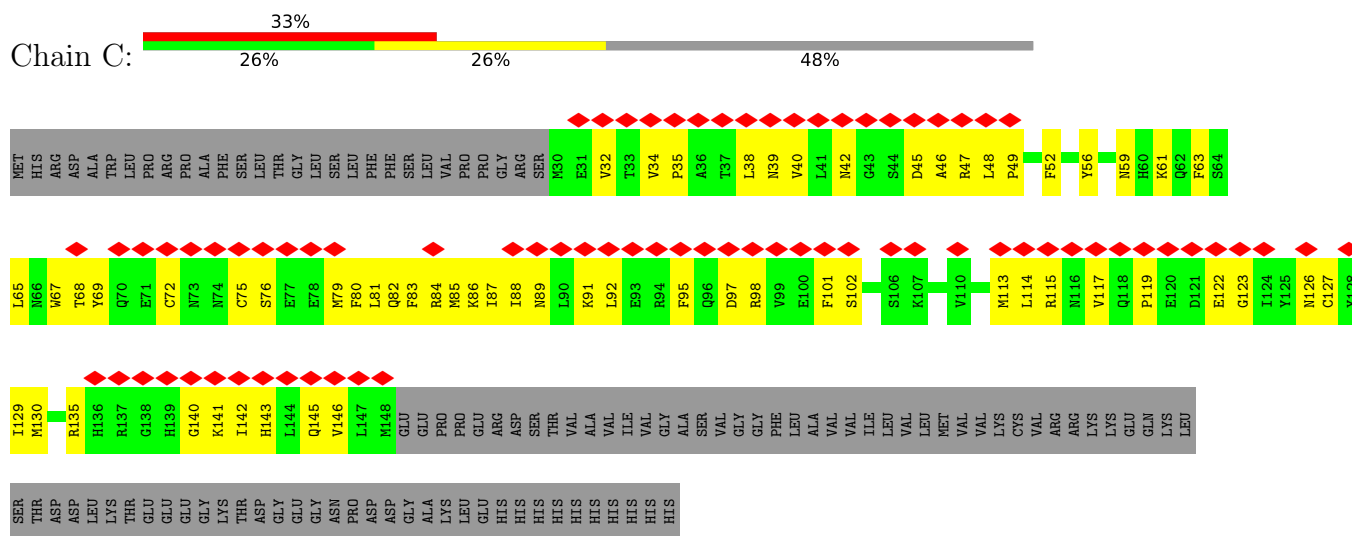




• Molecule 2: Sodium channel subunit beta-1



• Molecule 3: Sodium channel subunit beta-2



• 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

Chain E:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77511	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)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.416	Depositor
Minimum map value	-0.821	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	241.1712, 241.1712, 241.1712	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8374, 0.8374, 0.8374	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	11/10549 (0.1%)	0.84	25/14289 (0.2%)
2	B	0.38	0/1442	0.58	0/1949
3	C	0.30	0/1011	0.69	3/1367 (0.2%)
All	All	0.66	11/13002 (0.1%)	0.81	28/17605 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1588	ILE	C-O	-7.34	1.15	1.24
1	A	1440	PHE	CA-C	-6.89	1.44	1.52
1	A	1436	TYR	CA-C	-6.81	1.44	1.52
1	A	1367	ARG	CA-C	-6.52	1.44	1.52
1	A	1436	TYR	C-O	-6.22	1.16	1.24
1	A	1437	PHE	C-O	-6.19	1.16	1.24
1	A	956	ASN	N-CA	-5.33	1.39	1.46
1	A	381	PHE	CA-C	-5.26	1.46	1.52
1	A	336	ASN	CA-CB	-5.22	1.45	1.53
1	A	1440	PHE	C-O	-5.15	1.18	1.24
1	A	402	ALA	CA-C	-5.10	1.46	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	N-CA-C	-9.37	101.62	113.23
1	A	26	ARG	N-CA-C	-9.02	101.02	111.03
1	A	1436	TYR	N-CA-C	-8.71	101.73	111.14
3	C	76	SER	N-CA-C	8.65	122.69	110.50
1	A	1628	LYS	N-CA-C	-8.43	105.01	114.62
1	A	210	VAL	N-CA-C	-7.29	105.90	112.90
1	A	1596	ALA	N-CA-C	-6.61	104.16	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	THR	N-CA-C	6.37	119.47	110.23
1	A	956	ASN	N-CA-C	-6.36	104.42	111.36
1	A	780	ASN	N-CA-C	-6.12	104.53	111.07
1	A	863	VAL	N-CA-C	-6.08	106.80	113.43
1	A	1446	PHE	CA-C-N	-5.82	110.81	121.52
1	A	1446	PHE	C-N-CA	-5.82	110.81	121.52
1	A	951	VAL	CB-CA-C	-5.78	104.57	111.97
1	A	772	PHE	N-CA-C	-5.78	105.06	111.36
1	A	1581	PHE	N-CA-C	-5.76	105.00	111.28
1	A	385	VAL	N-CA-C	5.73	115.92	110.42
1	A	824	PHE	N-CA-C	5.73	120.14	113.20
3	C	92	LEU	N-CA-C	5.71	117.89	110.53
3	C	95	PHE	N-CA-C	-5.66	104.58	113.02
1	A	1444	GLY	CA-C-N	-5.43	113.72	122.24
1	A	1444	GLY	C-N-CA	-5.43	113.72	122.24
1	A	896	VAL	CB-CA-C	-5.38	103.39	112.16
1	A	1550	ILE	N-CA-C	-5.37	105.30	110.72
1	A	1601	THR	N-CA-C	5.34	117.18	111.36
1	A	784	THR	N-CA-C	-5.29	105.51	111.28
1	A	216	PHE	N-CA-C	-5.15	106.69	113.17
1	A	1366	ASN	N-CA-C	5.14	116.62	108.96

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	10299	0	10525	416	0
2	B	1416	0	1380	79	0
3	C	980	0	945	50	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
5	A	28	0	26	1	0
5	B	56	0	52	3	0
6	A	131	0	184	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	144	0	203	6	0
All	All	13110	0	13365	542	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 20.

All (542) 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:99:ARG:HD2	1:A:181:PHE:CZ	1.89	1.07
1:A:815:ILE:HG21	1:A:841:ARG:HD2	1.41	0.99
1:A:768:MET:HE3	1:A:773:LYS:HG2	1.46	0.94
1:A:1599:ILE:HD11	1:A:1605:SER:HB2	1.52	0.91
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.59	0.85
1:A:1347:PHE:HB3	1:A:1385:LEU:HD23	1.60	0.83
3:C:61:LYS:HA	3:C:85:MET:HE1	1.58	0.83
1:A:822:GLU:HG2	1:A:834:LEU:HG	1.65	0.79
1:A:133:MET:HB2	1:A:227:VAL:HG11	1.65	0.78
6:A:2004:LPE:H21	7:A:2005:PCW:H162	1.64	0.78
3:C:80:PHE:HD1	3:C:81:LEU:HD23	1.48	0.78
1:A:183:PHE:HD1	1:A:184:LEU:HD22	1.50	0.77
1:A:1732:ASN:HB3	1:A:1735:VAL:HG12	1.67	0.76
2:B:21:CYS:SG	2:B:102:GLN:NE2	2.59	0.76
1:A:66:ILE:HD12	1:A:67:PRO:HD2	1.66	0.75
1:A:1532:MET:SD	1:A:1616:ARG:NH1	2.60	0.75
1:A:1000:ASN:O	1:A:1004:GLN:HG2	1.87	0.74
3:C:45:ASP:OD2	3:C:115:ARG:NE	2.20	0.74
1:A:1232:ILE:HD11	2:B:163:MET:HA	1.68	0.74
1:A:970:SER:HA	1:A:974:ASP:HB2	1.71	0.73
3:C:98:ARG:HH21	3:C:114:LEU:HG	1.54	0.73
1:A:1485:MET:HB3	1:A:1639:MET:HE1	1.70	0.73
2:B:92:TRP:HH2	2:B:104:LEU:HD13	1.53	0.73
3:C:68:THR:OG1	3:C:126:ASN:ND2	2.21	0.72
1:A:149:PRO:HB2	1:A:151:TRP:HD1	1.53	0.72
1:A:1484:ALA:O	1:A:1487:LYS:HG3	1.89	0.72
1:A:1722:PRO:HB3	2:B:103:ASP:HB2	1.71	0.71
1:A:895:CYS:HA	3:C:56:TYR:HE2	1.55	0.71
1:A:942:ALA:O	1:A:946:ILE:HG13	1.91	0.71
1:A:895:CYS:HA	3:C:56:TYR:CE2	2.26	0.71
1:A:231:LEU:HD21	1:A:871:LEU:HD23	1.74	0.70
2:B:113:TYR:HA	2:B:146:VAL:HG11	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HA	1:A:63:TYR:HA	1.74	0.69
1:A:295:SER:HB3	1:A:298:ASP:HB2	1.74	0.69
2:B:112:THR:HG23	2:B:114:ASN:H	1.58	0.69
1:A:854:MET:O	1:A:858:ILE:HD12	1.92	0.68
1:A:244:LYS:O	1:A:244:LYS:NZ	2.25	0.68
1:A:362:TYR:HB3	1:A:929:ILE:HD11	1.74	0.68
1:A:376:LYS:HE3	1:A:1678:MET:HG3	1.75	0.68
1:A:1643:ALA:O	1:A:1647:ILE:HD12	1.94	0.67
2:B:43:CYS:HA	2:B:102:GLN:HE21	1.59	0.67
2:B:61:GLN:OE1	2:B:85:ARG:NH1	2.24	0.67
3:C:119:PRO:HA	3:C:146:VAL:HG21	1.77	0.66
1:A:1426:LYS:HB2	1:A:1429:TYR:HB2	1.78	0.66
2:B:78:LEU:HD21	2:B:80:LEU:HG	1.76	0.66
1:A:1741:VAL:O	1:A:1745:ILE:HD12	1.96	0.65
1:A:106:LEU:HD21	1:A:176:PHE:HB2	1.79	0.65
1:A:174:ARG:HG3	1:A:183:PHE:H	1.61	0.65
1:A:1217:GLU:HG2	2:B:24:VAL:HG11	1.79	0.65
1:A:116:ARG:O	1:A:120:ILE:HG12	1.96	0.65
1:A:1709:ASN:HB2	1:A:1714:ASP:HB3	1.79	0.65
3:C:68:THR:HG22	3:C:79:MET:HG2	1.78	0.65
1:A:834:LEU:HA	1:A:837:PHE:CE1	2.32	0.65
2:B:53:THR:HG21	2:B:125:ARG:NH1	2.12	0.65
1:A:112:PHE:HA	1:A:117:ARG:NH1	2.13	0.64
1:A:1218:ARG:HG3	2:B:24:VAL:HG22	1.79	0.64
1:A:158:THR:O	1:A:162:ILE:HG13	1.96	0.64
1:A:99:ARG:HD2	1:A:181:PHE:HZ	1.57	0.64
1:A:1381:ARG:NH2	1:A:1383:LYS:HD2	2.12	0.64
2:B:175:VAL:HA	2:B:178:MET:HG3	1.79	0.64
1:A:170:LYS:HD3	1:A:183:PHE:HE2	1.63	0.64
1:A:1416:VAL:HG11	1:A:1434:TYR:CD2	2.33	0.64
1:A:1519:ILE:O	1:A:1523:VAL:HG23	1.99	0.63
1:A:105:ALA:HB3	1:A:109:LEU:HB2	1.80	0.63
1:A:1502:ASN:HB3	1:A:1505:GLN:HG2	1.80	0.63
1:A:1416:VAL:HG11	1:A:1434:TYR:CE2	2.33	0.63
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.79	0.62
3:C:130:MET:HE3	3:C:135:ARG:HH22	1.63	0.62
1:A:188:TRP:CD1	1:A:232:LYS:HE2	2.35	0.62
1:A:314:LEU:HD23	1:A:373:ALA:HB2	1.82	0.62
1:A:1004:GLN:O	1:A:1008:GLU:HG2	2.00	0.61
2:B:148:ASP:OD2	2:B:149:LYS:N	2.33	0.61
2:B:175:VAL:O	2:B:179:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LEU:HD22	5:B:304:NAG:H82	1.83	0.61
1:A:1467:LEU:HD13	1:A:1470:GLN:HB2	1.83	0.61
1:A:140:CYS:SG	1:A:141:ILE:N	2.74	0.61
2:B:24:VAL:H	2:B:41:ILE:HD13	1.65	0.61
1:A:731:ILE:O	1:A:735:LYS:HG3	2.01	0.61
1:A:765:HIS:CE1	1:A:768:MET:HG3	2.36	0.61
1:A:1677:ASP:OD2	2:B:46:ARG:NH1	2.31	0.61
1:A:92:ASN:ND2	1:A:124:VAL:O	2.34	0.60
1:A:120:ILE:HD13	1:A:173:ALA:HB1	1.82	0.60
1:A:356:ARG:HH21	1:A:362:TYR:HD2	1.49	0.60
1:A:1756:ILE:O	1:A:1760:LEU:HG	2.01	0.60
1:A:192:ASP:HB3	1:A:223:LYS:NZ	2.16	0.60
3:C:135:ARG:HA	3:C:135:ARG:CZ	2.32	0.60
1:A:730:TRP:HA	1:A:733:PHE:CZ	2.36	0.60
1:A:929:ILE:O	1:A:932:MET:N	2.34	0.60
1:A:1387:VAL:HG11	1:A:1401:GLN:OE1	2.01	0.60
1:A:1574:PHE:HA	1:A:1580:ILE:HD11	1.84	0.60
1:A:119:SER:HB3	1:A:173:ALA:HB2	1.84	0.60
1:A:94:GLY:O	1:A:95:LYS:HG2	2.02	0.60
1:A:1333:LEU:O	1:A:1337:ILE:HG13	2.02	0.60
1:A:1672:GLU:HB2	1:A:1706:PRO:HB3	1.84	0.60
1:A:985:ALA:HB3	1:A:990:ILE:HD11	1.83	0.60
2:B:162:MET:HA	2:B:165:VAL:HG12	1.83	0.59
1:A:283:ASN:HB2	5:A:2002:NAG:H2	1.84	0.59
2:B:89:ARG:HH21	2:B:112:THR:HB	1.66	0.59
1:A:27:ILE:HG23	1:A:31:LYS:NZ	2.18	0.59
1:A:296:GLU:O	1:A:300:ARG:HG3	2.02	0.58
1:A:1230:ASP:O	1:A:1234:THR:HG23	2.03	0.58
1:A:300:ARG:HG2	1:A:305:TYR:CD1	2.39	0.58
1:A:357:LEU:HD23	1:A:363:TRP:HB2	1.85	0.58
1:A:149:PRO:HB2	1:A:151:TRP:CD1	2.37	0.58
1:A:286:LEU:HD11	1:A:333:ILE:HG21	1.85	0.58
1:A:327:GLY:HA2	2:B:134:HIS:CE1	2.39	0.58
1:A:192:ASP:HB3	1:A:223:LYS:HZ2	1.68	0.58
3:C:122:GLU:HG2	3:C:145:GLN:HA	1.85	0.58
1:A:736:CYS:O	1:A:740:ILE:HG12	2.04	0.58
1:A:192:ASP:O	1:A:196:ILE:HG12	2.03	0.58
1:A:29:GLU:O	1:A:33:LYS:HG2	2.03	0.57
1:A:327:GLY:C	1:A:328:TYR:HD1	2.11	0.57
1:A:276:PHE:CZ	1:A:280:LEU:HD21	2.39	0.57
1:A:120:ILE:O	1:A:124:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:ILE:HG21	1:A:1299:ARG:HE	1.70	0.57
1:A:192:ASP:OD2	1:A:192:ASP:N	2.36	0.57
1:A:730:TRP:HD1	1:A:733:PHE:HZ	1.51	0.57
2:B:29:GLU:N	2:B:29:GLU:OE2	2.38	0.56
1:A:16:THR:HG23	1:A:18:GLN:H	1.68	0.56
1:A:112:PHE:HA	1:A:117:ARG:HH11	1.68	0.56
1:A:118:ILE:O	1:A:122:ILE:HG12	2.05	0.56
1:A:835:ARG:HH21	1:A:835:ARG:HG3	1.71	0.56
1:A:838:ARG:O	1:A:841:ARG:NE	2.39	0.56
1:A:1500:PRO:HB2	1:A:1505:GLN:NE2	2.21	0.56
2:B:187:ALA:O	2:B:191:THR:HG23	2.06	0.56
1:A:13:VAL:HB	1:A:76:GLU:HG2	1.88	0.56
2:B:122:HIS:ND1	2:B:139:VAL:HG22	2.19	0.56
2:B:166:LEU:HA	2:B:169:VAL:HG12	1.88	0.56
1:A:1703:LEU:O	1:A:1706:PRO:HD2	2.05	0.56
1:A:304:TYR:HB2	1:A:328:TYR:CE2	2.41	0.56
1:A:322:GLY:HA2	1:A:1678:MET:HE1	1.87	0.55
1:A:395:ASN:ND2	1:A:1758:VAL:HG13	2.22	0.55
1:A:1408:TRP:H	1:A:1408:TRP:CD1	2.24	0.55
1:A:1504:ILE:O	1:A:1508:ILE:HG12	2.06	0.55
1:A:75:LEU:HD12	1:A:91:LEU:HD23	1.88	0.55
1:A:306:LEU:HD11	1:A:313:LEU:HD13	1.88	0.55
1:A:1400:LEU:HD21	1:A:1744:ILE:HD11	1.88	0.55
1:A:405:TYR:O	1:A:408:GLN:HG3	2.07	0.55
1:A:924:LEU:HD21	1:A:955:GLY:HA3	1.88	0.55
1:A:1371:PHE:HD2	1:A:1374:MET:CE	2.20	0.55
1:A:99:ARG:HB3	1:A:181:PHE:CE1	2.41	0.55
1:A:919:ILE:O	1:A:923:VAL:HG23	2.07	0.55
3:C:98:ARG:HH22	3:C:117:VAL:HA	1.72	0.55
1:A:295:SER:OG	1:A:297:GLU:N	2.40	0.54
1:A:1460:PHE:HD2	1:A:1756:ILE:HG21	1.71	0.54
1:A:747:ASP:O	1:A:751:THR:HG23	2.08	0.54
1:A:932:MET:SD	1:A:936:MET:HE3	2.47	0.54
1:A:1177:ILE:O	1:A:1181:ILE:HG13	2.06	0.54
3:C:63:PHE:HE1	3:C:129:ILE:HG23	1.72	0.54
1:A:20:LEU:HD11	1:A:112:PHE:HE2	1.73	0.54
1:A:188:TRP:HD1	1:A:232:LYS:HE2	1.72	0.54
1:A:304:TYR:HB2	1:A:328:TYR:CD2	2.42	0.54
1:A:732:LYS:HA	1:A:735:LYS:HE2	1.90	0.54
1:A:1295:LEU:HD22	1:A:1298:LEU:HD12	1.89	0.54
2:B:127:LEU:HB3	2:B:129:PHE:HE2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:ILE:O	1:A:1457:ILE:HG12	2.08	0.54
1:A:251:LEU:HB2	1:A:1630:ILE:HG12	1.89	0.54
1:A:266:LEU:HD11	1:A:1614:LEU:HD21	1.90	0.54
1:A:1187:LYS:HD2	1:A:1187:LYS:O	2.08	0.54
1:A:1656:PHE:HE1	6:A:2010:LPE:H112	1.73	0.54
3:C:84:ARG:HH21	3:C:88:ILE:HG13	1.72	0.54
1:A:180:GLU:O	1:A:185:ARG:HD2	2.08	0.54
1:A:1529:MET:O	1:A:1533:MET:HG3	2.08	0.54
1:A:297:GLU:O	1:A:301:LYS:HG3	2.08	0.54
1:A:1485:MET:CB	1:A:1639:MET:HE1	2.37	0.54
1:A:1492:LYS:HD3	1:A:1492:LYS:N	2.23	0.54
1:A:1680:ASN:OD1	1:A:1686:ASN:ND2	2.40	0.54
3:C:87:ILE:HG13	3:C:101:PHE:HD1	1.73	0.54
1:A:1402:VAL:HG22	1:A:1408:TRP:HB2	1.90	0.53
1:A:1001:TYR:O	1:A:1005:THR:HG23	2.08	0.53
1:A:1534:VAL:HG13	1:A:1547:LEU:HD21	1.90	0.53
1:A:306:LEU:HD12	1:A:306:LEU:H	1.72	0.53
1:A:348:SER:HB3	7:A:2008:PCW:H352	1.91	0.53
1:A:742:MET:HG2	1:A:744:PRO:HD2	1.90	0.53
2:B:36:PHE:HE2	2:B:144:ILE:HD12	1.72	0.53
1:A:737:ILE:HG13	1:A:796:ILE:HD11	1.90	0.53
2:B:54:PHE:CZ	2:B:124:TYR:HD2	2.26	0.53
1:A:1409:THR:HA	1:A:1412:MET:HE3	1.90	0.53
1:A:117:ARG:O	1:A:121:LYS:HG2	2.07	0.53
1:A:769:THR:O	1:A:773:LYS:HG3	2.09	0.53
2:B:168:VAL:O	2:B:171:THR:OG1	2.25	0.53
1:A:48:LYS:HD3	1:A:48:LYS:N	2.24	0.53
1:A:1675:ILE:HD12	1:A:1706:PRO:HG2	1.89	0.53
1:A:1742:SER:O	1:A:1746:ILE:HG13	2.08	0.53
1:A:794:LYS:HB2	1:A:803:TYR:OH	2.08	0.53
2:B:172:ILE:HA	2:B:175:VAL:HG22	1.91	0.53
1:A:1350:CYS:HA	1:A:1381:ARG:O	2.09	0.52
1:A:162:ILE:HA	1:A:165:PHE:CE2	2.44	0.52
1:A:1365:PRO:HG2	1:A:1366:ASN:OD1	2.10	0.52
1:A:82:TYR:HD1	1:A:85:LYS:HZ3	1.58	0.52
1:A:89:ILE:HG21	1:A:97:ILE:HG23	1.90	0.52
2:B:121:CYS:HB3	2:B:140:LYS:HB2	1.91	0.52
1:A:364:GLU:O	1:A:368:GLN:HG3	2.10	0.52
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.91	0.52
2:B:89:ARG:NH2	2:B:112:THR:HB	2.24	0.52
1:A:293:LEU:HB3	1:A:299:PHE:HE1	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1732:ASN:HB3	1:A:1735:VAL:CG1	2.36	0.52
3:C:46:ALA:HB3	3:C:114:LEU:HB3	1.91	0.52
1:A:275:CYS:HB3	1:A:328:TYR:HB3	1.91	0.52
3:C:84:ARG:O	3:C:85:MET:HE2	2.09	0.52
1:A:187:PRO:HA	1:A:190:TRP:HD1	1.75	0.51
1:A:730:TRP:HD1	1:A:733:PHE:CZ	2.27	0.51
1:A:994:ARG:HG2	1:A:994:ARG:HH11	1.75	0.51
1:A:1177:ILE:HD12	1:A:1177:ILE:H	1.74	0.51
1:A:234:ILE:HG21	1:A:872:VAL:HG21	1.92	0.51
1:A:1242:LEU:O	1:A:1246:ILE:HG12	2.11	0.51
1:A:1298:LEU:HD23	1:A:1301:LEU:HD11	1.92	0.51
1:A:1185:CYS:O	1:A:1189:VAL:HG22	2.10	0.51
1:A:1405:PHE:HA	1:A:1408:TRP:CD1	2.46	0.51
2:B:39:LEU:HD12	2:B:105:SER:HB3	1.93	0.51
1:A:936:MET:HE2	1:A:945:LEU:HG	1.92	0.51
2:B:87:GLU:HG2	2:B:88:GLY:H	1.76	0.51
1:A:50:SER:OG	1:A:53:LEU:HB2	2.11	0.51
1:A:276:PHE:HZ	1:A:280:LEU:HD21	1.75	0.51
1:A:332:LYS:NZ	1:A:1537:GLU:OE1	2.44	0.50
1:A:1185:CYS:SG	1:A:1246:ILE:HG13	2.51	0.50
1:A:1522:MET:HA	1:A:1525:ILE:HG12	1.92	0.50
1:A:1675:ILE:HD12	1:A:1706:PRO:CG	2.41	0.50
1:A:99:ARG:NH1	1:A:99:ARG:HB2	2.26	0.50
3:C:65:LEU:O	3:C:82:GLN:HG3	2.12	0.50
1:A:969:SER:O	1:A:974:ASP:N	2.44	0.50
1:A:1195:GLU:O	1:A:1199:VAL:HG23	2.11	0.50
1:A:1234:THR:O	1:A:1238:ILE:HG23	2.12	0.50
1:A:1656:PHE:O	1:A:1660:ILE:HG12	2.12	0.50
1:A:86:LYS:O	1:A:86:LYS:HG3	2.10	0.50
1:A:23:ILE:HD12	1:A:86:LYS:HB2	1.92	0.50
1:A:140:CYS:HA	1:A:143:MET:HG3	1.94	0.50
1:A:30:ARG:O	1:A:34:GLU:HG2	2.11	0.50
1:A:186:ASP:HB3	1:A:189:ASN:OD1	2.12	0.50
1:A:1409:THR:HA	1:A:1412:MET:CE	2.42	0.50
1:A:1521:ILE:O	1:A:1525:ILE:HG12	2.12	0.50
1:A:731:ILE:HD12	1:A:731:ILE:H	1.77	0.49
1:A:992:VAL:HA	1:A:995:ILE:HG12	1.94	0.49
1:A:1543:MET:HA	1:A:1546:VAL:HG22	1.93	0.49
2:B:64:THR:HG22	2:B:66:GLU:H	1.78	0.49
1:A:1251:LYS:HE3	1:A:1255:THR:HG21	1.93	0.49
3:C:40:VAL:HG13	3:C:117:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HD3	1:A:17:LYS:N	2.27	0.49
1:A:47:PRO:C	1:A:48:LYS:HD3	2.38	0.49
1:A:165:PHE:HA	1:A:168:LEU:HB3	1.94	0.49
1:A:1565:LYS:HE3	1:A:1569:LEU:HD11	1.95	0.49
2:B:185:ILE:HG13	2:B:186:ALA:N	2.27	0.49
1:A:210:VAL:HA	1:A:213:LEU:HD12	1.94	0.49
2:B:125:ARG:HH11	2:B:125:ARG:HG3	1.78	0.49
1:A:195:VAL:HG21	1:A:220:ARG:HG3	1.95	0.48
1:A:28:ALA:HA	1:A:31:LYS:NZ	2.29	0.48
1:A:742:MET:O	1:A:746:VAL:HG12	2.14	0.48
2:B:153:ASP:O	2:B:156:SER:OG	2.28	0.48
3:C:80:PHE:CD1	3:C:81:LEU:HD23	2.39	0.48
3:C:82:GLN:HG2	3:C:83:PHE:H	1.77	0.48
1:A:247:ASP:OD1	1:A:248:VAL:N	2.47	0.48
1:A:295:SER:HB3	1:A:298:ASP:H	1.79	0.48
1:A:843:PHE:CD1	1:A:856:ILE:HD11	2.48	0.48
1:A:1283:LEU:HG	1:A:1286:ILE:HD13	1.94	0.48
1:A:1488:LEU:HD23	1:A:1491:LYS:HZ3	1.78	0.48
1:A:228:ILE:HD12	1:A:228:ILE:H	1.79	0.48
2:B:65:GLU:OE2	2:B:65:GLU:N	2.47	0.48
1:A:1254:PHE:O	1:A:1260:TRP:NE1	2.39	0.48
1:A:1256:ASN:OD1	1:A:1257:ALA:N	2.47	0.48
1:A:1336:SER:O	1:A:1340:VAL:HG12	2.13	0.48
2:B:58:THR:OG1	2:B:67:PHE:HB3	2.14	0.48
1:A:1301:LEU:HD12	1:A:1301:LEU:H	1.78	0.48
1:A:1324:VAL:HG21	1:A:1455:VAL:CG2	2.37	0.48
2:B:173:TRP:O	2:B:177:GLU:HG2	2.13	0.48
1:A:155:VAL:HA	1:A:158:THR:HG22	1.96	0.48
1:A:1219:LYS:HZ3	6:A:2010:LPE:H2N3	1.79	0.48
1:A:222:LEU:HD23	1:A:222:LEU:O	2.14	0.47
1:A:1330:ILE:HD12	1:A:1333:LEU:HD23	1.96	0.47
1:A:50:SER:N	1:A:79:ASP:OD1	2.47	0.47
1:A:1240:GLU:OE2	1:A:1244:LYS:NZ	2.48	0.47
1:A:1539:GLN:HG3	1:A:1540:SER:H	1.78	0.47
1:A:1314:LEU:HD23	1:A:1314:LEU:O	2.14	0.47
1:A:191:LEU:HA	1:A:194:VAL:HG22	1.96	0.47
1:A:1232:ILE:O	1:A:1236:ILE:HG13	2.14	0.47
1:A:289:ILE:HG22	1:A:293:LEU:HD22	1.96	0.47
1:A:1430:SER:O	1:A:1430:SER:OG	2.25	0.47
2:B:93:ASN:OD1	5:B:301:NAG:N2	2.47	0.47
2:B:157:ILE:O	2:B:161:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:HG11	1:A:883:VAL:HG23	1.97	0.47
1:A:731:ILE:HA	1:A:734:LYS:HG2	1.97	0.47
1:A:1273:LEU:O	1:A:1277:THR:HG23	2.14	0.47
1:A:1387:VAL:HG13	1:A:1397:LEU:HD23	1.97	0.47
2:B:54:PHE:HB2	2:B:73:TYR:O	2.15	0.47
1:A:1241:MET:SD	1:A:1266:VAL:HG21	2.55	0.47
1:A:1504:ILE:HG13	1:A:1505:GLN:H	1.80	0.47
1:A:1543:MET:O	1:A:1547:LEU:HD12	2.15	0.47
1:A:986:ASN:OD1	1:A:988:LEU:HB3	2.15	0.47
1:A:1620:ILE:H	1:A:1620:ILE:HD12	1.80	0.47
3:C:67:TRP:CH2	3:C:127:CYS:HB3	2.50	0.47
3:C:72:CYS:N	3:C:75:CYS:SG	2.78	0.47
1:A:195:VAL:HG21	1:A:220:ARG:CG	2.45	0.47
1:A:203:GLU:HG2	1:A:204:PHE:HD1	1.80	0.47
1:A:852:LEU:HD12	1:A:852:LEU:HA	1.72	0.47
1:A:1423:LYS:HE3	1:A:1423:LYS:HA	1.96	0.47
2:B:73:TYR:HE2	2:B:76:GLU:C	2.22	0.47
2:B:87:GLU:CD	2:B:87:GLU:H	2.23	0.47
1:A:1283:LEU:HD23	1:A:1283:LEU:H	1.80	0.46
1:A:203:GLU:HG2	1:A:204:PHE:CD1	2.50	0.46
1:A:27:ILE:C	1:A:31:LYS:HZ3	2.23	0.46
1:A:326:GLU:HG3	2:B:45:ARG:HG3	1.97	0.46
1:A:1587:ILE:HD12	1:A:1587:ILE:HA	1.75	0.46
1:A:337:PRO:HG2	1:A:342:THR:OG1	2.15	0.46
1:A:1178:TRP:HA	1:A:1181:ILE:HD12	1.97	0.46
1:A:1366:ASN:OD1	1:A:1366:ASN:N	2.48	0.46
1:A:997:LYS:HD2	1:A:997:LYS:C	2.40	0.46
1:A:1264:LEU:O	1:A:1268:VAL:HG23	2.16	0.46
3:C:65:LEU:O	3:C:82:GLN:HA	2.14	0.46
3:C:126:ASN:HB2	3:C:141:LYS:NZ	2.31	0.46
2:B:174:LEU:O	2:B:178:MET:HG3	2.15	0.46
1:A:385:VAL:O	1:A:389:GLY:N	2.49	0.46
1:A:1307:MET:HE3	1:A:1307:MET:HB3	1.61	0.46
1:A:1337:ILE:HA	1:A:1340:VAL:HG12	1.97	0.46
1:A:290:MET:HE3	1:A:290:MET:O	2.16	0.46
1:A:1219:LYS:NZ	6:A:2010:LPE:H2N3	2.31	0.46
1:A:1348:TYR:HD1	1:A:1382:TRP:HE1	1.62	0.46
1:A:1366:ASN:HB3	1:A:1423:LYS:NZ	2.31	0.46
1:A:1654:VAL:HG22	6:A:2006:LPE:H211	1.98	0.46
1:A:907:ARG:HG2	1:A:1413:TYR:CZ	2.50	0.46
1:A:1012:LYS:HD3	1:A:1012:LYS:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:MET:HG2	1:A:1380:VAL:HB	1.98	0.46
2:B:34:MET:O	2:B:111:VAL:HG23	2.16	0.46
1:A:202:THR:HA	1:A:205:VAL:HG12	1.98	0.45
1:A:815:ILE:HD13	1:A:841:ARG:HG3	1.98	0.45
1:A:916:SER:O	1:A:920:VAL:HG23	2.16	0.45
1:A:1295:LEU:HD22	1:A:1298:LEU:CD1	2.46	0.45
1:A:1642:PRO:O	1:A:1645:PHE:HB3	2.16	0.45
2:B:46:ARG:HE	2:B:48:GLU:CD	2.24	0.45
1:A:730:TRP:O	1:A:734:LYS:HG2	2.17	0.45
2:B:166:LEU:O	2:B:170:LEU:HG	2.16	0.45
1:A:27:ILE:HG23	1:A:31:LYS:HZ2	1.78	0.45
1:A:193:PHE:O	1:A:197:VAL:HG13	2.17	0.45
1:A:318:SER:OG	1:A:319:THR:N	2.49	0.45
1:A:760:PHE:HA	1:A:763:MET:SD	2.55	0.45
1:A:1321:ILE:HG12	1:A:1452:PHE:HE1	1.81	0.45
1:A:82:TYR:HA	1:A:85:LYS:NZ	2.31	0.45
2:B:145:GLU:HA	2:B:145:GLU:OE2	2.17	0.45
3:C:89:ASN:OD1	3:C:91:LYS:N	2.44	0.45
1:A:99:ARG:CD	1:A:181:PHE:CZ	2.80	0.45
3:C:81:LEU:HD13	3:C:89:ASN:HA	1.98	0.45
1:A:1321:ILE:HD11	1:A:1456:ILE:HD11	1.98	0.45
1:A:1576:VAL:O	1:A:1580:ILE:HG12	2.16	0.45
2:B:143:HIS:NE2	2:B:145:GLU:OE1	2.50	0.45
2:B:168:VAL:O	2:B:172:ILE:HG23	2.16	0.45
3:C:59:ASN:OD1	3:C:61:LYS:HG2	2.17	0.45
1:A:118:ILE:HA	1:A:121:LYS:HG2	1.99	0.45
1:A:743:ASP:HB3	1:A:744:PRO:HD3	1.99	0.45
1:A:994:ARG:HG2	1:A:994:ARG:NH1	2.32	0.45
1:A:1206:SER:HA	1:A:1209:LEU:HD12	1.99	0.45
1:A:1524:LEU:HA	1:A:1527:LEU:HB2	1.99	0.45
2:B:74:GLU:O	2:B:74:GLU:HG3	2.17	0.45
2:B:87:GLU:OE1	2:B:87:GLU:N	2.42	0.45
3:C:102:SER:OG	3:C:113:MET:HE2	2.16	0.45
1:A:202:THR:HG22	1:A:213:LEU:HD13	1.99	0.45
1:A:943:MET:O	1:A:947:VAL:HG23	2.17	0.45
1:A:1453:ILE:HD13	1:A:1453:ILE:HA	1.85	0.45
1:A:246:SER:OG	1:A:247:ASP:N	2.48	0.45
1:A:768:MET:HE2	1:A:768:MET:HB3	1.82	0.45
1:A:1183:LYS:HD2	1:A:1183:LYS:HA	1.83	0.45
3:C:69:TYR:HE2	3:C:123:GLY:HA3	1.82	0.45
1:A:307:GLU:OE1	1:A:307:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HD11	2:B:86:PHE:HD1	1.82	0.45
3:C:34:VAL:HG12	3:C:49:PRO:O	2.17	0.45
1:A:1408:TRP:H	1:A:1408:TRP:HD1	1.63	0.44
1:A:1610:ARG:O	1:A:1614:LEU:HD13	2.17	0.44
3:C:42:ASN:HD21	3:C:119:PRO:HG3	1.82	0.44
1:A:162:ILE:HA	1:A:165:PHE:CD2	2.52	0.44
1:A:187:PRO:HA	1:A:190:TRP:CD1	2.52	0.44
1:A:1761:GLU:HA	1:A:1761:GLU:OE2	2.17	0.44
1:A:222:LEU:HD23	1:A:225:ILE:HD12	2.00	0.44
1:A:410:GLN:O	1:A:413:ILE:HG12	2.16	0.44
1:A:969:SER:HA	1:A:973:SER:HB2	1.99	0.44
1:A:1585:VAL:HA	1:A:1588:ILE:HG12	1.99	0.44
3:C:47:ARG:HG2	3:C:113:MET:HE1	1.98	0.44
1:A:24:GLU:O	1:A:28:ALA:N	2.49	0.44
1:A:1237:PHE:O	1:A:1240:GLU:HB3	2.17	0.44
1:A:1417:ASP:OD2	1:A:1428:GLU:N	2.40	0.44
2:B:86:PHE:CE2	2:B:115:HIS:CE1	3.06	0.44
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.74	0.44
1:A:1242:LEU:HD23	1:A:1242:LEU:HA	1.73	0.44
2:B:154:MET:O	2:B:158:VAL:HG23	2.18	0.44
1:A:111:PRO:HA	1:A:116:ARG:CD	2.48	0.44
1:A:1607:THR:O	1:A:1611:VAL:HG23	2.17	0.44
1:A:1755:TYR:O	1:A:1759:ILE:HD12	2.18	0.44
3:C:35:PRO:O	3:C:142:ILE:HG12	2.17	0.44
3:C:67:TRP:HB2	3:C:81:LEU:O	2.17	0.44
1:A:176:PHE:HB3	1:A:177:CYS:H	1.70	0.44
1:A:203:GLU:O	1:A:206:ASN:ND2	2.51	0.44
2:B:165:VAL:O	2:B:169:VAL:HG12	2.18	0.44
1:A:24:GLU:HA	1:A:27:ILE:HG22	2.00	0.43
1:A:412:ASN:O	1:A:415:GLU:HG2	2.18	0.43
1:A:992:VAL:HG13	1:A:996:LYS:HZ1	1.82	0.43
1:A:1366:ASN:O	1:A:1369:GLU:HB2	2.18	0.43
1:A:1367:ARG:O	1:A:1368:SER:C	2.59	0.43
1:A:1435:ILE:HD12	1:A:1435:ILE:H	1.83	0.43
1:A:1678:MET:HE3	1:A:1678:MET:HB2	1.71	0.43
2:B:69:LYS:NZ	2:B:72:ARG:HB2	2.33	0.43
3:C:38:LEU:N	3:C:143:HIS:O	2.41	0.43
3:C:47:ARG:HG2	3:C:113:MET:SD	2.58	0.43
1:A:417:LYS:HE2	1:A:417:LYS:HB3	1.77	0.43
1:A:798:MET:HE1	1:A:803:TYR:HA	1.99	0.43
1:A:1514:ASN:OD1	1:A:1516:ALA:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:HB2	1:A:75:LEU:C	2.43	0.43
1:A:165:PHE:O	1:A:169:VAL:HG13	2.18	0.43
1:A:202:THR:HG21	1:A:213:LEU:HB3	2.01	0.43
1:A:1204:LEU:HB3	1:A:1233:PHE:HZ	1.82	0.43
1:A:1348:TYR:CD1	1:A:1382:TRP:NE1	2.86	0.43
2:B:56:GLU:OE1	2:B:69:LYS:HD2	2.18	0.43
3:C:143:HIS:HB3	3:C:145:GLN:HE21	1.82	0.43
4:D:1:NAG:O6	4:D:2:NAG:O5	2.31	0.43
1:A:344:PHE:HE1	1:A:354:LEU:HD11	1.84	0.43
1:A:835:ARG:HG3	1:A:835:ARG:NH2	2.33	0.43
1:A:996:LYS:HA	1:A:999:ILE:HG12	2.00	0.43
1:A:1267:ASP:O	1:A:1271:VAL:HG23	2.19	0.43
2:B:112:THR:HG23	2:B:114:ASN:N	2.31	0.43
1:A:890:LYS:HE2	1:A:890:LYS:HB3	1.79	0.43
2:B:175:VAL:HA	2:B:178:MET:HE2	2.00	0.43
1:A:12:PHE:CZ	1:A:63:TYR:HB3	2.54	0.43
1:A:71:VAL:O	1:A:73:GLU:HG2	2.18	0.43
1:A:1502:ASN:H	1:A:1505:GLN:HE21	1.67	0.43
1:A:1672:GLU:O	1:A:1673:ASP:C	2.62	0.43
1:A:345:ASP:HB3	1:A:1537:GLU:HB2	2.01	0.43
1:A:419:LYS:HA	1:A:419:LYS:HD3	1.66	0.43
1:A:907:ARG:HG2	1:A:1413:TYR:CE1	2.54	0.43
1:A:989:GLN:O	1:A:992:VAL:HG12	2.18	0.43
6:A:2003:LPE:H141	6:A:2003:LPE:H112	1.47	0.43
3:C:48:LEU:HD23	3:C:142:ILE:HD12	2.00	0.43
1:A:328:TYR:HE1	2:B:132:TYR:CE2	2.36	0.43
1:A:840:LEU:HD12	1:A:840:LEU:H	1.84	0.43
1:A:1485:MET:HB3	1:A:1639:MET:CE	2.46	0.43
1:A:183:PHE:CZ	1:A:189:ASN:HB3	2.54	0.43
1:A:1260:TRP:O	1:A:1264:LEU:HD23	2.18	0.42
1:A:1445:SER:O	1:A:1449:LEU:HB2	2.19	0.42
1:A:20:LEU:HD11	1:A:112:PHE:CE2	2.53	0.42
1:A:86:LYS:HZ1	1:A:102:ALA:C	2.26	0.42
1:A:1177:ILE:HA	1:A:1180:ASN:OD1	2.19	0.42
1:A:1306:GLY:HA2	1:A:1309:VAL:HG12	2.01	0.42
2:B:51:ALA:HB2	2:B:127:LEU:HD23	2.00	0.42
2:B:154:MET:H	2:B:154:MET:HG2	1.66	0.42
3:C:143:HIS:O	3:C:145:GLN:NE2	2.52	0.42
1:A:124:VAL:O	1:A:124:VAL:HG22	2.19	0.42
1:A:174:ARG:HG3	1:A:183:PHE:N	2.33	0.42
2:B:42:SER:O	2:B:42:SER:OG	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:CD1	1:A:107:TYR:O	2.72	0.42
1:A:730:TRP:HA	1:A:733:PHE:CE2	2.55	0.42
1:A:791:MET:HE1	1:A:803:TYR:HE1	1.84	0.42
1:A:855:LEU:HA	1:A:858:ILE:HD13	2.01	0.42
3:C:32:VAL:HG11	3:C:140:GLY:HA3	2.00	0.42
3:C:141:LYS:HE3	3:C:141:LYS:HA	2.01	0.42
1:A:741:VAL:O	1:A:741:VAL:HG12	2.20	0.42
1:A:79:ASP:OD2	1:A:81:TYR:N	2.49	0.42
1:A:142:PHE:CE2	1:A:155:VAL:HG11	2.54	0.42
1:A:1343:PHE:HD1	1:A:1389:PHE:CD1	2.38	0.42
1:A:736:CYS:HA	1:A:739:PHE:CD1	2.55	0.42
1:A:1429:TYR:CD2	1:A:1429:TYR:C	2.98	0.42
1:A:1592:GLY:O	1:A:1593:MET:C	2.61	0.42
2:B:31:VAL:HG23	2:B:34:MET:HB2	2.02	0.42
2:B:129:PHE:HB2	2:B:132:TYR:O	2.19	0.42
1:A:250:ILE:HG22	1:A:1630:ILE:HD11	2.01	0.42
1:A:842:VAL:HB	1:A:1334:ILE:HD11	2.02	0.42
1:A:950:MET:HE2	1:A:950:MET:HA	2.01	0.42
7:A:2005:PCW:H361	7:A:2005:PCW:H181	2.01	0.42
1:A:22:LEU:HA	1:A:25:GLN:NE2	2.35	0.42
1:A:209:ASN:HB2	1:A:210:VAL:H	1.52	0.42
1:A:820:LEU:HA	1:A:820:LEU:HD13	1.62	0.42
1:A:1348:TYR:HE2	1:A:1384:ASN:HB2	1.85	0.42
1:A:1442:ILE:O	1:A:1446:PHE:HB3	2.19	0.42
2:B:162:MET:HA	2:B:165:VAL:CG1	2.49	0.42
1:A:235:VAL:O	1:A:239:ILE:HG12	2.19	0.42
1:A:285:THR:O	1:A:289:ILE:HG12	2.20	0.42
1:A:1195:GLU:OE2	1:A:1303:ARG:NE	2.50	0.42
1:A:1326:LEU:HA	1:A:1329:LEU:HD12	2.02	0.42
1:A:1358:ARG:NH2	1:A:1417:ASP:OD1	2.53	0.42
1:A:1408:TRP:CZ3	1:A:1441:ILE:HD11	2.55	0.42
1:A:1305:GLU:O	1:A:1306:GLY:C	2.62	0.41
1:A:1504:ILE:HG13	1:A:1505:GLN:N	2.35	0.41
1:A:1711:LYS:O	1:A:1712:PRO:C	2.63	0.41
3:C:52:PHE:CE1	3:C:129:ILE:HG21	2.55	0.41
1:A:62:ILE:HG13	1:A:63:TYR:CD1	2.55	0.41
1:A:404:ALA:O	1:A:405:TYR:C	2.61	0.41
2:B:46:ARG:O	2:B:49:THR:HG23	2.20	0.41
2:B:54:PHE:HE2	2:B:72:ARG:HE	1.68	0.41
1:A:347:PHE:C	1:A:347:PHE:CD2	2.99	0.41
1:A:1348:TYR:HD1	1:A:1382:TRP:NE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1641:LEU:HD23	1:A:1641:LEU:HA	1.89	0.41
1:A:101:ASN:HD21	1:A:181:PHE:H	1.69	0.41
1:A:752:ILE:O	1:A:756:LEU:HD23	2.20	0.41
1:A:1697:SER:O	1:A:1700:TRP:HD1	2.04	0.41
1:A:361:ASP:OD1	1:A:361:ASP:C	2.62	0.41
1:A:964:LEU:HD23	1:A:964:LEU:HA	1.88	0.41
1:A:991:ALA:O	1:A:995:ILE:HG12	2.20	0.41
1:A:1508:ILE:O	1:A:1512:VAL:HG13	2.21	0.41
7:A:2008:PCW:H20	7:A:2008:PCW:H231	1.91	0.41
2:B:33:GLY:C	5:B:302:NAG:H82	2.45	0.41
3:C:82:GLN:CG	3:C:83:PHE:H	2.33	0.41
7:A:2005:PCW:H63	7:A:2005:PCW:H42	1.91	0.41
1:A:1491:LYS:HB3	1:A:1491:LYS:HE3	1.81	0.41
1:A:1559:THR:HG22	1:A:1586:VAL:HG13	2.01	0.41
1:A:224:THR:HG21	1:A:875:ILE:HD11	2.02	0.41
1:A:322:GLY:CA	1:A:1678:MET:HE1	2.51	0.41
1:A:402:ALA:HA	1:A:964:LEU:HD13	2.03	0.41
1:A:855:LEU:O	1:A:859:ILE:HG12	2.21	0.41
1:A:1512:VAL:HA	1:A:1517:PHE:CD2	2.56	0.41
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.77	0.41
2:B:70:ILE:HG12	2:B:86:PHE:CD1	2.56	0.41
3:C:35:PRO:HD2	3:C:142:ILE:HD11	2.01	0.41
1:A:135:THR:HG21	1:A:162:ILE:HG21	2.03	0.41
1:A:327:GLY:O	1:A:328:TYR:HD1	2.04	0.41
1:A:924:LEU:HA	1:A:924:LEU:HD23	1.69	0.41
1:A:1232:ILE:HG13	2:B:163:MET:HG3	2.03	0.41
1:A:1248:TYR:HB3	1:A:1252:THR:OG1	2.21	0.41
1:A:1353:THR:OG1	1:A:1379:ASN:HB3	2.21	0.41
1:A:1378:GLN:HG3	1:A:1379:ASN:H	1.85	0.41
1:A:1394:LEU:HA	1:A:1394:LEU:HD23	1.88	0.41
1:A:1394:LEU:HD11	7:A:2005:PCW:H131	2.01	0.41
1:A:1406:LYS:HG3	1:A:1697:SER:O	2.21	0.41
2:B:28:THR:OG1	2:B:29:GLU:OE2	2.28	0.41
1:A:1213:ASP:OD1	1:A:1215:TYR:N	2.46	0.41
1:A:1500:PRO:HD2	1:A:1509:PHE:CD1	2.56	0.41
3:C:39:ASN:OD1	3:C:145:GLN:HB2	2.21	0.41
1:A:18:GLN:HA	1:A:21:ALA:HB3	2.03	0.40
1:A:77:ASP:HA	1:A:89:ILE:HD12	2.02	0.40
1:A:201:LEU:O	1:A:205:VAL:HG12	2.21	0.40
1:A:272:LYS:HB3	1:A:272:LYS:HE3	1.63	0.40
1:A:858:ILE:HD12	1:A:858:ILE:H	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:PHE:O	1:A:1305:GLU:C	2.64	0.40
1:A:1640:SER:O	1:A:1644:LEU:HD12	2.21	0.40
2:B:120:GLU:HA	2:B:140:LYS:O	2.21	0.40
3:C:86:LYS:HE3	3:C:86:LYS:HB3	1.86	0.40
3:C:98:ARG:NH2	3:C:117:VAL:HA	2.35	0.40
1:A:188:TRP:CE3	1:A:188:TRP:HA	2.56	0.40
1:A:1596:ALA:O	1:A:1597:ASP:C	2.62	0.40
1:A:336:ASN:HB3	1:A:337:PRO:HD2	2.02	0.40
1:A:1374:MET:CG	1:A:1380:VAL:HB	2.50	0.40
6:A:2003:LPE:H312	6:A:2003:LPE:H1N2	1.87	0.40
1:A:992:VAL:HG13	1:A:996:LYS:NZ	2.36	0.40
1:A:1320:SER:O	1:A:1321:ILE:C	2.64	0.40
1:A:1325:LEU:HD12	1:A:1325:LEU:O	2.22	0.40
1:A:1752:VAL:O	1:A:1756:ILE:HG12	2.21	0.40
3:C:86:LYS:HD2	3:C:87:ILE:N	2.37	0.40
1:A:1205:SER:N	1:A:1233:PHE:HE2	2.19	0.40
1:A:1324:VAL:HG21	1:A:1455:VAL:HG11	2.03	0.40
6:A:2010:LPE:H181	6:A:2010:LPE:H151	1.91	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	1265/2031 (62%)	1180 (93%)	83 (7%)	2 (0%)	43	70
2	B	171/230 (74%)	158 (92%)	13 (8%)	0	100	100
3	C	120/227 (53%)	112 (93%)	7 (6%)	1 (1%)	16	44
All	All	1556/2488 (62%)	1450 (93%)	103 (7%)	3 (0%)	44	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	PHE
1	A	183	PHE
3	C	97	ASP

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	1140/1810 (63%)	1107 (97%)	33 (3%)	37	60
2	B	157/202 (78%)	157 (100%)	0	100	100
3	C	114/205 (56%)	114 (100%)	0	100	100
All	All	1411/2217 (64%)	1378 (98%)	33 (2%)	44	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LYS
1	A	156	GLU
1	A	178	VAL
1	A	209	ASN
1	A	215	THR
1	A	293	LEU
1	A	326	GLU
1	A	358	MET
1	A	380	ILE
1	A	383	VAL
1	A	388	LEU
1	A	395	ASN
1	A	396	LEU
1	A	398	LEU
1	A	408	GLN
1	A	776	LEU
1	A	781	LEU
1	A	812	ASP
1	A	818	LEU
1	A	820	LEU

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	952	MET
1	A	957	LEU
1	A	967	LEU
1	A	1246	ILE
1	A	1449	LEU
1	A	1456	ILE
1	A	1466	LYS
1	A	1557	LEU
1	A	1569	LEU
1	A	1571	HIS
1	A	1599	ILE
1	A	1628	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	412	ASN
1	A	765	HIS
1	A	915	HIS
1	A	1461	ASN
1	A	1470	GLN
1	A	1505	GLN
1	A	1551	ASN
1	A	1693	GLN
2	B	102	GLN
2	B	115	HIS
3	C	39	ASN
3	C	139	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 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	4,1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
4	NAG	D	2	4	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	E	1	4,1	14,14,15	0.65	0	17,19,21	1.00	2 (11%)
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.56	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	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C1-O5-C5	2.95	116.15	112.19
4	E	1	NAG	O5-C5-C4	-2.24	105.39	110.83
4	E	1	NAG	C1-O5-C5	-2.12	109.34	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2

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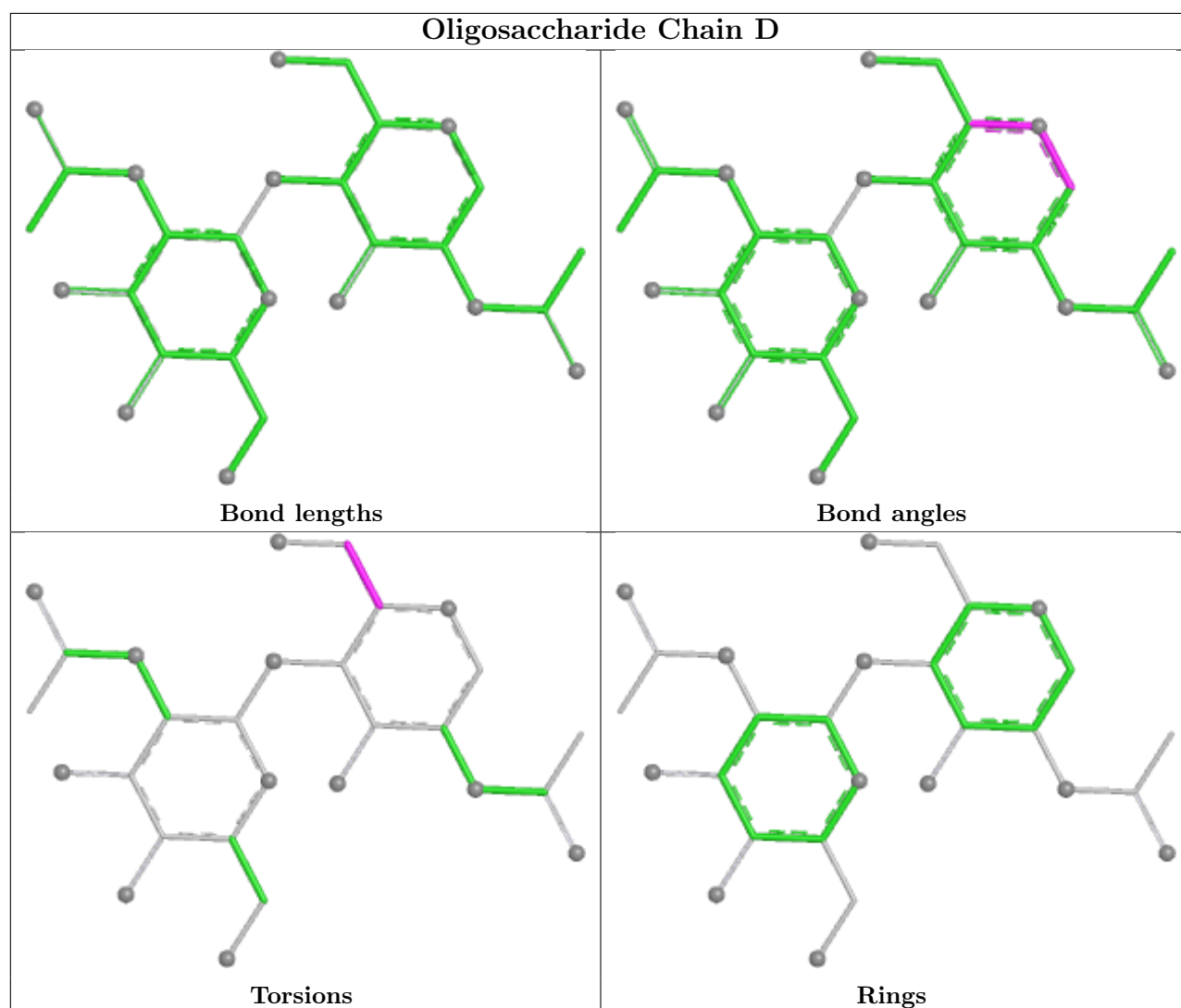
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

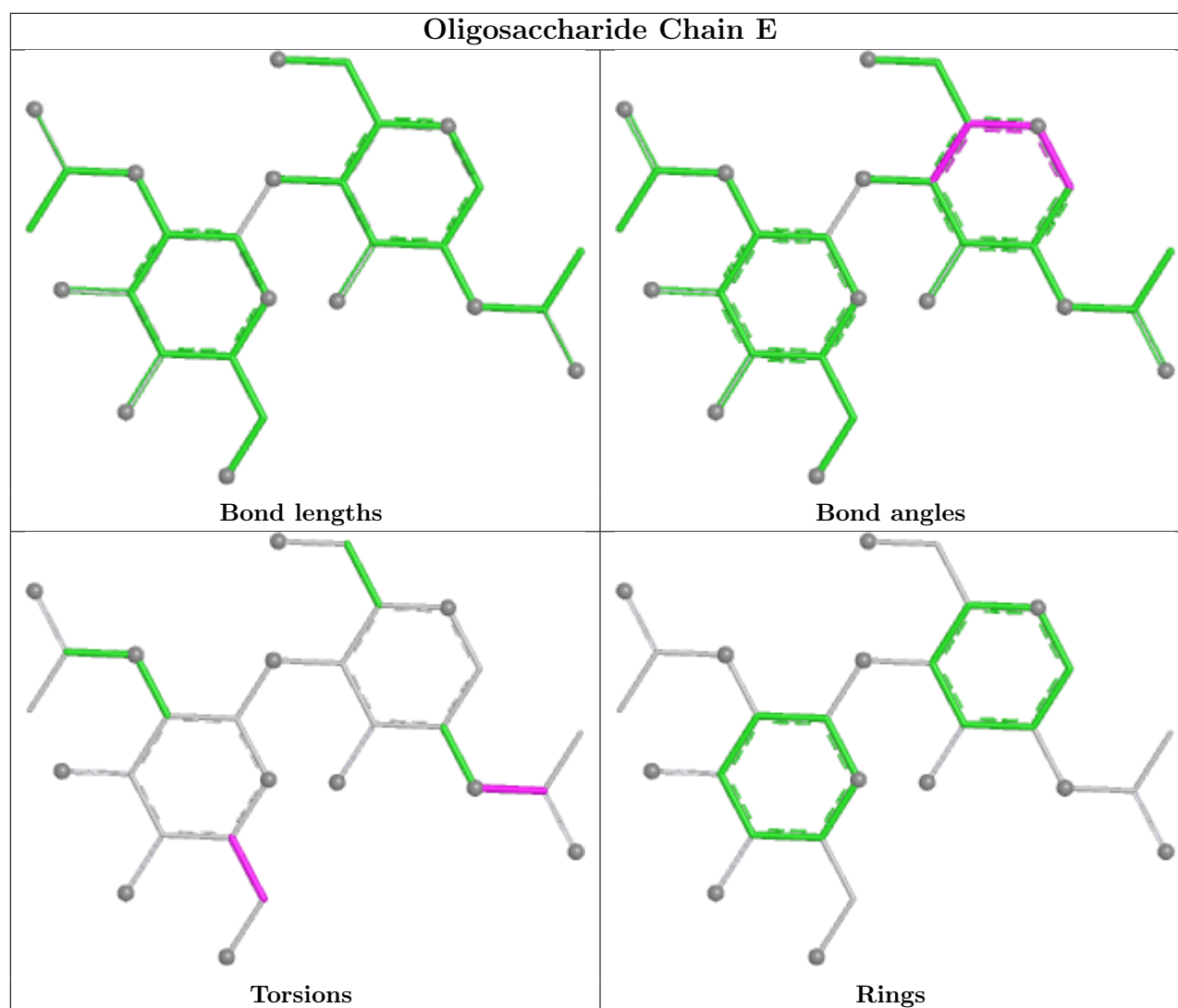
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	D	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	2002	1	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	A	2001	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	B	302	2	14,14,15	0.20	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PCW	A	2005	-	52,52,53	0.92	2 (3%)	58,60,61	1.06	6 (10%)
6	LPE	A	2003	-	24,24,33	0.55	0	28,30,39	0.73	0
6	LPE	A	2006	-	27,27,33	0.54	0	31,33,39	0.76	1 (3%)
5	NAG	B	303	2	14,14,15	0.33	0	17,19,21	0.56	0
7	PCW	A	2009	-	43,43,53	1.01	2 (4%)	49,51,61	1.21	4 (8%)
6	LPE	A	2007	-	27,27,33	0.53	0	31,33,39	0.66	1 (3%)
6	LPE	A	2004	-	24,24,33	0.34	0	25,27,39	0.70	0
7	PCW	A	2008	-	46,46,53	0.98	2 (4%)	52,54,61	1.24	4 (7%)
5	NAG	B	301	2	14,14,15	0.39	0	17,19,21	1.01	1 (5%)
5	NAG	B	304	2	14,14,15	0.19	0	17,19,21	0.81	1 (5%)
6	LPE	A	2010	-	24,24,33	0.56	0	28,30,39	0.62	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
7	PCW	A	2005	-	-	19/56/56/57	-
6	LPE	A	2003	-	-	10/25/25/34	-
6	LPE	A	2006	-	-	9/28/28/34	-
5	NAG	B	303	2	-	2/6/23/26	0/1/1/1
7	PCW	A	2009	-	-	11/47/47/57	-
6	LPE	A	2007	-	-	11/28/28/34	-
6	LPE	A	2004	-	-	10/25/25/34	-
7	PCW	A	2008	-	-	19/50/50/57	-
5	NAG	B	301	2	-	4/6/23/26	0/1/1/1
5	NAG	B	304	2	-	2/6/23/26	0/1/1/1
6	LPE	A	2010	-	-	10/25/25/34	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2008	PCW	O3-C11	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2005	PCW	O3-C11	4.15	1.45	1.33
7	A	2009	PCW	O3-C11	4.13	1.45	1.33
7	A	2009	PCW	O2-C31	3.98	1.45	1.34
7	A	2005	PCW	O2-C31	3.94	1.45	1.34
7	A	2008	PCW	O2-C31	3.83	1.45	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2008	PCW	O2-C31-C32	4.97	122.22	111.48
7	A	2009	PCW	O2-C31-C32	4.40	121.00	111.48
7	A	2005	PCW	O2-C31-C32	3.83	119.77	111.48
7	A	2009	PCW	C2-O2-C31	-3.65	109.06	117.80
5	B	301	NAG	C1-O5-C5	3.39	116.73	112.19
7	A	2009	PCW	O3-C11-C12	3.08	121.21	111.83
7	A	2008	PCW	C2-O2-C31	-3.07	110.44	117.80
5	B	304	NAG	C1-O5-C5	2.79	115.92	112.19
7	A	2005	PCW	O3-C11-C12	2.64	119.88	111.83
7	A	2008	PCW	O3-C11-C12	2.58	119.69	111.83
7	A	2008	PCW	O2-C31-O31	-2.57	117.69	123.70
7	A	2005	PCW	C2-O2-C31	-2.39	112.08	117.80
6	A	2010	LPE	C31-C32-N	-2.16	108.88	115.82
7	A	2005	PCW	C4-C5-N	-2.15	108.93	115.82
7	A	2005	PCW	O1P-P-O2P	2.11	122.25	112.44
6	A	2006	LPE	C31-C32-N	-2.10	109.07	115.82
7	A	2009	PCW	O2-C31-O31	-2.06	118.88	123.70
7	A	2005	PCW	O2-C31-O31	-2.02	118.98	123.70
6	A	2007	LPE	C31-C32-N	-2.01	109.36	115.82

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2003	LPE	C2-C3-O3-P
6	A	2003	LPE	C3-O3-P-O33
6	A	2003	LPE	C31-O33-P-O3
6	A	2003	LPE	C31-O33-P-O31
6	A	2004	LPE	O1-C1-C2-O2H
6	A	2004	LPE	C3-O3-P-O32
6	A	2004	LPE	C3-O3-P-O33
6	A	2004	LPE	C31-O33-P-O3
6	A	2004	LPE	C31-O33-P-O31

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Mol	Chain	Res	Type	Atoms
6	A	2004	LPE	C31-O33-P-O32
6	A	2006	LPE	C31-O33-P-O31
6	A	2007	LPE	C3-O3-P-O31
6	A	2007	LPE	C3-O3-P-O32
6	A	2007	LPE	C3-O3-P-O33
6	A	2007	LPE	C31-O33-P-O31
6	A	2010	LPE	O33-C31-C32-N
7	A	2005	PCW	C32-C31-O2-C2
7	A	2005	PCW	C1-O3P-P-O1P
7	A	2005	PCW	C1-O3P-P-O2P
7	A	2005	PCW	C1-O3P-P-O4P
7	A	2005	PCW	C4-O4P-P-O2P
7	A	2005	PCW	C4-O4P-P-O3P
7	A	2008	PCW	C1-O3P-P-O2P
7	A	2008	PCW	C4-O4P-P-O3P
7	A	2009	PCW	C4-O4P-P-O1P
7	A	2009	PCW	C4-O4P-P-O3P
7	A	2005	PCW	O31-C31-O2-C2
5	B	304	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
7	A	2009	PCW	C32-C31-O2-C2
5	B	303	NAG	O5-C5-C6-O6
5	B	304	NAG	O5-C5-C6-O6
5	A	2002	NAG	C4-C5-C6-O6
7	A	2009	PCW	O31-C31-O2-C2
5	A	2002	NAG	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
7	A	2009	PCW	C12-C11-O3-C3
5	B	303	NAG	C4-C5-C6-O6
7	A	2008	PCW	C4-C5-N-C6
7	A	2005	PCW	C12-C11-O3-C3
6	A	2007	LPE	C31-C32-N-C2N
6	A	2010	LPE	C31-C32-N-C1N
6	A	2010	LPE	C31-C32-N-C3N
7	A	2009	PCW	C4-C5-N-C6
7	A	2008	PCW	C12-C11-O3-C3
7	A	2009	PCW	O11-C11-O3-C3
6	A	2010	LPE	C31-C32-N-C2N
7	A	2005	PCW	O11-C11-O3-C3
6	A	2004	LPE	C14-C15-C16-C17
7	A	2008	PCW	O11-C11-O3-C3
6	A	2006	LPE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	A	2008	PCW	C32-C31-O2-C2
6	A	2003	LPE	C11-C12-C13-C14
6	A	2006	LPE	C31-C32-N-C1N
6	A	2007	LPE	C31-C32-N-C1N
7	A	2008	PCW	C4-C5-N-C7
7	A	2008	PCW	C4-C5-N-C8
7	A	2009	PCW	C4-C5-N-C7
7	A	2009	PCW	C4-C5-N-C8
7	A	2008	PCW	O31-C31-O2-C2
6	A	2003	LPE	C2-C1-O1-C11
7	A	2005	PCW	C16-C17-C18-C19
6	A	2006	LPE	C2-C1-O1-C11
6	A	2006	LPE	C31-C32-N-C3N
6	A	2007	LPE	C31-C32-N-C3N
6	A	2007	LPE	C2-C1-O1-C11
6	A	2004	LPE	O1-C1-C2-C3
6	A	2007	LPE	C12-C11-O1-C1
6	A	2003	LPE	O33-C31-C32-N
6	A	2006	LPE	O33-C31-C32-N
6	A	2007	LPE	O33-C31-C32-N
7	A	2005	PCW	O4P-C4-C5-N
7	A	2008	PCW	O4P-C4-C5-N
7	A	2008	PCW	C32-C33-C34-C35
6	A	2006	LPE	C12-C13-C14-C15
5	A	2001	NAG	C4-C5-C6-O6
6	A	2006	LPE	C31-C32-N-C2N
6	A	2010	LPE	C12-C11-O1-C1
5	B	301	NAG	C3-C2-N2-C7
6	A	2003	LPE	C3-O3-P-O31
6	A	2004	LPE	C3-O3-P-O31
6	A	2007	LPE	C31-O33-P-O3
6	A	2010	LPE	C31-O33-P-O31
7	A	2005	PCW	C4-O4P-P-O1P
7	A	2008	PCW	C4-O4P-P-O1P
7	A	2008	PCW	C4-O4P-P-O2P
6	A	2003	LPE	C12-C11-O1-C1
6	A	2010	LPE	C2-C1-O1-C11
6	A	2006	LPE	C12-C11-O1-C1
7	A	2008	PCW	C17-C18-C19-C20
6	A	2010	LPE	O2H-C2-C3-O3
7	A	2008	PCW	C39-C40-C41-C42
7	A	2009	PCW	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
6	A	2010	LPE	C14-C15-C16-C17
6	A	2003	LPE	C15-C16-C17-C18
7	A	2005	PCW	C12-C13-C14-C15
7	A	2005	PCW	C11-C12-C13-C14
5	B	301	NAG	C1-C2-N2-C7
6	A	2004	LPE	C2-C1-O1-C11
5	A	2001	NAG	O5-C5-C6-O6
6	A	2010	LPE	O1-C1-C2-O2H
7	A	2005	PCW	C37-C38-C39-C40
7	A	2005	PCW	C5-C4-O4P-P
7	A	2008	PCW	C37-C38-C39-C40
7	A	2005	PCW	C39-C40-C41-C42
7	A	2008	PCW	O2-C31-C32-C33
7	A	2005	PCW	C19-C20-C21-C22
7	A	2008	PCW	O31-C31-C32-C33
7	A	2008	PCW	C34-C35-C36-C37
7	A	2009	PCW	O3-C11-C12-C13
7	A	2005	PCW	C31-C32-C33-C34

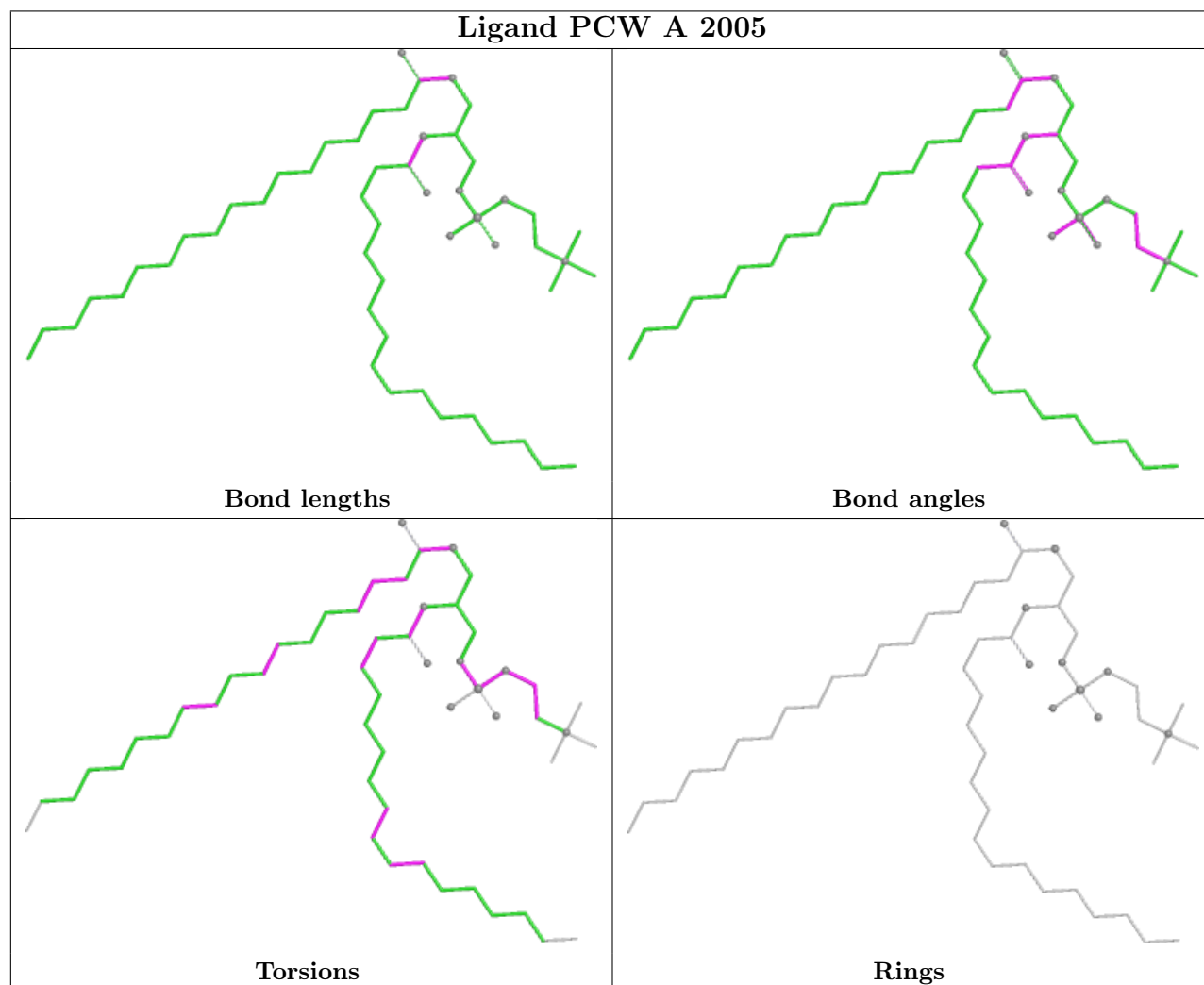
There are no ring outliers.

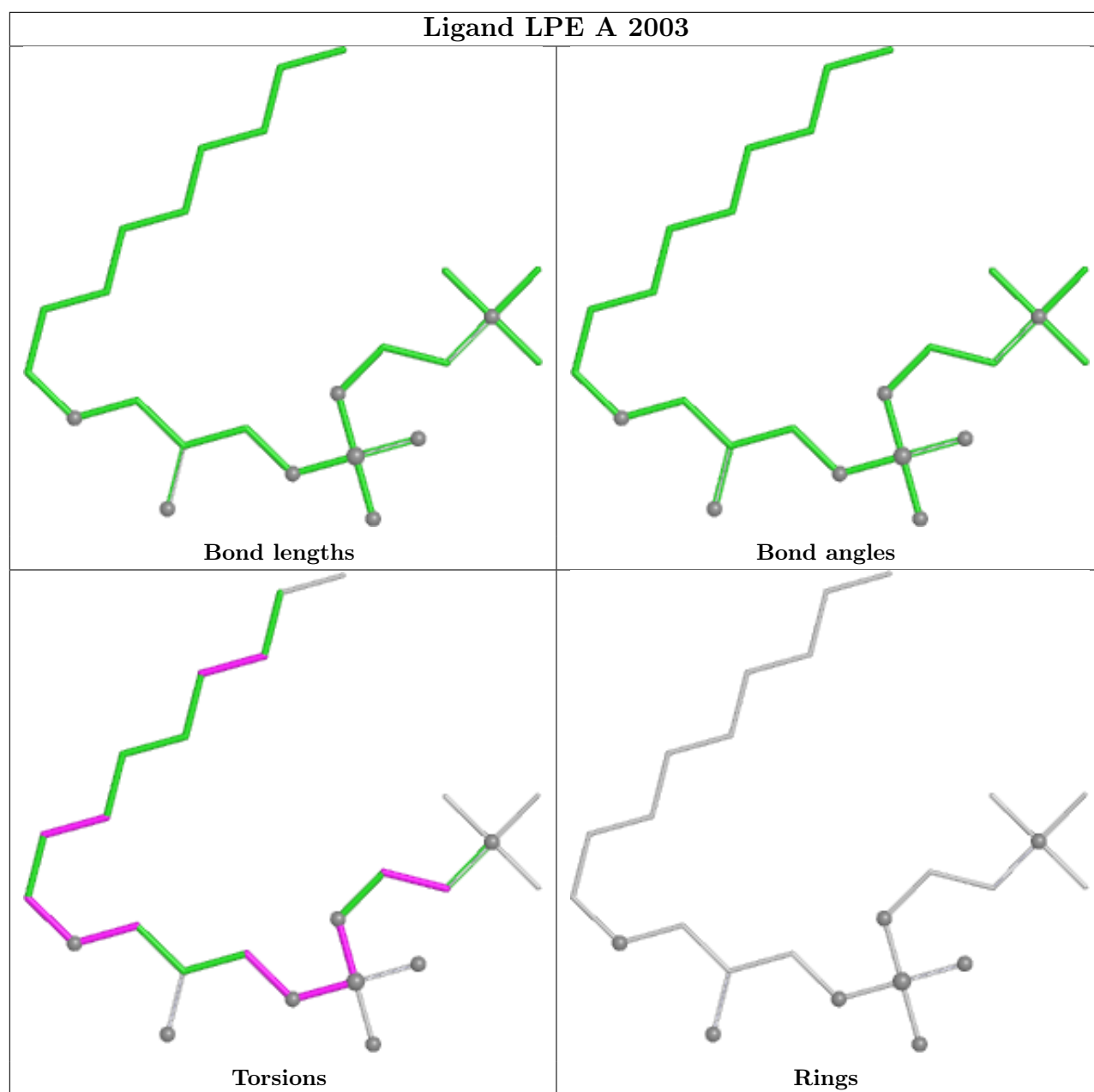
10 monomers are involved in 17 short contacts:

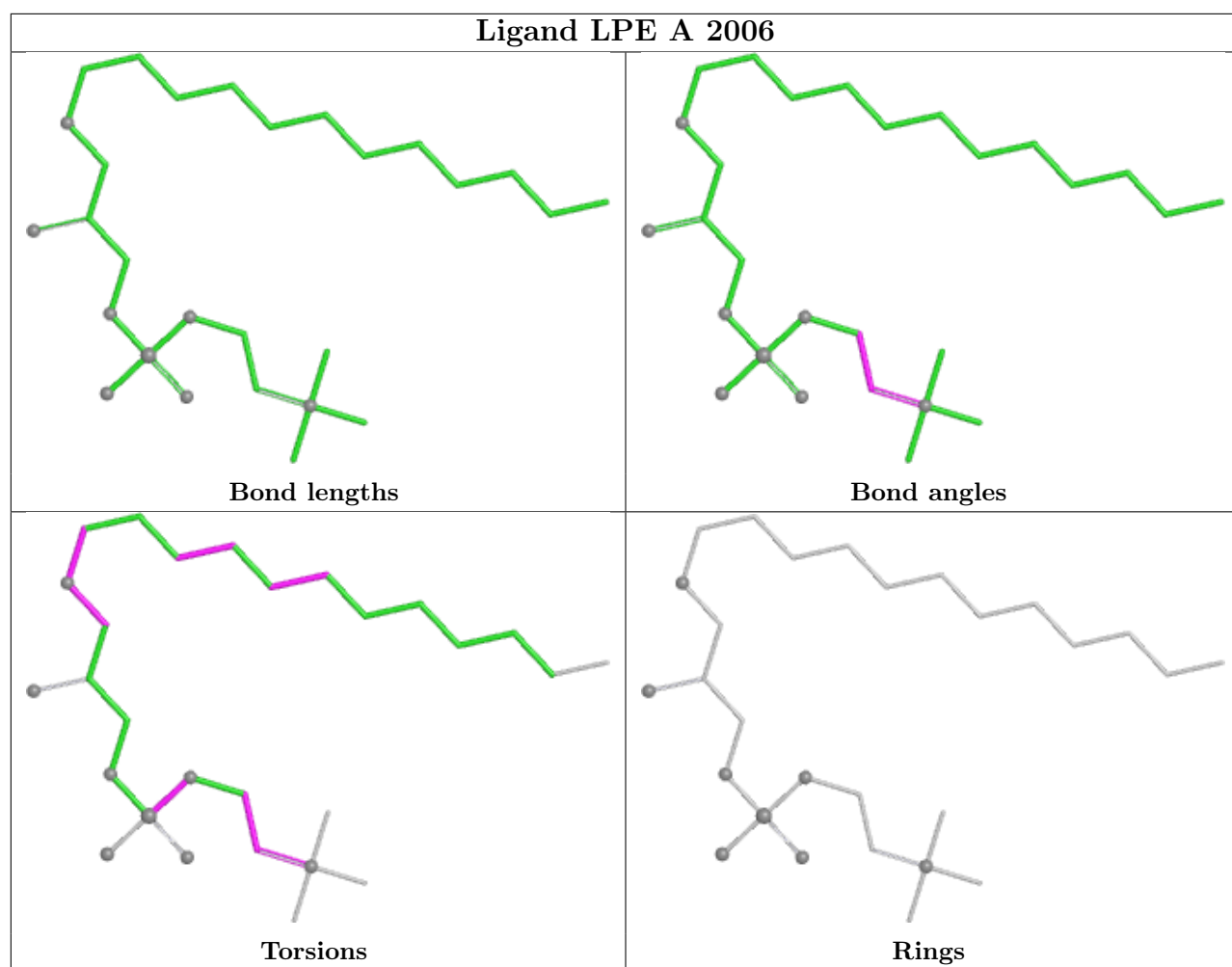
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2002	NAG	1	0
5	B	302	NAG	1	0
7	A	2005	PCW	4	0
6	A	2003	LPE	2	0
6	A	2006	LPE	1	0
6	A	2004	LPE	1	0
7	A	2008	PCW	2	0
5	B	301	NAG	1	0
5	B	304	NAG	1	0
6	A	2010	LPE	4	0

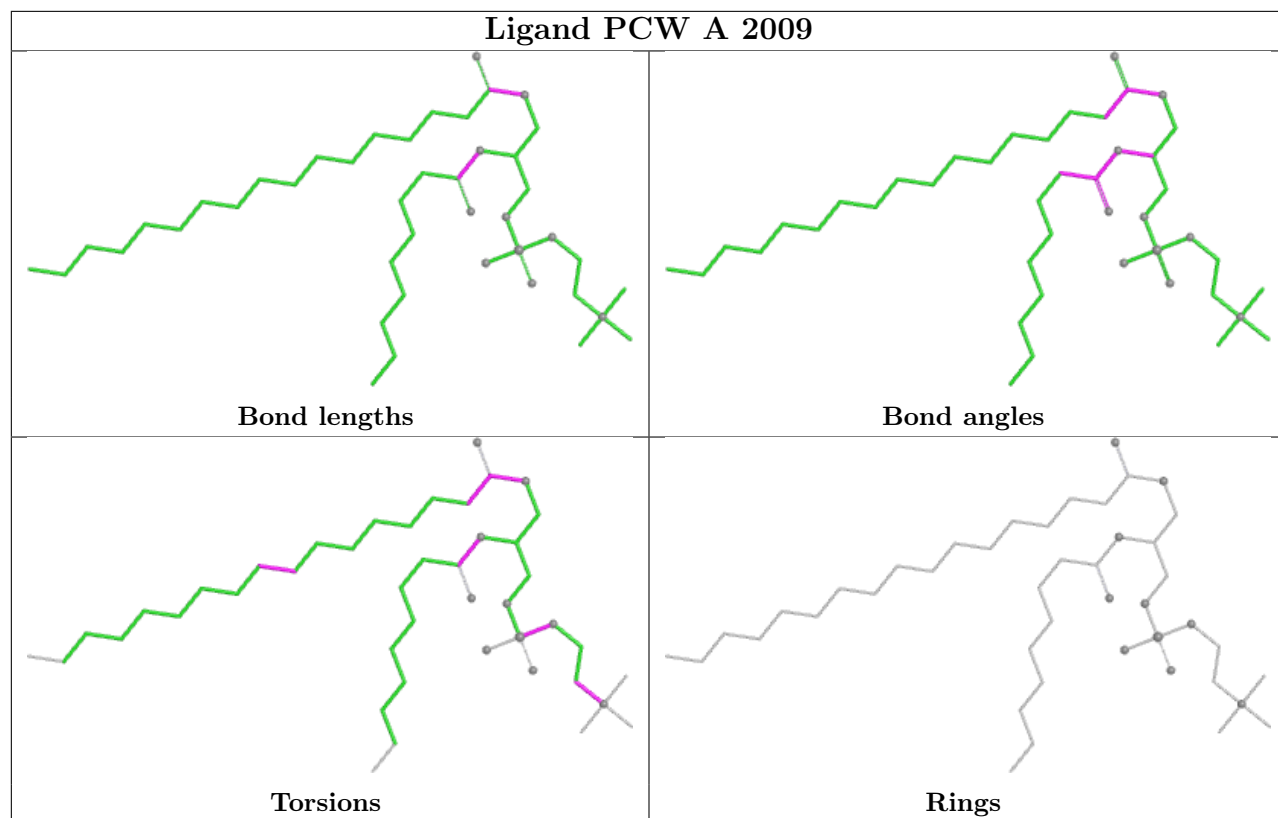
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

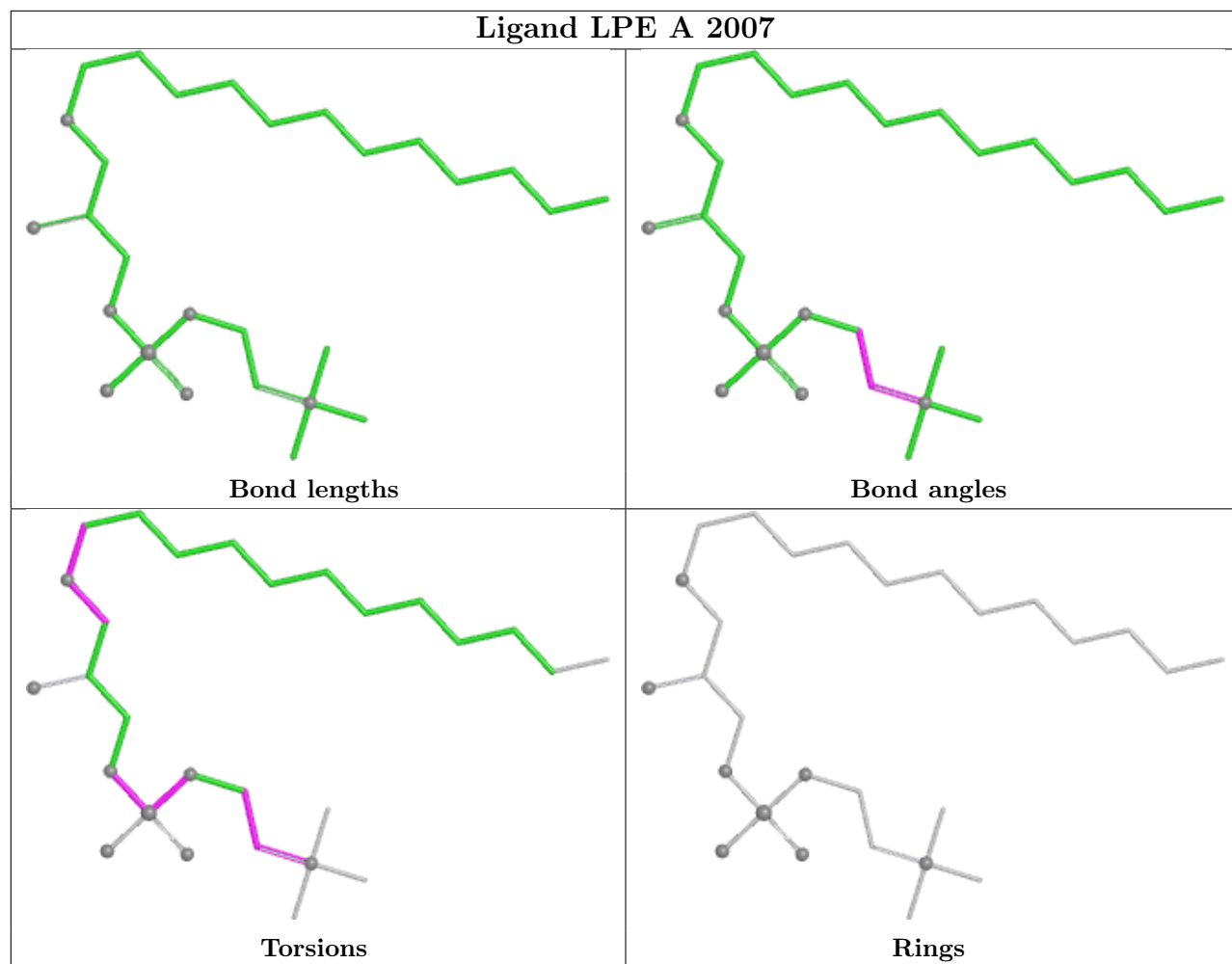
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

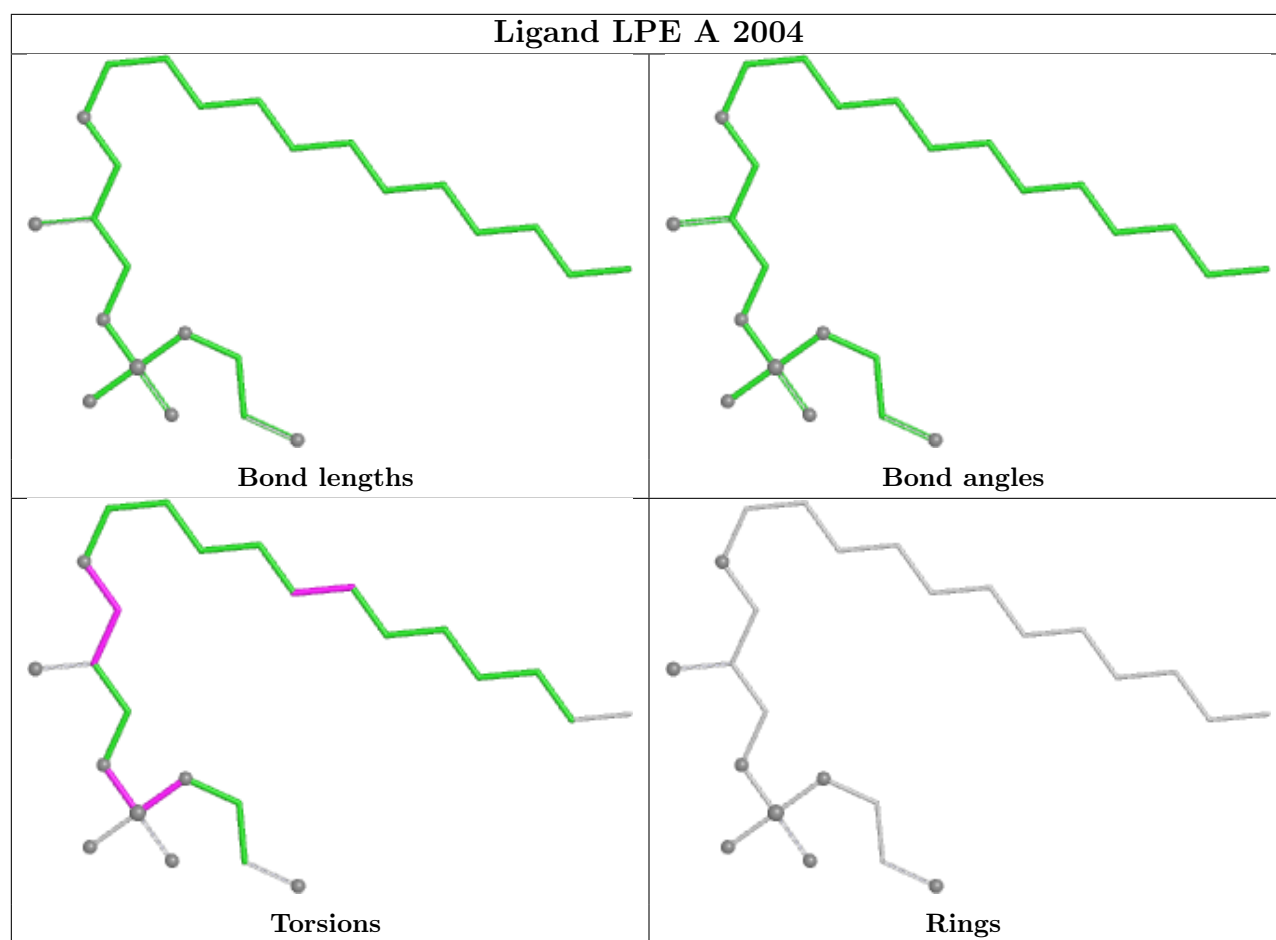


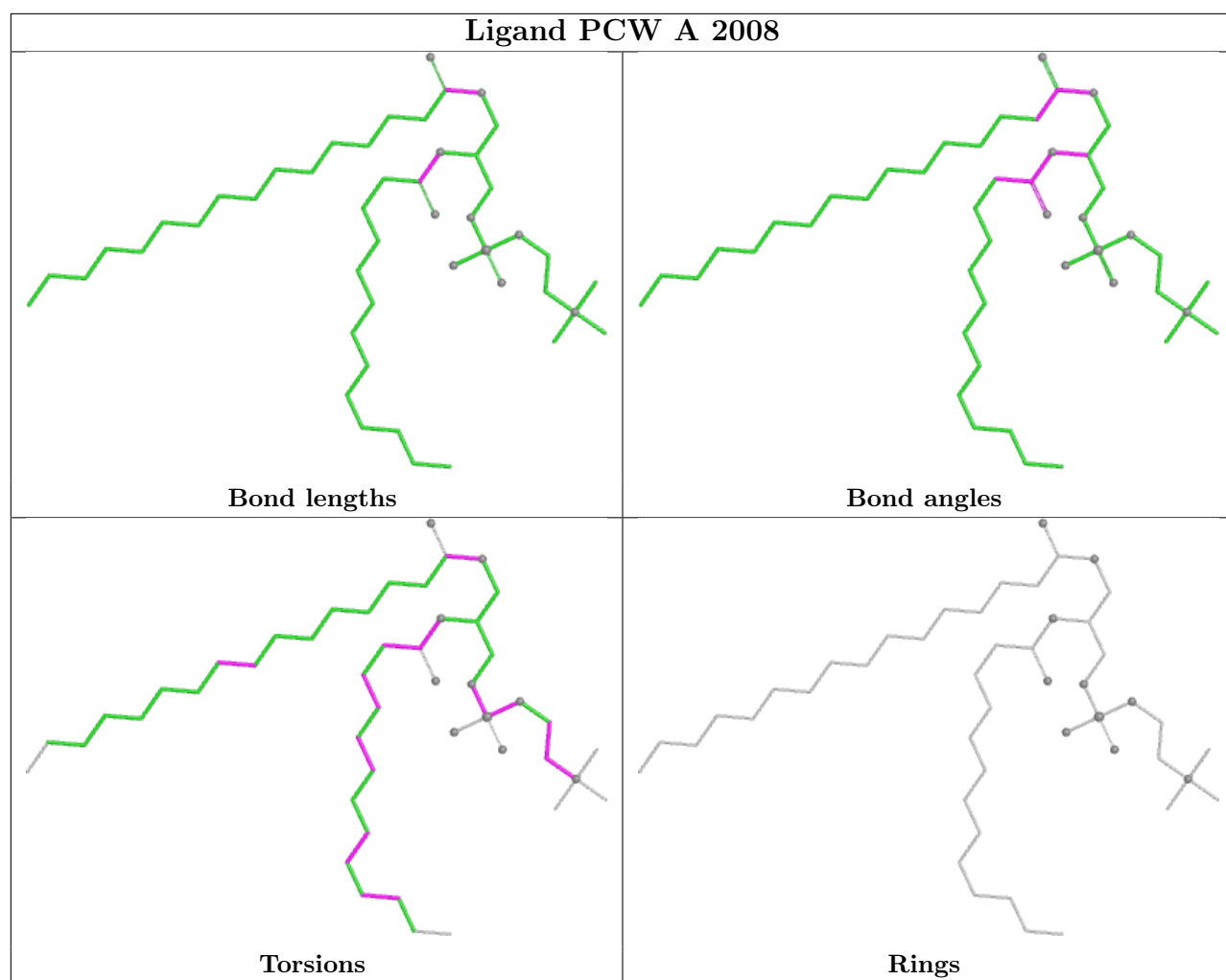


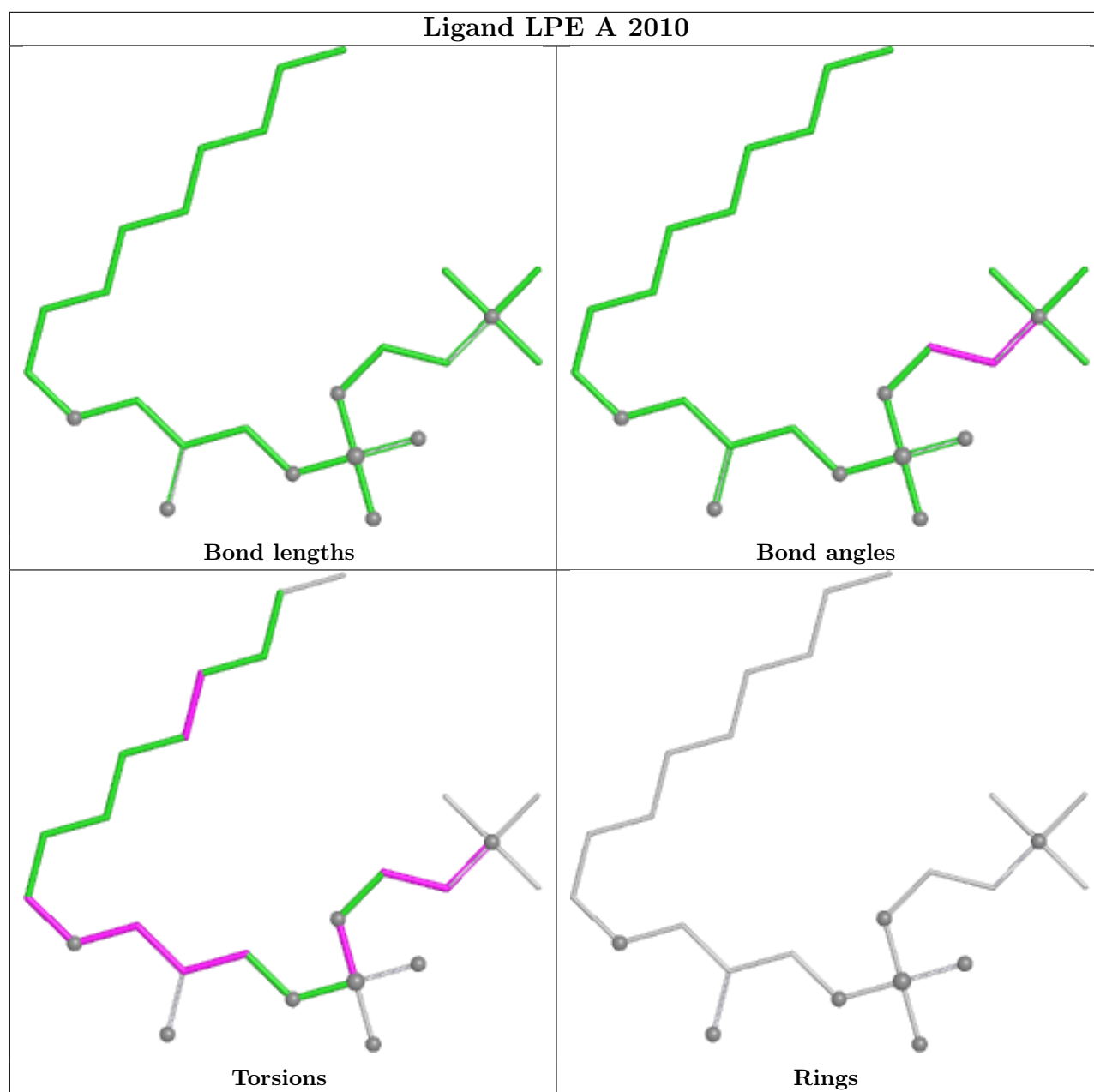












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

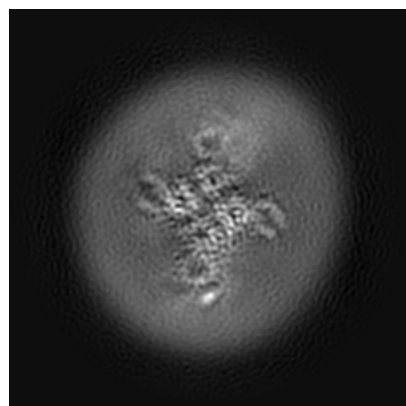
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38483. These allow visual inspection of the internal detail of the map and identification of artifacts.

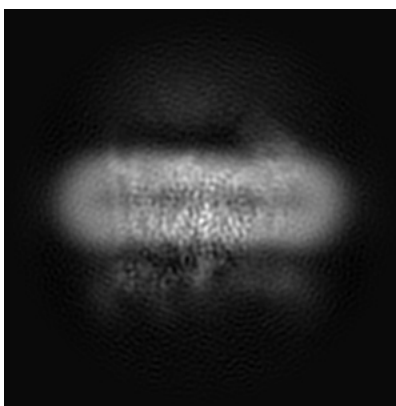
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

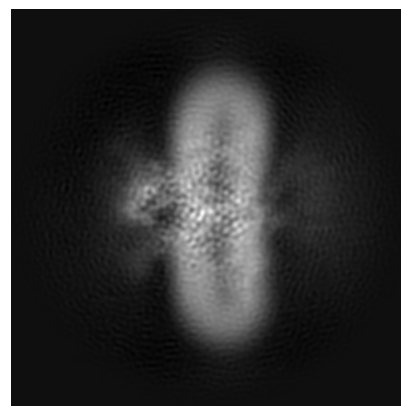
6.1.1 Primary map



X

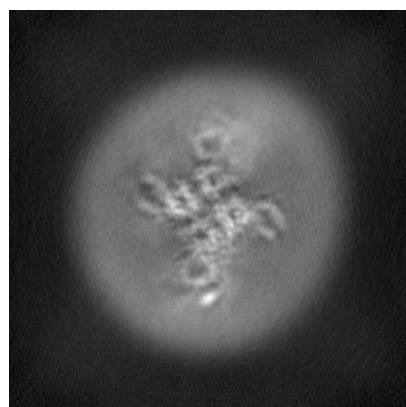


Y

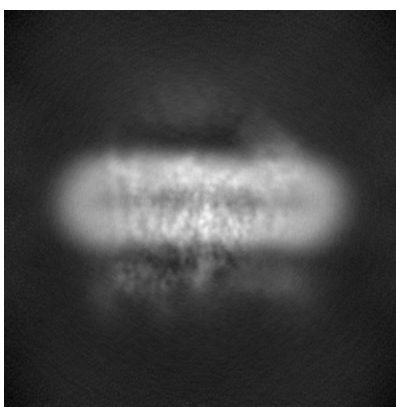


Z

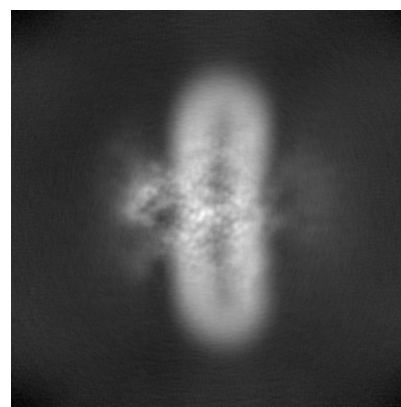
6.1.2 Raw map



X



Y

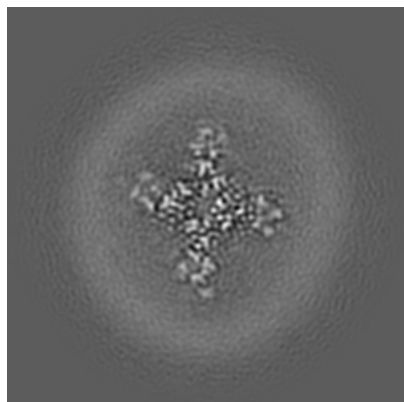


Z

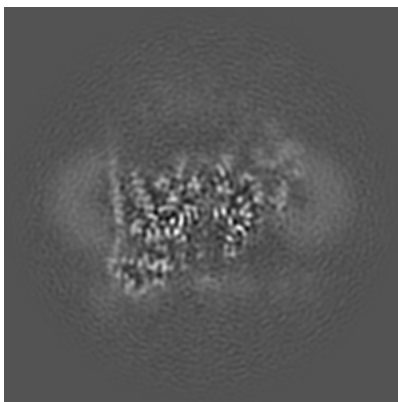
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

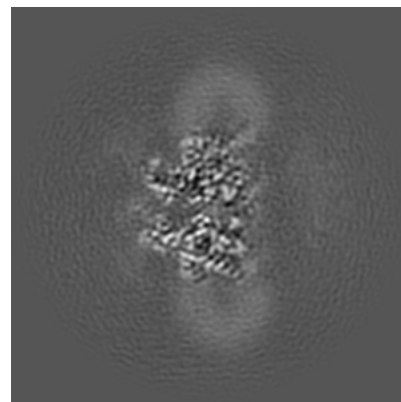
6.2.1 Primary map



X Index: 144

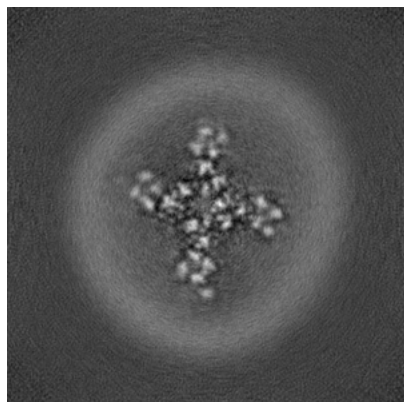


Y Index: 144

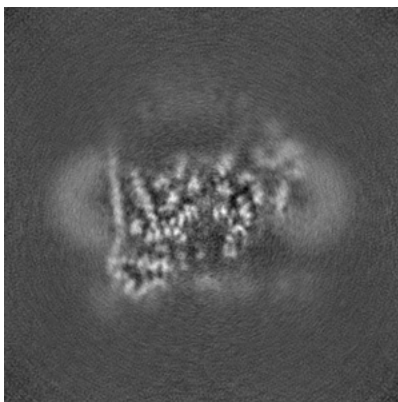


Z Index: 144

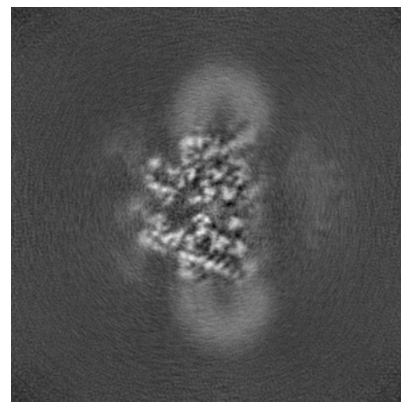
6.2.2 Raw map



X Index: 144



Y Index: 144

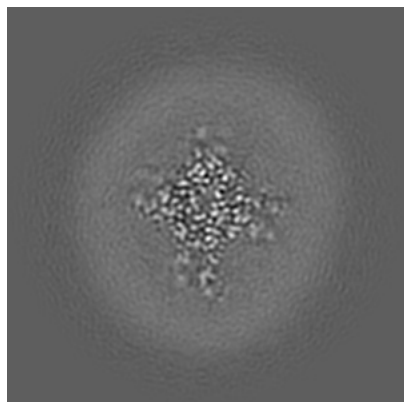


Z Index: 144

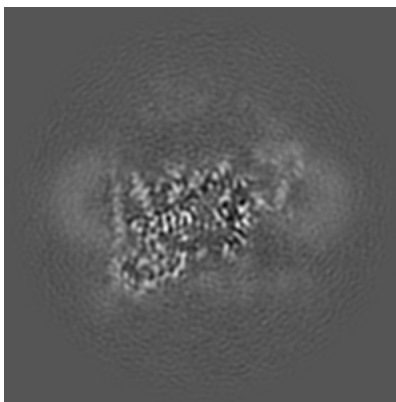
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

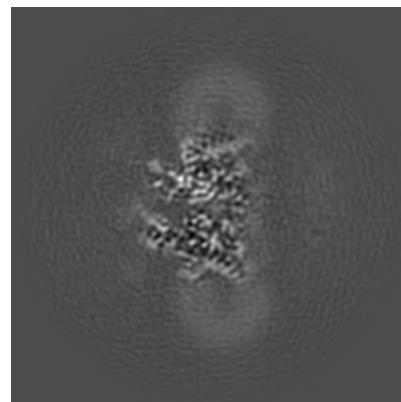
6.3.1 Primary map



X Index: 133

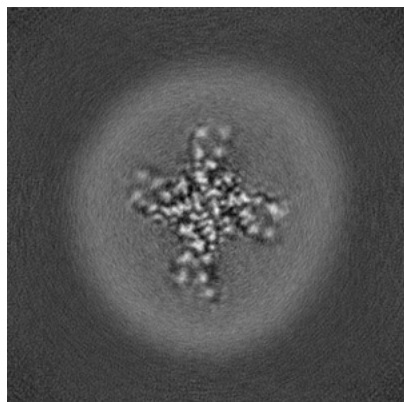


Y Index: 146

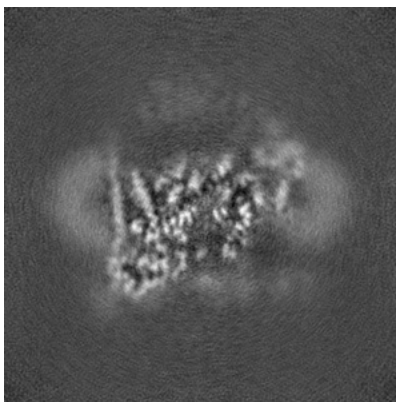


Z Index: 146

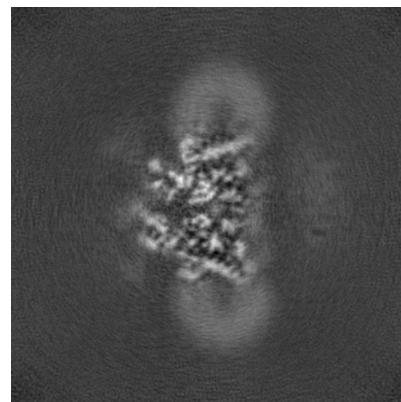
6.3.2 Raw map



X Index: 136



Y Index: 145

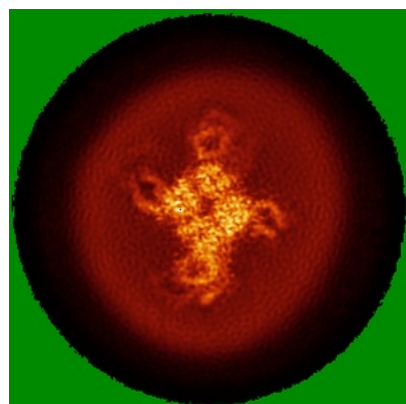


Z Index: 146

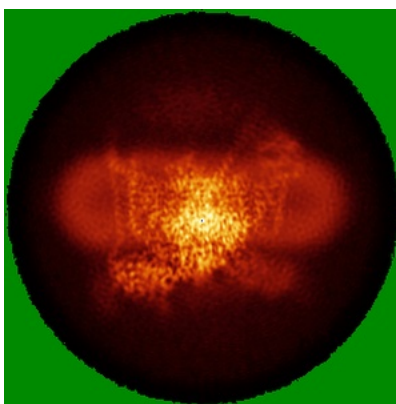
The images above show the largest variance slices of the map in three orthogonal directions.

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

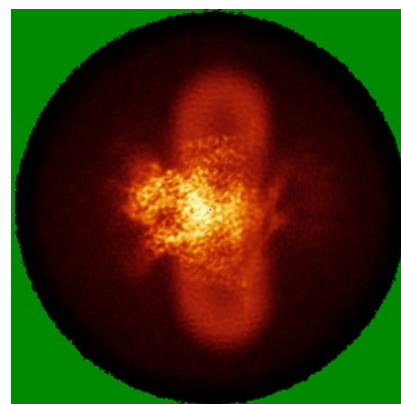
6.4.1 Primary map



X

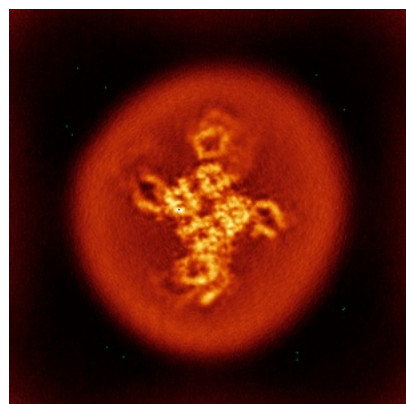


Y

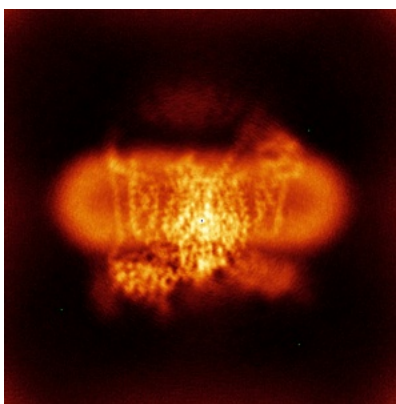


Z

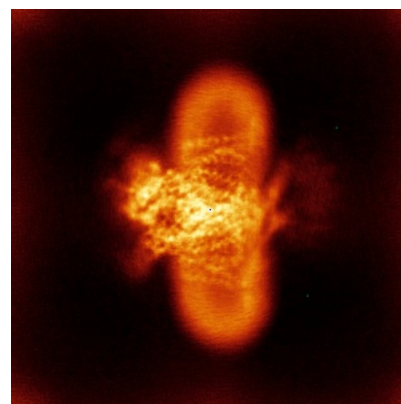
6.4.2 Raw map



X



Y

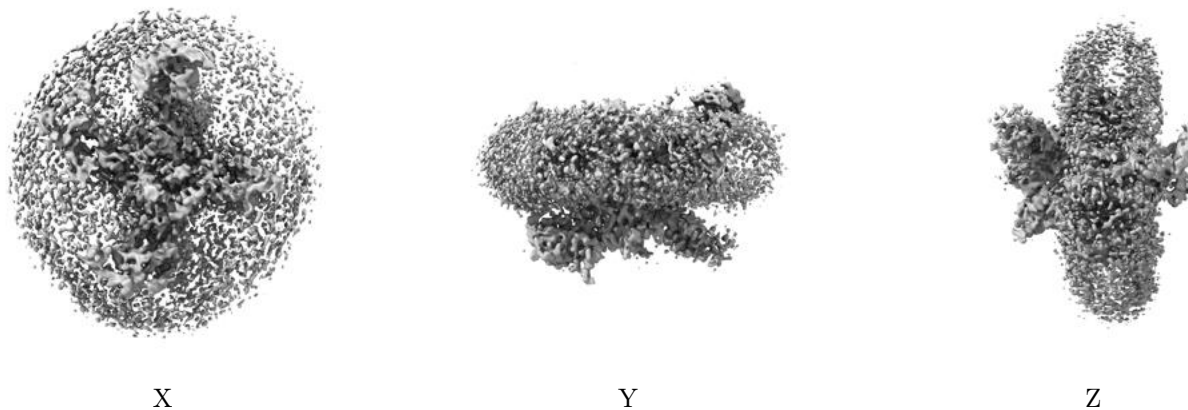


Z

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.

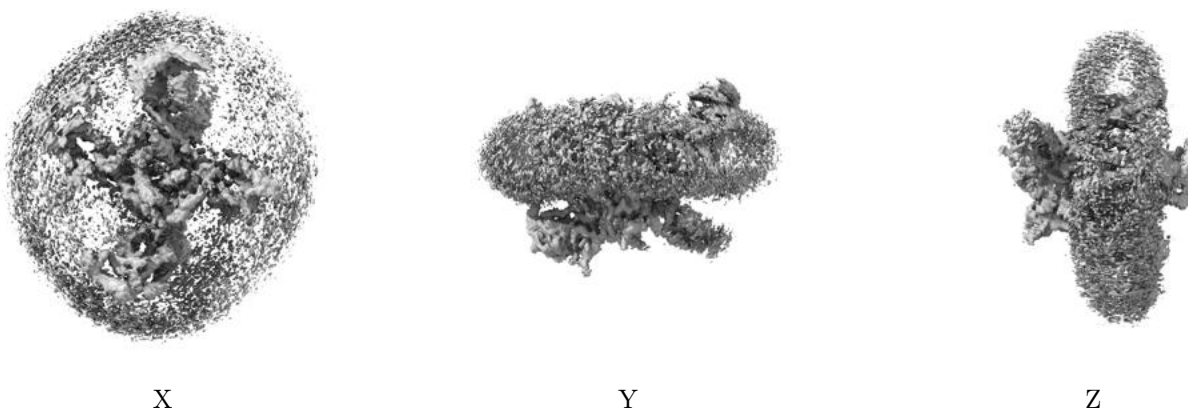
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

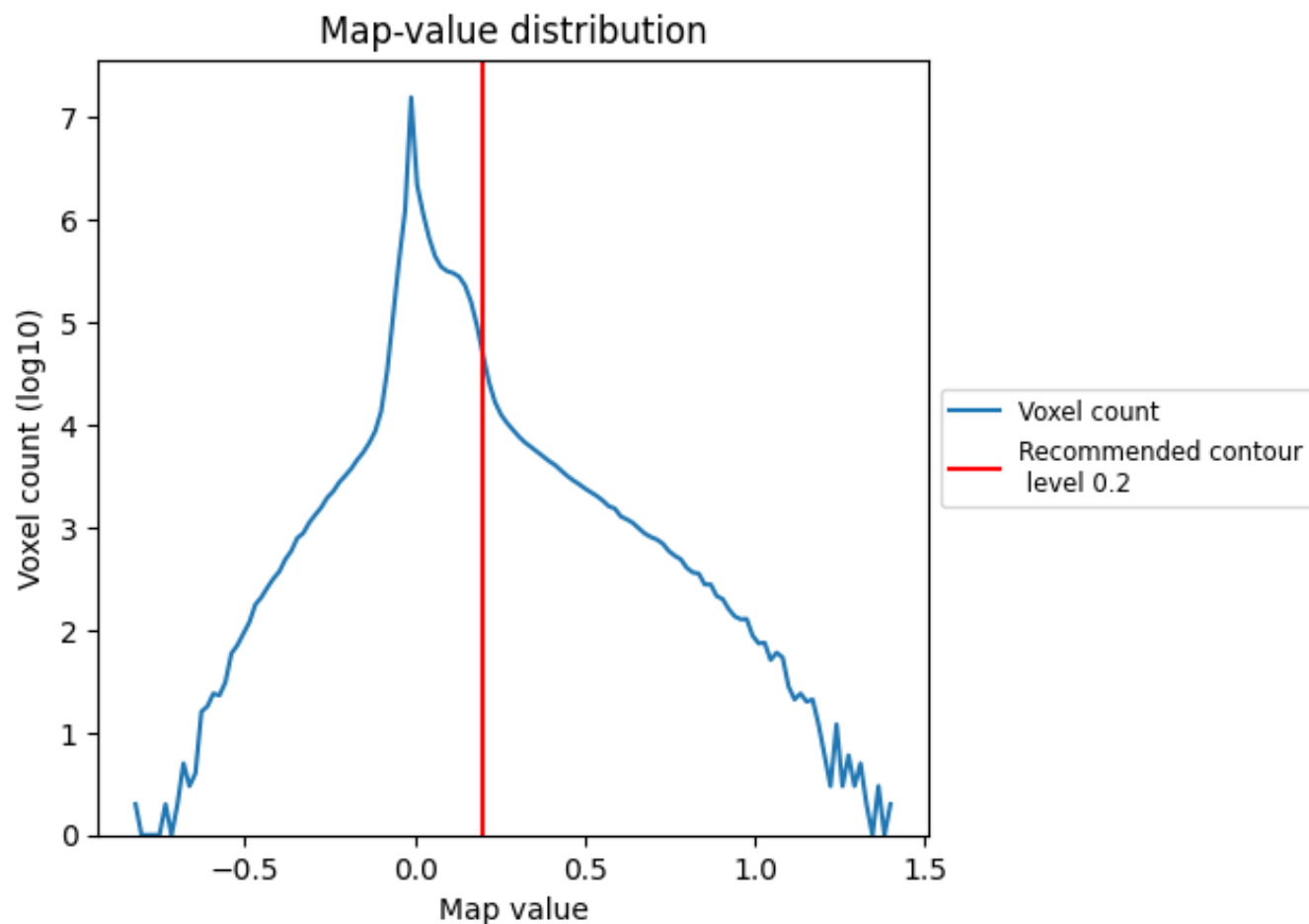
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

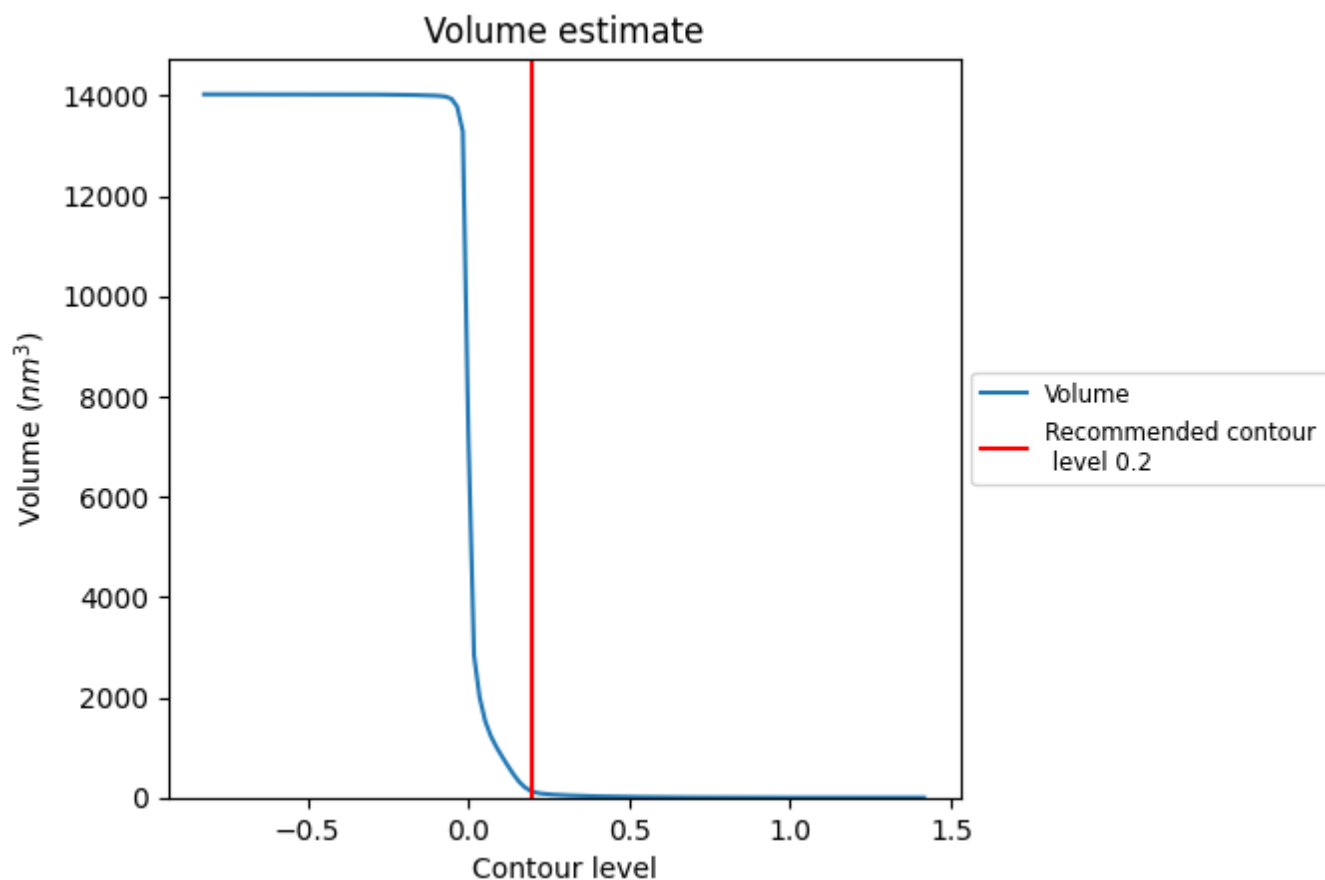
This section contains the results of statistical analysis of the map.

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.

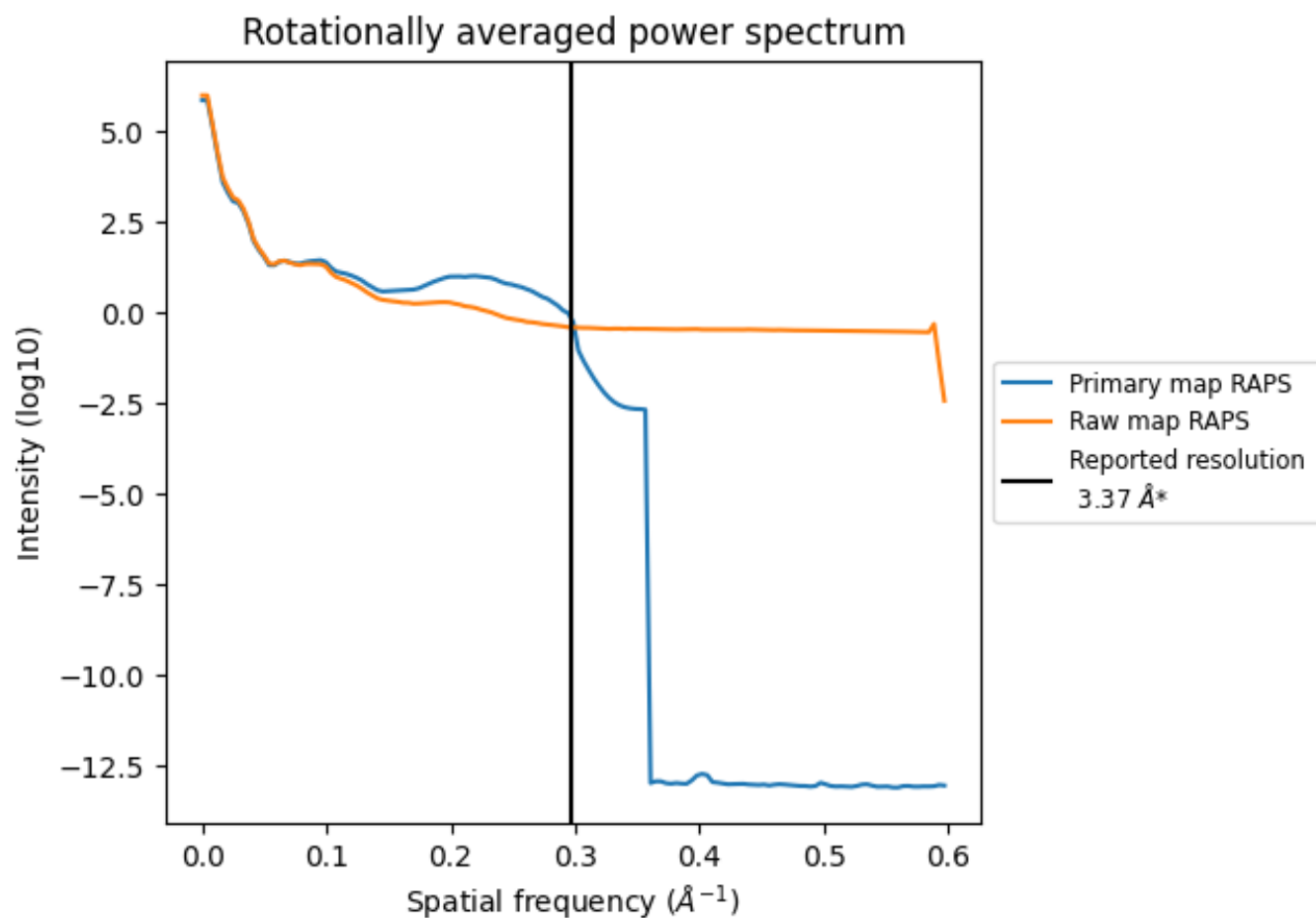
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 109 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 ⓘ

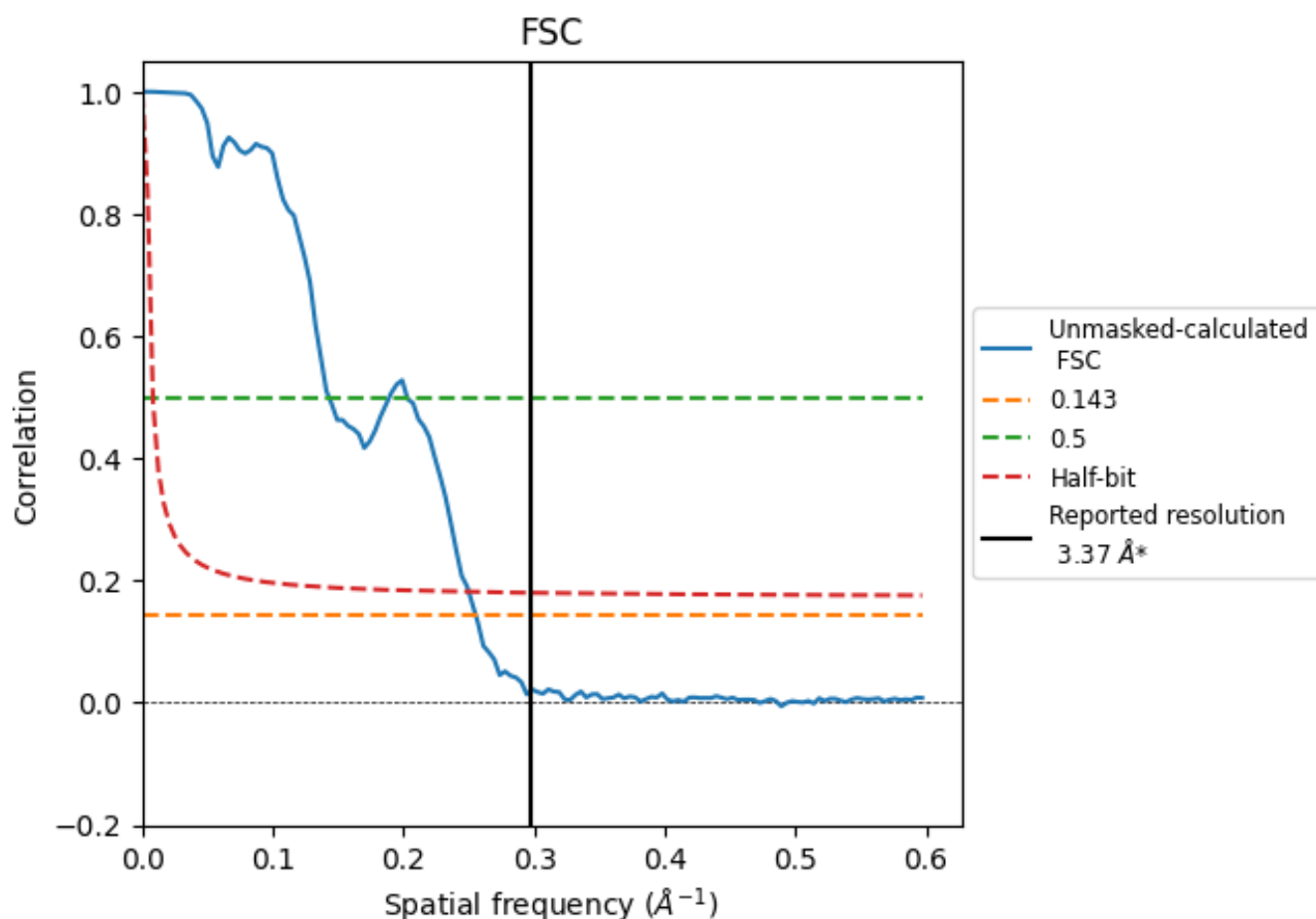


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 $0.297 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

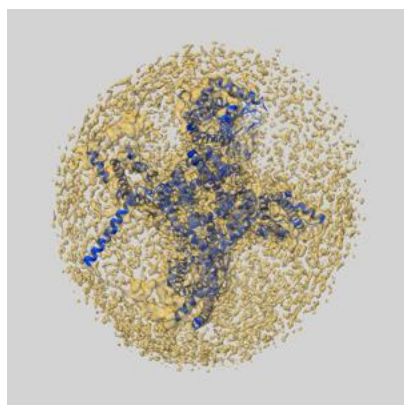
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.00	4.00

*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 3.92 differs from the reported value 3.37 by more than 10 %

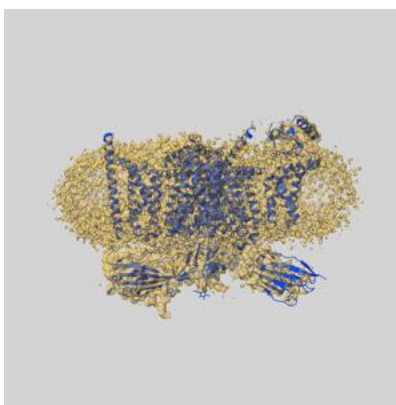
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38483 and PDB model 8XMN. Per-residue inclusion information can be found in section [3](#) on page [10](#).

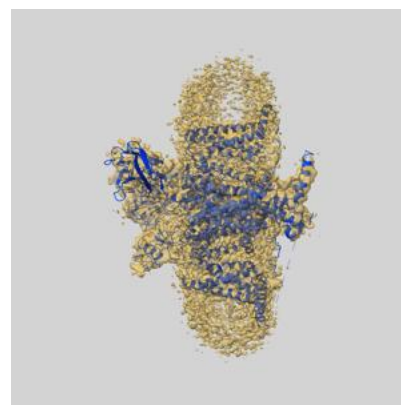
9.1 Map-model overlay [i](#)



X



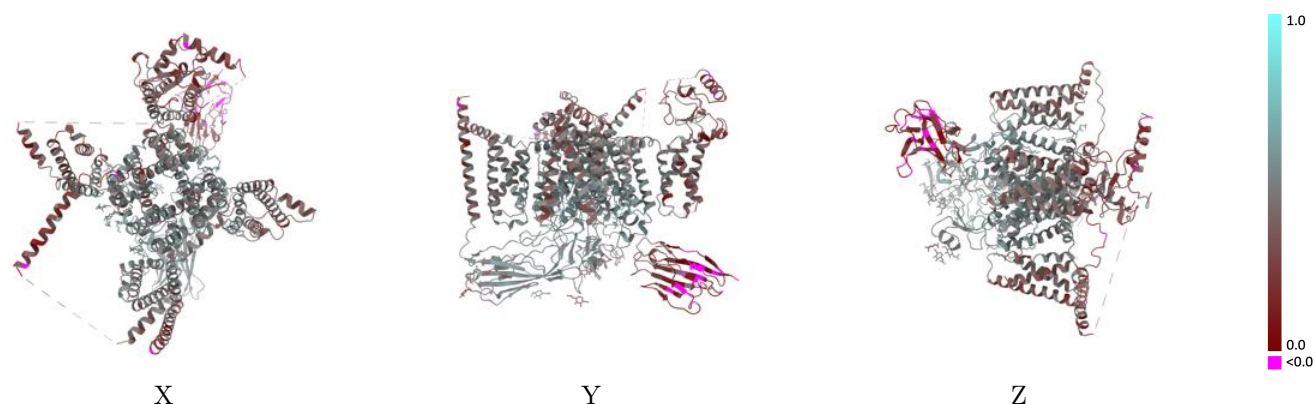
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

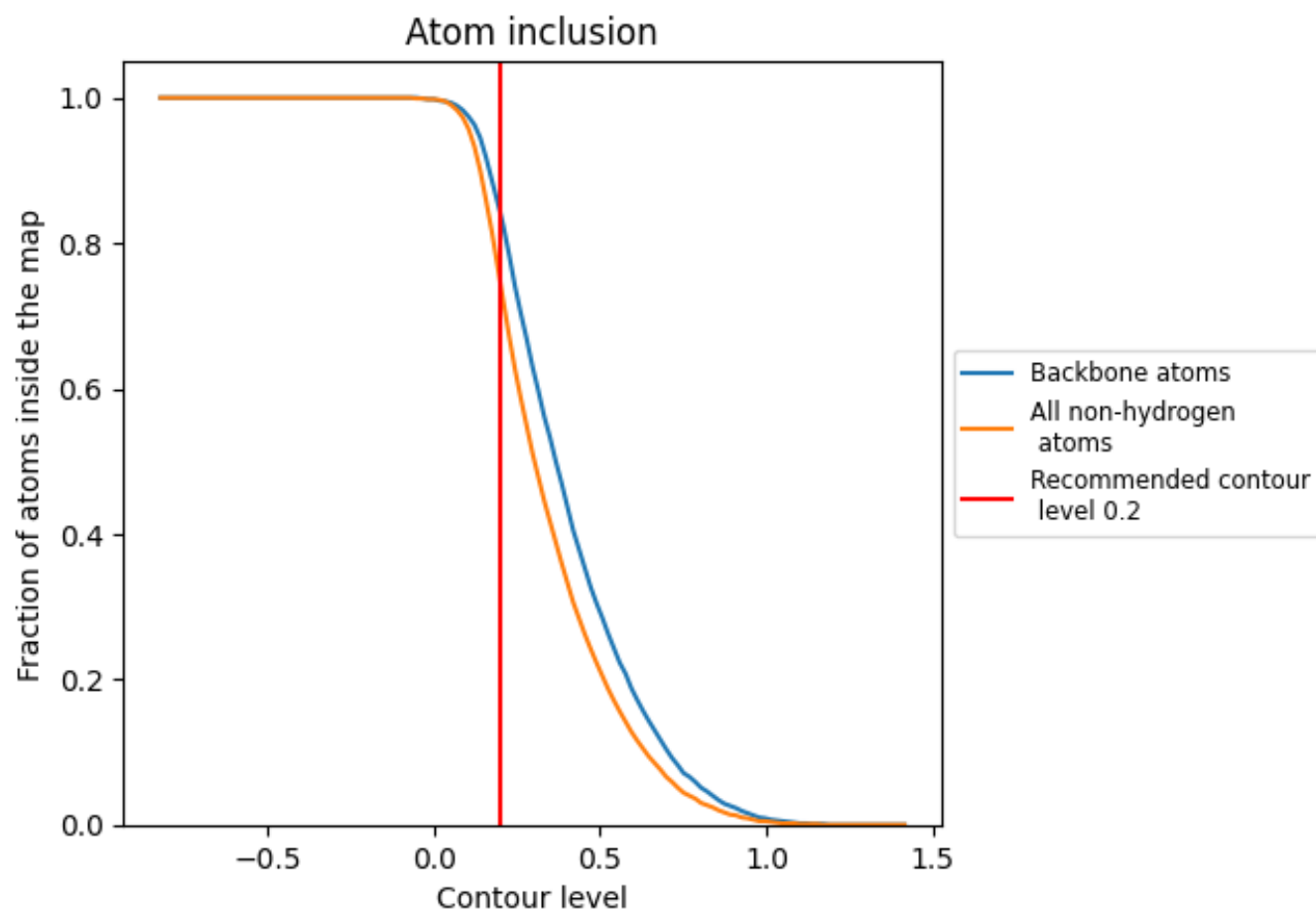


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.4310
A	0.7730	0.4510
B	0.8320	0.4690
C	0.3080	0.1480
D	0.8570	0.4480
E	0.7860	0.4950

