Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 06:32 PM JST

PDB ID	:	8X91
EMDB ID	:	EMD-38159
Title	:	P/Q type calcium channel in complex with omega-conotoxin MVIIC
Authors	:	Yan, N.; Li, Z.; Cong, Y.; Wu, T.; Wang, T.
Deposited on	:	2023-11-29
Resolution	:	3.11 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

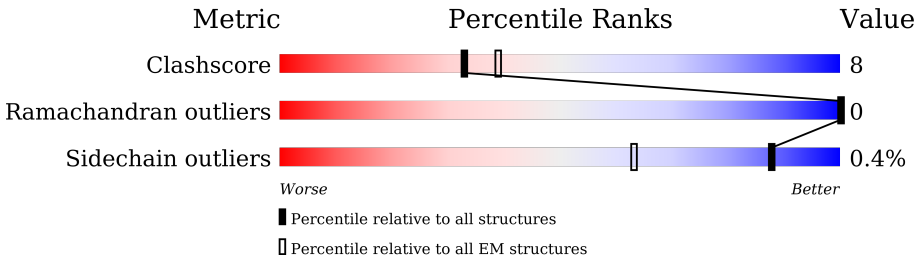
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	496	38% 50% 15% 35%
2	X	26	88% 8% .
3	B	1115	67% 19% 14%
4	A	2549	. 46% 8% 46%
5	E	3	33% 67%
6	F	2	100%
6	H	2	100%
6	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
7	G	4	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22269 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	485	LEU	-	expression tag	UNP P54284
C	486	GLU	-	expression tag	UNP P54284
C	487	HIS	-	expression tag	UNP P54284
C	488	HIS	-	expression tag	UNP P54284
C	489	HIS	-	expression tag	UNP P54284
C	490	HIS	-	expression tag	UNP P54284
C	491	HIS	-	expression tag	UNP P54284
C	492	HIS	-	expression tag	UNP P54284
C	493	HIS	-	expression tag	UNP P54284
C	494	HIS	-	expression tag	UNP P54284
C	495	HIS	-	expression tag	UNP P54284
C	496	HIS	-	expression tag	UNP P54284

- Molecule 2 is a protein called Omega-conotoxin MVIIC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	26	Total	C	N	O	S	0	0
			184	106	39	32	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	964	Total	C	N	O	S	0	0
			7695	4879	1289	1493	34		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1104	LEU	-	expression tag	UNP P54289
B	1105	GLU	-	expression tag	UNP P54289
B	1106	HIS	-	expression tag	UNP P54289
B	1107	HIS	-	expression tag	UNP P54289
B	1108	HIS	-	expression tag	UNP P54289
B	1109	HIS	-	expression tag	UNP P54289
B	1110	HIS	-	expression tag	UNP P54289
B	1111	HIS	-	expression tag	UNP P54289
B	1112	HIS	-	expression tag	UNP P54289
B	1113	HIS	-	expression tag	UNP P54289
B	1114	HIS	-	expression tag	UNP P54289
B	1115	HIS	-	expression tag	UNP P54289

- Molecule 4 is a protein called Voltage-dependent P/Q-type calcium channel subunit alpha-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1377	Total	C	N	O	S	1	0
			11202	7353	1819	1950	80		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP O00555
A	-41	ALA	-	expression tag	UNP O00555
A	-40	SER	-	expression tag	UNP O00555
A	-39	TRP	-	expression tag	UNP O00555
A	-38	SER	-	expression tag	UNP O00555
A	-37	HIS	-	expression tag	UNP O00555
A	-36	PRO	-	expression tag	UNP O00555
A	-35	GLN	-	expression tag	UNP O00555
A	-34	PHE	-	expression tag	UNP O00555
A	-33	GLU	-	expression tag	UNP O00555
A	-32	LYS	-	expression tag	UNP O00555
A	-31	GLY	-	expression tag	UNP O00555
A	-30	GLY	-	expression tag	UNP O00555
A	-29	GLY	-	expression tag	UNP O00555
A	-28	ALA	-	expression tag	UNP O00555
A	-27	ARG	-	expression tag	UNP O00555
A	-26	GLY	-	expression tag	UNP O00555
A	-25	GLY	-	expression tag	UNP O00555
A	-24	SER	-	expression tag	UNP O00555
A	-23	GLY	-	expression tag	UNP O00555

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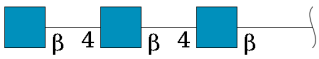
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP O00555
A	-21	GLY	-	expression tag	UNP O00555
A	-20	SER	-	expression tag	UNP O00555
A	-19	TRP	-	expression tag	UNP O00555
A	-18	SER	-	expression tag	UNP O00555
A	-17	HIS	-	expression tag	UNP O00555
A	-16	PRO	-	expression tag	UNP O00555
A	-15	GLN	-	expression tag	UNP O00555
A	-14	PHE	-	expression tag	UNP O00555
A	-13	GLU	-	expression tag	UNP O00555
A	-12	LYS	-	expression tag	UNP O00555
A	-11	GLY	-	expression tag	UNP O00555
A	-10	PHE	-	expression tag	UNP O00555
A	-9	ASP	-	expression tag	UNP O00555
A	-8	TYR	-	expression tag	UNP O00555
A	-7	LYS	-	expression tag	UNP O00555
A	-6	ASP	-	expression tag	UNP O00555
A	-5	ASP	-	expression tag	UNP O00555
A	-4	ASP	-	expression tag	UNP O00555
A	-3	ASP	-	expression tag	UNP O00555
A	-2	LYS	-	expression tag	UNP O00555
A	-1	GLY	-	expression tag	UNP O00555
A	0	THR	-	expression tag	UNP O00555

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	3	42	24	3	15	0	0

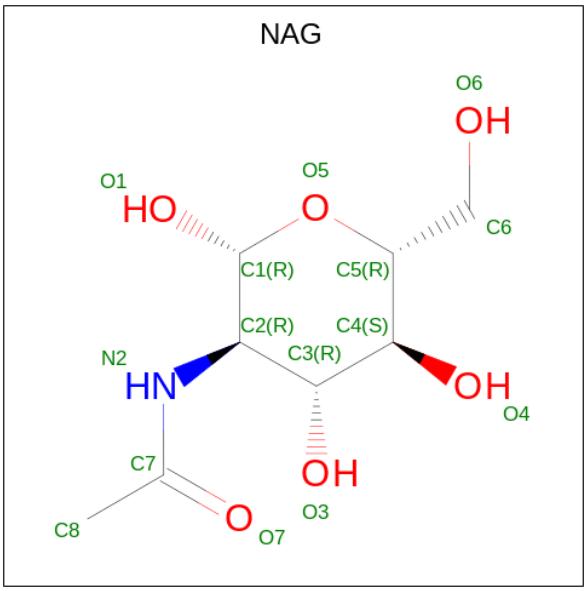
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	F	2	Total C N O 28 16 2 10	0	0
6	H	2	Total C N O 28 16 2 10	0	0
6	I	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	G	4	Total C N O 56 32 4 20	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

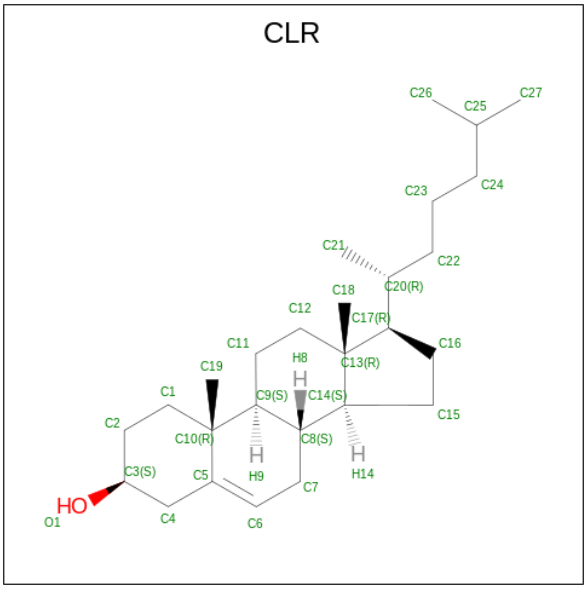


Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

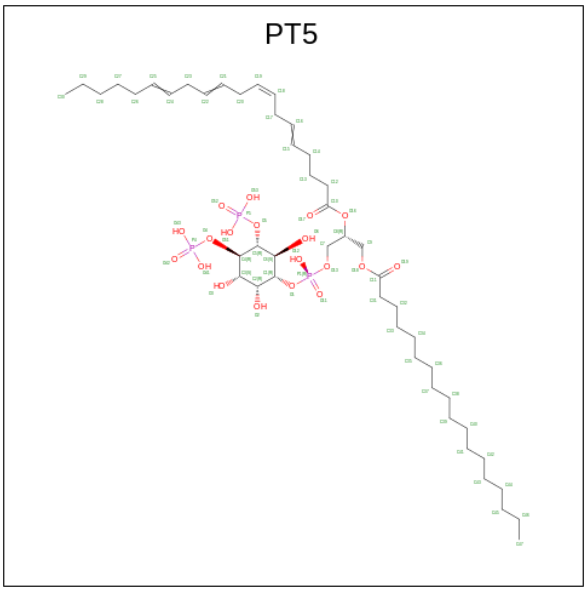
Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total Ca 1 1	0
9	A	2	Total Ca 2 2	0

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



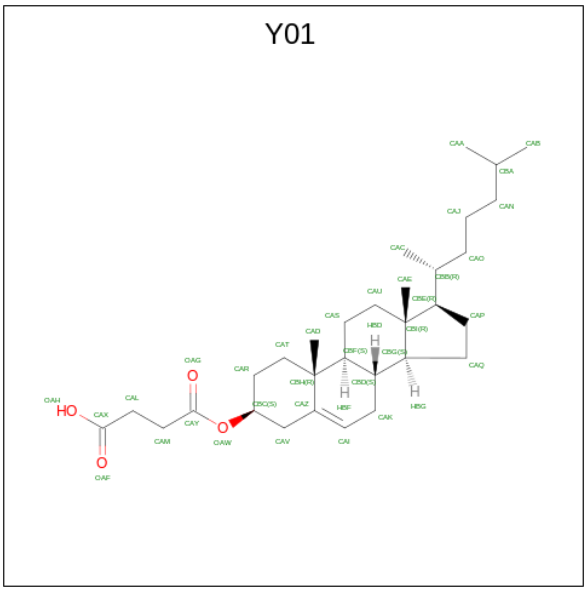
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 28 27 1	0
10	A	1	Total C O 28 27 1	0
10	A	1	Total C O 28 27 1	0
10	A	1	Total C O 28 27 1	0
10	A	1	Total C O 28 27 1	0

- Molecule 11 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



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

- Molecule 12 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			35	31	4	
12	A	1	Total	C	O	0
			35	31	4	

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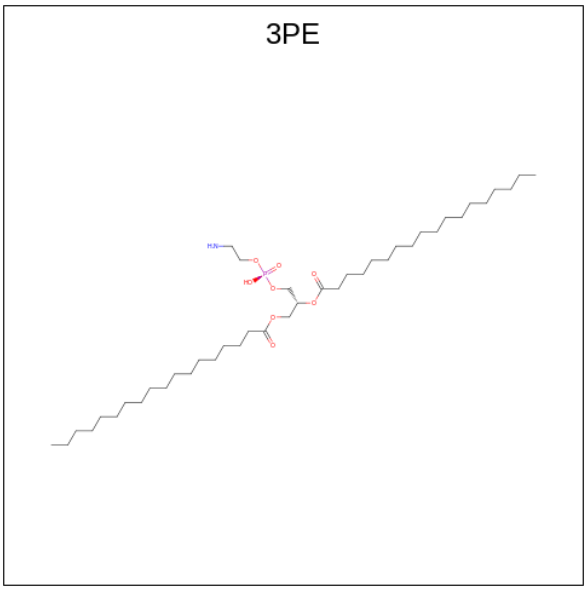
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			35	31	4	

- Molecule 13 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



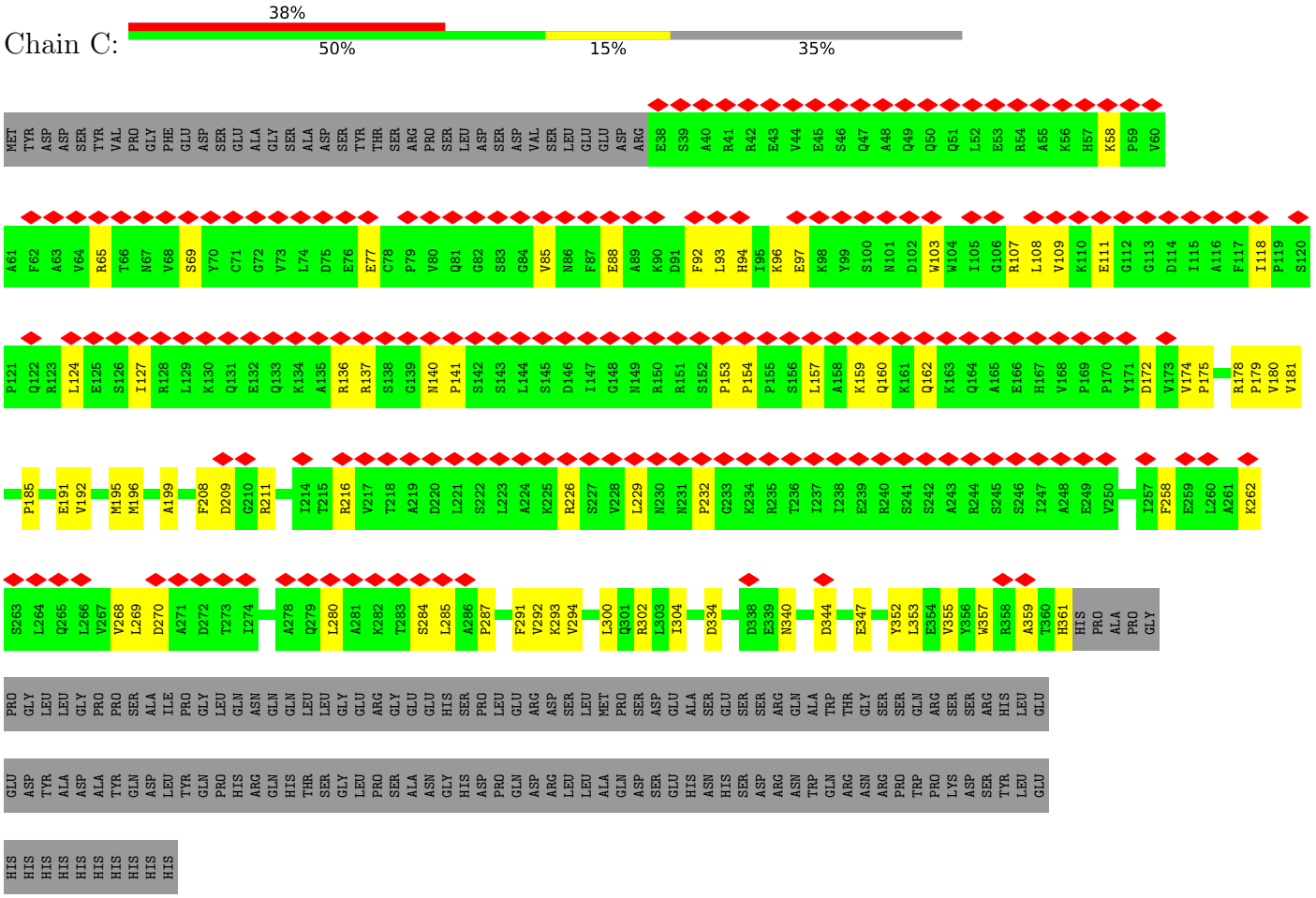
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
13	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

3 Residue-property plots (i)

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

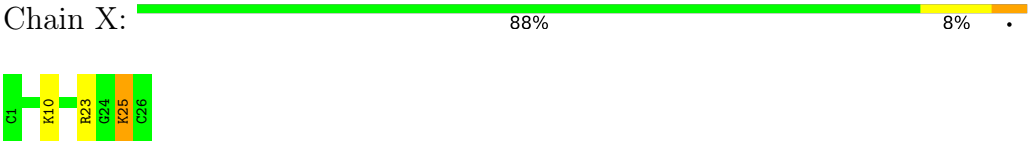
• Molecule 1: Voltage-dependent L-type calcium channel subunit beta-3

Chain C:



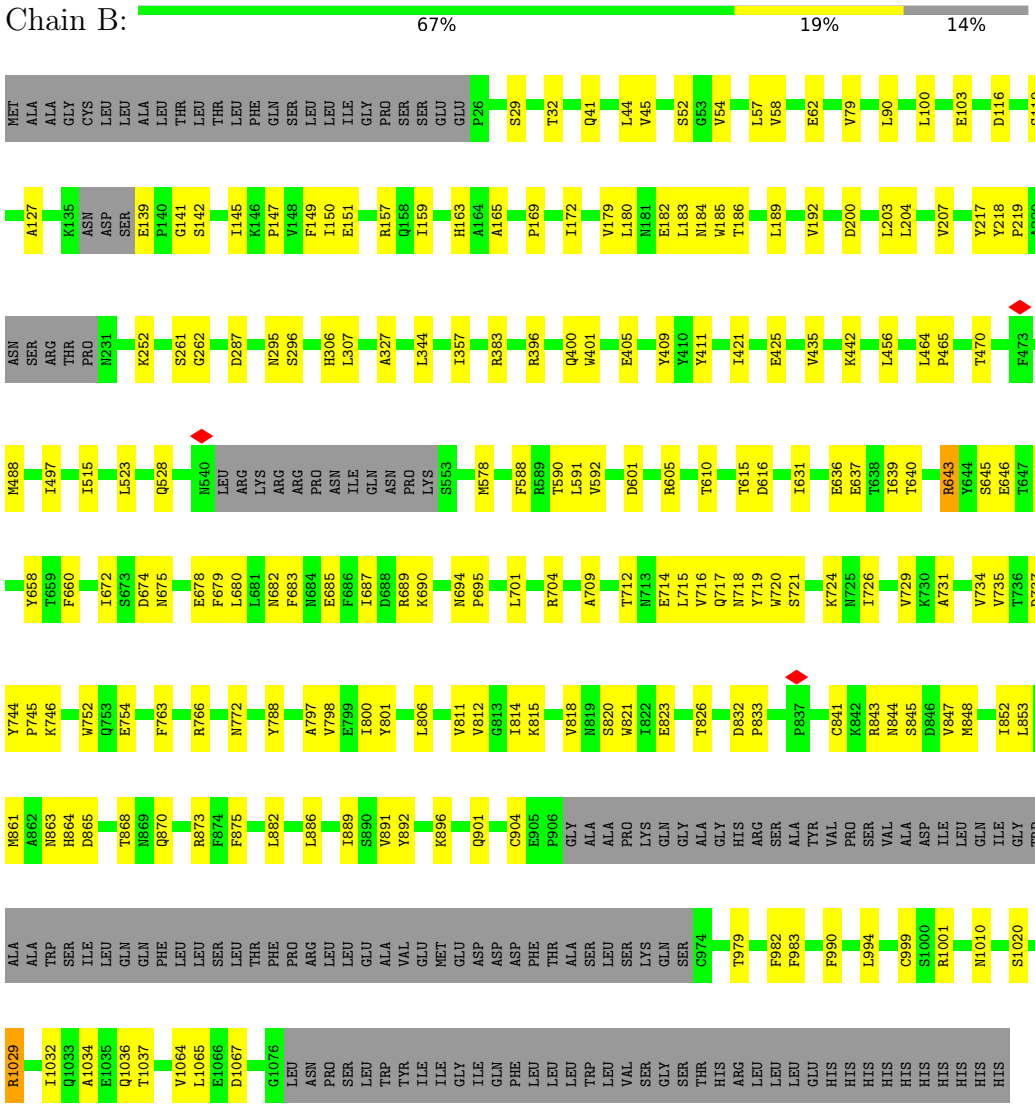
• Molecule 2: Omega-conotoxin MVIIC

Chain X:



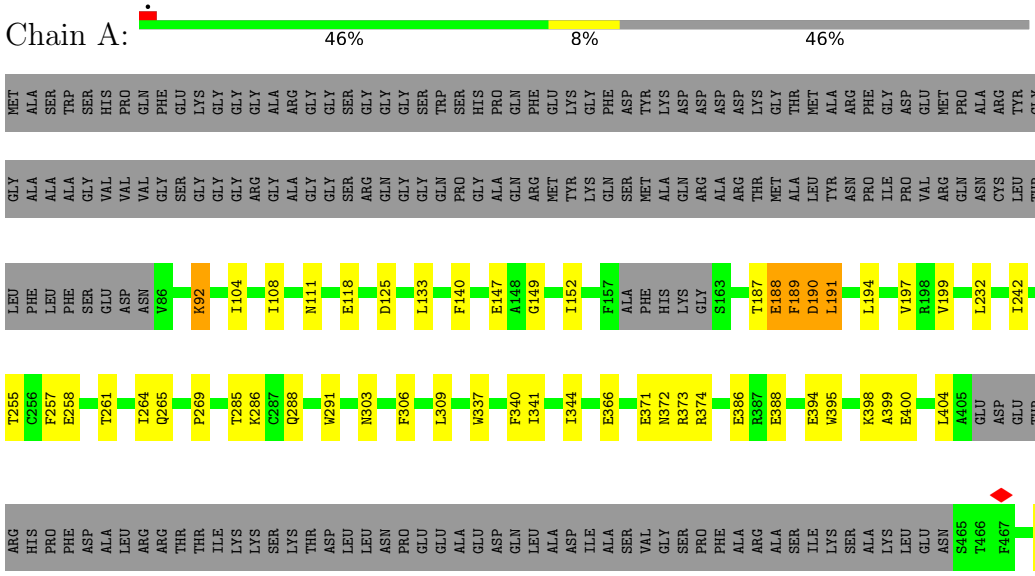
• Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1

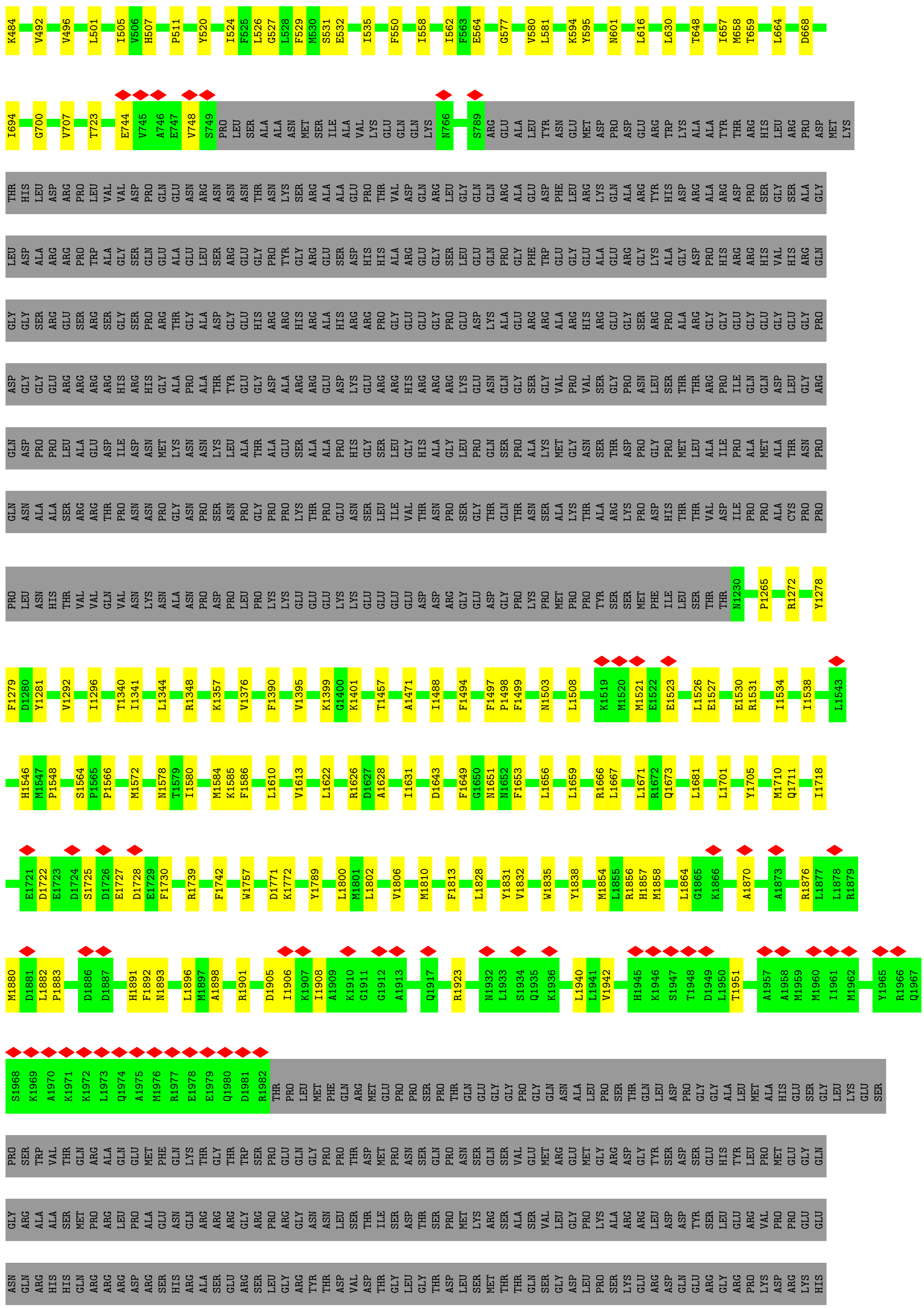
Chain B:

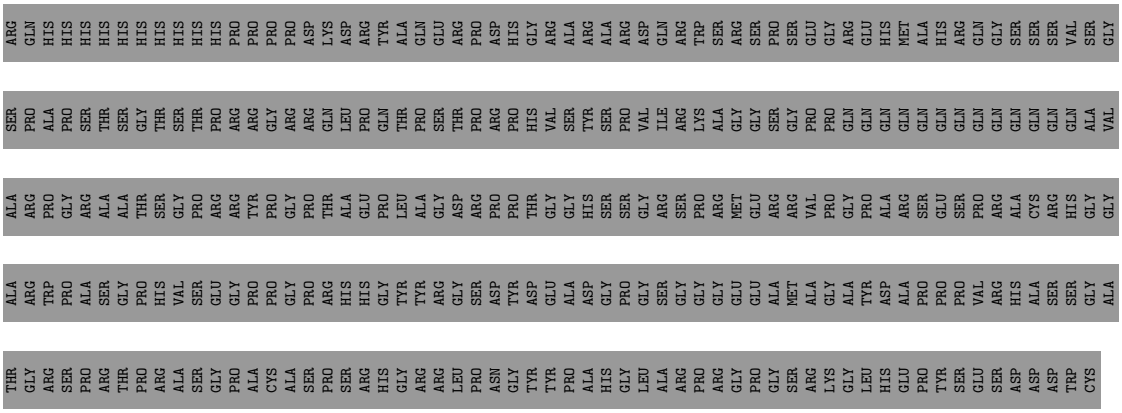


• Molecule 4: Voltage-dependent P/Q-type calcium channel subunit alpha-1A

Chain A:







• 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

Chain E:

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

Chain F:

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

Chain H:

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

Chain I:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:


NAG1
NAG2
NAG3
NAG4

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.301	Depositor
Minimum map value	-1.308	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	351.328, 351.328, 351.328	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, CA, 3PE, NAG, CLR, PT5

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	C	0.24	0/2624	0.50	0/3544
2	X	0.57	0/185	0.56	0/240
3	B	0.28	0/7858	0.50	0/10658
4	A	0.27	0/11478	0.45	0/15531
All	All	0.27	0/22145	0.47	0/29973

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	C	2575	0	2619	48	0
2	X	184	0	183	2	0
3	B	7695	0	7483	140	0
4	A	11202	0	11290	166	0
5	E	42	0	37	4	0
6	F	28	0	25	0	0
6	H	28	0	25	0	0
6	I	28	0	25	2	0
7	G	56	0	49	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	14	0	13	0	0
8	B	14	0	13	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
10	A	140	0	230	21	0
11	A	64	0	67	5	0
12	A	105	0	147	29	0
13	A	91	0	139	7	0
All	All	22269	0	22345	367	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 8.

All (367) 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)
3:B:184:ASN:O	5:E:1:NAG:H82	1.55	1.07
4:A:1586:PHE:CD1	10:A:2607:CLR:H21	1.98	0.98
4:A:658:MET:SD	12:A:2605:Y01:HAQ2	2.08	0.92
4:A:657:ILE:CG2	12:A:2605:Y01:HAP2	2.04	0.87
4:A:507:HIS:CE1	12:A:2608:Y01:HAR1	2.11	0.85
4:A:657:ILE:HG22	12:A:2605:Y01:HAP2	1.58	0.85
4:A:658:MET:SD	12:A:2605:Y01:CAQ	2.70	0.79
4:A:1580:ILE:HD12	10:A:2607:CLR:H242	1.62	0.78
1:C:196:MET:HA	4:A:395:TRP:HE1	1.49	0.78
3:B:631:ILE:HB	3:B:704:ARG:HH21	1.49	0.77
3:B:896:LYS:NZ	3:B:979:THR:OG1	2.20	0.75
3:B:119:SER:HA	3:B:141:GLY:HA2	1.68	0.74
3:B:157:ARG:NH2	3:B:222:PRO:O	2.21	0.74
4:A:507:HIS:CG	12:A:2608:Y01:HAR1	2.22	0.74
3:B:139:GLU:N	3:B:142:SER:HG	1.86	0.74
4:A:1586:PHE:CG	10:A:2607:CLR:H21	2.23	0.72
12:A:2609:Y01:HAA2	13:A:2612:3PE:H3I1	1.70	0.72
3:B:357:ILE:HG22	3:B:383:ARG:HB2	1.71	0.72
4:A:1580:ILE:CD1	10:A:2607:CLR:H242	2.18	0.72
4:A:483:VAL:HG23	4:A:484:LYS:HD3	1.72	0.71
4:A:1272:ARG:NH1	12:A:2609:Y01:CAD	2.53	0.71
3:B:57:LEU:HD13	3:B:715:LEU:HD22	1.73	0.71
3:B:646:GLU:O	3:B:652:ASN:ND2	2.24	0.70
4:A:507:HIS:CD2	12:A:2608:Y01:HAR1	2.26	0.70
1:C:178:ARG:NH1	1:C:285:LEU:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:704:ARG:NH1	3:B:737:ASP:O	2.25	0.69
3:B:994:LEU:HD12	3:B:1001:ARG:HB2	1.73	0.69
4:A:1272:ARG:NH1	12:A:2609:Y01:HAD1	2.07	0.69
1:C:93:LEU:HG	1:C:118:ILE:HD12	1.73	0.69
3:B:150:ILE:HG13	3:B:151:GLU:H	1.58	0.69
4:A:1742:PHE:CZ	12:A:2609:Y01:HAC1	2.29	0.67
3:B:766:ARG:NH2	3:B:855:ASP:OD1	2.23	0.67
4:A:511:PRO:HG3	12:A:2608:Y01:OAH	1.94	0.67
1:C:294:VAL:HG21	1:C:300:LEU:HB2	1.75	0.66
3:B:41:GLN:NE2	3:B:1010:ASN:OD1	2.29	0.66
4:A:1586:PHE:CD1	10:A:2607:CLR:C2	2.77	0.66
3:B:714:GLU:OE2	3:B:718:ASN:ND2	2.29	0.66
3:B:886:LEU:HD22	3:B:891:VAL:HG21	1.78	0.66
1:C:174:VAL:HB	1:C:178:ARG:HH22	1.62	0.65
4:A:507:HIS:ND1	12:A:2608:Y01:HAR1	2.11	0.65
3:B:127:ALA:HB2	3:B:165:ALA:HB1	1.79	0.64
4:A:1649:PHE:O	4:A:1651:ASN:ND2	2.30	0.64
4:A:394:GLU:OE2	4:A:398:LYS:NZ	2.30	0.64
3:B:726:ILE:HB	3:B:729:VAL:HG22	1.80	0.64
4:A:507:HIS:CE1	12:A:2608:Y01:CAR	2.81	0.64
4:A:1882:LEU:HD12	4:A:1883:PRO:HD2	1.79	0.63
3:B:731:ALA:HA	3:B:745:PRO:HG2	1.80	0.63
1:C:179:PRO:HG2	1:C:287:PRO:HB3	1.80	0.63
3:B:844:ASN:ND2	3:B:865:ASP:OD2	2.33	0.62
1:C:355:VAL:HG13	4:A:748:VAL:HG13	1.81	0.62
4:A:1832:VAL:HG22	4:A:1892:PHE:HZ	1.65	0.62
4:A:657:ILE:HG21	12:A:2605:Y01:HAP2	1.80	0.61
1:C:175:PRO:O	1:C:178:ARG:NH2	2.33	0.61
4:A:366:GLU:O	4:A:372:ASN:ND2	2.32	0.61
1:C:340:ASN:HD21	4:A:388:GLU:HG2	1.65	0.61
1:C:302:ARG:NH1	4:A:386:GLU:OE2	2.34	0.61
4:A:249:MET:SD	4:A:1585:LYS:NZ	2.66	0.60
3:B:982:PHE:HZ	6:I:1:NAG:H62	1.67	0.60
4:A:1923:ARG:NH2	4:A:1942:VAL:O	2.35	0.59
4:A:564:GLU:OE2	4:A:577:GLY:N	2.34	0.59
3:B:184:ASN:HB3	5:E:1:NAG:HN2	1.68	0.59
4:A:1497:PHE:HB2	4:A:1498:PRO:HD3	1.83	0.59
5:E:2:NAG:H83	5:E:2:NAG:H3	1.83	0.59
4:A:1835:TRP:HA	4:A:1854:MET:HE1	1.83	0.59
1:C:157:LEU:HD23	1:C:162:GLN:HG3	1.85	0.58
4:A:1272:ARG:HG3	10:A:2610:CLR:H191	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1838:TYR:HH	4:A:1857:HIS:HD1	1.49	0.58
3:B:845:SER:O	3:B:864:HIS:NE2	2.36	0.58
4:A:1488:ILE:HD11	12:A:2605:Y01:HAD2	1.86	0.58
3:B:482:GLN:HE22	3:B:1067:ASP:HB3	1.69	0.58
3:B:497:ILE:HG22	3:B:523:LEU:HD11	1.84	0.58
4:A:507:HIS:NE2	12:A:2608:Y01:HAR1	2.19	0.58
4:A:1586:PHE:CG	10:A:2607:CLR:C2	2.86	0.58
3:B:891:VAL:HG22	3:B:990:PHE:CE1	2.39	0.58
3:B:637:GLU:HG2	3:B:640:THR:HG23	1.84	0.58
4:A:1705:TYR:O	4:A:1789:TYR:OH	2.20	0.57
1:C:124:LEU:HA	1:C:127:ILE:HG22	1.86	0.57
4:A:404:LEU:HD11	4:A:476:ARG:HH22	1.68	0.57
4:A:257:PHE:HB2	4:A:288:GLN:HG3	1.86	0.57
4:A:1265:PRO:HG3	4:A:1710:MET:HE3	1.86	0.57
1:C:180:VAL:HB	1:C:268:VAL:HG12	1.87	0.57
3:B:122:VAL:HG21	3:B:180:LEU:HD22	1.85	0.56
3:B:515:ILE:HD12	3:B:578:MET:HE3	1.85	0.56
3:B:57:LEU:HD23	3:B:798:VAL:HG21	1.87	0.56
4:A:1580:ILE:HD11	10:A:2607:CLR:H262	1.88	0.56
1:C:209:ASP:O	1:C:211:ARG:NH1	2.38	0.56
3:B:207:VAL:HG22	3:B:217:TYR:HB3	1.87	0.56
1:C:109:VAL:O	1:C:359:ALA:HB1	2.06	0.55
4:A:1653:PHE:HE2	4:A:1656:LEU:HD13	1.71	0.55
3:B:1032:ILE:HG13	3:B:1034:ALA:H	1.70	0.55
4:A:658:MET:SD	12:A:2605:Y01:HAK1	2.47	0.54
3:B:90:LEU:HD12	3:B:615:THR:HG21	1.89	0.54
4:A:1898:ALA:HA	4:A:1901:ARG:HB3	1.90	0.54
3:B:889:ILE:HG13	3:B:891:VAL:HG23	1.90	0.54
4:A:1578:ASN:HD21	4:A:1666:ARG:HH11	1.55	0.54
3:B:442:LYS:NZ	3:B:465:PRO:O	2.41	0.54
3:B:169:PRO:HG2	3:B:172:ILE:HD12	1.88	0.54
4:A:658:MET:SD	12:A:2605:Y01:HAQ1	2.47	0.54
4:A:118:GLU:HG2	4:A:133:LEU:HD13	1.90	0.54
1:C:352:TYR:HD1	4:A:744:GLU:HB3	1.74	0.53
4:A:1722:ASP:HB3	4:A:1725:SER:O	2.08	0.53
4:A:1838:TYR:OH	4:A:1857:HIS:ND1	2.37	0.53
3:B:470:THR:O	3:B:477:THR:OG1	2.23	0.53
4:A:1488:ILE:HD11	12:A:2605:Y01:CAD	2.39	0.53
3:B:41:GLN:HE21	3:B:45:VAL:HG21	1.74	0.53
4:A:1831:TYR:HA	4:A:1858:MET:HE1	1.90	0.53
3:B:788:TYR:OH	3:B:868:THR:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:464:LEU:HD12	3:B:465:PRO:HD2	1.91	0.52
3:B:421:ILE:O	3:B:425:GLU:HG2	2.09	0.52
3:B:124:TYR:HE1	3:B:142:SER:HB2	1.74	0.52
4:A:1701:LEU:HD22	4:A:1800:LEU:HD12	1.92	0.52
3:B:826:THR:HG21	3:B:843:ARG:HD3	1.91	0.52
4:A:303:ASN:OD1	10:A:2607:CLR:H12	2.09	0.52
1:C:191:GLU:O	1:C:195:MET:HG2	2.09	0.52
1:C:199:ALA:HB2	4:A:399:ALA:HB2	1.91	0.52
3:B:832:ASP:HB3	3:B:833:PRO:HD3	1.91	0.52
3:B:295:ASN:OD1	3:B:296:SER:N	2.36	0.52
4:A:1742:PHE:CZ	12:A:2609:Y01:CAC	2.93	0.52
4:A:1880:MET:SD	4:A:1882:LEU:HB2	2.50	0.52
4:A:1901:ARG:NE	4:A:1906:ILE:O	2.43	0.52
4:A:1530:GLU:HG2	4:A:1906:ILE:HG12	1.93	0.51
13:A:2613:3PE:H251	13:A:2613:3PE:H351	1.92	0.51
4:A:1905:ASP:HA	4:A:1908:ILE:HD12	1.93	0.51
1:C:340:ASN:ND2	4:A:388:GLU:HA	2.26	0.51
3:B:147:PRO:HB3	3:B:163:HIS:NE2	2.26	0.51
4:A:1390:PHE:CE1	10:A:2606:CLR:H242	2.46	0.51
3:B:734:VAL:HG23	3:B:812:VAL:HG12	1.93	0.51
4:A:1856:ARG:NH2	4:A:1870:ALA:HA	2.25	0.51
3:B:401:TRP:CE2	3:B:405:GLU:HG3	2.46	0.51
4:A:1279:PHE:CD2	10:A:2610:CLR:H261	2.46	0.51
3:B:653:PHE:CE2	3:B:658:TYR:HD1	2.29	0.51
4:A:616:LEU:HD23	4:A:707:VAL:HG13	1.93	0.50
4:A:1340:THR:O	4:A:1344:LEU:HD12	2.11	0.50
4:A:303:ASN:HD22	4:A:306:PHE:HD2	1.57	0.50
4:A:476:ARG:HA	4:A:479:ILE:HG12	1.94	0.50
4:A:664:LEU:HD22	4:A:700:GLY:HA3	1.93	0.50
4:A:1376:VAL:HG12	4:A:1508:LEU:HD23	1.92	0.50
1:C:216:ARG:HA	1:C:270:ASP:HB3	1.93	0.50
4:A:1395:VAL:O	4:A:1399:LYS:HB2	2.12	0.50
4:A:1488:ILE:HG13	12:A:2605:Y01:HAD3	1.93	0.50
4:A:1856:ARG:HH22	4:A:1870:ALA:HA	1.76	0.50
4:A:1578:ASN:ND2	4:A:1666:ARG:HD2	2.27	0.50
1:C:58:LYS:HE3	1:C:96:LYS:HB3	1.94	0.50
3:B:788:TYR:HA	3:B:818:VAL:HG11	1.94	0.50
1:C:65:ARG:HH12	1:C:92:PHE:HE1	1.60	0.49
3:B:892:TYR:HE1	3:B:983:PHE:HE1	1.60	0.49
4:A:191:LEU:HG	4:A:194:LEU:HD12	1.94	0.49
1:C:226:ARG:HD2	1:C:284:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:653:PHE:O	3:B:746:LYS:NZ	2.35	0.49
4:A:309:LEU:HD13	4:A:694:ILE:HD11	1.93	0.49
3:B:52:SER:HB2	3:B:814:ILE:HG12	1.92	0.49
3:B:744:TYR:HB3	3:B:745:PRO:HD3	1.93	0.49
4:A:1521:MET:HB3	4:A:1523:GLU:HG2	1.94	0.49
4:A:265:GLN:HG3	4:A:285:THR:HG21	1.95	0.49
1:C:58:LYS:HE2	1:C:97:GLU:HB3	1.95	0.49
3:B:683:PHE:O	3:B:687:ILE:HG12	2.13	0.49
3:B:886:LEU:HB3	3:B:891:VAL:HB	1.94	0.49
3:B:182:GLU:HA	3:B:185:TRP:CD1	2.48	0.49
3:B:772:ASN:HB2	3:B:1010:ASN:O	2.12	0.49
3:B:79:VAL:HG22	3:B:610:THR:HG22	1.95	0.48
3:B:116:ASP:OD2	3:B:116:ASP:N	2.46	0.48
4:A:371:GLU:OE1	4:A:374:ARG:NH2	2.45	0.48
4:A:1628:ALA:HA	4:A:1631:ILE:HD12	1.94	0.48
4:A:1864:LEU:HD21	4:A:1876:ARG:HD3	1.94	0.48
10:A:2610:CLR:H221	10:A:2610:CLR:H162	1.37	0.48
1:C:185:PRO:HD3	1:C:292:VAL:HG23	1.96	0.48
3:B:797:ALA:HA	3:B:811:VAL:HG22	1.93	0.48
1:C:179:PRO:HB2	1:C:269:LEU:HG	1.95	0.48
3:B:200:ASP:HB3	3:B:203:LEU:HD23	1.96	0.48
4:A:501:LEU:O	4:A:505:ILE:HG12	2.14	0.48
4:A:1279:PHE:CE2	10:A:2610:CLR:H261	2.49	0.48
4:A:1718:ILE:HG12	4:A:1739:ARG:NH2	2.29	0.48
1:C:291:PHE:CZ	1:C:293:LYS:HB3	2.49	0.48
3:B:717:GLN:O	3:B:721:SER:HB2	2.14	0.48
1:C:229:LEU:HB3	1:C:232:PRO:HG3	1.95	0.48
4:A:1572:MET:HE1	4:A:1673:GLN:HG3	1.95	0.48
3:B:261:SER:O	3:B:327:ALA:HB1	2.14	0.47
4:A:1527:GLU:HG2	4:A:1531:ARG:HH11	1.79	0.47
3:B:1032:ILE:HG12	3:B:1036:GLN:NE2	2.30	0.47
1:C:65:ARG:HB3	1:C:172:ASP:HB2	1.95	0.47
3:B:672:ILE:HA	3:B:679:PHE:CE1	2.50	0.47
3:B:182:GLU:HG2	3:B:185:TRP:HE1	1.80	0.46
4:A:1580:ILE:O	4:A:1584:MET:HG3	2.16	0.46
4:A:264:ILE:HG21	4:A:269:PRO:HG3	1.96	0.46
1:C:94:HIS:HB2	1:C:107:ARG:HG2	1.97	0.46
1:C:136:ARG:O	1:C:137:ARG:NH1	2.39	0.46
4:A:242:ILE:HD12	4:A:1667:LEU:HD11	1.96	0.46
4:A:1457:THR:HG21	4:A:1757:TRP:HE1	1.81	0.46
12:A:2605:Y01:HBC	12:A:2605:Y01:HAM1	1.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:672:ILE:HA	3:B:679:PHE:HE1	1.81	0.46
1:C:159:LYS:HG2	1:C:160:GLN:H	1.81	0.46
3:B:123:VAL:HG12	3:B:145:ILE:HD11	1.98	0.46
3:B:159:ILE:HG22	3:B:221:SER:OG	2.16	0.46
3:B:262:GLY:HA3	4:A:125:ASP:HB2	1.98	0.46
3:B:528:GLN:O	3:B:901:GLN:NE2	2.48	0.46
4:A:1488:ILE:CG1	12:A:2605:Y01:HAD3	2.46	0.46
11:A:2602:PT5:H50	11:A:2602:PT5:H43	1.66	0.46
3:B:103:GLU:HG2	3:B:192:VAL:HG21	1.97	0.46
4:A:532:GLU:HA	4:A:535:ILE:HG22	1.98	0.46
3:B:720:TRP:CE3	3:B:744:TYR:HB2	2.51	0.46
1:C:180:VAL:H	1:C:268:VAL:HA	1.82	0.45
1:C:334:ASP:OD2	1:C:352:TYR:OH	2.32	0.45
3:B:891:VAL:HG22	3:B:990:PHE:CD1	2.50	0.45
3:B:29:SER:HB3	3:B:32:THR:HG23	1.98	0.45
1:C:181:VAL:HG22	1:C:269:LEU:HB2	1.98	0.45
3:B:674:ASP:OD1	3:B:675:ASN:N	2.50	0.45
3:B:719:TYR:HD2	3:B:720:TRP:CD1	2.35	0.45
3:B:999:CYS:HB3	3:B:1024:CYS:HB3	1.79	0.45
4:A:648:THR:HB	4:A:659:THR:HG23	1.99	0.45
10:A:2601:CLR:H182	10:A:2601:CLR:H8	1.65	0.45
1:C:208:PHE:CE2	1:C:353:LEU:HD11	2.52	0.45
4:A:188:GLU:H	4:A:188:GLU:HG2	1.59	0.45
4:A:1488:ILE:CG1	12:A:2605:Y01:CAD	2.95	0.45
10:A:2611:CLR:H182	10:A:2611:CLR:H8	1.74	0.45
1:C:192:VAL:HG11	1:C:304:ILE:HA	1.99	0.45
3:B:588:PHE:CE2	3:B:590:THR:HB	2.51	0.45
4:A:1810:MET:HA	4:A:1813:PHE:HB2	1.98	0.45
10:A:2611:CLR:H193	10:A:2611:CLR:H111	1.62	0.45
2:X:10:LYS:NZ	4:A:668:ASP:OD1	2.50	0.45
3:B:218:TYR:HB3	3:B:219:PRO:HD3	1.99	0.45
3:B:724:LYS:HE2	3:B:724:LYS:HB2	1.65	0.45
3:B:841:CYS:SG	3:B:863:ASN:ND2	2.90	0.45
3:B:1064:VAL:HG23	3:B:1065:LEU:HD22	1.98	0.45
5:E:1:NAG:O7	5:E:1:NAG:O3	2.30	0.45
3:B:179:VAL:O	3:B:183:LEU:HG	2.17	0.44
3:B:682:ASN:O	3:B:685:GLU:HG2	2.17	0.44
4:A:149:GLY:HA2	4:A:152:ILE:HG22	1.99	0.44
2:X:25:LYS:HB2	2:X:25:LYS:HE2	1.55	0.44
4:A:1499:PHE:O	4:A:1503:ASN:ND2	2.45	0.44
4:A:1891:HIS:CE1	4:A:1940:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:183:LEU:HA	3:B:186:THR:HG22	1.98	0.44
4:A:594:LYS:HZ2	4:A:595:TYR:HE1	1.64	0.44
1:C:69:SER:OG	1:C:88:GLU:OE1	2.30	0.44
1:C:140:ASN:OD1	1:C:141:PRO:HD3	2.17	0.44
3:B:139:GLU:N	3:B:142:SER:OG	2.48	0.44
4:A:1891:HIS:CE1	4:A:1893:ASN:HB2	2.53	0.44
4:A:92:LYS:H	4:A:92:LYS:HG3	1.47	0.44
4:A:247:PHE:CD2	13:A:2613:3PE:H322	2.53	0.44
4:A:1348:ARG:HH21	4:A:1711:GLN:HE22	1.65	0.44
4:A:1527:GLU:HG2	4:A:1531:ARG:NH1	2.33	0.44
4:A:1742:PHE:CE1	12:A:2609:Y01:CAC	3.00	0.44
3:B:147:PRO:HG2	3:B:149:PHE:CZ	2.52	0.44
4:A:1526:LEU:HD23	4:A:1526:LEU:HA	1.83	0.44
11:A:2602:PT5:H20	11:A:2602:PT5:H26	1.17	0.44
3:B:147:PRO:HB3	3:B:163:HIS:CE1	2.53	0.44
4:A:189:PHE:HB2	4:A:190:ASP:H	1.52	0.44
4:A:520:TYR:O	4:A:524:ILE:HD12	2.18	0.44
3:B:435:VAL:HG11	3:B:482:GLN:HA	2.00	0.44
4:A:258:GLU:HB2	4:A:261:THR:HB	2.00	0.44
4:A:1357:LYS:HE2	4:A:1357:LYS:HB3	1.84	0.44
4:A:1718:ILE:H	4:A:1739:ARG:NH2	2.16	0.44
11:A:2602:PT5:H31	11:A:2602:PT5:H27	1.51	0.44
3:B:601:ASP:OD1	3:B:766:ARG:NE	2.51	0.43
3:B:752:TRP:NE1	3:B:754:GLU:HB2	2.33	0.43
4:A:492:VAL:O	4:A:496:VAL:HG23	2.17	0.43
4:A:1564:SER:OG	4:A:1566:PRO:HD2	2.19	0.43
1:C:357:TRP:O	1:C:361:HIS:ND1	2.38	0.43
4:A:1401:LYS:HB3	4:A:1471:ALA:HB1	2.00	0.43
11:A:2602:PT5:H36	11:A:2602:PT5:H40	1.74	0.43
1:C:153:PRO:HA	1:C:154:PRO:HD3	1.92	0.43
3:B:678:GLU:OE1	3:B:678:GLU:N	2.50	0.43
13:A:2613:3PE:H292	13:A:2613:3PE:H262	1.83	0.43
3:B:875:PHE:HE2	3:B:882:LEU:HD22	1.82	0.43
3:B:591:LEU:HD11	6:I:1:NAG:H61	2.01	0.43
4:A:255:THR:HG22	4:A:291:TRP:HB2	2.01	0.43
4:A:550:PHE:HZ	11:A:2602:PT5:H17	1.83	0.43
1:C:77:GLU:HB2	1:C:103:TRP:HZ2	1.83	0.43
4:A:1580:ILE:HD11	10:A:2607:CLR:C26	2.49	0.43
4:A:1671:LEU:HD23	4:A:1671:LEU:HA	1.82	0.43
3:B:44:LEU:HD21	3:B:821:TRP:NE1	2.33	0.43
3:B:1001:ARG:NE	3:B:1020:SER:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:2613:3PE:H272	13:A:2613:3PE:H242	1.86	0.43
3:B:616:ASP:OD1	3:B:616:ASP:N	2.51	0.43
3:B:639:ILE:HG22	3:B:643:ARG:NH1	2.34	0.43
3:B:735:VAL:HG21	3:B:763:PHE:HZ	1.84	0.43
3:B:904:CYS:SG	3:B:1037:THR:OG1	2.64	0.43
4:A:1578:ASN:HD22	4:A:1666:ARG:HD2	1.83	0.43
4:A:1727:GLU:HB3	4:A:1730:PHE:CE1	2.54	0.43
3:B:100:LEU:HD22	3:B:488:MET:HE1	2.01	0.42
3:B:592:VAL:HG11	3:B:605:ARG:CZ	2.49	0.42
3:B:649:LYS:HB2	3:B:652:ASN:HB2	2.01	0.42
4:A:527:GLY:O	4:A:531:SER:N	2.50	0.42
10:A:2611:CLR:H183	10:A:2611:CLR:H20	1.80	0.42
1:C:195:MET:HE1	4:A:400:GLU:N	2.34	0.42
3:B:645:SER:HB2	3:B:687:ILE:HD12	2.02	0.42
4:A:1828:LEU:HD22	4:A:1896:LEU:HD11	2.00	0.42
4:A:1883:PRO:HA	4:A:1951:THR:HA	2.01	0.42
13:A:2612:3PE:H3F1	13:A:2612:3PE:H3I2	1.79	0.42
4:A:104:ILE:O	4:A:108:ILE:HG13	2.19	0.42
4:A:232:LEU:HD21	4:A:1681:LEU:HD21	2.01	0.42
4:A:529:PHE:HB3	4:A:558:ILE:HD11	2.01	0.42
4:A:1546:HIS:CE1	4:A:1548:PRO:HG3	2.54	0.42
4:A:1278:TYR:HA	4:A:1281:TYR:HD2	1.85	0.42
4:A:1742:PHE:CE1	12:A:2609:Y01:HAC1	2.53	0.42
4:A:1771:ASP:OD1	4:A:1772:LYS:N	2.53	0.42
4:A:526:LEU:HD21	4:A:562:ILE:HD13	2.02	0.42
4:A:1494:PHE:HA	4:A:1498:PRO:HD2	2.00	0.42
4:A:1880:MET:HG2	4:A:1898:ALA:HB1	2.02	0.42
1:C:111:GLU:HG3	4:A:748:VAL:HG12	2.02	0.42
3:B:62:GLU:OE2	3:B:800:ILE:HG13	2.20	0.42
3:B:344:LEU:HD23	3:B:344:LEU:HA	1.87	0.42
3:B:853:LEU:HD23	3:B:859:LEU:HA	2.02	0.42
3:B:865:ASP:HA	3:B:868:THR:HG22	2.02	0.42
4:A:104:ILE:HG13	4:A:147:GLU:HG3	2.00	0.42
4:A:1292:VAL:O	4:A:1296:ILE:HD12	2.20	0.42
4:A:1390:PHE:CE1	10:A:2606:CLR:C24	3.03	0.42
1:C:280:LEU:HD11	1:C:285:LEU:HD12	2.02	0.42
3:B:204:LEU:HD13	3:B:456:LEU:HD21	2.02	0.42
4:A:285:THR:O	4:A:286:LYS:HE2	2.19	0.42
4:A:1610:LEU:HA	4:A:1613:VAL:HG12	2.02	0.42
3:B:689:ARG:HD2	3:B:690:LYS:HG3	2.01	0.42
3:B:820:SER:O	3:B:823:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:340:PHE:O	4:A:344:ILE:HG12	2.20	0.42
4:A:373:ARG:HD2	4:A:373:ARG:HA	1.91	0.42
4:A:1340:THR:O	4:A:1341:ILE:C	2.58	0.42
4:A:1718:ILE:HG12	4:A:1739:ARG:CZ	2.50	0.42
4:A:1831:TYR:CD2	4:A:1896:LEU:HD13	2.55	0.42
3:B:653:PHE:CD2	3:B:658:TYR:HA	2.55	0.41
4:A:1622:LEU:O	4:A:1626:ARG:HG3	2.20	0.41
12:A:2609:Y01:HAP1	12:A:2609:Y01:HAO2	1.68	0.41
3:B:182:GLU:HA	3:B:185:TRP:NE1	2.34	0.41
3:B:639:ILE:HG22	3:B:643:ARG:HH11	1.85	0.41
3:B:801:TYR:CZ	3:B:806:LEU:HD13	2.55	0.41
4:A:111:ASN:ND2	4:A:140:PHE:HD2	2.18	0.41
4:A:1527:GLU:HA	4:A:1531:ARG:HB2	2.02	0.41
4:A:1534:ILE:O	4:A:1538:ILE:HG12	2.20	0.41
1:C:258:PHE:O	1:C:262:LYS:HG3	2.19	0.41
3:B:648:LEU:HD12	3:B:680:LEU:HD11	2.03	0.41
3:B:870:GLN:OE1	3:B:873:ARG:NH1	2.53	0.41
10:A:2601:CLR:H193	10:A:2601:CLR:H111	1.85	0.41
3:B:660:PHE:HB2	3:B:741:THR:HB	2.02	0.41
3:B:712:THR:O	3:B:716:VAL:HG12	2.21	0.41
3:B:852:ILE:HG22	3:B:861:MET:HB2	2.02	0.41
4:A:199:VAL:HG11	4:A:630:LEU:HB2	2.02	0.41
1:C:85:VAL:HG23	1:C:108:LEU:HD11	2.03	0.41
3:B:694:ASN:HB2	3:B:695:PRO:HD3	2.03	0.41
3:B:396:ARG:C	3:B:400:GLN:HE21	2.24	0.41
3:B:409:TYR:HD2	3:B:411:TYR:CZ	2.39	0.41
3:B:709:ALA:HA	3:B:740:ILE:HD13	2.03	0.41
3:B:1029:ARG:HG2	3:B:1029:ARG:O	2.21	0.41
4:A:1643:ASP:HB2	4:A:1659:LEU:HB3	2.03	0.41
4:A:1802:LEU:O	4:A:1806:VAL:HG23	2.20	0.41
12:A:2609:Y01:HAA3	12:A:2609:Y01:HAJ2	1.75	0.41
7:G:3:NAG:HN2	7:G:3:NAG:H5	1.86	0.41
3:B:252:LYS:N	3:B:287:ASP:OD1	2.43	0.41
3:B:636:GLU:HB3	3:B:640:THR:HG21	2.03	0.41
4:A:1272:ARG:HG3	10:A:2610:CLR:H8	2.03	0.41
3:B:401:TRP:CZ2	3:B:405:GLU:HG3	2.56	0.40
4:A:577:GLY:O	4:A:580:VAL:HG12	2.21	0.40
13:A:2613:3PE:H2B2	13:A:2613:3PE:H2E1	1.91	0.40
3:B:186:THR:HA	3:B:189:LEU:HD13	2.03	0.40
3:B:306:HIS:O	3:B:307:LEU:HG	2.21	0.40
3:B:823:GLU:HA	3:B:843:ARG:HH12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:847:VAL:HG13	3:B:848:MET:N	2.36	0.40
4:A:194:LEU:O	4:A:197:VAL:HG22	2.21	0.40
3:B:701:LEU:HD23	3:B:701:LEU:HA	1.97	0.40
3:B:731:ALA:HB3	3:B:815:LYS:HG3	2.02	0.40
3:B:1027:ASP:O	3:B:1029:ARG:NH1	2.54	0.40
4:A:337:TRP:HB2	4:A:341:ILE:HD12	2.04	0.40
4:A:601:ASN:ND2	4:A:723:THR:OG1	2.46	0.40
4:A:1722:ASP:O	4:A:1728:ASP:HB2	2.21	0.40
3:B:875:PHE:CE2	3:B:882:LEU:HD22	2.56	0.40
4:A:581:LEU:HD23	4:A:581:LEU:HA	1.93	0.40
4:A:1572:MET:HE3	4:A:1572:MET:HB2	1.99	0.40
1:C:344:ASP:O	1:C:347:GLU:HG3	2.22	0.40
3:B:41:GLN:NE2	3:B:45:VAL:HG21	2.36	0.40
3:B:54:VAL:O	3:B:58:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	322/496 (65%)	311 (97%)	11 (3%)	0	100	100
2	X	24/26 (92%)	24 (100%)	0	0	100	100
3	B	954/1115 (86%)	900 (94%)	54 (6%)	0	100	100
4	A	1368/2549 (54%)	1336 (98%)	32 (2%)	0	100	100
All	All	2668/4186 (64%)	2571 (96%)	97 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	287/438 (66%)	287 (100%)	0	100 100
2	X	20/20 (100%)	18 (90%)	2 (10%)	6 23
3	B	854/983 (87%)	852 (100%)	2 (0%)	92 96
4	A	1214/2154 (56%)	1208 (100%)	6 (0%)	86 92
All	All	2375/3595 (66%)	2365 (100%)	10 (0%)	88 94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	23	ARG
2	X	25	LYS
3	B	643	ARG
3	B	1029	ARG
4	A	92	LYS
4	A	187	THR
4	A	188	GLU
4	A	189	PHE
4	A	190	ASP
4	A	191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	340	ASN
3	B	41	GLN
3	B	1010	ASN
4	A	706	ASN
4	A	1332	ASN
4	A	1578	ASN
4	A	1651	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	1	3,5	14,14,15	0.88	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	E	2	5	14,14,15	0.42	0	17,19,21	1.25	1 (5%)
5	NAG	E	3	5	14,14,15	0.40	0	17,19,21	0.36	0
6	NAG	F	1	3,6	14,14,15	0.44	0	17,19,21	0.48	0
6	NAG	F	2	6	14,14,15	0.34	0	17,19,21	0.41	0
7	NAG	G	1	3,7	14,14,15	0.26	0	17,19,21	0.44	0
7	NAG	G	2	7	14,14,15	0.22	0	17,19,21	0.52	0
7	NAG	G	3	7	14,14,15	0.83	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	G	4	7	14,14,15	0.33	0	17,19,21	0.35	0
6	NAG	H	1	3,6	14,14,15	0.22	0	17,19,21	0.40	0
6	NAG	H	2	6	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	I	1	3,6	14,14,15	0.22	0	17,19,21	0.65	0
6	NAG	I	2	6	14,14,15	0.28	0	17,19,21	0.58	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	2	5	-	5/6/23/26	0/1/1/1
5	NAG	E	3	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	F	2	6	-	4/6/23/26	0/1/1/1
7	NAG	G	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	NAG	G	3	7	-	0/6/23/26	0/1/1/1
7	NAG	G	4	7	-	1/6/23/26	0/1/1/1
6	NAG	H	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	3/6/23/26	0/1/1/1
6	NAG	I	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	O5-C1	-2.26	1.40	1.43
7	G	3	NAG	C1-C2	2.26	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2	NAG	C2-N2-C7	4.26	128.97	122.90
7	G	3	NAG	C1-O5-C5	3.13	116.44	112.19
5	E	1	NAG	C4-C3-C2	2.54	114.74	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C1-C2-N2-C7
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
5	E	3	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6

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

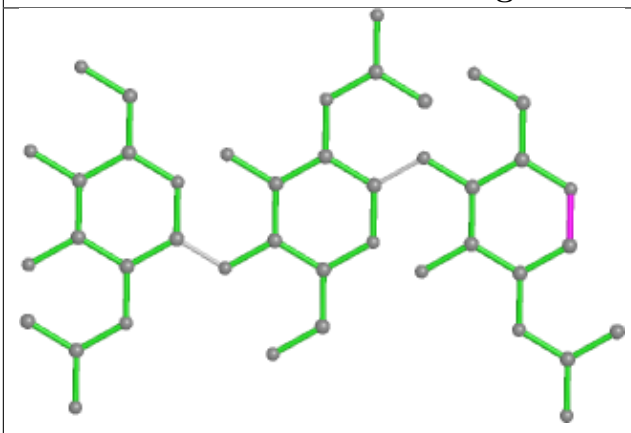
There are no ring outliers.

4 monomers are involved in 7 short contacts:

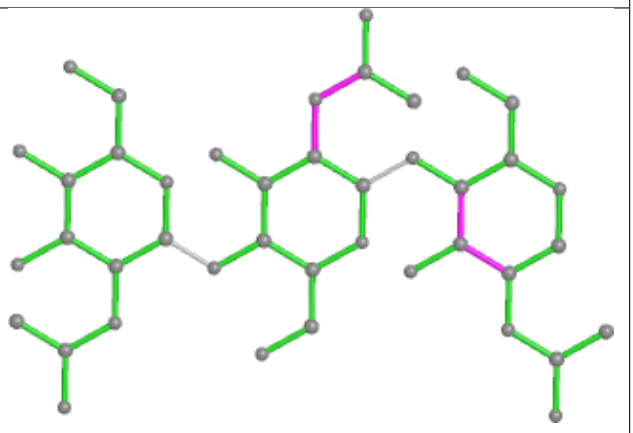
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	1	0
5	E	1	NAG	3	0
6	I	1	NAG	2	0
7	G	3	NAG	1	0

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

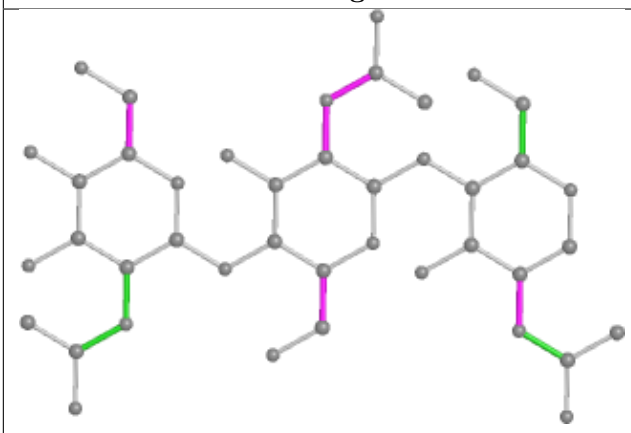
Oligosaccharide Chain E



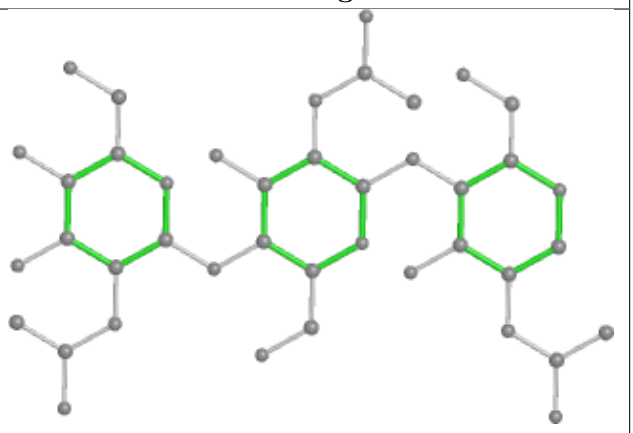
Bond lengths



Bond angles

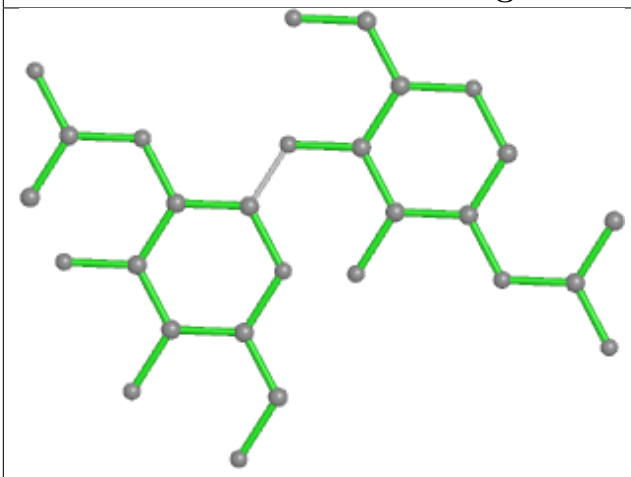


Torsions

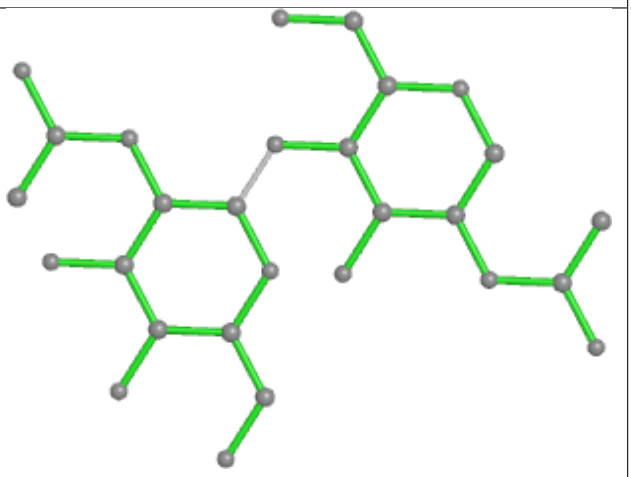


Rings

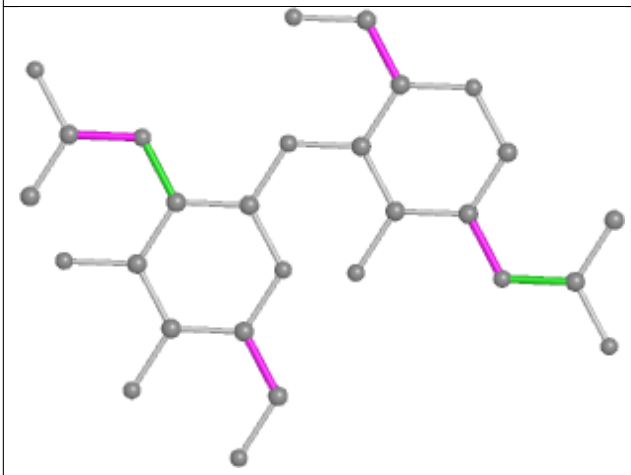
Oligosaccharide Chain F



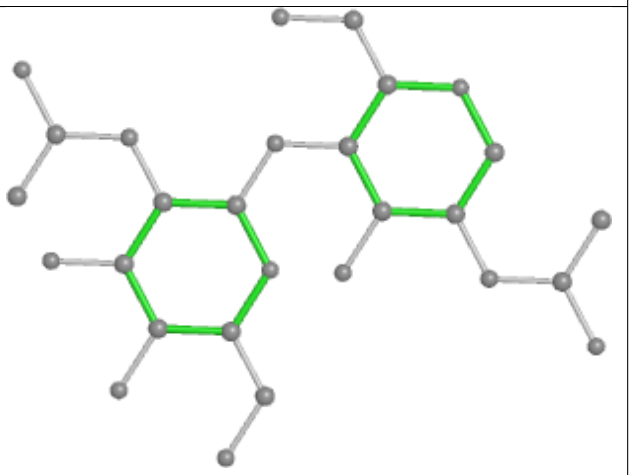
Bond lengths



Bond angles

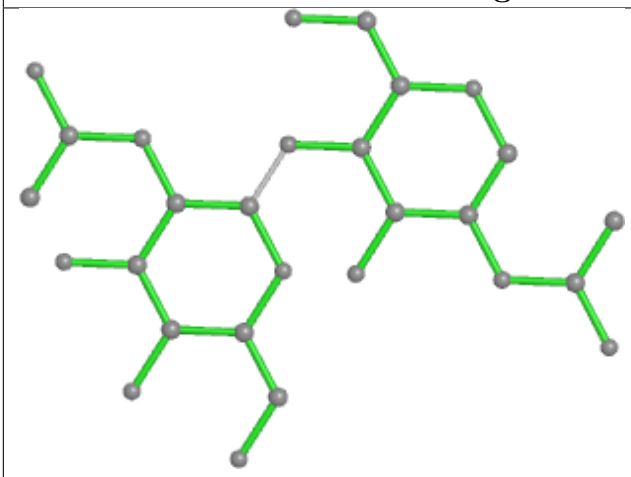


Torsions

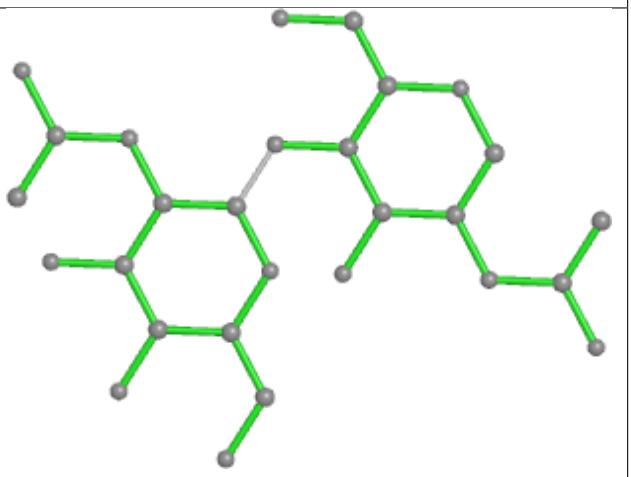


Rings

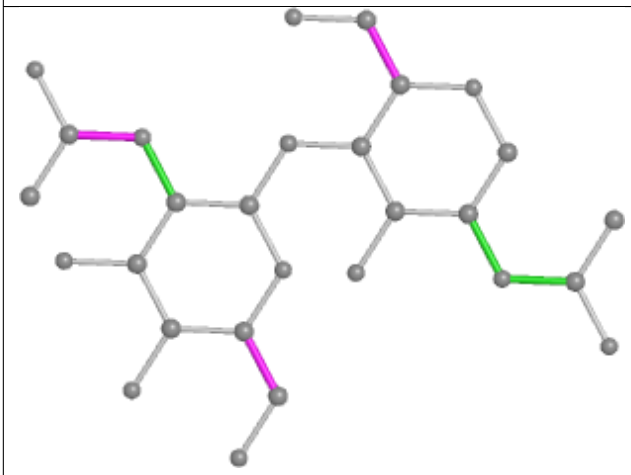
Oligosaccharide Chain H



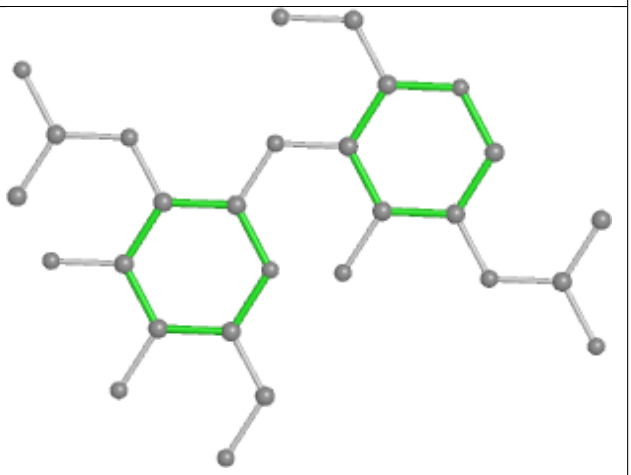
Bond lengths



Bond angles

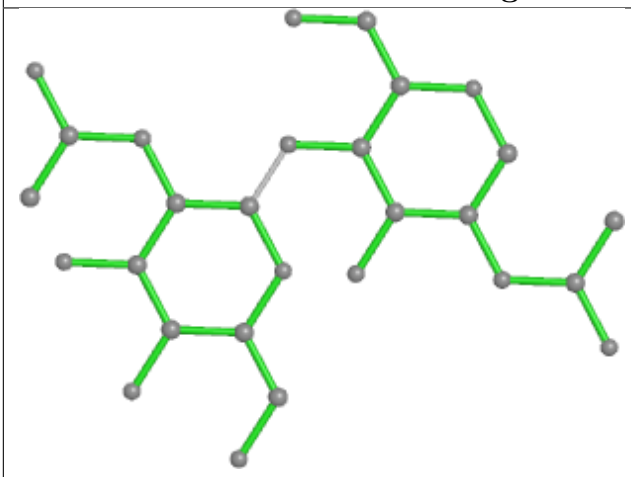


Torsions

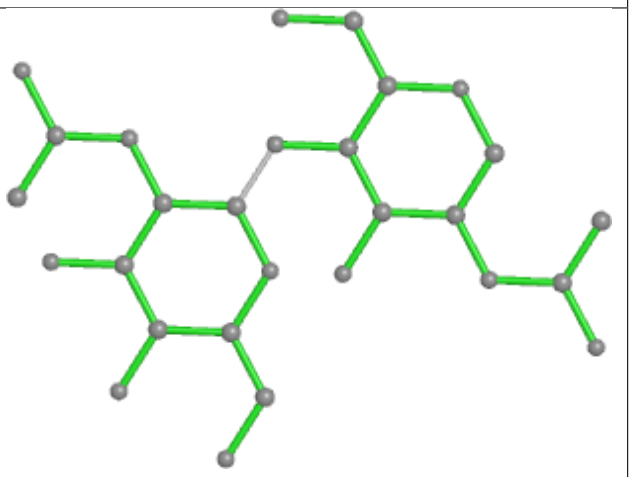


Rings

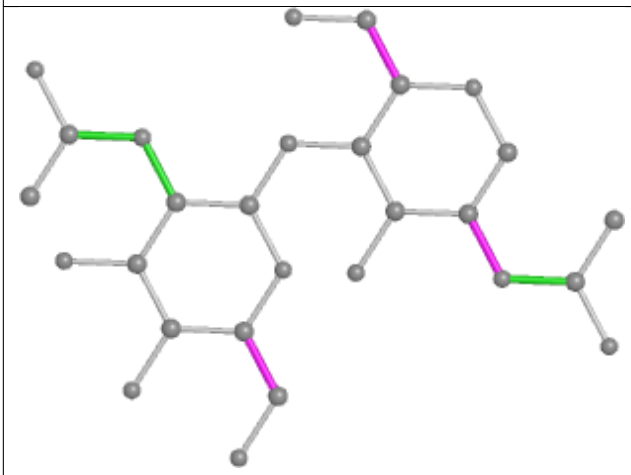
Oligosaccharide Chain I



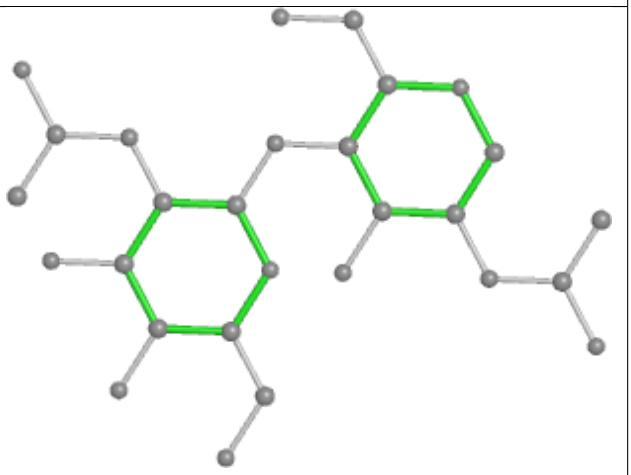
Bond lengths



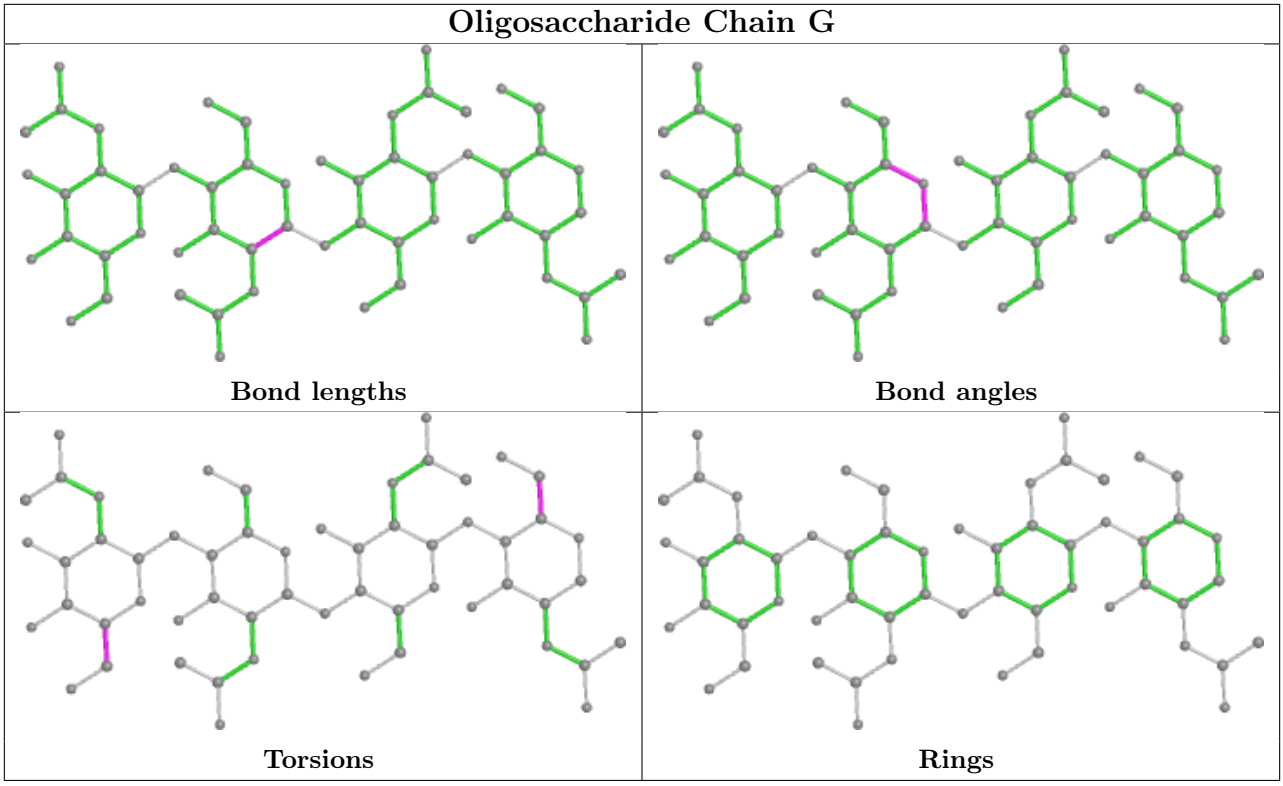
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	CLR	A	2611	-	31,31,31	0.97	2 (6%)	48,48,48	1.67	11 (22%)
8	NAG	A	2604	4	14,14,15	0.25	0	17,19,21	0.46	0
10	CLR	A	2606	-	31,31,31	0.31	0	48,48,48	0.46	0
10	CLR	A	2607	-	31,31,31	0.35	0	48,48,48	0.57	0
10	CLR	A	2601	-	31,31,31	0.96	2 (6%)	48,48,48	1.91	17 (35%)
11	PT5	A	2602	-	64,64,69	0.88	3 (4%)	78,82,87	1.28	9 (11%)
12	Y01	A	2605	-	38,38,38	0.46	0	57,57,57	0.51	0
13	3PE	A	2613	-	50,50,50	0.88	2 (4%)	53,55,55	1.02	2 (3%)
12	Y01	A	2608	-	38,38,38	0.45	0	57,57,57	0.66	0
10	CLR	A	2610	-	31,31,31	0.30	0	48,48,48	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	Y01	A	2609	-	38,38,38	0.45	0	57,57,57	0.48	0
13	3PE	A	2612	-	39,39,50	0.97	2 (5%)	42,44,55	1.21	4 (9%)
8	NAG	B	1201	3	14,14,15	0.24	0	17,19,21	0.54	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
10	CLR	A	2611	-	-	10/10/68/68	0/4/4/4
8	NAG	A	2604	4	-	2/6/23/26	0/1/1/1
10	CLR	A	2606	-	-	6/10/68/68	0/4/4/4
10	CLR	A	2607	-	-	10/10/68/68	0/4/4/4
10	CLR	A	2601	-	-	3/10/68/68	0/4/4/4
11	PT5	A	2602	-	-	34/61/85/90	0/1/1/1
12	Y01	A	2605	-	-	8/19/77/77	0/4/4/4
13	3PE	A	2613	-	-	30/54/54/54	-
12	Y01	A	2608	-	-	10/19/77/77	0/4/4/4
10	CLR	A	2610	-	-	9/10/68/68	0/4/4/4
12	Y01	A	2609	-	-	13/19/77/77	0/4/4/4
13	3PE	A	2612	-	-	22/43/43/54	-
8	NAG	B	1201	3	-	4/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2602	PT5	O18-C11	4.30	1.45	1.33
13	A	2613	3PE	O21-C21	4.12	1.45	1.34
13	A	2613	3PE	O31-C31	3.85	1.44	1.33
11	A	2602	PT5	O16-C10	3.80	1.45	1.34
13	A	2612	3PE	O21-C21	3.74	1.44	1.34
13	A	2612	3PE	O31-C31	3.69	1.44	1.33
10	A	2601	CLR	C13-C14	-2.68	1.49	1.55
10	A	2611	CLR	C13-C14	-2.58	1.50	1.55
10	A	2611	CLR	C10-C9	-2.13	1.52	1.56
10	A	2601	CLR	C10-C9	-2.11	1.52	1.56
11	A	2602	PT5	P4-O4	2.08	1.63	1.59

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2611	CLR	C8-C7-C6	-4.41	106.39	112.73
13	A	2613	3PE	O21-C21-C22	4.09	120.31	111.50
11	A	2602	PT5	O16-C10-C12	3.99	120.10	111.50
13	A	2612	3PE	O21-C21-C22	3.76	119.60	111.50
10	A	2601	CLR	C3-C4-C5	-3.56	105.98	112.03
10	A	2601	CLR	C7-C6-C5	-3.47	118.67	125.06
10	A	2601	CLR	C12-C11-C9	3.43	119.06	113.11
10	A	2601	CLR	C1-C10-C9	3.31	113.34	108.73
10	A	2611	CLR	C13-C14-C8	-3.29	109.51	114.38
10	A	2601	CLR	C21-C20-C22	-3.28	105.21	110.36
10	A	2601	CLR	C13-C14-C8	-3.13	109.75	114.38
11	A	2602	PT5	C5-C6-C1	3.08	115.36	108.96
10	A	2601	CLR	C8-C7-C6	-2.95	108.50	112.73
10	A	2611	CLR	C13-C17-C20	-2.86	115.01	119.49
10	A	2601	CLR	C14-C8-C9	-2.84	105.29	109.09
10	A	2601	CLR	C4-C5-C10	2.84	120.19	116.42
10	A	2611	CLR	C12-C11-C9	2.84	118.03	113.11
11	A	2602	PT5	C12-C13-C14	-2.78	108.26	113.23
10	A	2611	CLR	C19-C10-C9	-2.76	108.39	111.68
10	A	2611	CLR	C4-C5-C10	2.74	120.07	116.42
11	A	2602	PT5	O18-C11-C31	2.74	120.52	111.91
10	A	2611	CLR	C16-C17-C20	-2.70	107.96	112.15
13	A	2612	3PE	O31-C31-C32	2.69	120.35	111.91
13	A	2613	3PE	O31-C31-C32	2.67	120.29	111.91
13	A	2612	3PE	C2-O21-C21	-2.63	111.32	117.79
11	A	2602	PT5	O4-C4-C3	2.61	114.73	108.66
11	A	2602	PT5	C2-C3-C4	2.61	115.64	109.68
11	A	2602	PT5	C2-C1-C6	2.60	114.60	110.85
10	A	2611	CLR	C14-C8-C9	-2.52	105.72	109.09
10	A	2601	CLR	C7-C8-C9	2.52	112.76	109.71
10	A	2601	CLR	C10-C9-C8	-2.45	109.06	112.73
10	A	2611	CLR	C4-C5-C6	-2.43	117.10	120.61
10	A	2601	CLR	C15-C14-C8	-2.41	115.11	119.08
10	A	2601	CLR	C1-C2-C3	2.38	113.52	110.47
10	A	2611	CLR	C17-C13-C14	2.38	102.89	100.07
13	A	2612	3PE	O31-C31-O32	-2.32	117.73	123.59
11	A	2602	PT5	C9-O18-C11	2.26	125.51	117.12
10	A	2601	CLR	C10-C5-C6	-2.21	119.53	122.90
10	A	2601	CLR	C12-C13-C14	-2.15	103.94	107.27
11	A	2602	PT5	O18-C11-O19	-2.13	118.21	123.59
10	A	2601	CLR	C15-C14-C13	2.09	106.36	103.84
10	A	2611	CLR	C15-C14-C13	2.09	106.36	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2601	CLR	C16-C17-C20	-2.03	109.01	112.15

There are no chirality outliers.

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2610	CLR	C13-C17-C20-C21
10	A	2610	CLR	C16-C17-C20-C22
11	A	2602	PT5	C1-O1-P1-O12
11	A	2602	PT5	C1-O1-P1-O11
11	A	2602	PT5	C3-C4-O4-P4
11	A	2602	PT5	C12-C10-O16-C8
11	A	2602	PT5	O19-C11-O18-C9
11	A	2602	PT5	C12-C13-C14-C15
11	A	2602	PT5	C18-C19-C20-C21
12	A	2605	Y01	OAG-CAY-OAW-CBC
12	A	2605	Y01	CAM-CAY-OAW-CBC
12	A	2609	Y01	CAR-CBC-OAW-CAY
12	A	2609	Y01	CAM-CAY-OAW-CBC
13	A	2612	3PE	C1-O11-P-O14
13	A	2612	3PE	C11-O13-P-O14
13	A	2612	3PE	O13-C11-C12-N
13	A	2613	3PE	C11-O13-P-O14
13	A	2613	3PE	C22-C21-O21-C2
10	A	2610	CLR	C16-C17-C20-C21
12	A	2608	Y01	CAC-CBB-CBE-CAP
10	A	2611	CLR	C13-C17-C20-C21
12	A	2608	Y01	CAC-CBB-CBE-CBI
10	A	2610	CLR	C13-C17-C20-C22
11	A	2602	PT5	O17-C10-O16-C8
13	A	2613	3PE	O22-C21-O21-C2
11	A	2602	PT5	C31-C11-O18-C9
8	B	1201	NAG	O5-C5-C6-O6
10	A	2606	CLR	C21-C20-C22-C23
10	A	2607	CLR	C21-C20-C22-C23
10	A	2610	CLR	C21-C20-C22-C23
10	A	2611	CLR	C21-C20-C22-C23
10	A	2607	CLR	C16-C17-C20-C21
10	A	2611	CLR	C16-C17-C20-C21
10	A	2607	CLR	C13-C17-C20-C22
10	A	2611	CLR	C13-C17-C20-C22
12	A	2608	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
12	A	2605	Y01	CAX-CAL-CAM-CAY
12	A	2609	Y01	OAG-CAY-OAW-CBC
10	A	2607	CLR	C13-C17-C20-C21
10	A	2611	CLR	C16-C17-C20-C22
12	A	2608	Y01	CAO-CBB-CBE-CAP
13	A	2612	3PE	C22-C23-C24-C25
13	A	2613	3PE	C26-C27-C28-C29
12	A	2609	Y01	CAO-CBB-CBE-CBI
13	A	2613	3PE	C24-C25-C26-C27
10	A	2611	CLR	C17-C20-C22-C23
10	A	2601	CLR	C21-C20-C22-C23
8	A	2604	NAG	O5-C5-C6-O6
8	B	1201	NAG	C4-C5-C6-O6
10	A	2607	CLR	C16-C17-C20-C22
10	A	2601	CLR	C17-C20-C22-C23
10	A	2610	CLR	C17-C20-C22-C23
12	A	2609	Y01	CAJ-CAO-CBB-CBE
8	A	2604	NAG	C4-C5-C6-O6
12	A	2609	Y01	CAC-CBB-CBE-CBI
10	A	2607	CLR	C17-C20-C22-C23
8	B	1201	NAG	C8-C7-N2-C2
8	B	1201	NAG	O7-C7-N2-C2
10	A	2607	CLR	C22-C23-C24-C25
10	A	2606	CLR	C22-C23-C24-C25
11	A	2602	PT5	C10-C12-C13-C14
13	A	2613	3PE	C21-C22-C23-C24
12	A	2605	Y01	CAN-CAJ-CAO-CBB
11	A	2602	PT5	C11-C31-C32-C33
13	A	2612	3PE	C32-C33-C34-C35
10	A	2611	CLR	C20-C22-C23-C24
10	A	2611	CLR	C22-C23-C24-C25
13	A	2612	3PE	C22-C21-O21-C2
10	A	2601	CLR	C22-C23-C24-C25
12	A	2609	Y01	CAX-CAL-CAM-CAY
10	A	2607	CLR	C20-C22-C23-C24
12	A	2609	Y01	CAO-CAJ-CAN-CBA
12	A	2608	Y01	CAJ-CAO-CBB-CBE
13	A	2612	3PE	C1-O11-P-O13
13	A	2612	3PE	C11-O13-P-O11
13	A	2613	3PE	C11-O13-P-O11
13	A	2612	3PE	O22-C21-O21-C2
12	A	2609	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
10	A	2606	CLR	C20-C22-C23-C24
11	A	2602	PT5	C1-O1-P1-O13
11	A	2602	PT5	C36-C37-C38-C39
13	A	2612	3PE	C36-C37-C38-C39
13	A	2613	3PE	C29-C2A-C2B-C2C
12	A	2605	Y01	CAJ-CAN-CBA-CAB
11	A	2602	PT5	C33-C34-C35-C36
13	A	2613	3PE	C39-C3A-C3B-C3C
11	A	2602	PT5	C31-C32-C33-C34
11	A	2602	PT5	C27-C28-C29-C30
13	A	2613	3PE	C2E-C2F-C2G-C2H
12	A	2609	Y01	CAC-CBB-CBE-CAP
10	A	2606	CLR	C17-C20-C22-C23
13	A	2613	3PE	C37-C38-C39-C3A
12	A	2608	Y01	CAJ-CAO-CBB-CAC
13	A	2613	3PE	C2D-C2E-C2F-C2G
10	A	2606	CLR	C23-C24-C25-C26
12	A	2605	Y01	CAJ-CAN-CBA-CAA
11	A	2602	PT5	C35-C36-C37-C38
10	A	2607	CLR	C23-C24-C25-C27
13	A	2613	3PE	C23-C24-C25-C26
13	A	2612	3PE	C3F-C3G-C3H-C3I
13	A	2612	3PE	C24-C25-C26-C27
12	A	2609	Y01	CAO-CBB-CBE-CAP
13	A	2613	3PE	C28-C29-C2A-C2B
12	A	2605	Y01	CAJ-CAO-CBB-CBE
11	A	2602	PT5	C34-C35-C36-C37
10	A	2607	CLR	C23-C24-C25-C26
13	A	2612	3PE	C1-C2-C3-O31
10	A	2610	CLR	C23-C24-C25-C26
13	A	2613	3PE	C1-C2-O21-C21
13	A	2613	3PE	O21-C2-C3-O31
11	A	2602	PT5	C15-C16-C17-C18
12	A	2605	Y01	CAJ-CAO-CBB-CAC
11	A	2602	PT5	O13-C7-C8-O16
12	A	2608	Y01	CAL-CAM-CAY-OAW
13	A	2612	3PE	O21-C2-C3-O31
10	A	2606	CLR	C23-C24-C25-C27
10	A	2610	CLR	C23-C24-C25-C27
11	A	2602	PT5	C37-C38-C39-C40
11	A	2602	PT5	O13-C7-C8-C9
11	A	2602	PT5	C5-O5-P5-O52

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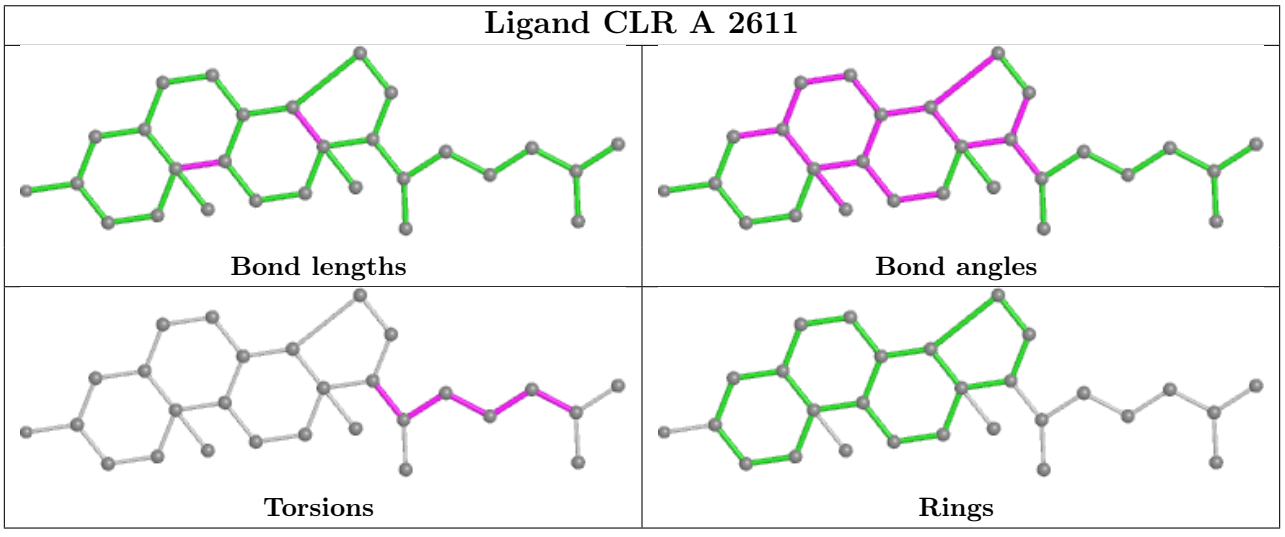
Mol	Chain	Res	Type	Atoms
10	A	2610	CLR	C22-C23-C24-C25
13	A	2613	3PE	C2-C1-O11-P
13	A	2613	3PE	O11-C1-C2-O21
10	A	2611	CLR	C23-C24-C25-C26
11	A	2602	PT5	C5-C4-O4-P4
11	A	2602	PT5	C6-C5-O5-P5
13	A	2613	3PE	C34-C35-C36-C37
12	A	2609	Y01	CAJ-CAN-CBA-CAA
13	A	2612	3PE	C1-O11-P-O12
13	A	2612	3PE	C11-O13-P-O12
13	A	2613	3PE	C11-O13-P-O12
13	A	2612	3PE	C3C-C3D-C3E-C3F
11	A	2602	PT5	C39-C40-C41-C42
10	A	2611	CLR	C23-C24-C25-C27
11	A	2602	PT5	C7-O13-P1-O1
13	A	2613	3PE	C1-O11-P-O13
13	A	2613	3PE	C38-C39-C3A-C3B
13	A	2612	3PE	C37-C38-C39-C3A
12	A	2609	Y01	CAJ-CAN-CBA-CAB
12	A	2608	Y01	CAN-CAJ-CAO-CBB
11	A	2602	PT5	C38-C39-C40-C41
13	A	2613	3PE	C32-C33-C34-C35
13	A	2613	3PE	C1-C2-C3-O31
13	A	2612	3PE	C35-C36-C37-C38
13	A	2613	3PE	C3F-C3G-C3H-C3I
13	A	2612	3PE	C3B-C3C-C3D-C3E
13	A	2613	3PE	O31-C31-C32-C33
13	A	2613	3PE	O11-C1-C2-C3
13	A	2612	3PE	O31-C31-C32-C33
11	A	2602	PT5	C13-C14-C15-C16
12	A	2608	Y01	CAL-CAM-CAY-OAG
11	A	2602	PT5	O18-C11-C31-C32
11	A	2602	PT5	C26-C27-C28-C29
13	A	2612	3PE	C38-C39-C3A-C3B
13	A	2613	3PE	C22-C23-C24-C25
11	A	2602	PT5	C4-O4-P4-O43
11	A	2602	PT5	C4-C5-O5-P5
11	A	2602	PT5	O19-C11-C31-C32
13	A	2613	3PE	C25-C26-C27-C28
13	A	2613	3PE	C3D-C3E-C3F-C3G
12	A	2608	Y01	CAO-CAJ-CAN-CBA

There are no ring outliers.

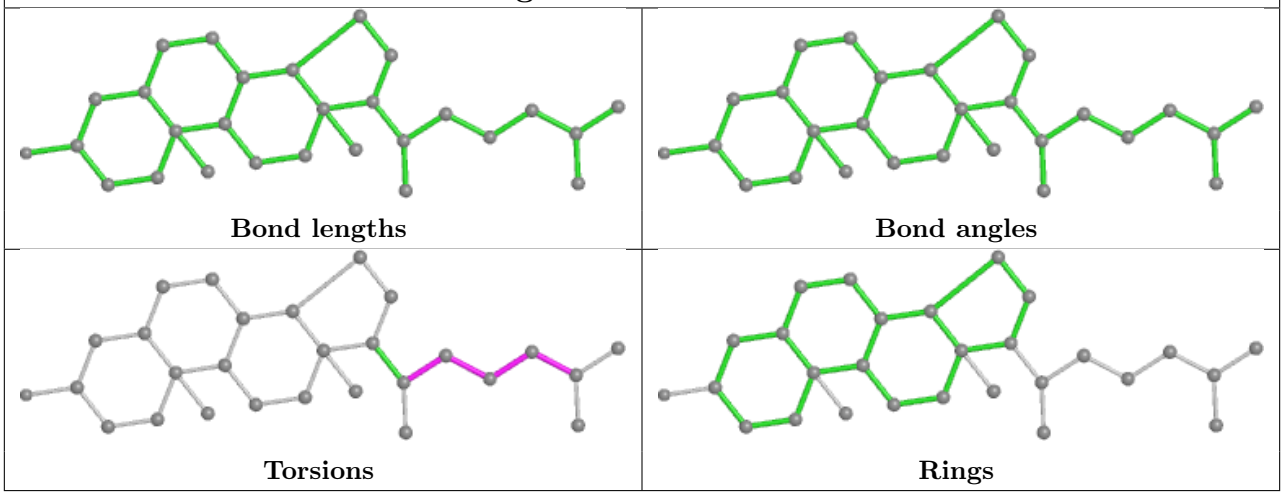
11 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2611	CLR	3	0
10	A	2606	CLR	2	0
10	A	2607	CLR	9	0
10	A	2601	CLR	2	0
11	A	2602	PT5	5	0
12	A	2605	Y01	13	0
13	A	2613	3PE	5	0
12	A	2608	Y01	7	0
10	A	2610	CLR	5	0
12	A	2609	Y01	9	0
13	A	2612	3PE	2	0

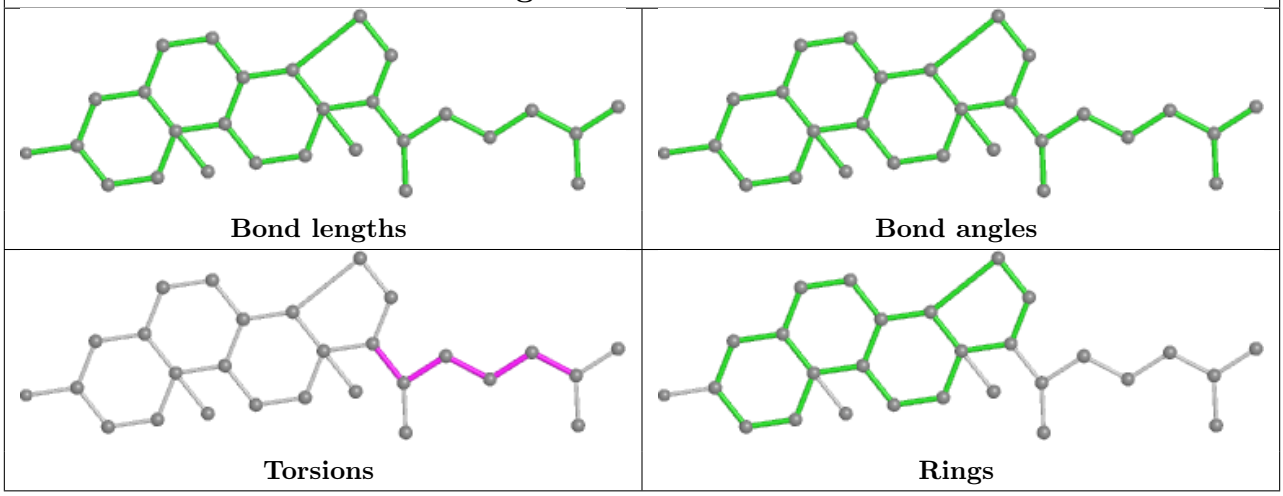
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



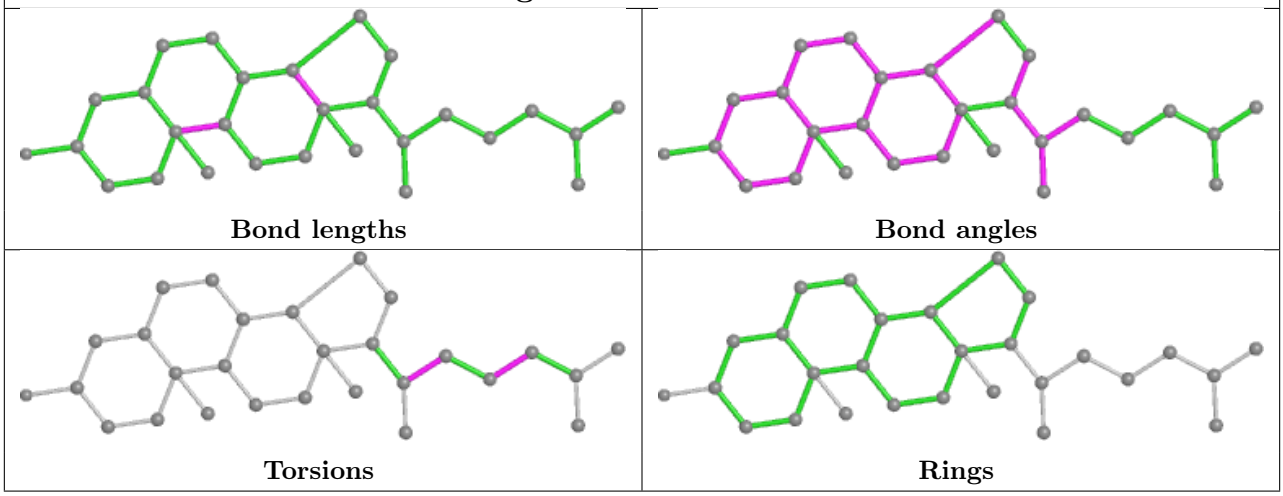
Ligand CLR A 2606



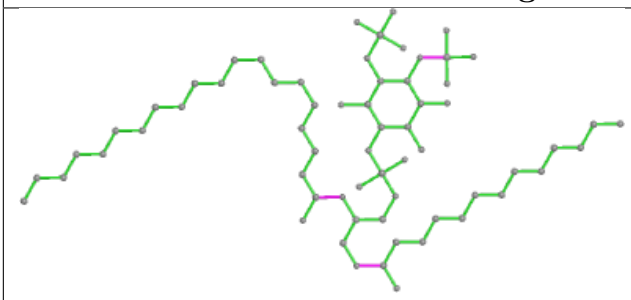
Ligand CLR A 2607



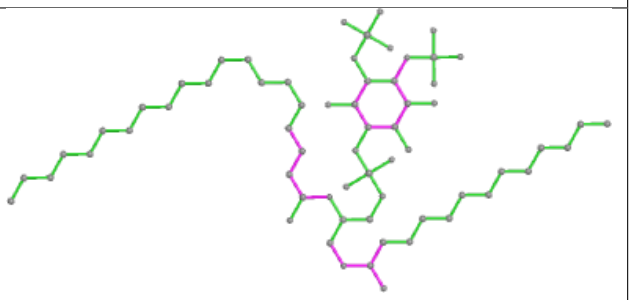
Ligand CLR A 2601



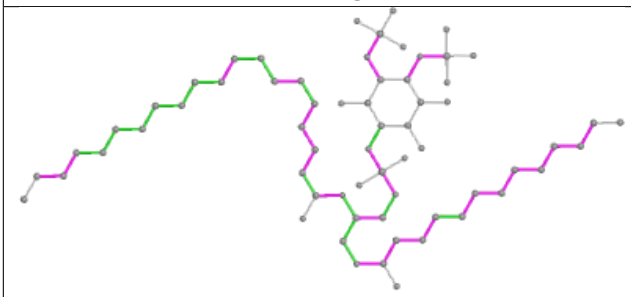
Ligand PT5 A 2602



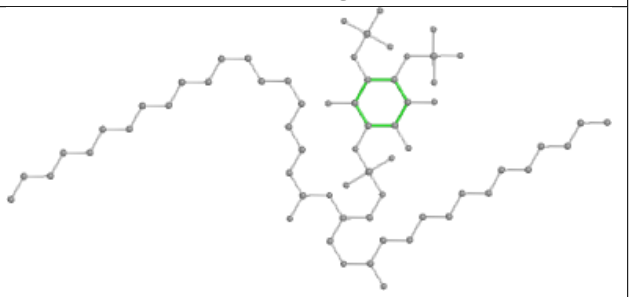
Bond lengths



Bond angles

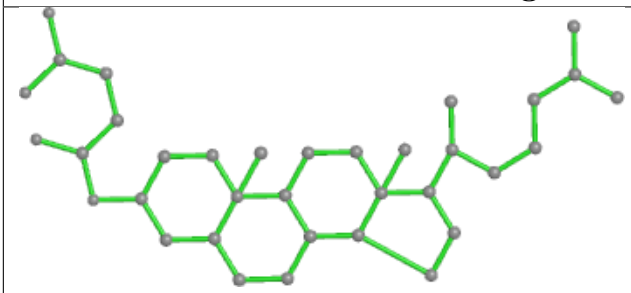


Torsions

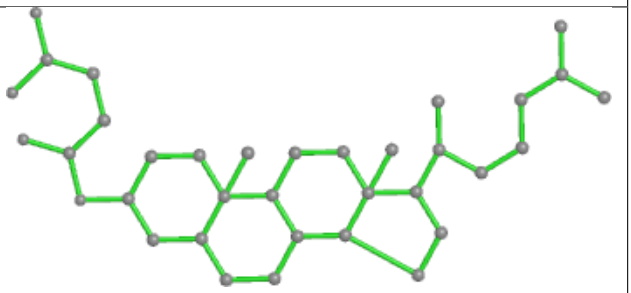


Rings

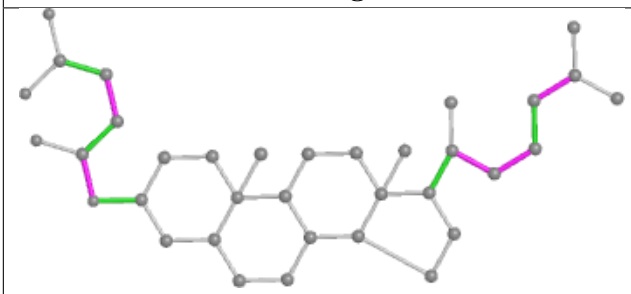
Ligand Y01 A 2605



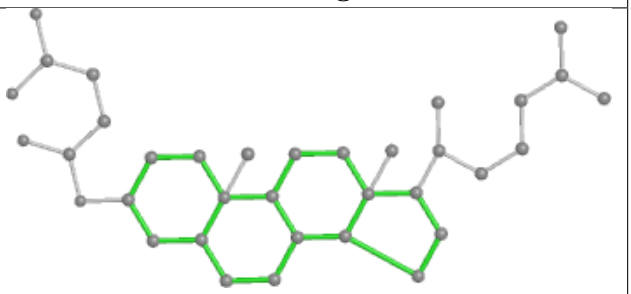
Bond lengths



Bond angles

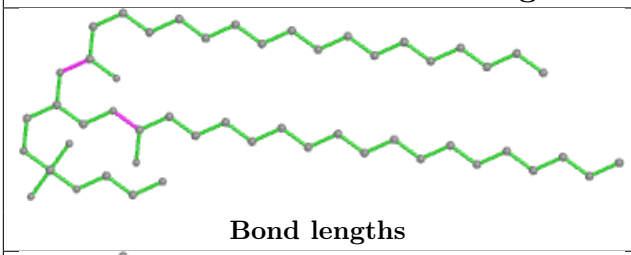


Torsions

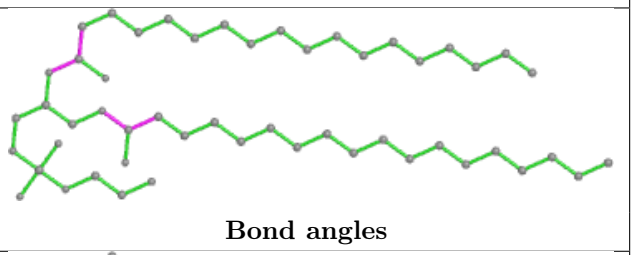


Rings

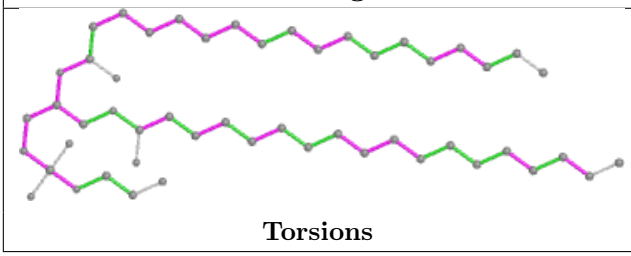
Ligand 3PE A 2613



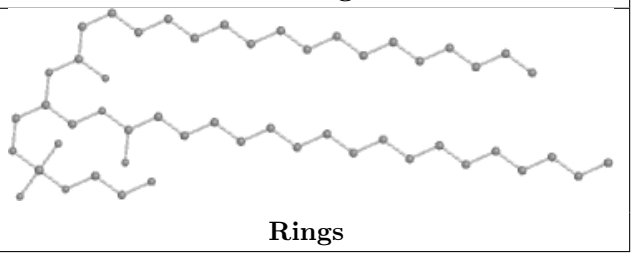
Bond lengths



Bond angles

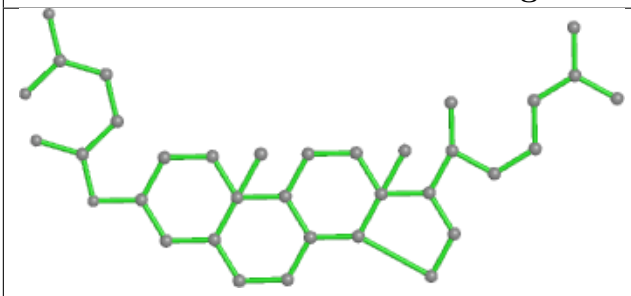


Torsions

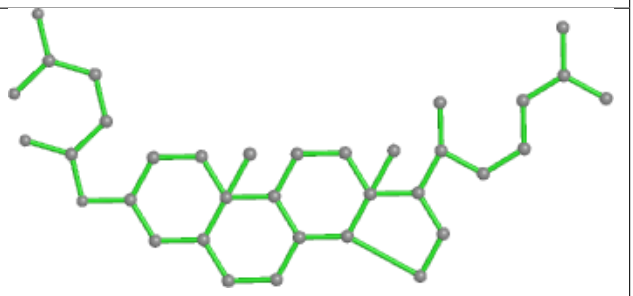


Rings

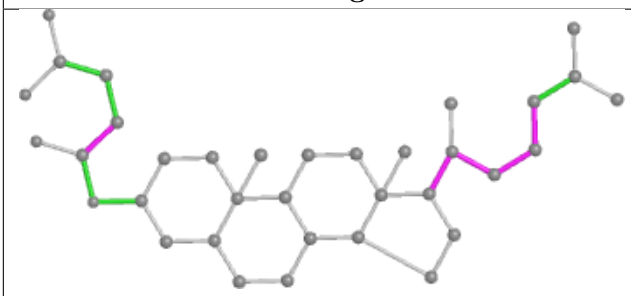
Ligand Y01 A 2608



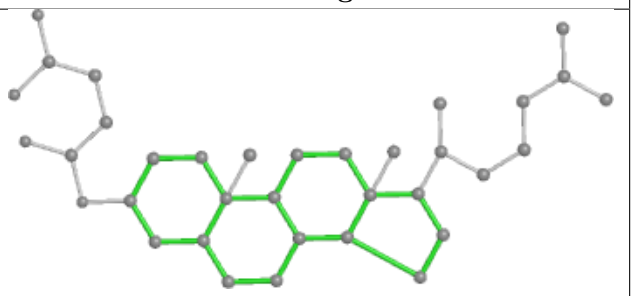
Bond lengths



Bond angles

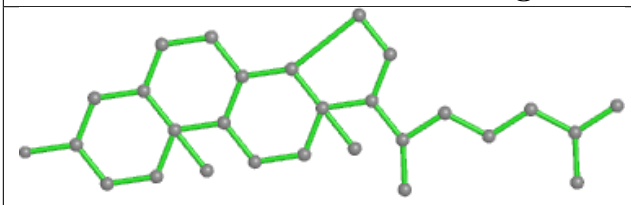


Torsions

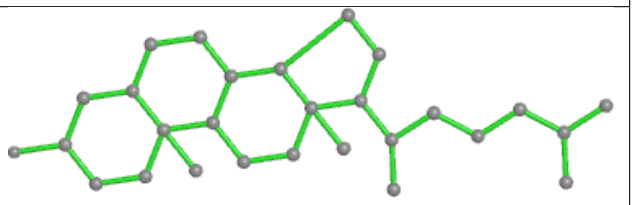


Rings

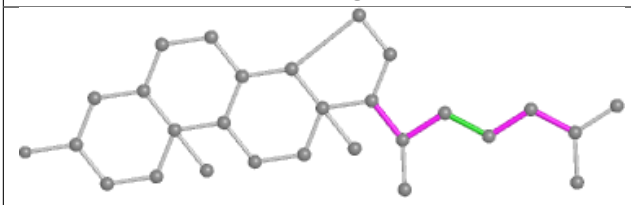
Ligand CLR A 2610



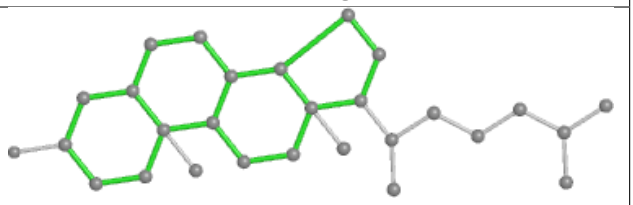
Bond lengths



Bond angles

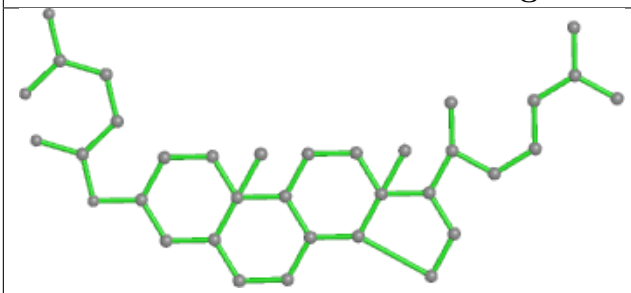


Torsions

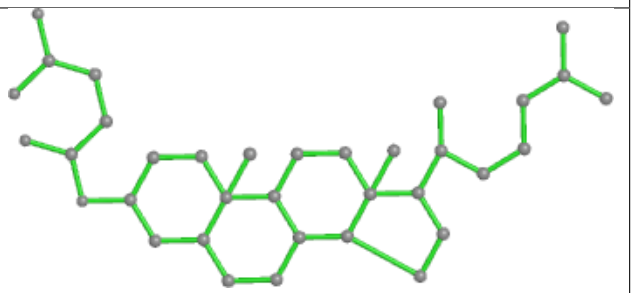


Rings

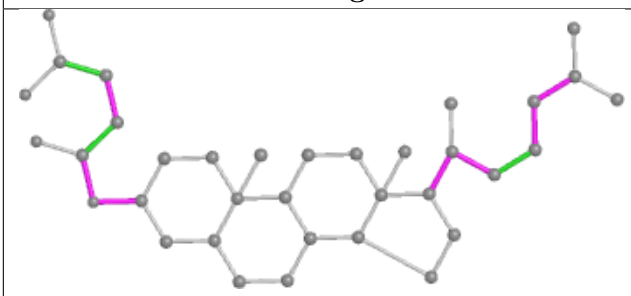
Ligand Y01 A 2609



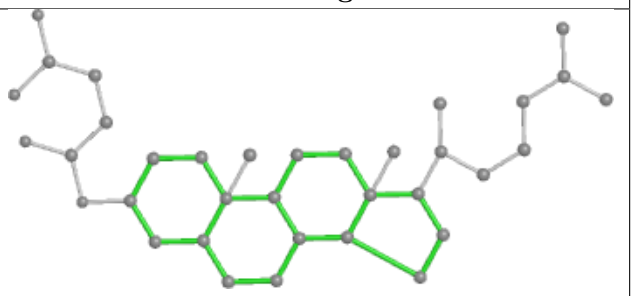
Bond lengths



Bond angles

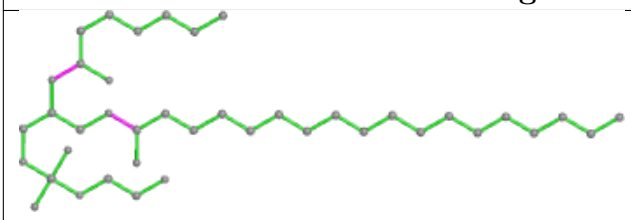


Torsions

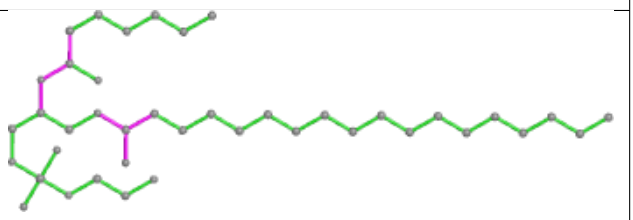


Rings

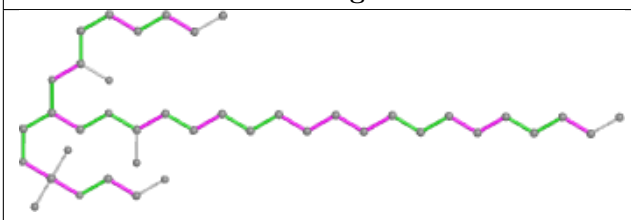
Ligand 3PE A 2612



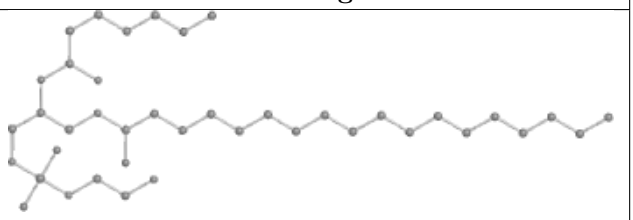
Bond lengths



Bond angles



Torsions



Rings

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.

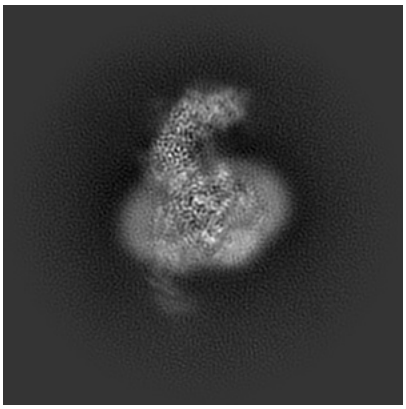
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38159. These allow visual inspection of the internal detail of the map and identification of artifacts.

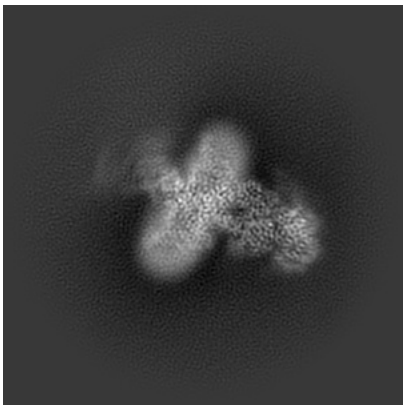
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

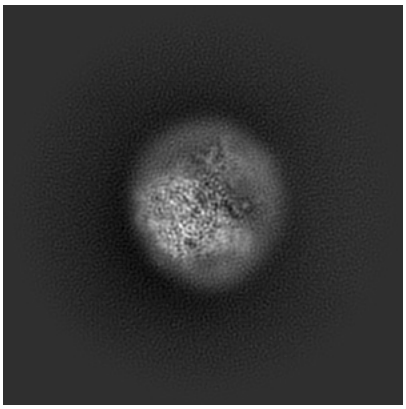
6.1.1 Primary map



X

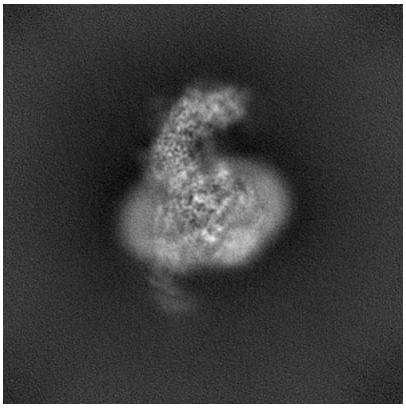


Y

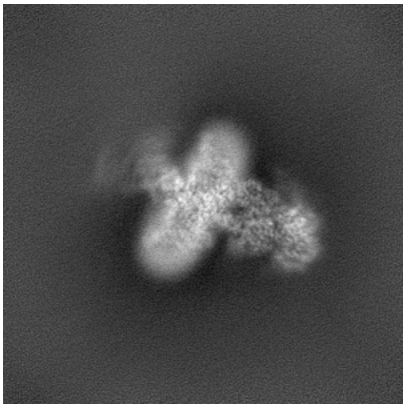


Z

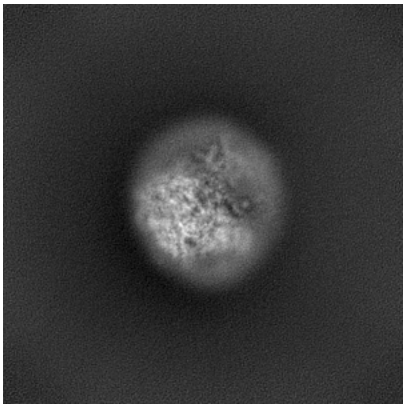
6.1.2 Raw map



X



Y

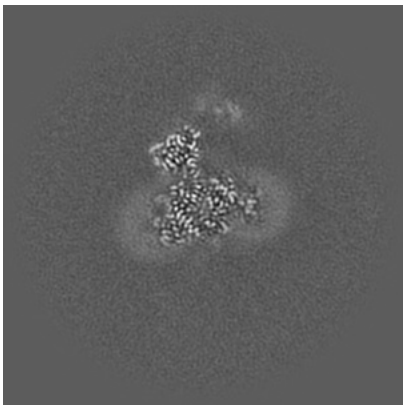


Z

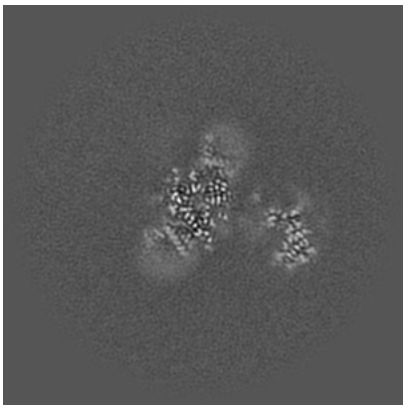
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

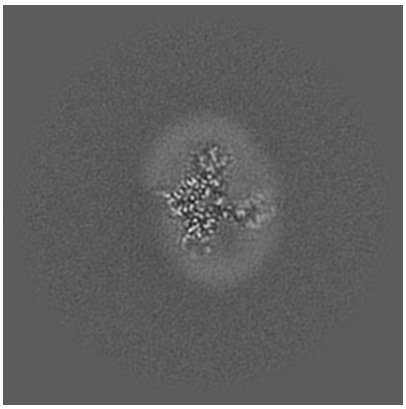
6.2.1 Primary map



X Index: 160

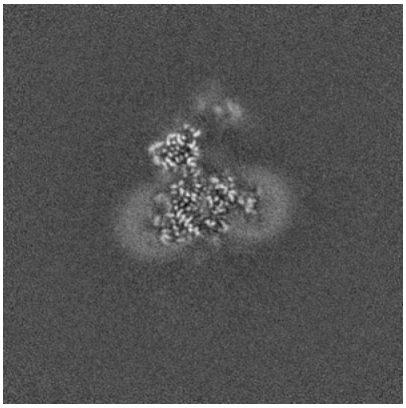


Y Index: 160



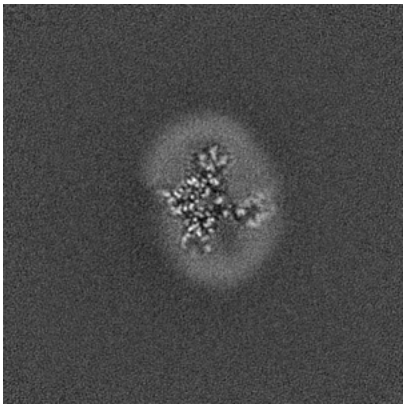
Z Index: 160

6.2.2 Raw map



X Index: 160

Y Index: 160

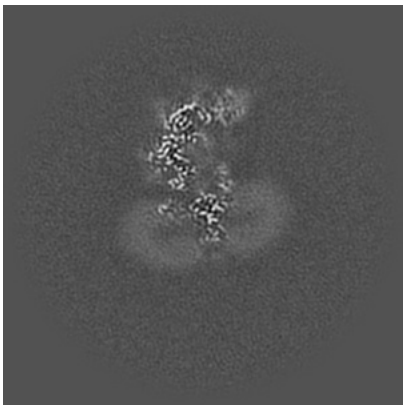


Z Index: 160

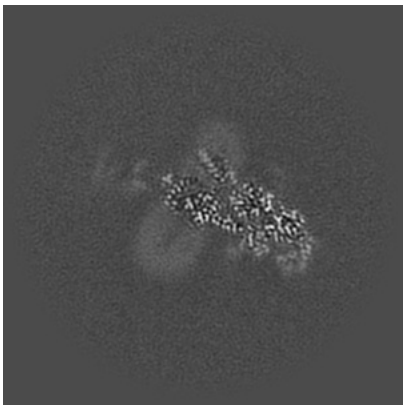
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

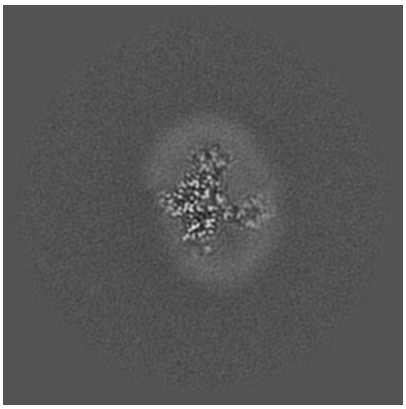
6.3.1 Primary map



X Index: 143

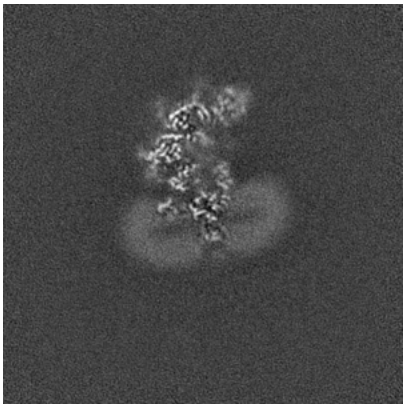


Y Index: 144

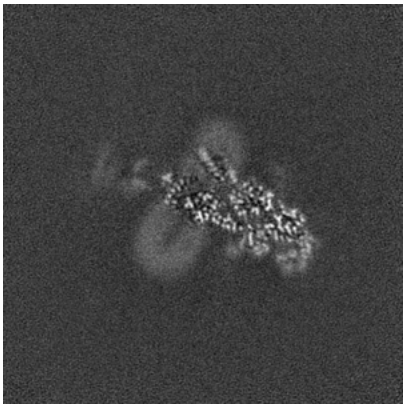


Z Index: 161

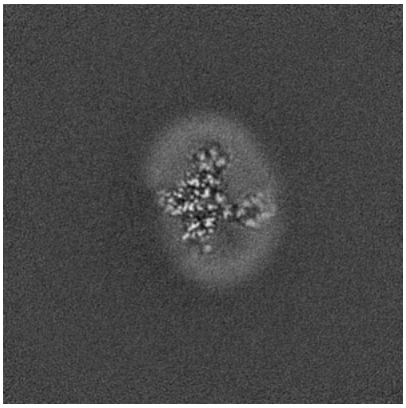
6.3.2 Raw map



X Index: 144



Y Index: 144

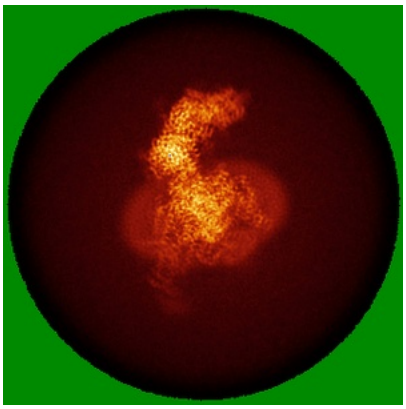


Z Index: 161

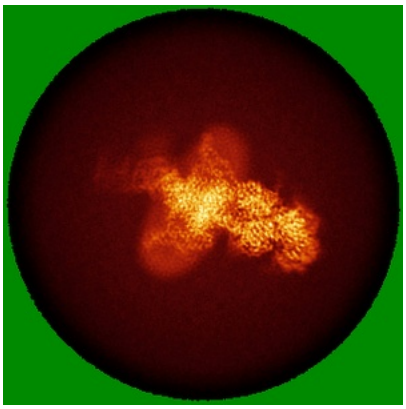
The images above show the largest variance slices of the map in three orthogonal directions.

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

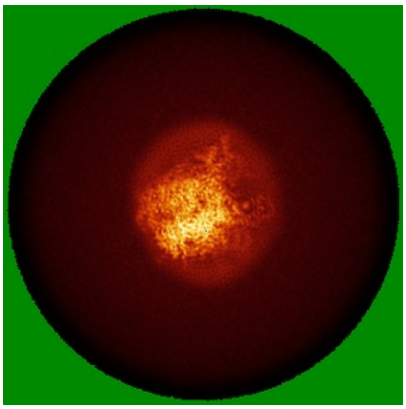
6.4.1 Primary map



X

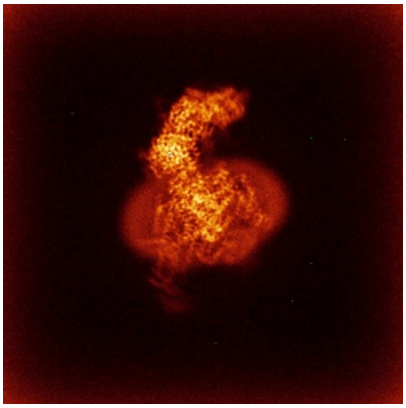


Y

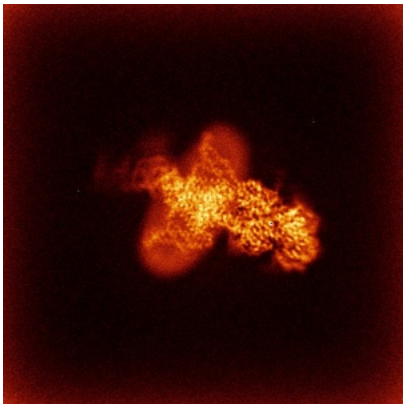


Z

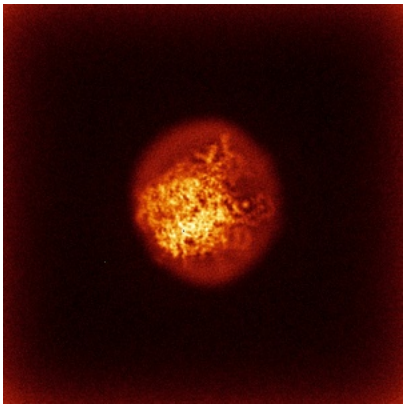
6.4.2 Raw map



X



Y



Z

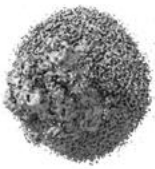
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y



Z

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

X

Y

Z

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

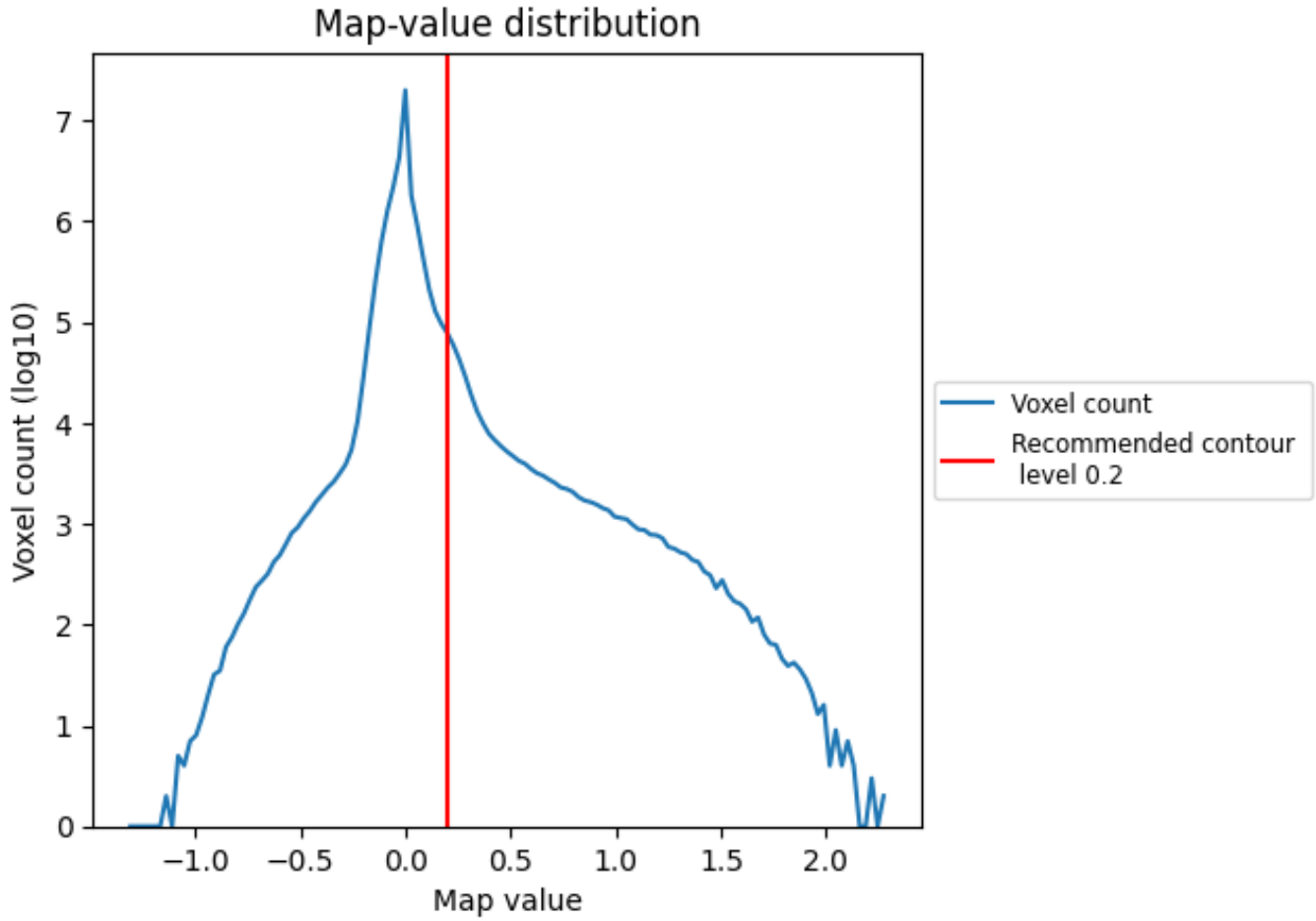
6.6 Mask visualisation (i)

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

7 Map analysis

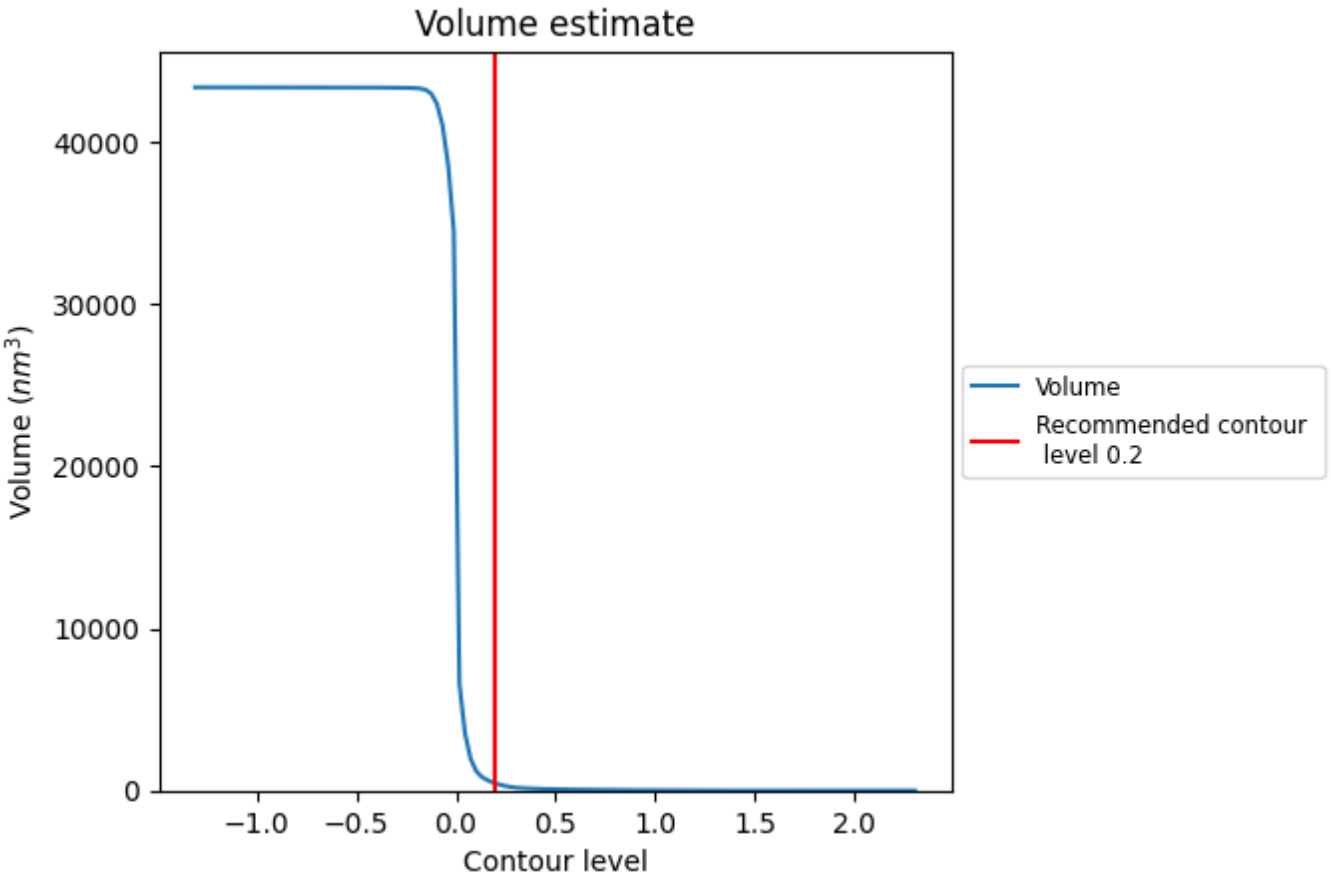
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

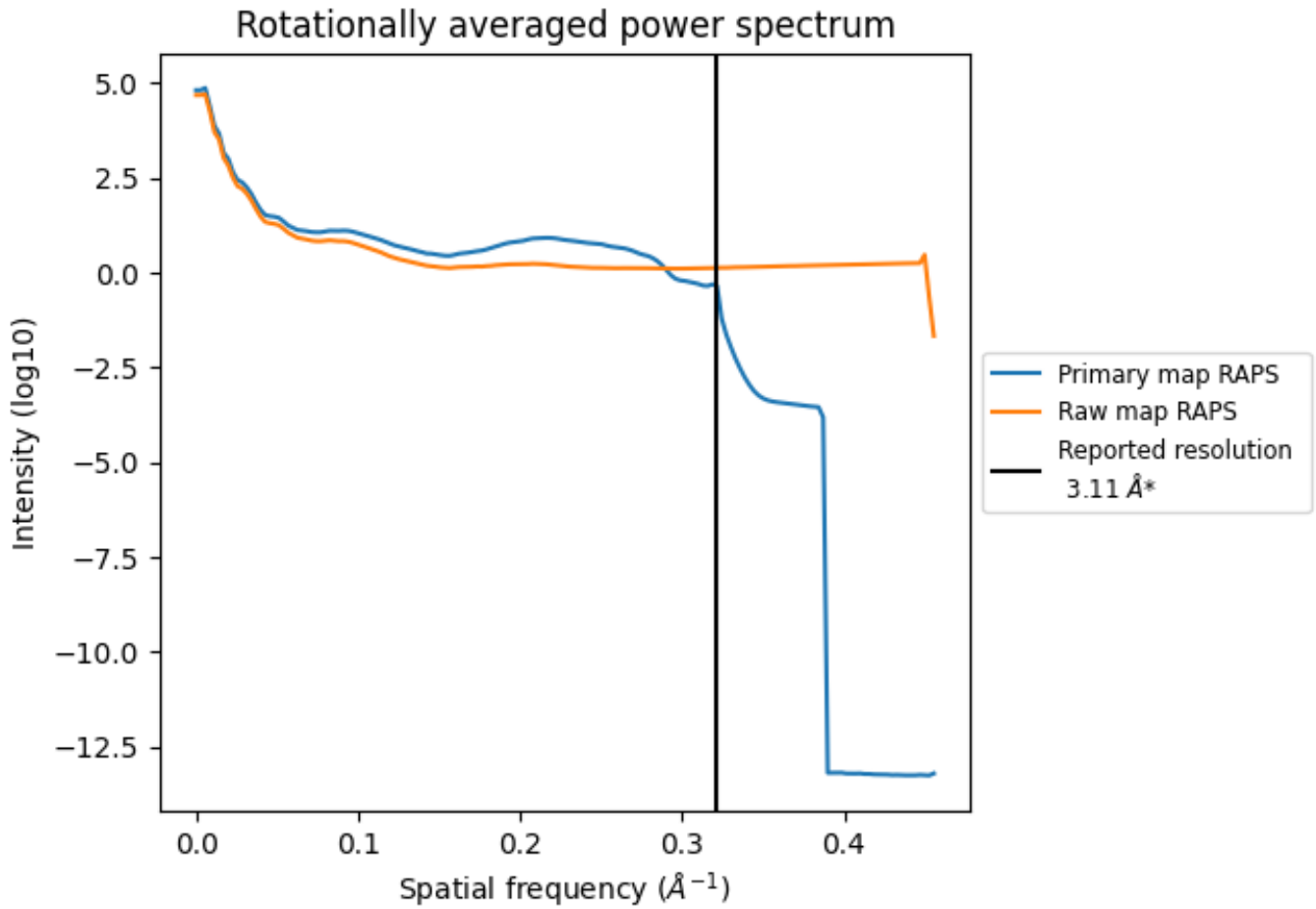
7.2 Volume estimate



The volume at the recommended contour level is 440 nm^3; this corresponds to an approximate mass of 398 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

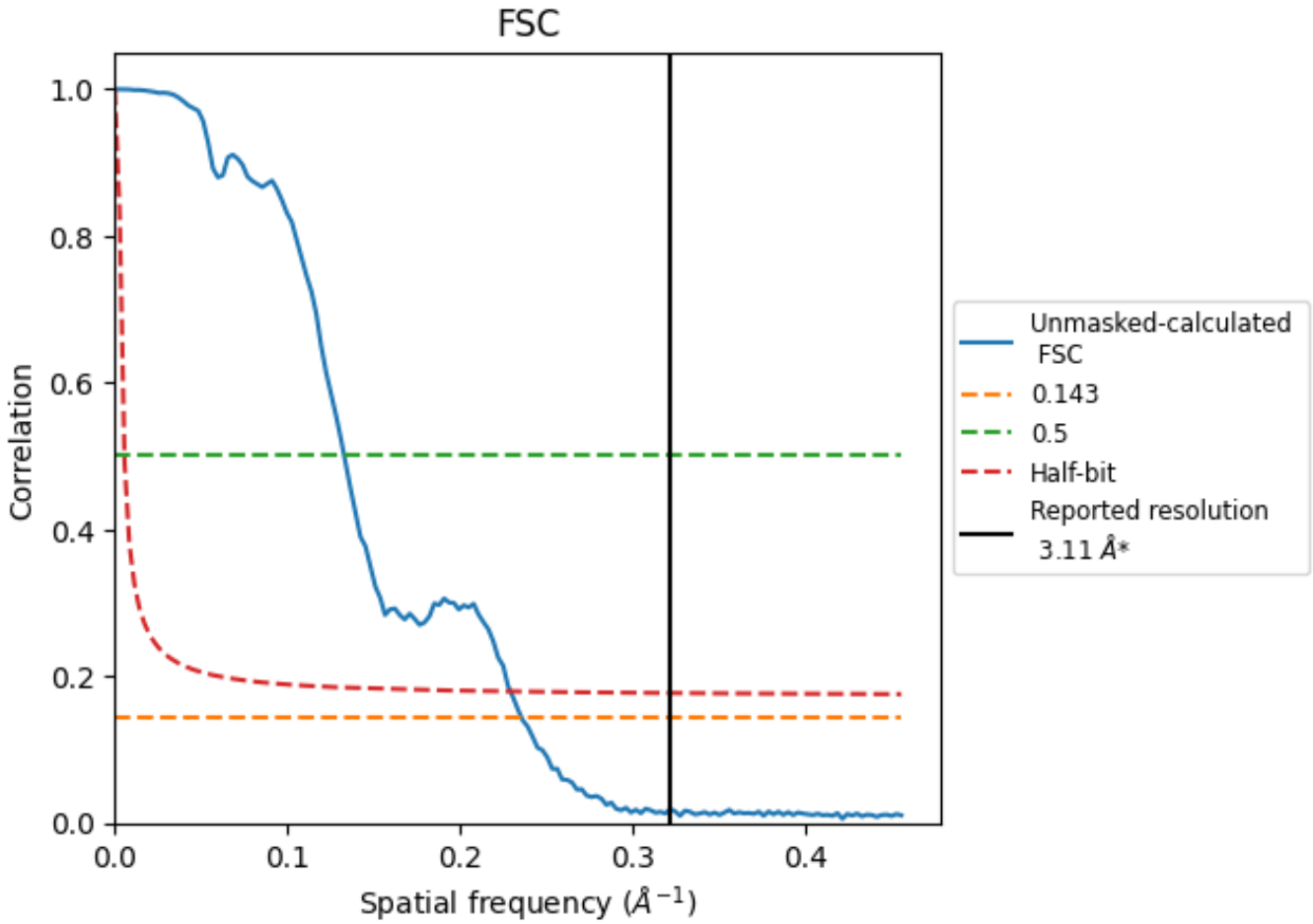


*Reported resolution corresponds to spatial frequency of 0.322 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.322 Å^{-1}

8.2 Resolution estimates (i)

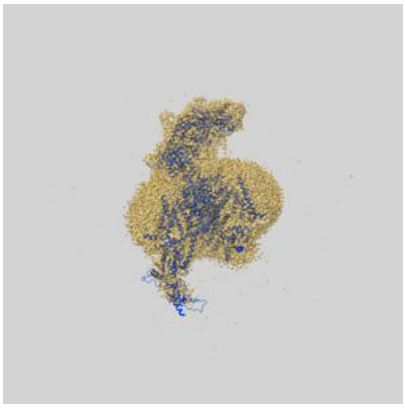
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.53	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.11 by more than 10 %

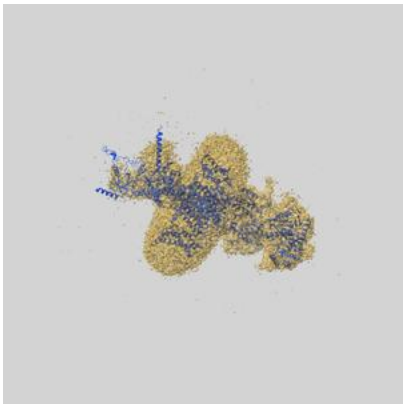
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38159 and PDB model 8X91. Per-residue inclusion information can be found in section 3 on page 11.

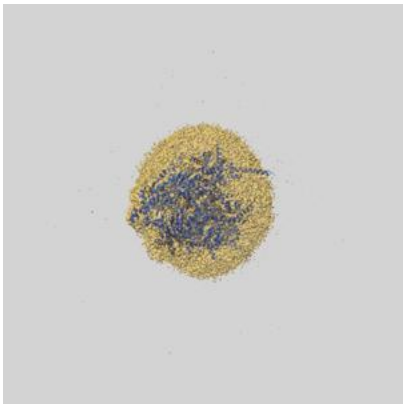
9.1 Map-model overlay



X



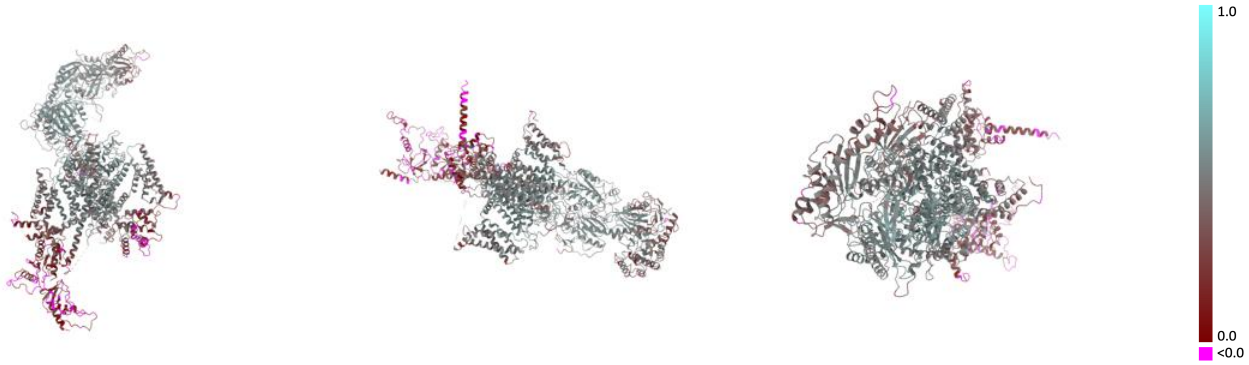
Y



Z

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

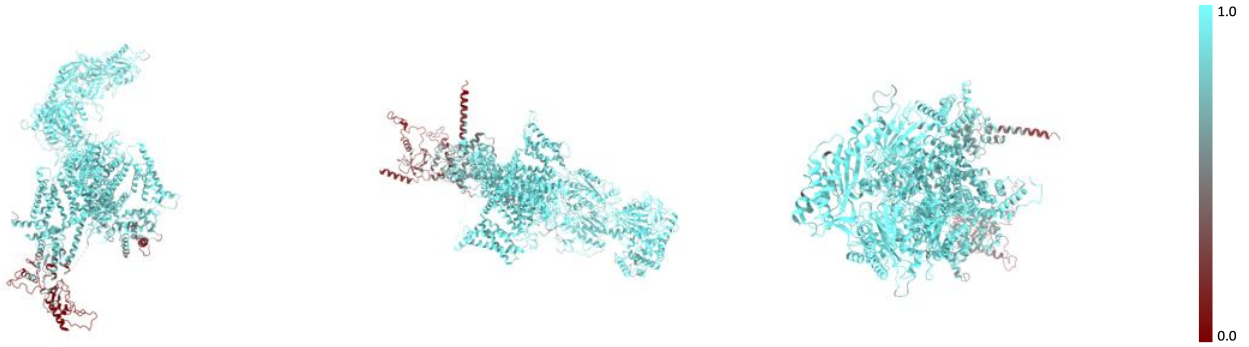
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

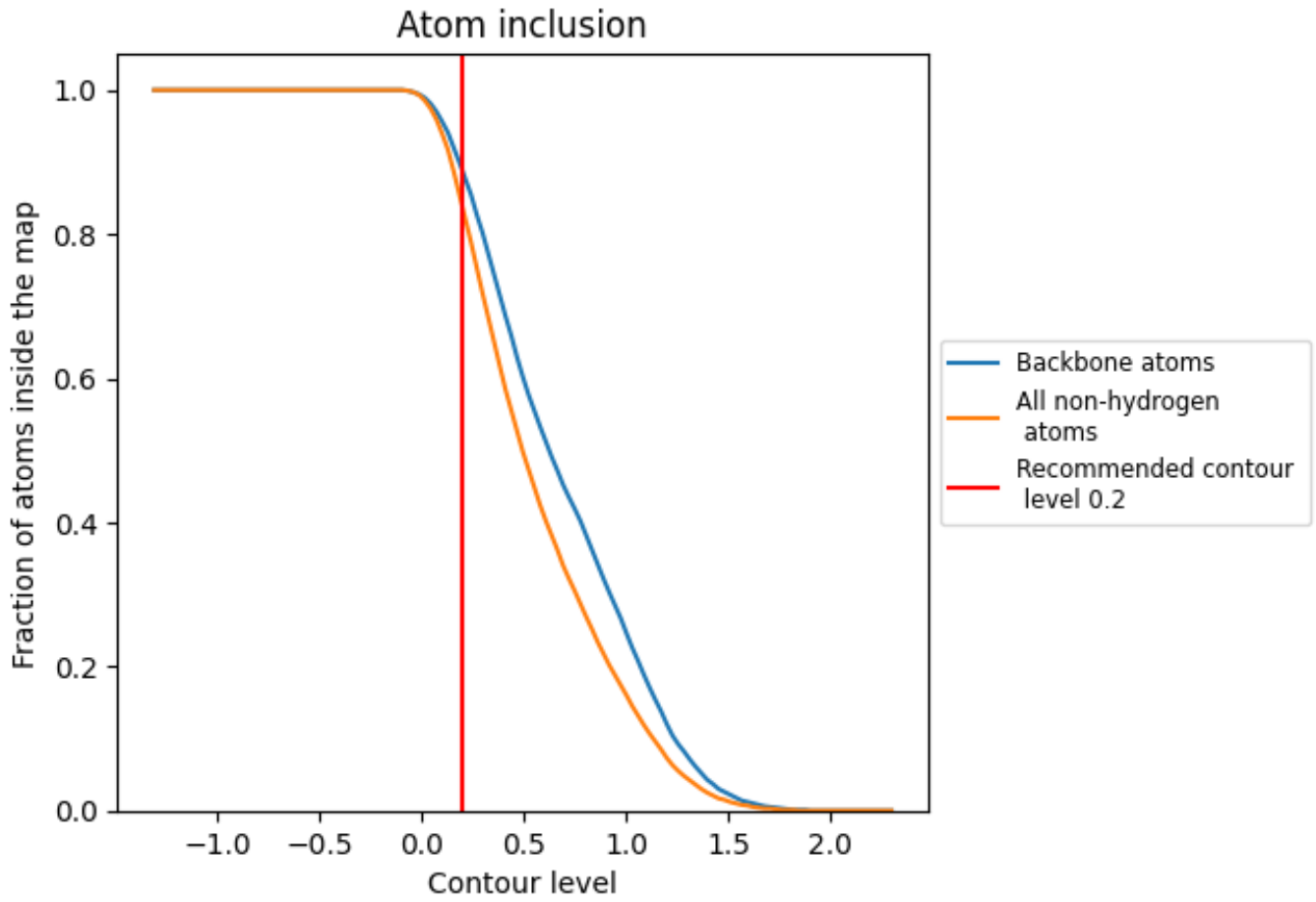
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% 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	0.8390	0.4170
A	0.8720	0.4380
B	0.9440	0.4760
C	0.3630	0.1420
E	0.8810	0.2900
F	0.8210	0.3010
G	0.9460	0.4330
H	0.8210	0.3210
I	0.7860	0.3170
X	0.9720	0.5450