



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:11 AM UTC

PDB ID : 7OCA / pdb_00007oca
EMDB ID : EMD-12802
Title : Resting state full-length GluA1/A2 heterotrimer in complex with TARP
gamma 8 and CNIH2
Authors : Zhang, D.; Watson, J.F.; Matthews, P.M.; Cais, O.; Greger, I.H.
Deposited on : 2021-04-26
Resolution : 3.40 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:

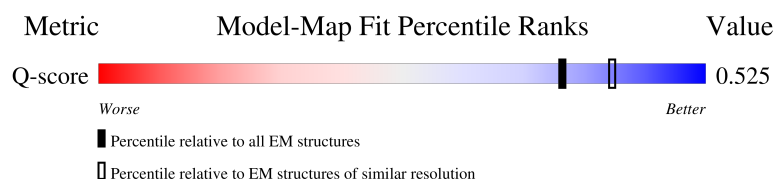
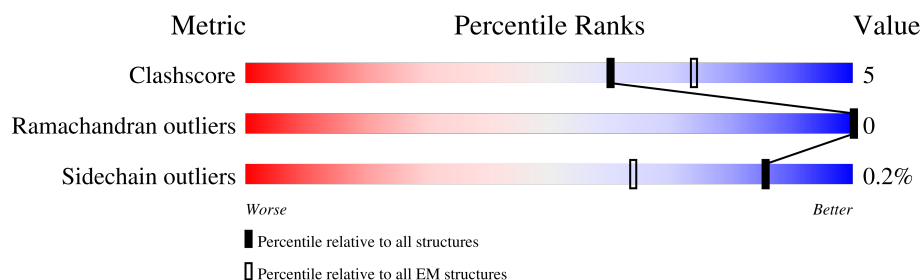
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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	915	 5% 75% 10% 15%
1	C	915	 5% 76% 9% 15%
2	B	860	 1% 81% 10% 9%
2	D	860	 1% 81% 10% 9%

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Mol	Chain	Length	Quality of chain
3	E	188	
3	G	188	
4	I	423	
4	J	423	
5	F	3	
5	M	3	
6	H	2	
6	K	2	
6	L	2	
6	N	2	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 29294 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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	775	Total	C	N	O	S	0	0
			5637	3660	939	1012	26		
1	C	775	Total	C	N	O	S	0	0
			5637	3660	939	1012	26		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	783	Total	C	N	O	S	0	0
			5815	3759	969	1060	27		
2	D	783	Total	C	N	O	S	0	0
			5815	3759	969	1060	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491

- Molecule 3 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	158	Total	C	N	O	S	0	0
			1248	841	193	201	13		
3	E	158	Total	C	N	O	S	0	0
			1248	841	193	201	13		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	161	GLU	-	expression tag	UNP Q5BJU5
G	162	ASN	-	expression tag	UNP Q5BJU5
G	163	LEU	-	expression tag	UNP Q5BJU5
G	164	TYR	-	expression tag	UNP Q5BJU5
G	165	PHE	-	expression tag	UNP Q5BJU5
G	166	GLN	-	expression tag	UNP Q5BJU5
G	167	SER	-	expression tag	UNP Q5BJU5
G	168	GLY	-	expression tag	UNP Q5BJU5
G	169	GLY	-	expression tag	UNP Q5BJU5
G	170	SER	-	expression tag	UNP Q5BJU5
G	171	THR	-	expression tag	UNP Q5BJU5
G	172	GLU	-	expression tag	UNP Q5BJU5
G	173	THR	-	expression tag	UNP Q5BJU5
G	174	SER	-	expression tag	UNP Q5BJU5
G	175	GLN	-	expression tag	UNP Q5BJU5
G	176	VAL	-	expression tag	UNP Q5BJU5
G	177	ALA	-	expression tag	UNP Q5BJU5
G	178	PRO	-	expression tag	UNP Q5BJU5
G	179	ALA	-	expression tag	UNP Q5BJU5
G	180	TYR	-	expression tag	UNP Q5BJU5
G	181	PRO	-	expression tag	UNP Q5BJU5
G	182	TYR	-	expression tag	UNP Q5BJU5
G	183	ASP	-	expression tag	UNP Q5BJU5
G	184	VAL	-	expression tag	UNP Q5BJU5
G	185	PRO	-	expression tag	UNP Q5BJU5
G	186	ASP	-	expression tag	UNP Q5BJU5
G	187	TYR	-	expression tag	UNP Q5BJU5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	188	ALA	-	expression tag	UNP Q5BJU5
E	161	GLU	-	expression tag	UNP Q5BJU5
E	162	ASN	-	expression tag	UNP Q5BJU5
E	163	LEU	-	expression tag	UNP Q5BJU5
E	164	TYR	-	expression tag	UNP Q5BJU5
E	165	PHE	-	expression tag	UNP Q5BJU5
E	166	GLN	-	expression tag	UNP Q5BJU5
E	167	SER	-	expression tag	UNP Q5BJU5
E	168	GLY	-	expression tag	UNP Q5BJU5
E	169	GLY	-	expression tag	UNP Q5BJU5
E	170	SER	-	expression tag	UNP Q5BJU5
E	171	THR	-	expression tag	UNP Q5BJU5
E	172	GLU	-	expression tag	UNP Q5BJU5
E	173	THR	-	expression tag	UNP Q5BJU5
E	174	SER	-	expression tag	UNP Q5BJU5
E	175	GLN	-	expression tag	UNP Q5BJU5
E	176	VAL	-	expression tag	UNP Q5BJU5
E	177	ALA	-	expression tag	UNP Q5BJU5
E	178	PRO	-	expression tag	UNP Q5BJU5
E	179	ALA	-	expression tag	UNP Q5BJU5
E	180	TYR	-	expression tag	UNP Q5BJU5
E	181	PRO	-	expression tag	UNP Q5BJU5
E	182	TYR	-	expression tag	UNP Q5BJU5
E	183	ASP	-	expression tag	UNP Q5BJU5
E	184	VAL	-	expression tag	UNP Q5BJU5
E	185	PRO	-	expression tag	UNP Q5BJU5
E	186	ASP	-	expression tag	UNP Q5BJU5
E	187	TYR	-	expression tag	UNP Q5BJU5
E	188	ALA	-	expression tag	UNP Q5BJU5

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	185	Total	C	N	O	S	0	0
			1284	843	212	222	7		
4	J	185	Total	C	N	O	S	0	0
			1284	843	212	222	7		

There are 14 discrepancies between the modelled and reference sequences:

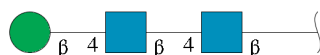
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		

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



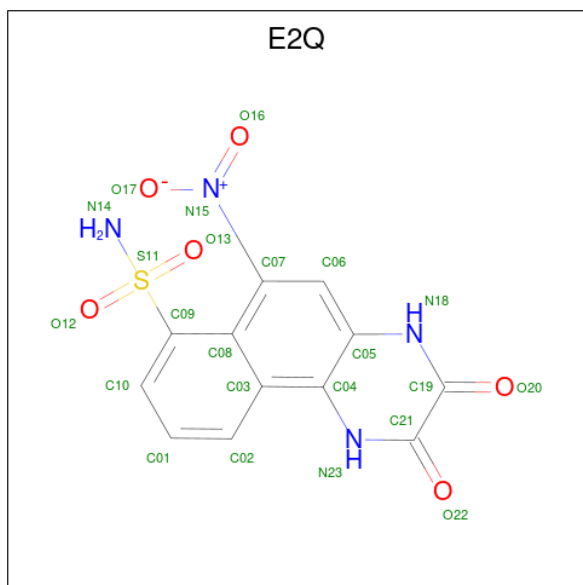
Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	L	2	Total	C	N	O	0	0
			28	16	2	10		

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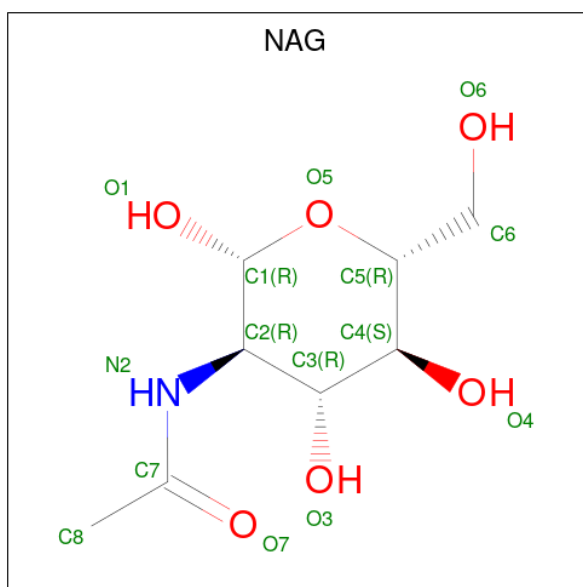
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 6-nitro-2,3-bis(oxidanylidene)-1,4-dihydrobenzo[f]quinoxaline-7-sulfonamide (CCD ID: E2Q) (formula: C₁₂H₈N₄O₆S).



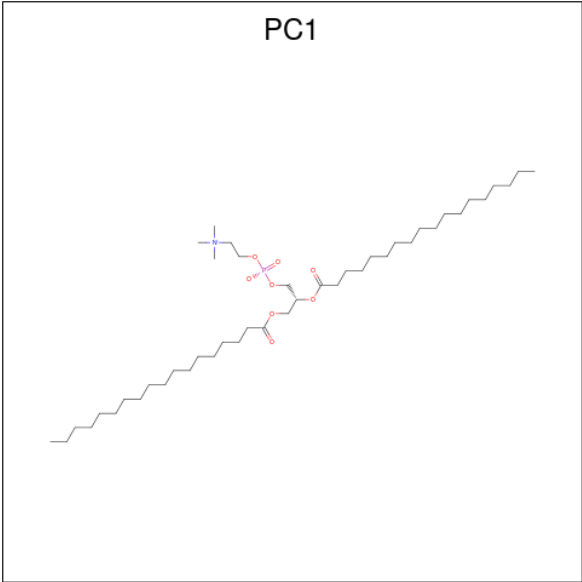
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	S	0
			23	12	4	6	1	
7	B	1	Total	C	N	O	S	0
			23	12	4	6	1	
7	D	1	Total	C	N	O	S	0
			23	12	4	6	1	
7	C	1	Total	C	N	O	S	0
			23	12	4	6	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			20	18	2	
9	A	1	Total	C	O	0
			18	16	2	
9	A	1	Total	C	O	0
			20	18	2	
9	A	1	Total	C	O	0
			18	16	2	
9	A	1	Total	C	O	0
			25	21	4	
9	A	1	Total	C	O	0
			18	16	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			16	14	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			18	16	2	
9	B	1	Total	C	O	0
			25	21	4	

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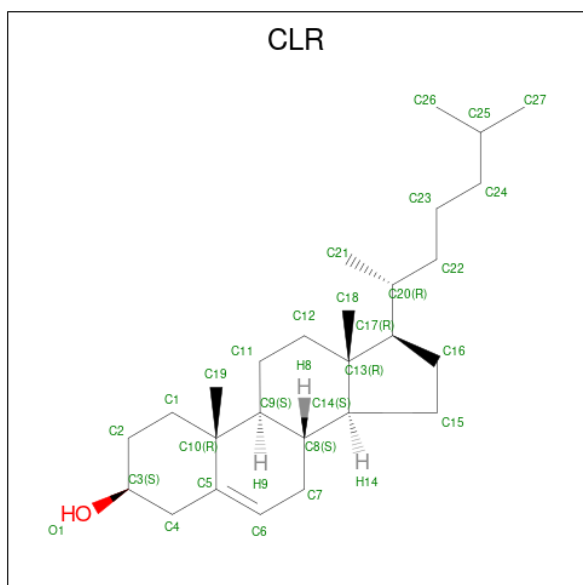
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			20	18	2	
9	G	1	Total	C	O	0
			20	18	2	
9	G	1	Total	C	O	0
			18	16	2	
9	G	1	Total	C	O	0
			20	18	2	
9	I	1	Total	C	O	0
			18	16	2	
9	I	1	Total	C	O	0
			20	18	2	
9	I	1	Total	C	O	0
			20	18	2	
9	I	1	Total	C	O	0
			20	18	2	
9	I	1	Total	C	O	0
			18	16	2	
9	D	1	Total	C	O	0
			16	14	2	
9	D	1	Total	C	O	0
			20	18	2	
9	D	1	Total	C	O	0
			20	18	2	
9	D	1	Total	C	O	0
			20	18	2	
9	D	1	Total	C	O	0
			20	18	2	
9	D	1	Total	C	O	0
			18	16	2	
9	D	1	Total	C	O	0
			25	21	4	
9	D	1	Total	C	O	0
			20	18	2	
9	D	1	Total	C	O	0
			20	18	2	
9	J	1	Total	C	O	0
			20	18	2	
9	J	1	Total	C	O	0
			20	18	2	
9	J	1	Total	C	O	0
			20	18	2	

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Mol	Chain	Residues	Atoms			AltConf
9	J	1	Total	C	O	0
			18	16	2	
9	J	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			20	18	2	
9	C	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			20	18	2	
9	C	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			25	21	4	
9	E	1	Total	C	O	0
			18	16	2	
9	E	1	Total	C	O	0
			20	18	2	
9	E	1	Total	C	O	0
			20	18	2	

- Molecule 10 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

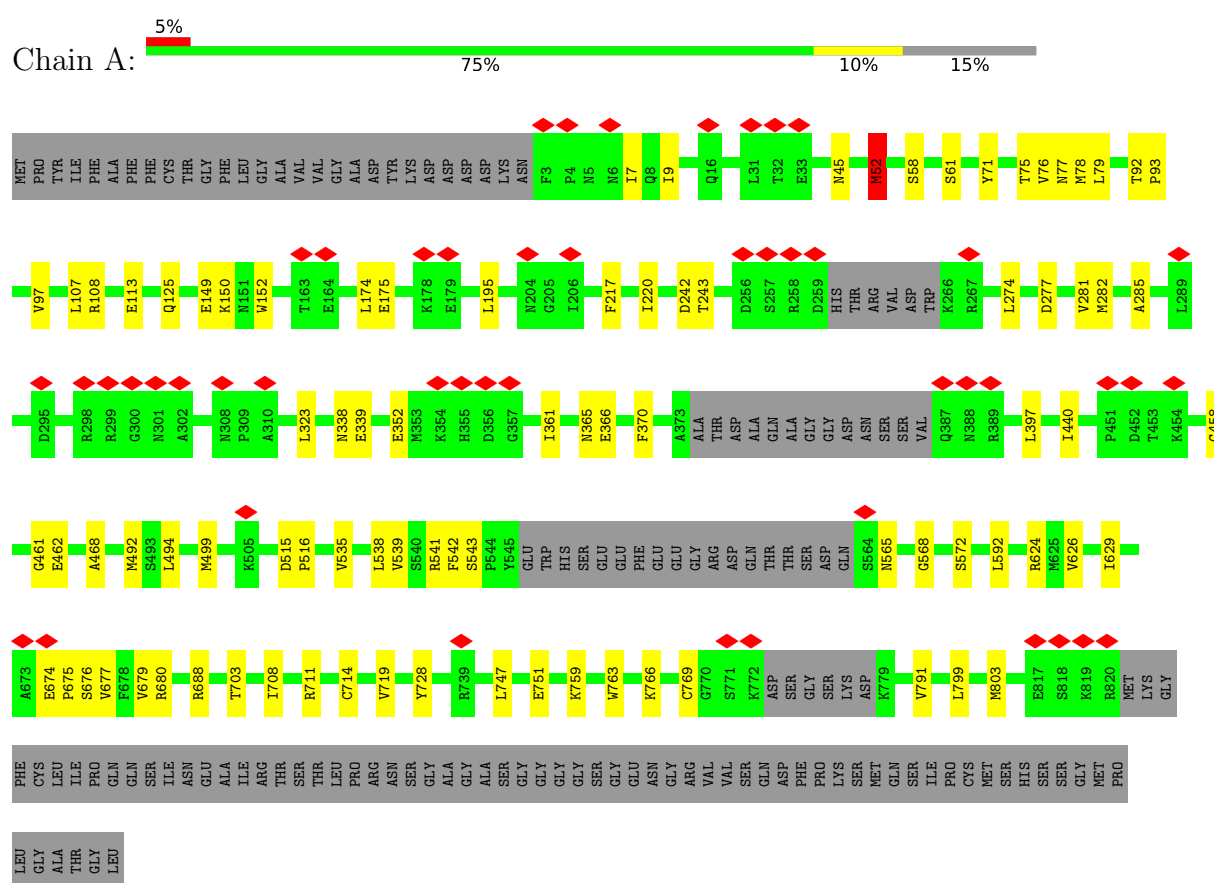


Mol	Chain	Residues	Atoms			AltConf
10	G	1	Total	C	O	0
			28	27	1	
10	E	1	Total	C	O	0
			28	27	1	

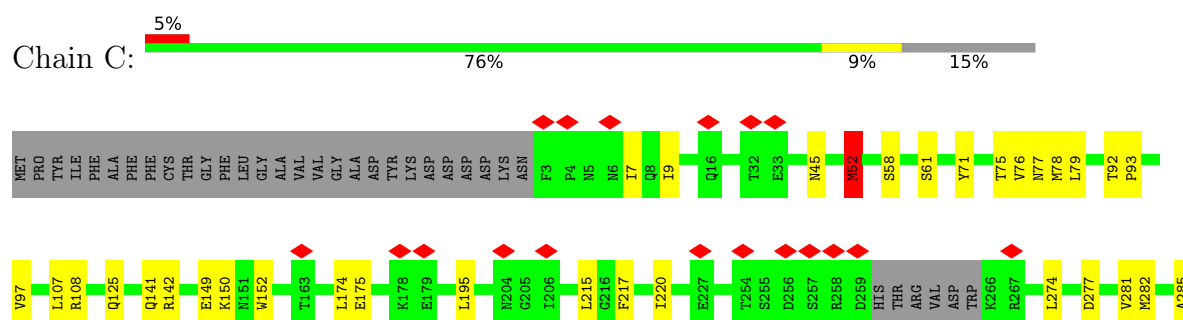
3 Residue-property plots

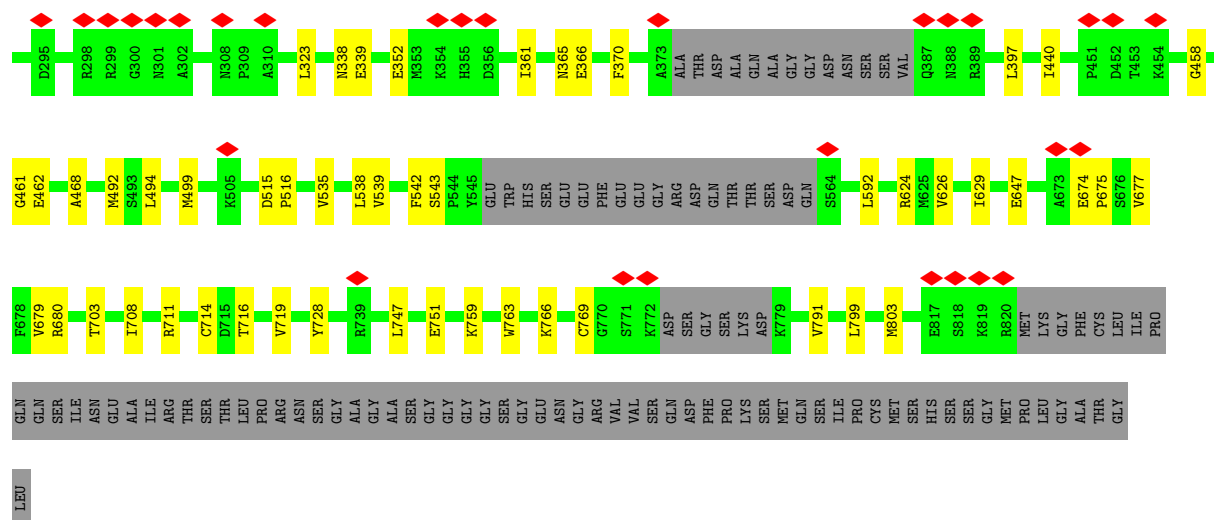
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor 1



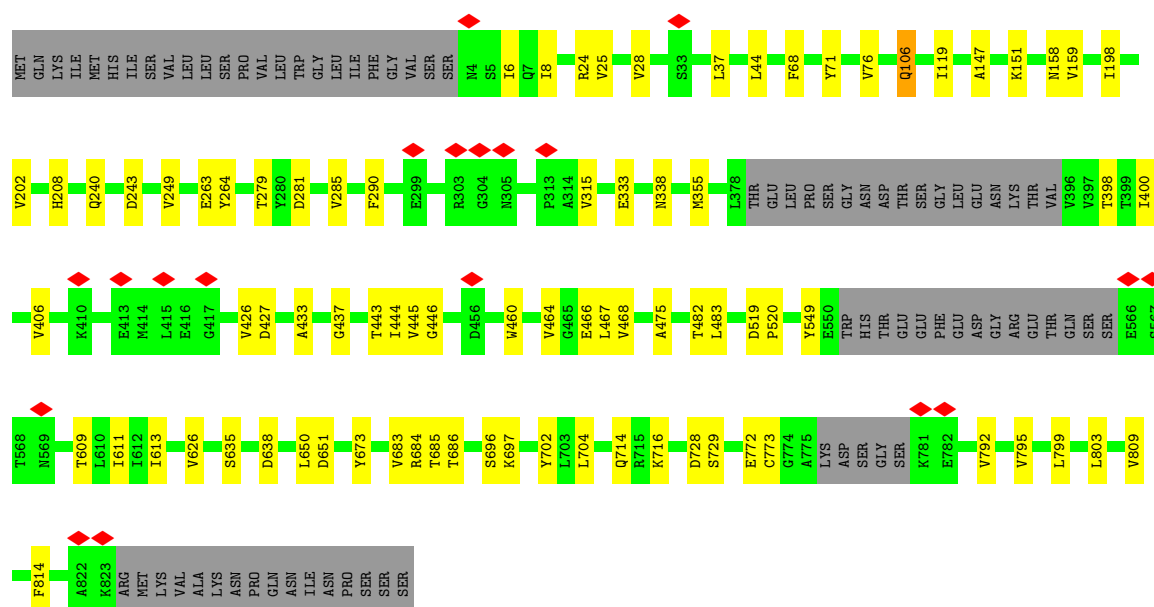
• Molecule 1: Glutamate receptor 1





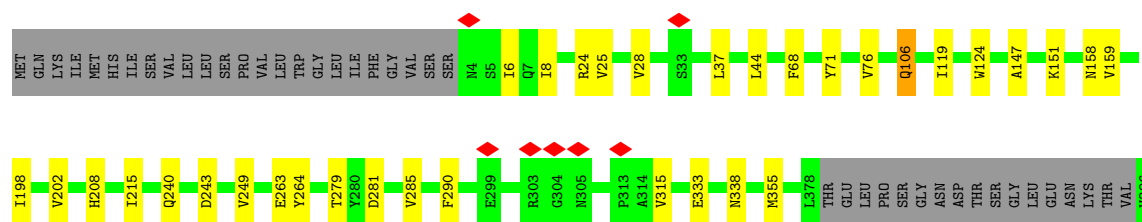
• Molecule 2: Glutamate receptor 2

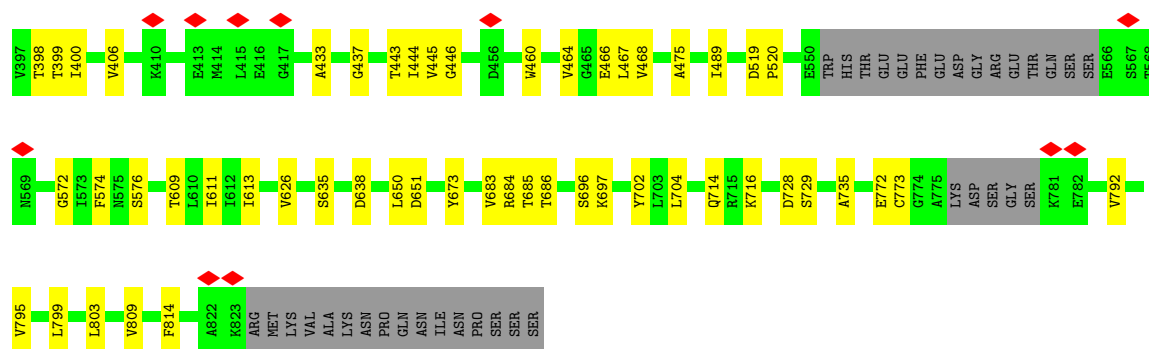
Chain B: 81% 10% 9%



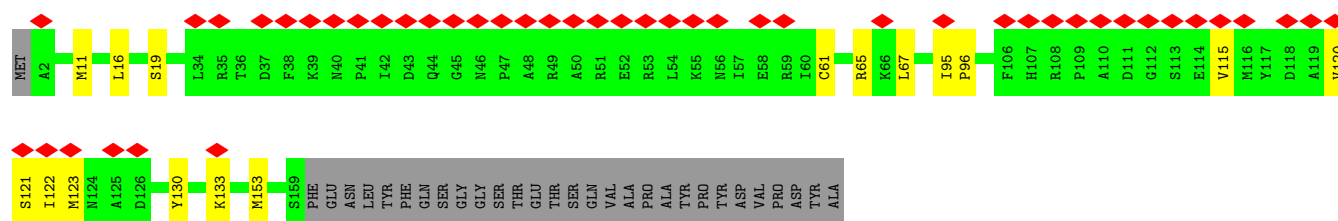
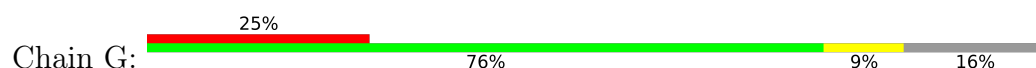
• Molecule 2: Glutamate receptor 2

Chain D: 81% 10% 9%

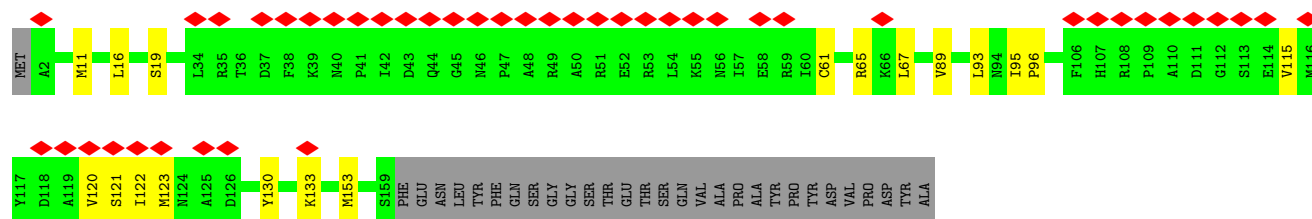
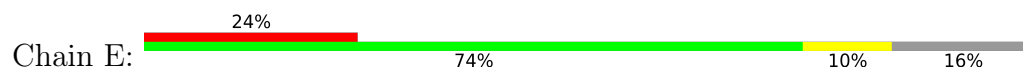




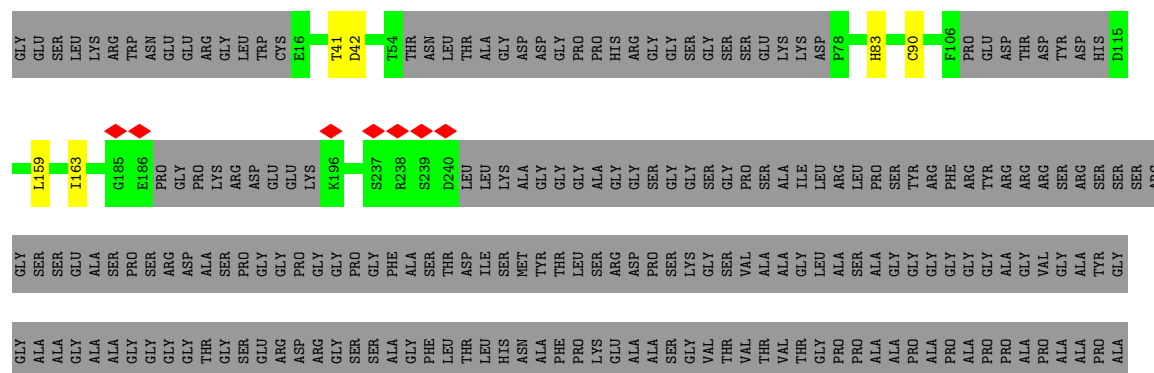
• Molecule 3: Protein cornichon homolog 2



• Molecule 3: Protein cornichon homolog 2



• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit



PRO GLY THR SER LYS GLU ALA ALA SER ASN THR ASN THR LEU ASN ARG LYS LEU VAL PHE GLN

- Molecule 4: Voltage-dependent calcium channel gamma-8 subunit

Chain J:



GLY GLU SER LEU LYS ARG TRP ASN GLU GLU ALA SER ASN THR TRP CYS E16 T41 D42 T47 R48 T54 THR ASN LEU THR ALA GLY ASP ASP GLY PRO PRO HIS ARG GLY GLY SER SER SER GLU LYS LYS ASP P78 H83 C90 F106 PRO GLU ASP THR TYR

ASP HIS D115 L159 L163 G185 E186 PRO PRO LYS ARG ASP GLU LYS K196 N224 S237 R238 S239 D240 LEU LEU LYS ASP THR ILE SER MET TYR THR LEU SER ARG GLY GLY SER GLY GLY PRO SER VAL VAL ALA ALA GLY LEU ARG LEU PRO PRO ALA ALA GLY TYR ARG PHE ARG ARG ARG ARG ARG

ARG SER SER SER ARG GLY SER SER ALA ALA SER PRO ARG ASP THR SER PRO GLY PRO GLY PHE ALA PHE SER ASP THR ILE SER MET TYR THR LEU SER ARG GLY GLY SER GLY GLY PRO SER VAL VAL ALA ALA GLY LEU ARG LEU PRO PRO ALA ALA GLY TYR ARG PHE ARG ARG ARG ARG

VAL GLY ALA TYR PRO GLY ALA ALA GLY LEU SER LYS GLU ALA ALA GLY THR GLY SER THR ASN ASN THR LEU ASN ARG LYS LEU GLU VAL PHE GLN

PRO ALA ALA PRO PRO GLY THR SER LYS GLU ALA ALA ALA SER ASN THR ASN THR LEU ASN ARG LYS LEU GLU VAL PHE GLN

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



NAG1 NAG2 BM43

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



NAG1 NAG2 BM43

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



NAG1 NAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain N:  50%
100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218320	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: PC1, E2Q, CLR, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/5766	0.37	1/7872 (0.0%)
1	C	0.29	0/5766	0.37	1/7872 (0.0%)
2	B	0.37	0/5945	0.36	0/8088
2	D	0.37	0/5945	0.36	0/8088
3	E	0.15	0/1289	0.29	0/1760
3	G	0.15	0/1289	0.29	0/1760
4	I	0.25	0/1305	0.32	0/1782
4	J	0.25	0/1305	0.32	0/1782
All	All	0.31	0/28610	0.35	2/39004 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	MET	CB-CG-SD	10.13	143.10	112.70
1	A	52	MET	CB-CG-SD	10.12	143.05	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5637	0	5182	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5637	0	5182	61	0
2	B	5815	0	5490	52	0
2	D	5815	0	5490	54	0
3	E	1248	0	1186	13	0
3	G	1248	0	1186	12	0
4	I	1284	0	1219	3	0
4	J	1284	0	1219	5	0
5	F	39	0	34	1	0
5	M	39	0	34	1	0
6	H	28	0	25	0	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
6	N	28	0	25	0	0
7	A	23	0	0	0	0
7	B	23	0	0	1	0
7	C	23	0	0	0	0
7	D	23	0	0	1	0
8	A	28	0	26	0	0
8	B	14	0	13	1	0
8	C	28	0	26	0	0
8	D	14	0	13	1	0
9	A	119	0	194	0	0
9	B	179	0	302	1	0
9	C	119	0	194	0	0
9	D	179	0	302	1	0
9	E	58	0	98	0	0
9	G	58	0	98	0	0
9	I	96	0	161	0	0
9	J	96	0	161	1	0
10	E	28	0	46	3	0
10	G	28	0	46	3	0
All	All	29294	0	28002	259	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 5.

All (259) 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)
2:B:716:LYS:N	2:B:772:GLU:OE2	2.10	0.84
2:D:716:LYS:N	2:D:772:GLU:OE2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:NH2	2:B:626:VAL:O	2.12	0.83
2:B:728:ASP:OD2	2:B:729:SER:N	2.14	0.81
2:D:626:VAL:O	1:C:624:ARG:NH2	2.13	0.81
2:D:728:ASP:OD2	2:D:729:SER:N	2.14	0.80
1:A:71:TYR:HE1	1:A:92:THR:HG21	1.53	0.73
1:C:71:TYR:HE1	1:C:92:THR:HG21	1.53	0.73
1:A:9:ILE:HG21	1:A:282:MET:HE1	1.75	0.68
1:C:9:ILE:HG21	1:C:282:MET:HE1	1.76	0.68
2:B:635:SER:OG	2:B:638:ASP:OD1	2.12	0.66
1:A:107:LEU:O	1:A:274:LEU:HD22	1.95	0.66
1:C:107:LEU:O	1:C:274:LEU:HD22	1.95	0.66
2:D:635:SER:OG	2:D:638:ASP:OD1	2.12	0.66
2:D:398:THR:OG1	2:D:466:GLU:OE2	2.08	0.63
2:D:333:GLU:OE2	2:D:338:ASN:ND2	2.32	0.63
2:B:333:GLU:OE2	2:B:338:ASN:ND2	2.32	0.62
1:C:711:ARG:NH2	1:C:766:LYS:O	2.34	0.61
1:A:711:ARG:NH2	1:A:766:LYS:O	2.34	0.60
3:E:16:LEU:O	3:E:19:SER:OG	2.19	0.60
1:C:9:ILE:HG21	1:C:282:MET:CE	2.31	0.60
1:A:9:ILE:HG21	1:A:282:MET:CE	2.31	0.60
10:G:3103:CLR:H192	10:G:3103:CLR:O1	2.02	0.60
1:C:458:GLY:O	1:C:461:GLY:N	2.34	0.60
3:G:16:LEU:O	3:G:19:SER:OG	2.19	0.59
1:A:458:GLY:O	1:A:461:GLY:N	2.34	0.59
2:B:24:ARG:NH2	2:B:263:GLU:O	2.35	0.59
10:E:3103:CLR:H192	10:E:3103:CLR:O1	2.02	0.59
2:D:24:ARG:NH2	2:D:263:GLU:O	2.35	0.58
1:A:52:MET:HE2	1:A:75:THR:HG21	1.87	0.57
2:B:814:PHE:HB2	1:C:542:PHE:HE2	1.70	0.57
1:C:52:MET:CE	1:C:75:THR:HG21	2.35	0.56
2:B:71:TYR:CD2	2:B:76:VAL:HG22	2.40	0.56
1:C:150:LYS:HE3	1:C:152:TRP:CH2	2.41	0.56
2:D:71:TYR:CD2	2:D:76:VAL:HG22	2.40	0.56
1:C:58:SER:O	1:C:61:SER:OG	2.14	0.56
1:A:52:MET:CE	1:A:75:THR:HG21	2.35	0.55
1:A:150:LYS:HE3	1:A:152:TRP:CZ3	2.41	0.55
1:C:150:LYS:HE3	1:C:152:TRP:CZ3	2.41	0.55
1:A:542:PHE:HE2	2:D:814:PHE:HB2	1.71	0.55
1:A:150:LYS:HE3	1:A:152:TRP:CH2	2.41	0.55
1:C:45:ASN:ND2	5:M:1:NAG:O6	2.39	0.55
3:E:65:ARG:HE	3:E:115:VAL:HB	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:ND2	5:F:1:NAG:O6	2.39	0.55
2:B:398:THR:OG1	2:B:466:GLU:OE2	2.15	0.55
1:C:52:MET:HE2	1:C:75:THR:HG21	1.87	0.55
3:G:65:ARG:HE	3:G:115:VAL:HB	1.72	0.54
2:B:8:ILE:HG13	2:B:37:LEU:HD22	1.90	0.54
2:D:8:ILE:HG13	2:D:37:LEU:HD22	1.90	0.54
1:C:462:GLU:O	1:C:468:ALA:N	2.42	0.53
1:A:462:GLU:O	1:A:468:ALA:N	2.42	0.53
1:A:58:SER:O	1:A:61:SER:OG	2.14	0.53
2:D:433:ALA:O	2:D:437:GLY:N	2.34	0.52
1:A:626:VAL:HG13	1:A:626:VAL:O	2.09	0.52
1:C:626:VAL:HG13	1:C:626:VAL:O	2.09	0.52
2:B:433:ALA:O	2:B:437:GLY:N	2.34	0.51
1:A:365:ASN:OD1	1:A:366:GLU:N	2.43	0.51
1:A:679:VAL:HG12	1:A:680:ARG:N	2.27	0.50
1:C:499:MET:HE1	1:C:708:ILE:HG21	1.93	0.50
1:C:365:ASN:OD1	1:C:366:GLU:N	2.43	0.50
1:C:747:LEU:O	1:C:751:GLU:HG2	2.12	0.49
1:A:499:MET:HE1	1:A:708:ILE:HG21	1.93	0.49
4:I:83:HIS:CE1	4:I:90:CYS:HB2	2.47	0.49
1:C:679:VAL:HG12	1:C:680:ARG:N	2.27	0.49
3:G:61:CYS:SG	3:G:65:ARG:NH2	2.86	0.49
1:A:338:ASN:OD1	1:A:339:GLU:N	2.43	0.49
2:D:467:LEU:HD11	2:D:475:ALA:HB2	1.95	0.49
1:C:338:ASN:OD1	1:C:339:GLU:N	2.43	0.49
3:E:133:LYS:CB	10:E:3103:CLR:H71	2.43	0.49
2:B:467:LEU:HD11	2:B:475:ALA:HB2	1.95	0.49
1:C:674:GLU:CB	1:C:677:VAL:HG13	2.43	0.49
1:A:747:LEU:O	1:A:751:GLU:HG2	2.12	0.49
3:G:133:LYS:CB	10:G:3103:CLR:H71	2.42	0.49
1:A:674:GLU:CB	1:A:677:VAL:HG13	2.43	0.48
4:J:83:HIS:CE1	4:J:90:CYS:HB2	2.47	0.48
3:E:61:CYS:SG	3:E:65:ARG:NH2	2.86	0.48
2:D:572:GLY:O	2:D:576:SER:OG	2.24	0.48
1:A:78:MET:HE3	1:A:79:LEU:N	2.29	0.48
1:A:93:PRO:O	1:A:108:ARG:NE	2.46	0.48
2:D:208:HIS:CG	2:D:208:HIS:O	2.66	0.48
1:A:71:TYR:CE2	1:A:76:VAL:HG23	2.49	0.48
1:A:462:GLU:OE1	1:A:462:GLU:N	2.47	0.48
2:B:208:HIS:CG	2:B:208:HIS:O	2.66	0.47
1:C:71:TYR:CE2	1:C:76:VAL:HG23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:OE2	1:A:175:GLU:HA	2.14	0.47
1:A:535:VAL:O	1:A:539:VAL:HG22	2.15	0.47
2:D:443:THR:O	2:D:444:ILE:HD13	2.14	0.47
1:C:78:MET:HE3	1:C:79:LEU:N	2.29	0.47
1:C:175:GLU:OE2	1:C:175:GLU:HA	2.14	0.47
4:J:224:ASN:ND2	9:J:2502:PC1:O22	2.48	0.47
1:A:71:TYR:CE1	1:A:92:THR:HG21	2.43	0.47
2:B:467:LEU:HD11	2:B:475:ALA:CB	2.45	0.47
2:B:809:VAL:HG11	1:C:592:LEU:HD23	1.97	0.47
1:C:535:VAL:O	1:C:539:VAL:HG22	2.15	0.47
2:D:400:ILE:O	2:D:406:VAL:HB	2.15	0.46
2:B:400:ILE:O	2:B:406:VAL:HB	2.15	0.46
2:D:467:LEU:HD11	2:D:475:ALA:CB	2.45	0.46
1:C:195:LEU:HD12	1:C:220:ILE:HD11	1.97	0.46
2:B:443:THR:O	2:B:444:ILE:HD13	2.14	0.46
2:B:683:VAL:HG12	2:B:685:THR:H	1.81	0.46
1:C:629:ILE:O	1:C:719:VAL:HG21	2.16	0.46
1:A:515:ASP:N	1:A:516:PRO:CD	2.79	0.46
1:A:370:PHE:CG	1:A:370:PHE:O	2.69	0.46
1:C:370:PHE:O	1:C:370:PHE:CG	2.69	0.46
1:C:462:GLU:OE1	1:C:462:GLU:N	2.47	0.46
1:A:629:ILE:O	1:A:719:VAL:HG21	2.16	0.46
2:B:460:TRP:CE3	2:B:464:VAL:HG11	2.51	0.46
2:B:519:ASP:N	2:B:520:PRO:CD	2.79	0.46
2:D:315:VAL:HG23	2:D:315:VAL:O	2.16	0.46
2:B:714:GLN:NE2	2:B:773:CYS:O	2.50	0.45
3:G:122:ILE:HG22	3:G:123:MET:N	2.30	0.45
2:D:460:TRP:CE3	2:D:464:VAL:HG11	2.51	0.45
3:E:122:ILE:HG22	3:E:123:MET:N	2.30	0.45
1:C:149:GLU:HA	1:C:149:GLU:OE2	2.17	0.45
1:C:515:ASP:N	1:C:516:PRO:CD	2.79	0.45
2:B:315:VAL:HG23	2:B:315:VAL:O	2.16	0.45
2:D:519:ASP:N	2:D:520:PRO:CD	2.79	0.45
8:D:902:NAG:H83	8:D:902:NAG:C1	2.46	0.45
1:C:125:GLN:O	1:C:152:TRP:HB2	2.17	0.45
8:B:2903:NAG:H83	8:B:2903:NAG:C1	2.46	0.45
3:E:95:ILE:N	3:E:96:PRO:HD2	2.32	0.45
1:A:592:LEU:HD23	2:D:809:VAL:HG11	1.98	0.45
2:D:714:GLN:NE2	2:D:773:CYS:O	2.50	0.45
1:C:492:MET:SD	1:C:703:THR:HG21	2.56	0.45
2:D:683:VAL:HG12	2:D:685:THR:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:MET:SD	1:A:703:THR:HG21	2.57	0.45
1:A:149:GLU:OE2	1:A:149:GLU:HA	2.17	0.45
1:A:195:LEU:HD12	1:A:220:ILE:HD11	1.97	0.45
2:D:792:VAL:O	2:D:795:VAL:HG22	2.17	0.44
1:C:76:VAL:HG13	1:C:77:ASN:N	2.33	0.44
1:C:674:GLU:N	1:C:675:PRO:CA	2.80	0.44
3:G:95:ILE:N	3:G:96:PRO:HD2	2.32	0.44
4:I:41:THR:HG22	4:I:42:ASP:N	2.32	0.44
1:A:76:VAL:HG13	1:A:77:ASN:N	2.33	0.44
2:B:464:VAL:O	2:B:468:VAL:HG23	2.18	0.44
1:A:714:CYS:HB2	1:A:769:CYS:HB2	1.86	0.44
1:C:494:LEU:HD13	1:C:728:TYR:CZ	2.53	0.44
1:A:125:GLN:O	1:A:152:TRP:HB2	2.17	0.44
2:D:464:VAL:O	2:D:468:VAL:HG23	2.18	0.44
3:G:67:LEU:HD23	3:G:67:LEU:O	2.18	0.44
2:D:68:PHE:CZ	2:D:279:THR:HG23	2.53	0.44
3:E:67:LEU:O	3:E:67:LEU:HD23	2.18	0.44
2:B:792:VAL:O	2:B:795:VAL:HG22	2.18	0.44
2:B:68:PHE:CZ	2:B:279:THR:HG23	2.53	0.43
1:C:93:PRO:O	1:C:108:ARG:NH2	2.49	0.43
3:E:123:MET:HE3	3:E:123:MET:HA	2.00	0.43
2:D:696:SER:OG	2:D:697:LYS:N	2.50	0.43
2:D:799:LEU:O	2:D:803:LEU:HG	2.18	0.43
4:J:41:THR:HG22	4:J:42:ASP:N	2.32	0.43
1:A:674:GLU:N	1:A:675:PRO:CA	2.80	0.43
2:B:696:SER:OG	2:B:697:LYS:N	2.50	0.43
1:A:494:LEU:HD13	1:A:728:TYR:CZ	2.53	0.43
3:E:130:TYR:CE2	10:E:3103:CLR:H152	2.53	0.43
1:A:93:PRO:O	1:A:108:ARG:NH2	2.50	0.43
3:G:123:MET:HE3	3:G:123:MET:HA	2.00	0.43
2:D:6:ILE:HG21	2:D:290:PHE:CE1	2.53	0.43
2:D:243:ASP:O	2:D:249:VAL:HG21	2.19	0.43
2:D:673:TYR:CD1	2:D:673:TYR:C	2.97	0.43
2:B:6:ILE:HG21	2:B:290:PHE:CE1	2.53	0.43
2:B:650:LEU:HD23	2:B:651:ASP:N	2.34	0.43
2:B:702:TYR:CE2	2:B:704:LEU:HB3	2.53	0.43
3:G:130:TYR:CE2	10:G:3103:CLR:H152	2.54	0.43
2:D:650:LEU:HD23	2:D:651:ASP:N	2.34	0.43
2:B:25:VAL:O	2:B:28:VAL:HG22	2.18	0.43
1:C:71:TYR:CE1	1:C:92:THR:HG21	2.43	0.43
1:A:799:LEU:O	1:A:803:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:120:VAL:HG23	3:E:121:SER:N	2.34	0.43
1:A:674:GLU:N	1:A:675:PRO:HA	2.34	0.42
2:B:243:ASP:O	2:B:249:VAL:HG21	2.18	0.42
2:B:673:TYR:CD1	2:B:673:TYR:C	2.97	0.42
2:B:799:LEU:O	2:B:803:LEU:HG	2.19	0.42
4:I:159:LEU:O	4:I:163:ILE:HG12	2.19	0.42
1:C:93:PRO:O	1:C:108:ARG:NE	2.46	0.42
1:C:352:GLU:HB2	1:C:361:ILE:HD11	2.02	0.42
3:G:120:VAL:HG23	3:G:121:SER:N	2.34	0.42
2:D:71:TYR:CE2	2:D:76:VAL:HG22	2.55	0.42
1:C:647:GLU:N	1:C:679:VAL:O	2.43	0.42
1:C:799:LEU:O	1:C:803:MET:HG3	2.19	0.42
2:B:445:VAL:HG13	2:B:446:GLY:N	2.35	0.42
2:D:25:VAL:O	2:D:28:VAL:HG22	2.19	0.42
1:A:542:PHE:CG	1:A:543:SER:N	2.87	0.42
2:D:702:TYR:CE2	2:D:704:LEU:HB3	2.53	0.42
1:C:277:ASP:O	1:C:281:VAL:HG23	2.20	0.42
1:A:217:PHE:O	1:A:220:ILE:HG22	2.19	0.42
2:B:106:GLN:HE21	2:B:106:GLN:N	2.18	0.42
3:E:11:MET:HG3	3:E:153:MET:HG3	2.02	0.42
1:A:7:ILE:O	1:A:7:ILE:HG22	2.20	0.42
2:B:8:ILE:CG1	2:B:37:LEU:HD22	2.49	0.42
2:D:106:GLN:HE21	2:D:106:GLN:N	2.18	0.42
1:C:542:PHE:CG	1:C:543:SER:N	2.87	0.42
1:A:397:LEU:HD21	1:A:440:ILE:CD1	2.50	0.42
2:D:8:ILE:CG1	2:D:37:LEU:HD22	2.49	0.42
2:D:147:ALA:O	2:D:151:LYS:N	2.53	0.42
1:A:538:LEU:O	1:A:542:PHE:HD1	2.03	0.42
2:B:119:ILE:HG22	2:B:119:ILE:O	2.19	0.42
2:B:147:ALA:O	2:B:151:LYS:N	2.53	0.42
3:G:11:MET:HG3	3:G:153:MET:HG3	2.02	0.42
4:J:159:LEU:O	4:J:163:ILE:HG12	2.20	0.42
1:C:7:ILE:O	1:C:7:ILE:HG22	2.20	0.42
1:C:76:VAL:HG21	1:C:97:VAL:HG11	2.02	0.42
1:C:397:LEU:HD21	1:C:440:ILE:CD1	2.50	0.42
2:B:71:TYR:CE2	2:B:76:VAL:HG22	2.54	0.41
2:D:445:VAL:HG13	2:D:446:GLY:N	2.35	0.41
2:D:609:THR:O	2:D:613:ILE:HG12	2.20	0.41
1:A:352:GLU:HB2	1:A:361:ILE:HD11	2.01	0.41
2:B:158:ASN:OD1	2:B:159:VAL:N	2.53	0.41
2:B:281:ASP:O	2:B:285:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:THR:O	2:B:613:ILE:HG12	2.20	0.41
1:C:538:LEU:O	1:C:542:PHE:HD1	2.02	0.41
1:C:674:GLU:N	1:C:675:PRO:HA	2.35	0.41
1:C:714:CYS:HB2	1:C:769:CYS:HB2	1.86	0.41
2:B:683:VAL:HG12	2:B:684:ARG:N	2.35	0.41
2:D:158:ASN:OD1	2:D:159:VAL:N	2.53	0.41
1:C:141:GLN:O	1:C:142:ARG:C	2.63	0.41
2:D:398:THR:HG22	2:D:399:THR:N	2.36	0.41
1:A:676:SER:O	1:A:688:ARG:NH1	2.47	0.41
2:D:198:ILE:O	2:D:202:VAL:HG23	2.20	0.41
2:D:683:VAL:HG12	2:D:684:ARG:N	2.36	0.41
3:E:89:VAL:O	3:E:93:LEU:HD13	2.21	0.41
1:A:541:ARG:NH1	1:A:565:ASN:O	2.44	0.41
1:A:568:GLY:O	1:A:572:SER:OG	2.19	0.41
2:B:198:ILE:O	2:B:202:VAL:HG23	2.20	0.41
2:D:685:THR:HG22	2:D:686:THR:N	2.36	0.41
1:C:285:ALA:CB	1:C:323:LEU:HD23	2.50	0.41
1:C:499:MET:HE2	1:C:716:THR:HG21	2.03	0.41
1:A:76:VAL:HG21	1:A:97:VAL:HG11	2.02	0.41
1:A:759:LYS:O	1:A:763:TRP:HB2	2.21	0.41
2:B:426:VAL:HG23	2:B:427:ASP:N	2.36	0.41
2:B:685:THR:HG22	2:B:686:THR:N	2.35	0.41
1:A:174:LEU:C	1:A:174:LEU:HD23	2.46	0.41
2:D:119:ILE:O	2:D:119:ILE:HG22	2.19	0.41
1:C:217:PHE:O	1:C:220:ILE:HG22	2.19	0.41
1:C:759:LYS:O	1:C:763:TRP:HB2	2.21	0.41
1:A:285:ALA:CB	1:A:323:LEU:HD23	2.50	0.41
1:C:77:ASN:O	1:C:78:MET:C	2.64	0.41
1:A:113:GLU:HA	1:A:113:GLU:OE1	2.20	0.40
1:A:277:ASP:O	1:A:281:VAL:HG23	2.20	0.40
2:B:240:GLN:OE1	2:B:355:MET:SD	2.80	0.40
2:D:281:ASP:O	2:D:285:VAL:HG23	2.21	0.40
2:B:24:ARG:NH2	2:B:264:TYR:CD2	2.89	0.40
2:D:124:TRP:CH2	2:D:215:ILE:HD12	2.56	0.40
2:D:240:GLN:OE1	2:D:355:MET:SD	2.80	0.40
2:D:489:ILE:HD12	2:D:735:ALA:HB1	2.03	0.40
4:J:47:THR:OG1	4:J:48:ARG:N	2.54	0.40
2:D:24:ARG:NH2	2:D:264:TYR:CD2	2.90	0.40
2:D:611:ILE:HG21	1:C:791:VAL:HG21	2.03	0.40
3:E:122:ILE:CG2	3:E:123:MET:N	2.84	0.40
1:A:242:ASP:OD1	1:A:243:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:VAL:HG21	2:B:611:ILE:HG21	2.02	0.40
2:B:44:LEU:HD23	2:B:44:LEU:N	2.37	0.40
7:B:2902:E2Q:N15	7:B:2902:E2Q:S11	2.95	0.40
2:D:574:PHE:CD2	9:D:909:PC1:H3I1	2.56	0.40
7:D:901:E2Q:S11	7:D:901:E2Q:N15	2.95	0.40
1:C:174:LEU:C	1:C:174:LEU:HD23	2.46	0.40
1:C:215:LEU:HD23	1:C:215:LEU:HA	1.95	0.40
2:B:482:THR:HG22	2:B:483:LEU:N	2.36	0.40
2:B:549:TYR:HE1	9:B:2901:PC1:H221	1.87	0.40
3:G:122:ILE:CG2	3:G:123:MET:N	2.84	0.40
2:D:44:LEU:HD23	2:D:44:LEU:N	2.37	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	765/915 (84%)	741 (97%)	24 (3%)	0	100	100
1	C	765/915 (84%)	741 (97%)	24 (3%)	0	100	100
2	B	775/860 (90%)	743 (96%)	32 (4%)	0	100	100
2	D	775/860 (90%)	743 (96%)	32 (4%)	0	100	100
3	E	156/188 (83%)	153 (98%)	3 (2%)	0	100	100
3	G	156/188 (83%)	153 (98%)	3 (2%)	0	100	100
4	I	177/423 (42%)	170 (96%)	7 (4%)	0	100	100
4	J	177/423 (42%)	170 (96%)	7 (4%)	0	100	100
All	All	3746/4772 (78%)	3614 (96%)	132 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	517/778 (66%)	516 (100%)	1 (0%)	87	85
1	C	517/778 (66%)	516 (100%)	1 (0%)	87	85
2	B	563/737 (76%)	562 (100%)	1 (0%)	87	85
2	D	563/737 (76%)	562 (100%)	1 (0%)	87	85
3	E	123/166 (74%)	123 (100%)	0	100	100
3	G	123/166 (74%)	123 (100%)	0	100	100
4	I	114/309 (37%)	114 (100%)	0	100	100
4	J	114/309 (37%)	114 (100%)	0	100	100
All	All	2634/3980 (66%)	2630 (100%)	4 (0%)	85	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
2	B	106	GLN
2	D	106	GLN
1	C	52	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	710	GLN
2	B	101	HIS
2	B	106	GLN
2	B	714	GLN
2	D	106	GLN
2	D	213	HIS
2	D	714	GLN
1	C	101	ASN
1	C	324	GLN

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Mol	Chain	Res	Type
1	C	710	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 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	F	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	1.54	1 (5%)
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.70	0
6	NAG	H	1	6,1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	H	2	6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	K	1	6,2	14,14,15	0.43	0	17,19,21	0.65	0
6	NAG	K	2	6	14,14,15	0.46	0	17,19,21	0.61	0
6	NAG	L	1	6,2	14,14,15	0.42	0	17,19,21	0.65	0
6	NAG	L	2	6	14,14,15	0.46	0	17,19,21	0.60	0
5	NAG	M	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	1.53	1 (5%)
5	NAG	M	2	5	14,14,15	0.26	0	17,19,21	0.41	0
5	BMA	M	3	5	11,11,12	0.58	0	15,15,17	0.69	0
6	NAG	N	1	6,1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	N	2	6	14,14,15	0.25	0	17,19,21	0.43	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	F	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1
6	NAG	L	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	O5-C1	2.71	1.48	1.43
5	F	1	NAG	O5-C1	2.63	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	6.01	120.24	112.19
5	M	1	NAG	C1-O5-C5	5.99	120.21	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C1-C2-N2-C7
6	L	2	NAG	C1-C2-N2-C7
6	H	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6

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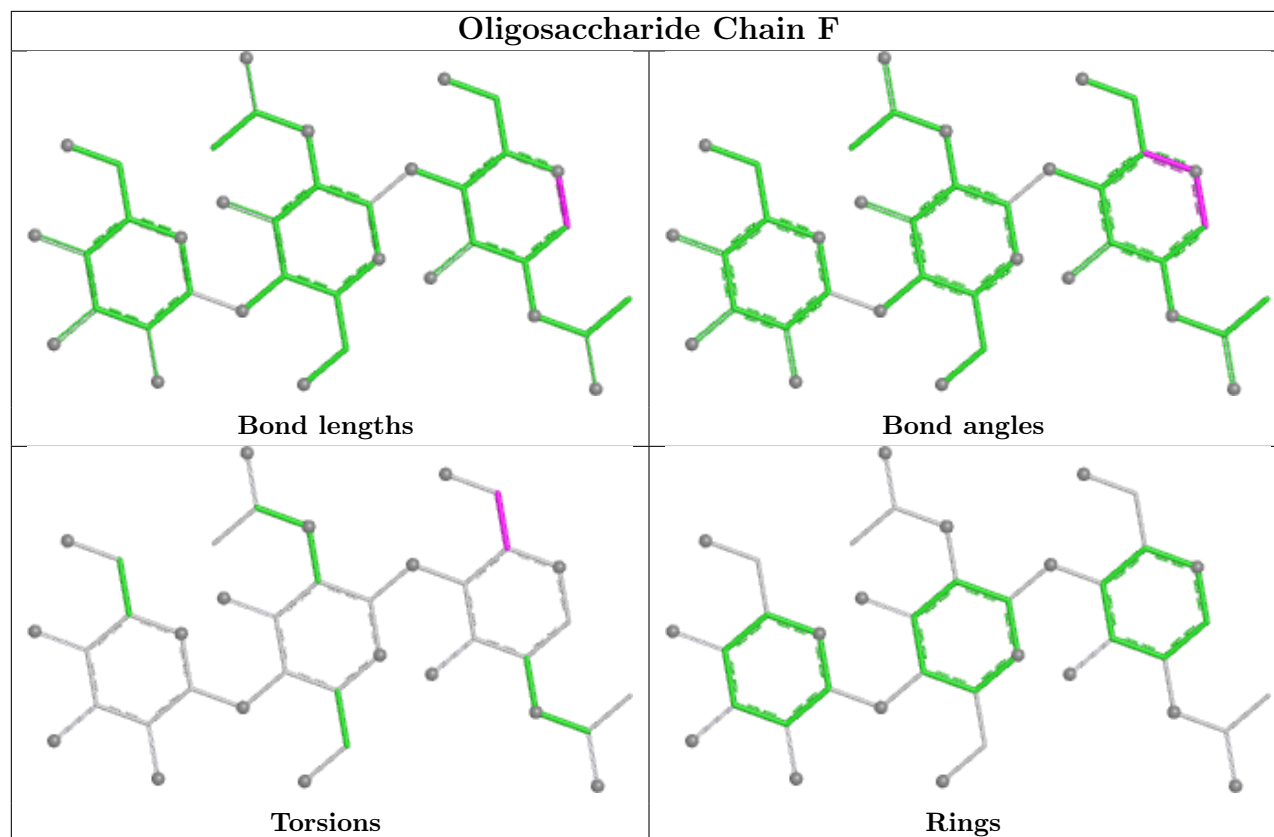
Mol	Chain	Res	Type	Atoms
6	N	1	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C3-C2-N2-C7
6	L	2	NAG	C3-C2-N2-C7

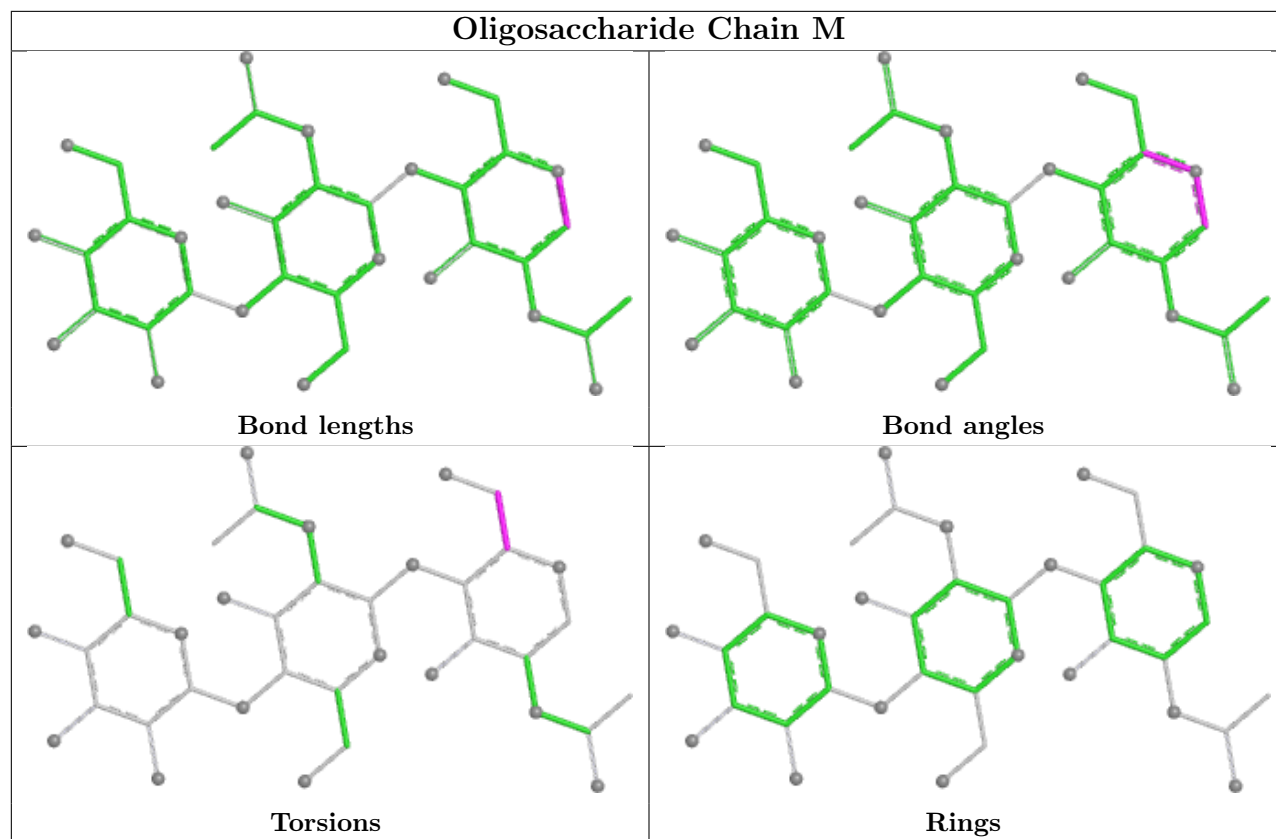
There are no ring outliers.

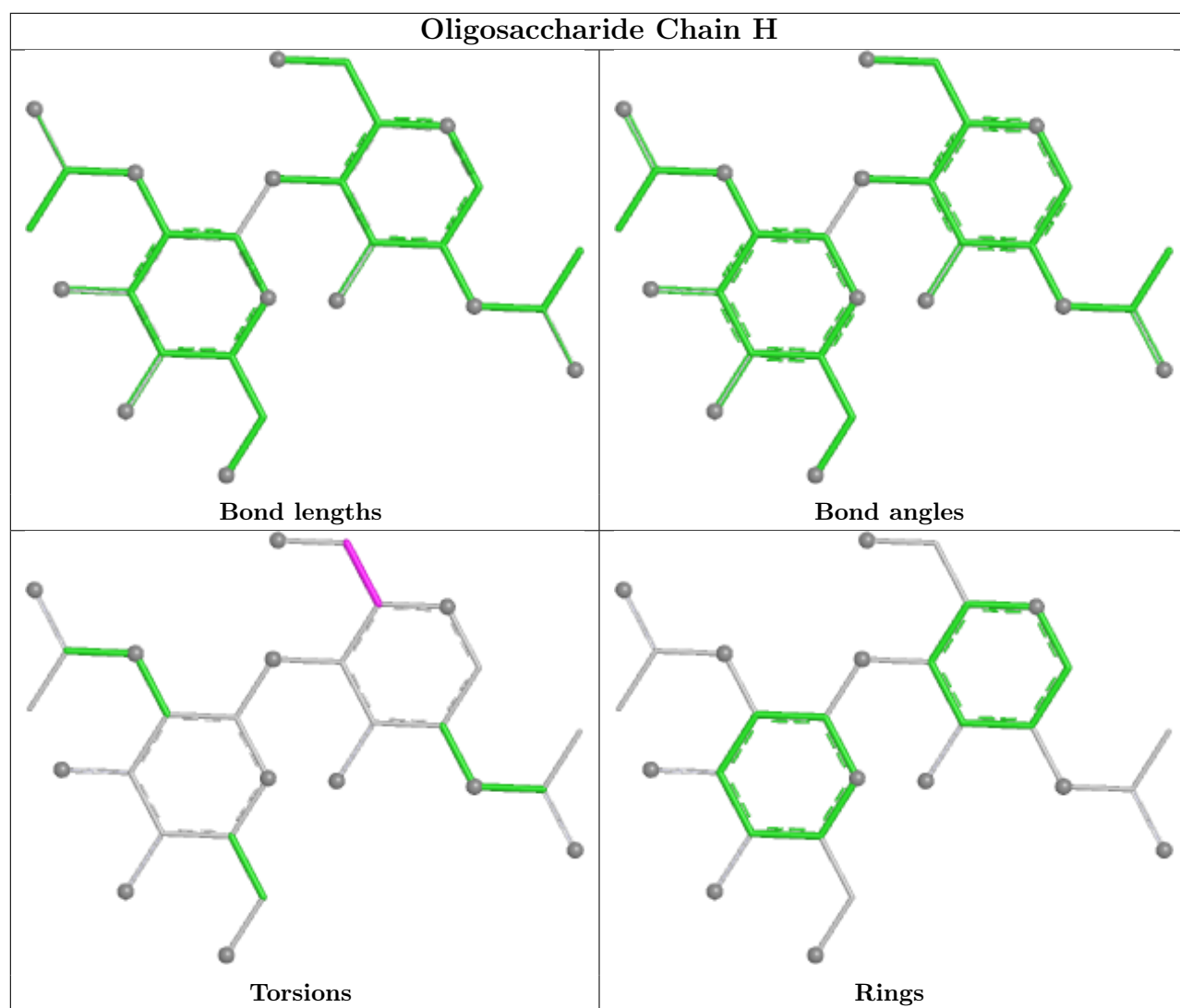
2 monomers are involved in 2 short contacts:

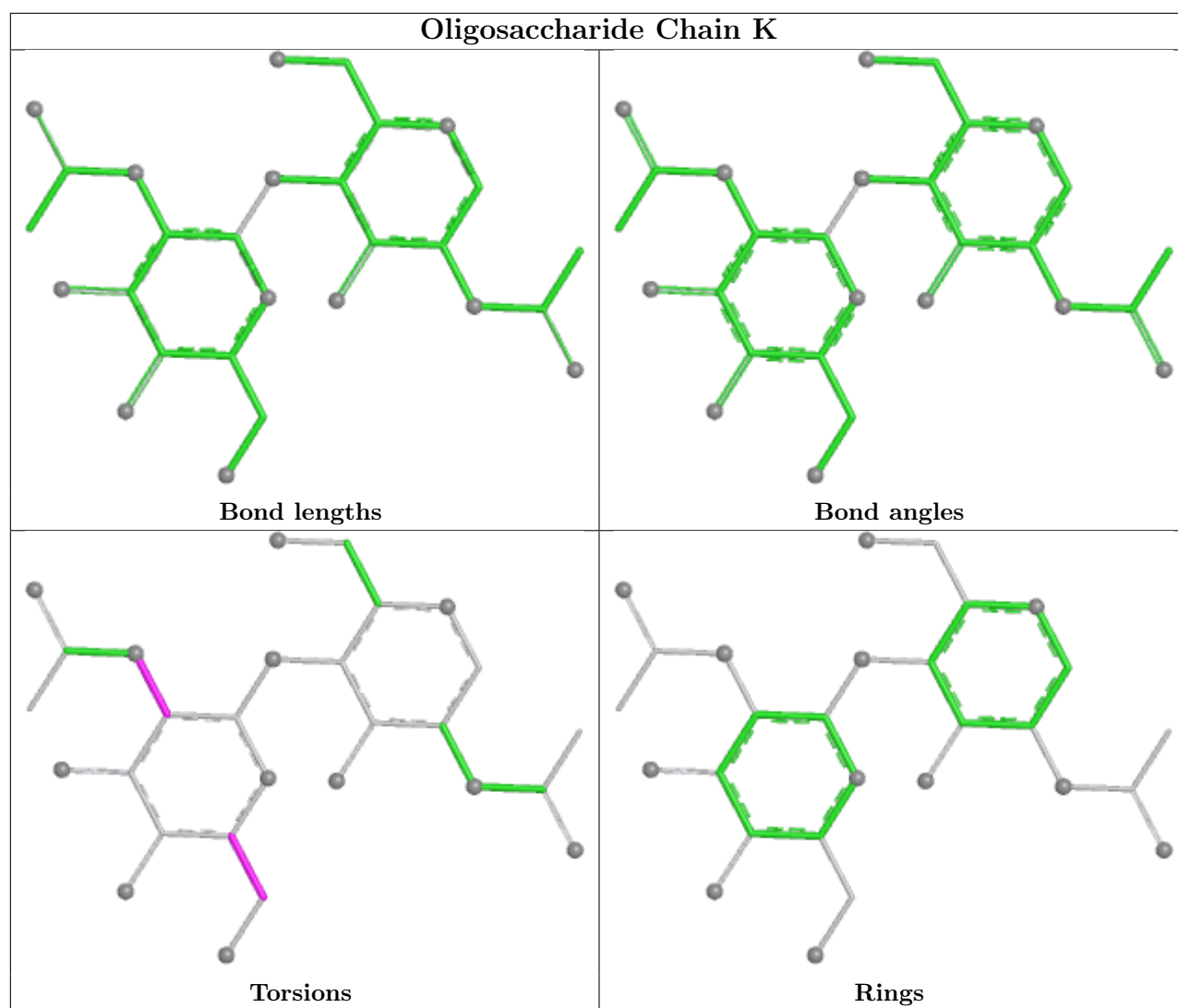
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1	NAG	1	0
5	F	1	NAG	1	0

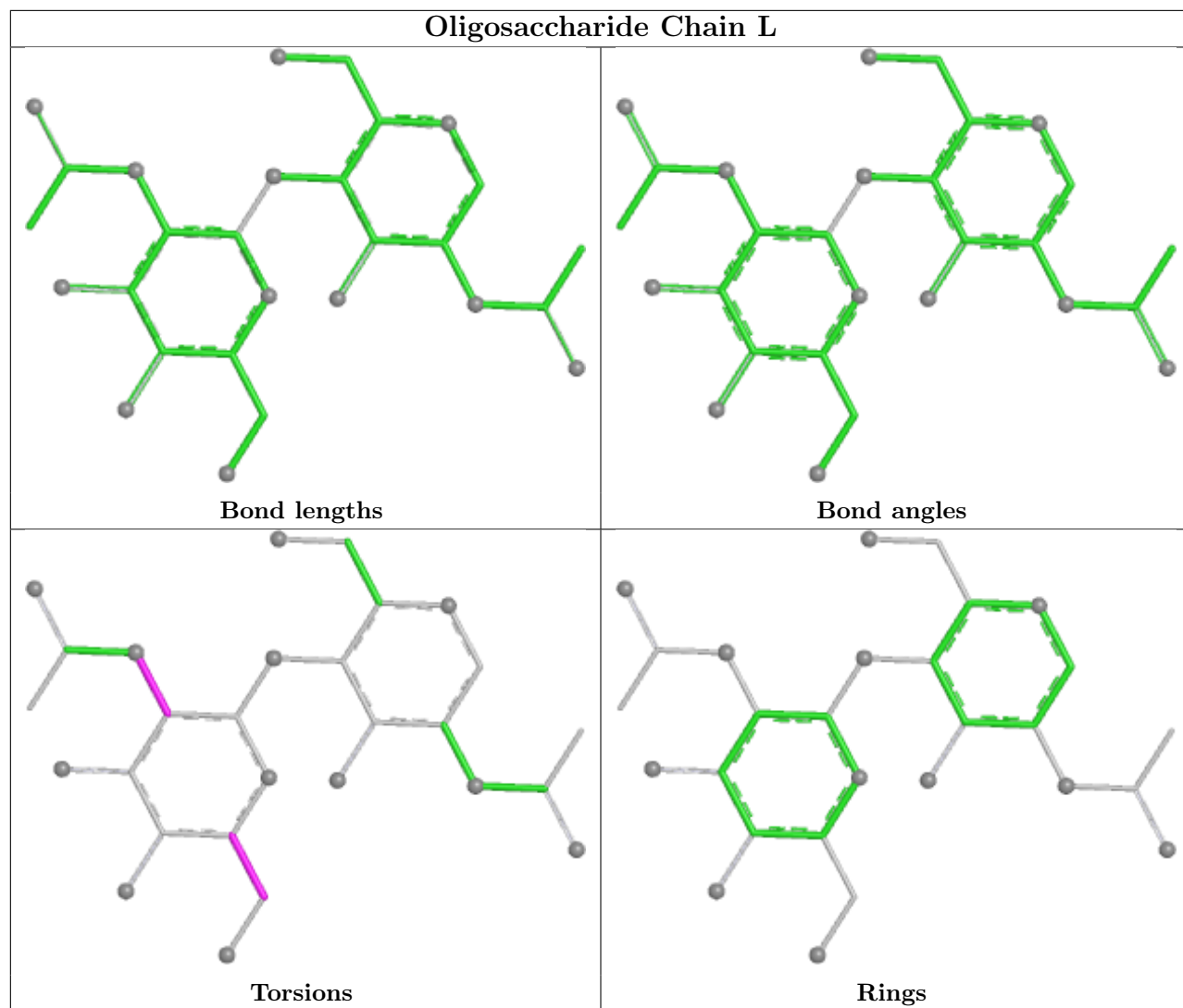
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

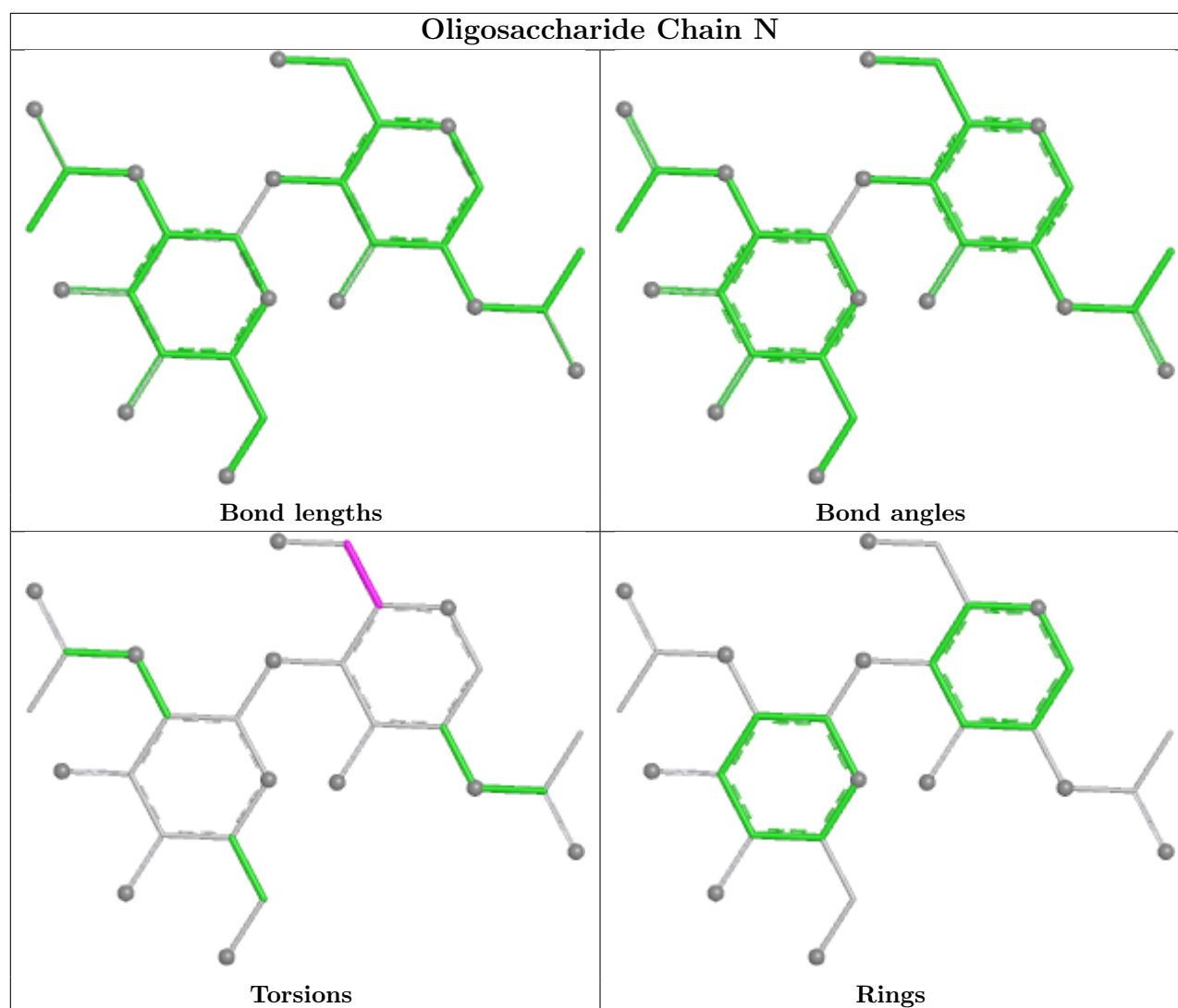












5.6 Ligand geometry [i](#)

58 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	$\# Z > 2$
7	E2Q	A	901	-	25,25,25	1.77	6 (24%)	32,39,39	2.20	12 (37%)
8	NAG	D	902	2	14,14,15	0.42	0	17,19,21	0.48	0
8	NAG	A	902	1	14,14,15	0.53	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	B	2908	-	19,19,53	0.79	1 (5%)	19,19,61	0.96	0
9	PC1	D	904	-	19,19,53	0.79	1 (5%)	19,19,61	1.05	1 (5%)
9	PC1	E	3101	-	17,17,53	0.85	1 (5%)	17,17,61	1.03	0
9	PC1	G	3104	-	19,19,53	0.79	1 (5%)	19,19,61	1.07	0
9	PC1	C	2709	-	24,24,53	0.81	2 (8%)	25,25,61	1.04	1 (4%)
9	PC1	E	3102	-	19,19,53	0.79	1 (5%)	19,19,61	1.04	0
9	PC1	B	2904	-	15,15,53	0.85	1 (6%)	15,15,61	1.09	0
9	PC1	J	2501	-	19,19,53	0.79	1 (5%)	19,19,61	1.10	1 (5%)
9	PC1	D	905	-	19,19,53	0.79	1 (5%)	19,19,61	1.02	0
9	PC1	B	2907	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
9	PC1	B	2909	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
9	PC1	D	903	-	15,15,53	0.84	1 (6%)	15,15,61	1.09	0
9	PC1	I	3001	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	0
9	PC1	J	2502	-	19,19,53	0.78	1 (5%)	19,19,61	1.02	0
9	PC1	J	2503	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	0
9	PC1	I	3005	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
9	PC1	B	2910	-	24,24,53	0.80	2 (8%)	25,25,61	1.05	1 (4%)
9	PC1	I	3002	-	19,19,53	0.78	1 (5%)	19,19,61	1.10	1 (5%)
10	CLR	E	3103	-	31,31,31	0.31	0	48,48,48	0.63	1 (2%)
9	PC1	C	2706	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	0
9	PC1	I	3004	-	19,19,53	0.79	1 (5%)	19,19,61	1.06	0
9	PC1	A	906	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
8	NAG	A	903	1	14,14,15	0.17	0	17,19,21	0.45	0
9	PC1	B	2901	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	0
8	NAG	B	2903	2	14,14,15	0.41	0	17,19,21	0.50	0
9	PC1	G	3101	-	19,19,53	0.79	1 (5%)	19,19,61	1.04	0
9	PC1	D	907	-	19,19,53	0.79	1 (5%)	19,19,61	0.96	0
8	NAG	C	2703	1	14,14,15	0.55	0	17,19,21	0.40	0
9	PC1	D	908	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
9	PC1	C	2701	-	17,17,53	0.83	1 (5%)	17,17,61	0.96	0
8	NAG	C	2704	1	14,14,15	0.18	0	17,19,21	0.46	0
7	E2Q	D	901	-	25,25,25	1.78	6 (24%)	32,39,39	2.17	11 (34%)
7	E2Q	C	2702	-	25,25,25	1.77	6 (24%)	32,39,39	2.20	12 (37%)
9	PC1	G	3102	-	17,17,53	0.84	1 (5%)	17,17,61	1.02	0
9	PC1	J	2505	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	A	904	-	19,19,53	0.77	1 (5%)	19,19,61	1.03	0
9	PC1	J	2504	-	17,17,53	0.83	1 (5%)	17,17,61	1.08	0
9	PC1	D	910	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	1 (5%)
9	PC1	A	907	-	17,17,53	0.82	1 (5%)	17,17,61	1.05	0
9	PC1	C	2708	-	17,17,53	0.82	1 (5%)	17,17,61	1.05	0
9	PC1	A	908	-	24,24,53	0.82	2 (8%)	25,25,61	1.04	1 (4%)
9	PC1	D	909	-	24,24,53	0.79	2 (8%)	25,25,61	1.05	1 (4%)
9	PC1	A	905	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	0
9	PC1	I	3003	-	19,19,53	0.78	1 (5%)	19,19,61	1.02	0
9	PC1	D	906	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
9	PC1	B	2906	-	19,19,53	0.80	1 (5%)	19,19,61	1.02	0
9	PC1	A	909	-	17,17,53	0.84	1 (5%)	17,17,61	0.97	0
9	PC1	D	911	-	19,19,53	0.77	1 (5%)	19,19,61	0.93	0
9	PC1	C	2707	-	19,19,53	0.78	1 (5%)	19,19,61	1.05	0
9	PC1	E	3104	-	19,19,53	0.79	1 (5%)	19,19,61	1.07	0
10	CLR	G	3103	-	31,31,31	0.31	0	48,48,48	0.63	1 (2%)
9	PC1	C	2705	-	19,19,53	0.77	1 (5%)	19,19,61	1.04	0
9	PC1	B	2911	-	19,19,53	0.77	1 (5%)	19,19,61	0.92	0
7	E2Q	B	2902	-	25,25,25	1.78	6 (24%)	32,39,39	2.18	11 (34%)
9	PC1	B	2905	-	19,19,53	0.78	1 (5%)	19,19,61	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	E2Q	A	901	-	-	3/8/10/10	0/3/3/3
8	NAG	D	902	2	-	3/6/23/26	0/1/1/1
8	NAG	A	902	1	-	2/6/23/26	0/1/1/1
9	PC1	B	2908	-	-	5/17/17/57	-
9	PC1	D	904	-	-	8/17/17/57	-
9	PC1	E	3101	-	-	2/15/15/57	-
9	PC1	G	3104	-	-	6/17/17/57	-
9	PC1	C	2709	-	-	12/24/24/57	-
9	PC1	E	3102	-	-	6/17/17/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	B	2904	-	-	5/13/13/57	-
9	PC1	J	2501	-	-	2/17/17/57	-
9	PC1	D	905	-	-	3/17/17/57	-
9	PC1	B	2907	-	-	4/17/17/57	-
9	PC1	B	2909	-	-	5/15/15/57	-
9	PC1	D	903	-	-	5/13/13/57	-
9	PC1	I	3001	-	-	5/15/15/57	-
9	PC1	J	2502	-	-	6/17/17/57	-
9	PC1	J	2503	-	-	4/17/17/57	-
9	PC1	I	3005	-	-	7/15/15/57	-
9	PC1	B	2910	-	-	10/24/24/57	-
9	PC1	I	3002	-	-	2/17/17/57	-
10	CLR	E	3103	-	-	4/10/68/68	0/4/4/4
9	PC1	C	2706	-	-	8/15/15/57	-
9	PC1	I	3004	-	-	4/17/17/57	-
9	PC1	A	906	-	-	5/17/17/57	-
8	NAG	A	903	1	-	2/6/23/26	0/1/1/1
9	PC1	B	2901	-	-	6/17/17/57	-
8	NAG	B	2903	2	-	3/6/23/26	0/1/1/1
9	PC1	G	3101	-	-	6/17/17/57	-
9	PC1	D	907	-	-	6/17/17/57	-
8	NAG	C	2703	1	-	2/6/23/26	0/1/1/1
9	PC1	D	908	-	-	5/15/15/57	-
9	PC1	C	2701	-	-	11/15/15/57	-
8	NAG	C	2704	1	-	2/6/23/26	0/1/1/1
7	E2Q	D	901	-	-	3/8/10/10	0/3/3/3
7	E2Q	C	2702	-	-	3/8/10/10	0/3/3/3
9	PC1	G	3102	-	-	2/15/15/57	-
9	PC1	J	2505	-	-	5/15/15/57	-
9	PC1	A	904	-	-	6/17/17/57	-
9	PC1	J	2504	-	-	7/15/15/57	-
9	PC1	D	910	-	-	6/17/17/57	-
9	PC1	A	907	-	-	3/15/15/57	-
9	PC1	C	2708	-	-	3/15/15/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	A	908	-	-	12/24/24/57	-
9	PC1	D	909	-	-	10/24/24/57	-
9	PC1	A	905	-	-	8/15/15/57	-
9	PC1	I	3003	-	-	6/17/17/57	-
9	PC1	D	906	-	-	4/17/17/57	-
9	PC1	B	2906	-	-	3/17/17/57	-
9	PC1	A	909	-	-	11/15/15/57	-
9	PC1	D	911	-	-	9/17/17/57	-
9	PC1	C	2707	-	-	5/17/17/57	-
9	PC1	E	3104	-	-	6/17/17/57	-
10	CLR	G	3103	-	-	4/10/68/68	0/4/4/4
9	PC1	C	2705	-	-	6/17/17/57	-
9	PC1	B	2911	-	-	9/17/17/57	-
7	E2Q	B	2902	-	-	3/8/10/10	0/3/3/3
9	PC1	B	2905	-	-	8/17/17/57	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2702	E2Q	C09-S11	-5.79	1.69	1.77
7	D	901	E2Q	C09-S11	-5.74	1.69	1.77
7	A	901	E2Q	C09-S11	-5.73	1.69	1.77
7	B	2902	E2Q	C09-S11	-5.72	1.69	1.77
7	A	901	E2Q	C21-N23	3.21	1.40	1.35
7	C	2702	E2Q	C21-N23	3.21	1.40	1.35
7	D	901	E2Q	C21-N23	3.21	1.40	1.35
7	B	2902	E2Q	C21-N23	3.15	1.40	1.35
9	I	3004	PC1	O21-C21	2.91	1.40	1.30
9	G	3102	PC1	O21-C21	2.91	1.40	1.30
9	B	2909	PC1	O21-C21	2.91	1.40	1.30
9	D	907	PC1	O21-C21	2.90	1.40	1.30
9	D	905	PC1	O21-C21	2.90	1.40	1.30
9	E	3104	PC1	O21-C21	2.90	1.40	1.30
9	E	3101	PC1	O21-C21	2.90	1.40	1.30
9	B	2906	PC1	O21-C21	2.89	1.40	1.30
9	J	2503	PC1	O21-C21	2.89	1.40	1.30
9	D	908	PC1	O21-C21	2.89	1.40	1.30
9	E	3102	PC1	O21-C21	2.89	1.40	1.30
9	D	904	PC1	O21-C21	2.89	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2706	PC1	O21-C21	2.89	1.40	1.30
9	J	2504	PC1	O21-C21	2.89	1.40	1.30
9	A	905	PC1	O21-C21	2.89	1.40	1.30
9	B	2905	PC1	O21-C21	2.89	1.40	1.30
9	I	3003	PC1	O21-C21	2.88	1.40	1.30
7	A	901	E2Q	C19-N18	2.88	1.39	1.35
9	A	909	PC1	O21-C21	2.88	1.40	1.30
9	I	3005	PC1	O21-C21	2.88	1.40	1.30
9	B	2901	PC1	O21-C21	2.88	1.40	1.30
9	D	910	PC1	O21-C21	2.88	1.40	1.30
9	J	2505	PC1	O21-C21	2.87	1.40	1.30
9	G	3104	PC1	O21-C21	2.87	1.40	1.30
9	G	3101	PC1	O21-C21	2.87	1.40	1.30
9	A	906	PC1	O21-C21	2.87	1.40	1.30
9	I	3001	PC1	O21-C21	2.87	1.40	1.30
9	C	2707	PC1	O21-C21	2.87	1.40	1.30
9	C	2701	PC1	O21-C21	2.87	1.40	1.30
9	B	2908	PC1	O21-C21	2.86	1.40	1.30
9	I	3002	PC1	O21-C21	2.86	1.40	1.30
9	J	2501	PC1	O21-C21	2.86	1.40	1.30
9	B	2904	PC1	O21-C21	2.86	1.40	1.30
9	J	2502	PC1	O21-C21	2.85	1.40	1.30
9	D	906	PC1	O21-C21	2.84	1.40	1.30
9	B	2911	PC1	O21-C21	2.84	1.40	1.30
9	D	903	PC1	O21-C21	2.84	1.40	1.30
9	D	911	PC1	O21-C21	2.83	1.40	1.30
9	A	907	PC1	O21-C21	2.83	1.40	1.30
9	B	2907	PC1	O21-C21	2.82	1.40	1.30
9	C	2708	PC1	O21-C21	2.82	1.40	1.30
7	C	2702	E2Q	C19-N18	2.82	1.39	1.35
9	A	904	PC1	O21-C21	2.80	1.40	1.30
9	C	2705	PC1	O21-C21	2.80	1.40	1.30
7	B	2902	E2Q	C19-N18	2.76	1.39	1.35
7	D	901	E2Q	C19-N18	2.74	1.39	1.35
7	B	2902	E2Q	C06-C07	-2.50	1.36	1.38
9	C	2709	PC1	O31-C31	2.48	1.40	1.33
9	A	908	PC1	O31-C31	2.47	1.40	1.33
7	B	2902	E2Q	C07-N15	2.44	1.50	1.45
7	D	901	E2Q	C07-N15	2.43	1.50	1.45
7	D	901	E2Q	O17-N15	-2.43	1.19	1.35
7	B	2902	E2Q	O17-N15	-2.41	1.19	1.35
7	C	2702	E2Q	O17-N15	-2.41	1.19	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	901	E2Q	O17-N15	-2.41	1.19	1.35
7	D	901	E2Q	C06-C07	-2.40	1.36	1.38
7	A	901	E2Q	C07-N15	2.32	1.50	1.45
9	B	2910	PC1	O31-C3	-2.31	1.40	1.45
9	B	2910	PC1	O31-C31	2.30	1.40	1.33
7	C	2702	E2Q	C07-N15	2.29	1.49	1.45
9	D	909	PC1	O31-C31	2.28	1.40	1.33
7	C	2702	E2Q	C06-C07	-2.28	1.36	1.38
9	D	909	PC1	O31-C3	-2.26	1.40	1.45
7	A	901	E2Q	C06-C07	-2.23	1.36	1.38
9	A	908	PC1	O31-C3	-2.16	1.40	1.45
9	C	2709	PC1	O31-C3	-2.12	1.40	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	901	E2Q	C09-C08-C03	5.44	119.76	116.78
7	C	2702	E2Q	C09-C08-C03	5.37	119.72	116.78
7	B	2902	E2Q	C09-C08-C03	5.37	119.72	116.78
7	D	901	E2Q	C09-C08-C03	5.34	119.71	116.78
7	C	2702	E2Q	O22-C21-C19	3.79	122.98	119.62
7	A	901	E2Q	O22-C21-C19	3.75	122.94	119.62
7	D	901	E2Q	O22-C21-C19	3.72	122.92	119.62
7	B	2902	E2Q	O22-C21-C19	3.71	122.90	119.62
7	A	901	E2Q	O13-S11-O12	3.53	124.23	118.80
7	B	2902	E2Q	O13-S11-O12	3.53	124.23	118.80
7	D	901	E2Q	O13-S11-O12	3.52	124.22	118.80
7	C	2702	E2Q	O13-S11-O12	3.51	124.20	118.80
7	D	901	E2Q	C01-C10-C09	3.51	124.27	120.37
7	B	2902	E2Q	C01-C10-C09	3.50	124.27	120.37
7	A	901	E2Q	C01-C10-C09	3.50	124.26	120.37
7	C	2702	E2Q	C01-C10-C09	3.48	124.25	120.37
7	D	901	E2Q	C02-C03-C04	-3.46	118.48	124.70
7	C	2702	E2Q	C04-C05-N18	3.45	121.89	118.59
7	B	2902	E2Q	C02-C03-C04	-3.44	118.51	124.70
7	C	2702	E2Q	C02-C03-C04	-3.41	118.56	124.70
7	A	901	E2Q	C02-C03-C04	-3.39	118.59	124.70
7	A	901	E2Q	C04-C05-N18	3.37	121.82	118.59
7	B	2902	E2Q	C04-C05-N18	3.33	121.78	118.59
7	D	901	E2Q	C04-C05-N18	3.20	121.65	118.59
9	C	2709	PC1	O31-C31-C32	3.00	120.99	111.83
9	A	908	PC1	O31-C31-C32	2.99	120.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	901	E2Q	C08-C09-S11	2.97	125.43	121.74
7	C	2702	E2Q	C08-C09-S11	2.91	125.36	121.74
7	D	901	E2Q	O20-C19-C21	2.89	122.19	119.62
7	A	901	E2Q	O20-C19-C21	2.89	122.18	119.62
7	B	2902	E2Q	O20-C19-C21	2.87	122.16	119.62
7	C	2702	E2Q	O20-C19-C21	2.85	122.15	119.62
7	A	901	E2Q	C10-C09-C08	-2.74	116.01	120.18
7	D	901	E2Q	C10-C09-C08	-2.73	116.03	120.18
9	D	909	PC1	O31-C31-C32	2.73	120.14	111.83
9	B	2910	PC1	O31-C31-C32	2.72	120.12	111.83
7	C	2702	E2Q	C10-C09-C08	-2.71	116.06	120.18
7	B	2902	E2Q	C10-C09-C08	-2.70	116.07	120.18
7	C	2702	E2Q	O16-N15-C07	-2.62	114.55	119.03
7	A	901	E2Q	O16-N15-C07	-2.61	114.56	119.03
7	D	901	E2Q	O16-N15-C07	-2.60	114.59	119.03
7	B	2902	E2Q	O16-N15-C07	-2.55	114.66	119.03
7	D	901	E2Q	C08-C09-S11	2.52	124.87	121.74
7	C	2702	E2Q	C05-N18-C19	-2.52	121.30	124.82
7	B	2902	E2Q	C08-C09-S11	2.51	124.86	121.74
7	A	901	E2Q	C05-N18-C19	-2.48	121.35	124.82
7	B	2902	E2Q	C05-N18-C19	-2.43	121.41	124.82
7	D	901	E2Q	C05-N18-C19	-2.41	121.44	124.82
10	G	3103	CLR	C1-C2-C3	2.38	113.63	110.48
10	E	3103	CLR	C1-C2-C3	2.37	113.63	110.48
9	J	2501	PC1	C23-C22-C21	-2.10	109.03	114.51
9	I	3002	PC1	C23-C22-C21	-2.09	109.07	114.51
7	C	2702	E2Q	O13-S11-N14	-2.04	104.41	107.35
7	A	901	E2Q	O13-S11-N14	-2.03	104.42	107.35
9	D	904	PC1	O21-C21-C22	2.03	120.41	114.00
9	D	910	PC1	O21-C21-C22	2.01	120.34	114.00
9	B	2905	PC1	O21-C21-C22	2.00	120.33	114.00

There are no chirality outliers.

All (311) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	901	E2Q	C06-C07-N15-O16
7	A	901	E2Q	C08-C07-N15-O16
7	B	2902	E2Q	C06-C07-N15-O16
7	B	2902	E2Q	C08-C07-N15-O16
7	D	901	E2Q	C06-C07-N15-O16
7	D	901	E2Q	C08-C07-N15-O16

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Mol	Chain	Res	Type	Atoms
7	C	2702	E2Q	C06-C07-N15-O16
7	C	2702	E2Q	C08-C07-N15-O16
9	A	908	PC1	C1-C2-C3-O31
9	B	2910	PC1	C1-C2-C3-O31
9	B	2910	PC1	O21-C2-C3-O31
9	D	909	PC1	C1-C2-C3-O31
9	D	909	PC1	O21-C2-C3-O31
9	C	2709	PC1	C1-C2-C3-O31
9	A	908	PC1	O32-C31-O31-C3
9	C	2709	PC1	O32-C31-O31-C3
9	A	908	PC1	C32-C31-O31-C3
9	B	2910	PC1	C32-C31-O31-C3
9	D	909	PC1	C32-C31-O31-C3
9	C	2709	PC1	C32-C31-O31-C3
9	B	2910	PC1	O32-C31-O31-C3
9	D	909	PC1	O32-C31-O31-C3
9	A	908	PC1	O21-C2-C3-O31
9	C	2709	PC1	O21-C2-C3-O31
10	G	3103	CLR	C17-C20-C22-C23
10	E	3103	CLR	C17-C20-C22-C23
9	B	2905	PC1	C21-C22-C23-C24
9	D	904	PC1	C21-C22-C23-C24
8	A	903	NAG	O5-C5-C6-O6
8	C	2704	NAG	O5-C5-C6-O6
8	A	902	NAG	C8-C7-N2-C2
8	A	902	NAG	O7-C7-N2-C2
8	B	2903	NAG	C8-C7-N2-C2
8	B	2903	NAG	O7-C7-N2-C2
8	D	902	NAG	C8-C7-N2-C2
8	D	902	NAG	O7-C7-N2-C2
8	C	2703	NAG	C8-C7-N2-C2
8	C	2703	NAG	O7-C7-N2-C2
10	G	3103	CLR	C21-C20-C22-C23
10	E	3103	CLR	C21-C20-C22-C23
9	A	909	PC1	C21-C22-C23-C24
9	C	2701	PC1	C21-C22-C23-C24
9	B	2910	PC1	C31-C32-C33-C34
9	D	909	PC1	C31-C32-C33-C34
9	I	3004	PC1	C22-C23-C24-C25
9	J	2503	PC1	C22-C23-C24-C25
9	A	909	PC1	C27-C28-C29-C2A
9	C	2701	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
9	B	2905	PC1	C2C-C2D-C2E-C2F
9	D	904	PC1	C2C-C2D-C2E-C2F
10	G	3103	CLR	C20-C22-C23-C24
10	E	3103	CLR	C20-C22-C23-C24
9	A	906	PC1	C24-C25-C26-C27
9	C	2707	PC1	C24-C25-C26-C27
9	B	2904	PC1	C23-C24-C25-C26
9	B	2911	PC1	C23-C24-C25-C26
9	D	903	PC1	C23-C24-C25-C26
9	D	911	PC1	C23-C24-C25-C26
9	B	2907	PC1	C21-C22-C23-C24
9	D	906	PC1	C21-C22-C23-C24
9	A	905	PC1	C22-C23-C24-C25
9	C	2706	PC1	C22-C23-C24-C25
9	B	2905	PC1	C23-C24-C25-C26
9	D	909	PC1	C37-C38-C39-C3A
9	B	2910	PC1	C37-C38-C39-C3A
9	D	904	PC1	C23-C24-C25-C26
9	B	2901	PC1	C27-C28-C29-C2A
9	D	910	PC1	C27-C28-C29-C2A
9	A	906	PC1	C25-C26-C27-C28
9	C	2707	PC1	C25-C26-C27-C28
9	J	2503	PC1	C26-C27-C28-C29
9	C	2709	PC1	C39-C3A-C3B-C3C
9	A	908	PC1	C39-C3A-C3B-C3C
9	A	909	PC1	C29-C2A-C2B-C2C
9	I	3004	PC1	C26-C27-C28-C29
9	I	3003	PC1	C28-C29-C2A-C2B
9	J	2502	PC1	C28-C29-C2A-C2B
9	C	2701	PC1	C29-C2A-C2B-C2C
9	A	908	PC1	C38-C39-C3A-C3B
9	C	2709	PC1	C38-C39-C3A-C3B
9	B	2910	PC1	C36-C37-C38-C39
9	D	909	PC1	C36-C37-C38-C39
9	A	908	PC1	C3C-C3D-C3E-C3F
9	C	2709	PC1	C3C-C3D-C3E-C3F
9	B	2909	PC1	C22-C23-C24-C25
9	D	908	PC1	C22-C23-C24-C25
9	B	2911	PC1	C27-C28-C29-C2A
9	D	905	PC1	C23-C24-C25-C26
9	D	911	PC1	C27-C28-C29-C2A
9	B	2906	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
9	A	905	PC1	C23-C24-C25-C26
9	C	2706	PC1	C23-C24-C25-C26
9	J	2502	PC1	C24-C25-C26-C27
9	A	904	PC1	C2D-C2E-C2F-C2G
9	I	3003	PC1	C24-C25-C26-C27
9	C	2705	PC1	C2D-C2E-C2F-C2G
8	A	903	NAG	C4-C5-C6-O6
8	C	2704	NAG	C4-C5-C6-O6
9	J	2504	PC1	C25-C26-C27-C28
9	I	3005	PC1	C25-C26-C27-C28
9	A	909	PC1	C26-C27-C28-C29
9	C	2701	PC1	C26-C27-C28-C29
9	A	904	PC1	C28-C29-C2A-C2B
9	A	907	PC1	C26-C27-C28-C29
9	C	2705	PC1	C28-C29-C2A-C2B
9	C	2708	PC1	C26-C27-C28-C29
9	A	909	PC1	C2B-C2C-C2D-C2E
9	C	2701	PC1	C2B-C2C-C2D-C2E
9	B	2906	PC1	C27-C28-C29-C2A
9	D	905	PC1	C27-C28-C29-C2A
9	D	911	PC1	C2C-C2D-C2E-C2F
9	B	2911	PC1	C2C-C2D-C2E-C2F
9	B	2911	PC1	C29-C2A-C2B-C2C
9	D	911	PC1	C29-C2A-C2B-C2C
9	E	3104	PC1	C2B-C2C-C2D-C2E
9	G	3104	PC1	C2B-C2C-C2D-C2E
9	A	908	PC1	C3E-C3F-C3G-C3H
9	C	2709	PC1	C3E-C3F-C3G-C3H
9	G	3101	PC1	C28-C29-C2A-C2B
9	E	3102	PC1	C28-C29-C2A-C2B
9	B	2905	PC1	C29-C2A-C2B-C2C
9	D	904	PC1	C29-C2A-C2B-C2C
9	B	2907	PC1	C25-C26-C27-C28
9	D	906	PC1	C25-C26-C27-C28
7	A	901	E2Q	C08-C09-S11-O12
7	B	2902	E2Q	C08-C09-S11-O13
7	D	901	E2Q	C08-C09-S11-O13
7	C	2702	E2Q	C08-C09-S11-O12
9	G	3104	PC1	C25-C26-C27-C28
9	E	3104	PC1	C25-C26-C27-C28
9	I	3003	PC1	C23-C24-C25-C26
9	J	2502	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
9	B	2909	PC1	C2C-C2D-C2E-C2F
9	A	908	PC1	C3A-C3B-C3C-C3D
9	B	2901	PC1	C2D-C2E-C2F-C2G
9	D	910	PC1	C2D-C2E-C2F-C2G
9	C	2709	PC1	C3A-C3B-C3C-C3D
9	D	908	PC1	C27-C28-C29-C2A
9	B	2909	PC1	C27-C28-C29-C2A
9	B	2904	PC1	C26-C27-C28-C29
9	D	903	PC1	C26-C27-C28-C29
9	D	910	PC1	C23-C24-C25-C26
9	B	2901	PC1	C23-C24-C25-C26
9	B	2908	PC1	C26-C27-C28-C29
9	D	907	PC1	C26-C27-C28-C29
9	D	908	PC1	C2C-C2D-C2E-C2F
9	J	2504	PC1	C21-C22-C23-C24
9	I	3005	PC1	C21-C22-C23-C24
9	I	3005	PC1	C29-C2A-C2B-C2C
9	J	2504	PC1	C29-C2A-C2B-C2C
9	C	2701	PC1	C23-C24-C25-C26
9	A	909	PC1	C23-C24-C25-C26
9	B	2911	PC1	C2A-C2B-C2C-C2D
9	D	911	PC1	C2A-C2B-C2C-C2D
9	G	3104	PC1	C22-C23-C24-C25
9	D	903	PC1	C25-C26-C27-C28
9	E	3104	PC1	C22-C23-C24-C25
9	B	2904	PC1	C25-C26-C27-C28
9	I	3005	PC1	C23-C24-C25-C26
9	J	2504	PC1	C23-C24-C25-C26
9	C	2701	PC1	C28-C29-C2A-C2B
9	A	909	PC1	C28-C29-C2A-C2B
9	D	911	PC1	C28-C29-C2A-C2B
9	B	2911	PC1	C28-C29-C2A-C2B
9	A	907	PC1	C28-C29-C2A-C2B
9	C	2708	PC1	C28-C29-C2A-C2B
9	D	907	PC1	C2B-C2C-C2D-C2E
9	B	2908	PC1	C2B-C2C-C2D-C2E
9	D	909	PC1	C32-C33-C34-C35
9	D	904	PC1	C2F-C2G-C2H-C2I
9	B	2910	PC1	C32-C33-C34-C35
9	D	904	PC1	C27-C28-C29-C2A
9	B	2905	PC1	C27-C28-C29-C2A
9	B	2905	PC1	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
9	E	3101	PC1	C27-C28-C29-C2A
9	G	3102	PC1	C27-C28-C29-C2A
9	J	2505	PC1	C24-C25-C26-C27
9	I	3001	PC1	C26-C27-C28-C29
9	B	2904	PC1	C29-C2A-C2B-C2C
9	D	903	PC1	C29-C2A-C2B-C2C
9	J	2505	PC1	C26-C27-C28-C29
9	I	3001	PC1	C24-C25-C26-C27
9	E	3104	PC1	C2C-C2D-C2E-C2F
9	A	905	PC1	C2D-C2E-C2F-C2G
9	C	2706	PC1	C2D-C2E-C2F-C2G
9	G	3104	PC1	C2C-C2D-C2E-C2F
9	E	3102	PC1	C27-C28-C29-C2A
9	G	3101	PC1	C27-C28-C29-C2A
9	I	3003	PC1	C2C-C2D-C2E-C2F
9	D	911	PC1	C22-C23-C24-C25
9	J	2502	PC1	C2C-C2D-C2E-C2F
9	B	2911	PC1	C22-C23-C24-C25
9	B	2904	PC1	C2B-C2C-C2D-C2E
9	D	903	PC1	C2B-C2C-C2D-C2E
9	E	3102	PC1	C2E-C2F-C2G-C2H
9	G	3101	PC1	C2E-C2F-C2G-C2H
9	I	3001	PC1	C22-C23-C24-C25
9	B	2908	PC1	C23-C24-C25-C26
9	D	907	PC1	C23-C24-C25-C26
9	I	3003	PC1	C29-C2A-C2B-C2C
9	J	2502	PC1	C29-C2A-C2B-C2C
9	A	904	PC1	C29-C2A-C2B-C2C
9	C	2705	PC1	C29-C2A-C2B-C2C
9	D	907	PC1	C28-C29-C2A-C2B
9	B	2908	PC1	C28-C29-C2A-C2B
9	J	2505	PC1	C22-C23-C24-C25
9	A	905	PC1	C25-C26-C27-C28
9	J	2503	PC1	C2B-C2C-C2D-C2E
9	C	2705	PC1	C2A-C2B-C2C-C2D
9	C	2706	PC1	C25-C26-C27-C28
9	A	904	PC1	C2A-C2B-C2C-C2D
9	I	3004	PC1	C2B-C2C-C2D-C2E
9	I	3001	PC1	O22-C21-C22-C23
9	J	2505	PC1	O22-C21-C22-C23
9	A	905	PC1	C29-C2A-C2B-C2C
9	C	2706	PC1	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
9	B	2910	PC1	C39-C3A-C3B-C3C
9	A	906	PC1	O21-C21-C22-C23
9	C	2707	PC1	O21-C21-C22-C23
9	A	906	PC1	O22-C21-C22-C23
9	I	3002	PC1	O22-C21-C22-C23
9	J	2501	PC1	O22-C21-C22-C23
9	B	2905	PC1	C2A-C2B-C2C-C2D
9	D	909	PC1	C39-C3A-C3B-C3C
9	A	907	PC1	C2B-C2C-C2D-C2E
9	D	904	PC1	C2A-C2B-C2C-C2D
9	A	905	PC1	O21-C21-C22-C23
9	J	2505	PC1	O21-C21-C22-C23
9	C	2707	PC1	O22-C21-C22-C23
9	C	2708	PC1	C2B-C2C-C2D-C2E
9	C	2706	PC1	O21-C21-C22-C23
9	A	909	PC1	C25-C26-C27-C28
9	C	2705	PC1	C2E-C2F-C2G-C2H
9	I	3001	PC1	O21-C21-C22-C23
9	A	904	PC1	C2E-C2F-C2G-C2H
9	D	909	PC1	C38-C39-C3A-C3B
9	C	2701	PC1	C25-C26-C27-C28
9	B	2910	PC1	C38-C39-C3A-C3B
9	I	3002	PC1	O21-C21-C22-C23
9	J	2501	PC1	O21-C21-C22-C23
9	A	904	PC1	C2B-C2C-C2D-C2E
9	C	2705	PC1	C2B-C2C-C2D-C2E
9	B	2905	PC1	C2E-C2F-C2G-C2H
9	D	904	PC1	C2E-C2F-C2G-C2H
9	A	905	PC1	O22-C21-C22-C23
9	I	3005	PC1	O21-C21-C22-C23
9	J	2504	PC1	O21-C21-C22-C23
9	B	2906	PC1	C28-C29-C2A-C2B
9	C	2706	PC1	O22-C21-C22-C23
9	A	909	PC1	C2A-C2B-C2C-C2D
8	B	2903	NAG	C1-C2-N2-C7
8	D	902	NAG	C1-C2-N2-C7
9	A	908	PC1	C32-C33-C34-C35
9	C	2709	PC1	C32-C33-C34-C35
9	C	2701	PC1	C2A-C2B-C2C-C2D
9	D	905	PC1	C28-C29-C2A-C2B
9	I	3005	PC1	C28-C29-C2A-C2B
9	J	2504	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
9	A	908	PC1	O11-C1-C2-O21
9	C	2709	PC1	O11-C1-C2-O21
9	I	3005	PC1	O22-C21-C22-C23
9	J	2504	PC1	O22-C21-C22-C23
9	G	3102	PC1	C25-C26-C27-C28
9	E	3101	PC1	C25-C26-C27-C28
9	D	906	PC1	O22-C21-C22-C23
9	B	2907	PC1	O22-C21-C22-C23
9	C	2707	PC1	C22-C23-C24-C25
9	A	906	PC1	C22-C23-C24-C25
9	A	909	PC1	O21-C21-C22-C23
9	A	909	PC1	O22-C21-C22-C23
9	C	2701	PC1	O22-C21-C22-C23
9	C	2701	PC1	O21-C21-C22-C23
9	G	3104	PC1	O22-C21-C22-C23
9	E	3104	PC1	O22-C21-C22-C23
9	G	3104	PC1	O21-C21-C22-C23
9	E	3104	PC1	O21-C21-C22-C23
9	G	3101	PC1	C24-C25-C26-C27
9	E	3102	PC1	C24-C25-C26-C27
9	B	2911	PC1	O21-C21-C22-C23
9	C	2706	PC1	C24-C25-C26-C27
9	D	911	PC1	O21-C21-C22-C23
9	A	905	PC1	C24-C25-C26-C27
9	B	2909	PC1	C23-C24-C25-C26
9	D	906	PC1	O21-C21-C22-C23
9	D	908	PC1	C23-C24-C25-C26
9	D	910	PC1	C25-C26-C27-C28
9	E	3102	PC1	O21-C21-C22-C23
9	E	3102	PC1	O22-C21-C22-C23
9	B	2901	PC1	C25-C26-C27-C28
9	B	2907	PC1	O21-C21-C22-C23
9	G	3101	PC1	O22-C21-C22-C23
9	G	3101	PC1	O21-C21-C22-C23
9	J	2502	PC1	C25-C26-C27-C28
9	I	3003	PC1	C25-C26-C27-C28
9	D	911	PC1	O22-C21-C22-C23
10	G	3103	CLR	C22-C23-C24-C25
10	E	3103	CLR	C22-C23-C24-C25
9	B	2911	PC1	O22-C21-C22-C23
9	I	3004	PC1	C25-C26-C27-C28
9	J	2503	PC1	C25-C26-C27-C28

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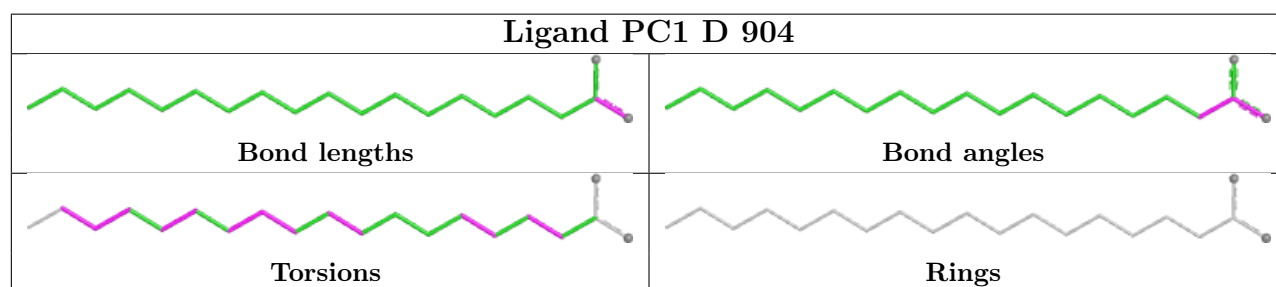
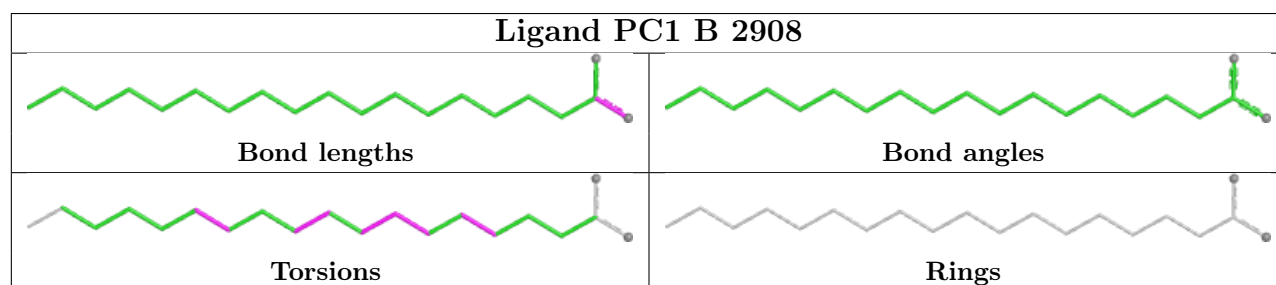
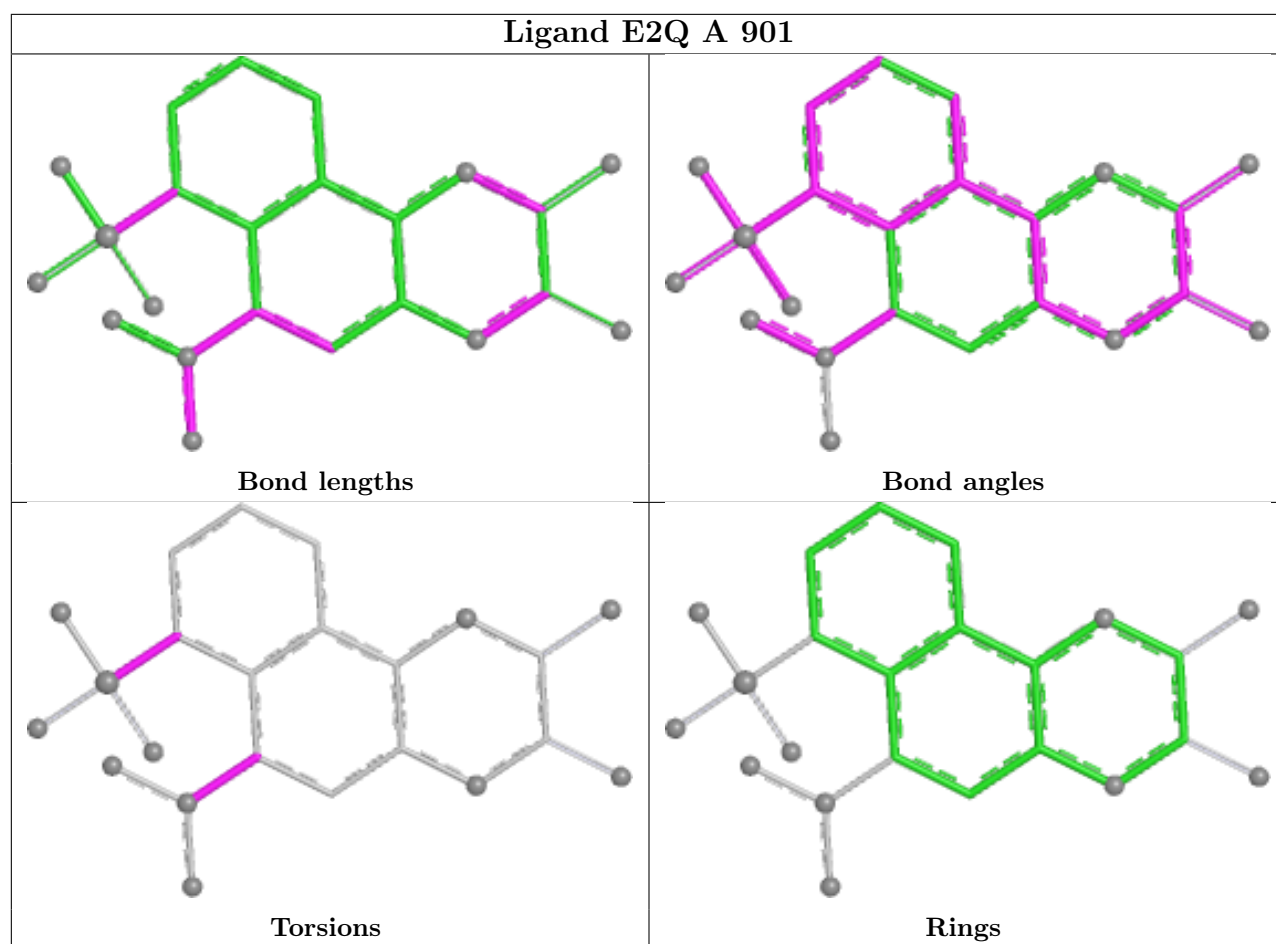
Mol	Chain	Res	Type	Atoms
9	A	908	PC1	C35-C36-C37-C38
9	C	2709	PC1	C35-C36-C37-C38
9	D	907	PC1	C25-C26-C27-C28
9	B	2908	PC1	C25-C26-C27-C28
9	D	910	PC1	C22-C23-C24-C25
9	B	2901	PC1	C22-C23-C24-C25
9	D	910	PC1	O21-C21-C22-C23
9	B	2901	PC1	O21-C21-C22-C23
9	B	2909	PC1	O21-C21-C22-C23
9	D	908	PC1	O21-C21-C22-C23
9	D	907	PC1	C2D-C2E-C2F-C2G

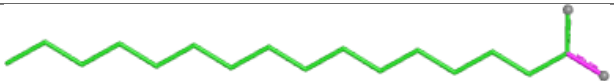
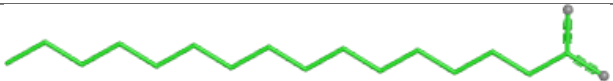
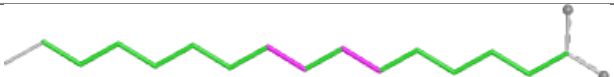
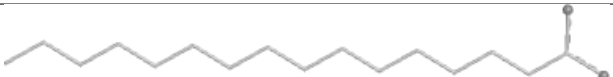
There are no ring outliers.

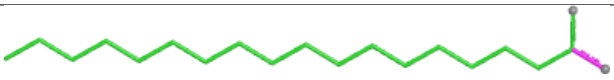
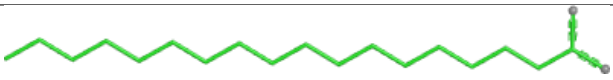
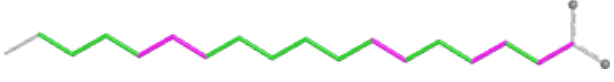
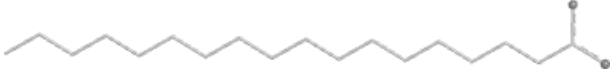
9 monomers are involved in 13 short contacts:

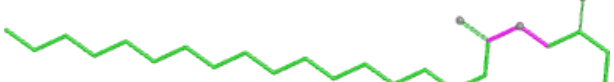
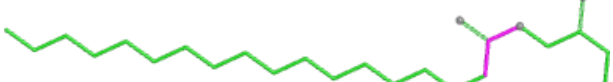
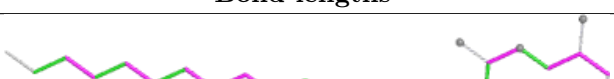
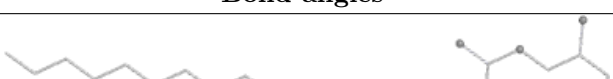
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	902	NAG	1	0
9	J	2502	PC1	1	0
10	E	3103	CLR	3	0
9	B	2901	PC1	1	0
8	B	2903	NAG	1	0
7	D	901	E2Q	1	0
9	D	909	PC1	1	0
10	G	3103	CLR	3	0
7	B	2902	E2Q	1	0

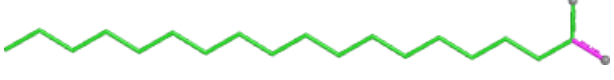
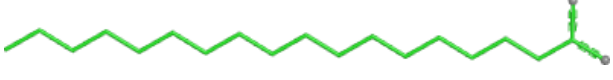
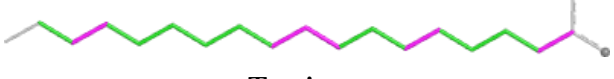
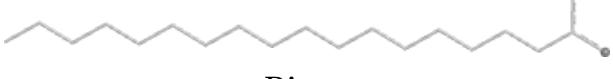
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

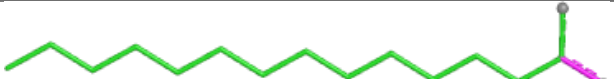
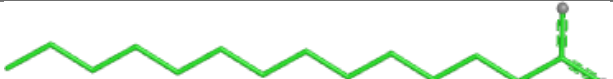


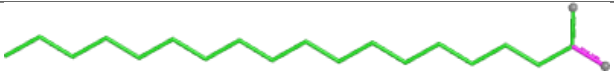
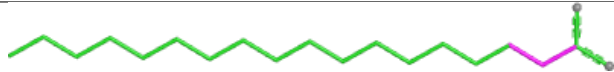
Ligand PC1 E 3101	
 Bond lengths	 Bond angles
 Torsions	 Rings

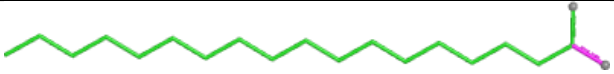
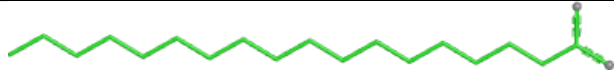
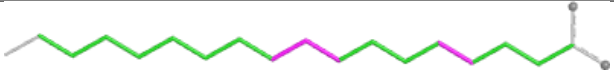
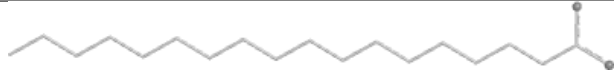
Ligand PC1 G 3104	
 Bond lengths	 Bond angles
 Torsions	 Rings

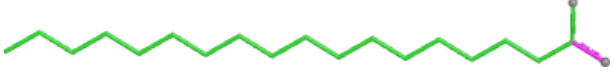
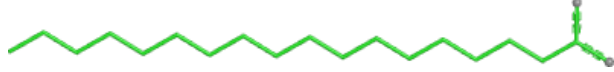
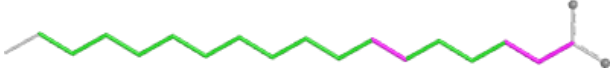
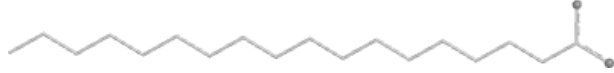
Ligand PC1 C 2709	
 Bond lengths	 Bond angles
 Torsions	 Rings

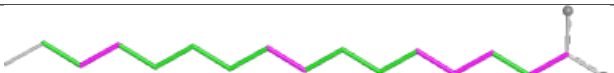
Ligand PC1 E 3102	
 Bond lengths	 Bond angles
 Torsions	 Rings

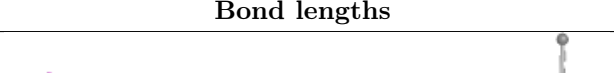
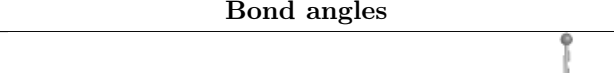
Ligand PC1 B 2904	
 Bond lengths	 Bond angles
 Torsions	 Rings

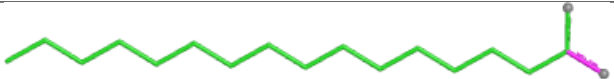
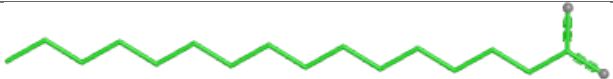
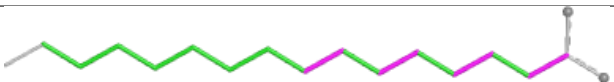
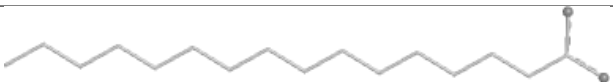
Ligand PC1 J 2501			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

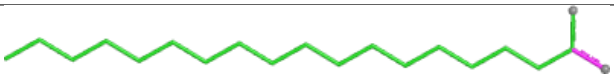
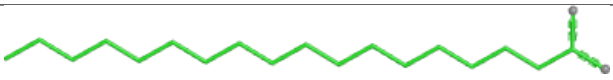
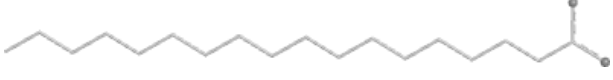
Ligand PC1 D 905			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

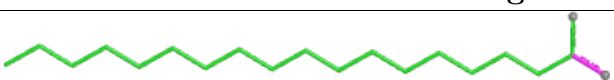
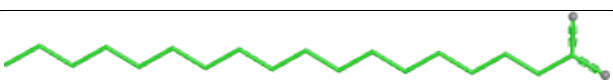
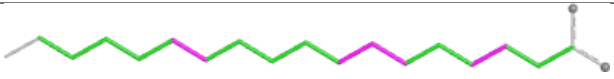
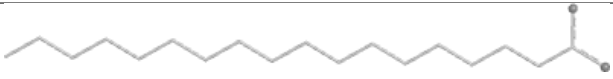
Ligand PC1 B 2907			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

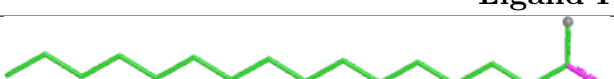
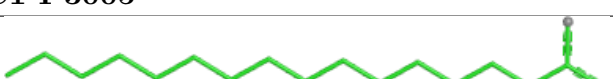
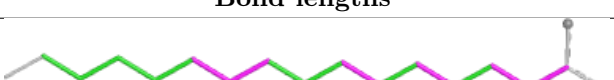
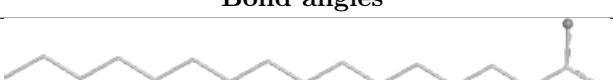
Ligand PC1 B 2909			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

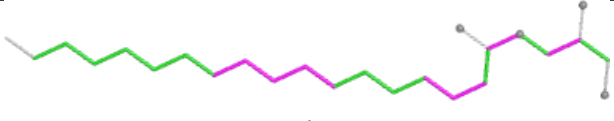
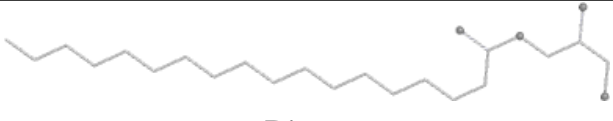
Ligand PC1 D 903			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

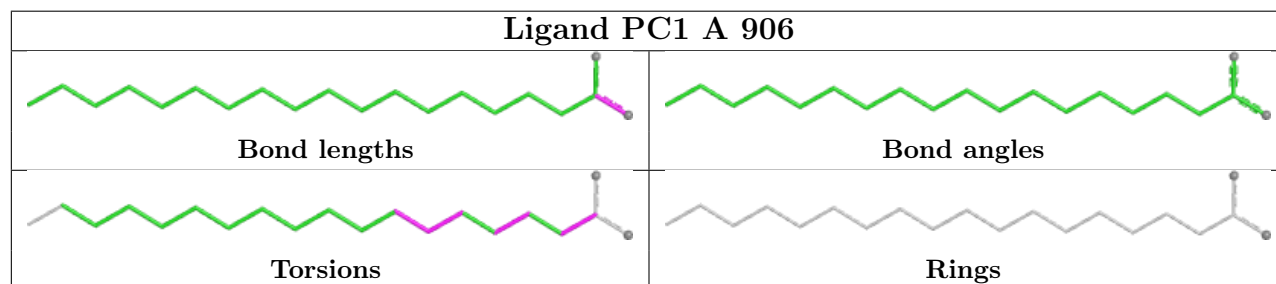
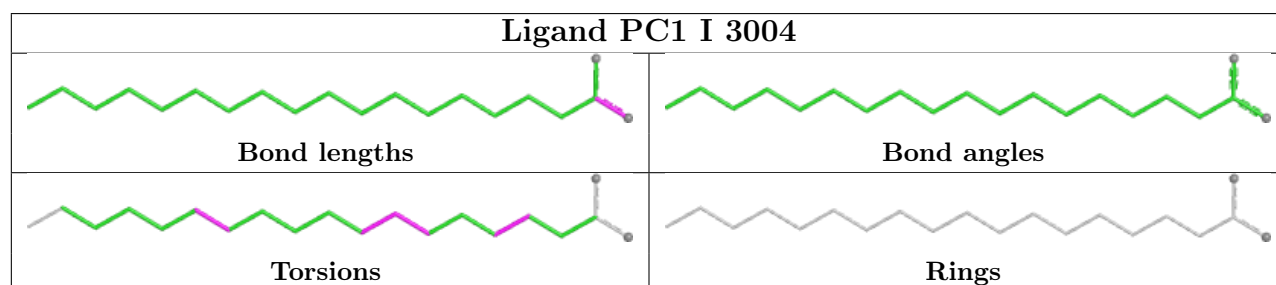
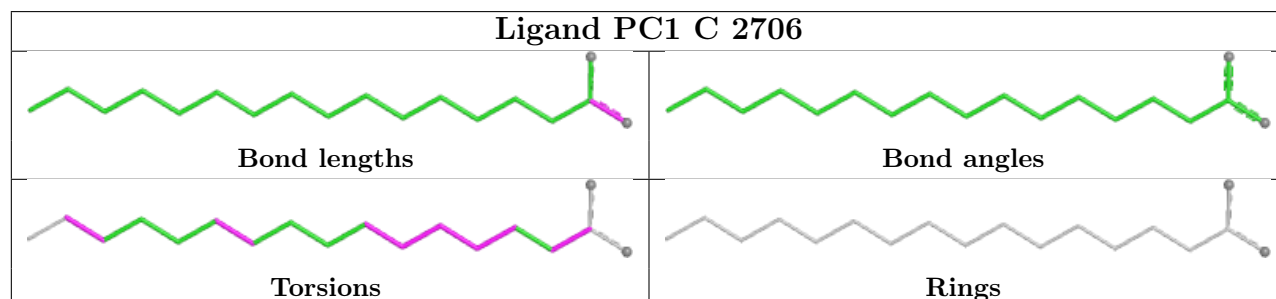
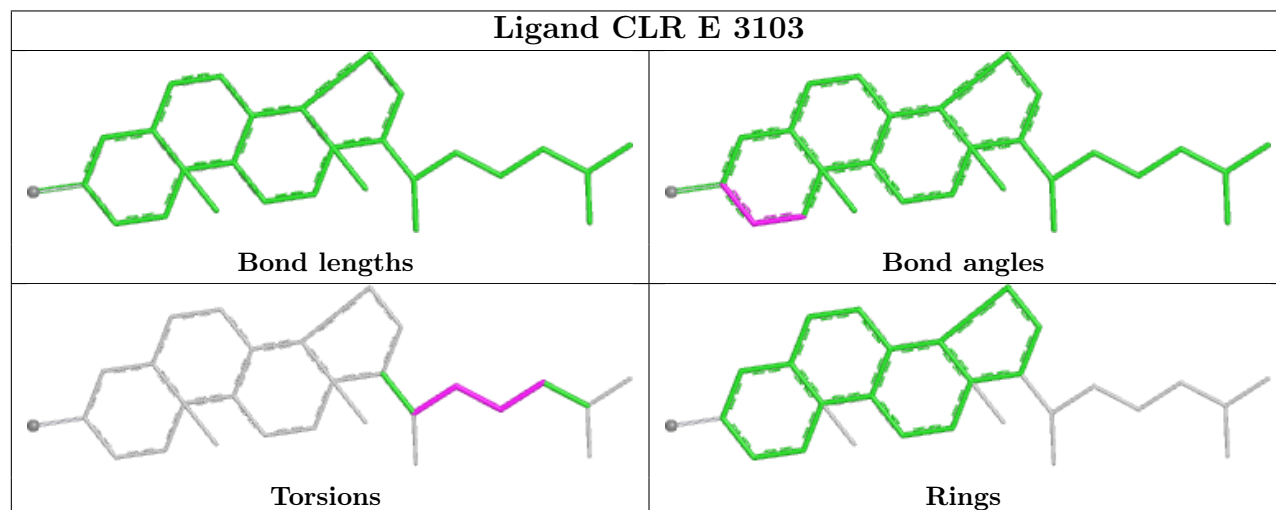
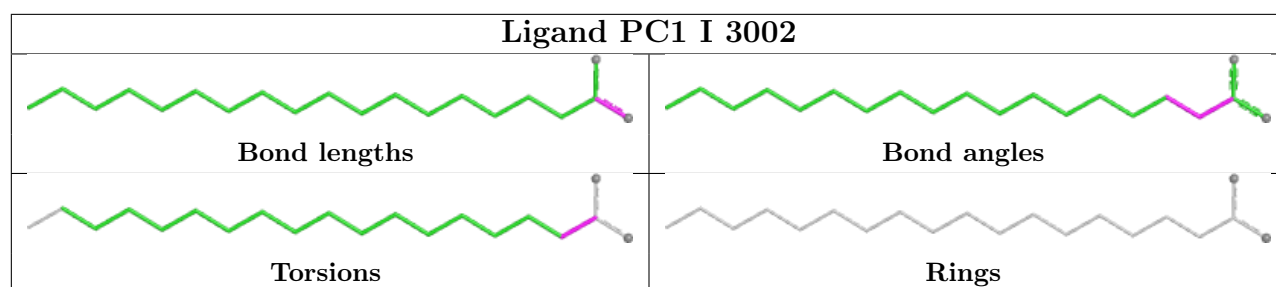
Ligand PC1 I 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

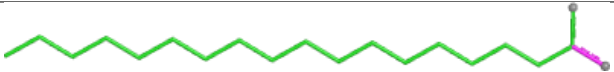
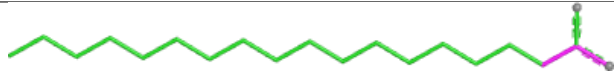
Ligand PC1 J 2502	
 Bond lengths	 Bond angles
 Torsions	 Rings

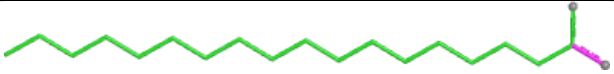
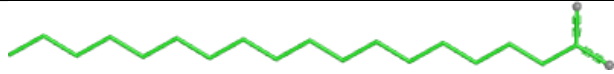
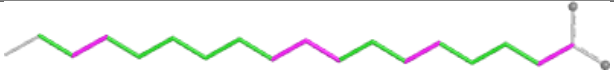
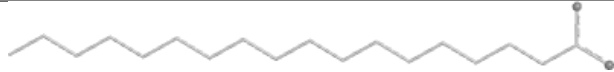
Ligand PC1 J 2503	
 Bond lengths	 Bond angles
 Torsions	 Rings

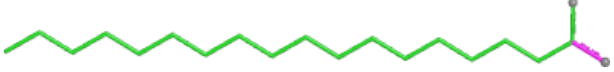
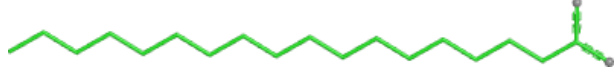
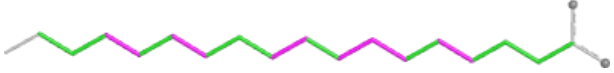
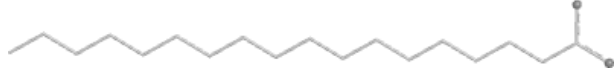
Ligand PC1 I 3005	
 Bond lengths	 Bond angles
 Torsions	 Rings

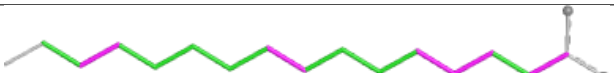
Ligand PC1 B 2910	
 Bond lengths	 Bond angles
 Torsions	 Rings

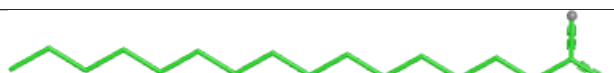
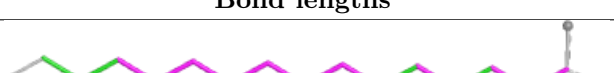
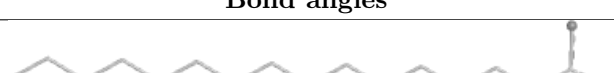


Ligand PC1 B 2901	
 Bond lengths	 Bond angles
 Torsions	 Rings

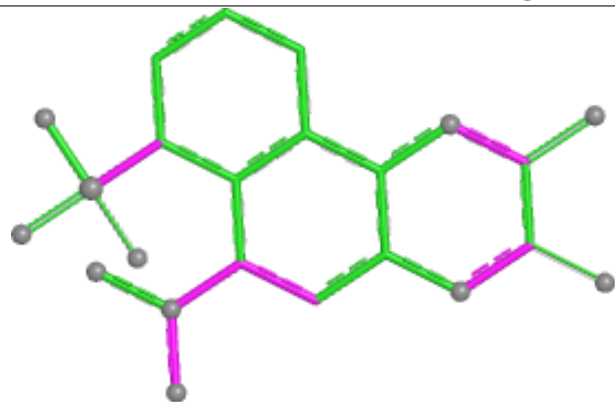
Ligand PC1 G 3101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 D 907	
 Bond lengths	 Bond angles
 Torsions	 Rings

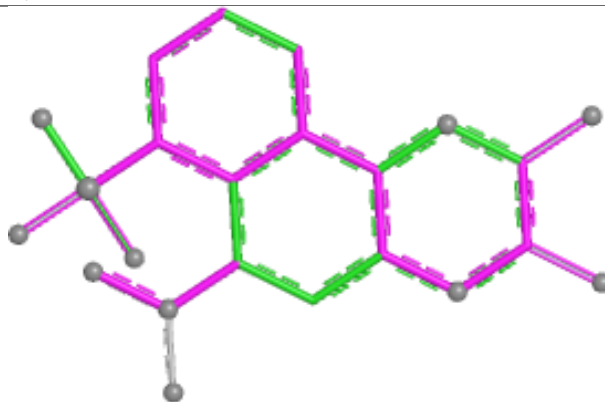
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 C 2701	
 Bond lengths	 Bond angles
 Torsions	 Rings

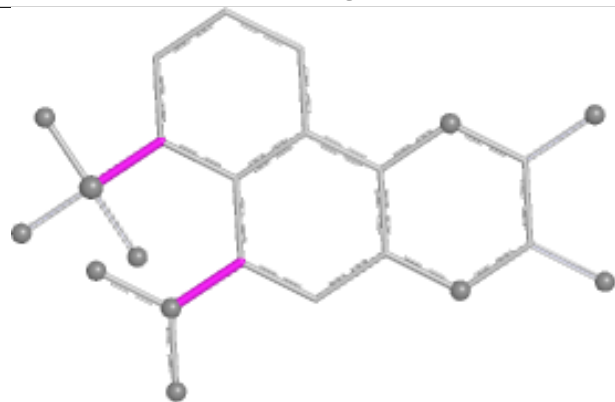
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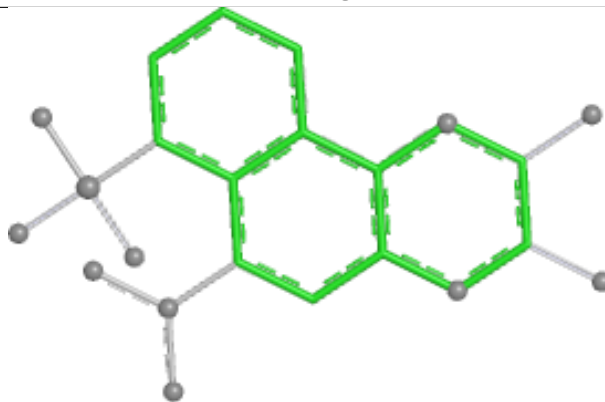
Bond lengths



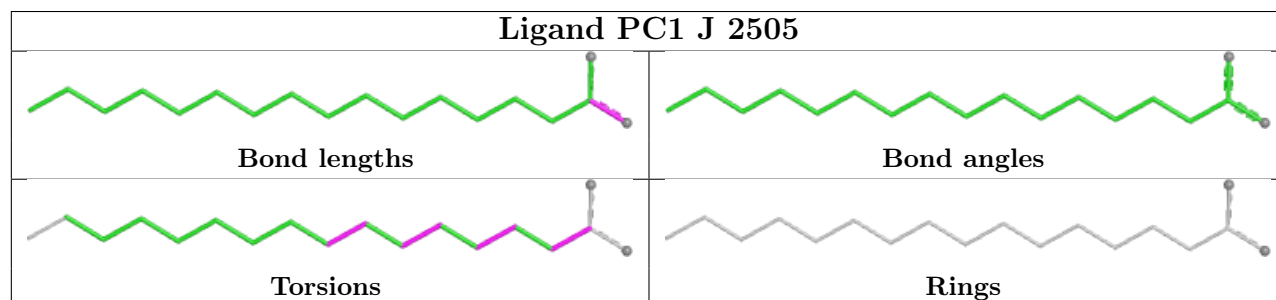
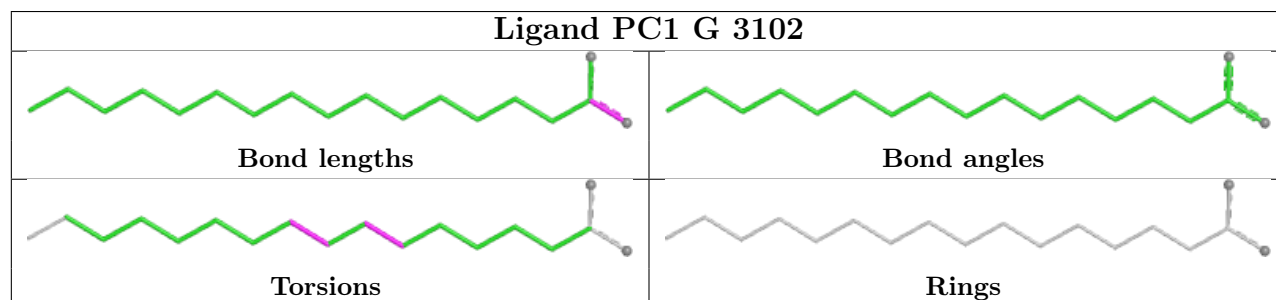
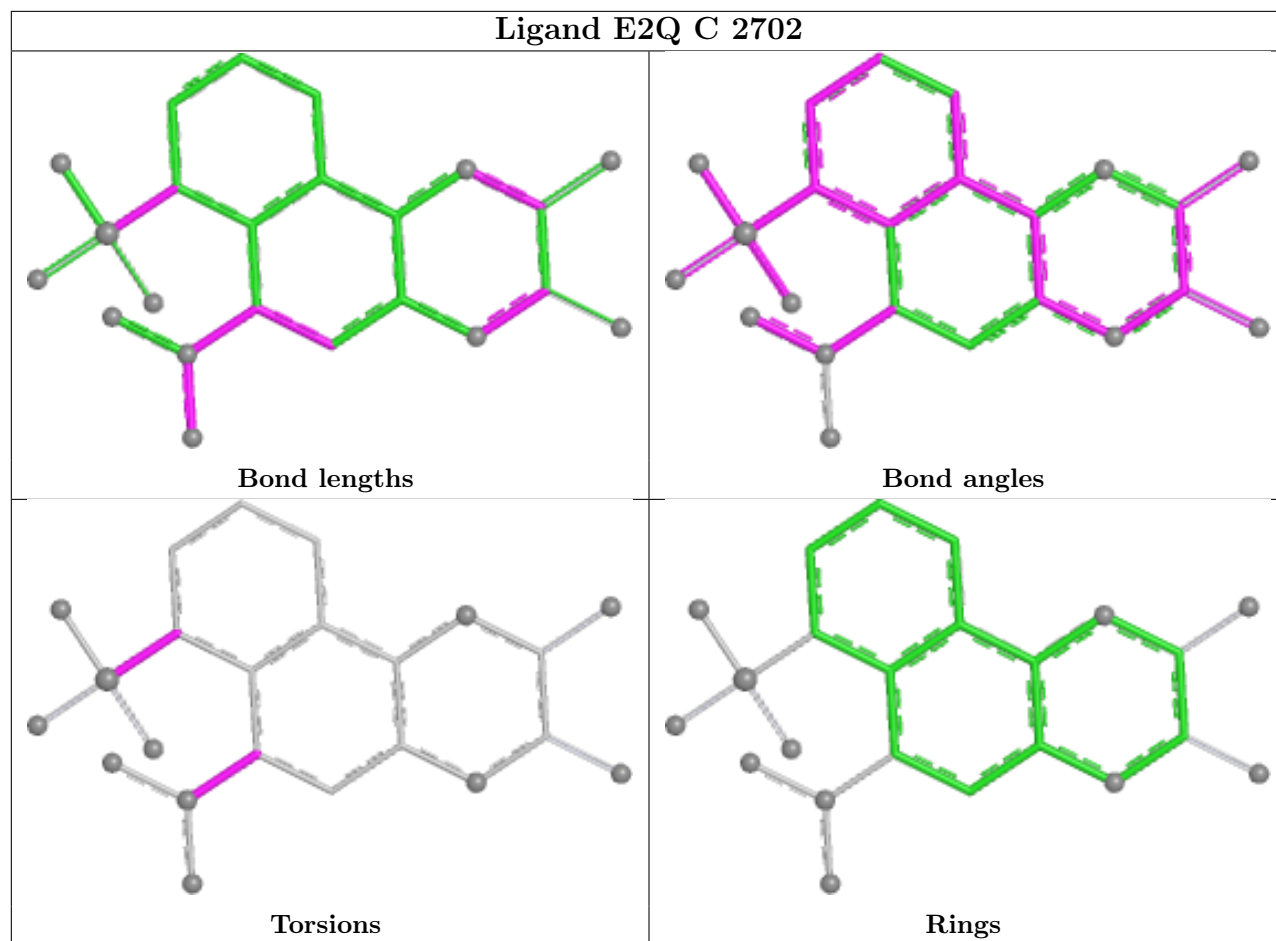
Bond angles

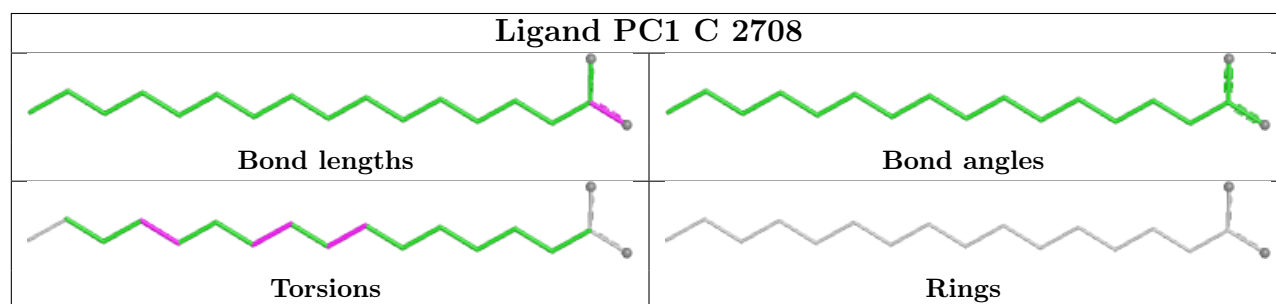
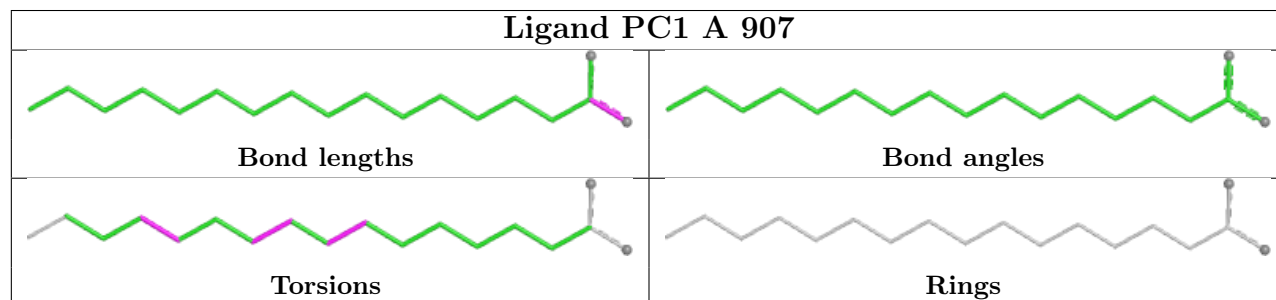
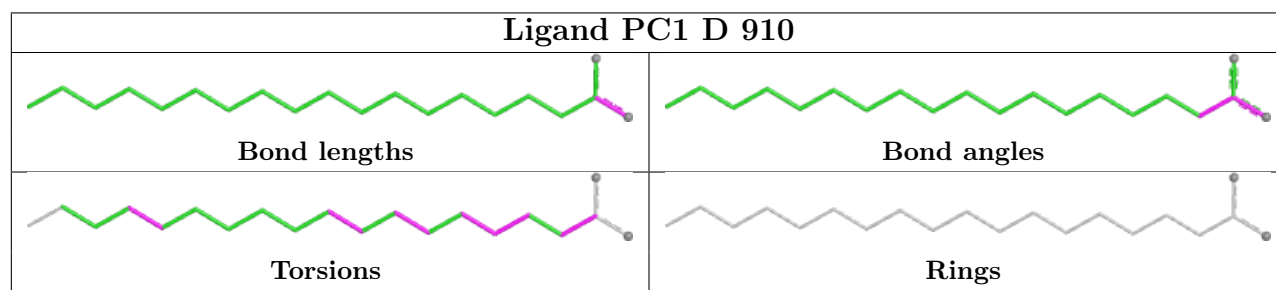
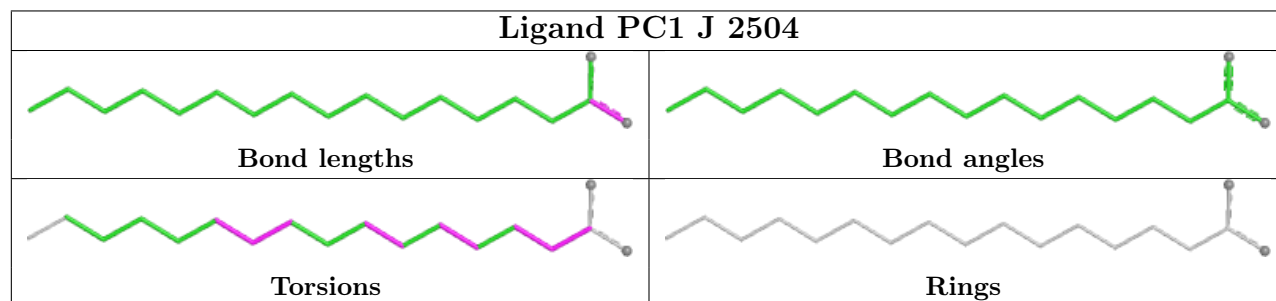
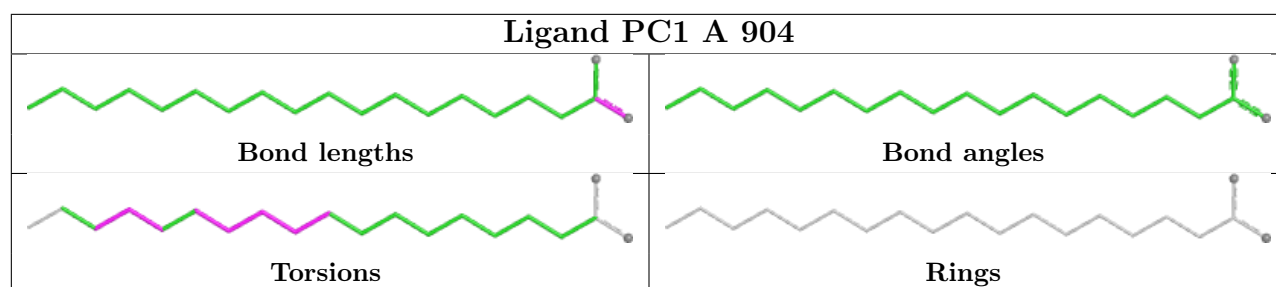


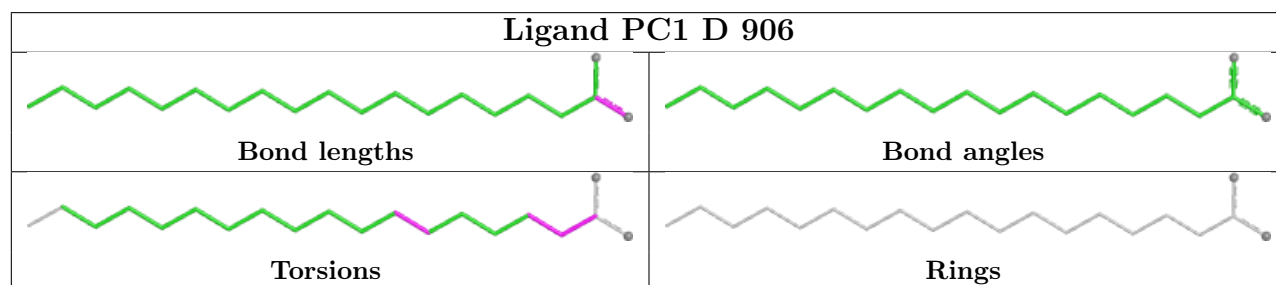
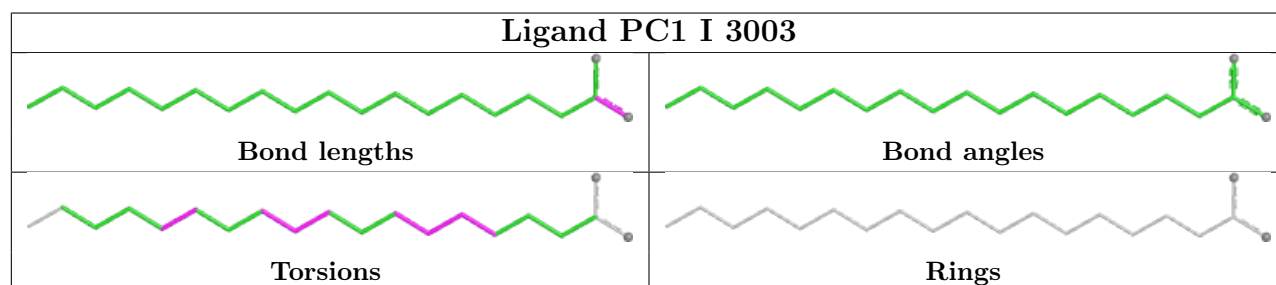
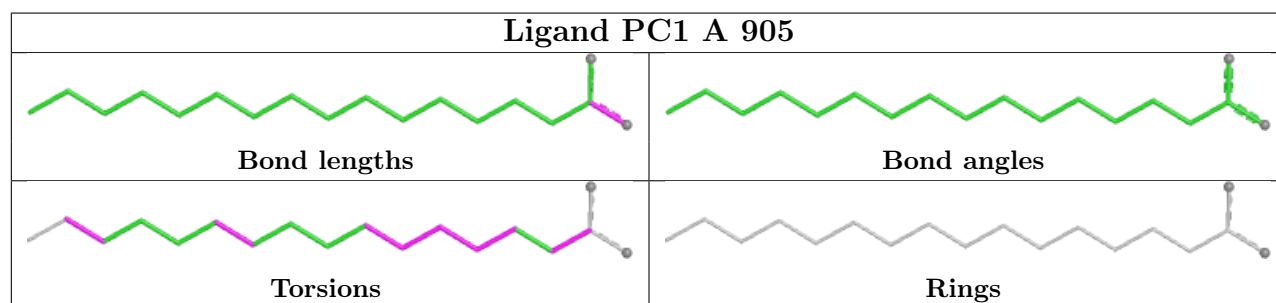
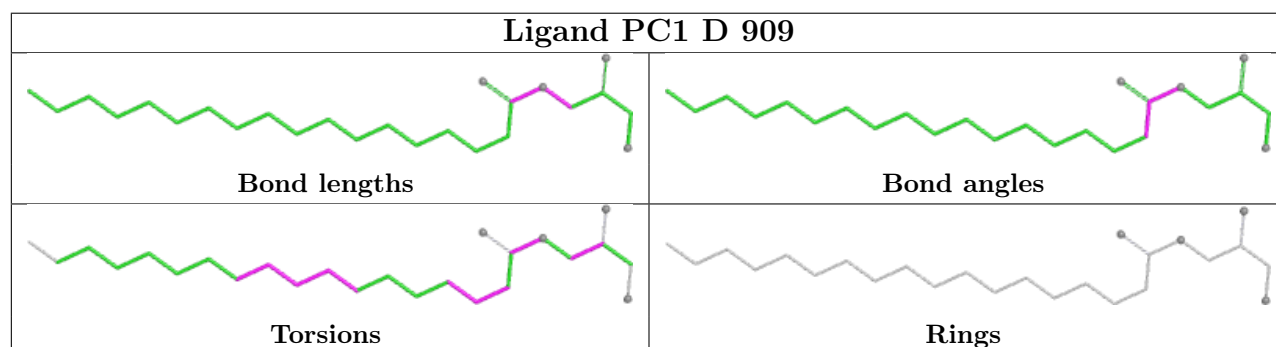
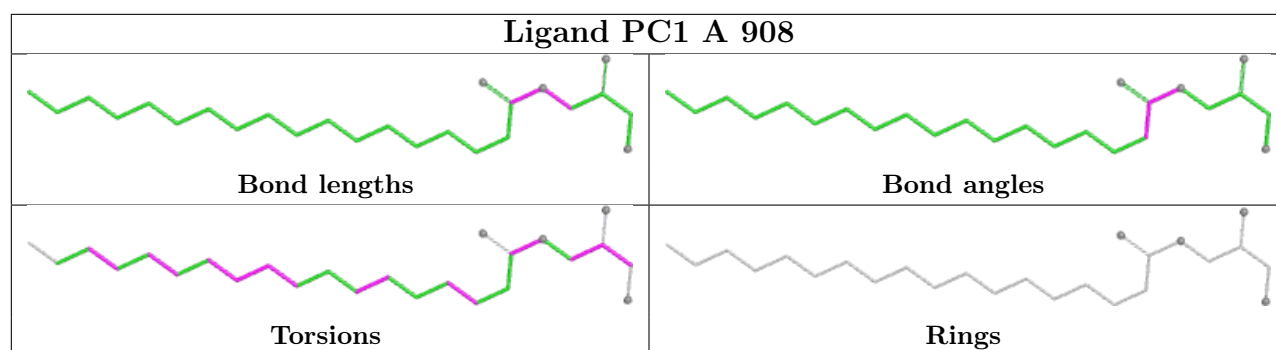
Torsions

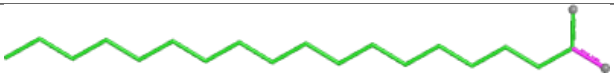
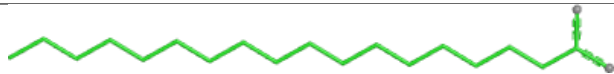
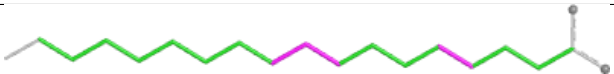


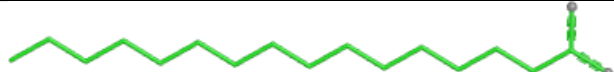
Rings

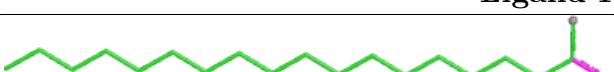
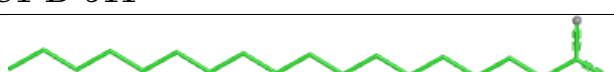
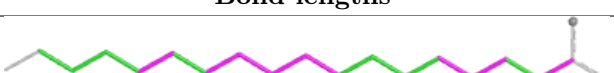


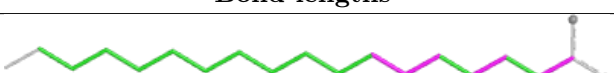


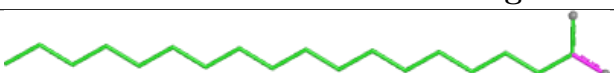
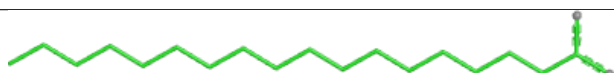
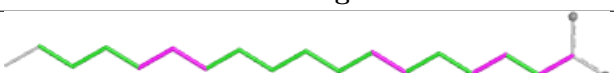
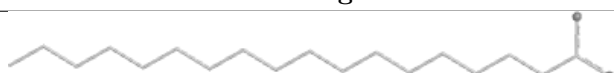


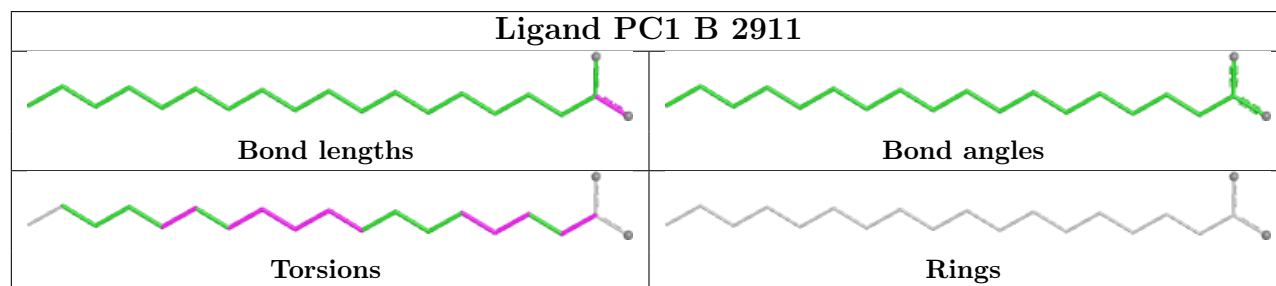
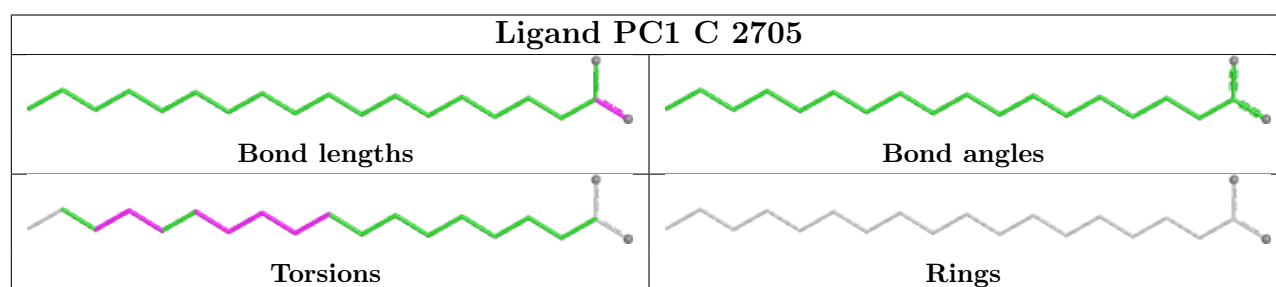
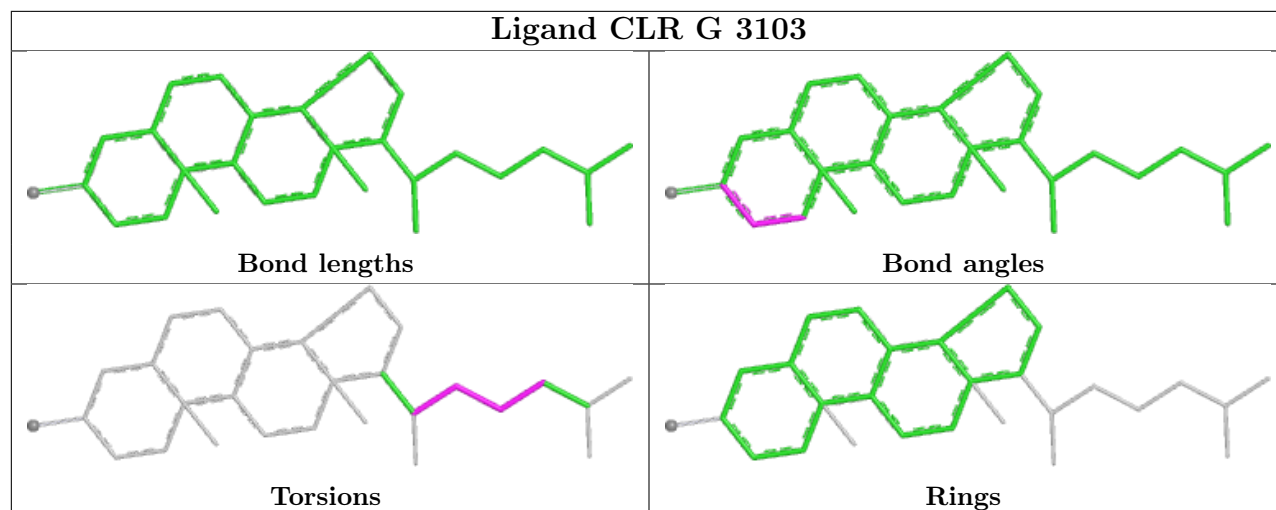
Ligand PC1 B 2906			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

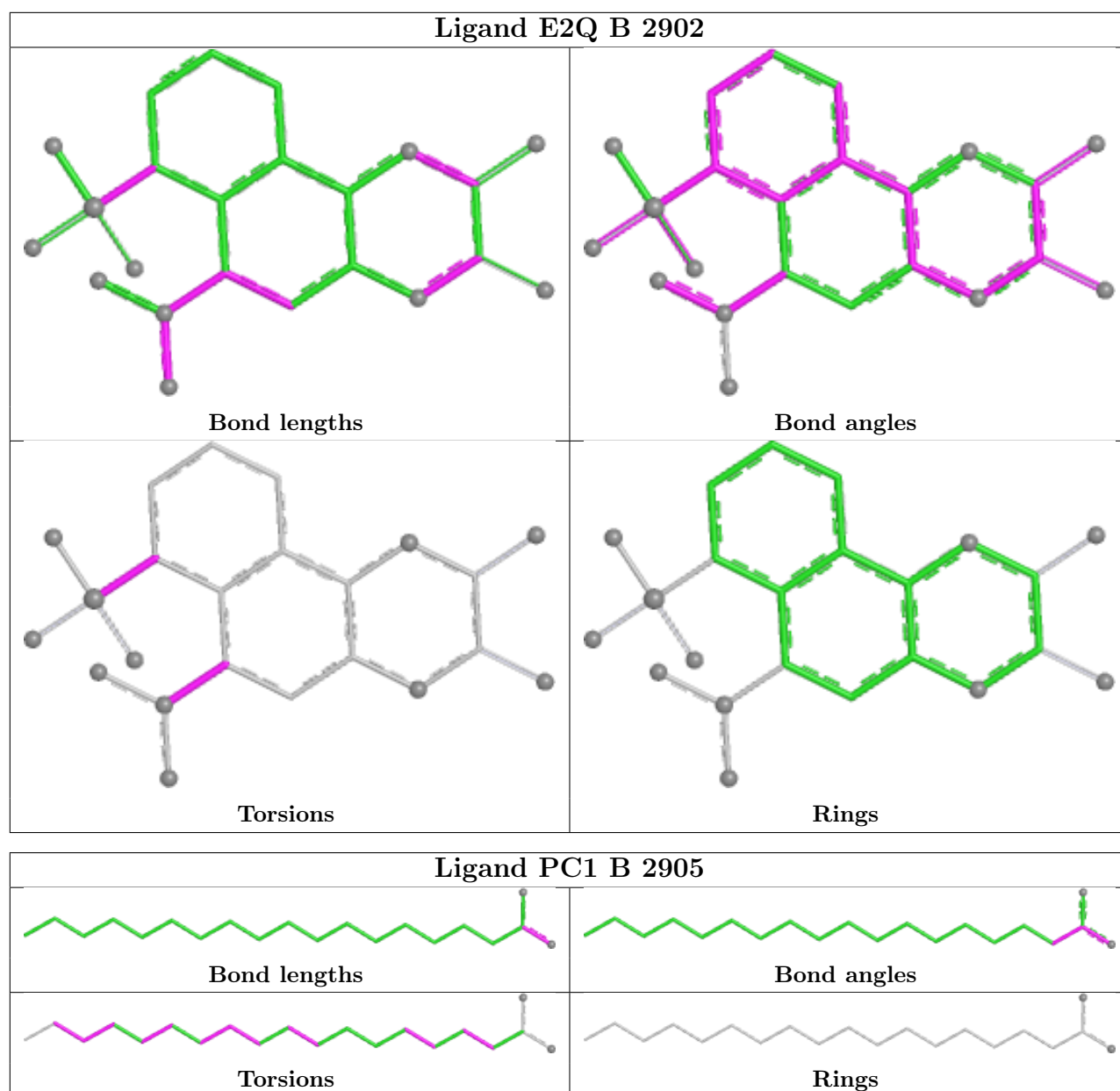
Ligand PC1 A 909			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 D 911			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 C 2707			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 E 3104			
 Bond lengths		 Bond angles	
 Torsions		 Rings	





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.

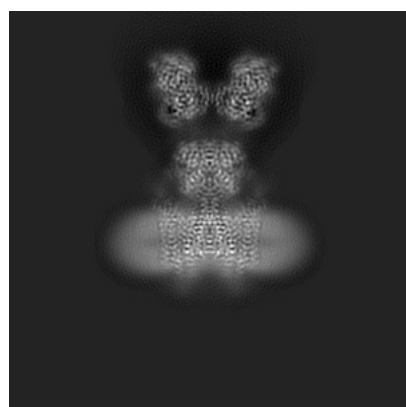
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12802. These allow visual inspection of the internal detail of the map and identification of artifacts.

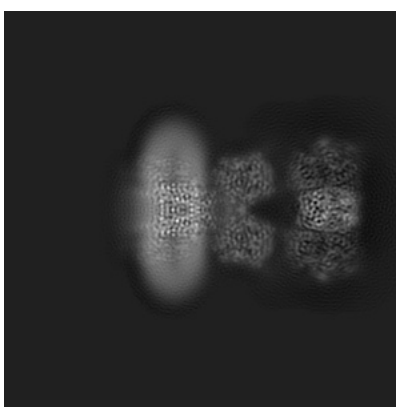
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

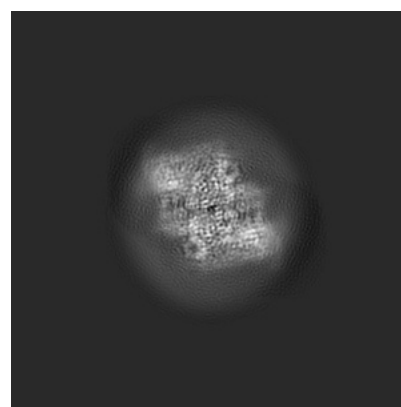
6.1.1 Primary map



X



Y

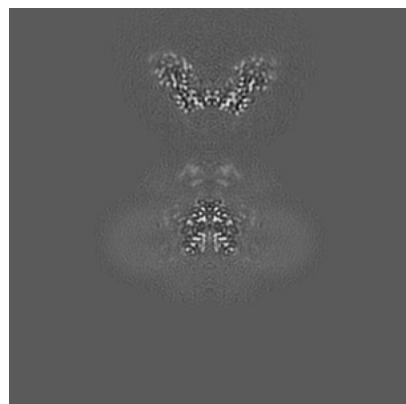


Z

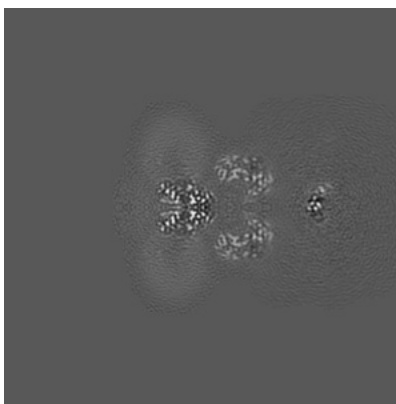
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

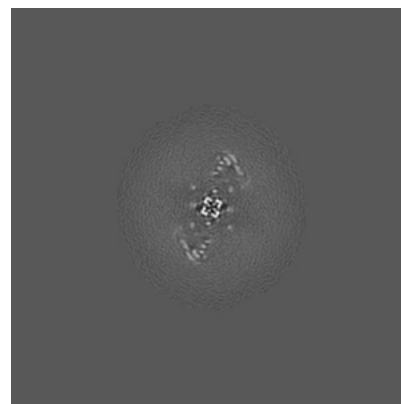
6.2.1 Primary map



X Index: 160



Y Index: 160

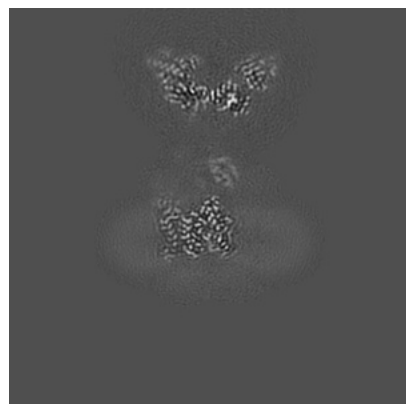


Z Index: 160

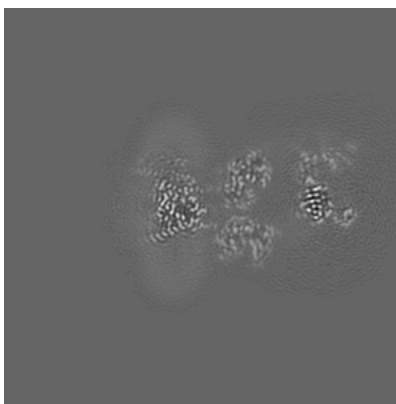
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

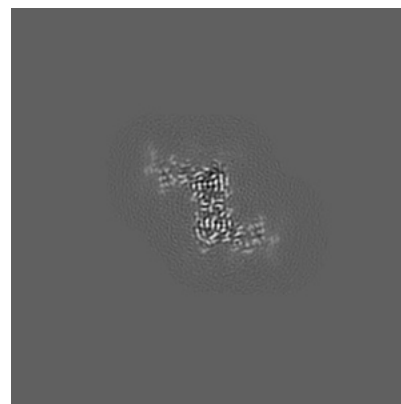
6.3.1 Primary map



X Index: 155



Y Index: 147

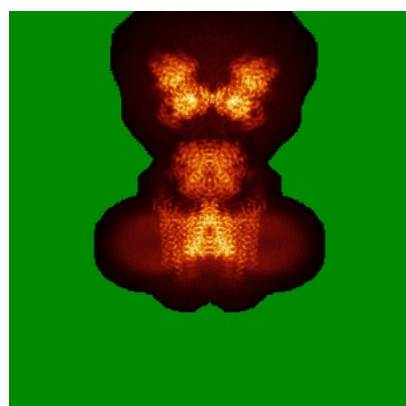


Z Index: 248

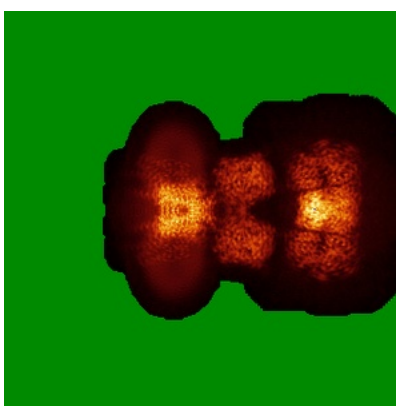
The images above show the largest variance slices of the map in three orthogonal directions.

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

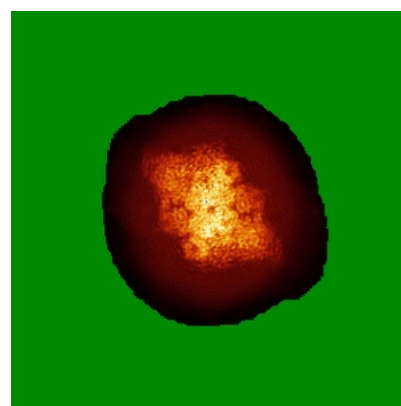
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

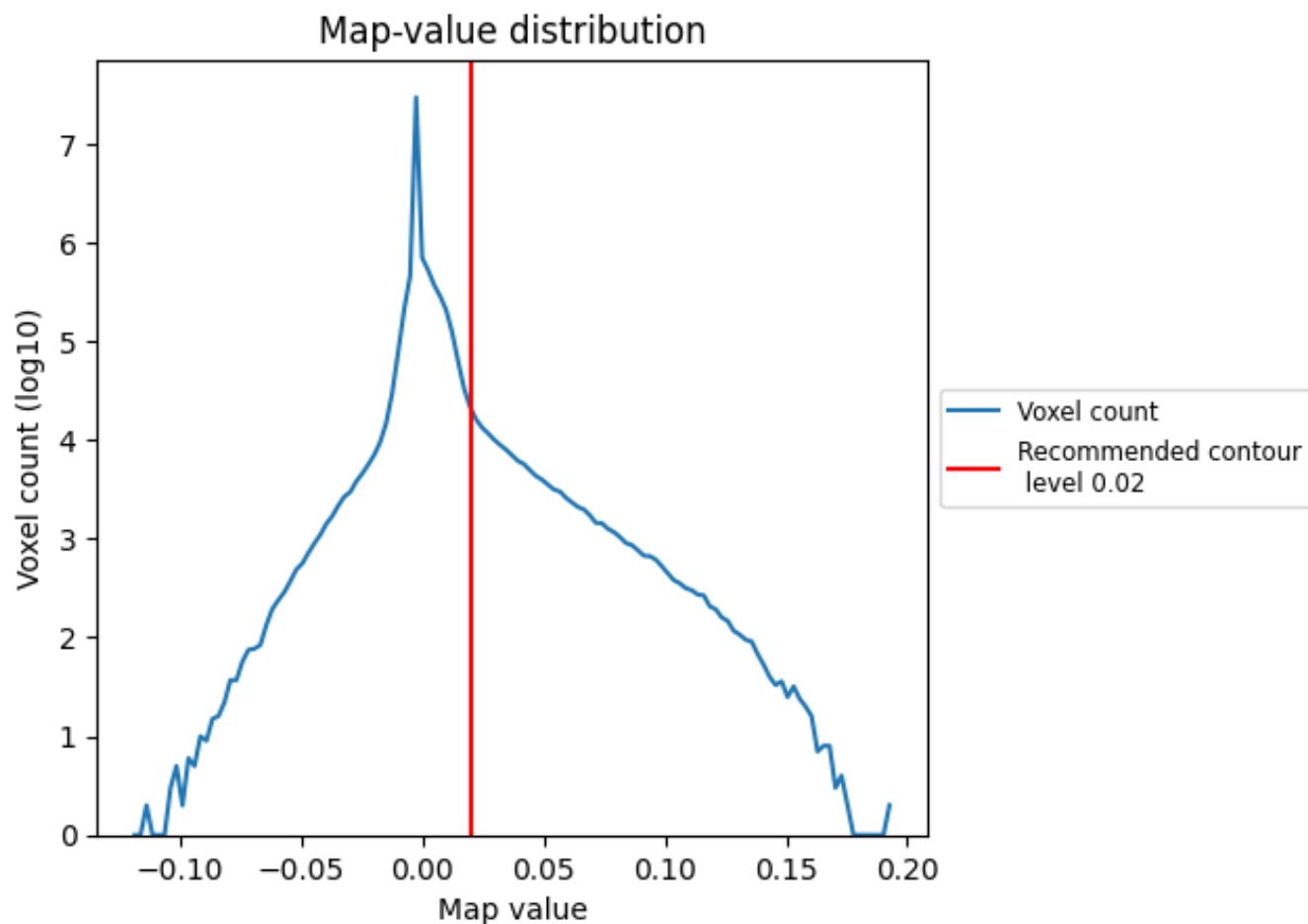
6.6 Mask visualisation

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

7 Map analysis [i](#)

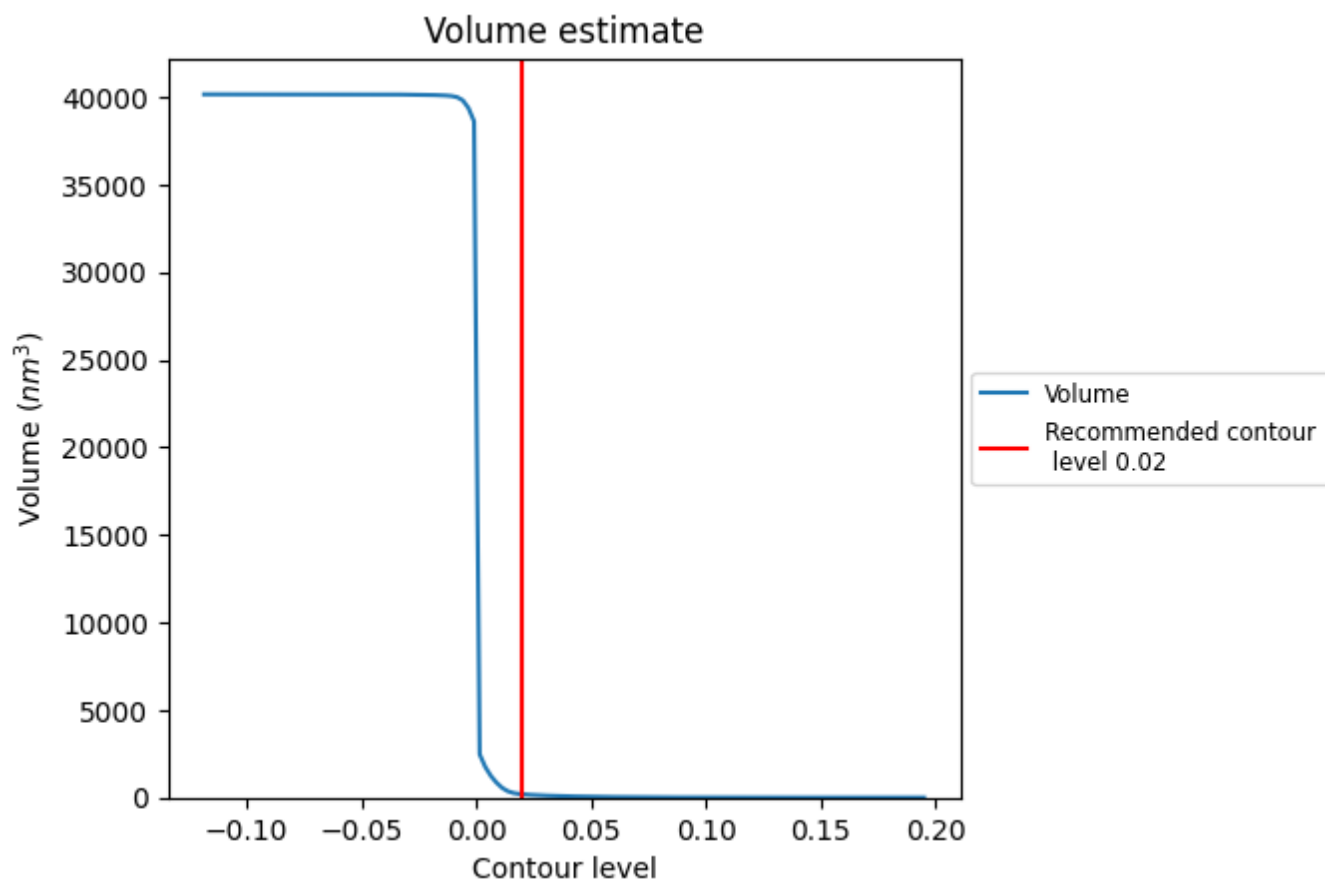
This section contains the results of statistical analysis of the map.

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.

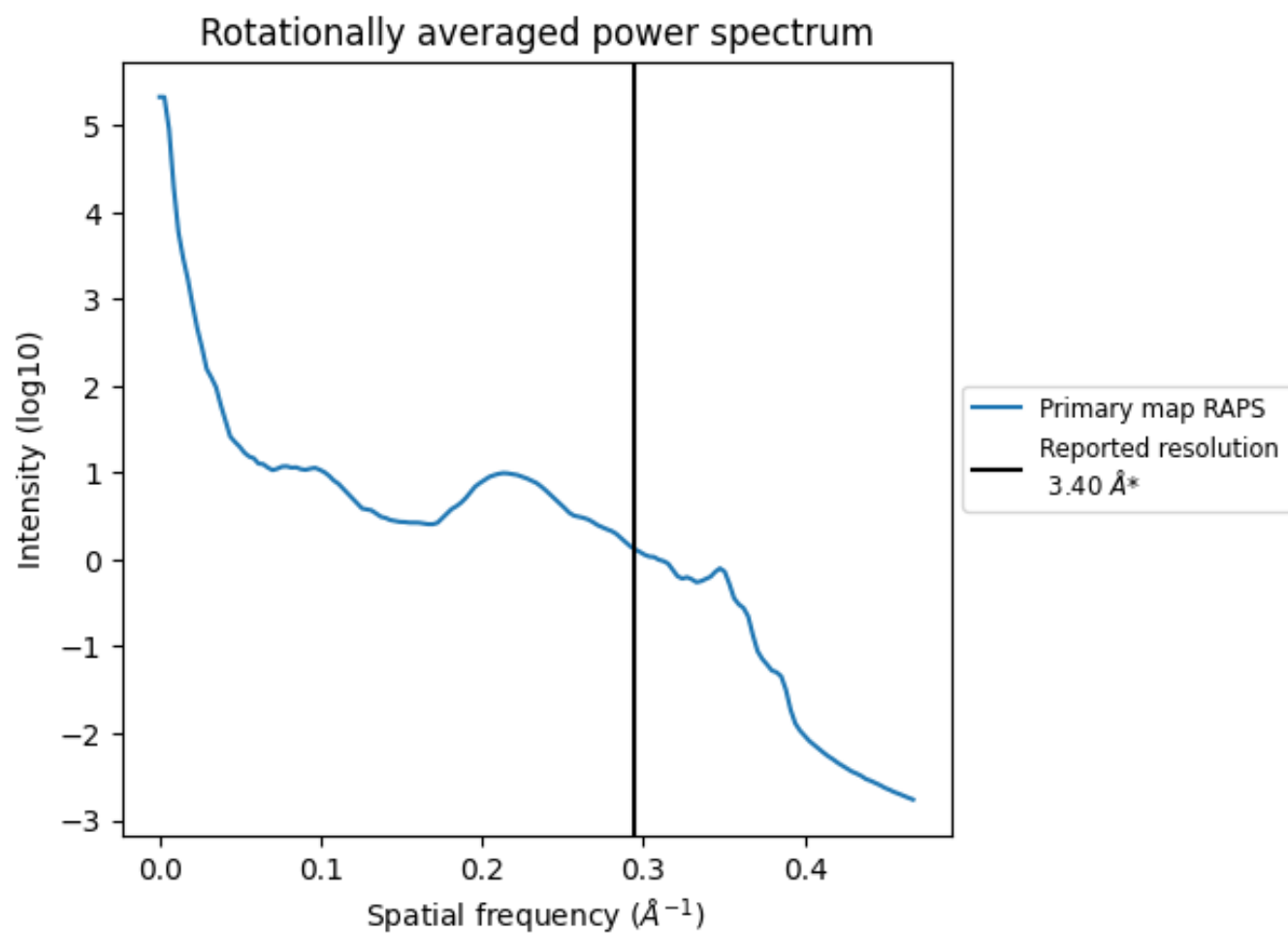
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 173 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 0.294 Å⁻¹

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

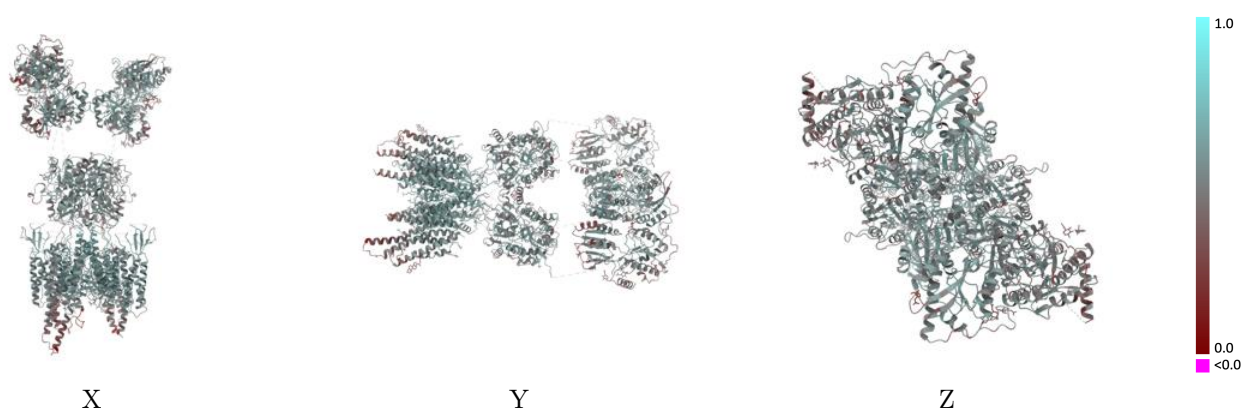
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-12802 and PDB model 7OCA. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

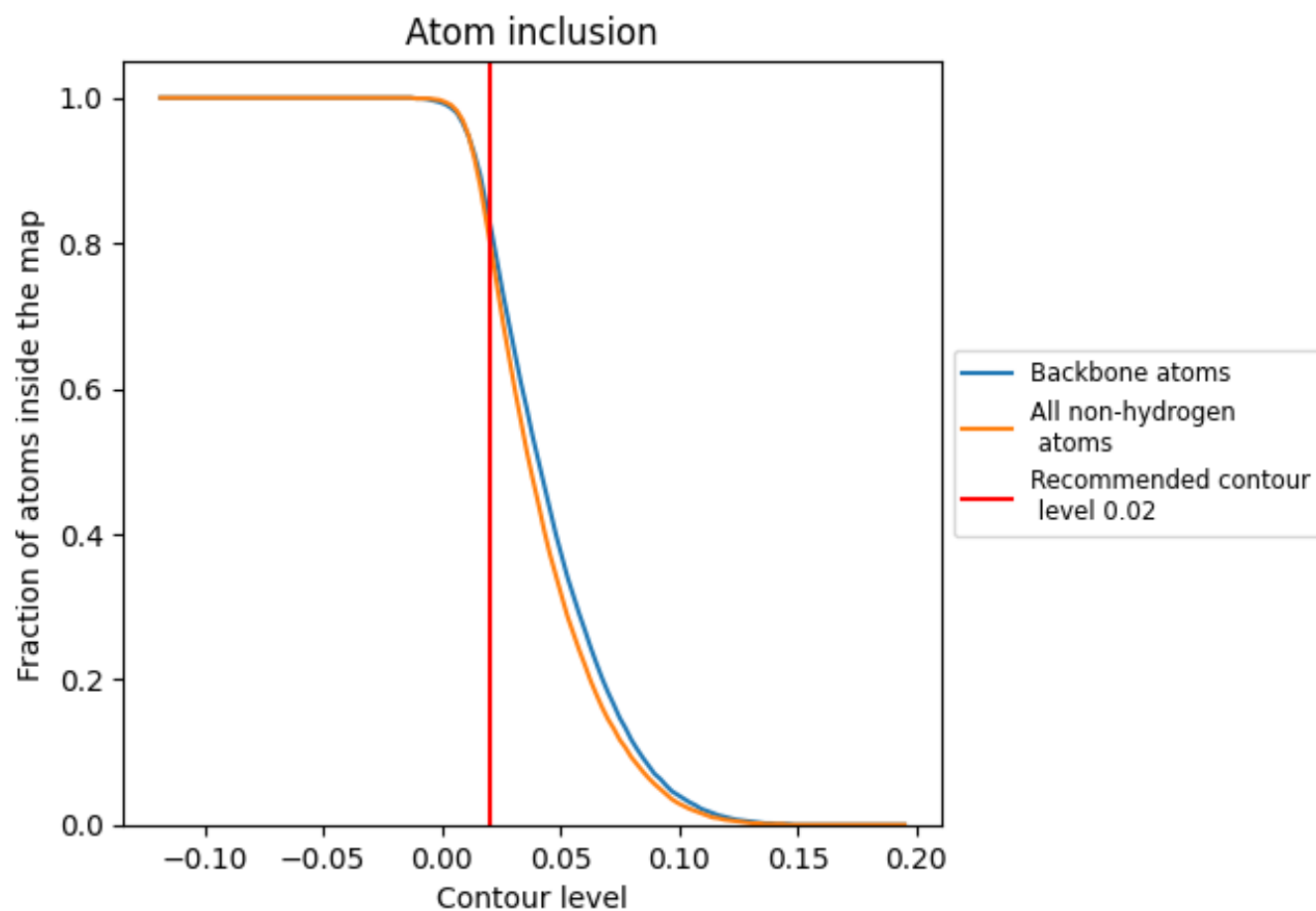


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 81% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.5250
A	0.8130	0.5170
B	0.8630	0.5460
C	0.8160	0.5180
D	0.8620	0.5460
E	0.5500	0.4560
F	0.2050	0.3300
G	0.5420	0.4530
H	0.4290	0.3870
I	0.8230	0.5490
J	0.8180	0.5470
K	0.7140	0.4350
L	0.6790	0.4400
M	0.2050	0.3050
N	0.3570	0.4080

1.0

0.0

<0.0