Full wwPDB EM Validation Report ⓘ

Aug 8, 2023 – 12:19 PM JST

PDB ID	:	8JFZ
EMDB ID	:	EMD-36220
Title	:	Cryo-EM structure of Na+,K+-ATPase in the E1.Mg2+ state.
Authors	:	Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on	:	2023-05-19
Resolution	:	3.50 Å(reported)
Based on initial model	:	8JBM

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:

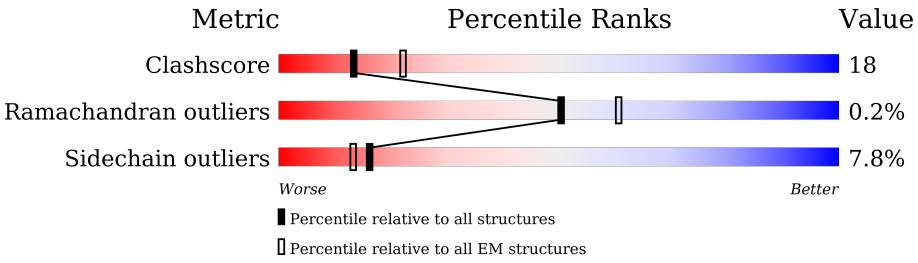
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	305	62% 30%
1	D	305	61% 31% 5%
2	A	1028	21% 60% 34%
2	C	1028	23% 60% 34%
3	E	94	33% 10% 57%
3	G	94	33% 10% 57%
4	F	6	67% 83% 17%
4	K	6	67% 83% 17%

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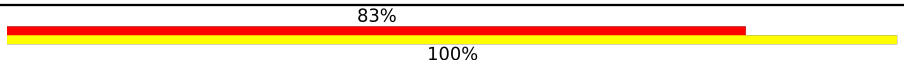
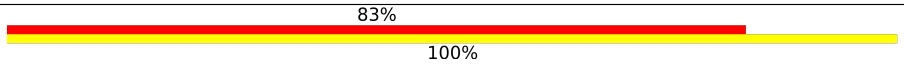
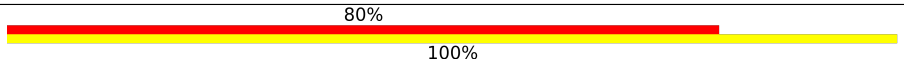
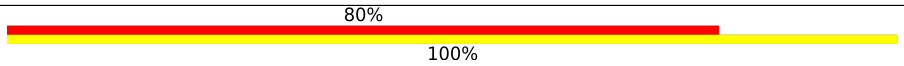
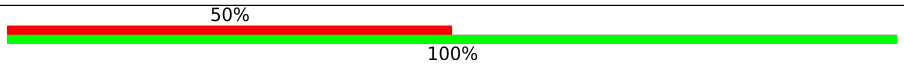
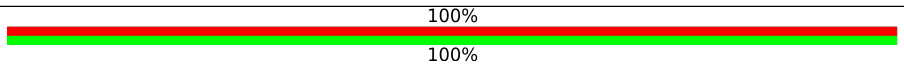
Mol	Chain	Length	Quality of chain
5	H	6	
5	L	6	
6	I	5	
6	M	5	
7	J	2	
7	N	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22340 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 Na+,K+-ATPase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	294	Total	C	N	O	S	0	0
			2399	1551	394	443	11		
1	B	294	Total	C	N	O	S	0	0
			2399	1551	394	443	11		

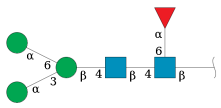
- Molecule 2 is a protein called Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	987	Total	C	N	O	S	0	0
			7633	4859	1284	1444	46		
2	A	987	Total	C	N	O	S	0	0
			7633	4859	1284	1444	46		

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	40	Total	C	N	O	S	0	0
			311	203	51	55	2		
3	G	40	Total	C	N	O	S	0	0
			311	203	51	55	2		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	6	Total	C	N	O	0	0
			71	40	2	29		

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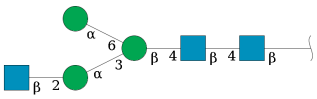
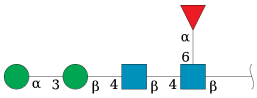
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	H	6	Total	C	N	O	0	0
			75	42	3	30		
5	L	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	5	Total	C	N	O	0	0
			60	34	2	24		
6	M	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 7 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
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

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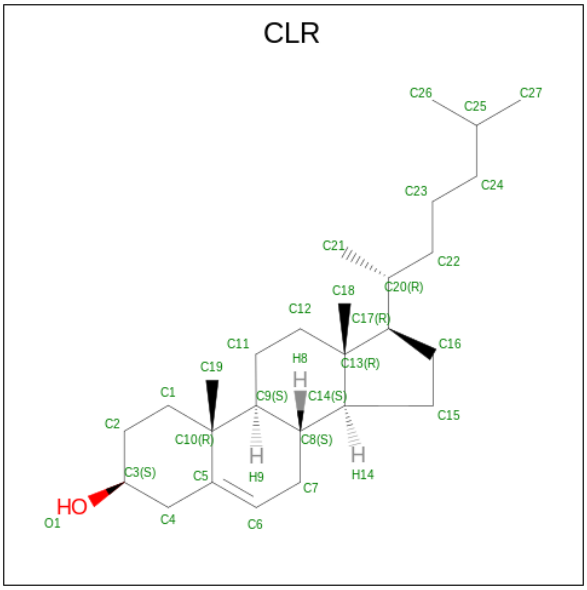
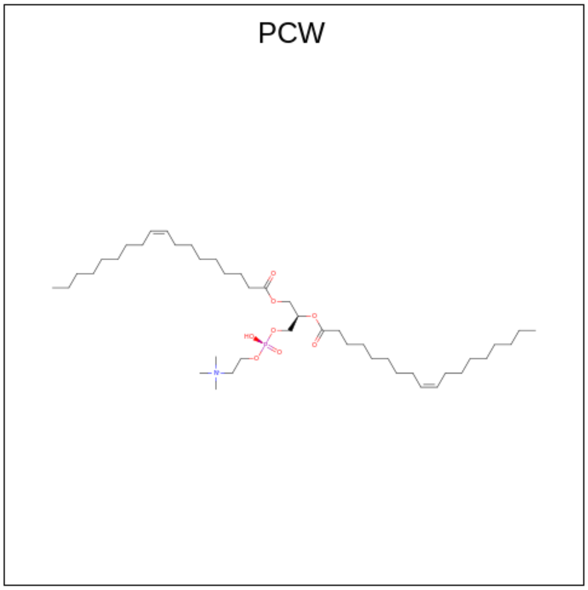
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			28	27	1	
8	C	1	Total	C	O	0
			28	27	1	
8	E	1	Total	C	O	0
			28	27	1	
8	B	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	
8	A	1	Total	C	O	0
			28	27	1	
8	G	1	Total	C	O	0
			28	27	1	

- Molecule 9 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total C N O P 22 12 1 8 1	0
9	C	1	Total C N O P 22 12 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	C	1	Total C N O P 54 44 1 8 1	0
9	E	1	Total C N O P 54 44 1 8 1	0
9	A	1	Total C N O P 22 12 1 8 1	0
9	A	1	Total C N O P 22 12 1 8 1	0
9	A	1	Total C N O P 54 44 1 8 1	0
9	A	1	Total C N O P 54 44 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	C	2	Total	Mg	0
			2	2	
10	A	2	Total	Mg	0
			2	2	

- Molecule 11 is water.

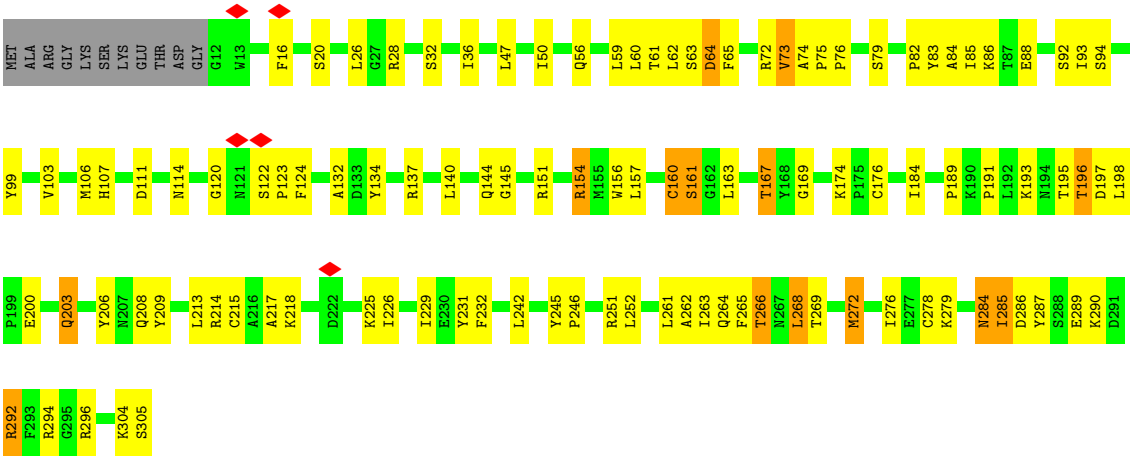
Mol	Chain	Residues	Atoms		AltConf
11	C	3	Total	O	0
			3	3	
11	A	3	Total	O	0
			3	3	

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.

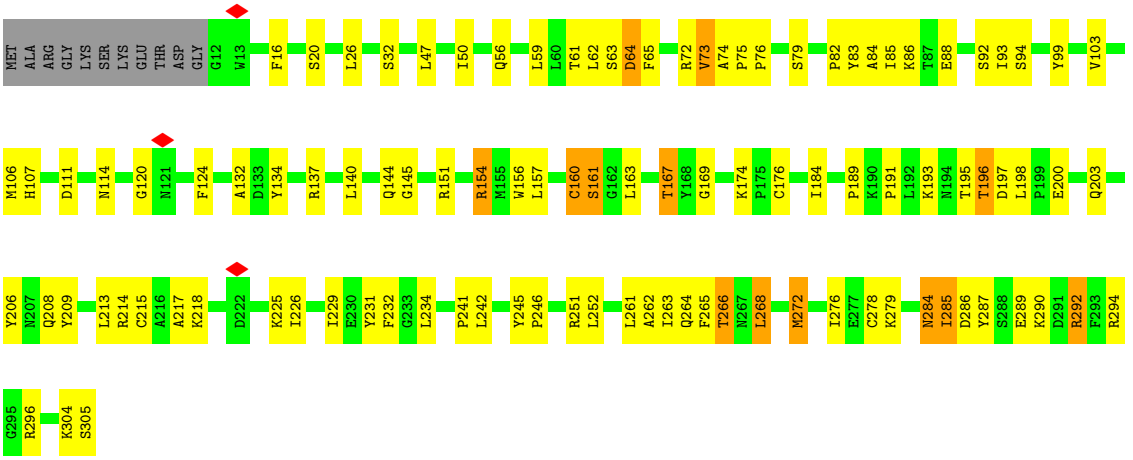
• Molecule 1: Na+,K+-ATPase beta subunit

Chain D:



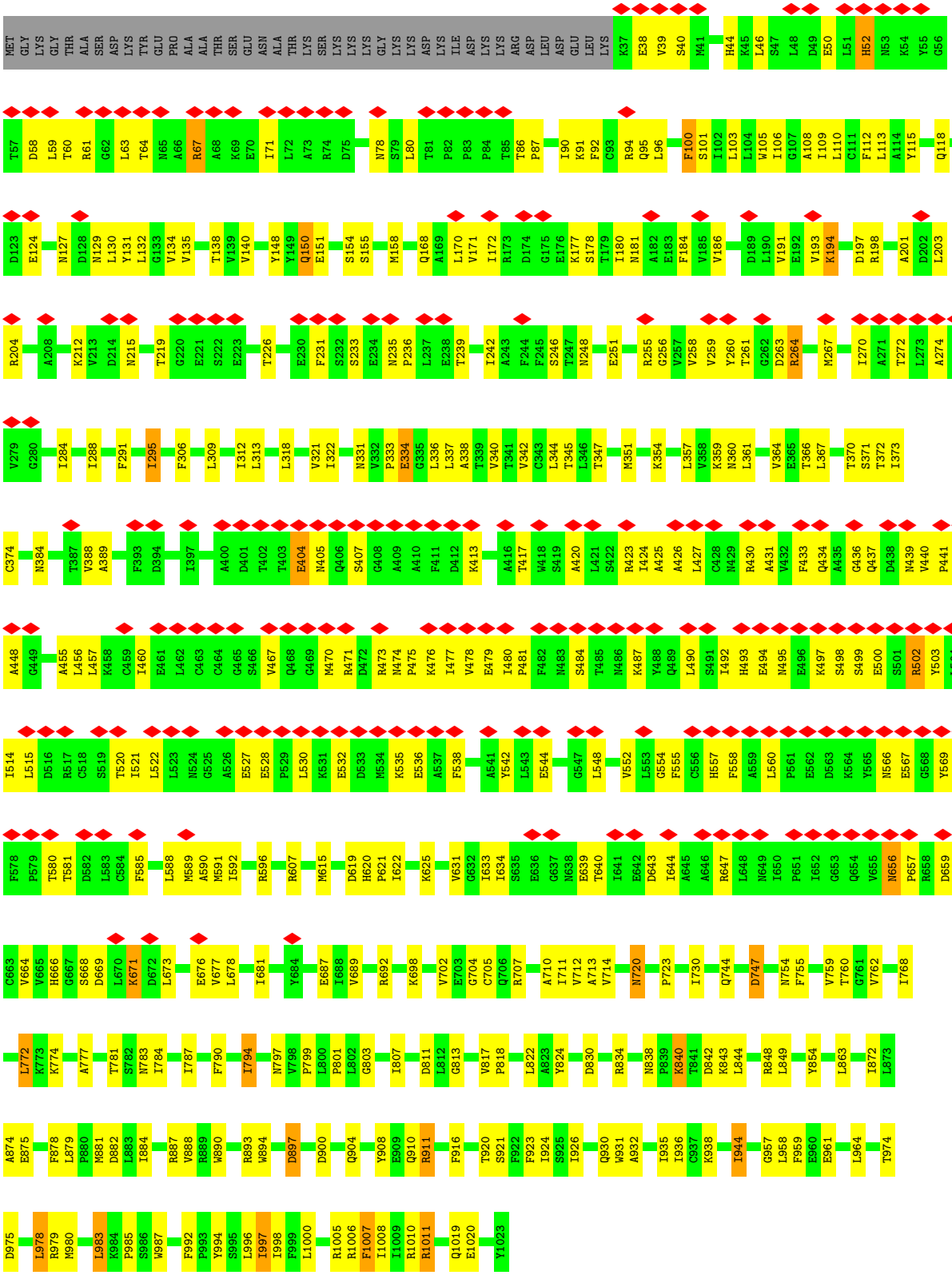
• Molecule 1: Na+,K+-ATPase beta subunit

Chain B:

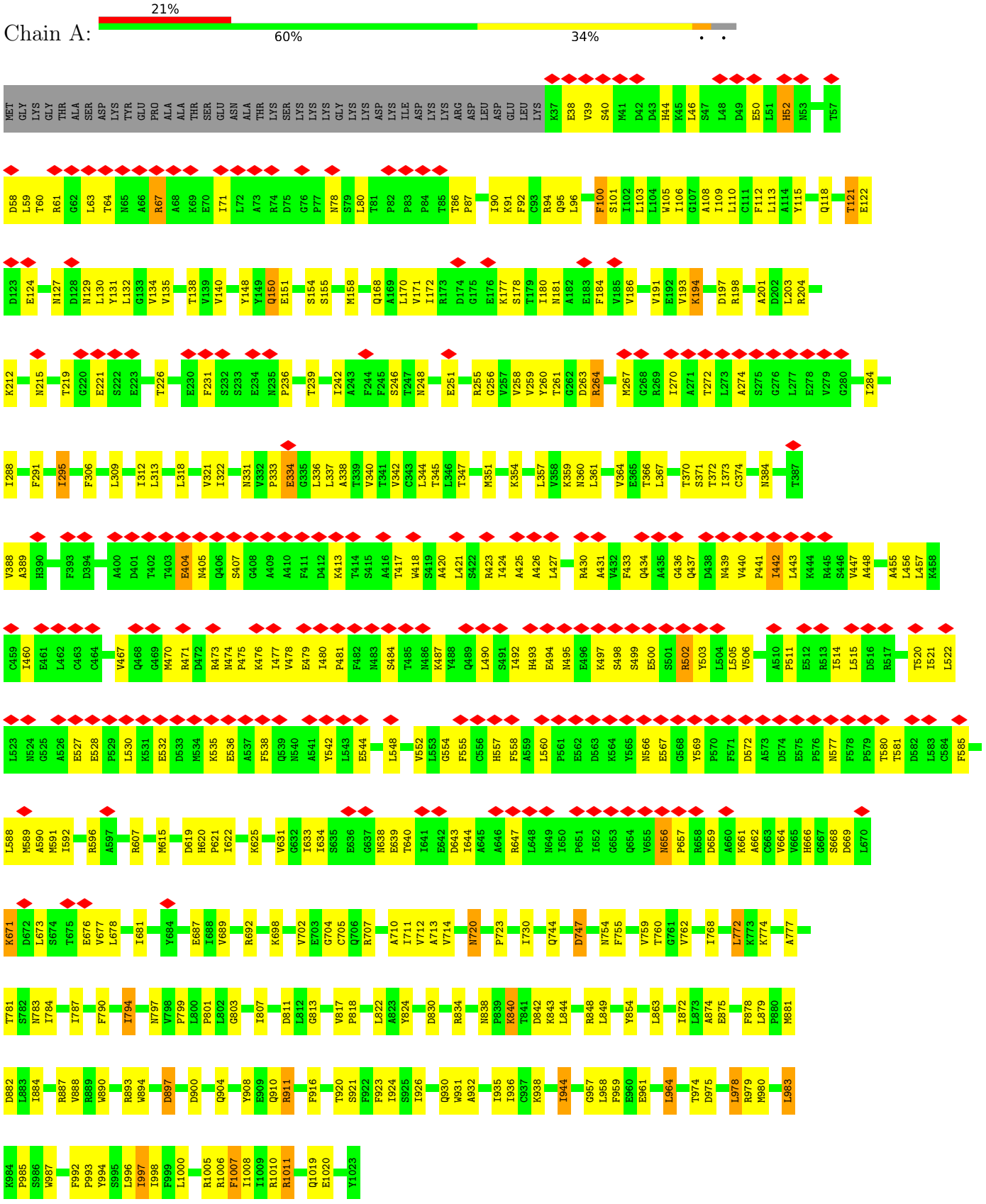


• Molecule 2: Na, K-ATPase alpha subunit

Chain C:



- Molecule 2: Na, K-ATPase alpha subunit



• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:

• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

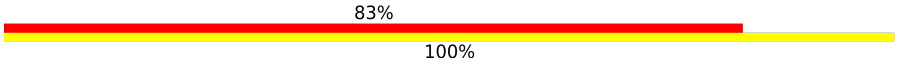
Chain K:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

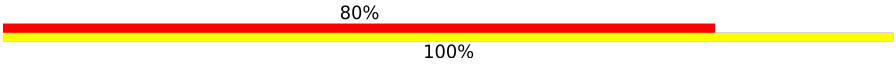


• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain J:

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

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	36635	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	258.24, 258.24, 258.24	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG, MAN, FUC, CLR, PCW, 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	B	0.34	0/2462	0.73	0/3317
1	D	0.34	0/2462	0.73	0/3317
2	A	0.38	0/7783	0.72	0/10560
2	C	0.38	0/7783	0.72	0/10560
3	E	0.30	0/315	0.54	0/427
3	G	0.30	0/315	0.54	0/427
All	All	0.37	0/21120	0.72	0/28608

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	B	2399	0	2354	73	0
1	D	2399	0	2354	75	0
2	A	7633	0	7654	327	0
2	C	7633	0	7654	323	0
3	E	311	0	323	5	0
3	G	311	0	323	5	0
4	F	71	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	71	0	61	1	0
5	H	75	0	64	0	0
5	L	75	0	64	0	0
6	I	60	0	52	0	0
6	M	60	0	52	0	0
7	J	28	0	25	0	0
7	N	28	0	25	0	0
8	A	84	0	138	16	0
8	B	28	0	46	0	0
8	C	28	0	46	0	0
8	D	28	0	46	1	0
8	E	28	0	46	8	0
8	G	28	0	46	8	0
9	A	422	0	624	51	0
9	C	422	0	624	55	0
9	E	54	0	84	1	0
9	G	54	0	84	1	0
10	A	2	0	0	0	0
10	C	2	0	0	0	0
11	A	3	0	0	0	0
11	C	3	0	0	0	0
All	All	22340	0	22850	817	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 18.

All (817) 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)
8:A:1101:CLR:H273	9:A:1108:PCW:H271	1.32	1.12
2:C:138:THR:HG21	9:C:1107:PCW:H20	1.44	0.99
9:C:1107:PCW:H372	9:E:1302:PCW:H39	1.41	0.98
2:A:138:THR:HG21	9:A:1109:PCW:H20	1.44	0.98
9:A:1109:PCW:H372	9:G:1302:PCW:H39	1.41	0.98
3:G:26:VAL:HG11	8:G:1301:CLR:H71	1.41	0.97
3:E:26:VAL:HG11	8:E:1301:CLR:H71	1.41	0.96
9:A:1107:PCW:H441	8:G:1301:CLR:H273	1.54	0.89
2:A:558:PHE:HD2	2:A:560:LEU:HD12	1.37	0.88
9:C:1105:PCW:H441	8:E:1301:CLR:H273	1.54	0.88
2:C:673:LEU:HD22	2:C:677:VAL:HG11	1.57	0.87
2:A:673:LEU:HD22	2:A:677:VAL:HG11	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:558:PHE:HD2	2:C:560:LEU:HD12	1.37	0.86
2:C:480:ILE:HD12	2:C:490:LEU:HD23	1.58	0.85
2:A:239:THR:HG21	2:A:242:ILE:HD12	1.58	0.85
2:A:52:HIS:HB2	2:A:59:LEU:HD21	1.59	0.84
2:C:372:THR:HB	2:C:712:VAL:HG12	1.60	0.84
2:A:480:ILE:HD12	2:A:490:LEU:HD23	1.58	0.84
2:C:52:HIS:HB2	2:C:59:LEU:HD21	1.59	0.84
2:C:997:ILE:HG21	9:C:1104:PCW:H272	1.61	0.83
2:C:239:THR:HG21	2:C:242:ILE:HD12	1.58	0.82
2:A:372:THR:HB	2:A:712:VAL:HG12	1.60	0.82
2:A:997:ILE:HG21	9:A:1106:PCW:H272	1.61	0.82
2:C:121:THR:HG22	2:C:122:GLU:H	1.47	0.80
1:D:124:PHE:HB3	1:D:151:ARG:HG2	1.64	0.80
1:B:76:PRO:HG3	1:B:184:ILE:HD12	1.63	0.80
2:A:121:THR:HG22	2:A:122:GLU:H	1.47	0.79
2:C:500:GLU:HG2	2:C:502:ARG:H	1.47	0.79
1:D:76:PRO:HG3	1:D:184:ILE:HD12	1.63	0.79
2:A:490:LEU:HD11	2:A:505:LEU:HD11	1.65	0.78
9:C:1106:PCW:H272	2:A:996:LEU:HD23	1.65	0.78
1:B:124:PHE:HB3	1:B:151:ARG:HG2	1.64	0.78
2:A:500:GLU:HG2	2:A:502:ARG:H	1.47	0.78
1:D:47:LEU:HD22	2:C:863:LEU:HD12	1.66	0.78
2:C:490:LEU:HD11	2:C:505:LEU:HD11	1.65	0.77
2:A:40:SER:HB3	2:A:236:PRO:HG3	1.67	0.77
2:C:1007:PHE:CE2	9:C:1106:PCW:H12	2.20	0.76
2:A:1007:PHE:CE2	9:A:1108:PCW:H12	2.20	0.76
1:B:47:LEU:HD22	2:A:863:LEU:HD12	1.66	0.76
2:A:86:THR:HB	2:A:90:ILE:HD11	1.68	0.75
2:C:456:LEU:O	2:C:460:ILE:HG12	1.87	0.75
9:C:1104:PCW:H462	8:A:1103:CLR:H263	1.68	0.75
1:B:161:SER:HB3	1:B:163:LEU:HD12	1.69	0.75
2:C:840:LYS:H	2:C:840:LYS:HD2	1.52	0.75
2:C:40:SER:HB3	2:C:236:PRO:HG3	1.67	0.74
2:A:840:LYS:H	2:A:840:LYS:HD2	1.52	0.74
2:C:86:THR:HB	2:C:90:ILE:HD11	1.68	0.74
2:A:366:THR:HG22	2:A:730:ILE:HD11	1.70	0.73
2:C:193:VAL:HG23	2:C:197:ASP:HB2	1.70	0.73
2:A:193:VAL:HG23	2:A:197:ASP:HB2	1.70	0.73
8:A:1101:CLR:H71	9:A:1108:PCW:H172	1.68	0.73
2:A:456:LEU:O	2:A:460:ILE:HG12	1.87	0.73
2:C:478:VAL:HG23	2:C:492:ILE:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1007:PHE:CZ	1:B:61:THR:HA	2.24	0.73
1:D:161:SER:HB3	1:D:163:LEU:HD12	1.69	0.72
2:A:838:ASN:HD22	2:A:840:LYS:HD3	1.54	0.72
2:C:366:THR:HG22	2:C:730:ILE:HD11	1.70	0.72
2:A:309:LEU:HD23	2:A:312:ILE:HD11	1.72	0.71
2:A:478:VAL:HG23	2:A:492:ILE:HD13	1.71	0.71
1:D:176:CYS:SG	1:D:264:GLN:HG3	2.31	0.71
2:C:669:ASP:O	2:C:673:LEU:HG	1.91	0.71
1:B:73:VAL:HG12	2:A:910:GLN:HE21	1.55	0.71
2:A:669:ASP:O	2:A:673:LEU:HG	1.91	0.71
2:C:309:LEU:HD23	2:C:312:ILE:HD11	1.72	0.71
2:C:838:ASN:HD22	2:C:840:LYS:HD3	1.54	0.70
9:C:1106:PCW:H242	9:A:1107:PCW:H272	1.74	0.70
2:A:333:PRO:HB2	2:A:336:LEU:HD13	1.74	0.70
2:C:503:TYR:CE2	2:C:560:LEU:HD13	2.26	0.70
2:C:783:ASN:O	2:C:787:ILE:HG12	1.91	0.70
8:A:1101:CLR:H273	9:A:1108:PCW:C27	2.18	0.70
2:A:181:ASN:HB3	2:A:184:PHE:CD1	2.27	0.70
1:B:176:CYS:SG	1:B:264:GLN:HG3	2.31	0.70
2:A:783:ASN:O	2:A:787:ILE:HG12	1.91	0.70
2:C:181:ASN:HB3	2:C:184:PHE:CD1	2.27	0.69
2:C:333:PRO:HB2	2:C:336:LEU:HD13	1.74	0.69
2:C:420:ALA:HA	2:C:423:ARG:NH1	2.08	0.69
2:A:872:ILE:HD11	2:A:921:SER:OG	1.93	0.69
1:D:73:VAL:HG12	2:C:910:GLN:HE21	1.56	0.69
2:A:503:TYR:CE2	2:A:560:LEU:HD13	2.26	0.69
2:A:420:ALA:HA	2:A:423:ARG:NH1	2.08	0.68
2:C:872:ILE:HD11	2:C:921:SER:OG	1.93	0.68
2:A:1011:ARG:HD3	9:A:1108:PCW:H73	1.76	0.68
2:C:442:ILE:HD13	2:C:442:ILE:H	1.59	0.67
9:A:1107:PCW:H482	8:G:1301:CLR:H222	1.76	0.67
2:A:360:ASN:HD21	2:A:747:ASP:HB3	1.60	0.67
2:C:181:ASN:HB3	2:C:184:PHE:HD1	1.60	0.67
2:A:181:ASN:HB3	2:A:184:PHE:HD1	1.59	0.67
2:A:442:ILE:HD13	2:A:442:ILE:H	1.59	0.67
1:D:290:LYS:NZ	2:C:979:ARG:HH12	1.92	0.67
2:A:520:THR:CG2	2:A:527:GLU:HG2	2.25	0.67
1:B:290:LYS:NZ	2:A:979:ARG:HH12	1.92	0.67
2:A:198:ARG:HA	2:A:248:ASN:HD22	1.60	0.66
1:D:73:VAL:HG12	2:C:910:GLN:NE2	2.11	0.66
2:C:1011:ARG:HD3	9:C:1106:PCW:H73	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:ARG:HA	2:C:248:ASN:HD22	1.59	0.66
9:C:1105:PCW:H482	8:E:1301:CLR:H222	1.76	0.66
2:C:520:THR:CG2	2:C:527:GLU:HG2	2.25	0.66
2:C:360:ASN:HD21	2:C:747:ASP:HB3	1.60	0.65
2:C:503:TYR:HE2	2:C:560:LEU:HD13	1.62	0.65
2:C:361:LEU:O	2:C:364:VAL:HG12	1.96	0.65
2:A:935:ILE:HD11	2:A:958:LEU:HD11	1.78	0.65
2:C:644:ILE:O	2:C:647:ARG:HG2	1.97	0.65
2:C:935:ILE:HD11	2:C:958:LEU:HD11	1.78	0.65
2:A:997:ILE:HD13	9:A:1106:PCW:H261	1.79	0.65
1:B:213:LEU:HD23	1:B:261:LEU:HD13	1.79	0.65
1:D:213:LEU:HD23	1:D:261:LEU:HD13	1.79	0.64
2:C:430:ARG:HH12	2:C:481:PRO:HB3	1.63	0.64
1:B:73:VAL:HG12	2:A:910:GLN:NE2	2.11	0.64
2:C:997:ILE:HD13	9:C:1104:PCW:H261	1.79	0.64
2:A:430:ARG:HH12	2:A:481:PRO:HB3	1.63	0.64
2:A:361:LEU:O	2:A:364:VAL:HG12	1.96	0.64
2:A:997:ILE:HD13	9:A:1106:PCW:H282	1.80	0.64
2:A:424:ILE:HD12	2:A:555:PHE:HB3	1.79	0.64
2:C:424:ILE:HD12	2:C:555:PHE:HB3	1.79	0.63
9:C:1106:PCW:H282	2:A:996:LEU:HB3	1.78	0.63
2:C:476:LYS:HD2	2:C:479:GLU:HB3	1.81	0.63
1:D:290:LYS:HZ3	2:C:979:ARG:HH12	1.45	0.63
2:C:318:LEU:O	2:C:322:ILE:HG12	1.99	0.63
1:D:209:TYR:HA	1:D:242:LEU:HD22	1.81	0.63
2:A:644:ILE:O	2:A:647:ARG:HG2	1.97	0.63
2:C:433:PHE:HB3	2:C:437:GLN:OE1	1.99	0.63
2:A:318:LEU:O	2:A:322:ILE:HG12	1.99	0.63
9:C:1106:PCW:H63	1:B:63:SER:HA	1.81	0.63
1:B:290:LYS:HZ3	2:A:979:ARG:HH12	1.45	0.63
2:A:44:HIS:HD2	2:A:231:PHE:HE1	1.47	0.62
2:C:997:ILE:HD13	9:C:1104:PCW:H282	1.80	0.62
1:D:61:THR:HA	2:A:1007:PHE:HZ	1.64	0.62
1:D:217:ALA:HB2	1:D:226:ILE:HD12	1.81	0.62
2:C:246:SER:OG	2:C:267:MET:HG2	1.99	0.62
1:D:56:GLN:HE22	1:D:59:LEU:HD12	1.65	0.62
2:A:442:ILE:HG12	2:A:443:LEU:HD12	1.80	0.62
2:C:442:ILE:HG12	2:C:443:LEU:HD12	1.80	0.62
1:B:56:GLN:HE22	1:B:59:LEU:HD12	1.65	0.62
2:A:433:PHE:HB3	2:A:437:GLN:OE1	1.99	0.61
2:A:503:TYR:HE2	2:A:560:LEU:HD13	1.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:270:ILE:O	2:A:274:ALA:HB3	2.00	0.61
1:B:209:TYR:HA	1:B:242:LEU:HD22	1.81	0.61
2:A:246:SER:OG	2:A:267:MET:HG2	1.99	0.61
2:A:476:LYS:HD2	2:A:479:GLU:HB3	1.81	0.61
1:D:47:LEU:CD2	9:C:1104:PCW:H271	2.30	0.61
2:C:270:ILE:O	2:C:274:ALA:HB3	2.00	0.61
2:C:495:ASN:HD21	2:C:497:LYS:NZ	1.98	0.61
3:G:18:ARG:O	3:G:22:VAL:HG23	2.00	0.61
2:C:520:THR:HG22	2:C:527:GLU:HG2	1.83	0.61
1:D:206:TYR:O	1:D:206:TYR:CD1	2.54	0.61
2:C:44:HIS:HD2	2:C:231:PHE:HE1	1.47	0.61
2:C:105:TRP:NE1	2:C:140:VAL:HG11	2.15	0.61
2:A:495:ASN:HD21	2:A:497:LYS:NZ	1.98	0.61
8:A:1101:CLR:H71	9:A:1108:PCW:C17	2.30	0.61
2:C:389:ALA:HB2	2:C:592:ILE:HG13	1.83	0.60
3:E:18:ARG:O	3:E:22:VAL:HG23	2.00	0.60
1:B:217:ALA:HB2	1:B:226:ILE:HD12	1.81	0.60
2:A:926:ILE:O	2:A:930:GLN:HG2	2.00	0.60
1:B:47:LEU:CD2	9:A:1106:PCW:H271	2.30	0.60
2:C:424:ILE:CD1	2:C:555:PHE:HB3	2.31	0.60
2:A:105:TRP:NE1	2:A:140:VAL:HG11	2.15	0.60
2:A:389:ALA:HB2	2:A:592:ILE:HG13	1.83	0.60
2:A:424:ILE:CD1	2:A:555:PHE:HB3	2.31	0.60
1:B:206:TYR:O	1:B:206:TYR:CD1	2.54	0.60
2:A:580:THR:HG23	2:A:581:THR:HG23	1.83	0.60
2:C:566:ASN:OD1	2:C:569:TYR:HB2	2.02	0.60
2:C:926:ILE:O	2:C:930:GLN:HG2	2.00	0.60
2:C:702:VAL:HG22	2:C:714:VAL:HG21	1.83	0.60
2:A:520:THR:HG22	2:A:527:GLU:HG2	1.83	0.60
1:D:63:SER:HA	9:A:1108:PCW:H63	1.84	0.60
2:C:131:TYR:O	2:C:135:VAL:HG23	2.02	0.60
2:C:558:PHE:CD2	2:C:560:LEU:HD12	2.29	0.59
2:A:702:VAL:HG22	2:A:714:VAL:HG21	1.83	0.59
2:C:212:LYS:HB2	2:C:251:GLU:HG2	1.85	0.59
2:A:291:PHE:CZ	2:A:295:ILE:HD12	2.37	0.59
2:A:566:ASN:OD1	2:A:569:TYR:HB2	2.02	0.59
2:A:720:ASN:ND2	2:A:720:ASN:H	2.00	0.59
2:C:720:ASN:ND2	2:C:720:ASN:H	2.00	0.59
2:C:291:PHE:CZ	2:C:295:ILE:HD12	2.37	0.59
2:A:1011:ARG:HD3	9:A:1108:PCW:H62	1.85	0.58
1:D:61:THR:HA	2:A:1007:PHE:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:705:CYS:HB3	2:C:712:VAL:HG11	1.86	0.58
1:B:61:THR:HG21	8:A:1103:CLR:H21	1.85	0.58
2:C:580:THR:HG23	2:C:581:THR:HG23	1.83	0.58
1:D:64:ASP:N	1:D:64:ASP:OD1	2.36	0.58
2:C:433:PHE:CE1	2:C:447:VAL:HG22	2.38	0.58
2:A:46:LEU:HD22	2:A:50:GLU:HB3	1.86	0.58
2:A:131:TYR:O	2:A:135:VAL:HG23	2.02	0.58
2:A:784:ILE:HD11	2:A:854:TYR:CD2	2.39	0.58
1:D:60:LEU:HB3	2:A:1007:PHE:CD1	2.38	0.58
2:C:784:ILE:HD11	2:C:854:TYR:CD2	2.39	0.58
3:E:21:VAL:O	3:E:25:ILE:HG12	2.03	0.58
2:A:212:LYS:HB2	2:A:251:GLU:HG2	1.85	0.58
2:A:678:LEU:HD12	2:A:681:ILE:HD11	1.86	0.58
2:A:705:CYS:HB3	2:A:712:VAL:HG11	1.85	0.58
2:C:625:LYS:HE2	2:C:640:THR:HG21	1.86	0.57
2:C:306:PHE:CZ	2:C:794:ILE:HD13	2.39	0.57
2:A:433:PHE:CE1	2:A:447:VAL:HG22	2.38	0.57
1:D:61:THR:HG21	8:A:1101:CLR:H21	1.85	0.57
2:A:1000:LEU:HD23	9:A:1106:PCW:H461	1.86	0.57
3:G:21:VAL:O	3:G:25:ILE:HG12	2.03	0.57
2:A:306:PHE:CZ	2:A:794:ILE:HD13	2.39	0.57
2:A:625:LYS:HE2	2:A:640:THR:HG21	1.86	0.57
2:C:1000:LEU:CD2	8:A:1103:CLR:H241	2.34	0.57
2:C:1011:ARG:HD3	9:C:1106:PCW:H62	1.85	0.57
1:B:64:ASP:N	1:B:64:ASP:OD1	2.36	0.57
2:C:46:LEU:HD22	2:C:50:GLU:HB3	1.86	0.57
2:C:838:ASN:ND2	2:C:840:LYS:HD3	2.20	0.57
2:A:172:ILE:CD1	2:A:177:LYS:HG2	2.35	0.57
2:A:295:ILE:HG21	2:A:333:PRO:HD2	1.87	0.57
1:D:47:LEU:HD23	9:C:1104:PCW:H271	1.87	0.57
2:C:154:SER:HA	2:C:345:THR:HG21	1.87	0.57
2:C:848:ARG:HG2	2:C:1020:GLU:O	2.05	0.56
2:C:1000:LEU:HD23	9:C:1104:PCW:H461	1.86	0.56
2:C:1007:PHE:CE1	1:B:61:THR:HA	2.40	0.56
2:A:511:PRO:HB2	2:A:542:TYR:HE2	1.71	0.56
2:A:634:ILE:HA	2:A:687:GLU:OE1	2.06	0.56
2:A:838:ASN:ND2	2:A:840:LYS:HD3	2.20	0.56
2:C:997:ILE:CG2	9:C:1104:PCW:H272	2.35	0.56
2:C:634:ILE:HA	2:C:687:GLU:OE1	2.06	0.56
2:A:154:SER:HA	2:A:345:THR:HG21	1.86	0.56
2:C:511:PRO:HB2	2:C:542:TYR:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:678:LEU:HD12	2:C:681:ILE:HD11	1.86	0.56
9:A:1107:PCW:H472	8:G:1301:CLR:H242	1.87	0.56
2:A:620:HIS:CG	2:A:621:PRO:HD2	2.41	0.55
2:C:172:ILE:CD1	2:C:177:LYS:HG2	2.35	0.55
2:C:625:LYS:HG2	2:C:664:VAL:HG21	1.89	0.55
2:C:944:ILE:HD11	9:C:1105:PCW:H142	1.88	0.55
9:C:1105:PCW:H472	8:E:1301:CLR:H242	1.87	0.55
2:A:848:ARG:HG2	2:A:1020:GLU:O	2.05	0.55
2:A:997:ILE:CG2	9:A:1106:PCW:H272	2.35	0.55
2:C:620:HIS:CG	2:C:621:PRO:HD2	2.41	0.55
2:C:924:ILE:HD12	2:C:983:LEU:HD22	1.89	0.55
2:A:924:ILE:HD12	2:A:983:LEU:HD22	1.89	0.55
2:C:295:ILE:HG21	2:C:333:PRO:HD2	1.87	0.55
2:C:897:ASP:OD1	2:C:897:ASP:N	2.40	0.55
1:B:47:LEU:HD23	9:A:1106:PCW:H271	1.87	0.55
1:B:174:LYS:HD3	1:B:266:THR:HG23	1.89	0.55
2:A:340:VAL:HG12	2:A:772:LEU:HD21	1.89	0.55
2:A:503:TYR:CD2	2:A:560:LEU:HB2	2.42	0.55
2:C:992:PHE:HD2	9:C:1105:PCW:H261	1.72	0.54
2:A:558:PHE:CD2	2:A:560:LEU:HD12	2.29	0.54
2:A:625:LYS:HG2	2:A:664:VAL:HG21	1.89	0.54
9:A:1111:PCW:O31	8:G:1301:CLR:H11	2.08	0.54
1:D:72:ARG:O	2:C:910:GLN:HG2	2.08	0.54
2:C:777:ALA:O	2:C:781:THR:HG23	2.08	0.54
2:C:340:VAL:HG12	2:C:772:LEU:CD2	2.38	0.54
2:C:340:VAL:HG12	2:C:772:LEU:HD21	1.89	0.54
2:C:474:ASN:HB3	2:C:493:HIS:HB3	1.89	0.54
2:A:890:TRP:HA	2:A:911:ARG:HH11	1.72	0.54
1:D:174:LYS:HD3	1:D:266:THR:HG23	1.89	0.54
2:A:215:ASN:O	2:A:219:THR:HG22	2.07	0.54
2:A:544:GLU:O	2:A:548:LEU:HG	2.08	0.54
2:A:474:ASN:HB3	2:A:493:HIS:HB3	1.88	0.54
1:D:279:LYS:HG3	1:D:296:ARG:HB3	1.90	0.54
2:C:521:ILE:HB	2:C:530:LEU:HD21	1.90	0.54
2:A:367:LEU:HD21	2:A:730:ILE:HG21	1.90	0.54
2:C:367:LEU:HD21	2:C:730:ILE:HG21	1.90	0.53
2:A:340:VAL:HG12	2:A:772:LEU:CD2	2.38	0.53
2:C:890:TRP:HA	2:C:911:ARG:HH11	1.72	0.53
2:C:931:TRP:O	2:C:935:ILE:HG12	2.09	0.53
2:A:944:ILE:HD11	9:A:1107:PCW:H142	1.88	0.53
2:C:503:TYR:CD2	2:C:560:LEU:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:544:GLU:O	2:C:548:LEU:HG	2.08	0.53
2:C:974:THR:HG23	2:C:978:LEU:HB2	1.90	0.53
2:A:521:ILE:HB	2:A:530:LEU:HD21	1.90	0.53
2:A:797:ASN:OD1	2:A:887:ARG:NH1	2.42	0.53
2:A:897:ASP:OD1	2:A:897:ASP:N	2.40	0.53
2:C:495:ASN:HB3	2:C:500:GLU:HG3	1.90	0.53
2:C:370:THR:HG21	2:C:373:ILE:HD11	1.90	0.53
2:A:495:ASN:HB3	2:A:500:GLU:HG3	1.90	0.53
2:A:511:PRO:HB2	2:A:542:TYR:CE2	2.44	0.53
2:A:992:PHE:HD2	9:A:1107:PCW:H261	1.72	0.53
1:D:47:LEU:HD22	2:C:863:LEU:CD1	2.37	0.53
2:C:215:ASN:O	2:C:219:THR:HG22	2.08	0.53
2:C:784:ILE:N	2:C:784:ILE:HD12	2.24	0.53
2:C:996:LEU:HD23	9:A:1108:PCW:H272	1.91	0.53
9:C:1109:PCW:O31	8:E:1301:CLR:H11	2.08	0.53
1:B:279:LYS:HG3	1:B:296:ARG:HB3	1.90	0.53
2:A:768:ILE:O	2:A:772:LEU:HD12	2.09	0.53
2:C:511:PRO:HB2	2:C:542:TYR:CE2	2.44	0.53
2:A:974:THR:HG23	2:A:978:LEU:HB2	1.90	0.53
2:C:430:ARG:NH1	2:C:481:PRO:HB3	2.24	0.53
2:C:797:ASN:OD1	2:C:887:ARG:NH1	2.42	0.53
2:A:370:THR:HG21	2:A:373:ILE:HD11	1.90	0.53
2:A:492:ILE:HG23	2:A:503:TYR:CE1	2.44	0.53
2:A:777:ALA:O	2:A:781:THR:HG23	2.08	0.53
2:C:492:ILE:HG23	2:C:503:TYR:CE1	2.44	0.52
2:C:572:ASP:HB2	2:C:577:ASN:ND2	2.24	0.52
1:B:47:LEU:HD22	2:A:863:LEU:CD1	2.37	0.52
2:A:931:TRP:O	2:A:935:ILE:HG12	2.09	0.52
2:C:103:LEU:O	2:C:106:ILE:HG22	2.09	0.52
2:A:313:LEU:HD22	2:A:887:ARG:HH22	1.75	0.52
2:A:784:ILE:HD12	2:A:784:ILE:N	2.24	0.52
1:B:72:ARG:O	2:A:910:GLN:HG2	2.08	0.52
2:A:473:ARG:O	2:A:475:PRO:HD3	2.09	0.52
2:C:473:ARG:O	2:C:475:PRO:HD3	2.09	0.52
9:C:1106:PCW:H63	1:B:63:SER:HB2	1.90	0.52
2:A:103:LEU:O	2:A:106:ILE:HG22	2.09	0.52
2:A:520:THR:HG21	2:A:527:GLU:HG2	1.91	0.52
1:B:92:SER:HA	1:B:304:LYS:O	2.10	0.52
2:A:172:ILE:HG13	2:A:255:ARG:HH12	1.74	0.52
2:A:572:ASP:HB2	2:A:577:ASN:ND2	2.24	0.52
2:C:768:ILE:O	2:C:772:LEU:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:LYS:O	2:A:94:ARG:N	2.43	0.52
2:C:520:THR:HG21	2:C:527:GLU:HG2	1.91	0.52
2:C:671:LYS:HD2	2:C:671:LYS:C	2.30	0.52
1:B:16:PHE:CZ	9:A:1112:PCW:H62	2.45	0.52
2:A:520:THR:HG23	2:A:528:GLU:O	2.10	0.52
1:D:92:SER:HA	1:D:304:LYS:O	2.10	0.52
2:C:313:LEU:HD22	2:C:887:ARG:HH22	1.75	0.52
2:C:620:HIS:CD2	2:C:622:ILE:H	2.28	0.52
2:C:997:ILE:HG21	9:C:1104:PCW:C27	2.37	0.52
2:A:284:ILE:O	2:A:288:ILE:HD13	2.10	0.52
2:C:425:ALA:HB2	2:C:589:MET:HE1	1.92	0.51
2:A:442:ILE:H	2:A:442:ILE:CD1	2.23	0.51
2:C:172:ILE:HG13	2:C:255:ARG:NH1	2.25	0.51
1:D:16:PHE:CZ	9:C:1110:PCW:H62	2.45	0.51
2:C:172:ILE:HG13	2:C:255:ARG:HH12	1.74	0.51
2:C:698:LYS:O	2:C:702:VAL:HG23	2.10	0.51
1:B:75:PRO:HG2	1:B:286:ASP:N	2.26	0.51
2:A:193:VAL:HG23	2:A:197:ASP:CB	2.40	0.51
2:A:430:ARG:NH1	2:A:481:PRO:HB3	2.24	0.51
2:A:620:HIS:CD2	2:A:622:ILE:H	2.29	0.51
2:C:193:VAL:HG23	2:C:197:ASP:CB	2.40	0.51
2:C:434:GLN:HB2	2:C:437:GLN:NE2	2.25	0.51
2:C:520:THR:HG23	2:C:528:GLU:O	2.10	0.51
2:A:434:GLN:HB2	2:A:437:GLN:NE2	2.26	0.51
3:G:17:TYR:O	3:G:21:VAL:HG23	2.10	0.51
2:A:172:ILE:HG13	2:A:255:ARG:NH1	2.25	0.51
2:A:698:LYS:O	2:A:702:VAL:HG23	2.10	0.51
2:C:838:ASN:HB2	2:C:840:LYS:HD3	1.93	0.51
2:C:848:ARG:HD3	2:C:1019:GLN:O	2.11	0.51
2:A:180:ILE:HG12	2:A:184:PHE:HB2	1.93	0.51
2:A:671:LYS:C	2:A:671:LYS:HD2	2.30	0.51
2:A:893:ARG:HA	2:A:908:TYR:CD1	2.46	0.51
2:C:620:HIS:HD2	2:C:622:ILE:H	1.59	0.51
2:C:656:ASN:HD22	2:C:657:PRO:HD2	1.75	0.51
2:A:389:ALA:CB	2:A:592:ILE:HG13	2.41	0.51
2:A:656:ASN:HD22	2:A:657:PRO:HD2	1.75	0.51
3:E:17:TYR:O	3:E:21:VAL:HG23	2.10	0.51
2:A:371:SER:OG	2:A:710:ALA:HB1	2.11	0.50
1:D:75:PRO:HG2	1:D:286:ASP:N	2.26	0.50
2:C:284:ILE:O	2:C:288:ILE:HD13	2.10	0.50
2:A:848:ARG:HD3	2:A:1019:GLN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44:HIS:HD2	2:C:231:PHE:CE1	2.28	0.50
2:C:371:SER:OG	2:C:710:ALA:HB1	2.11	0.50
2:C:713:ALA:HA	2:C:730:ILE:O	2.12	0.50
2:C:893:ARG:HA	2:C:908:TYR:CD1	2.46	0.50
2:A:713:ALA:HA	2:A:730:ILE:O	2.12	0.50
2:C:442:ILE:H	2:C:442:ILE:CD1	2.23	0.50
2:C:91:LYS:O	2:C:94:ARG:N	2.43	0.50
2:C:480:ILE:HB	2:C:490:LEU:HB3	1.94	0.50
2:C:515:LEU:HD21	2:C:535:LYS:HG2	1.94	0.50
2:A:838:ASN:HB2	2:A:840:LYS:HD3	1.93	0.50
2:C:118:GLN:NE2	2:C:129:ASN:OD1	2.45	0.50
2:C:425:ALA:HB2	2:C:589:MET:CE	2.42	0.50
9:C:1105:PCW:H482	8:E:1301:CLR:H161	1.94	0.50
9:C:1106:PCW:H63	1:B:63:SER:CA	2.41	0.50
2:A:118:GLN:NE2	2:A:129:ASN:OD1	2.45	0.50
2:C:180:ILE:HG12	2:C:184:PHE:HB2	1.93	0.49
2:C:803:GLY:O	2:C:807:ILE:HG13	2.13	0.49
2:C:203:LEU:HD23	2:C:258:VAL:HA	1.94	0.49
2:A:44:HIS:HD2	2:A:231:PHE:CE1	2.28	0.49
2:A:620:HIS:HD2	2:A:622:ILE:H	1.59	0.49
9:C:1106:PCW:C6	1:B:63:SER:HA	2.42	0.49
2:A:92:PHE:CZ	2:A:96:LEU:HD21	2.47	0.49
2:A:359:LYS:NZ	2:A:744:GLN:HA	2.28	0.49
1:B:83:TYR:HE1	2:A:894:TRP:CB	2.25	0.49
2:C:431:ALA:O	2:C:457:LEU:HD11	2.13	0.49
2:A:106:ILE:O	2:A:110:LEU:HG	2.13	0.49
2:A:425:ALA:HB2	2:A:589:MET:CE	2.42	0.49
1:D:60:LEU:HB3	2:A:1007:PHE:CE1	2.48	0.49
2:C:477:ILE:HG22	2:C:478:VAL:HG13	1.94	0.49
2:C:720:ASN:O	2:C:723:PRO:HD2	2.13	0.49
2:A:239:THR:CG2	2:A:242:ILE:HD12	2.38	0.49
2:C:92:PHE:CZ	2:C:96:LEU:HD21	2.47	0.49
2:A:803:GLY:O	2:A:807:ILE:HG13	2.13	0.49
2:C:389:ALA:CB	2:C:592:ILE:HG13	2.41	0.49
2:A:515:LEU:HD21	2:A:535:LYS:HG2	1.94	0.49
2:A:115:TYR:OH	2:A:127:ASN:ND2	2.46	0.49
1:D:83:TYR:HE1	2:C:894:TRP:CB	2.25	0.48
2:A:373:ILE:HD13	2:A:713:ALA:HB3	1.95	0.48
9:A:1107:PCW:H482	8:G:1301:CLR:H161	1.94	0.48
2:C:359:LYS:NZ	2:C:744:GLN:HA	2.28	0.48
2:A:38:GLU:HG3	2:A:39:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:ILE:HG13	2:A:91:LYS:N	2.28	0.48
2:A:619:ASP:O	2:A:692:ARG:HG2	2.14	0.48
2:A:997:ILE:HG21	9:A:1106:PCW:C27	2.37	0.48
2:C:38:GLU:HG3	2:C:39:VAL:HG23	1.95	0.48
2:C:201:ALA:HB1	2:C:260:TYR:O	2.13	0.48
2:C:552:VAL:HG11	2:C:588:LEU:HD13	1.95	0.48
1:B:47:LEU:HD21	9:A:1106:PCW:H271	1.95	0.48
2:A:480:ILE:HB	2:A:490:LEU:HB3	1.94	0.48
2:A:552:VAL:HG11	2:A:588:LEU:HD13	1.95	0.48
2:A:838:ASN:HB2	2:A:840:LYS:CD	2.44	0.48
2:C:90:ILE:HG13	2:C:91:LYS:N	2.28	0.48
2:C:115:TYR:OH	2:C:127:ASN:ND2	2.46	0.48
2:C:420:ALA:HA	2:C:423:ARG:HH12	1.76	0.48
2:C:1000:LEU:HD21	8:A:1103:CLR:H241	1.94	0.48
2:A:477:ILE:HG22	2:A:478:VAL:HG13	1.94	0.48
2:A:596:ARG:HG2	2:A:754:ASN:ND2	2.29	0.48
9:C:1104:PCW:H483	8:A:1103:CLR:C27	2.44	0.48
1:B:85:ILE:O	1:B:86:LYS:HB2	2.13	0.48
2:A:201:ALA:HB1	2:A:260:TYR:O	2.13	0.48
2:A:431:ALA:O	2:A:457:LEU:HD11	2.13	0.48
2:C:106:ILE:O	2:C:110:LEU:HG	2.13	0.48
2:C:388:VAL:HG23	2:C:455:ALA:HB1	1.96	0.48
2:C:1007:PHE:HZ	1:B:61:THR:HA	1.76	0.48
2:A:720:ASN:O	2:A:723:PRO:HD2	2.13	0.48
2:C:338:ALA:O	2:C:342:VAL:HG23	2.14	0.48
2:A:87:PRO:HD2	2:A:90:ILE:HD13	1.95	0.48
2:C:87:PRO:HD2	2:C:90:ILE:HD13	1.95	0.48
2:C:596:ARG:HG2	2:C:754:ASN:ND2	2.29	0.48
2:C:784:ILE:HD12	2:C:784:ILE:H	1.79	0.48
2:C:790:PHE:HE2	2:C:807:ILE:HD11	1.79	0.48
2:A:203:LEU:HD23	2:A:258:VAL:HA	1.94	0.48
2:A:1008:ILE:HD13	9:A:1106:PCW:H361	1.95	0.48
2:C:959:PHE:HE2	9:C:1109:PCW:H231	1.79	0.48
2:A:447:VAL:HG12	2:A:448:ALA:N	2.29	0.48
2:A:992:PHE:CD2	9:A:1107:PCW:H261	2.49	0.48
1:D:85:ILE:O	1:D:86:LYS:HB2	2.13	0.47
9:C:1104:PCW:C40	9:C:1104:PCW:H20	2.44	0.47
2:A:180:ILE:HD11	2:A:184:PHE:HB3	1.95	0.47
2:A:784:ILE:HD12	2:A:784:ILE:H	1.79	0.47
1:D:134:TYR:HE1	1:D:242:LEU:HG	1.79	0.47
2:C:373:ILE:HD13	2:C:713:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1109:PCW:H432	8:E:1301:CLR:H263	1.95	0.47
1:B:132:ALA:O	1:B:209:TYR:HB3	2.14	0.47
9:A:1106:PCW:C40	9:A:1106:PCW:H20	2.44	0.47
1:D:132:ALA:O	1:D:209:TYR:HB3	2.14	0.47
2:C:404:GLU:HG2	2:C:443:LEU:HD13	1.96	0.47
2:C:768:ILE:HG22	2:C:772:LEU:HD12	1.96	0.47
2:A:959:PHE:HE2	9:A:1111:PCW:H231	1.79	0.47
2:C:180:ILE:HD11	2:C:184:PHE:HB3	1.95	0.47
2:C:619:ASP:O	2:C:692:ARG:HG2	2.14	0.47
2:C:774:LYS:HB3	2:C:822:LEU:HD12	1.96	0.47
2:A:774:LYS:HB3	2:A:822:LEU:HD12	1.96	0.47
9:A:1111:PCW:H432	8:G:1301:CLR:H263	1.95	0.47
2:C:108:ALA:O	2:C:112:PHE:HD2	1.98	0.47
2:C:447:VAL:HG12	2:C:448:ALA:N	2.29	0.47
2:C:514:ILE:HG13	2:C:515:LEU:N	2.30	0.47
2:C:1008:ILE:HD13	9:C:1104:PCW:H361	1.95	0.47
2:C:132:LEU:HD21	2:C:322:ILE:HD12	1.97	0.47
2:C:838:ASN:HB2	2:C:840:LYS:CD	2.44	0.47
2:C:1011:ARG:HD3	9:C:1106:PCW:C7	2.43	0.47
1:B:120:GLY:O	1:B:151:ARG:NH2	2.47	0.47
2:C:260:TYR:HD1	2:C:264:ARG:HB3	1.80	0.47
9:C:1106:PCW:H272	2:A:996:LEU:CD2	2.40	0.47
1:B:134:TYR:HE1	1:B:242:LEU:HG	1.79	0.47
2:A:404:GLU:HG2	2:A:443:LEU:HD13	1.96	0.47
2:A:420:ALA:HA	2:A:423:ARG:HH12	1.76	0.47
2:A:426:ALA:HB3	2:A:470:MET:SD	2.55	0.47
2:A:514:ILE:HG13	2:A:515:LEU:N	2.30	0.47
2:C:64:THR:HG23	2:C:67:ARG:H	1.80	0.47
2:C:109:ILE:O	2:C:113:LEU:HD13	2.15	0.47
2:C:171:VAL:HG12	2:C:191:VAL:HG22	1.97	0.47
2:C:702:VAL:CG2	2:C:714:VAL:HG21	2.45	0.47
2:A:260:TYR:HD1	2:A:264:ARG:HB3	1.80	0.47
2:A:615:MET:HB3	2:A:689:VAL:HG13	1.97	0.47
9:A:1109:PCW:H122	9:A:1109:PCW:H152	1.59	0.47
1:D:120:GLY:O	1:D:151:ARG:NH2	2.47	0.47
1:D:225:LYS:HD2	1:D:272:MET:SD	2.55	0.47
2:C:170:LEU:HD12	2:C:178:SER:O	2.15	0.47
2:C:212:LYS:HD3	2:C:226:THR:HA	1.97	0.47
2:C:424:ILE:HG22	2:C:506:VAL:HG12	1.97	0.47
2:C:503:TYR:CE2	2:C:505:LEU:HB2	2.50	0.47
2:C:615:MET:HB3	2:C:689:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:424:ILE:HG22	2:A:506:VAL:HG12	1.97	0.47
2:A:436:GLY:O	2:A:439:ASN:ND2	2.48	0.47
2:C:44:HIS:HB3	2:C:242:ILE:HD11	1.97	0.47
2:A:212:LYS:HD3	2:A:226:THR:HA	1.97	0.47
2:A:337:LEU:O	2:A:340:VAL:HG22	2.15	0.47
2:A:790:PHE:HE2	2:A:807:ILE:HD11	1.79	0.47
2:C:337:LEU:O	2:C:340:VAL:HG22	2.15	0.46
2:C:992:PHE:CD2	9:C:1105:PCW:H261	2.49	0.46
1:B:225:LYS:HD2	1:B:272:MET:SD	2.55	0.46
2:A:92:PHE:O	2:A:96:LEU:HD23	2.16	0.46
2:A:288:ILE:HD11	2:A:844:LEU:HD22	1.98	0.46
2:A:427:LEU:HD11	2:A:474:ASN:HD22	1.80	0.46
2:A:702:VAL:CG2	2:A:714:VAL:HG21	2.45	0.46
2:C:495:ASN:HD21	2:C:497:LYS:HZ2	1.60	0.46
1:B:163:LEU:HD23	4:K:6:FUC:H61	1.97	0.46
2:A:388:VAL:HG23	2:A:455:ALA:HB1	1.96	0.46
2:C:92:PHE:O	2:C:96:LEU:HD23	2.16	0.46
2:A:100:PHE:CD1	2:A:100:PHE:C	2.88	0.46
2:A:132:LEU:HD21	2:A:322:ILE:HD12	1.97	0.46
2:A:484:SER:O	2:A:487:LYS:HG3	2.15	0.46
2:A:664:VAL:HA	2:A:689:VAL:O	2.16	0.46
2:A:964:LEU:HD23	2:A:964:LEU:HA	1.80	0.46
2:A:1011:ARG:HD3	9:A:1108:PCW:C7	2.43	0.46
2:C:426:ALA:HB3	2:C:470:MET:SD	2.55	0.46
2:C:664:VAL:HA	2:C:689:VAL:O	2.16	0.46
9:C:1106:PCW:H242	9:A:1107:PCW:C27	2.44	0.46
1:B:140:LEU:HD23	1:B:252:LEU:HD12	1.98	0.46
2:A:338:ALA:O	2:A:342:VAL:HG23	2.14	0.46
2:C:318:LEU:O	2:C:321:VAL:HG22	2.16	0.46
2:A:109:ILE:O	2:A:113:LEU:HD13	2.15	0.46
2:A:916:PHE:HE2	2:A:979:ARG:HH21	1.63	0.46
2:C:87:PRO:HD2	2:C:90:ILE:CD1	2.45	0.46
2:A:171:VAL:HG12	2:A:191:VAL:HG22	1.97	0.46
2:A:318:LEU:O	2:A:321:VAL:HG22	2.16	0.46
2:A:503:TYR:CE2	2:A:505:LEU:HB2	2.50	0.46
1:D:47:LEU:HD21	9:C:1104:PCW:H271	1.95	0.46
2:C:436:GLY:O	2:C:439:ASN:ND2	2.48	0.46
2:A:58:ASP:HB3	2:A:61:ARG:HB2	1.98	0.46
2:A:108:ALA:O	2:A:112:PHE:HD2	1.98	0.46
2:A:170:LEU:HD12	2:A:178:SER:O	2.15	0.46
2:A:514:ILE:HD11	2:A:585:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1101:CLR:C27	9:A:1108:PCW:H271	2.24	0.46
1:D:203:GLN:HE21	1:D:203:GLN:HB2	1.57	0.46
1:D:229:ILE:HD13	1:D:231:TYR:OH	2.16	0.46
2:C:38:GLU:HG3	2:C:39:VAL:N	2.31	0.46
2:C:514:ILE:HD11	2:C:585:PHE:CE2	2.50	0.46
2:A:44:HIS:HB3	2:A:242:ILE:HD11	1.97	0.46
2:A:388:VAL:HG22	2:A:591:MET:HG2	1.98	0.46
2:A:427:LEU:HD11	2:A:474:ASN:ND2	2.31	0.46
2:C:239:THR:CG2	2:C:242:ILE:HD12	2.38	0.46
2:C:475:PRO:HD2	2:C:494:GLU:O	2.16	0.46
2:A:900:ASP:OD2	2:A:904:GLN:HB2	2.16	0.46
2:C:44:HIS:CD2	2:C:231:PHE:HE1	2.31	0.46
2:A:495:ASN:HD21	2:A:497:LYS:HZ2	1.61	0.46
2:A:768:ILE:HG22	2:A:772:LEU:HD12	1.96	0.46
1:D:215:CYS:SG	1:D:263:ILE:HD13	2.56	0.45
2:C:80:LEU:HD23	2:C:272:THR:HG23	1.98	0.45
2:C:427:LEU:HD11	2:C:474:ASN:HD22	1.80	0.45
2:C:439:ASN:HD22	2:C:439:ASN:H	1.64	0.45
2:A:874:ALA:HA	2:A:878:PHE:O	2.17	0.45
2:A:1000:LEU:CD2	8:A:1101:CLR:H241	2.47	0.45
2:C:484:SER:O	2:C:487:LYS:HG3	2.15	0.45
2:C:662:ALA:HA	2:C:687:GLU:O	2.16	0.45
1:B:82:PRO:HD3	1:B:106:MET:SD	2.56	0.45
2:A:87:PRO:HD2	2:A:90:ILE:CD1	2.45	0.45
1:D:82:PRO:HD3	1:D:106:MET:SD	2.56	0.45
1:D:140:LEU:HD23	1:D:252:LEU:HD12	1.98	0.45
1:B:232:PHE:HB2	1:B:262:ALA:HB3	1.98	0.45
2:A:38:GLU:HG3	2:A:39:VAL:N	2.31	0.45
2:A:475:PRO:HD2	2:A:494:GLU:O	2.16	0.45
2:A:538:PHE:CE2	2:A:588:LEU:HD11	2.52	0.45
2:A:824:TYR:OH	9:A:1104:PCW:H73	2.17	0.45
2:A:875:GLU:OE1	2:A:987:TRP:NE1	2.44	0.45
2:C:58:ASP:OD1	2:C:60:THR:HG22	2.16	0.45
2:C:639:GLU:HB3	2:C:643:ASP:HB2	1.98	0.45
2:C:874:ALA:HA	2:C:878:PHE:O	2.16	0.45
9:C:1107:PCW:H241	9:C:1107:PCW:H271	1.67	0.45
2:A:64:THR:HG23	2:A:67:ARG:H	1.80	0.45
1:D:167:THR:HG22	1:D:169:GLY:H	1.82	0.45
2:C:388:VAL:HA	2:C:591:MET:HG2	1.99	0.45
2:C:644:ILE:HA	2:C:647:ARG:CD	2.47	0.45
2:C:817:VAL:HB	2:C:818:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:CYS:SG	1:B:263:ILE:HD13	2.56	0.45
2:A:194:LYS:HG2	2:A:197:ASP:OD2	2.16	0.45
2:A:884:ILE:HD11	9:A:1110:PCW:H131	1.99	0.45
2:A:1007:PHE:HE2	9:A:1108:PCW:H12	1.74	0.45
9:A:1107:PCW:H182	9:A:1107:PCW:H212	1.71	0.45
2:C:78:ASN:HD21	2:C:201:ALA:HB2	1.82	0.45
2:C:194:LYS:HG2	2:C:197:ASP:OD2	2.16	0.45
2:C:538:PHE:CE2	2:C:588:LEU:HD11	2.52	0.45
1:B:215:CYS:HA	1:B:278:CYS:HA	1.98	0.45
1:B:290:LYS:NZ	2:A:979:ARG:NH1	2.63	0.45
2:A:78:ASN:HD21	2:A:201:ALA:HB2	1.82	0.45
2:A:662:ALA:HA	2:A:687:GLU:O	2.16	0.45
9:A:1110:PCW:H483	9:A:1110:PCW:H451	1.66	0.45
2:C:388:VAL:HG22	2:C:591:MET:HG2	1.98	0.45
2:A:417:THR:OG1	2:A:522:LEU:HD22	2.17	0.45
2:A:639:GLU:HB3	2:A:643:ASP:HB2	1.98	0.45
2:C:427:LEU:HD11	2:C:474:ASN:ND2	2.31	0.45
2:C:447:VAL:HG12	2:C:448:ALA:H	1.82	0.45
2:C:656:ASN:HD22	2:C:657:PRO:CD	2.29	0.45
2:C:884:ILE:HD11	9:C:1108:PCW:H131	1.99	0.45
1:B:193:LYS:HA	1:B:206:TYR:OH	2.17	0.45
2:A:705:CYS:CB	2:A:712:VAL:HG11	2.46	0.45
2:A:754:ASN:OD1	2:A:755:PHE:N	2.50	0.45
1:D:265:PHE:CZ	1:D:276:ILE:HD12	2.52	0.45
2:C:340:VAL:O	2:C:344:LEU:HD13	2.17	0.45
2:C:900:ASP:OD2	2:C:904:GLN:HB2	2.16	0.45
2:C:921:SER:OG	2:C:983:LEU:HD11	2.16	0.45
9:C:1109:PCW:H332	8:E:1301:CLR:H112	1.99	0.45
2:A:799:PRO:O	2:A:801:PRO:HD3	2.17	0.45
2:A:872:ILE:HD11	2:A:921:SER:CB	2.47	0.45
1:D:163:LEU:HD23	4:F:6:FUC:H61	1.98	0.45
2:C:288:ILE:HD11	2:C:844:LEU:HD22	1.98	0.45
2:C:754:ASN:OD1	2:C:755:PHE:N	2.50	0.45
1:B:265:PHE:CZ	1:B:276:ILE:HD12	2.52	0.45
2:A:656:ASN:HD22	2:A:657:PRO:CD	2.29	0.45
2:C:58:ASP:HB3	2:C:61:ARG:HB2	1.98	0.44
2:C:457:LEU:HD23	2:C:460:ILE:HD11	1.99	0.44
2:A:58:ASP:OD1	2:A:60:THR:HG22	2.16	0.44
2:A:340:VAL:O	2:A:344:LEU:HD13	2.17	0.44
2:A:439:ASN:HD22	2:A:439:ASN:H	1.65	0.44
2:A:921:SER:OG	2:A:983:LEU:HD11	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LYS:HA	1:D:206:TYR:OH	2.17	0.44
1:D:215:CYS:HA	1:D:278:CYS:HA	1.98	0.44
1:D:232:PHE:HB2	1:D:262:ALA:HB3	1.99	0.44
1:D:290:LYS:NZ	2:C:979:ARG:NH1	2.63	0.44
2:C:100:PHE:CD1	2:C:100:PHE:C	2.88	0.44
2:C:284:ILE:HD11	2:C:844:LEU:HD21	2.00	0.44
2:C:417:THR:OG1	2:C:522:LEU:HD22	2.17	0.44
2:A:284:ILE:HD11	2:A:844:LEU:HD21	2.00	0.44
2:C:824:TYR:OH	9:C:1102:PCW:H73	2.17	0.44
2:A:421:LEU:HG	2:A:589:MET:HE2	1.99	0.44
2:C:101:SER:O	2:C:105:TRP:HD1	2.01	0.44
1:B:167:THR:HG22	1:B:169:GLY:H	1.82	0.44
8:A:1101:CLR:H161	8:A:1101:CLR:H222	1.96	0.44
9:A:1111:PCW:H332	8:G:1301:CLR:H112	1.99	0.44
2:C:351:MET:O	2:C:354:LYS:N	2.50	0.44
2:A:80:LEU:HD23	2:A:272:THR:HG23	1.98	0.44
2:A:457:LEU:HD23	2:A:460:ILE:HD11	1.99	0.44
2:A:974:THR:CG2	2:A:980:MET:HB2	2.48	0.44
2:C:532:GLU:O	2:C:536:GLU:HG3	2.18	0.44
9:C:1106:PCW:H283	2:A:993:PRO:HA	2.00	0.44
2:A:101:SER:O	2:A:105:TRP:HD1	2.01	0.44
2:C:433:PHE:CD1	2:C:447:VAL:HG22	2.53	0.44
2:C:440:VAL:CG2	2:C:441:PRO:HD2	2.48	0.44
1:B:74:ALA:HA	1:B:75:PRO:C	2.38	0.44
1:B:191:PRO:HG3	1:B:208:GLN:O	2.18	0.44
2:A:388:VAL:HA	2:A:591:MET:HG2	1.99	0.44
2:A:440:VAL:CG2	2:A:441:PRO:HD2	2.48	0.44
1:D:191:PRO:HG3	1:D:208:GLN:O	2.18	0.44
2:C:155:SER:HA	2:C:158:MET:CE	2.48	0.44
2:C:661:LYS:HD3	2:C:661:LYS:N	2.33	0.44
2:C:759:VAL:O	2:C:762:VAL:HG22	2.18	0.44
1:B:229:ILE:HD13	1:B:231:TYR:OH	2.16	0.44
2:A:473:ARG:NH2	2:A:497:LYS:HG3	2.33	0.44
2:A:532:GLU:O	2:A:536:GLU:HG3	2.18	0.44
2:A:817:VAL:HB	2:A:818:PRO:HD3	1.98	0.44
1:D:74:ALA:HA	1:D:75:PRO:C	2.38	0.43
2:C:872:ILE:HD11	2:C:921:SER:CB	2.47	0.43
2:A:644:ILE:HA	2:A:647:ARG:CD	2.47	0.43
2:C:95:GLN:HG3	2:C:148:TYR:HB2	2.00	0.43
2:C:473:ARG:NH2	2:C:497:LYS:HG3	2.33	0.43
1:B:189:PRO:HG2	1:B:245:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:LYS:O	2:A:92:PHE:C	2.57	0.43
2:A:92:PHE:CE2	2:A:96:LEU:HD21	2.53	0.43
2:C:442:ILE:HD13	2:C:442:ILE:N	2.32	0.43
2:C:460:ILE:HD12	2:C:467:VAL:HG22	2.00	0.43
2:C:503:TYR:OH	2:C:505:LEU:HD13	2.18	0.43
2:C:520:THR:HG23	2:C:528:GLU:C	2.38	0.43
1:B:160:CYS:SG	1:B:262:ALA:HB1	2.59	0.43
2:A:44:HIS:CD2	2:A:231:PHE:HE1	2.31	0.43
2:A:447:VAL:HG12	2:A:448:ALA:H	1.82	0.43
2:A:503:TYR:OH	2:A:505:LEU:HD13	2.18	0.43
2:C:631:VAL:HG23	2:C:633:ILE:HG12	2.01	0.43
2:C:640:THR:HG22	2:C:662:ALA:O	2.19	0.43
2:C:974:THR:HG22	2:C:980:MET:HB2	2.00	0.43
2:A:498:SER:O	2:A:499:SER:HB3	2.19	0.43
2:A:520:THR:HG23	2:A:528:GLU:C	2.38	0.43
2:A:552:VAL:HG22	2:A:590:ALA:HB2	1.99	0.43
2:A:661:LYS:HD3	2:A:661:LYS:N	2.33	0.43
2:A:784:ILE:HD11	2:A:854:TYR:HA	2.00	0.43
2:C:71:ILE:CG2	2:C:186:VAL:HB	2.48	0.43
2:C:784:ILE:HD11	2:C:854:TYR:HA	2.00	0.43
2:C:799:PRO:O	2:C:801:PRO:HD3	2.17	0.43
2:C:974:THR:CG2	2:C:980:MET:HB2	2.48	0.43
1:B:206:TYR:O	1:B:206:TYR:HD1	2.01	0.43
2:A:155:SER:HA	2:A:158:MET:CE	2.48	0.43
2:A:759:VAL:O	2:A:762:VAL:HG22	2.18	0.43
8:A:1101:CLR:H161	9:A:1108:PCW:H232	2.00	0.43
1:D:189:PRO:HG2	1:D:245:TYR:CD2	2.54	0.43
1:D:193:LYS:O	1:D:198:LEU:HD13	2.19	0.43
1:D:206:TYR:O	1:D:206:TYR:HD1	2.01	0.43
2:C:92:PHE:CE2	2:C:96:LEU:HD21	2.53	0.43
2:C:259:VAL:HG23	2:C:260:TYR:HD2	1.83	0.43
2:C:705:CYS:CB	2:C:712:VAL:HG11	2.46	0.43
2:C:1007:PHE:HE2	9:C:1106:PCW:H12	1.74	0.43
9:C:1108:PCW:H361	9:C:1108:PCW:H332	1.34	0.43
2:A:71:ILE:CG2	2:A:186:VAL:HB	2.48	0.43
1:D:160:CYS:SG	1:D:262:ALA:HB1	2.59	0.43
2:C:1011:ARG:HD3	9:C:1106:PCW:C6	2.49	0.43
1:B:229:ILE:H	1:B:229:ILE:HG13	1.52	0.43
2:A:354:LYS:HD3	2:A:760:THR:CG2	2.48	0.43
2:A:704:GLY:HA2	2:A:707:ARG:NH1	2.34	0.43
2:C:476:LYS:HB2	2:C:493:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:SER:O	2:C:499:SER:HB3	2.19	0.43
2:C:552:VAL:HG22	2:C:590:ALA:HB2	1.99	0.43
2:C:656:ASN:HB3	2:C:659:ASP:OD2	2.19	0.43
9:C:1106:PCW:C28	2:A:993:PRO:HA	2.48	0.43
2:A:78:ASN:CG	2:A:261:THR:HG23	2.39	0.43
2:A:259:VAL:HG23	2:A:260:TYR:HD2	1.83	0.43
2:A:351:MET:O	2:A:354:LYS:N	2.50	0.43
2:C:78:ASN:CG	2:C:261:THR:HG23	2.39	0.43
2:C:916:PHE:HE2	2:C:979:ARG:HH21	1.63	0.43
9:C:1105:PCW:H212	9:C:1105:PCW:H182	1.71	0.43
1:B:99:TYR:O	1:B:103:VAL:HG23	2.19	0.43
2:A:95:GLN:HG3	2:A:148:TYR:HB2	2.00	0.43
2:A:433:PHE:CD1	2:A:447:VAL:HG22	2.53	0.43
1:D:28:ARG:NH2	2:C:1020:GLU:OE2	2.45	0.42
2:C:354:LYS:HD3	2:C:760:THR:CG2	2.49	0.42
2:A:638:ASN:ND2	2:A:687:GLU:OE2	2.50	0.42
2:A:938:LYS:HB3	2:A:938:LYS:HE3	1.87	0.42
2:C:460:ILE:HD12	2:C:467:VAL:CG2	2.49	0.42
2:C:500:GLU:HG2	2:C:502:ARG:N	2.25	0.42
2:C:774:LYS:CB	2:C:822:LEU:HD12	2.49	0.42
1:B:114:ASN:OD1	1:B:154:ARG:NH1	2.53	0.42
2:C:704:GLY:HA2	2:C:707:ARG:NH1	2.34	0.42
1:B:229:ILE:HD12	1:B:229:ILE:O	2.19	0.42
2:A:974:THR:HG22	2:A:980:MET:HB2	2.00	0.42
1:D:292:ARG:NH2	2:C:124:GLU:OE2	2.53	0.42
2:C:91:LYS:O	2:C:92:PHE:C	2.57	0.42
1:B:84:ALA:HB1	1:B:88:GLU:O	2.20	0.42
1:B:193:LYS:O	1:B:198:LEU:HD13	2.19	0.42
1:B:292:ARG:NH2	2:A:124:GLU:OE2	2.53	0.42
2:A:460:ILE:HD12	2:A:467:VAL:CG2	2.49	0.42
2:A:666:HIS:HD2	2:A:668:SER:H	1.68	0.42
2:A:774:LYS:CB	2:A:822:LEU:HD12	2.49	0.42
2:C:554:GLY:HA2	2:C:588:LEU:HD23	2.02	0.42
2:C:920:THR:O	2:C:923:PHE:HB3	2.20	0.42
1:D:229:ILE:HD12	1:D:229:ILE:O	2.19	0.42
2:C:938:LYS:HB3	2:C:938:LYS:HE3	1.87	0.42
2:A:80:LEU:HA	2:A:263:ASP:OD1	2.20	0.42
2:A:631:VAL:HG23	2:A:633:ILE:HG12	2.01	0.42
9:A:1109:PCW:H411	9:A:1109:PCW:H381	1.85	0.42
1:D:114:ASN:OD1	1:D:154:ARG:NH1	2.53	0.42
2:C:467:VAL:CG1	2:C:471:ARG:HE	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:666:HIS:HD2	2:C:668:SER:H	1.68	0.42
2:A:259:VAL:HG23	2:A:260:TYR:CD2	2.54	0.42
2:A:309:LEU:HA	2:A:312:ILE:HG12	2.02	0.42
2:A:640:THR:HG22	2:A:662:ALA:O	2.19	0.42
2:A:932:ALA:O	2:A:936:ILE:HG12	2.19	0.42
2:C:259:VAL:HG23	2:C:260:TYR:CD2	2.54	0.42
2:C:374:CYS:HB2	2:C:714:VAL:HG22	2.02	0.42
2:C:662:ALA:HB2	2:C:687:GLU:HB2	2.02	0.42
2:A:1011:ARG:HD3	9:A:1108:PCW:C6	2.49	0.42
1:D:284:ASN:O	1:D:285:ILE:HD12	2.20	0.42
2:C:875:GLU:OE1	2:C:987:TRP:NE1	2.44	0.42
2:A:100:PHE:CZ	2:A:334:GLU:HG2	2.55	0.42
2:A:476:LYS:HB2	2:A:493:HIS:CE1	2.54	0.42
2:A:944:ILE:O	2:A:944:ILE:HG13	2.20	0.42
1:D:56:GLN:NE2	1:D:59:LEU:HD12	2.33	0.41
1:D:265:PHE:HB3	1:D:268:LEU:HD12	2.02	0.41
2:C:932:ALA:O	2:C:936:ILE:HG12	2.19	0.41
2:C:985:PRO:HD3	3:E:19:LEU:HD11	2.02	0.41
2:A:460:ILE:HD12	2:A:467:VAL:HG22	2.00	0.41
2:A:656:ASN:HB3	2:A:659:ASP:OD2	2.19	0.41
1:D:99:TYR:O	1:D:103:VAL:HG23	2.19	0.41
2:C:309:LEU:HA	2:C:312:ILE:HG12	2.02	0.41
2:C:347:THR:HG21	2:C:768:ILE:CG1	2.50	0.41
9:C:1105:PCW:H20	9:C:1105:PCW:H231	1.83	0.41
9:C:1106:PCW:H63	1:B:63:SER:CB	2.50	0.41
1:B:50:ILE:HD12	9:A:1106:PCW:H262	2.03	0.41
1:B:234:LEU:HG	1:B:241:PRO:HG3	2.02	0.41
1:D:84:ALA:HB1	1:D:88:GLU:O	2.20	0.41
2:C:502:ARG:HG2	2:C:567:GLU:HG2	2.02	0.41
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.87	0.41
1:B:245:TYR:HB3	1:B:246:PRO:HA	2.02	0.41
2:A:347:THR:HG21	2:A:768:ILE:CG1	2.50	0.41
2:A:467:VAL:CG1	2:A:471:ARG:HE	2.33	0.41
2:C:130:LEU:O	2:C:134:VAL:HG23	2.21	0.41
2:C:887:ARG:HG2	2:C:888:VAL:N	2.35	0.41
2:A:371:SER:OG	2:A:711:ILE:N	2.54	0.41
1:D:50:ILE:HD12	9:C:1104:PCW:H262	2.03	0.41
1:D:107:HIS:O	1:D:111:ASP:HB2	2.20	0.41
1:D:245:TYR:HB3	1:D:246:PRO:HA	2.02	0.41
2:A:475:PRO:O	2:A:493:HIS:HA	2.20	0.41
2:A:503:TYR:HE2	2:A:505:LEU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:662:ALA:HB2	2:A:687:GLU:HB2	2.02	0.41
2:A:887:ARG:HG2	2:A:888:VAL:N	2.35	0.41
2:C:100:PHE:CZ	2:C:334:GLU:HG2	2.55	0.41
2:C:170:LEU:HD21	2:C:177:LYS:NZ	2.36	0.41
2:C:994:TYR:O	2:C:998:ILE:HG13	2.21	0.41
2:C:373:ILE:HG21	2:C:755:PHE:HE1	1.86	0.41
2:C:433:PHE:HE1	2:C:447:VAL:HG22	1.86	0.41
2:C:957:GLY:O	2:C:961:GLU:HG2	2.21	0.41
9:C:1106:PCW:H271	8:A:1103:CLR:H273	2.02	0.41
1:B:107:HIS:O	1:B:111:ASP:HB2	2.20	0.41
2:A:920:THR:O	2:A:923:PHE:HB3	2.20	0.41
1:D:122:SER:HA	1:D:123:PRO:HA	1.74	0.41
2:C:172:ILE:HD12	2:C:177:LYS:HG2	2.03	0.41
2:C:495:ASN:HD21	2:C:497:LYS:HZ1	1.68	0.41
2:C:503:TYR:HE2	2:C:505:LEU:HB2	1.84	0.41
2:A:204:ARG:O	2:A:256:GLY:HA2	2.21	0.41
2:A:994:TYR:O	2:A:998:ILE:HG13	2.21	0.41
2:C:233:SER:OG	2:C:235:ASN:ND2	2.54	0.41
2:C:475:PRO:O	2:C:493:HIS:HA	2.20	0.41
1:B:265:PHE:HB3	1:B:268:LEU:CD1	2.51	0.41
1:B:284:ASN:O	1:B:285:ILE:HD12	2.20	0.41
2:A:121:THR:HG22	2:A:122:GLU:N	2.25	0.41
2:A:130:LEU:O	2:A:134:VAL:HG23	2.21	0.41
2:A:150:GLN:HG3	2:A:342:VAL:HG22	2.03	0.41
2:A:424:ILE:HG22	2:A:506:VAL:CG1	2.51	0.41
2:A:433:PHE:CZ	2:A:457:LEU:HB3	2.56	0.41
2:A:442:ILE:HD13	2:A:442:ILE:N	2.32	0.41
2:A:924:ILE:CD1	2:A:983:LEU:HD22	2.50	0.41
2:A:985:PRO:HD3	3:G:19:LEU:HD11	2.02	0.41
1:D:36:ILE:HD12	1:D:36:ILE:HA	1.90	0.41
1:D:195:THR:HG22	1:D:196:THR:N	2.36	0.41
2:C:80:LEU:HA	2:C:263:ASP:OD1	2.20	0.41
2:C:204:ARG:O	2:C:256:GLY:HA2	2.21	0.41
2:C:371:SER:OG	2:C:711:ILE:N	2.53	0.41
2:C:433:PHE:CZ	2:C:457:LEU:HB3	2.56	0.41
9:C:1107:PCW:H152	9:C:1107:PCW:H122	1.59	0.41
2:C:150:GLN:HG3	2:C:342:VAL:HG22	2.03	0.40
2:A:105:TRP:HE1	2:A:140:VAL:HG11	1.86	0.40
2:A:554:GLY:HA2	2:A:588:LEU:HD23	2.02	0.40
2:A:768:ILE:HG22	2:A:772:LEU:CD1	2.51	0.40
1:D:59:LEU:HD23	1:D:59:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:THR:HG22	2:C:122:GLU:N	2.25	0.40
1:B:195:THR:HG22	1:B:196:THR:N	2.36	0.40
2:A:219:THR:HG23	2:A:221:GLU:H	1.86	0.40
2:A:502:ARG:HG2	2:A:567:GLU:HG2	2.02	0.40
2:A:813:GLY:CA	9:A:1109:PCW:H261	2.52	0.40
8:A:1101:CLR:H151	9:A:1108:PCW:H211	2.02	0.40
1:D:93:ILE:HB	1:D:305:SER:OG	2.20	0.40
2:C:759:VAL:HA	2:C:762:VAL:HG22	2.03	0.40
2:C:813:GLY:CA	9:C:1107:PCW:H261	2.52	0.40
2:C:944:ILE:O	2:C:944:ILE:HG13	2.20	0.40
1:B:93:ILE:HB	1:B:305:SER:OG	2.20	0.40
2:A:170:LEU:HD21	2:A:177:LYS:NZ	2.36	0.40
2:A:418:TRP:CZ3	2:A:421:LEU:HD23	2.56	0.40
1:D:265:PHE:HB3	1:D:268:LEU:CD1	2.51	0.40
2:C:768:ILE:HG22	2:C:772:LEU:CD1	2.51	0.40
1:B:85:ILE:HG23	2:A:894:TRP:NE1	2.36	0.40
2:A:367:LEU:HD23	2:A:367:LEU:HA	1.94	0.40
2:A:373:ILE:HG21	2:A:755:PHE:HE1	1.86	0.40
2:A:374:CYS:HB2	2:A:714:VAL:HG22	2.02	0.40
1:D:56:GLN:HG3	8:D:401:CLR:C6	2.52	0.40
1:D:229:ILE:H	1:D:229:ILE:HG13	1.53	0.40
2:C:424:ILE:HG22	2:C:506:VAL:CG1	2.51	0.40
2:C:515:LEU:HD22	2:C:538:PHE:CD1	2.56	0.40
2:C:924:ILE:CD1	2:C:983:LEU:HD22	2.51	0.40
2:A:957:GLY:O	2:A:961:GLU:HG2	2.21	0.40
2:A:1007:PHE:HE2	9:A:1108:PCW:O31	2.05	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	B	292/305 (96%)	258 (88%)	33 (11%)	1 (0%)	41 75
1	D	292/305 (96%)	258 (88%)	33 (11%)	1 (0%)	41 75
2	A	985/1028 (96%)	941 (96%)	43 (4%)	1 (0%)	51 84
2	C	985/1028 (96%)	941 (96%)	43 (4%)	1 (0%)	51 84
3	E	38/94 (40%)	37 (97%)	1 (3%)	0	100 100
3	G	38/94 (40%)	37 (97%)	1 (3%)	0	100 100
All	All	2630/2854 (92%)	2472 (94%)	154 (6%)	4 (0%)	50 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	145	GLY
1	B	145	GLY
2	C	121	THR
2	A	121	THR

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	B	258/266 (97%)	225 (87%)	33 (13%)	4 22
1	D	258/266 (97%)	224 (87%)	34 (13%)	4 21
2	A	835/869 (96%)	783 (94%)	52 (6%)	18 51
2	C	835/869 (96%)	783 (94%)	52 (6%)	18 51
3	E	33/75 (44%)	31 (94%)	2 (6%)	18 51
3	G	33/75 (44%)	31 (94%)	2 (6%)	18 51
All	All	2252/2420 (93%)	2077 (92%)	175 (8%)	16 42

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	SER

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Mol	Chain	Res	Type
1	D	26	LEU
1	D	32	SER
1	D	62	LEU
1	D	64	ASP
1	D	65	PHE
1	D	73	VAL
1	D	79	SER
1	D	94	SER
1	D	137	ARG
1	D	144	GLN
1	D	154	ARG
1	D	156	TRP
1	D	157	LEU
1	D	160	CYS
1	D	161	SER
1	D	167	THR
1	D	196	THR
1	D	197	ASP
1	D	200	GLU
1	D	203	GLN
1	D	214	ARG
1	D	218	LYS
1	D	251	ARG
1	D	266	THR
1	D	268	LEU
1	D	269	THR
1	D	272	MET
1	D	284	ASN
1	D	285	ILE
1	D	287	TYR
1	D	289	GLU
1	D	292	ARG
1	D	294	ARG
2	C	52	HIS
2	C	63	LEU
2	C	67	ARG
2	C	100	PHE
2	C	150	GLN
2	C	151	GLU
2	C	168	GLN
2	C	194	LYS
2	C	264	ARG

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Mol	Chain	Res	Type
2	C	295	ILE
2	C	331	ASN
2	C	334	GLU
2	C	357	LEU
2	C	384	ASN
2	C	404	GLU
2	C	405	ASN
2	C	407	SER
2	C	413	LYS
2	C	442	ILE
2	C	502	ARG
2	C	557	HIS
2	C	607	ARG
2	C	656	ASN
2	C	671	LYS
2	C	676	GLU
2	C	720	ASN
2	C	747	ASP
2	C	772	LEU
2	C	794	ILE
2	C	811	ASP
2	C	830	ASP
2	C	834	ARG
2	C	840	LYS
2	C	842	ASP
2	C	843	LYS
2	C	849	LEU
2	C	879	LEU
2	C	881	MET
2	C	882	ASP
2	C	897	ASP
2	C	911	ARG
2	C	944	ILE
2	C	964	LEU
2	C	975	ASP
2	C	978	LEU
2	C	983	LEU
2	C	997	ILE
2	C	1005	ARG
2	C	1006	ARG
2	C	1007	PHE
2	C	1010	ARG

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Mol	Chain	Res	Type
2	C	1011	ARG
3	E	13	THR
3	E	33	ILE
1	B	20	SER
1	B	26	LEU
1	B	32	SER
1	B	62	LEU
1	B	64	ASP
1	B	65	PHE
1	B	73	VAL
1	B	79	SER
1	B	94	SER
1	B	137	ARG
1	B	144	GLN
1	B	154	ARG
1	B	156	TRP
1	B	157	LEU
1	B	160	CYS
1	B	161	SER
1	B	167	THR
1	B	196	THR
1	B	197	ASP
1	B	200	GLU
1	B	203	GLN
1	B	214	ARG
1	B	218	LYS
1	B	251	ARG
1	B	266	THR
1	B	268	LEU
1	B	272	MET
1	B	284	ASN
1	B	285	ILE
1	B	287	TYR
1	B	289	GLU
1	B	292	ARG
1	B	294	ARG
2	A	52	HIS
2	A	63	LEU
2	A	67	ARG
2	A	100	PHE
2	A	150	GLN
2	A	151	GLU

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Mol	Chain	Res	Type
2	A	168	GLN
2	A	194	LYS
2	A	264	ARG
2	A	295	ILE
2	A	331	ASN
2	A	334	GLU
2	A	357	LEU
2	A	384	ASN
2	A	404	GLU
2	A	405	ASN
2	A	407	SER
2	A	413	LYS
2	A	442	ILE
2	A	502	ARG
2	A	557	HIS
2	A	607	ARG
2	A	656	ASN
2	A	671	LYS
2	A	676	GLU
2	A	720	ASN
2	A	747	ASP
2	A	772	LEU
2	A	794	ILE
2	A	811	ASP
2	A	830	ASP
2	A	834	ARG
2	A	840	LYS
2	A	842	ASP
2	A	843	LYS
2	A	849	LEU
2	A	879	LEU
2	A	881	MET
2	A	882	ASP
2	A	897	ASP
2	A	911	ARG
2	A	944	ILE
2	A	964	LEU
2	A	975	ASP
2	A	978	LEU
2	A	983	LEU
2	A	997	ILE
2	A	1005	ARG

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Mol	Chain	Res	Type
2	A	1006	ARG
2	A	1007	PHE
2	A	1010	ARG
2	A	1011	ARG
3	G	13	THR
3	G	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
1	D	203	GLN
1	D	258	GLN
2	C	118	GLN
2	C	127	ASN
2	C	129	ASN
2	C	215	ASN
2	C	235	ASN
2	C	248	ASN
2	C	396	GLN
2	C	434	GLN
2	C	439	ASN
2	C	474	ASN
2	C	483	ASN
2	C	489	GLN
2	C	495	ASN
2	C	539	GLN
2	C	577	ASN
2	C	620	HIS
2	C	654	GLN
2	C	656	ASN
2	C	666	HIS
2	C	708	GLN
2	C	720	ASN
2	C	783	ASN
2	C	905	GLN
2	C	910	GLN
2	C	942	ASN
1	B	56	GLN
1	B	203	GLN
1	B	258	GLN
2	A	118	GLN

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Mol	Chain	Res	Type
2	A	127	ASN
2	A	129	ASN
2	A	215	ASN
2	A	235	ASN
2	A	248	ASN
2	A	396	GLN
2	A	405	ASN
2	A	434	GLN
2	A	439	ASN
2	A	474	ASN
2	A	483	ASN
2	A	489	GLN
2	A	495	ASN
2	A	539	GLN
2	A	577	ASN
2	A	620	HIS
2	A	654	GLN
2	A	656	ASN
2	A	666	HIS
2	A	708	GLN
2	A	720	ASN
2	A	783	ASN
2	A	905	GLN
2	A	910	GLN
2	A	942	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

38 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	1,4	14,14,15	1.11	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.62	1 (5%)
4	BMA	F	3	4	11,11,12	0.74	0	15,15,17	1.33	2 (13%)
4	MAN	F	4	4	11,11,12	0.74	0	15,15,17	0.99	2 (13%)
4	MAN	F	5	4	11,11,12	0.69	0	15,15,17	0.93	2 (13%)
4	FUC	F	6	4	10,10,11	1.08	1 (10%)	14,14,16	0.72	0
5	NAG	H	1	1,5	14,14,15	0.57	0	17,19,21	1.12	2 (11%)
5	NAG	H	2	5	14,14,15	0.32	0	17,19,21	1.50	2 (11%)
5	BMA	H	3	5	11,11,12	1.24	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	H	4	5	11,11,12	1.44	3 (27%)	15,15,17	1.40	2 (13%)
5	NAG	H	5	5	14,14,15	0.72	0	17,19,21	0.82	1 (5%)
5	MAN	H	6	5	11,11,12	0.72	0	15,15,17	0.95	2 (13%)
6	NAG	I	1	1,6	14,14,15	0.76	1 (7%)	17,19,21	1.55	1 (5%)
6	NAG	I	2	6	14,14,15	0.21	0	17,19,21	0.60	1 (5%)
6	BMA	I	3	6	11,11,12	0.58	0	15,15,17	1.28	2 (13%)
6	MAN	I	4	6	11,11,12	0.69	0	15,15,17	0.96	2 (13%)
6	FUC	I	5	6	10,10,11	1.05	1 (10%)	14,14,16	0.71	0
7	NAG	J	1	1,7	14,14,15	0.51	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.37	0
4	NAG	K	1	1,4	14,14,15	1.10	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	K	2	4	14,14,15	0.22	0	17,19,21	0.61	1 (5%)
4	BMA	K	3	4	11,11,12	0.75	0	15,15,17	1.34	2 (13%)
4	MAN	K	4	4	11,11,12	0.74	0	15,15,17	0.98	2 (13%)
4	MAN	K	5	4	11,11,12	0.69	0	15,15,17	0.93	2 (13%)
4	FUC	K	6	4	10,10,11	1.10	1 (10%)	14,14,16	0.72	0
5	NAG	L	1	1,5	14,14,15	0.56	0	17,19,21	1.13	2 (11%)
5	NAG	L	2	5	14,14,15	0.32	0	17,19,21	1.50	2 (11%)
5	BMA	L	3	5	11,11,12	1.23	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	L	4	5	11,11,12	1.44	3 (27%)	15,15,17	1.40	2 (13%)
5	NAG	L	5	5	14,14,15	0.72	0	17,19,21	0.82	1 (5%)
5	MAN	L	6	5	11,11,12	0.74	0	15,15,17	0.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	M	1	1,6	14,14,15	0.76	1 (7%)	17,19,21	1.55	1 (5%)
6	NAG	M	2	6	14,14,15	0.19	0	17,19,21	0.59	1 (5%)
6	BMA	M	3	6	11,11,12	0.57	0	15,15,17	1.28	2 (13%)
6	MAN	M	4	6	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
6	FUC	M	5	6	10,10,11	1.05	1 (10%)	14,14,16	0.71	0
7	NAG	N	1	1,7	14,14,15	0.52	0	17,19,21	0.62	0
7	NAG	N	2	7	14,14,15	0.20	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	FUC	F	6	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	4/6/23/26	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	FUC	I	5	6	-	-	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	0/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
4	FUC	K	6	4	-	-	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	NAG	L	5	5	-	4/6/23/26	0/1/1/1
5	MAN	L	6	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	FUC	M	5	6	-	-	0/1/1/1
7	NAG	N	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	3.71	1.49	1.43
4	K	1	NAG	O5-C1	3.70	1.49	1.43
5	H	4	MAN	O2-C2	3.02	1.49	1.43
5	L	4	MAN	O2-C2	2.99	1.49	1.43
4	K	6	FUC	O5-C1	-2.87	1.39	1.43
4	F	6	FUC	O5-C1	-2.82	1.39	1.43
6	I	5	FUC	O5-C1	-2.52	1.39	1.43
6	M	5	FUC	O5-C1	-2.50	1.39	1.43
6	I	1	NAG	O5-C1	2.40	1.47	1.43
6	M	1	NAG	O5-C1	2.40	1.47	1.43
5	L	4	MAN	C1-C2	2.24	1.57	1.52
5	H	4	MAN	C1-C2	2.21	1.57	1.52
5	H	3	BMA	C2-C3	2.19	1.55	1.52
5	L	3	BMA	C2-C3	2.15	1.55	1.52
5	L	4	MAN	C2-C3	2.12	1.55	1.52
5	H	4	MAN	C2-C3	2.11	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1	NAG	C1-O5-C5	5.89	120.18	112.19
6	I	1	NAG	C1-O5-C5	5.87	120.15	112.19
4	K	1	NAG	C1-O5-C5	4.66	118.51	112.19
4	F	1	NAG	C1-O5-C5	4.66	118.51	112.19
5	H	2	NAG	C1-O5-C5	4.44	118.20	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	2	NAG	C1-O5-C5	4.40	118.16	112.19
5	L	4	MAN	O2-C2-C1	4.22	117.78	109.15
5	H	4	MAN	O2-C2-C1	4.22	117.78	109.15
5	H	2	NAG	C2-N2-C7	3.64	128.09	122.90
5	L	2	NAG	C2-N2-C7	3.62	128.06	122.90
5	H	3	BMA	O3-C3-C2	3.26	116.24	109.99
5	L	3	BMA	O3-C3-C2	3.26	116.24	109.99
5	L	5	NAG	C1-O5-C5	3.15	116.46	112.19
5	H	5	NAG	C1-O5-C5	3.14	116.45	112.19
5	L	1	NAG	O4-C4-C5	3.05	116.88	109.30
5	H	1	NAG	O4-C4-C5	3.04	116.85	109.30
4	F	3	BMA	O5-C5-C6	2.75	111.51	107.20
4	K	3	BMA	O5-C5-C6	2.74	111.49	107.20
5	H	4	MAN	C1-O5-C5	2.73	115.89	112.19
5	L	4	MAN	C1-O5-C5	2.72	115.88	112.19
5	L	1	NAG	C1-O5-C5	2.68	115.82	112.19
5	H	1	NAG	C1-O5-C5	2.64	115.77	112.19
6	I	3	BMA	O5-C5-C6	2.36	110.91	107.20
6	M	3	BMA	O5-C5-C6	2.36	110.90	107.20
6	I	3	BMA	C3-C4-C5	-2.32	106.11	110.24
6	M	3	BMA	C3-C4-C5	-2.29	106.16	110.24
4	K	5	MAN	O2-C2-C3	-2.27	105.58	110.14
4	F	5	MAN	O2-C2-C3	-2.27	105.59	110.14
4	F	4	MAN	O2-C2-C3	-2.26	105.61	110.14
5	L	6	MAN	O2-C2-C3	-2.25	105.62	110.14
4	K	4	MAN	O2-C2-C3	-2.24	105.64	110.14
5	H	6	MAN	O2-C2-C3	-2.24	105.64	110.14
4	K	3	BMA	C3-C4-C5	-2.22	106.28	110.24
6	M	4	MAN	O2-C2-C3	-2.22	105.70	110.14
4	F	3	BMA	C3-C4-C5	-2.21	106.29	110.24
6	M	4	MAN	C1-O5-C5	2.20	115.17	112.19
6	I	4	MAN	O2-C2-C3	-2.20	105.73	110.14
5	H	6	MAN	C1-O5-C5	2.19	115.16	112.19
4	F	2	NAG	C1-O5-C5	2.18	115.15	112.19
5	L	6	MAN	C1-O5-C5	2.18	115.15	112.19
4	K	2	NAG	C1-O5-C5	2.15	115.11	112.19
6	I	4	MAN	C1-O5-C5	2.15	115.10	112.19
4	K	4	MAN	C1-O5-C5	2.14	115.10	112.19
4	F	4	MAN	C1-O5-C5	2.13	115.07	112.19
6	I	2	NAG	C1-O5-C5	2.07	115.00	112.19
6	M	2	NAG	C1-O5-C5	2.05	114.97	112.19
4	K	5	MAN	C1-O5-C5	2.01	114.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
5	H	5	NAG	O5-C5-C6-O6
5	L	5	NAG	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
5	H	5	NAG	C4-C5-C6-O6
5	L	5	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	H	5	NAG	C8-C7-N2-C2
5	H	5	NAG	O7-C7-N2-C2
5	L	5	NAG	C8-C7-N2-C2
5	L	5	NAG	O7-C7-N2-C2
5	H	3	BMA	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6

There are no ring outliers.

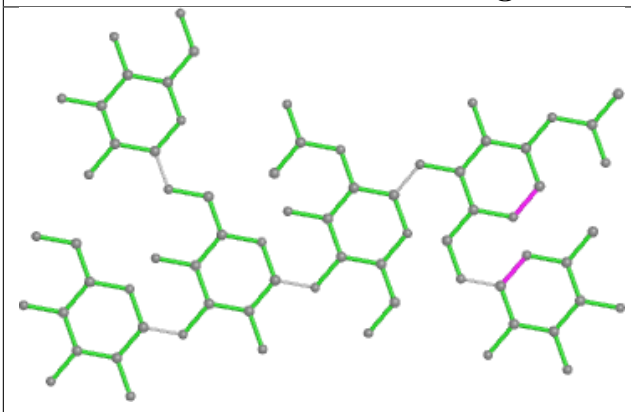
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	6	FUC	1	0
4	F	6	FUC	1	0

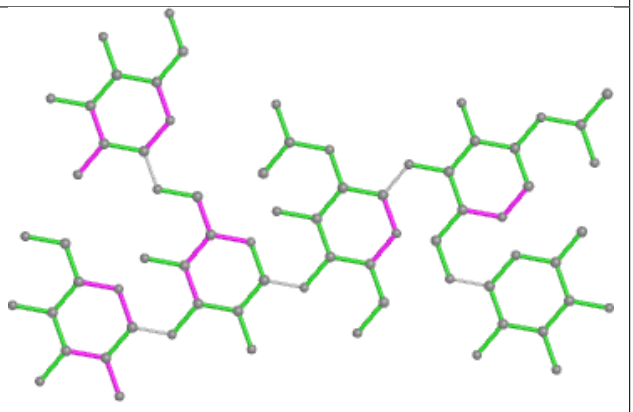
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

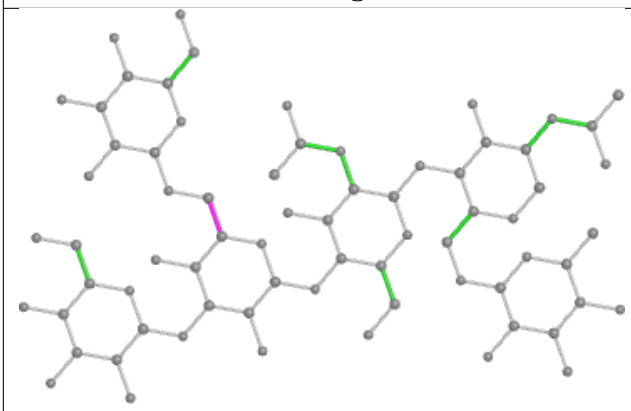
Oligosaccharide Chain F



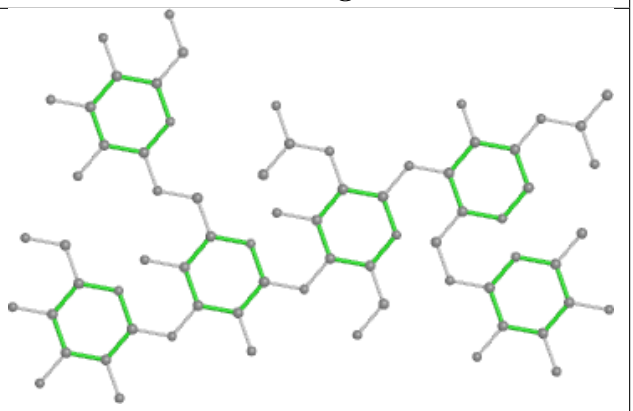
Bond lengths



Bond angles

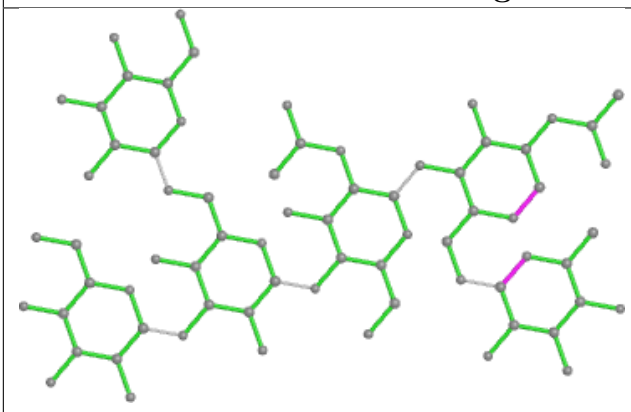


Torsions

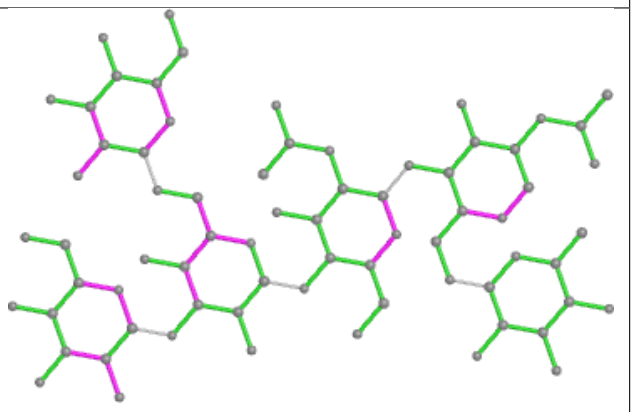


Rings

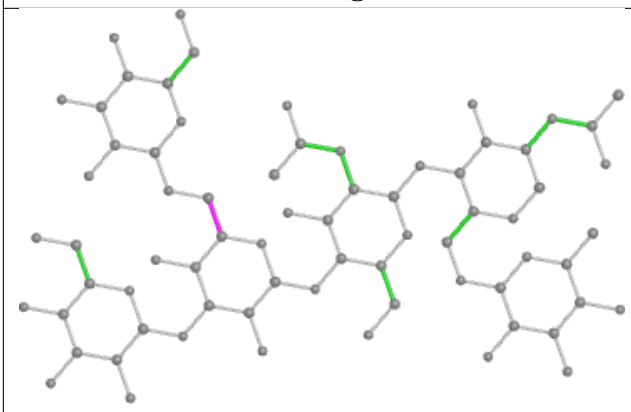
Oligosaccharide Chain K



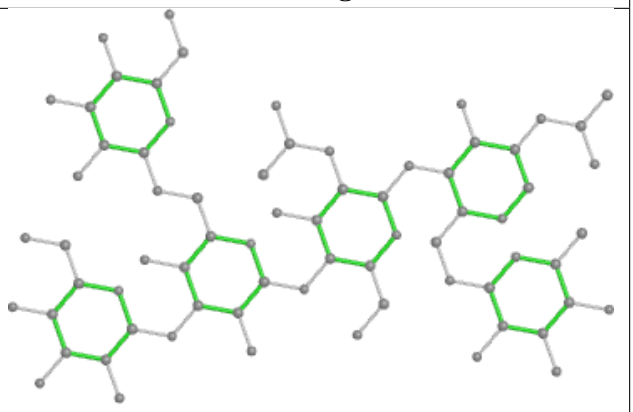
Bond lengths



Bond angles

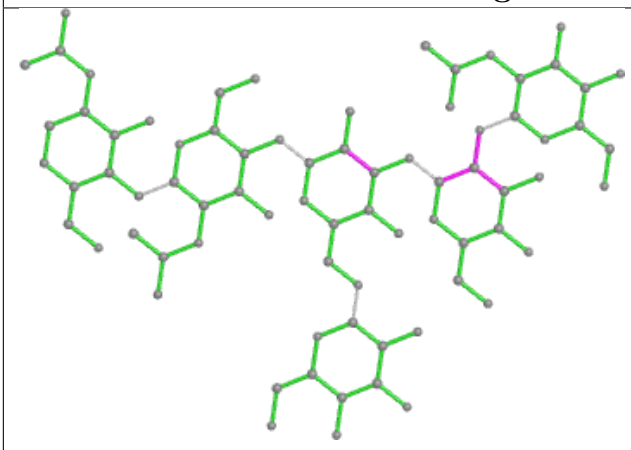


Torsions

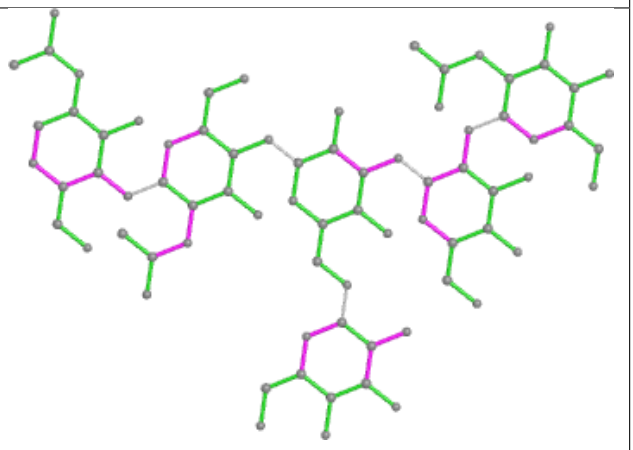


Rings

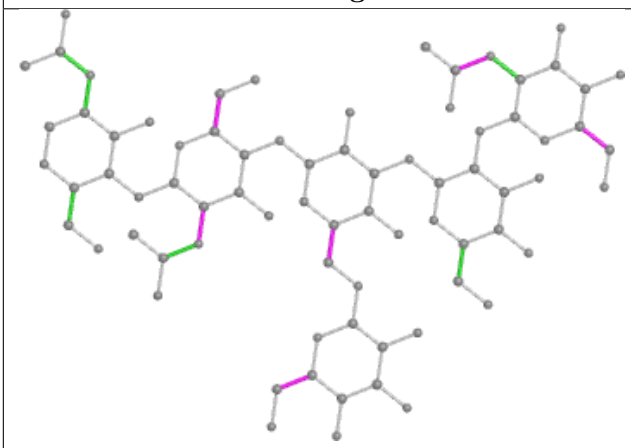
Oligosaccharide Chain H



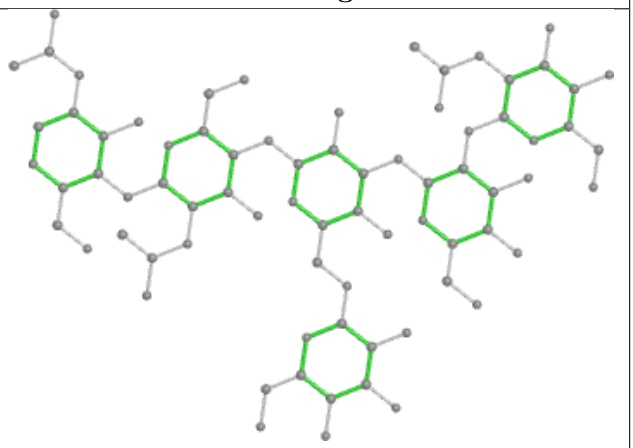
Bond lengths



Bond angles

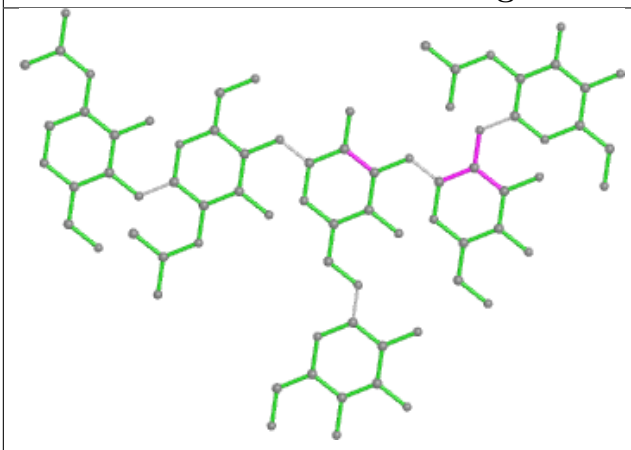


Torsions

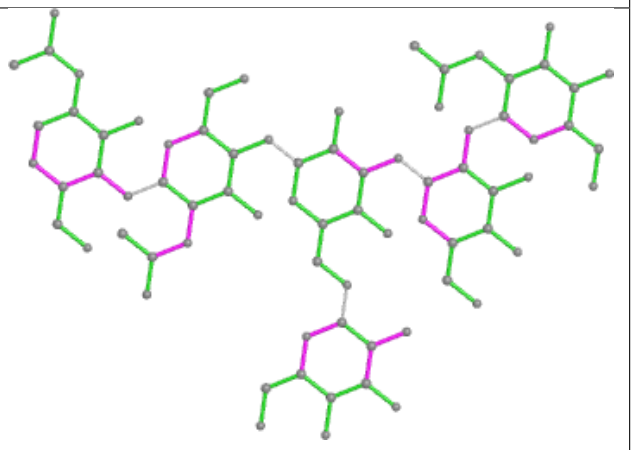


Rings

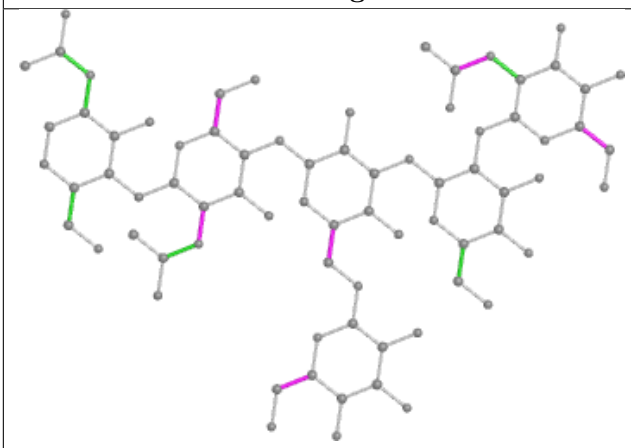
Oligosaccharide Chain L



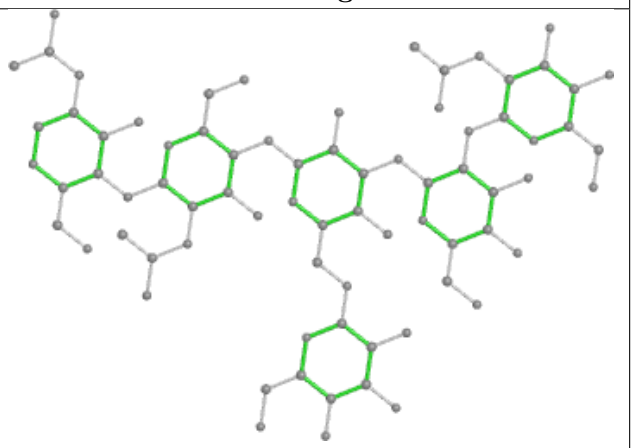
Bond lengths



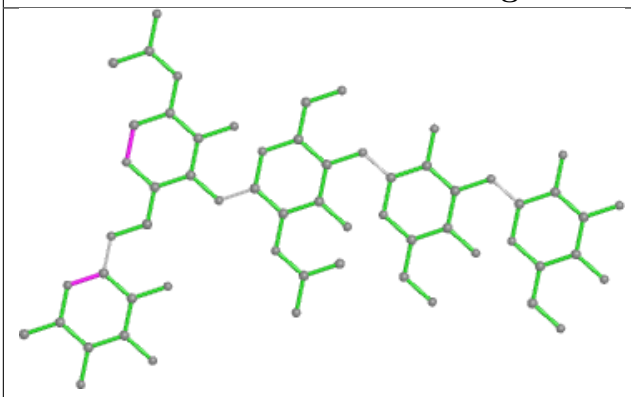
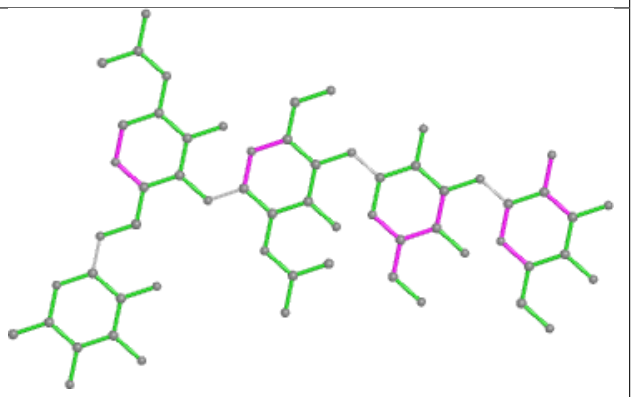
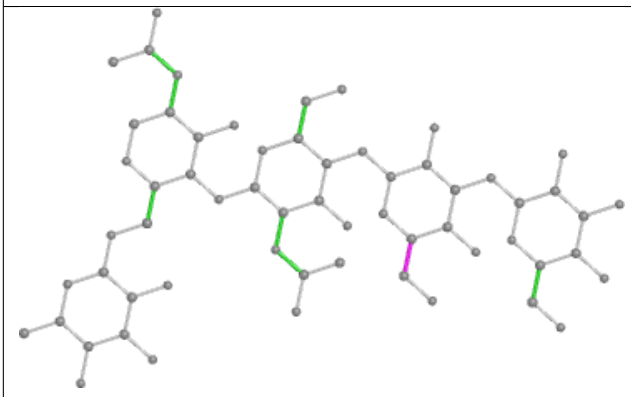
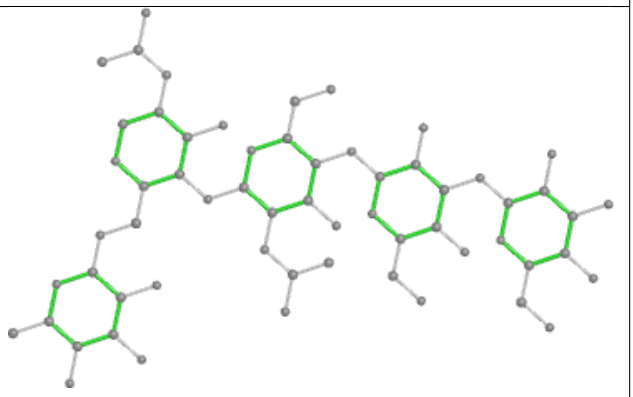
Bond angles

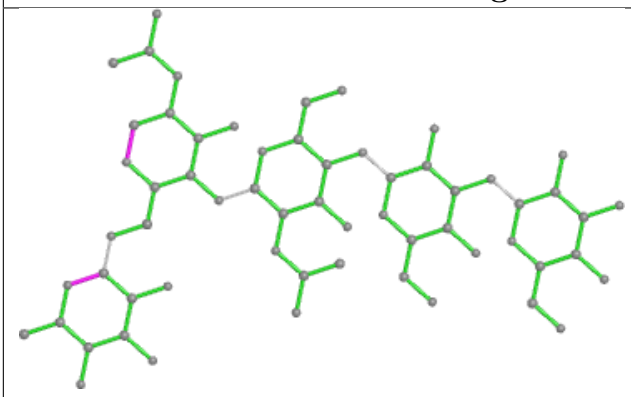
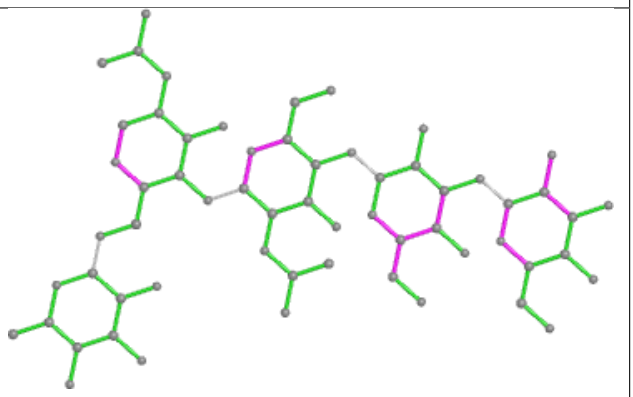
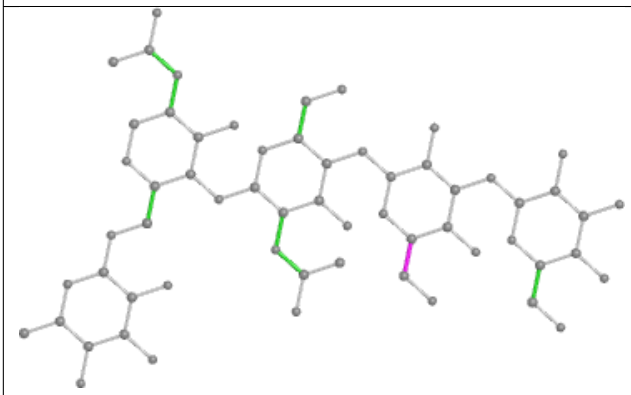
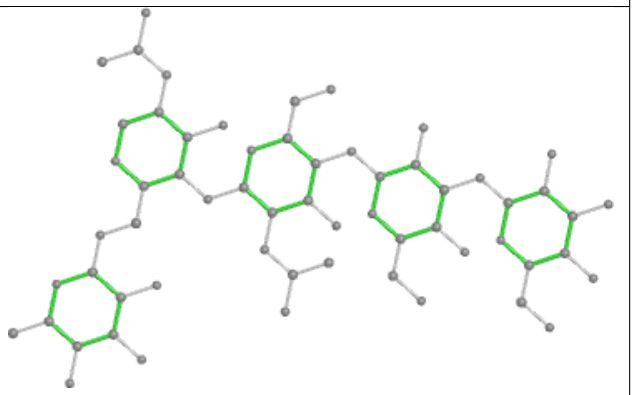


Torsions

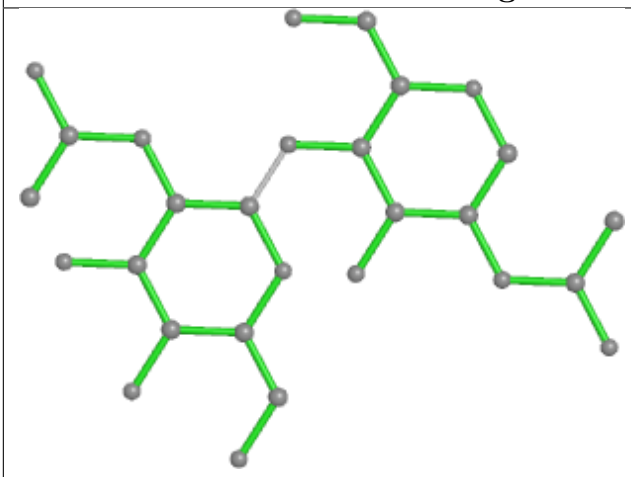


Rings

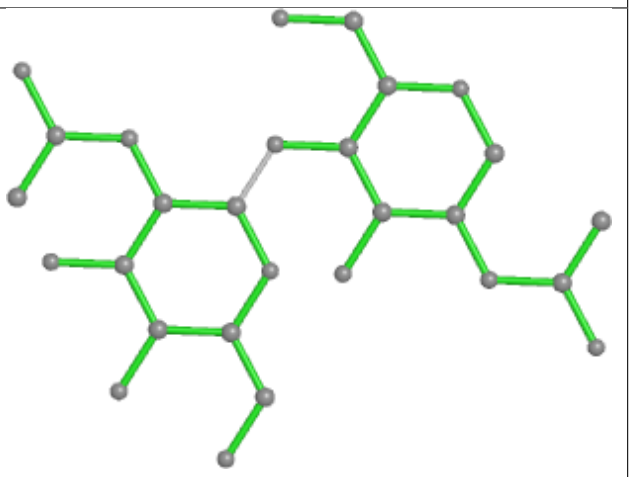
Oligosaccharide Chain I	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain M	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

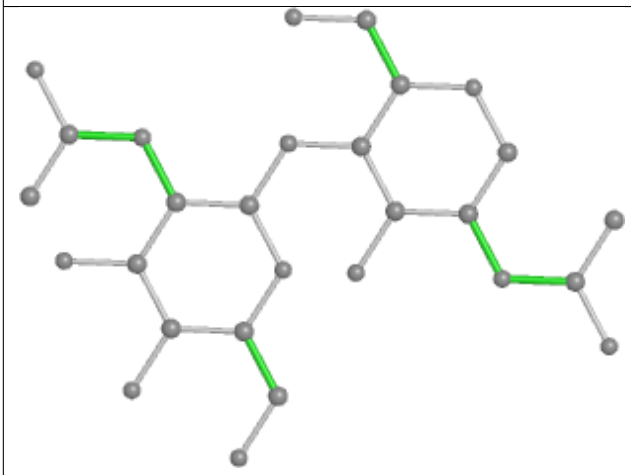
Oligosaccharide Chain J



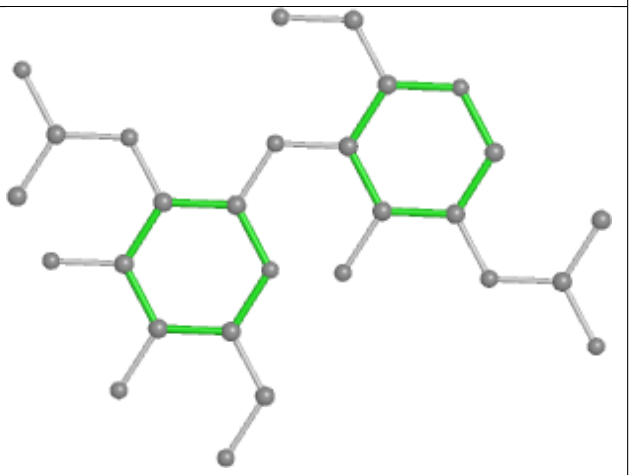
Bond lengths



Bond angles

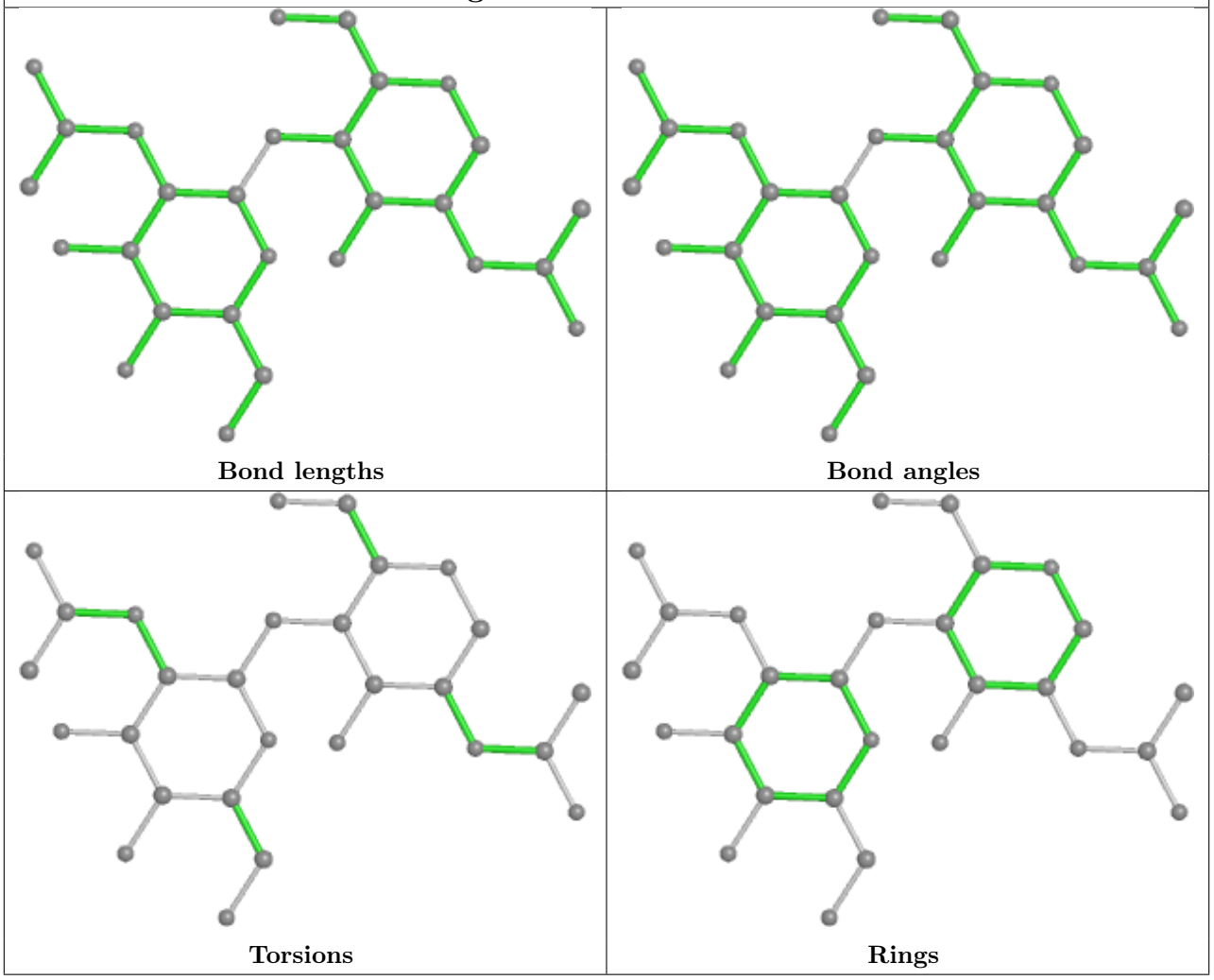


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	CLR	B	401	-	31,31,31	1.22	2 (6%)	48,48,48	1.37	5 (10%)
9	PCW	C	1105	-	53,53,53	0.97	2 (3%)	59,61,61	0.77	0
8	CLR	A	1103	-	31,31,31	1.19	2 (6%)	48,48,48	1.36	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PCW	C	1109	-	53,53,53	0.97	2 (3%)	59,61,61	0.73	0
8	CLR	C	1101	-	31,31,31	1.23	2 (6%)	48,48,48	1.36	6 (12%)
9	PCW	C	1106	-	53,53,53	0.96	2 (3%)	59,61,61	0.97	0
9	PCW	A	1109	-	53,53,53	0.95	2 (3%)	59,61,61	0.75	0
9	PCW	E	1302	-	53,53,53	0.98	2 (3%)	59,61,61	0.74	0
9	PCW	C	1110	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	0
9	PCW	A	1108	-	53,53,53	0.96	2 (3%)	59,61,61	0.97	0
9	PCW	G	1302	-	53,53,53	0.98	2 (3%)	59,61,61	0.74	0
9	PCW	C	1103	-	21,21,53	0.86	0	27,29,61	1.06	3 (11%)
8	CLR	D	401	-	31,31,31	1.21	2 (6%)	48,48,48	1.36	5 (10%)
8	CLR	A	1102	-	31,31,31	1.24	2 (6%)	48,48,48	1.36	6 (12%)
8	CLR	A	1101	-	31,31,31	1.20	2 (6%)	48,48,48	1.37	8 (16%)
9	PCW	C	1104	-	53,53,53	0.94	2 (3%)	59,61,61	0.76	0
9	PCW	A	1105	-	21,21,53	0.86	0	27,29,61	1.06	3 (11%)
9	PCW	A	1106	-	53,53,53	0.94	2 (3%)	59,61,61	0.76	0
9	PCW	A	1111	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	0
9	PCW	C	1107	-	53,53,53	0.95	2 (3%)	59,61,61	0.75	0
9	PCW	A	1104	-	21,21,53	0.94	0	27,29,61	1.13	3 (11%)
9	PCW	A	1110	-	53,53,53	0.96	2 (3%)	59,61,61	0.88	1 (1%)
9	PCW	A	1107	-	53,53,53	0.97	2 (3%)	59,61,61	0.77	0
9	PCW	C	1108	-	53,53,53	0.96	2 (3%)	59,61,61	0.87	1 (1%)
8	CLR	G	1301	-	31,31,31	1.25	2 (6%)	48,48,48	1.36	7 (14%)
9	PCW	C	1102	-	21,21,53	0.94	0	27,29,61	1.13	3 (11%)
8	CLR	E	1301	-	31,31,31	1.25	2 (6%)	48,48,48	1.36	7 (14%)
9	PCW	A	1112	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	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
8	CLR	B	401	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1105	-	-	18/57/57/57	-
8	CLR	A	1103	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1109	-	-	18/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	C	1101	-	-	1/10/68/68	0/4/4/4
9	PCW	C	1106	-	-	18/57/57/57	-
9	PCW	A	1109	-	-	27/57/57/57	-
9	PCW	E	1302	-	-	22/57/57/57	-
9	PCW	C	1110	-	-	17/57/57/57	-
9	PCW	A	1108	-	-	18/57/57/57	-
9	PCW	G	1302	-	-	22/57/57/57	-
9	PCW	C	1103	-	-	13/23/23/57	-
8	CLR	D	401	-	-	0/10/68/68	0/4/4/4
8	CLR	A	1102	-	-	1/10/68/68	0/4/4/4
8	CLR	A	1101	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1104	-	-	22/57/57/57	-
9	PCW	A	1105	-	-	13/23/23/57	-
9	PCW	A	1106	-	-	22/57/57/57	-
9	PCW	A	1111	-	-	18/57/57/57	-
9	PCW	C	1107	-	-	27/57/57/57	-
9	PCW	A	1104	-	-	9/23/23/57	-
9	PCW	A	1110	-	-	27/57/57/57	-
9	PCW	A	1107	-	-	18/57/57/57	-
9	PCW	C	1108	-	-	27/57/57/57	-
8	CLR	G	1301	-	-	0/10/68/68	0/4/4/4
9	PCW	C	1102	-	-	9/23/23/57	-
8	CLR	E	1301	-	-	0/10/68/68	0/4/4/4
9	PCW	A	1112	-	-	17/57/57/57	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1111	PCW	C40-C39	3.92	1.54	1.31
9	C	1109	PCW	C40-C39	3.92	1.54	1.31
9	C	1106	PCW	C40-C39	3.86	1.54	1.31
9	A	1108	PCW	C40-C39	3.86	1.54	1.31
9	C	1107	PCW	C40-C39	3.86	1.54	1.31
9	C	1105	PCW	C20-C19	3.85	1.54	1.31
9	A	1111	PCW	C20-C19	3.85	1.54	1.31
9	A	1109	PCW	C40-C39	3.85	1.54	1.31
9	A	1107	PCW	C20-C19	3.84	1.54	1.31
9	G	1302	PCW	C20-C19	3.84	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1108	PCW	C40-C39	3.84	1.54	1.31
9	A	1110	PCW	C40-C39	3.83	1.54	1.31
9	G	1302	PCW	C40-C39	3.83	1.54	1.31
9	A	1112	PCW	C20-C19	3.82	1.53	1.31
9	C	1110	PCW	C20-C19	3.82	1.53	1.31
9	E	1302	PCW	C40-C39	3.82	1.53	1.31
9	C	1109	PCW	C20-C19	3.82	1.53	1.31
9	E	1302	PCW	C20-C19	3.81	1.53	1.31
9	A	1108	PCW	C20-C19	3.80	1.53	1.31
9	C	1106	PCW	C20-C19	3.80	1.53	1.31
9	A	1112	PCW	C40-C39	3.80	1.53	1.31
9	C	1110	PCW	C40-C39	3.79	1.53	1.31
9	C	1105	PCW	C40-C39	3.79	1.53	1.31
9	A	1107	PCW	C40-C39	3.78	1.53	1.31
9	A	1106	PCW	C20-C19	3.74	1.53	1.31
9	C	1104	PCW	C20-C19	3.73	1.53	1.31
9	A	1110	PCW	C20-C19	3.72	1.53	1.31
9	C	1108	PCW	C20-C19	3.71	1.53	1.31
9	A	1106	PCW	C40-C39	3.71	1.53	1.31
9	A	1109	PCW	C20-C19	3.70	1.53	1.31
9	C	1104	PCW	C40-C39	3.70	1.53	1.31
9	C	1107	PCW	C20-C19	3.69	1.53	1.31
8	E	1301	CLR	C16-C17	3.20	1.61	1.54
8	G	1301	CLR	C16-C17	3.16	1.60	1.54
8	C	1101	CLR	C16-C17	3.16	1.60	1.54
8	A	1102	CLR	C16-C17	3.16	1.60	1.54
8	A	1101	CLR	C16-C17	3.12	1.60	1.54
8	D	401	CLR	C16-C17	3.11	1.60	1.54
8	B	401	CLR	C16-C17	3.10	1.60	1.54
8	A	1103	CLR	C16-C17	3.08	1.60	1.54
8	B	401	CLR	C7-C8	2.42	1.57	1.53
8	D	401	CLR	C7-C8	2.39	1.57	1.53
8	G	1301	CLR	C7-C8	2.37	1.57	1.53
8	E	1301	CLR	C7-C8	2.37	1.57	1.53
8	A	1102	CLR	C7-C8	2.30	1.57	1.53
8	A	1101	CLR	C7-C8	2.29	1.57	1.53
8	C	1101	CLR	C7-C8	2.28	1.57	1.53
8	A	1103	CLR	C7-C8	2.27	1.57	1.53

All (66) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1104	PCW	C2-O2-C31	-3.73	110.95	117.90
9	C	1102	PCW	C2-O2-C31	-3.69	111.02	117.90
9	A	1105	PCW	C2-O2-C31	-3.68	111.03	117.90
9	C	1103	PCW	C2-O2-C31	-3.68	111.04	117.90
8	A	1103	CLR	C22-C20-C17	-2.95	104.19	110.28
8	A	1101	CLR	C22-C20-C17	-2.91	104.27	110.28
8	D	401	CLR	C22-C20-C17	-2.90	104.30	110.28
8	B	401	CLR	C22-C20-C17	-2.87	104.35	110.28
8	E	1301	CLR	C22-C20-C17	-2.78	104.54	110.28
8	A	1102	CLR	C22-C20-C17	-2.77	104.57	110.28
9	A	1110	PCW	C2-O2-C31	-2.77	110.98	117.79
8	C	1101	CLR	C22-C20-C17	-2.76	104.58	110.28
8	G	1301	CLR	C22-C20-C17	-2.75	104.60	110.28
9	C	1108	PCW	C2-O2-C31	-2.75	111.03	117.79
9	C	1102	PCW	C3-O3-C11	-2.40	111.08	117.10
8	D	401	CLR	C7-C8-C14	-2.39	107.44	110.91
9	A	1104	PCW	C3-O3-C11	-2.39	111.09	117.10
8	B	401	CLR	C7-C8-C14	-2.37	107.48	110.91
8	A	1101	CLR	C7-C8-C14	-2.35	107.50	110.91
8	A	1103	CLR	C7-C8-C14	-2.34	107.52	110.91
8	B	401	CLR	C19-C10-C9	-2.30	108.94	111.68
8	G	1301	CLR	C18-C13-C12	2.29	114.21	110.59
8	G	1301	CLR	C7-C8-C14	-2.29	107.58	110.91
8	A	1102	CLR	C13-C17-C20	-2.29	115.90	119.49
8	C	1101	CLR	C18-C13-C12	2.29	114.20	110.59
8	D	401	CLR	C13-C17-C20	-2.28	115.92	119.49
8	E	1301	CLR	C18-C13-C12	2.28	114.18	110.59
8	B	401	CLR	C18-C13-C12	2.27	114.18	110.59
8	B	401	CLR	C13-C17-C20	-2.27	115.94	119.49
8	C	1101	CLR	C13-C17-C20	-2.26	115.94	119.49
8	A	1103	CLR	C13-C17-C20	-2.26	115.94	119.49
8	A	1102	CLR	C18-C13-C12	2.26	114.16	110.59
8	A	1103	CLR	C18-C13-C12	2.26	114.16	110.59
8	E	1301	CLR	C7-C8-C14	-2.25	107.64	110.91
8	D	401	CLR	C19-C10-C9	-2.25	109.00	111.68
8	A	1102	CLR	C7-C8-C14	-2.25	107.65	110.91
8	A	1101	CLR	C18-C13-C12	2.25	114.14	110.59
8	A	1101	CLR	C13-C17-C20	-2.25	115.97	119.49
8	C	1101	CLR	C7-C8-C14	-2.25	107.65	110.91
8	A	1102	CLR	C19-C10-C9	-2.24	109.01	111.68
8	D	401	CLR	C18-C13-C12	2.24	114.12	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1105	PCW	C3-O3-C11	-2.23	111.50	117.10
9	C	1103	PCW	C3-O3-C11	-2.23	111.51	117.10
8	C	1101	CLR	C19-C10-C9	-2.22	109.03	111.68
8	E	1301	CLR	C13-C17-C20	-2.22	116.01	119.49
8	G	1301	CLR	C13-C17-C20	-2.21	116.03	119.49
8	G	1301	CLR	C19-C10-C9	-2.19	109.07	111.68
8	E	1301	CLR	C19-C10-C9	-2.18	109.08	111.68
8	E	1301	CLR	C15-C14-C13	2.16	106.44	103.84
8	G	1301	CLR	C15-C14-C13	2.13	106.40	103.84
8	A	1101	CLR	C16-C17-C20	-2.10	108.89	112.15
9	C	1102	PCW	O2-C31-C32	2.09	114.94	111.09
8	C	1101	CLR	C15-C14-C13	2.09	106.36	103.84
9	A	1104	PCW	O2-C31-C32	2.07	114.90	111.09
8	A	1101	CLR	C15-C14-C13	2.07	106.33	103.84
8	A	1103	CLR	C15-C14-C13	2.07	106.33	103.84
8	A	1102	CLR	C15-C14-C13	2.06	106.33	103.84
8	A	1103	CLR	C16-C17-C20	-2.06	108.96	112.15
8	E	1301	CLR	C16-C17-C20	-2.04	108.98	112.15
8	G	1301	CLR	C16-C17-C20	-2.04	108.99	112.15
9	C	1103	PCW	O2-C31-C32	2.03	114.83	111.09
8	A	1103	CLR	C19-C10-C9	-2.03	109.26	111.68
8	A	1101	CLR	C19-C10-C9	-2.02	109.27	111.68
9	A	1105	PCW	O2-C31-C32	2.02	114.81	111.09
8	A	1103	CLR	C24-C23-C22	-2.01	104.01	113.24
8	A	1101	CLR	C24-C23-C22	-2.00	104.05	113.24

There are no chirality outliers.

All (384) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1102	PCW	C1-O3P-P-O1P
9	C	1103	PCW	C4-O4P-P-O2P
9	C	1104	PCW	C1-O3P-P-O2P
9	C	1104	PCW	C4-O4P-P-O1P
9	C	1105	PCW	O3P-C1-C2-O2
9	C	1106	PCW	C1-O3P-P-O1P
9	C	1106	PCW	C1-O3P-P-O2P
9	C	1106	PCW	C1-O3P-P-O4P
9	C	1107	PCW	C1-O3P-P-O1P
9	C	1107	PCW	C1-O3P-P-O2P
9	C	1107	PCW	C1-O3P-P-O4P
9	C	1108	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
9	C	1108	PCW	C1-O3P-P-O2P
9	C	1108	PCW	C1-O3P-P-O4P
9	C	1108	PCW	C4-O4P-P-O3P
9	E	1302	PCW	O2-C2-C3-O3
9	E	1302	PCW	O4P-C4-C5-N
9	E	1302	PCW	C1-O3P-P-O2P
9	A	1105	PCW	C4-O4P-P-O2P
9	A	1106	PCW	C1-O3P-P-O2P
9	A	1106	PCW	C4-O4P-P-O1P
9	A	1107	PCW	O3P-C1-C2-O2
9	A	1108	PCW	C1-O3P-P-O1P
9	A	1108	PCW	C1-O3P-P-O2P
9	A	1108	PCW	C1-O3P-P-O4P
9	A	1109	PCW	C1-O3P-P-O1P
9	A	1109	PCW	C1-O3P-P-O2P
9	A	1109	PCW	C1-O3P-P-O4P
9	A	1110	PCW	C1-O3P-P-O1P
9	A	1110	PCW	C1-O3P-P-O2P
9	A	1110	PCW	C1-O3P-P-O4P
9	A	1110	PCW	C4-O4P-P-O3P
9	G	1302	PCW	O2-C2-C3-O3
9	G	1302	PCW	O4P-C4-C5-N
9	G	1302	PCW	C1-O3P-P-O2P
9	C	1108	PCW	C4-C5-N-C8
9	A	1110	PCW	C4-C5-N-C8
9	C	1108	PCW	C23-C24-C25-C26
9	A	1110	PCW	C23-C24-C25-C26
9	C	1107	PCW	C24-C25-C26-C27
9	A	1109	PCW	C24-C25-C26-C27
9	C	1108	PCW	C33-C34-C35-C36
9	A	1110	PCW	C33-C34-C35-C36
9	C	1107	PCW	C4-C5-N-C8
9	C	1110	PCW	C4-C5-N-C8
9	A	1109	PCW	C4-C5-N-C8
9	A	1112	PCW	C4-C5-N-C8
9	C	1104	PCW	C31-C32-C33-C34
9	A	1106	PCW	C31-C32-C33-C34
9	C	1104	PCW	C11-C12-C13-C14
9	C	1106	PCW	C31-C32-C33-C34
9	C	1108	PCW	C31-C32-C33-C34
9	A	1106	PCW	C11-C12-C13-C14
9	A	1108	PCW	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
9	A	1110	PCW	C31-C32-C33-C34
9	C	1107	PCW	C31-C32-C33-C34
9	E	1302	PCW	C11-C12-C13-C14
9	A	1109	PCW	C31-C32-C33-C34
9	G	1302	PCW	C11-C12-C13-C14
9	C	1102	PCW	C1-O3P-P-O4P
9	C	1103	PCW	C4-O4P-P-O3P
9	C	1104	PCW	C4-O4P-P-O3P
9	C	1110	PCW	C4-O4P-P-O3P
9	E	1302	PCW	C1-O3P-P-O4P
9	A	1104	PCW	C1-O3P-P-O4P
9	A	1105	PCW	C4-O4P-P-O3P
9	A	1106	PCW	C4-O4P-P-O3P
9	A	1112	PCW	C4-O4P-P-O3P
9	G	1302	PCW	C1-O3P-P-O4P
9	C	1108	PCW	C11-C12-C13-C14
9	A	1110	PCW	C11-C12-C13-C14
9	C	1107	PCW	C4-C5-N-C6
9	C	1107	PCW	C4-C5-N-C7
9	C	1108	PCW	C4-C5-N-C6
9	C	1109	PCW	C4-C5-N-C6
9	C	1109	PCW	C4-C5-N-C7
9	C	1109	PCW	C4-C5-N-C8
9	C	1110	PCW	C4-C5-N-C6
9	C	1110	PCW	C4-C5-N-C7
9	A	1109	PCW	C4-C5-N-C6
9	A	1109	PCW	C4-C5-N-C7
9	A	1110	PCW	C4-C5-N-C6
9	A	1111	PCW	C4-C5-N-C6
9	A	1111	PCW	C4-C5-N-C7
9	A	1111	PCW	C4-C5-N-C8
9	A	1112	PCW	C4-C5-N-C6
9	A	1112	PCW	C4-C5-N-C7
9	C	1109	PCW	C41-C42-C43-C44
9	A	1111	PCW	C41-C42-C43-C44
9	C	1109	PCW	C34-C35-C36-C37
9	A	1110	PCW	C13-C14-C15-C16
9	A	1111	PCW	C34-C35-C36-C37
9	C	1108	PCW	C13-C14-C15-C16
9	C	1107	PCW	C42-C43-C44-C45
9	A	1109	PCW	C42-C43-C44-C45
9	C	1105	PCW	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
9	A	1107	PCW	C44-C45-C46-C47
9	C	1107	PCW	C13-C14-C15-C16
9	A	1109	PCW	C13-C14-C15-C16
9	C	1109	PCW	C21-C22-C23-C24
9	A	1111	PCW	C21-C22-C23-C24
9	C	1107	PCW	C40-C41-C42-C43
9	A	1109	PCW	C40-C41-C42-C43
9	C	1110	PCW	C14-C15-C16-C17
9	A	1109	PCW	C12-C13-C14-C15
9	A	1112	PCW	C14-C15-C16-C17
9	C	1108	PCW	C4-C5-N-C7
9	A	1110	PCW	C4-C5-N-C7
9	C	1104	PCW	C33-C34-C35-C36
9	C	1107	PCW	C12-C13-C14-C15
9	C	1107	PCW	C35-C36-C37-C38
9	A	1106	PCW	C33-C34-C35-C36
9	A	1109	PCW	C35-C36-C37-C38
9	C	1106	PCW	C15-C16-C17-C18
9	C	1106	PCW	C34-C35-C36-C37
9	A	1108	PCW	C15-C16-C17-C18
9	A	1108	PCW	C34-C35-C36-C37
9	C	1110	PCW	C1-C2-C3-O3
9	A	1112	PCW	C1-C2-C3-O3
9	C	1109	PCW	C33-C34-C35-C36
9	A	1111	PCW	C33-C34-C35-C36
9	C	1107	PCW	C33-C34-C35-C36
9	A	1109	PCW	C33-C34-C35-C36
9	A	1110	PCW	C15-C16-C17-C18
9	C	1108	PCW	C15-C16-C17-C18
9	C	1106	PCW	C41-C42-C43-C44
9	A	1108	PCW	C41-C42-C43-C44
9	E	1302	PCW	C13-C14-C15-C16
9	G	1302	PCW	C13-C14-C15-C16
9	C	1104	PCW	C16-C17-C18-C19
9	C	1104	PCW	C20-C21-C22-C23
9	C	1104	PCW	C40-C41-C42-C43
9	C	1110	PCW	C36-C37-C38-C39
9	A	1106	PCW	C16-C17-C18-C19
9	A	1106	PCW	C20-C21-C22-C23
9	A	1106	PCW	C40-C41-C42-C43
9	A	1112	PCW	C36-C37-C38-C39
9	C	1105	PCW	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
9	C	1109	PCW	C42-C43-C44-C45
9	A	1107	PCW	C42-C43-C44-C45
9	A	1111	PCW	C42-C43-C44-C45
9	C	1108	PCW	C12-C13-C14-C15
9	A	1110	PCW	C12-C13-C14-C15
9	C	1105	PCW	C40-C41-C42-C43
9	C	1107	PCW	C36-C37-C38-C39
9	C	1108	PCW	C16-C17-C18-C19
9	A	1107	PCW	C40-C41-C42-C43
9	A	1109	PCW	C36-C37-C38-C39
9	A	1110	PCW	C16-C17-C18-C19
9	C	1108	PCW	C32-C33-C34-C35
9	A	1110	PCW	C32-C33-C34-C35
9	C	1105	PCW	O3P-C1-C2-C3
9	C	1107	PCW	O3P-C1-C2-C3
9	C	1108	PCW	O3P-C1-C2-C3
9	C	1109	PCW	O3P-C1-C2-C3
9	E	1302	PCW	O3P-C1-C2-C3
9	A	1107	PCW	O3P-C1-C2-C3
9	A	1109	PCW	O3P-C1-C2-C3
9	A	1110	PCW	O3P-C1-C2-C3
9	A	1111	PCW	O3P-C1-C2-C3
9	G	1302	PCW	O3P-C1-C2-C3
9	C	1109	PCW	C11-C12-C13-C14
9	A	1111	PCW	C11-C12-C13-C14
9	C	1106	PCW	C40-C41-C42-C43
9	A	1108	PCW	C40-C41-C42-C43
9	G	1302	PCW	C35-C36-C37-C38
9	E	1302	PCW	C35-C36-C37-C38
9	C	1103	PCW	C1-C2-C3-O3
9	A	1105	PCW	C1-C2-C3-O3
9	C	1109	PCW	C16-C17-C18-C19
9	A	1111	PCW	C16-C17-C18-C19
9	C	1107	PCW	C14-C15-C16-C17
9	A	1109	PCW	C14-C15-C16-C17
9	C	1109	PCW	C31-C32-C33-C34
9	A	1111	PCW	C31-C32-C33-C34
9	E	1302	PCW	C45-C46-C47-C48
9	G	1302	PCW	C45-C46-C47-C48
9	C	1107	PCW	C25-C26-C27-C28
9	A	1109	PCW	C25-C26-C27-C28
9	C	1102	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	C	1103	PCW	O3P-C1-C2-C3
9	A	1104	PCW	O3P-C1-C2-C3
9	A	1105	PCW	O3P-C1-C2-C3
9	C	1105	PCW	C1-C2-C3-O3
9	A	1107	PCW	C1-C2-C3-O3
9	C	1102	PCW	O3P-C1-C2-O2
9	C	1103	PCW	O3P-C1-C2-O2
9	E	1302	PCW	O3P-C1-C2-O2
9	A	1104	PCW	O3P-C1-C2-O2
9	A	1105	PCW	O3P-C1-C2-O2
9	G	1302	PCW	O3P-C1-C2-O2
9	C	1107	PCW	C20-C21-C22-C23
9	A	1109	PCW	C20-C21-C22-C23
9	C	1102	PCW	O2-C2-C3-O3
9	C	1103	PCW	O2-C2-C3-O3
9	C	1104	PCW	O2-C2-C3-O3
9	A	1104	PCW	O2-C2-C3-O3
9	A	1105	PCW	O2-C2-C3-O3
9	A	1106	PCW	O2-C2-C3-O3
9	C	1110	PCW	C45-C46-C47-C48
9	A	1112	PCW	C45-C46-C47-C48
9	C	1105	PCW	C22-C23-C24-C25
9	A	1107	PCW	C22-C23-C24-C25
9	C	1104	PCW	C1-C2-C3-O3
9	E	1302	PCW	C1-C2-C3-O3
9	A	1106	PCW	C1-C2-C3-O3
9	G	1302	PCW	C1-C2-C3-O3
9	C	1105	PCW	O2-C2-C3-O3
9	A	1107	PCW	O2-C2-C3-O3
9	C	1106	PCW	C36-C37-C38-C39
9	A	1108	PCW	C36-C37-C38-C39
9	C	1105	PCW	C13-C14-C15-C16
9	A	1107	PCW	C13-C14-C15-C16
9	E	1302	PCW	C16-C17-C18-C19
9	G	1302	PCW	C16-C17-C18-C19
9	C	1106	PCW	C32-C33-C34-C35
9	A	1108	PCW	C32-C33-C34-C35
9	C	1103	PCW	C4-C5-N-C6
9	C	1103	PCW	C4-O4P-P-O1P
9	C	1108	PCW	C4-O4P-P-O1P
9	C	1110	PCW	C4-O4P-P-O2P
9	E	1302	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
9	A	1104	PCW	C1-O3P-P-O1P
9	A	1105	PCW	C4-C5-N-C6
9	A	1105	PCW	C4-O4P-P-O1P
9	A	1110	PCW	C4-O4P-P-O1P
9	A	1112	PCW	C4-O4P-P-O2P
9	G	1302	PCW	C1-O3P-P-O1P
9	A	1110	PCW	C14-C15-C16-C17
9	C	1108	PCW	C14-C15-C16-C17
9	C	1108	PCW	O3P-C1-C2-O2
9	A	1110	PCW	O3P-C1-C2-O2
9	C	1110	PCW	C35-C36-C37-C38
9	A	1112	PCW	C35-C36-C37-C38
9	C	1102	PCW	O4P-C4-C5-N
9	C	1103	PCW	O4P-C4-C5-N
9	C	1104	PCW	O4P-C4-C5-N
9	C	1105	PCW	O4P-C4-C5-N
9	C	1106	PCW	O4P-C4-C5-N
9	C	1107	PCW	O4P-C4-C5-N
9	C	1108	PCW	O4P-C4-C5-N
9	C	1109	PCW	O4P-C4-C5-N
9	C	1110	PCW	O4P-C4-C5-N
9	A	1104	PCW	O4P-C4-C5-N
9	A	1105	PCW	O4P-C4-C5-N
9	A	1106	PCW	O4P-C4-C5-N
9	A	1107	PCW	O4P-C4-C5-N
9	A	1108	PCW	O4P-C4-C5-N
9	A	1109	PCW	O4P-C4-C5-N
9	A	1110	PCW	O4P-C4-C5-N
9	A	1111	PCW	O4P-C4-C5-N
9	A	1112	PCW	O4P-C4-C5-N
9	C	1110	PCW	O2-C2-C3-O3
9	A	1112	PCW	O2-C2-C3-O3
9	A	1108	PCW	C14-C15-C16-C17
9	C	1106	PCW	C14-C15-C16-C17
9	E	1302	PCW	C2-C1-O3P-P
9	G	1302	PCW	C2-C1-O3P-P
9	C	1108	PCW	C40-C41-C42-C43
9	A	1110	PCW	C40-C41-C42-C43
9	A	1106	PCW	C35-C36-C37-C38
9	C	1104	PCW	C35-C36-C37-C38
9	E	1302	PCW	C43-C44-C45-C46
9	G	1302	PCW	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
9	C	1107	PCW	O3P-C1-C2-O2
9	C	1109	PCW	O3P-C1-C2-O2
9	A	1109	PCW	O3P-C1-C2-O2
9	A	1111	PCW	O3P-C1-C2-O2
9	C	1103	PCW	C4-C5-N-C8
9	A	1105	PCW	C4-C5-N-C8
9	C	1102	PCW	C4-O4P-P-O3P
9	C	1103	PCW	C1-O3P-P-O4P
9	C	1104	PCW	C1-O3P-P-O4P
9	C	1105	PCW	C4-O4P-P-O3P
9	C	1106	PCW	C4-O4P-P-O3P
9	C	1107	PCW	C4-O4P-P-O3P
9	E	1302	PCW	C4-O4P-P-O3P
9	A	1104	PCW	C4-O4P-P-O3P
9	A	1105	PCW	C1-O3P-P-O4P
9	A	1106	PCW	C1-O3P-P-O4P
9	A	1107	PCW	C4-O4P-P-O3P
9	A	1108	PCW	C4-O4P-P-O3P
9	A	1109	PCW	C4-O4P-P-O3P
9	G	1302	PCW	C4-O4P-P-O3P
9	C	1104	PCW	C2-C1-O3P-P
9	A	1106	PCW	C2-C1-O3P-P
9	E	1302	PCW	C33-C34-C35-C36
9	G	1302	PCW	C33-C34-C35-C36
9	C	1104	PCW	O3P-C1-C2-C3
9	A	1106	PCW	O3P-C1-C2-C3
9	C	1109	PCW	C20-C21-C22-C23
9	A	1111	PCW	C20-C21-C22-C23
9	C	1105	PCW	C15-C16-C17-C18
9	A	1107	PCW	C15-C16-C17-C18
9	C	1106	PCW	O2-C2-C3-O3
9	A	1108	PCW	O2-C2-C3-O3
9	A	1112	PCW	C41-C42-C43-C44
9	C	1110	PCW	C41-C42-C43-C44
9	C	1106	PCW	C1-C2-C3-O3
9	A	1108	PCW	C1-C2-C3-O3
9	C	1108	PCW	C21-C22-C23-C24
9	A	1110	PCW	C21-C22-C23-C24
9	C	1103	PCW	C4-C5-N-C7
9	A	1105	PCW	C4-C5-N-C7
9	C	1109	PCW	C36-C37-C38-C39
9	A	1111	PCW	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
9	C	1110	PCW	C43-C44-C45-C46
9	A	1112	PCW	C43-C44-C45-C46
8	C	1101	CLR	C23-C24-C25-C27
8	A	1102	CLR	C23-C24-C25-C27
9	E	1302	PCW	C20-C21-C22-C23
9	G	1302	PCW	C20-C21-C22-C23
9	E	1302	PCW	C14-C15-C16-C17
9	G	1302	PCW	C14-C15-C16-C17
9	C	1106	PCW	C39-C40-C41-C42
9	C	1110	PCW	C19-C20-C21-C22
9	A	1108	PCW	C39-C40-C41-C42
9	A	1112	PCW	C19-C20-C21-C22
9	C	1104	PCW	O3P-C1-C2-O2
9	A	1106	PCW	O3P-C1-C2-O2
9	C	1109	PCW	C19-C20-C21-C22
9	A	1111	PCW	C19-C20-C21-C22
9	A	1110	PCW	C20-C21-C22-C23
9	C	1105	PCW	O2-C31-C32-C33
9	A	1107	PCW	O2-C31-C32-C33
9	C	1108	PCW	C20-C21-C22-C23
9	C	1104	PCW	C19-C20-C21-C22
9	C	1109	PCW	C37-C38-C39-C40
9	E	1302	PCW	C17-C18-C19-C20
9	A	1106	PCW	C19-C20-C21-C22
9	A	1111	PCW	C37-C38-C39-C40
9	G	1302	PCW	C17-C18-C19-C20
9	C	1104	PCW	O2-C31-C32-C33
9	A	1106	PCW	O2-C31-C32-C33
9	C	1107	PCW	C17-C18-C19-C20
9	C	1108	PCW	C39-C40-C41-C42
9	A	1109	PCW	C17-C18-C19-C20
9	A	1110	PCW	C39-C40-C41-C42
9	A	1112	PCW	C37-C38-C39-C40
9	C	1105	PCW	C36-C37-C38-C39
9	C	1102	PCW	C1-C2-C3-O3
9	A	1104	PCW	C1-C2-C3-O3
9	C	1104	PCW	C4-C5-N-C7
9	A	1106	PCW	C4-C5-N-C7
9	C	1106	PCW	C19-C20-C21-C22
9	C	1108	PCW	C19-C20-C21-C22
9	C	1110	PCW	C37-C38-C39-C40
9	A	1108	PCW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
9	A	1110	PCW	C19-C20-C21-C22
9	A	1107	PCW	C36-C37-C38-C39
9	C	1107	PCW	O2-C31-C32-C33
9	A	1109	PCW	O2-C31-C32-C33
9	C	1104	PCW	C37-C38-C39-C40
9	A	1106	PCW	C37-C38-C39-C40
9	C	1108	PCW	C34-C35-C36-C37
9	A	1110	PCW	C34-C35-C36-C37
9	C	1105	PCW	C37-C38-C39-C40
9	C	1107	PCW	C19-C20-C21-C22
9	A	1107	PCW	C37-C38-C39-C40
9	A	1109	PCW	C19-C20-C21-C22
9	C	1105	PCW	C23-C24-C25-C26
9	A	1107	PCW	C23-C24-C25-C26
9	A	1106	PCW	O31-C31-C32-C33
9	C	1105	PCW	C20-C21-C22-C23
9	A	1107	PCW	C20-C21-C22-C23
9	C	1104	PCW	O31-C31-C32-C33
9	C	1105	PCW	O31-C31-C32-C33
9	A	1107	PCW	O31-C31-C32-C33
9	C	1102	PCW	C4-O4P-P-O2P
9	C	1103	PCW	C1-O3P-P-O2P
9	C	1106	PCW	C4-O4P-P-O2P
9	C	1107	PCW	C4-O4P-P-O2P
9	C	1110	PCW	C1-O3P-P-O2P
9	E	1302	PCW	C4-O4P-P-O2P
9	A	1104	PCW	C4-O4P-P-O2P
9	A	1105	PCW	C1-O3P-P-O2P
9	A	1108	PCW	C4-O4P-P-O2P
9	A	1109	PCW	C4-O4P-P-O2P
9	A	1112	PCW	C1-O3P-P-O2P
9	G	1302	PCW	C4-O4P-P-O2P
9	C	1107	PCW	O31-C31-C32-C33
9	A	1109	PCW	O31-C31-C32-C33
9	E	1302	PCW	C5-C4-O4P-P
9	G	1302	PCW	C5-C4-O4P-P

There are no ring outliers.

23 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1105	PCW	9	0

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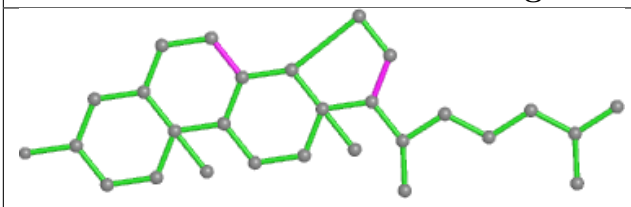
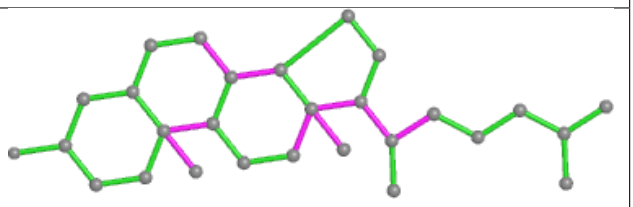
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1103	CLR	6	0
9	C	1109	PCW	4	0
9	C	1106	PCW	19	0
9	A	1109	PCW	5	0
9	E	1302	PCW	1	0
9	C	1110	PCW	1	0
9	A	1108	PCW	16	0
9	G	1302	PCW	1	0
8	D	401	CLR	1	0
8	A	1101	CLR	10	0
9	C	1104	PCW	14	0
9	A	1106	PCW	12	0
9	A	1111	PCW	4	0
9	C	1107	PCW	5	0
9	A	1104	PCW	1	0
9	A	1110	PCW	2	0
9	A	1107	PCW	10	0
9	C	1108	PCW	2	0
8	G	1301	CLR	8	0
9	C	1102	PCW	1	0
8	E	1301	CLR	8	0
9	A	1112	PCW	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 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.

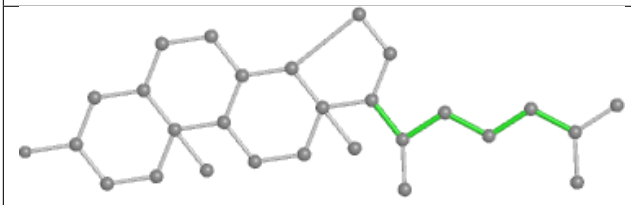
Ligand CLR B 401



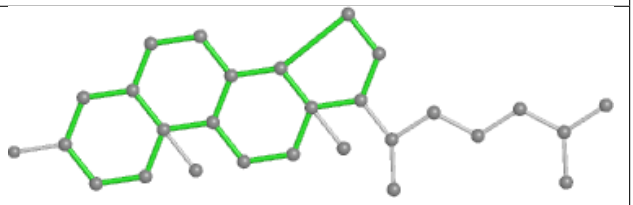
Bond lengths



Bond angles

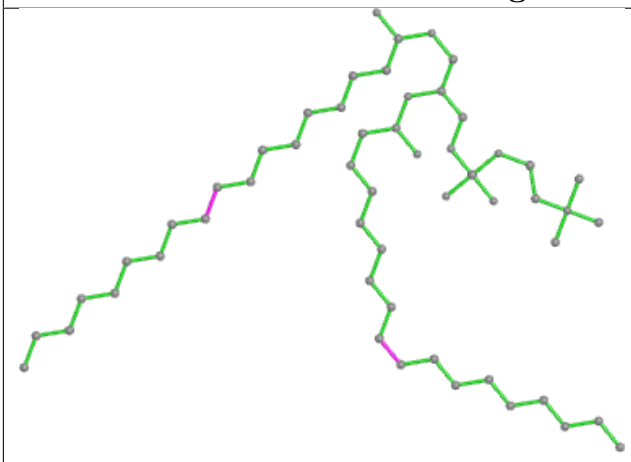


Torsions

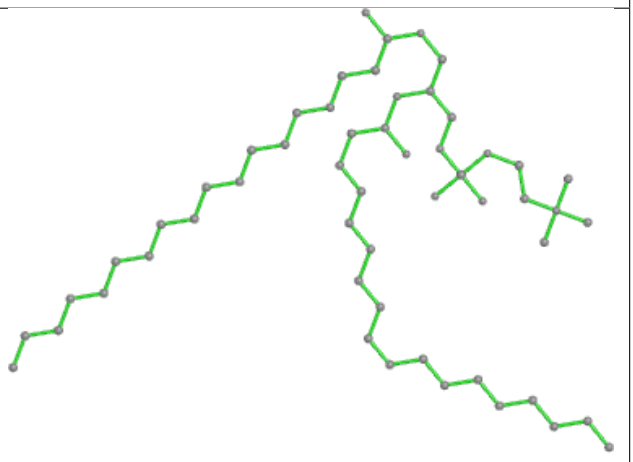


Rings

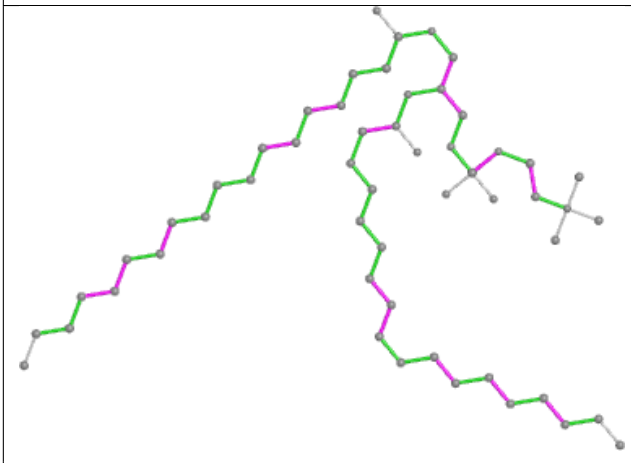
Ligand PCW C 1105



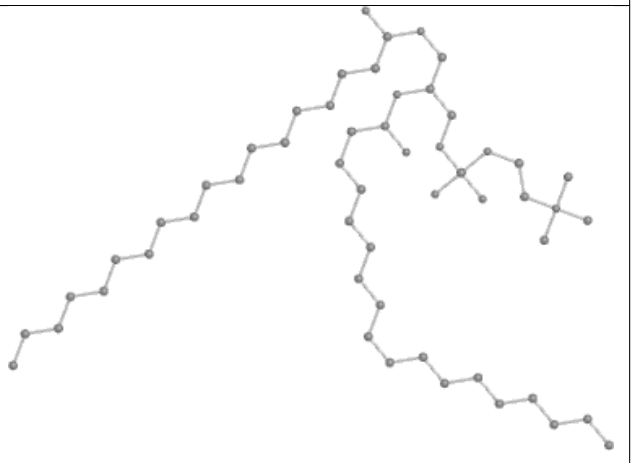
Bond lengths



Bond angles

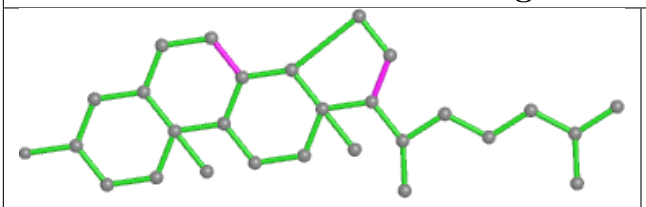


Torsions

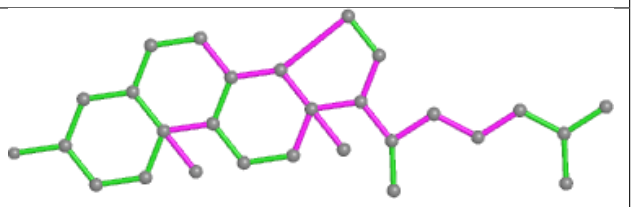


Rings

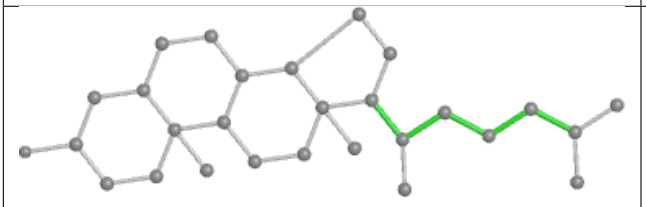
Ligand CLR A 1103



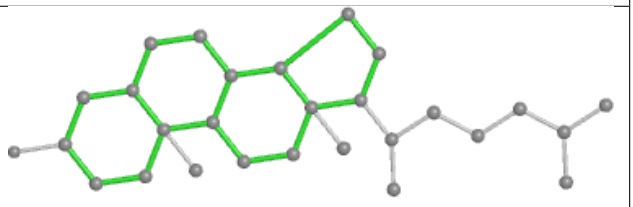
Bond lengths



Bond angles

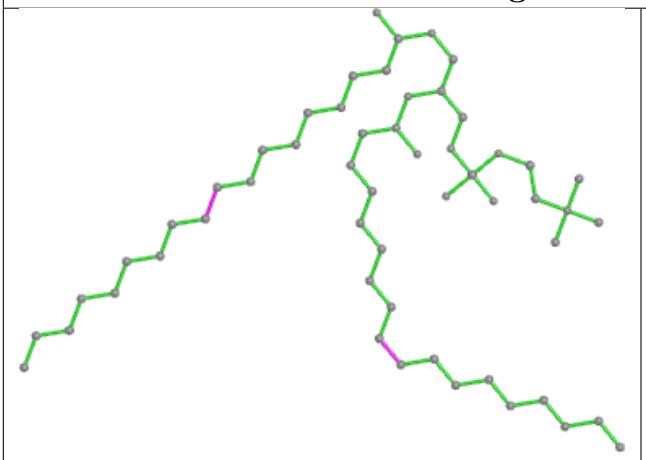


Torsions



Rings

Ligand PCW C 1109



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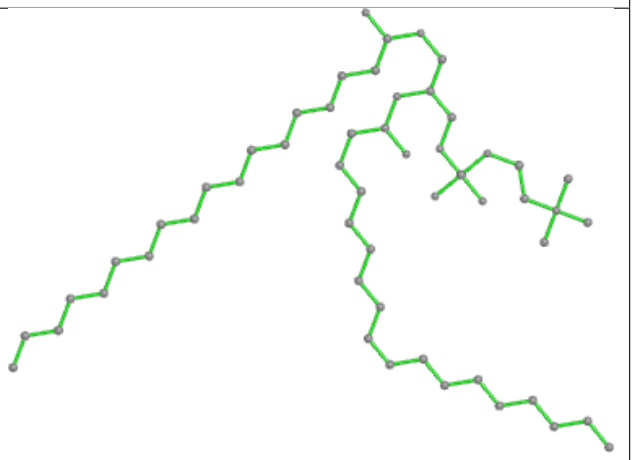
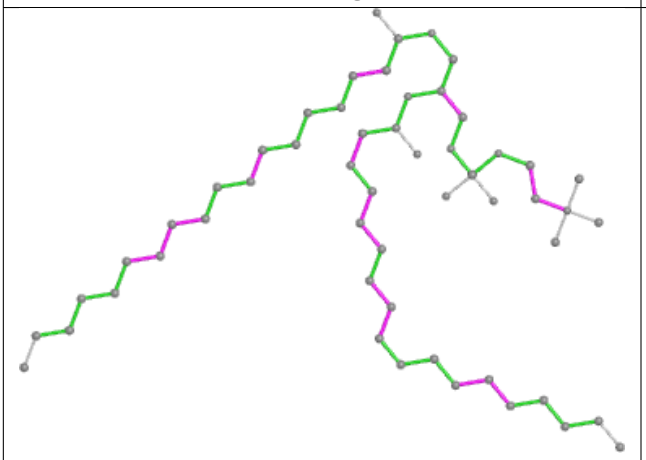


Bond angles



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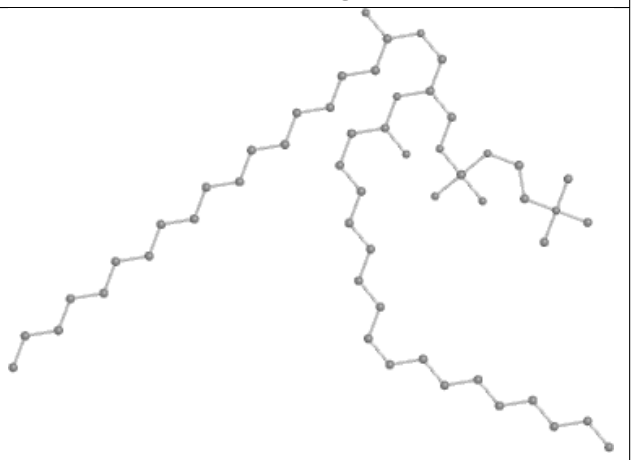
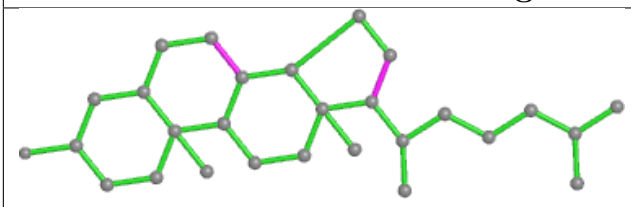


Rings

Ligand CLR C 1101



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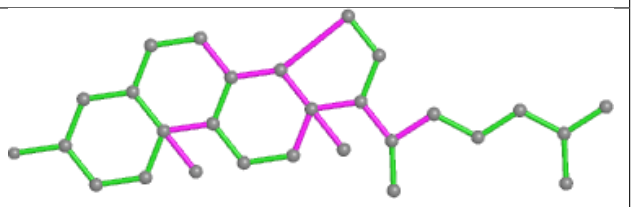
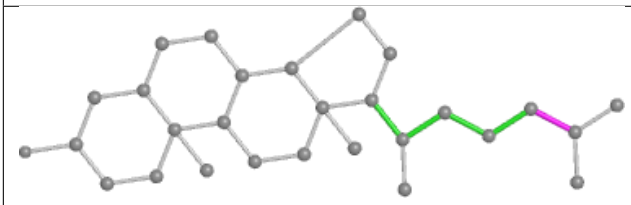
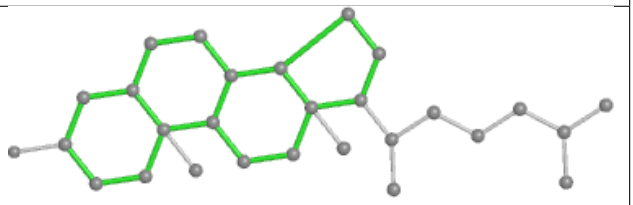


Bond angles

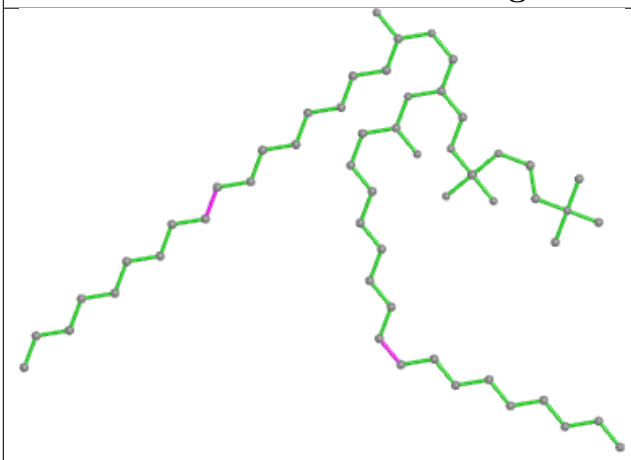


Torsions



Rings

Ligand PCW C 1106



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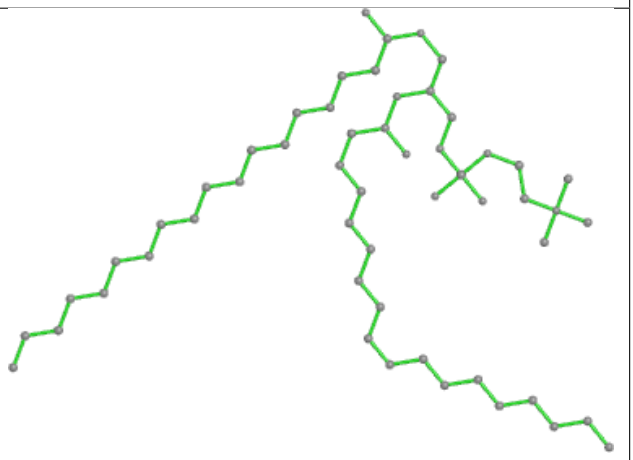
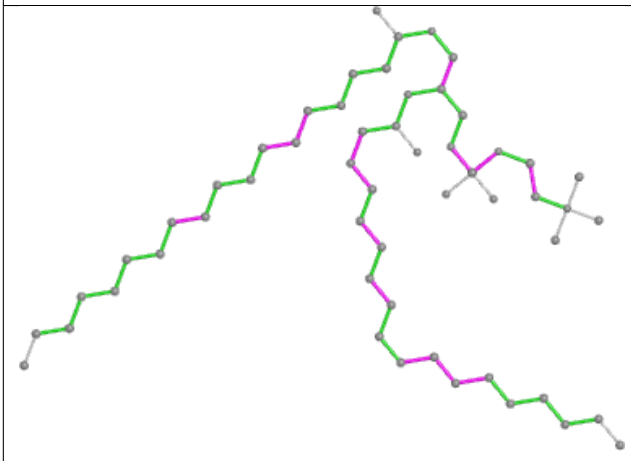


Bond angles



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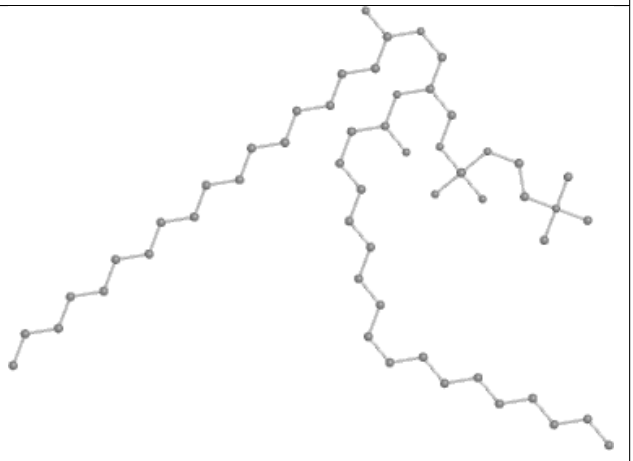
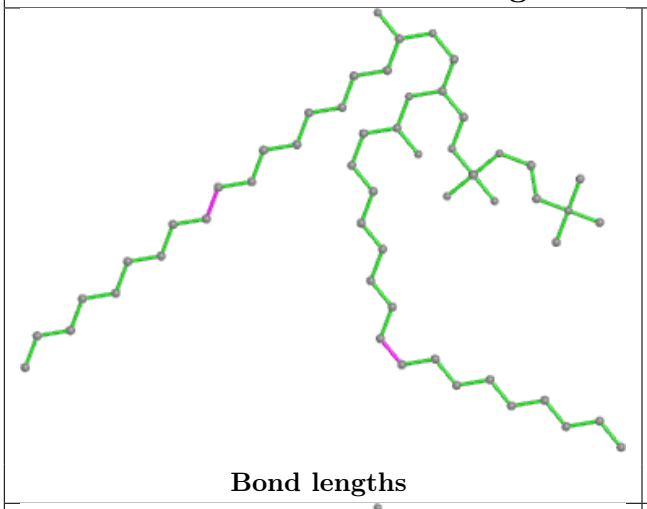


Rings

Ligand PCW A 1109



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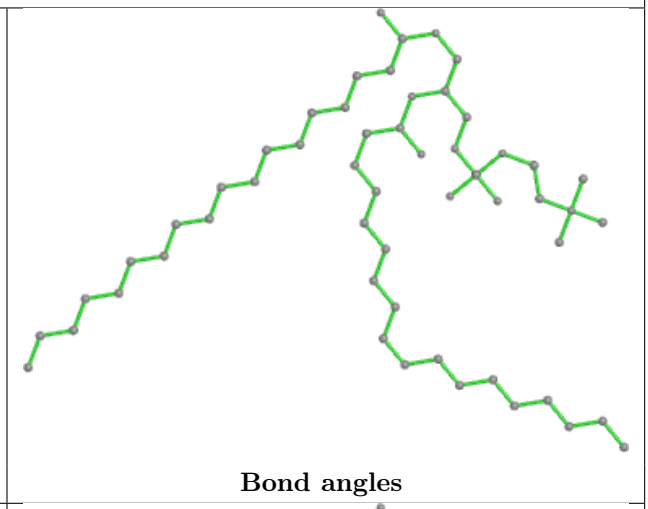
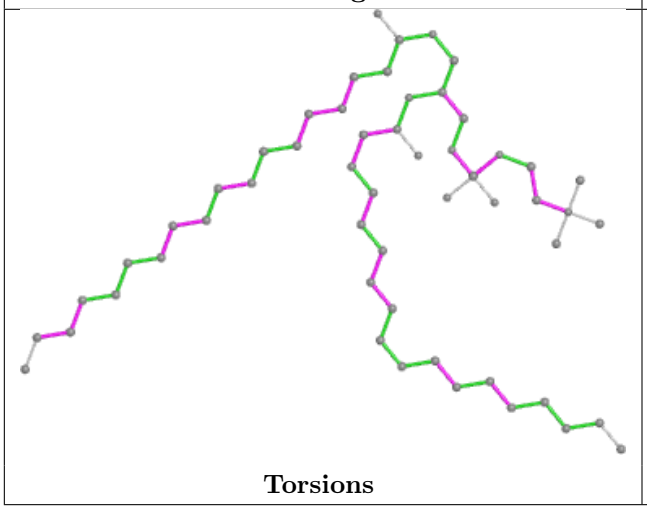
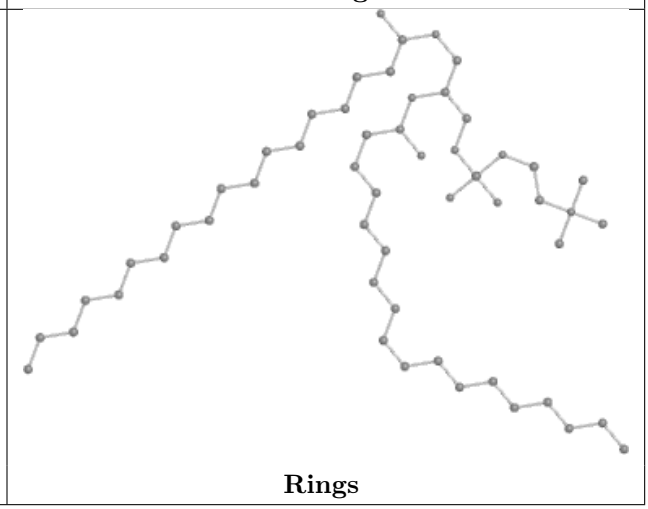


Bond angles

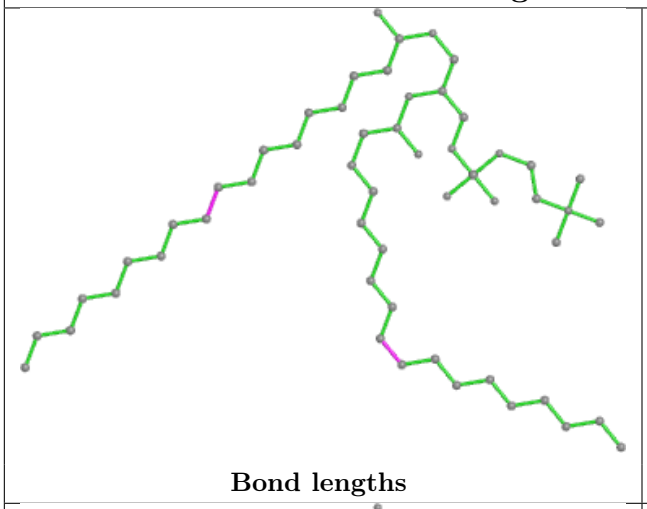


Torsions



Rings

Ligand PCW E 1302



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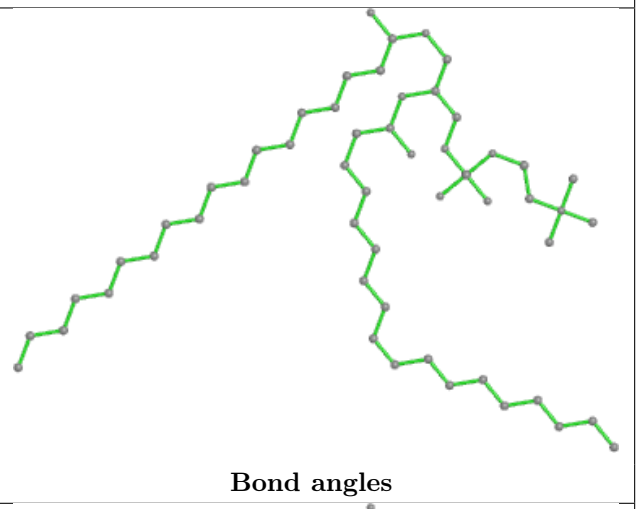
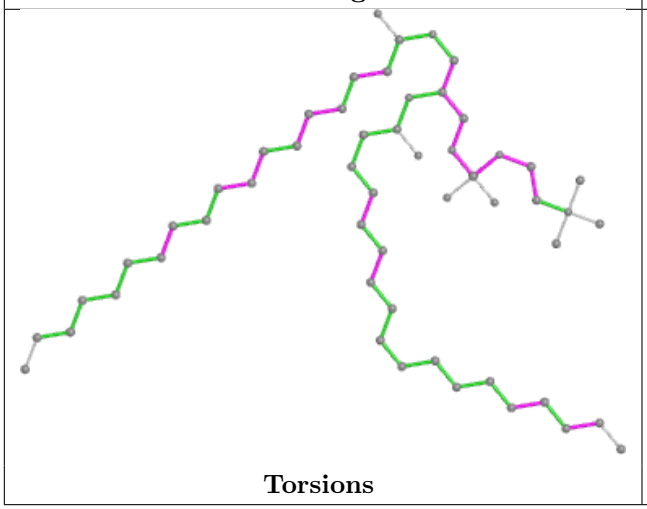
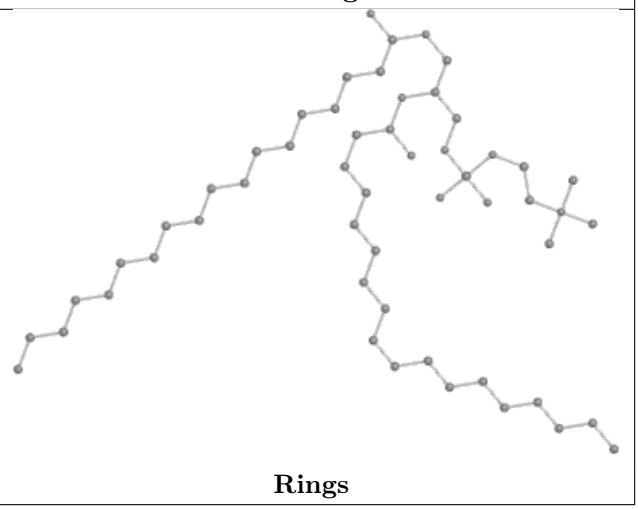


Bond angles

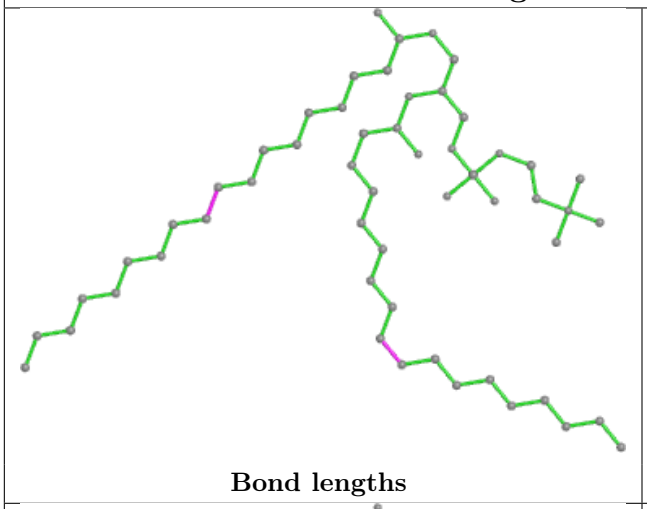


Torsions



Rings

Ligand PCW C 1110



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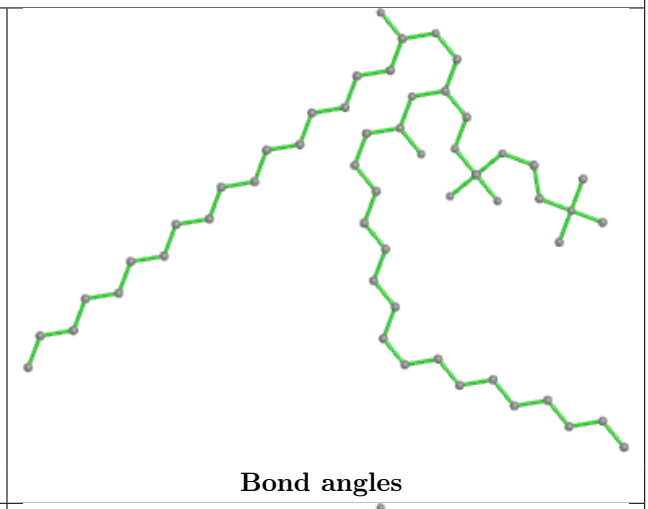
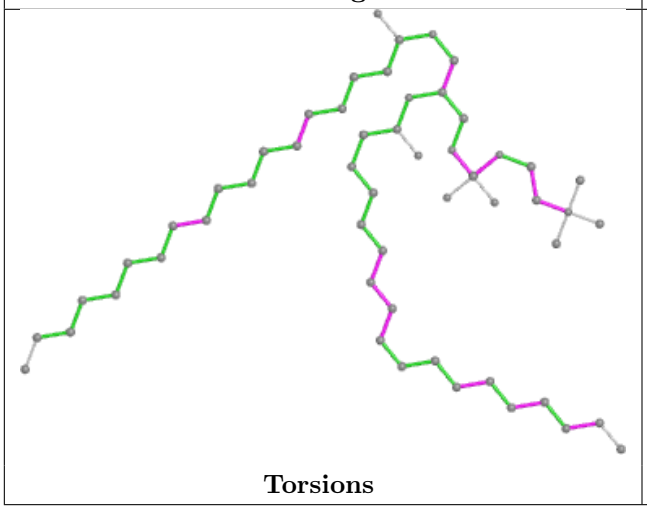
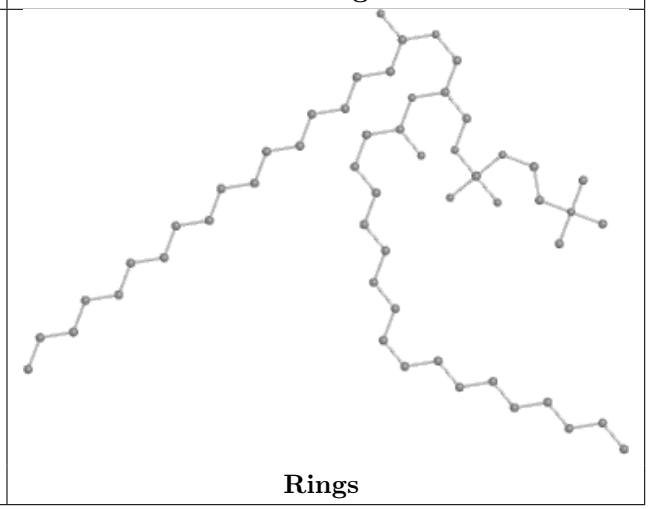


Bond angles

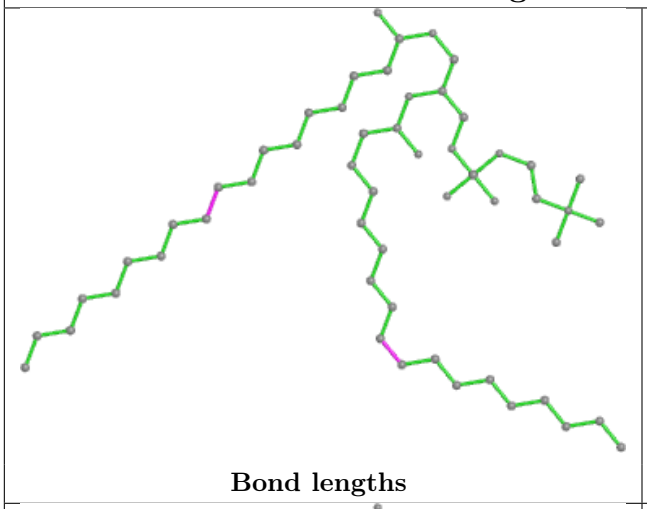


Torsions

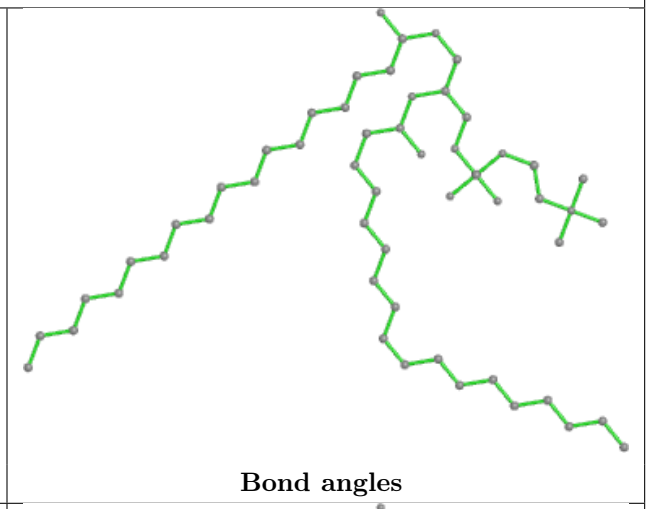


Rings

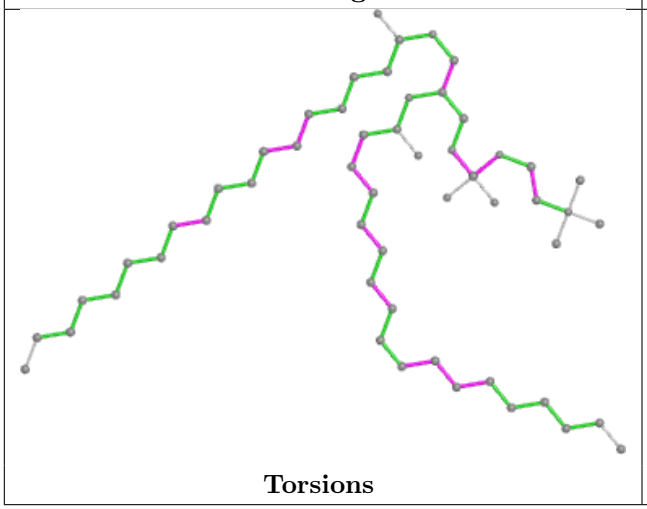
Ligand PCW A 1108



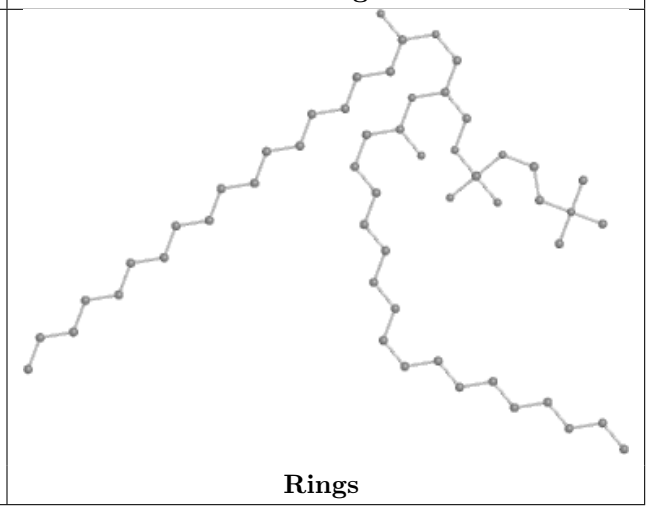
Bond lengths



Bond angles

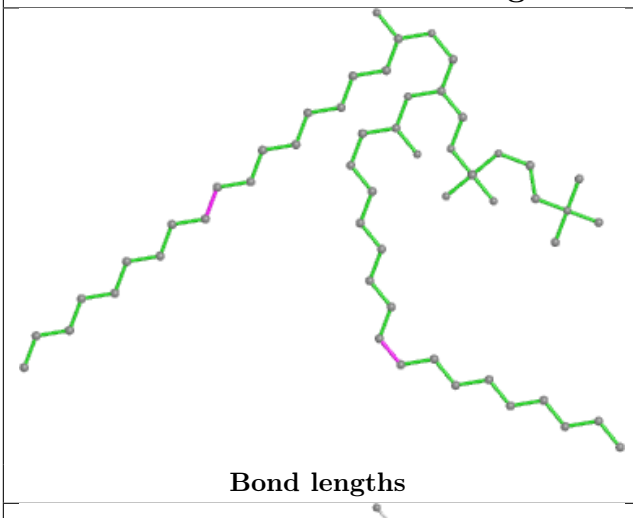


Torsions



Rings

Ligand PCW G 1302



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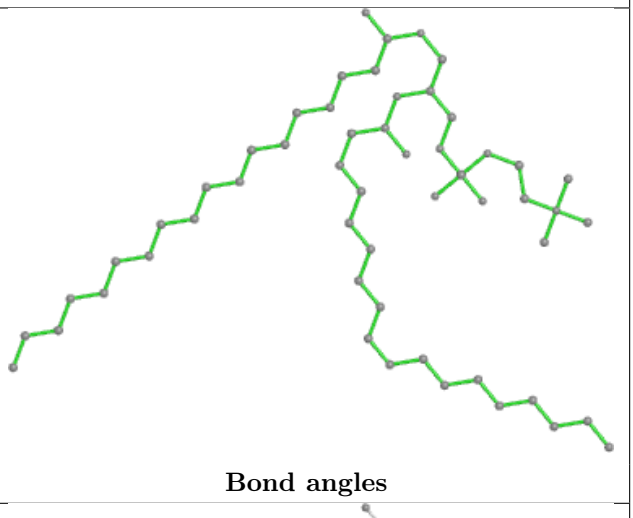
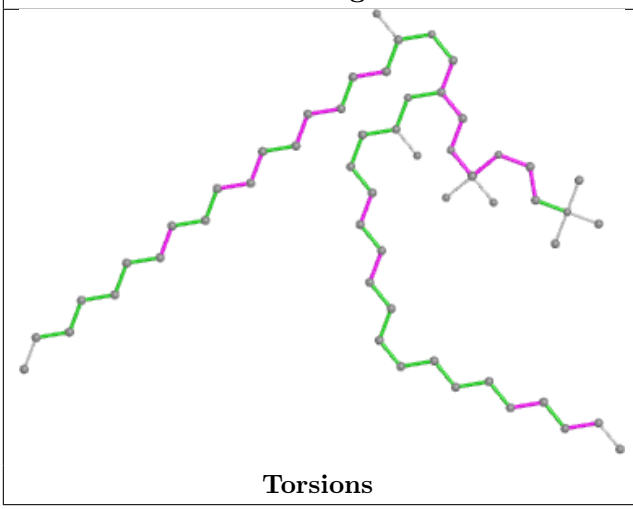
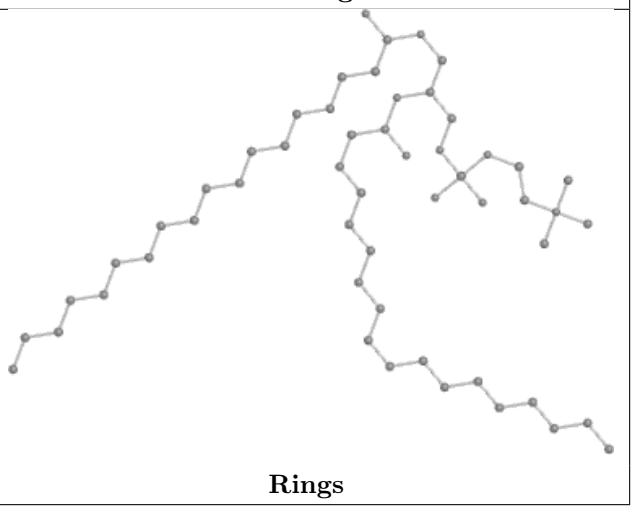


Bond angles

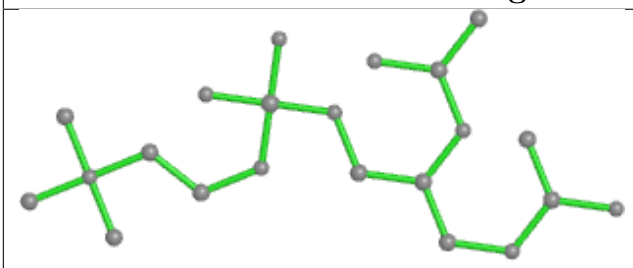


Torsions

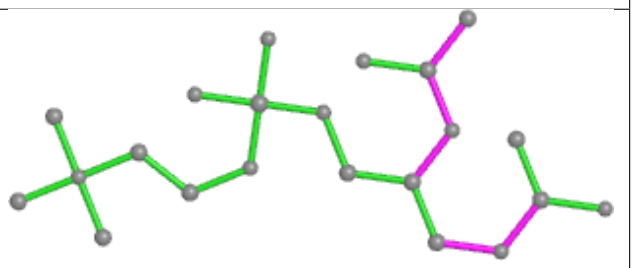


Rings

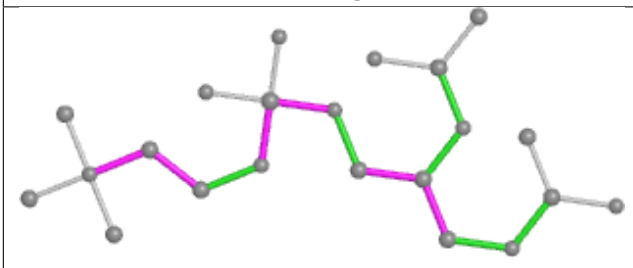
Ligand PCW C 1103



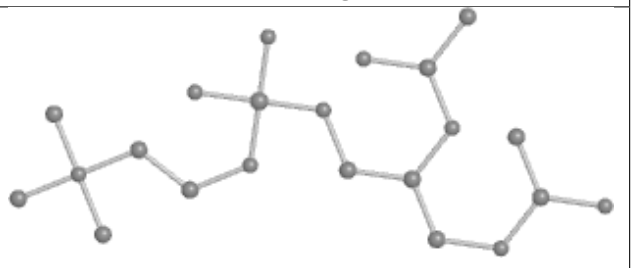
Bond lengths



Bond angles

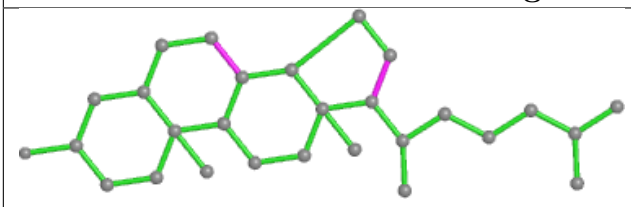


Torsions

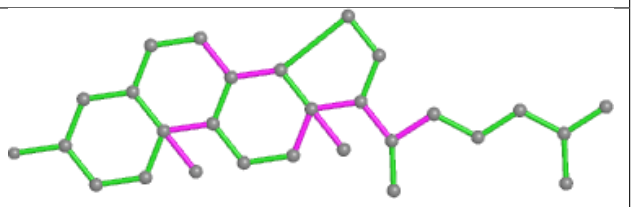


Rings

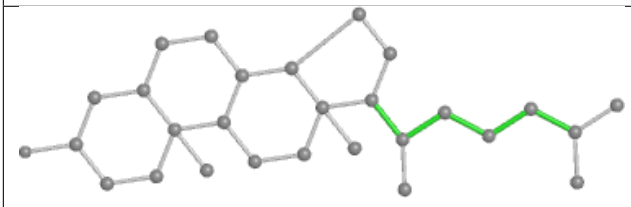
Ligand CLR D 401



Bond lengths



Bond angles



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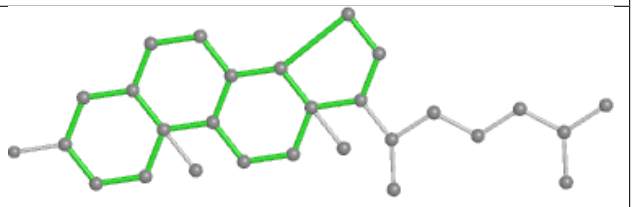
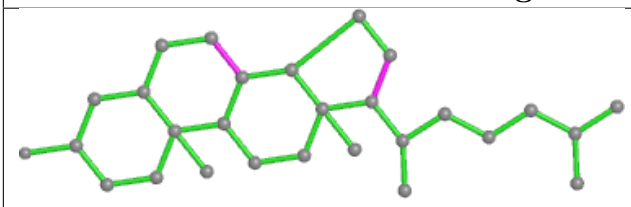


Rings

Ligand CLR A 1102



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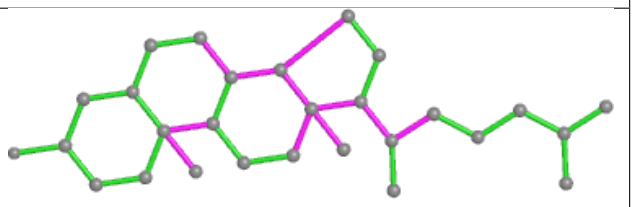
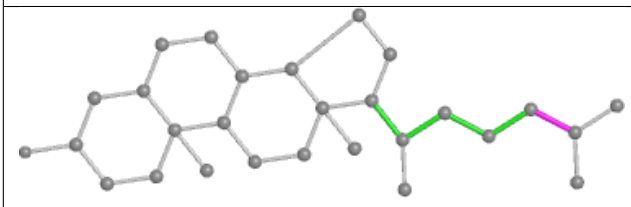
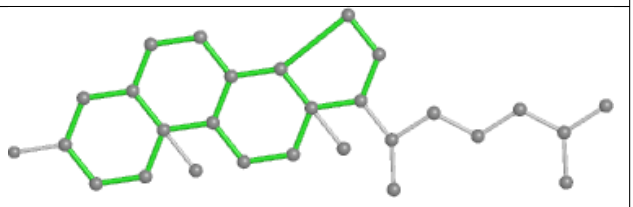


Bond angles

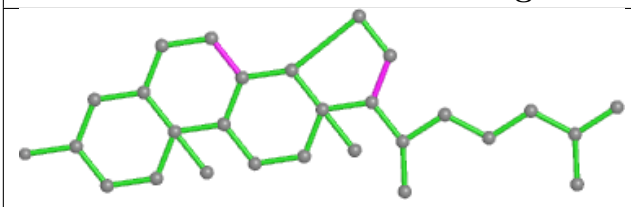


Torsions

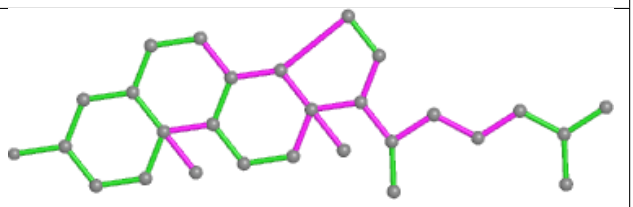


Rings

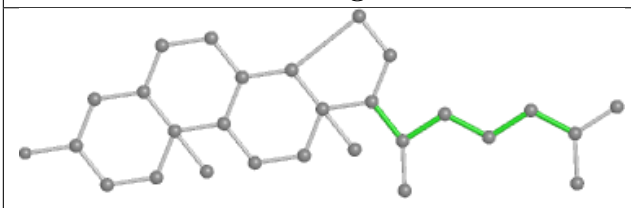
Ligand CLR A 1101



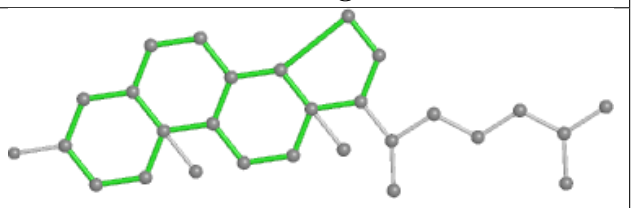
Bond lengths



Bond angles

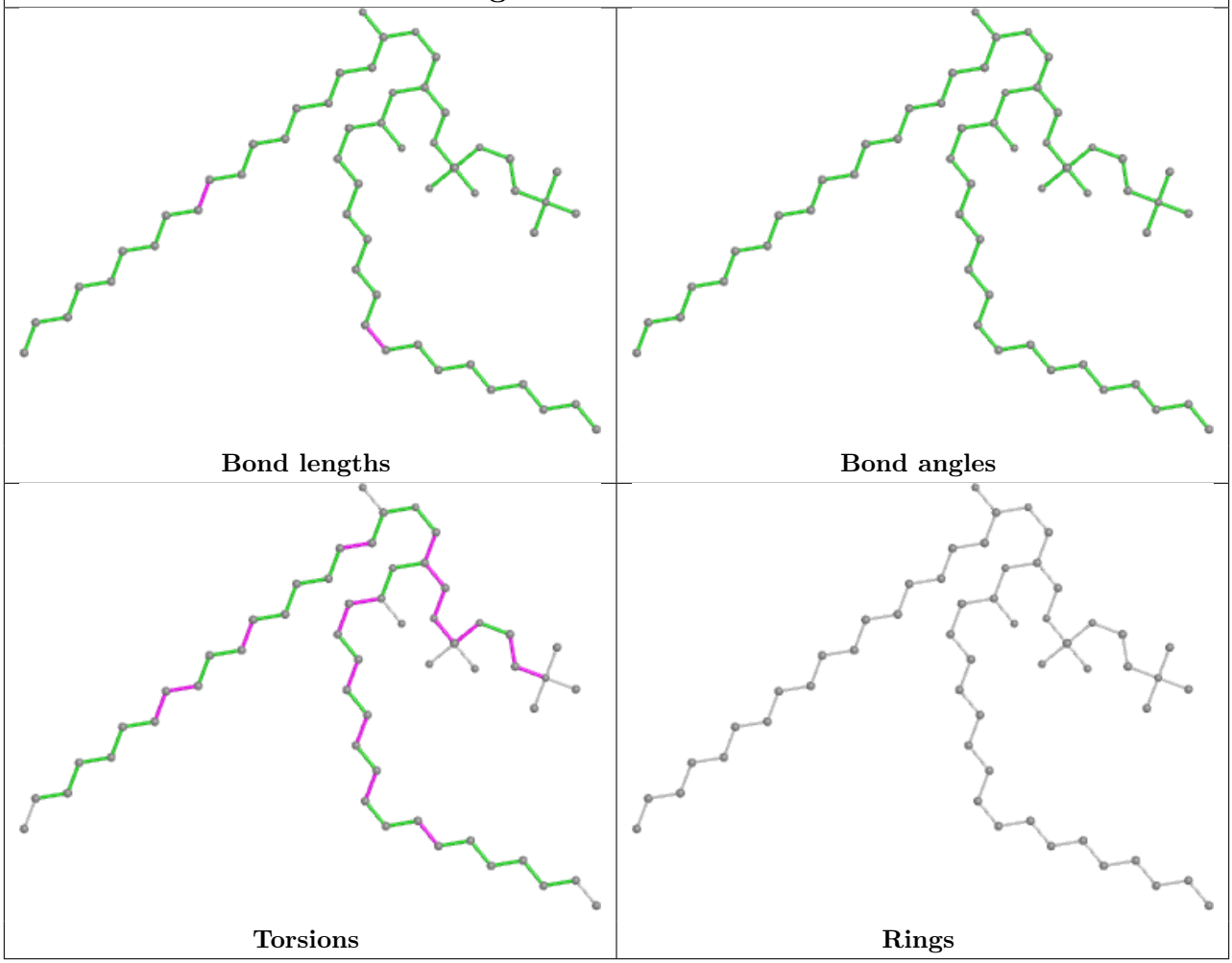


Torsions

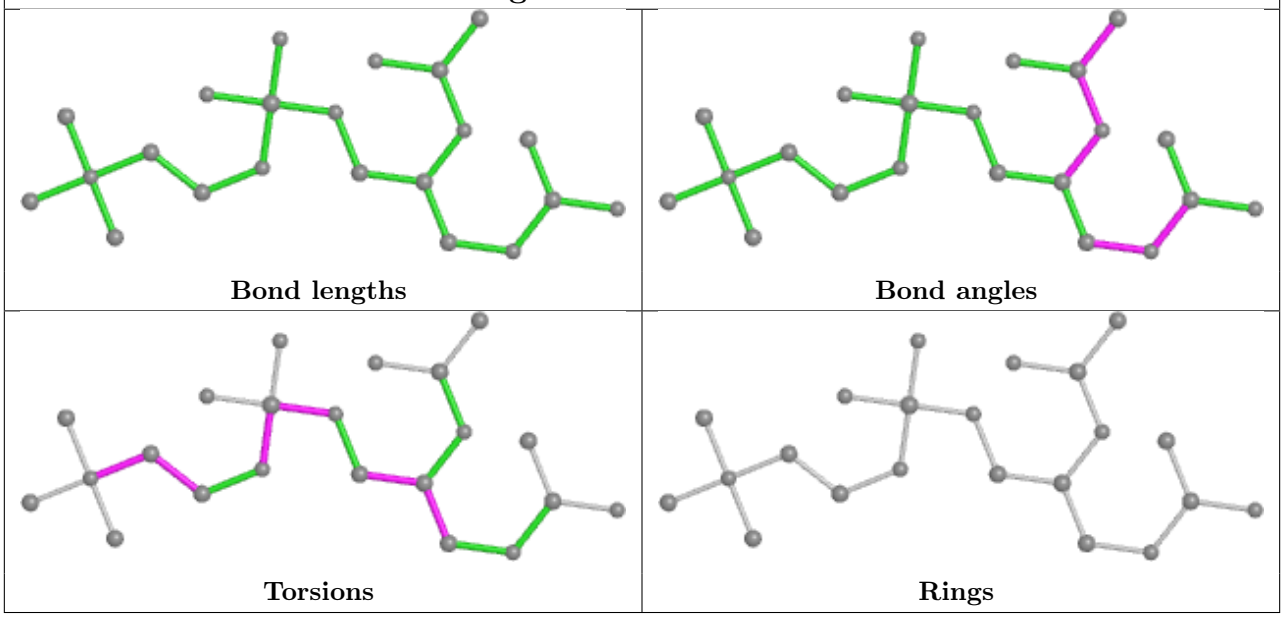


Rings

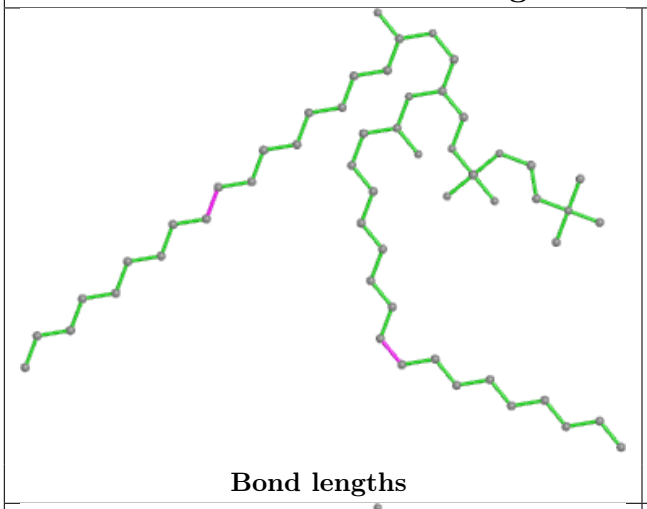
Ligand PCW C 1104



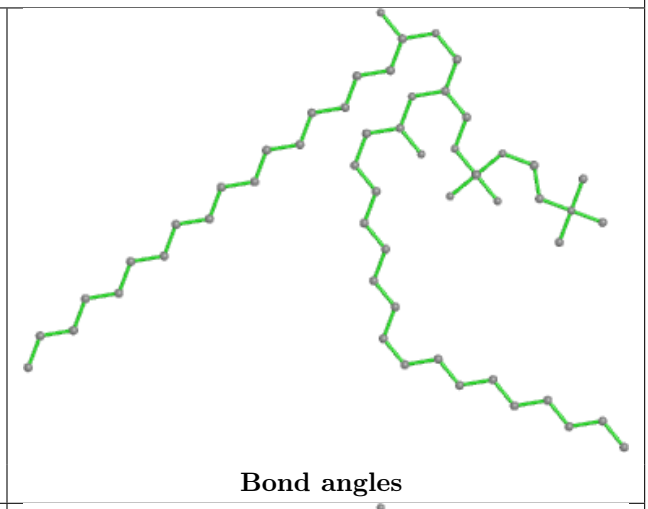
Ligand PCW A 1105



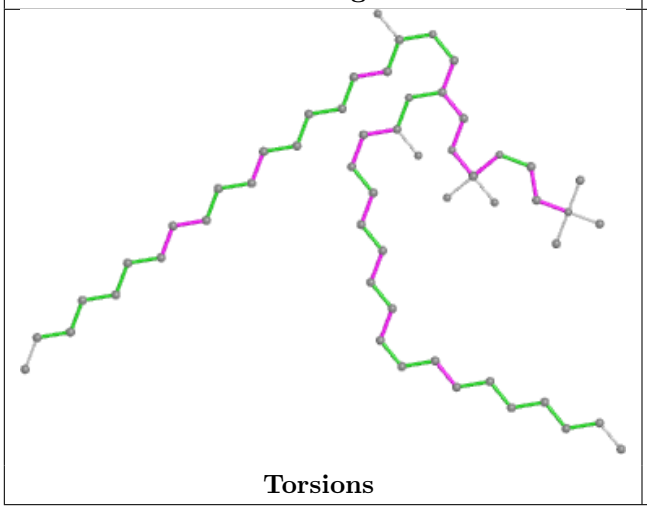
Ligand PCW A 1106



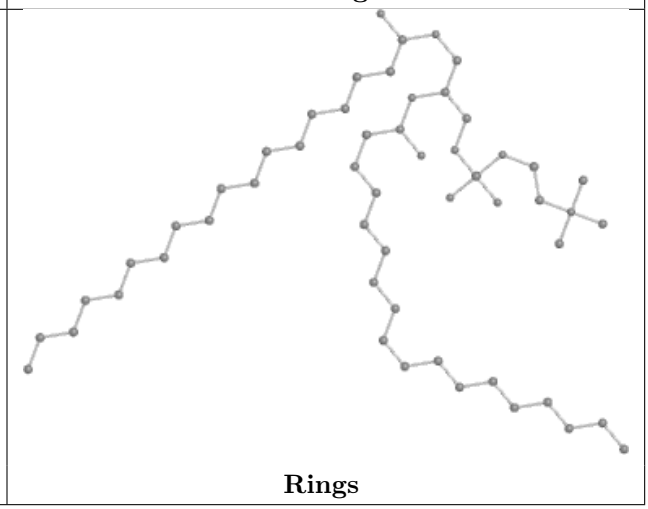
Bond lengths



Bond angles

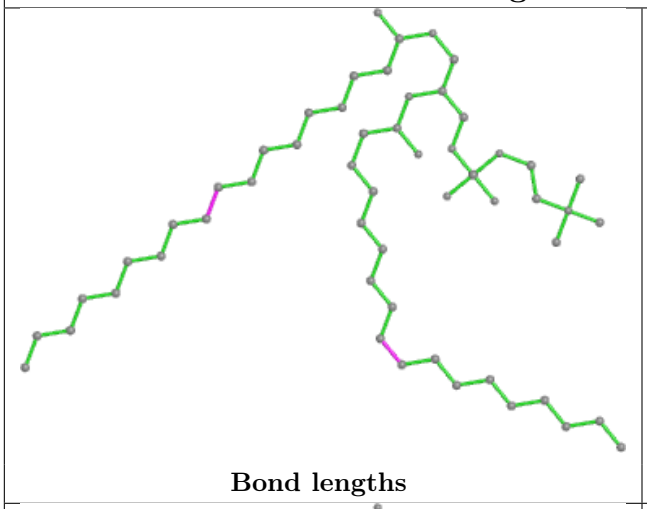


Torsions

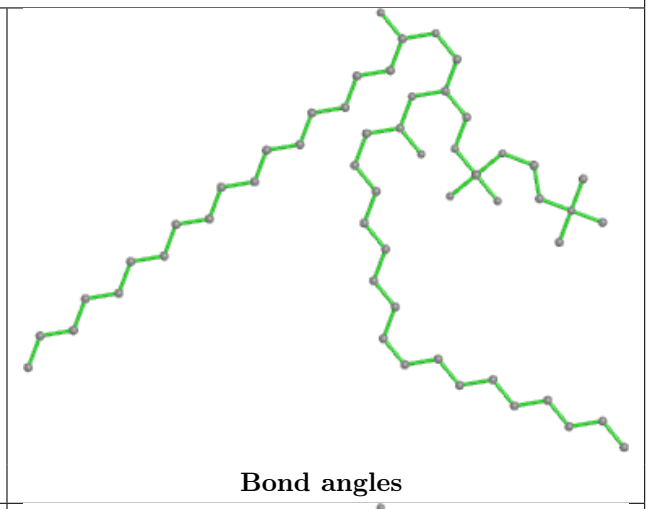


Rings

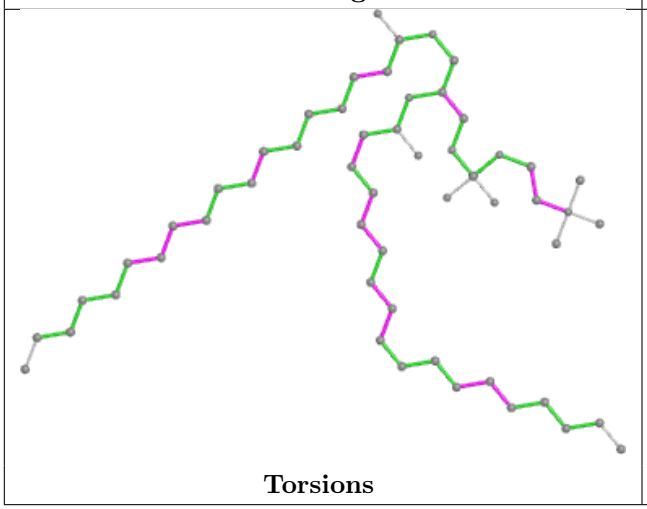
Ligand PCW A 1111



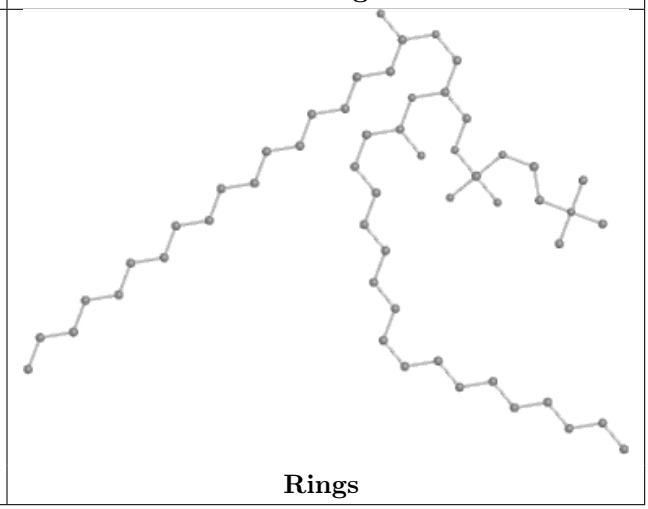
Bond lengths



Bond angles

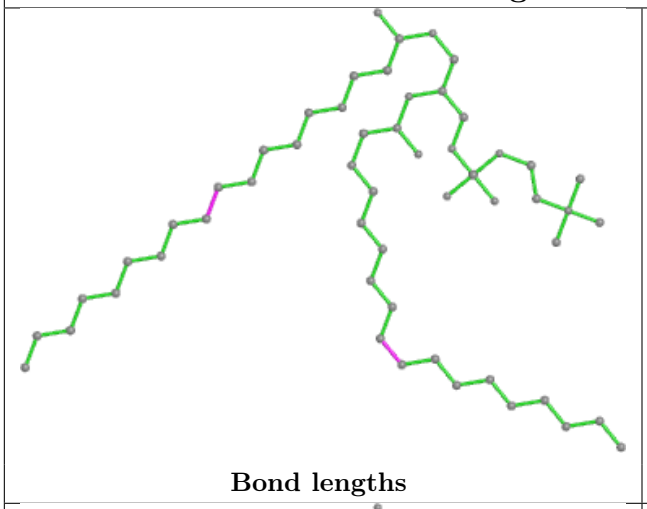


Torsions

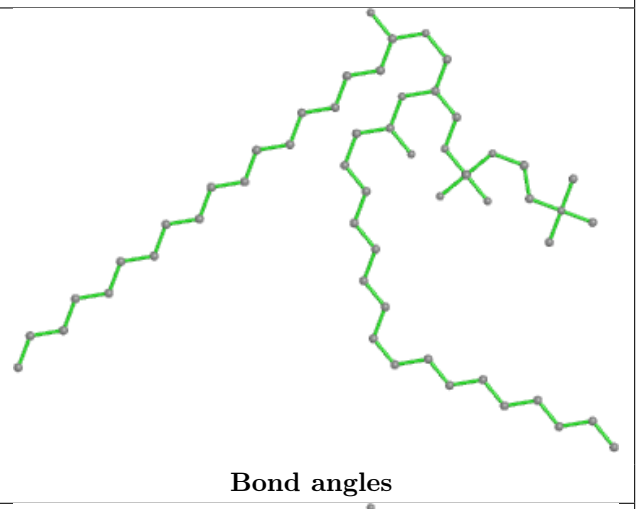


Rings

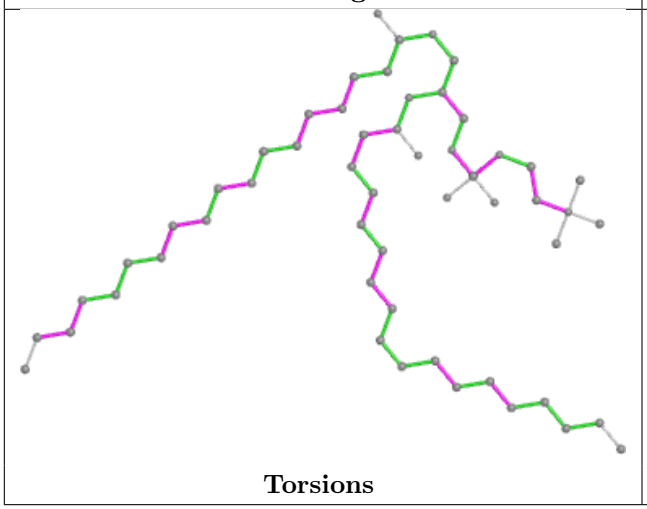
Ligand PCW C 1107



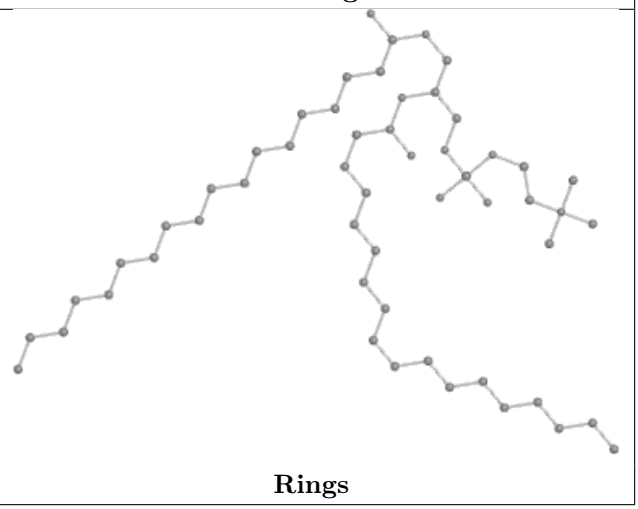
Bond lengths



Bond angles

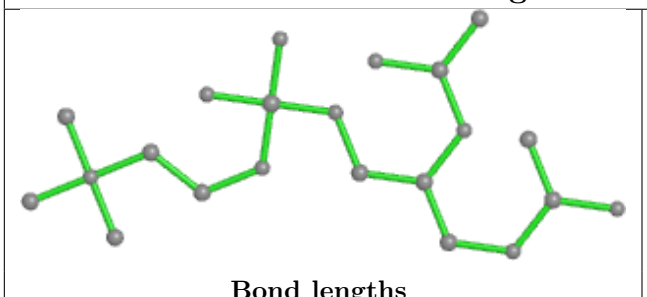


Torsions

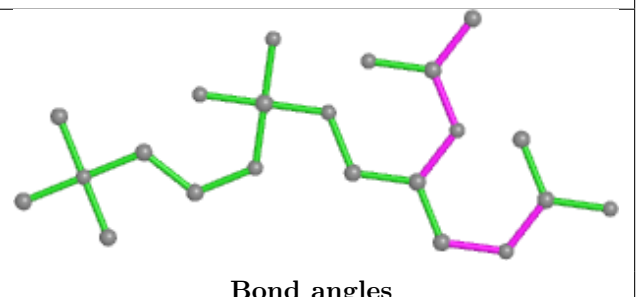


Rings

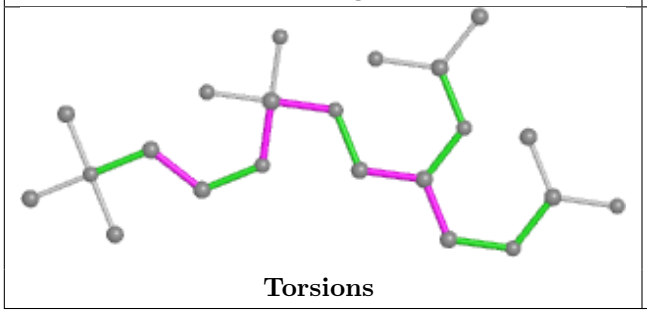
Ligand PCW A 1104



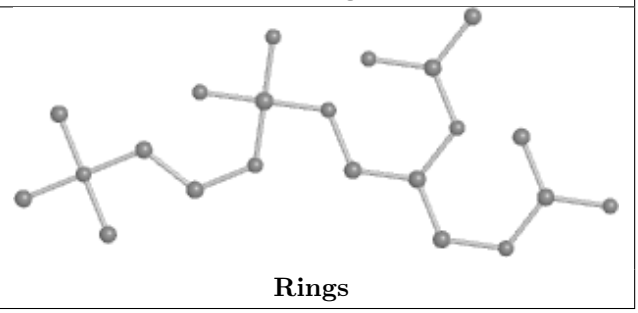
Bond lengths



Bond angles

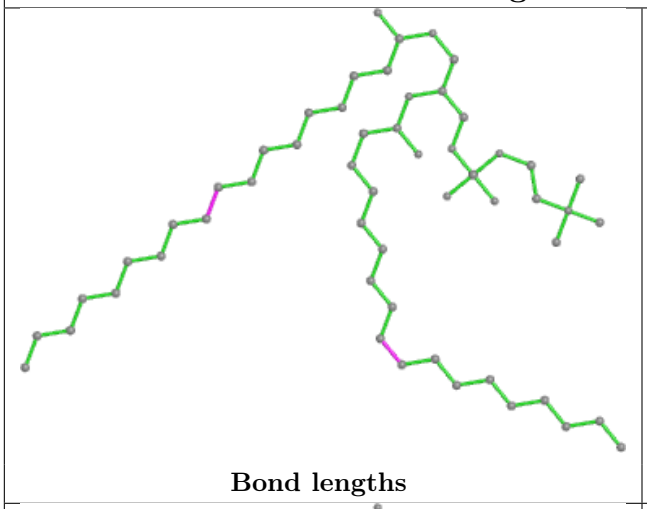


Torsions

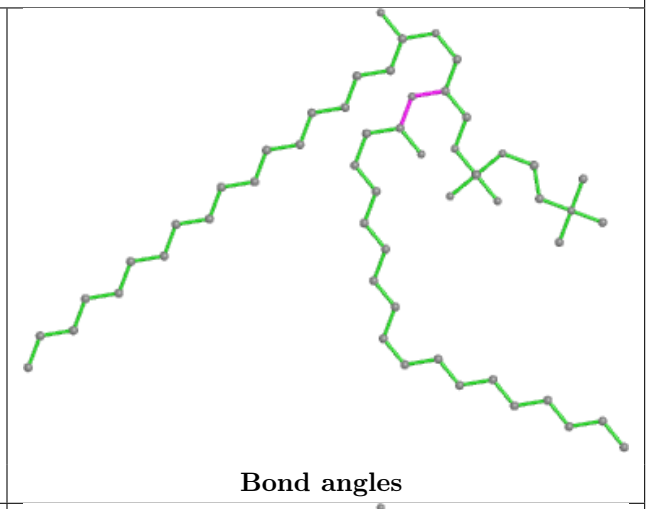


Rings

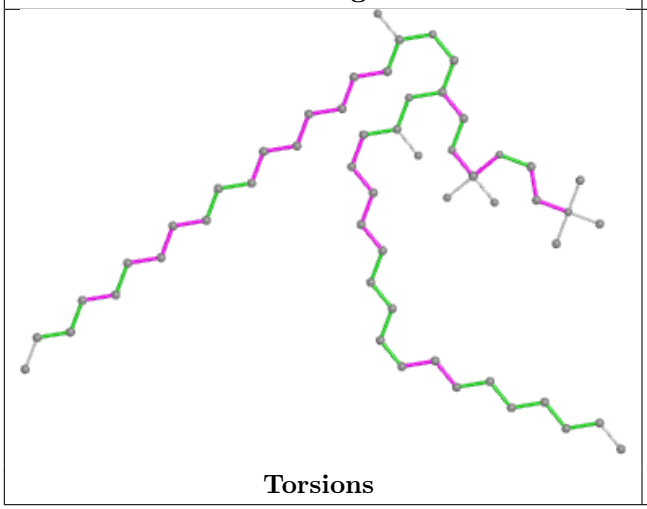
Ligand PCW A 1110



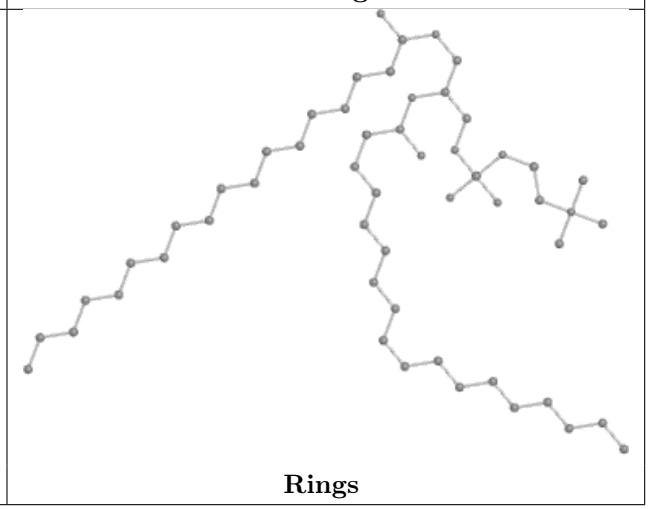
Bond lengths



Bond angles

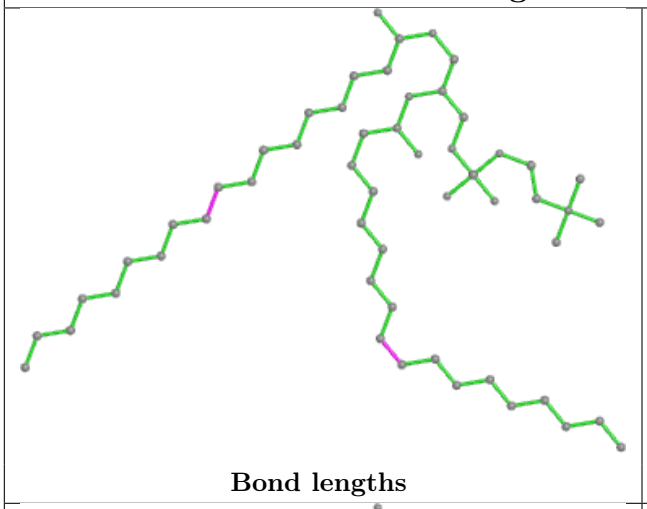


Torsions

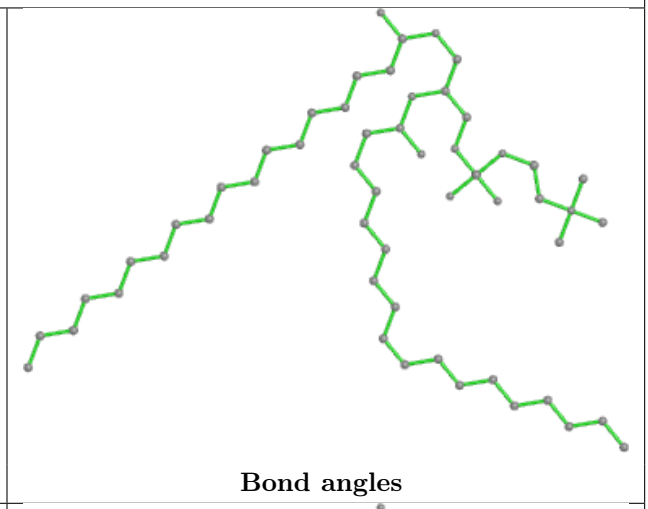


Rings

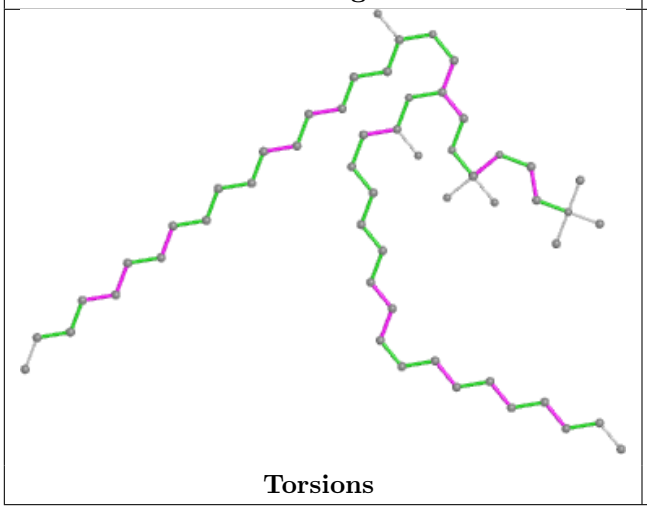
Ligand PCW A 1107



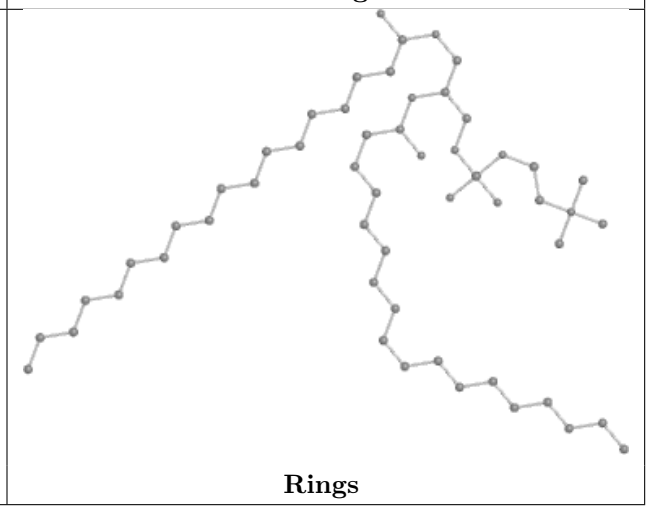
Bond lengths



Bond angles

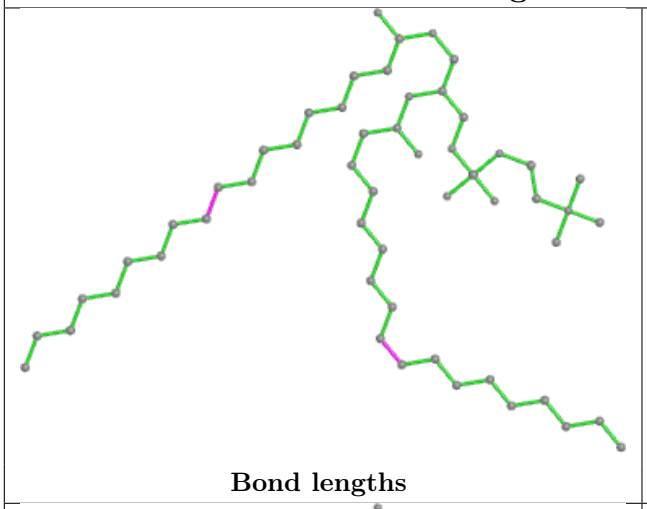


Torsions

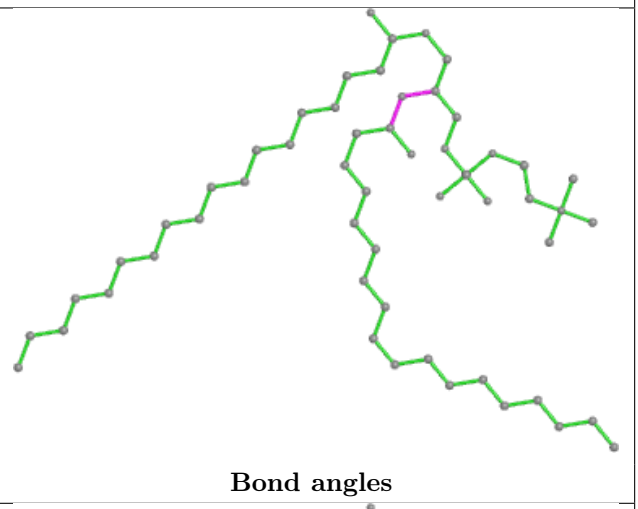


Rings

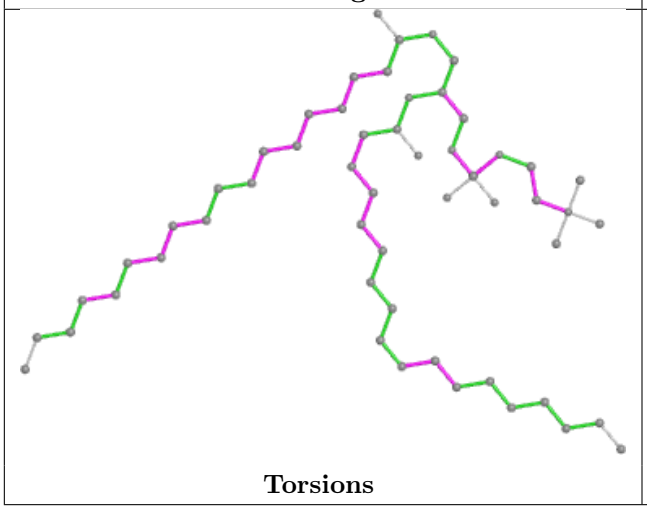
Ligand PCW C 1108



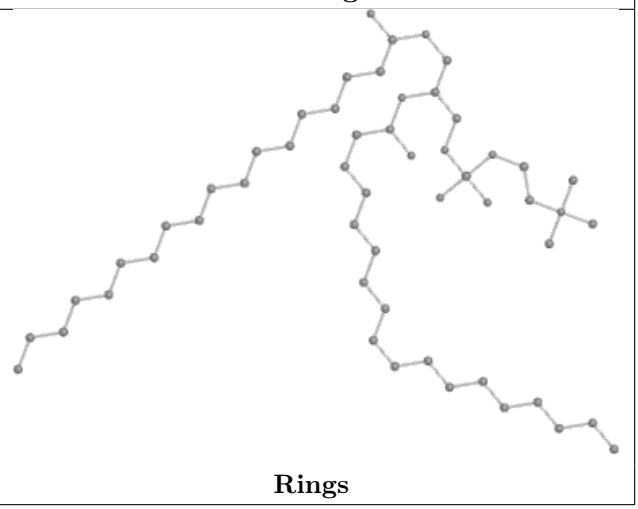
Bond lengths



Bond angles

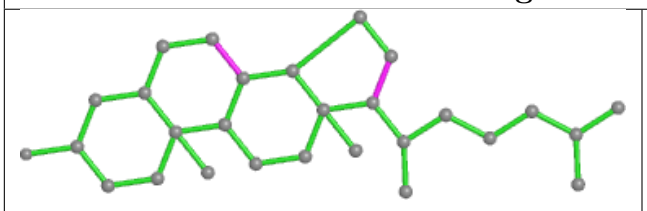


Torsions

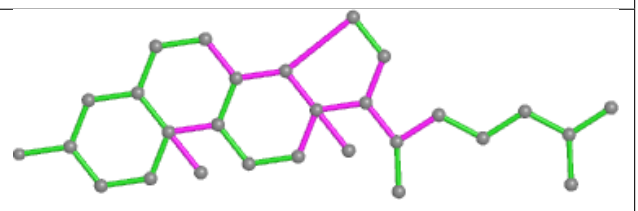


Rings

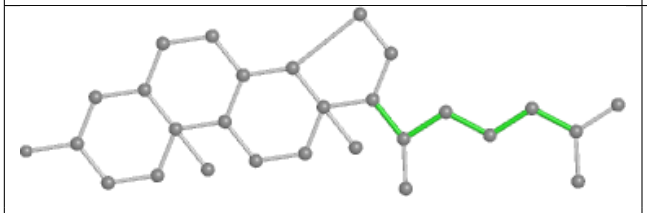
Ligand CLR G 1301



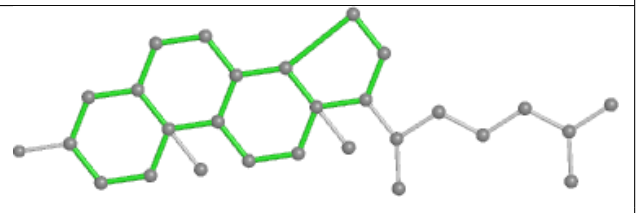
Bond lengths



Bond angles

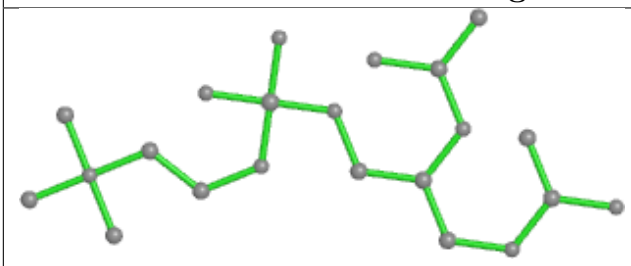


Torsions

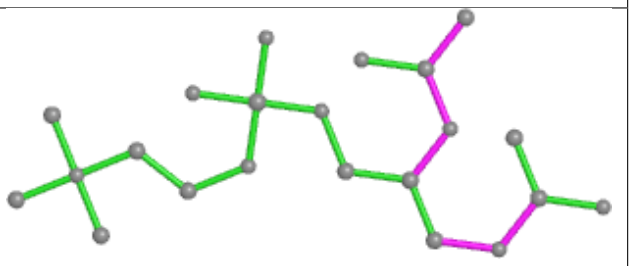


Rings

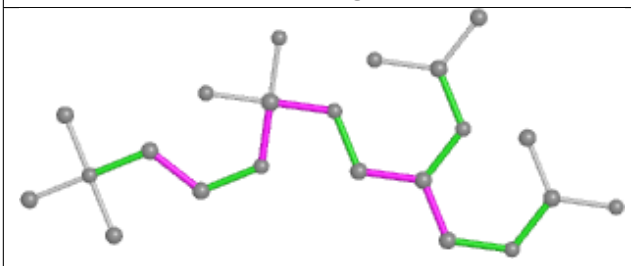
Ligand PCW C 1102



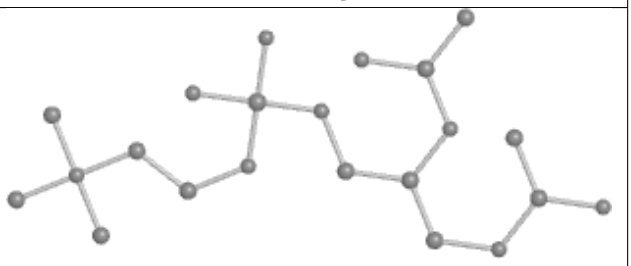
Bond lengths



Bond angles

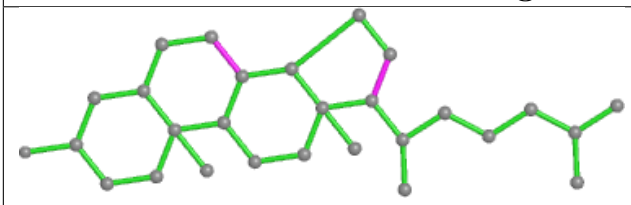


Torsions

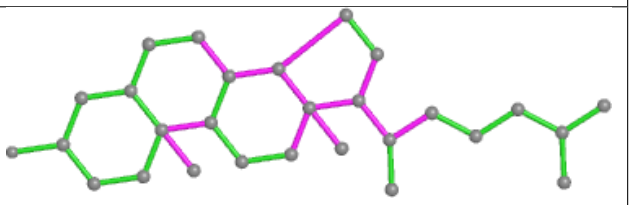


Rings

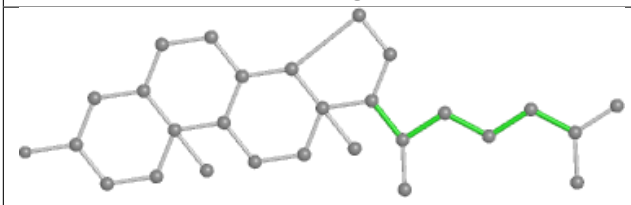
Ligand CLR E 1301



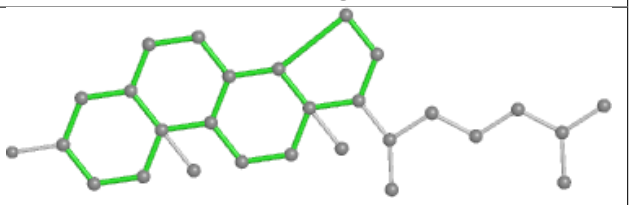
Bond lengths



Bond angles

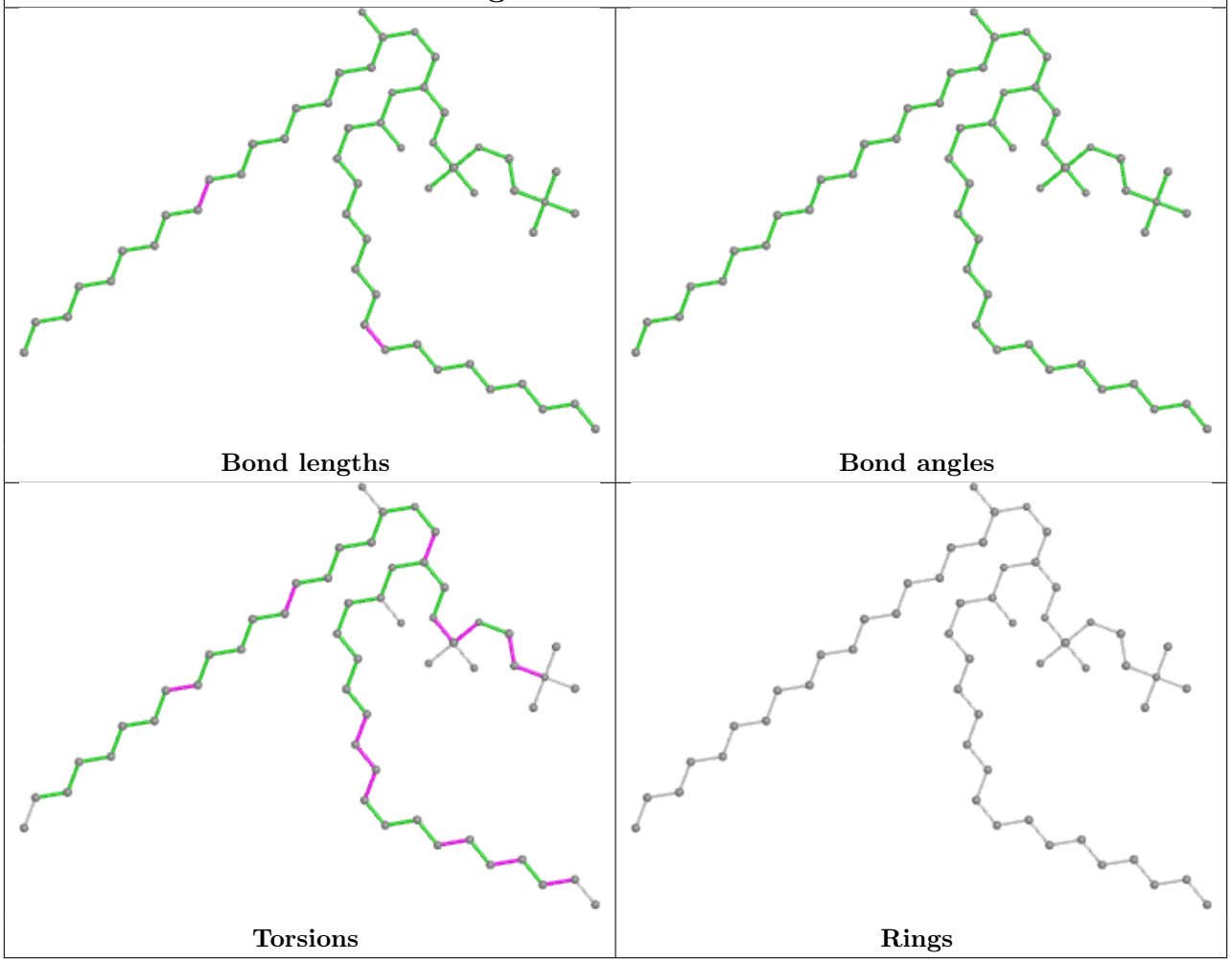


Torsions



Rings

Ligand PCW A 1112



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.

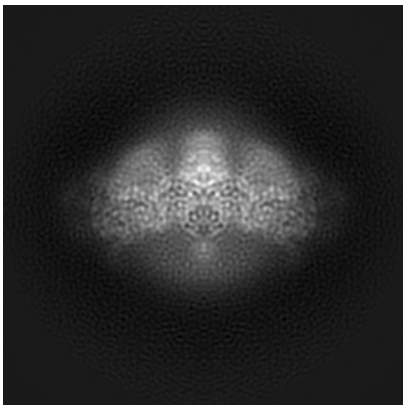
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36220. These allow visual inspection of the internal detail of the map and identification of artifacts.

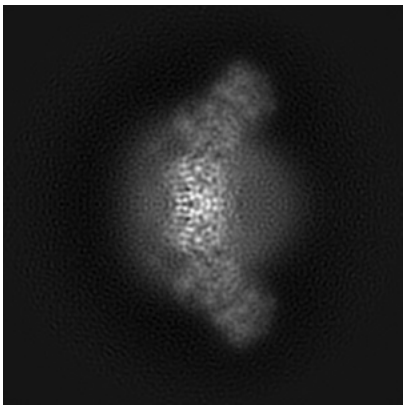
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

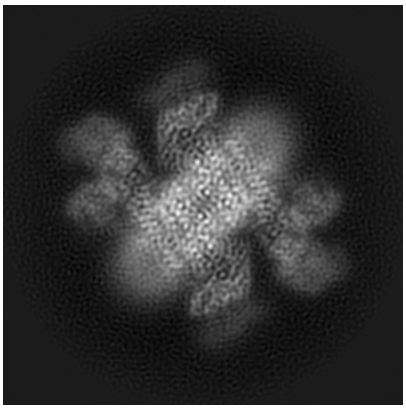
6.1.1 Primary map



X

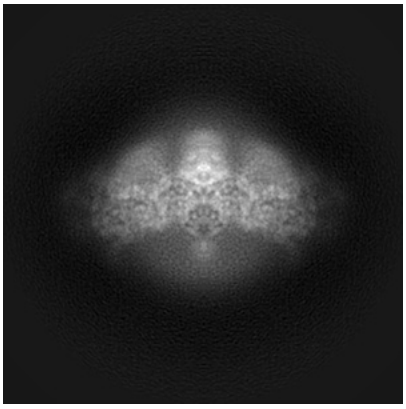


Y

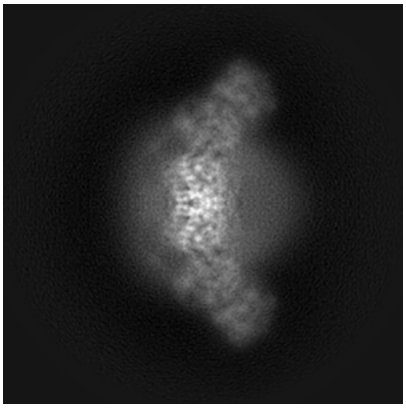


Z

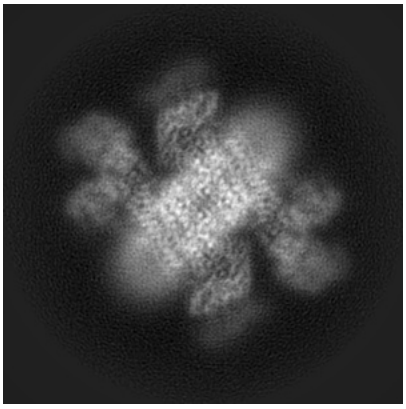
6.1.2 Raw map



X



Y

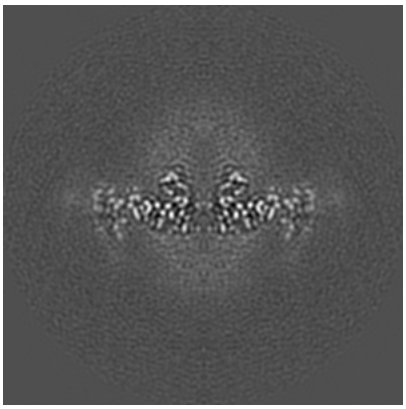


Z

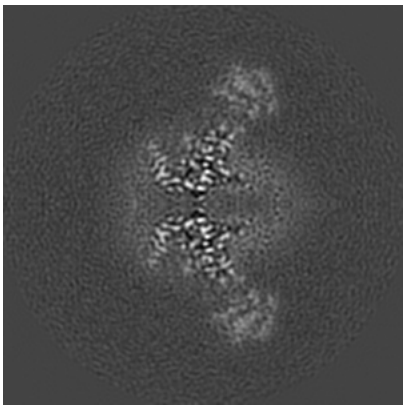
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

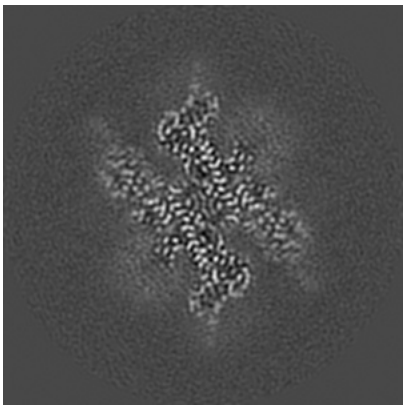
6.2.1 Primary map



X Index: 120

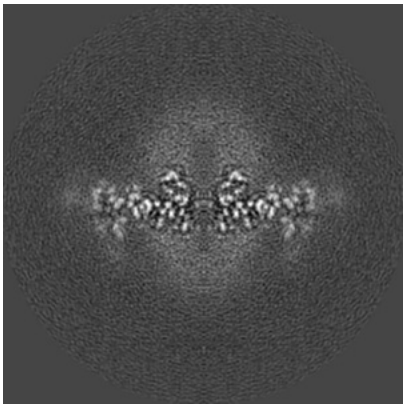


Y Index: 120

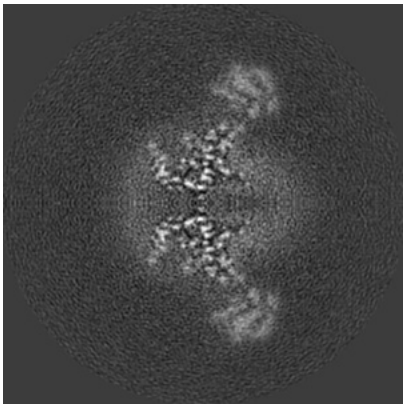


Z Index: 120

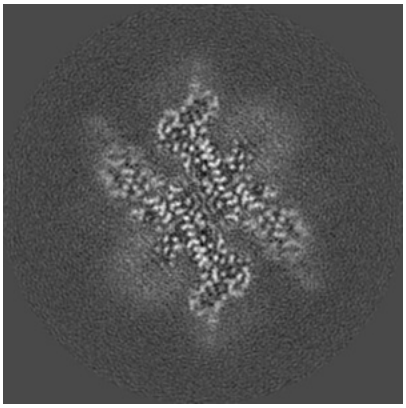
6.2.2 Raw map



X Index: 120



Y Index: 120

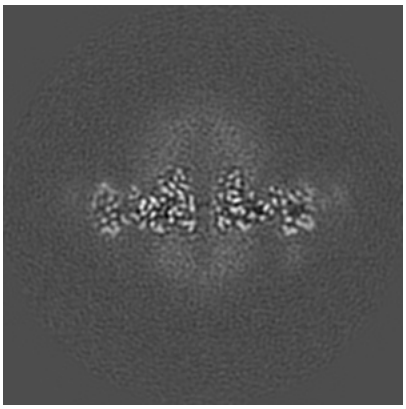


Z Index: 120

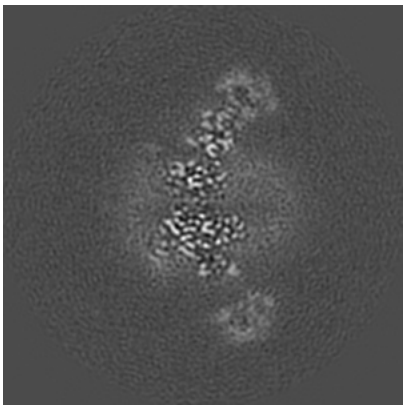
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

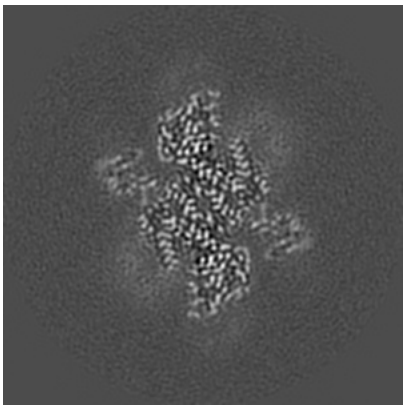
6.3.1 Primary map



X Index: 118

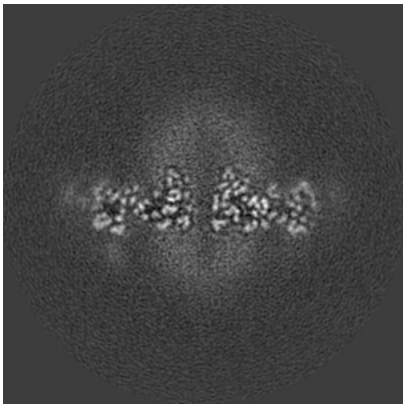


Y Index: 115

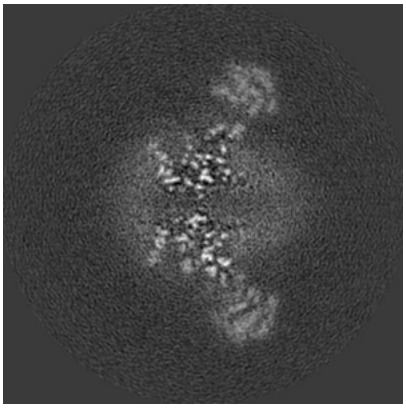


Z Index: 116

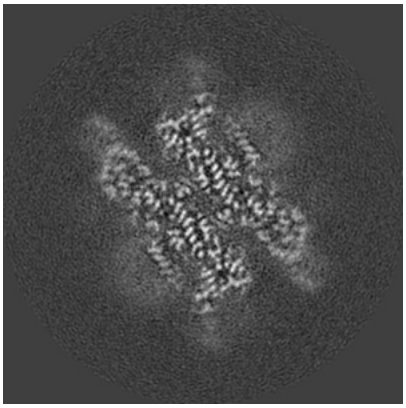
6.3.2 Raw map



X Index: 122



Y Index: 121

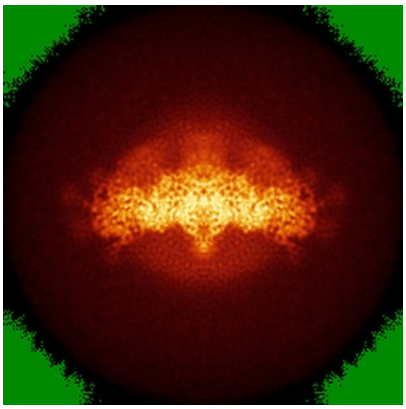


Z Index: 123

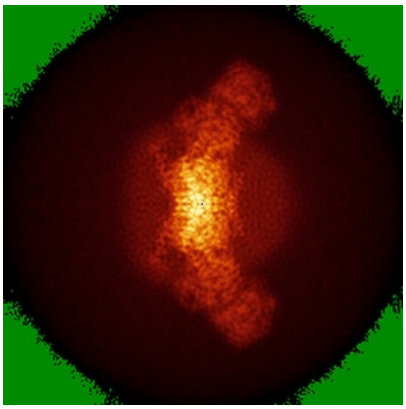
The images above show the largest variance slices of the map in three orthogonal directions.

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

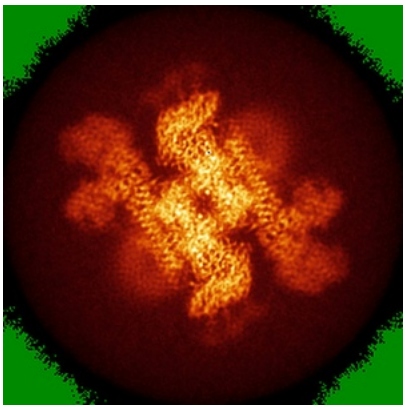
6.4.1 Primary map



X

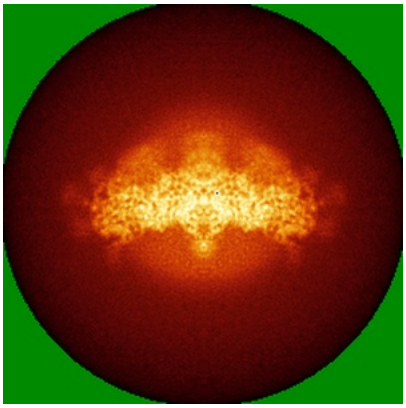


Y

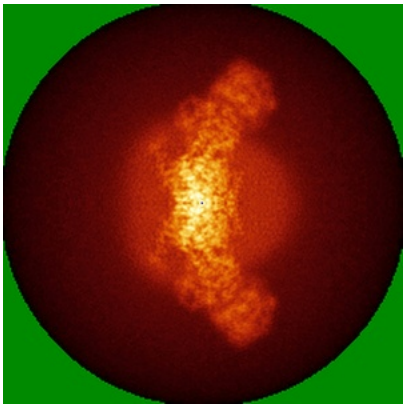


Z

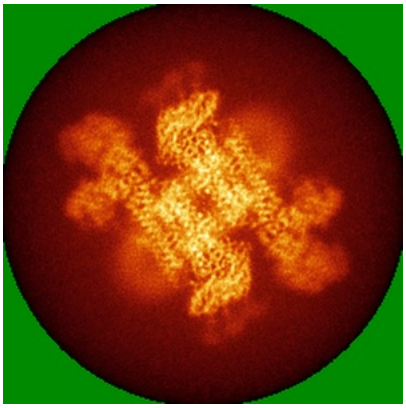
6.4.2 Raw map



X



Y

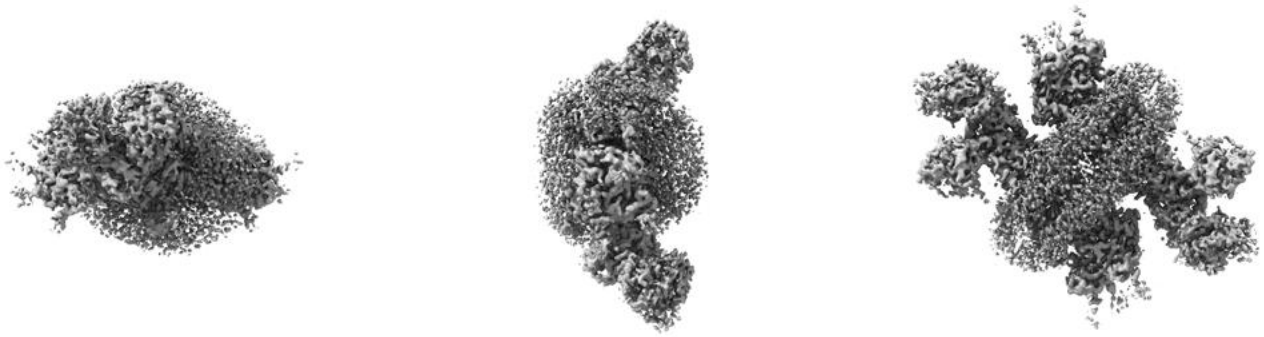


Z

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)

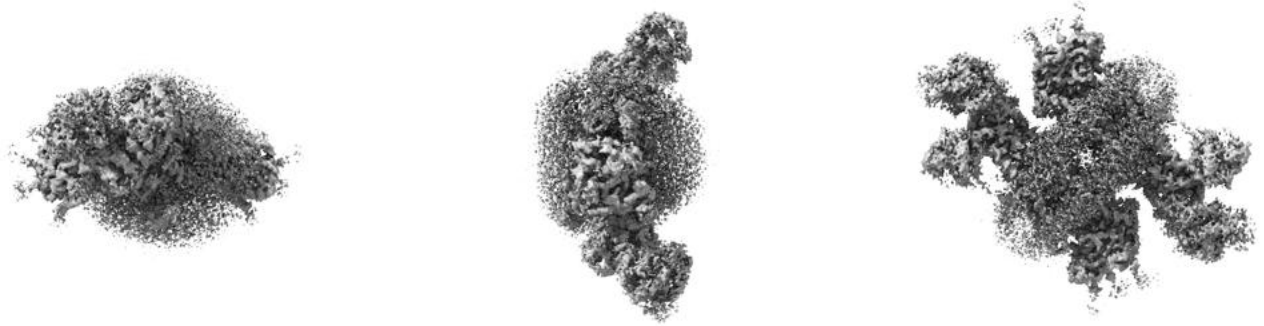
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

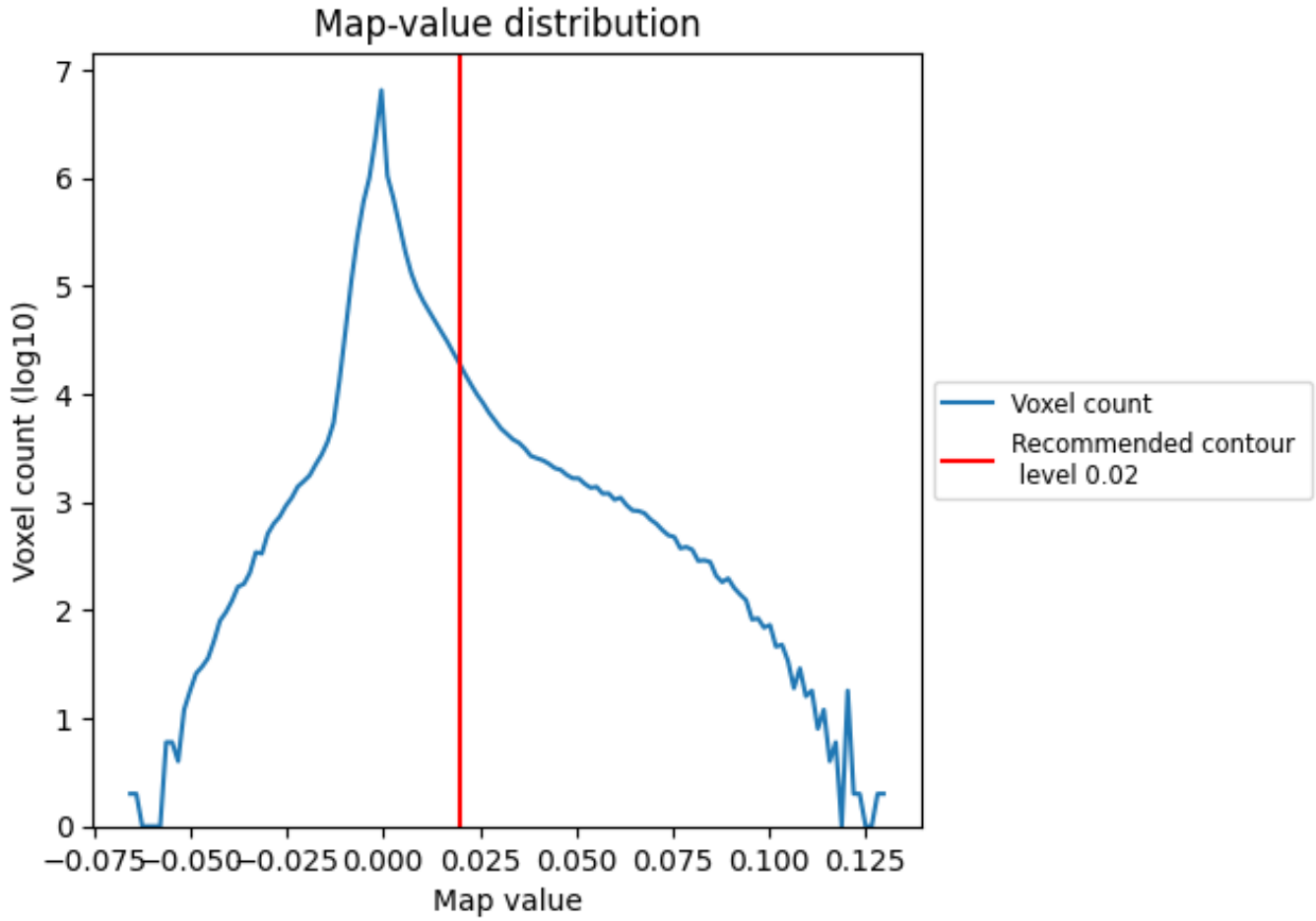
6.6 Mask visualisation (i)

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

7 Map analysis

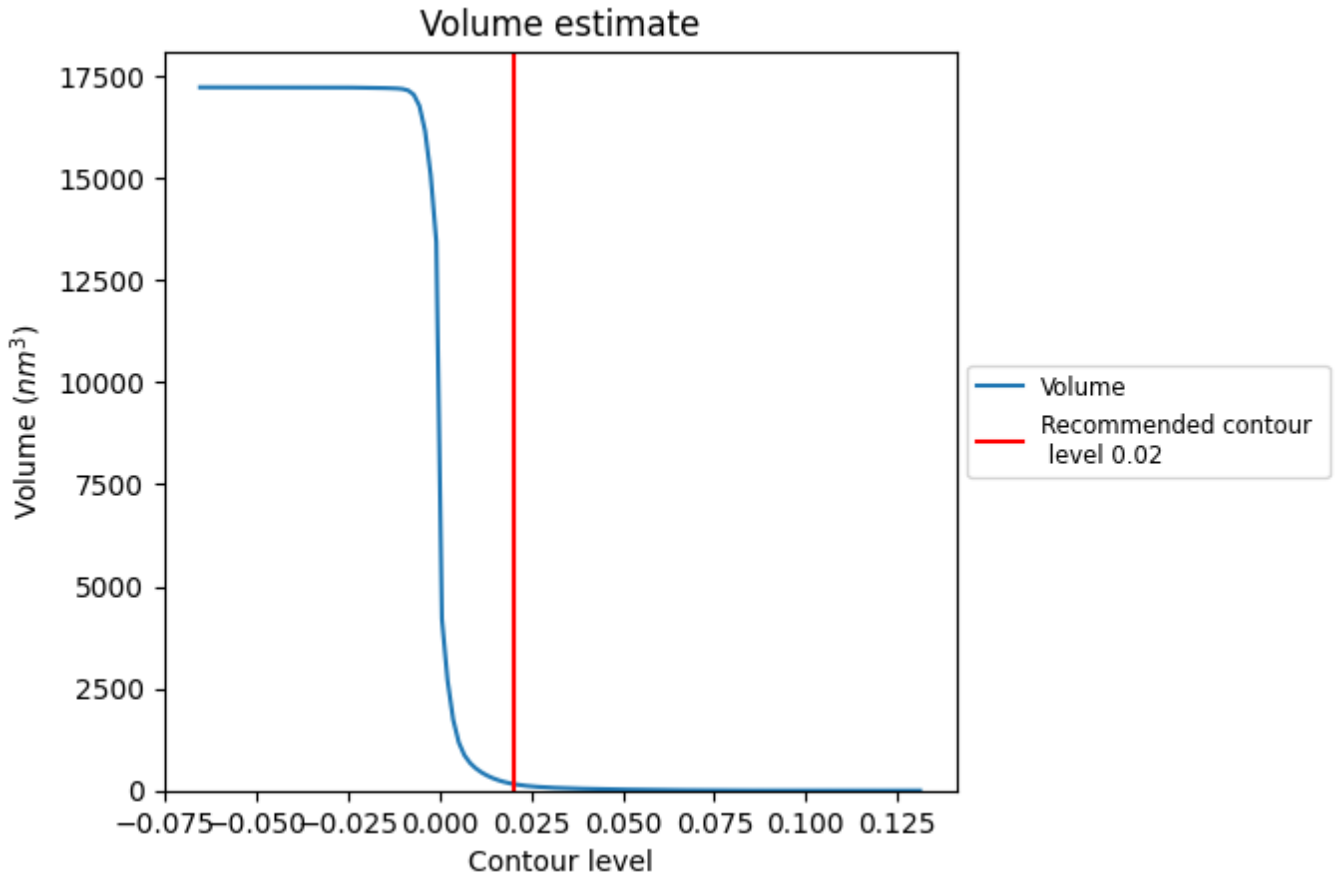
This section contains the results of statistical analysis of the map.

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.

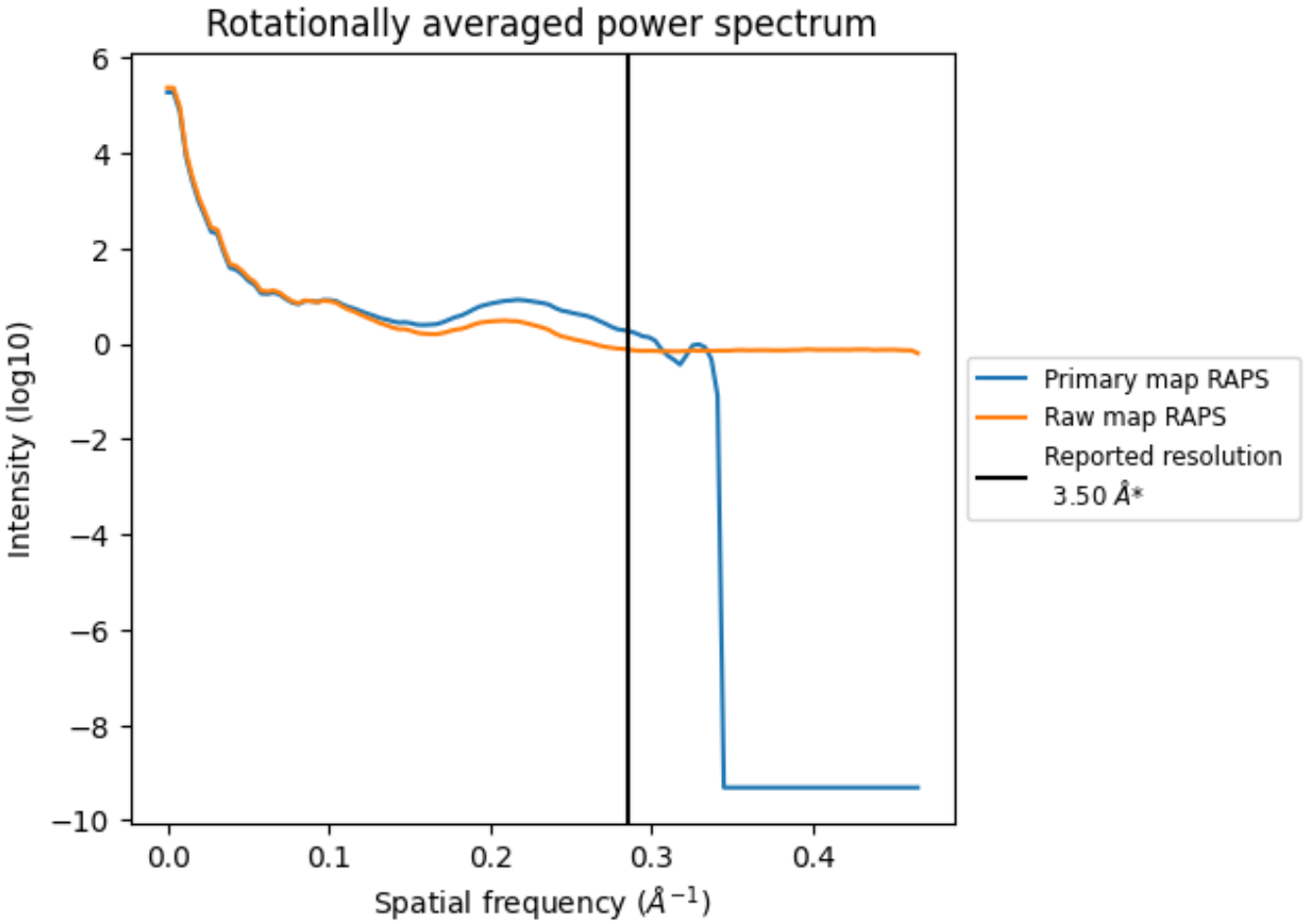
7.2 Volume estimate



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 147 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)

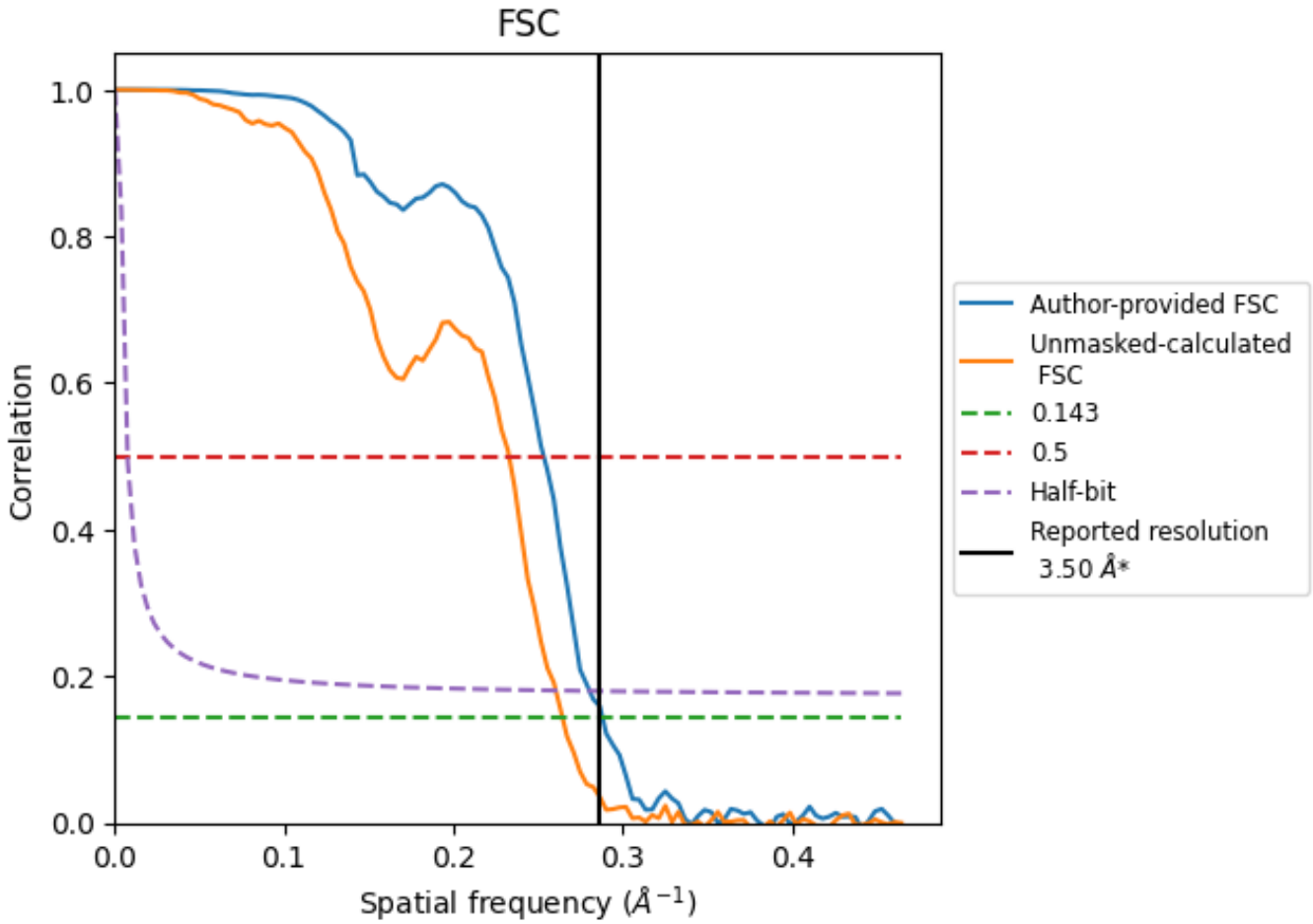


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

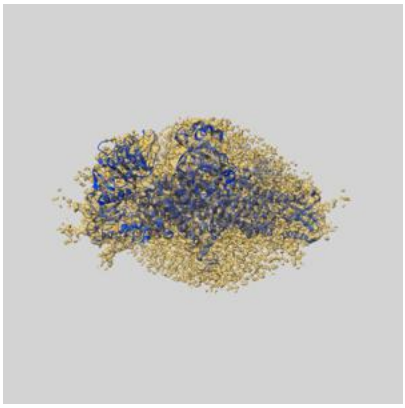
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.95	3.56
Unmasked-calculated*	3.78	4.29	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

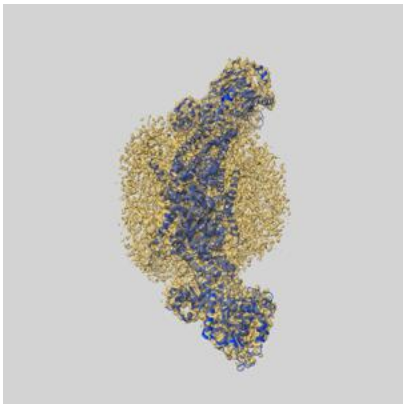
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36220 and PDB model 8JFZ. Per-residue inclusion information can be found in section 3 on page 9.

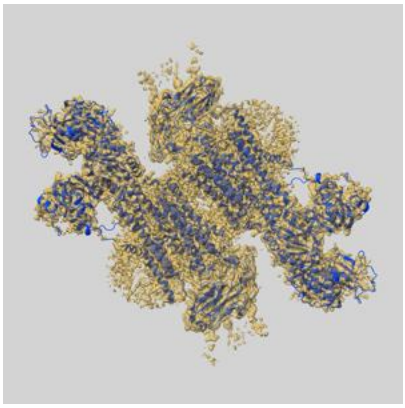
9.1 Map-model overlay



X



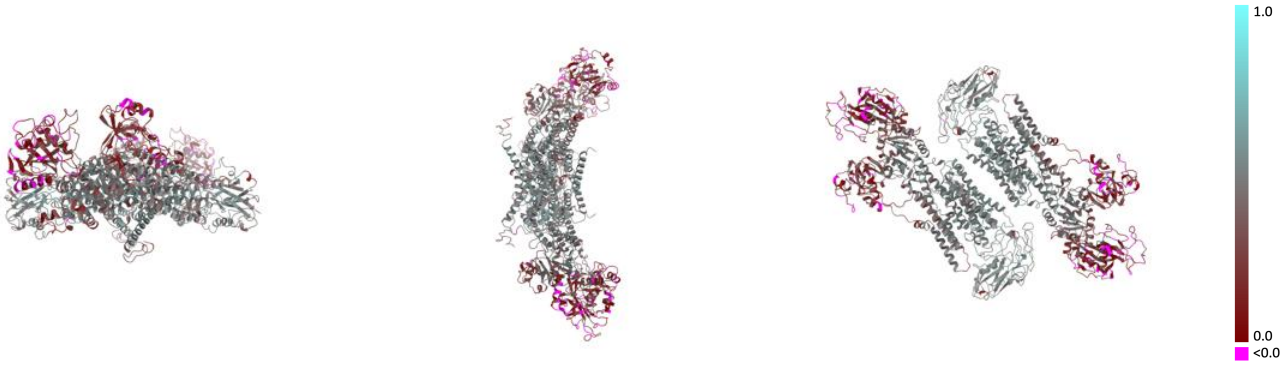
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

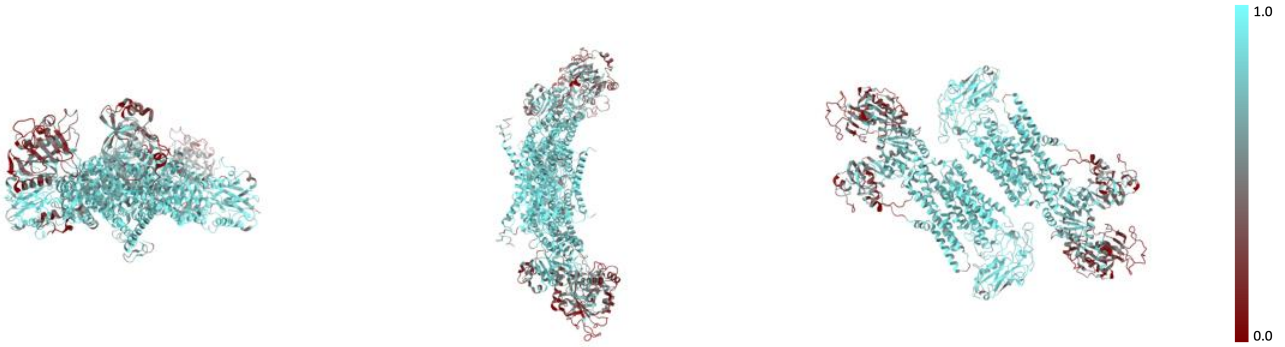
9.2 Q-score mapped to coordinate model (i)



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.

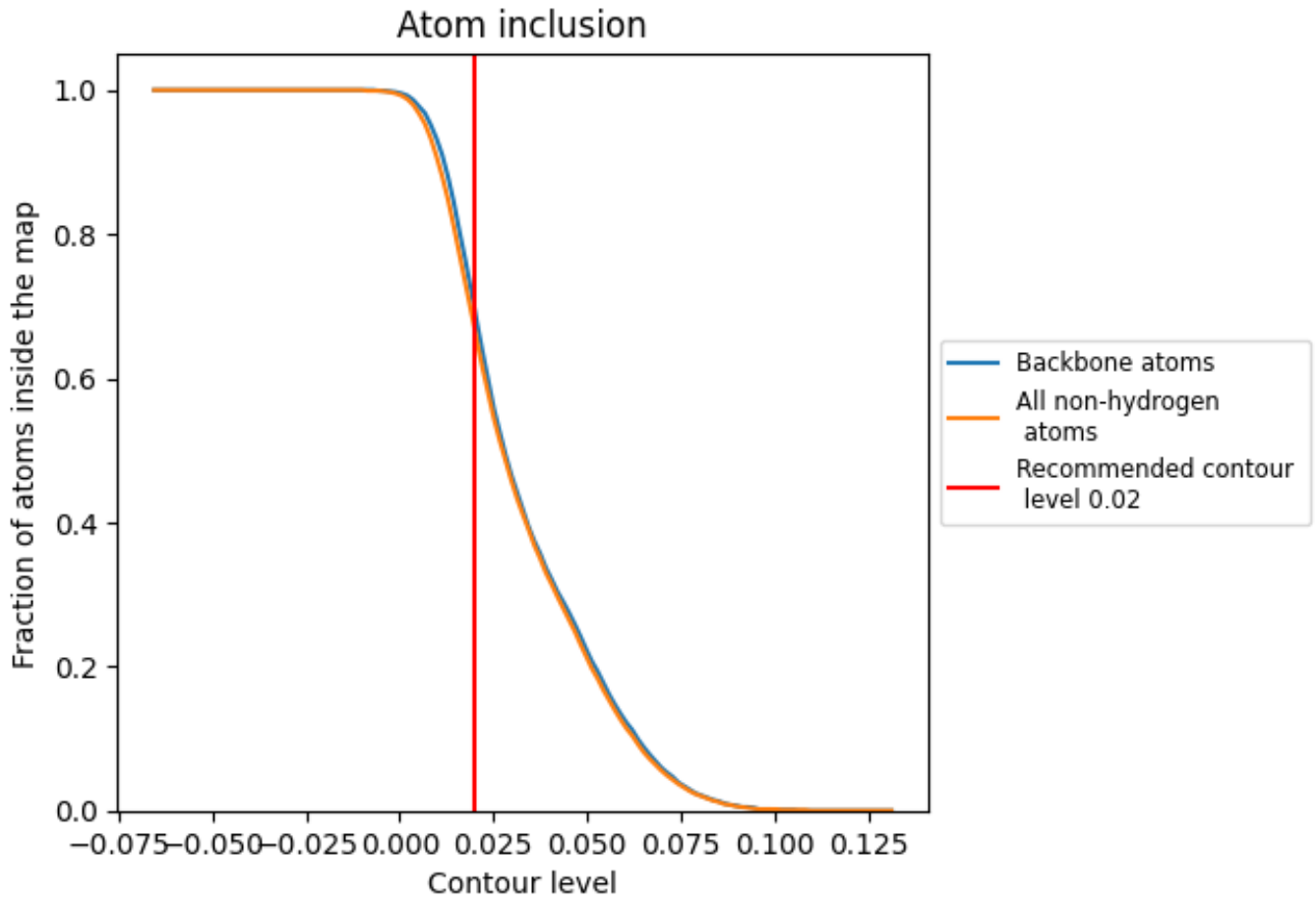
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 67% 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	0.6680	0.3830
A	0.6370	0.3590
B	0.8270	0.4850
C	0.6260	0.3480
D	0.8210	0.4730
E	0.7860	0.4920
F	0.4220	0.2310
G	0.8200	0.4820
H	0.2000	0.2050
I	0.3330	0.1910
J	0.2860	0.1480
K	0.4220	0.2280
L	0.2270	0.1980
M	0.3330	0.1950
N	0.2140	0.1580