



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:21 AM UTC

PDB ID : 8JBM / pdb_00008jbm
Title : Crystal structure of Na⁺,K⁺-ATPase in the E1.Mn²⁺ state
Authors : Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2023-05-09
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

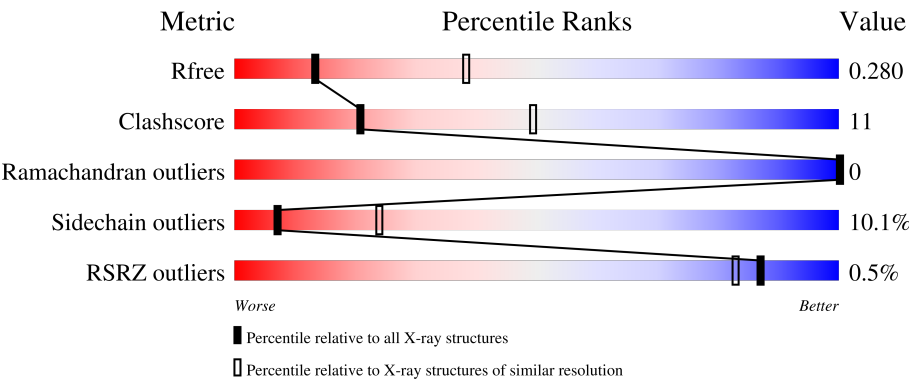
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1021	
1	C	1021	
2	B	303	
2	D	303	
3	E	65	

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Mol	Chain	Length	Quality of chain
3	G	65	 37% 17% 46%
4	F	6	 33% 67%
5	H	5	 80% 20%
6	I	2	 50% 50%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21682 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7723	4923	1301	1452	47			
1	C	995	Total	C	N	O	S	0	0	0
			7723	4923	1301	1452	47			

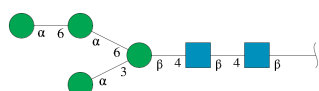
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			
2	D	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	35	Total	C	N	O	0	0	0
			285	192	46	47			
3	E	33	Total	C	N	O	0	0	0
			262	179	38	45			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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				ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

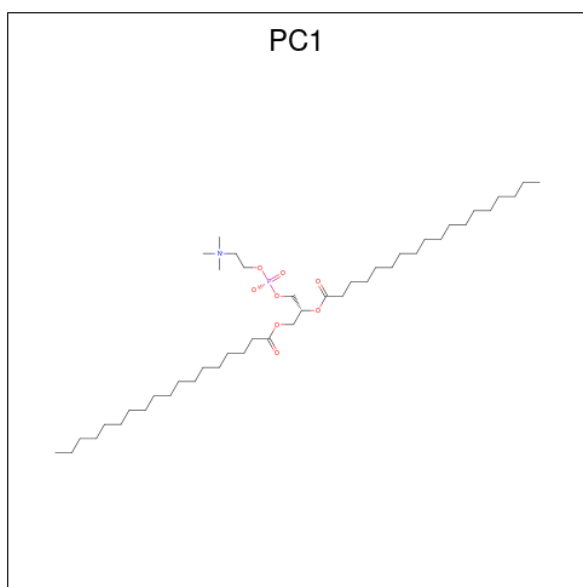
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Mn	0	0
			3	3		
7	C	3	Total	Mn	0	0
			3	3		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



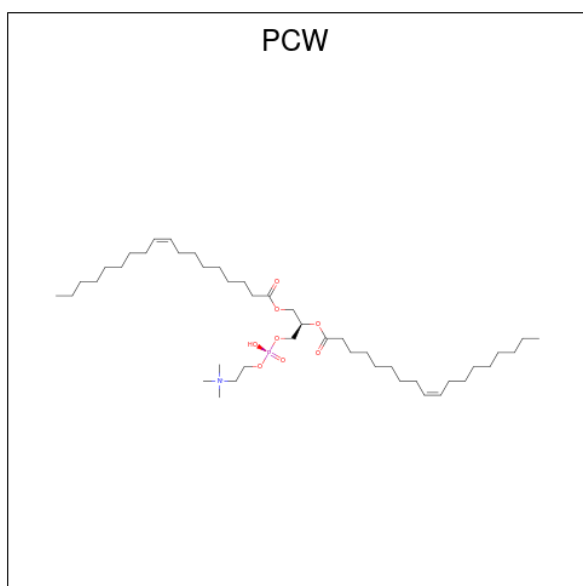
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	G	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	D	1	Total	C	O	0	0
			28	27	1		
8	E	1	Total	C	O	0	0
			28	27	1		

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



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

- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



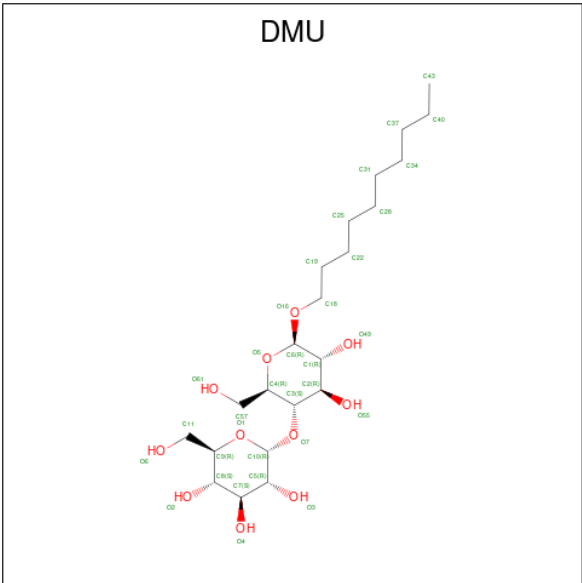
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	B	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	C	O	0	0
			33	22	11		

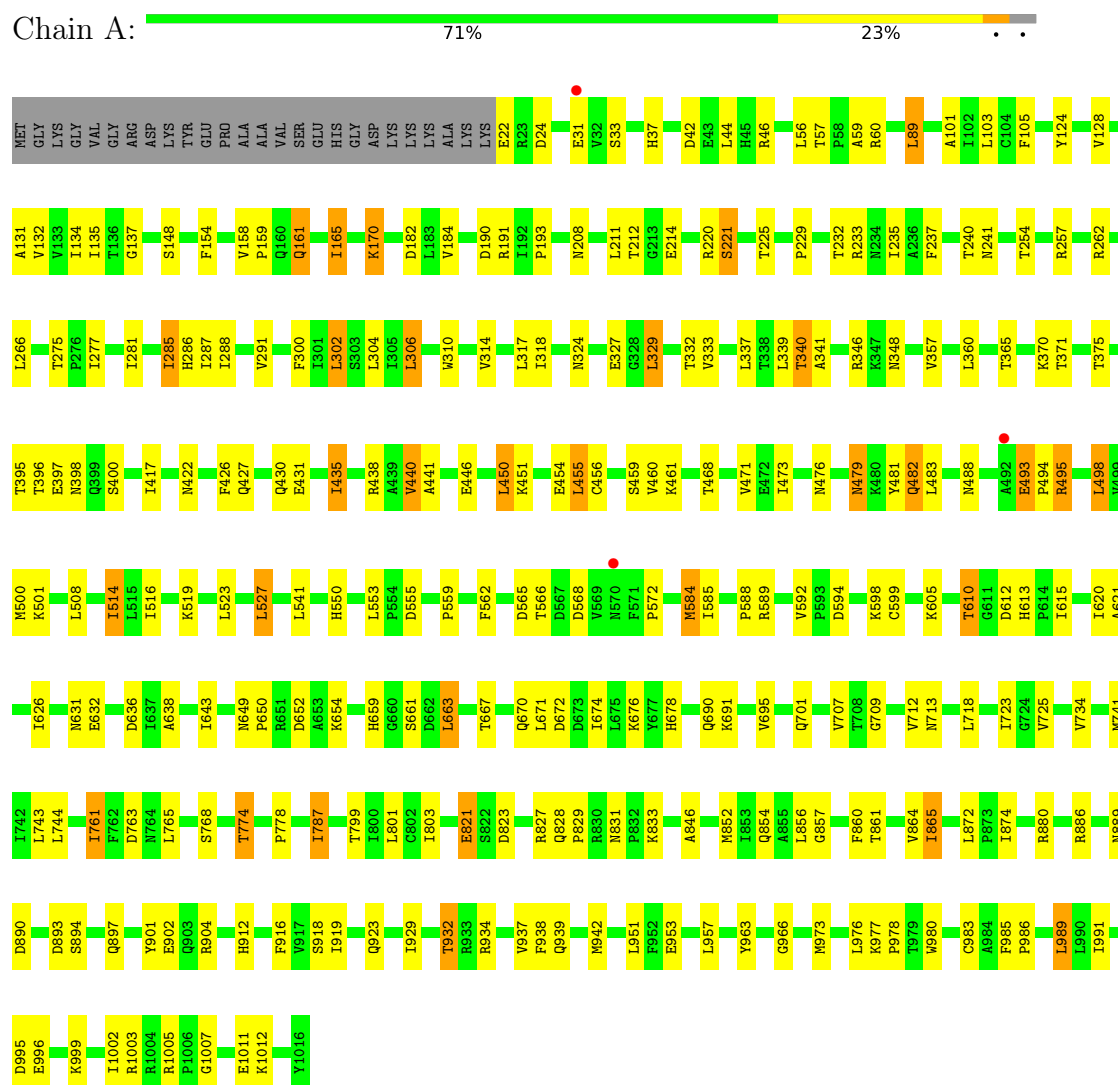
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	19	Total 19	O 19	0	0
13	C	12	Total 12	O 12	0	0
13	D	2	Total 2	O 2	0	0

3 Residue-property plots

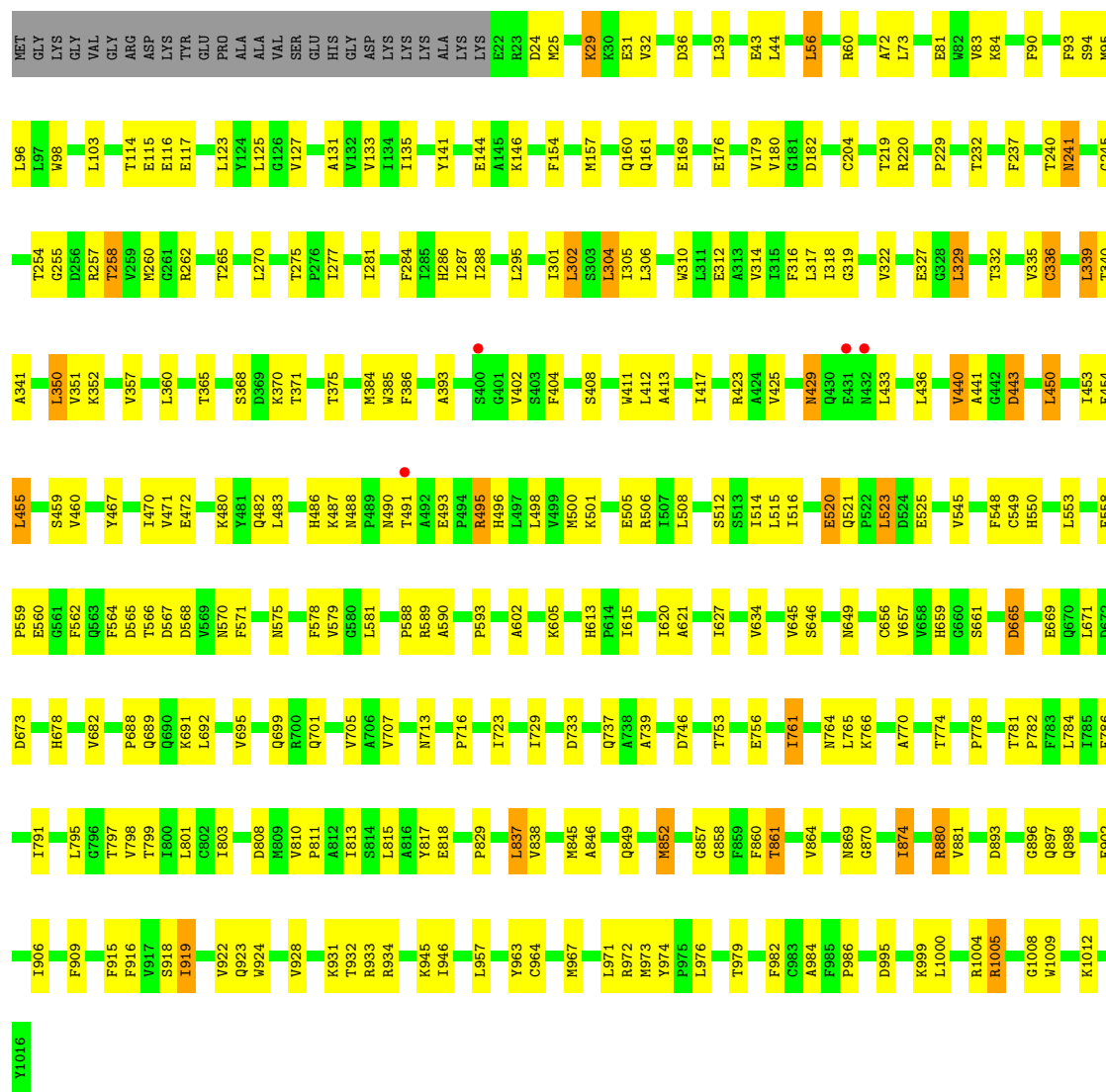
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

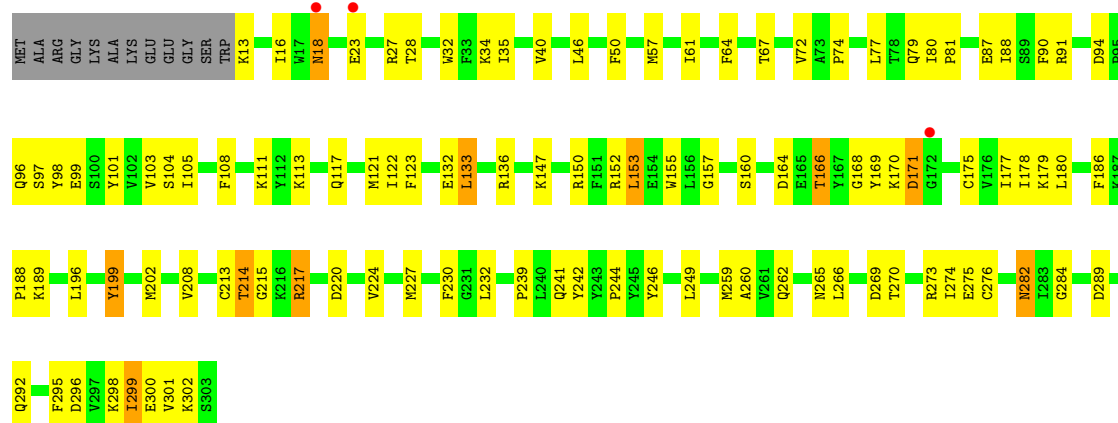


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

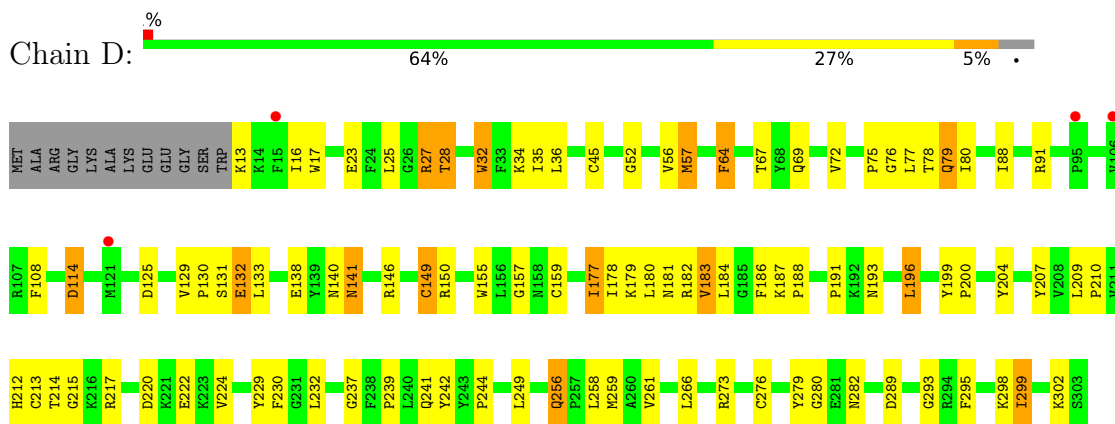




• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



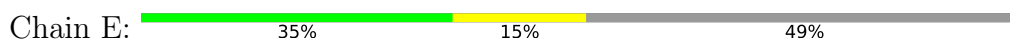
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



- Molecule 3: FXYD domain-containing ion transport regulator



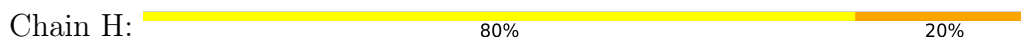
- Molecule 3: FXYD domain-containing ion transport regulator



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



- Molecule 5: 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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	196.98Å 74.43Å 162.98Å 90.00° 116.33° 90.00°	Depositor
Resolution (Å)	12.00 – 2.90 12.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	57.4 (12.00-2.90) 56.6 (12.00-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.278 0.230 , 0.280	Depositor DCC
R_{free} test set	2745 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21682	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, MN, PCW, NAG, BMA, PC1, DMU, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/7873	0.45	0/10683
1	C	0.24	0/7873	0.44	0/10683
2	B	0.20	0/2449	0.43	0/3301
2	D	0.20	0/2449	0.42	0/3301
3	E	0.26	0/268	0.35	0/364
3	G	0.24	0/291	0.43	0/393
All	All	0.23	0/21203	0.44	0/28725

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7723	0	7775	163	0
1	C	7723	0	7775	170	0
2	B	2386	0	2362	66	0
2	D	2386	0	2362	62	0
3	E	262	0	268	8	0
3	G	285	0	296	12	0
4	F	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	61	0	52	1	0
6	I	28	0	25	0	0
7	A	3	0	0	0	0
7	C	3	0	0	0	0
8	A	56	0	92	2	0
8	C	28	0	46	2	0
8	D	28	0	46	3	0
8	E	28	0	46	3	0
8	G	28	0	46	3	0
9	A	162	0	264	21	0
10	A	164	0	174	8	0
10	B	22	0	18	2	0
10	C	154	0	126	6	0
11	D	14	0	13	0	0
12	E	33	0	42	3	0
13	A	19	0	0	0	0
13	C	12	0	0	0	0
13	D	2	0	0	0	0
All	All	21682	0	21889	485	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 11.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:PRO:HG2	8:A:1104:CLR:H181	1.52	0.91
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.57	0.86
9:A:1107:PC1:H372	8:C:1104:CLR:H71	1.61	0.82
1:C:114:THR:HG22	1:C:115:GLU:H	1.46	0.78
1:A:340:THR:HG21	1:A:761:ILE:HG12	1.66	0.78
1:C:254:THR:HG23	1:C:257:ARG:HH21	1.49	0.78
9:A:1107:PC1:H3A2	9:A:1107:PC1:H2E2	1.66	0.78
2:D:131:SER:HB2	2:D:241:GLN:HB3	1.65	0.77
1:C:845:MET:SD	1:C:849:GLN:NE2	2.59	0.75
1:A:1005:ARG:HH22	10:A:1112:PCW:H72	1.51	0.74
1:C:613:HIS:HD2	1:C:615:ILE:H	1.35	0.73
10:B:401:PCW:H61	10:C:1107:PCW:H52	1.71	0.73
1:C:559:PRO:HD2	1:C:562:PHE:HB2	1.70	0.73
1:A:488:ASN:HB3	1:A:493:GLU:OE2	1.89	0.73
1:C:370:LYS:HE2	1:C:620:ILE:HG13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ARG:HB3	10:A:1111:PCW:H52	1.71	0.72
2:D:13:LYS:HD3	2:D:16:ILE:HD12	1.70	0.71
2:B:282:ASN:OD1	2:B:282:ASN:N	2.21	0.71
2:D:273:ARG:HG2	2:D:298:LYS:HB3	1.71	0.71
1:C:436:LEU:HD11	1:C:455:LEU:HD22	1.73	0.71
1:A:370:LYS:HB3	1:A:610:THR:HB	1.74	0.70
1:C:659:HIS:HD2	1:C:661:SER:H	1.39	0.69
1:A:33:SER:HB3	1:A:229:PRO:HG3	1.75	0.69
1:C:365:THR:HB	1:C:705:VAL:HG12	1.76	0.67
1:A:1007:GLY:HA2	1:A:1012:LYS:HE2	1.76	0.67
2:B:166:THR:HG23	2:B:168:GLY:H	1.59	0.67
1:A:135:ILE:HD12	10:A:1114:PCW:H261	1.77	0.66
2:D:75:PRO:HG3	2:D:183:VAL:HG21	1.77	0.66
2:D:76:GLY:HA2	2:D:293:GLY:H	1.61	0.66
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.76	0.66
1:C:384:MET:HE1	1:C:393:ALA:HB3	1.77	0.66
1:C:335:VAL:HG11	1:C:813:ILE:HG23	1.78	0.65
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.77	0.65
1:A:360:LEU:HD23	1:A:723:ILE:HD13	1.79	0.65
1:C:470:ILE:HD11	1:C:487:LYS:HG3	1.78	0.65
1:A:473:ILE:HB	1:A:483:LEU:HB3	1.78	0.64
1:A:856:LEU:HD13	2:B:50:PHE:HB2	1.79	0.64
1:C:495:ARG:HG2	1:C:560:GLU:HG3	1.78	0.64
1:C:204:CYS:HA	1:C:245:GLY:HA3	1.80	0.64
9:A:1107:PC1:H3H1	1:C:986:PRO:HB3	1.79	0.64
2:B:217:ARG:HG3	2:B:220:ASP:OD2	1.97	0.63
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.79	0.63
1:C:512:SER:HB2	1:C:575:ASN:HA	1.81	0.63
3:G:47:SER:HB2	3:G:50:LEU:HB2	1.80	0.63
1:C:945:LYS:HG3	1:C:946:ILE:HD12	1.79	0.63
1:A:89:LEU:HD11	1:A:134:ILE:HD13	1.79	0.63
1:A:493:GLU:OE2	1:A:495:ARG:HA	2.00	0.62
1:C:995:ASP:OD2	1:C:999:LYS:HE2	1.99	0.62
2:D:27:ARG:HG3	2:D:32:TRP:HD1	1.63	0.62
1:A:22:GLU:HB3	1:A:24:ASP:OD2	1.98	0.62
3:G:44:ILE:HD13	3:G:50:LEU:HD13	1.81	0.62
1:C:467:TYR:HB3	1:C:486:HIS:HB3	1.82	0.62
2:B:171:ASP:OD1	2:B:171:ASP:N	2.32	0.62
1:A:191:ARG:HA	1:A:241:ASN:HD22	1.64	0.62
1:A:435:ILE:HA	1:A:438:ARG:HE	1.64	0.62
10:A:1114:PCW:H20	10:A:1114:PCW:H451	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:ILE:HD11	2:D:258:LEU:HD22	1.82	0.61
1:C:514:ILE:HG12	1:C:578:PHE:HB3	1.83	0.61
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.81	0.61
1:A:938:PHE:CD1	9:A:1107:PC1:H342	2.35	0.61
1:C:803:ILE:HD13	1:C:919:ILE:HG21	1.82	0.61
2:B:61:ILE:HG23	2:B:67:THR:HG23	1.83	0.61
1:C:659:HIS:CD2	1:C:661:SER:H	2.18	0.61
1:A:996:GLU:HB3	9:A:1107:PC1:H292	1.82	0.61
1:C:766:LYS:HD2	1:C:933:ARG:HH22	1.67	0.60
1:C:408:SER:HB3	1:C:411:TRP:HB3	1.83	0.60
9:A:1110:PC1:H292	1:C:982:PHE:HE1	1.67	0.60
1:A:281:ILE:HG13	1:A:333:VAL:HG21	1.84	0.59
1:A:778:PRO:HG3	1:A:854:GLN:HE21	1.66	0.59
2:B:239:PRO:HB2	2:B:241:GLN:HG2	1.84	0.59
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.84	0.59
1:A:985:PHE:HE2	8:G:101:CLR:H241	1.68	0.59
3:G:40:VAL:HG21	3:E:36:LEU:HD11	1.84	0.59
1:A:302:LEU:HD13	1:A:787:ILE:HG12	1.86	0.58
1:C:482:GLN:HE21	1:C:501:LYS:HE2	1.68	0.58
1:A:942:MET:HB2	12:E:102:DMU:H6	1.85	0.58
9:A:1110:PC1:H231	12:E:102:DMU:H8	1.86	0.57
2:D:79:GLN:H	2:D:79:GLN:HE21	1.51	0.57
1:A:254:THR:HG23	1:A:257:ARG:HH21	1.67	0.57
2:D:178:ILE:HB	2:D:259:MET:HE2	1.86	0.57
1:C:340:THR:HG21	1:C:761:ILE:HG12	1.84	0.57
1:A:89:LEU:HD22	1:A:137:GLY:HA3	1.86	0.57
1:A:435:ILE:HG13	1:A:455:LEU:HG	1.87	0.57
1:C:490:ASN:HB3	1:C:493:GLU:HG2	1.87	0.57
1:A:131:ALA:O	1:A:135:ILE:HG12	2.04	0.57
2:D:217:ARG:HH12	2:D:273:ARG:HE	1.52	0.57
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.86	0.57
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.39	0.57
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.87	0.56
1:C:558:PHE:HZ	1:C:571:PHE:HA	1.70	0.56
1:C:692:LEU:HD22	1:C:716:PRO:HB2	1.87	0.56
1:C:919:ILE:O	1:C:923:GLN:HG2	2.05	0.56
1:A:454:GLU:OE2	1:A:459:SER:HA	2.05	0.56
2:B:178:ILE:HB	2:B:259:MET:HE3	1.87	0.56
1:C:93:PHE:HZ	1:C:322:VAL:HA	1.70	0.56
2:D:213:CYS:HA	2:D:276:CYS:HA	1.86	0.56
2:D:220:ASP:O	2:D:224:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:ASN:HB2	1:A:833:LYS:HD2	1.88	0.56
1:A:985:PHE:CE2	8:G:101:CLR:H241	2.40	0.56
1:C:90:PHE:HB3	1:C:95:MET:HE2	1.87	0.56
1:C:116:GLU:OE2	1:C:117:GLU:HG3	2.06	0.56
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.89	0.55
2:D:23:GLU:HG2	2:D:28:THR:HG22	1.89	0.55
1:A:613:HIS:HD2	1:A:615:ILE:H	1.53	0.55
1:C:861:THR:HG21	1:C:918:SER:OG	2.06	0.55
2:D:32:TRP:O	2:D:36:LEU:HB2	2.06	0.55
1:A:778:PRO:HG3	1:A:854:GLN:NE2	2.22	0.55
1:A:939:GLN:HG2	9:A:1107:PC1:H12	1.89	0.55
1:C:691:LYS:O	1:C:695:VAL:HG23	2.05	0.55
1:C:972:ARG:NH2	1:C:974:TYR:OH	2.39	0.55
1:A:42:ASP:OD2	1:A:46:ARG:NH1	2.39	0.55
2:B:213:CYS:HA	2:B:276:CYS:HA	1.89	0.55
1:A:919:ILE:O	1:A:923:GLN:HG2	2.07	0.55
1:C:896:GLY:O	2:D:182:ARG:NH2	2.40	0.55
2:B:289:ASP:OD2	2:B:292:GLN:HB2	2.07	0.54
1:C:852:MET:HE1	8:D:401:CLR:H232	1.90	0.54
1:A:132:VAL:HG11	1:A:801:LEU:HD23	1.90	0.54
1:A:165:ILE:HD13	1:A:170:LYS:HB3	1.88	0.54
1:C:483:LEU:HD13	1:C:500:MET:HB3	1.89	0.54
1:A:938:PHE:HA	9:A:1110:PC1:H12	1.89	0.54
1:C:496:HIS:HB3	1:C:553:LEU:HD12	1.89	0.54
1:A:103:LEU:HD22	1:A:310:TRP:HZ3	1.73	0.54
1:A:417:ILE:HG21	1:A:550:HIS:HB3	1.90	0.54
1:A:916:PHE:HD2	1:A:973:MET:HE1	1.73	0.54
1:C:766:LYS:HE2	1:C:837:LEU:HA	1.90	0.54
2:B:23:GLU:HA	2:B:28:THR:HA	1.90	0.53
1:A:774:THR:HG23	1:A:846:ALA:HA	1.90	0.53
1:C:514:ILE:HG13	1:C:523:LEU:HG	1.91	0.53
2:D:80:ILE:HG21	2:D:108:PHE:HD2	1.74	0.53
1:A:890:ASP:OD1	1:A:890:ASP:N	2.41	0.53
1:A:1007:GLY:H	1:A:1011:GLU:CD	2.17	0.53
2:D:157:GLY:H	2:D:230:PHE:HB3	1.74	0.53
1:A:709:GLY:HA3	1:A:718:LEU:HD21	1.89	0.53
1:A:902:GLU:HB2	2:B:289:ASP:HB2	1.91	0.53
1:A:916:PHE:CD2	1:A:973:MET:HE1	2.44	0.53
2:B:164:ASP:OD1	2:B:166:THR:HG22	2.08	0.53
1:A:494:PRO:HB3	1:A:555:ASP:HB2	1.90	0.52
1:A:621:ALA:HB1	1:A:626:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.23	0.52
1:C:565:ASP:HB2	1:C:570:ASN:HD22	1.74	0.52
1:C:339:LEU:HD11	1:C:817:TYR:CD1	2.44	0.52
1:C:774:THR:HG22	1:C:846:ALA:HA	1.90	0.52
1:A:398:ASN:HD21	1:A:400:SER:HB2	1.74	0.52
1:C:454:GLU:OE2	1:C:460:VAL:HG22	2.09	0.52
1:C:505:GLU:CD	1:C:505:GLU:H	2.17	0.52
1:C:1008:GLY:O	1:C:1012:LYS:HG2	2.09	0.52
1:A:827:ARG:HE	1:A:934:ARG:HE	1.56	0.52
2:B:177:ILE:HA	2:B:260:ALA:HA	1.92	0.52
1:A:886:ARG:HG2	1:A:901:TYR:CZ	2.43	0.52
2:B:90:PHE:CD2	2:B:98:TYR:HB3	2.44	0.52
1:C:1005:ARG:NE	10:C:1109:PCW:O1P	2.43	0.52
2:D:183:VAL:HB	2:D:186:PHE:HB2	1.90	0.52
1:C:454:GLU:HG2	1:C:460:VAL:HG13	1.92	0.52
2:D:179:LYS:HD2	2:D:256:GLN:CD	2.35	0.52
1:C:423:ARG:NE	1:C:472:GLU:OE2	2.40	0.52
1:C:440:VAL:HG12	1:C:441:ALA:H	1.75	0.52
1:C:613:HIS:CD2	1:C:615:ILE:H	2.21	0.52
2:D:80:ILE:HG21	2:D:108:PHE:CD2	2.45	0.52
2:B:155:TRP:CD1	2:B:232:LEU:HA	2.45	0.52
1:C:799:THR:HG22	1:C:973:MET:HE2	1.91	0.52
1:C:898:GLN:NE2	2:D:181:ASN:HA	2.25	0.52
1:A:211:LEU:HD23	1:A:212:THR:HG23	1.92	0.51
1:A:426:PHE:CZ	1:A:438:ARG:HD2	2.44	0.51
3:G:49:ARG:HB2	3:E:28:ASN:HD21	1.74	0.51
1:C:778:PRO:HB2	1:C:919:ILE:HD11	1.92	0.51
2:B:123:PHE:HB3	2:B:150:ARG:HD3	1.92	0.51
1:A:375:THR:HA	1:A:588:PRO:HA	1.92	0.51
9:A:1107:PC1:O32	9:A:1110:PC1:H121	2.10	0.51
1:A:827:ARG:HE	1:A:934:ARG:NE	2.09	0.51
1:A:999:LYS:O	1:A:1003:ARG:HG3	2.11	0.51
2:D:232:LEU:HD13	2:D:239:PRO:HG3	1.93	0.51
1:A:659:HIS:HD2	1:A:661:SER:H	1.58	0.51
1:C:553:LEU:HB3	1:C:558:PHE:CD2	2.46	0.51
1:A:649:ASN:HD22	1:A:650:PRO:HD2	1.75	0.50
1:C:281:ILE:HD11	1:C:837:LEU:HD23	1.92	0.50
1:A:225:THR:HG21	1:A:233:ARG:HD2	1.93	0.50
3:G:33:PHE:CZ	8:G:101:CLR:H151	2.47	0.50
1:C:131:ALA:O	1:C:135:ILE:HG12	2.12	0.50
1:A:57:THR:HG22	1:A:59:ALA:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TYR:O	1:A:128:VAL:HG23	2.11	0.50
1:A:488:ASN:HD22	1:A:493:GLU:HG3	1.76	0.50
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.92	0.50
1:C:39:LEU:HD12	1:C:44:LEU:HD23	1.93	0.50
1:C:602:ALA:O	1:C:829:PRO:HD3	2.11	0.50
1:C:550:HIS:C	1:C:550:HIS:CD2	2.90	0.50
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.94	0.50
1:A:594:ASP:O	1:A:598:LYS:HG3	2.12	0.49
1:A:893:ASP:OD1	1:A:897:GLN:N	2.41	0.49
2:B:13:LYS:HA	2:B:16:ILE:HD12	1.93	0.49
1:C:304:LEU:HD21	1:C:310:TRP:HA	1.94	0.49
2:D:141:ASN:O	2:D:141:ASN:ND2	2.45	0.49
1:A:370:LYS:HE2	1:A:620:ILE:HD12	1.93	0.49
1:A:631:ASN:OD1	1:A:654:LYS:HD2	2.12	0.49
2:B:244:PRO:HG2	2:B:246:TYR:HE1	1.78	0.49
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.94	0.49
1:A:426:PHE:CD1	1:A:440:VAL:HG13	2.47	0.49
1:C:94:SER:HB2	1:C:133:VAL:HG13	1.94	0.49
1:C:488:ASN:CG	1:C:493:GLU:HG3	2.37	0.49
1:C:695:VAL:HG12	1:C:699:GLN:OE1	2.13	0.49
1:C:946:ILE:HD12	1:C:946:ILE:H	1.78	0.49
2:B:275:GLU:HB2	2:B:296:ASP:OD1	2.13	0.49
1:A:348:ASN:HA	1:A:744:LEU:HD12	1.95	0.49
1:A:893:ASP:OD2	1:A:897:GLN:HB2	2.13	0.49
2:B:27:ARG:HH12	2:B:35:ILE:HG21	1.77	0.49
2:B:132:GLU:HG3	2:B:133:LEU:HD12	1.94	0.49
1:A:482:GLN:NE2	1:A:501:LYS:HE3	2.28	0.48
2:D:138:GLU:O	2:D:146:ARG:NH2	2.46	0.48
2:B:217:ARG:HH21	2:B:273:ARG:HD2	1.76	0.48
1:A:426:PHE:CZ	1:A:450:LEU:HD22	2.49	0.48
1:A:287:ILE:O	1:A:291:VAL:HG13	2.14	0.48
2:B:27:ARG:NH1	2:B:35:ILE:HG21	2.29	0.48
1:C:764:ASN:OD1	1:C:818:GLU:HB3	2.13	0.48
2:D:69:GLN:HE22	2:D:184:LEU:HB3	1.79	0.48
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.49	0.48
1:A:300:PHE:CD1	1:A:317:LEU:HD12	2.49	0.48
2:B:94:ASP:HB3	2:B:97:SER:OG	2.13	0.48
1:C:93:PHE:CZ	1:C:322:VAL:HA	2.49	0.48
1:C:902:GLU:O	1:C:906:ILE:HG12	2.13	0.48
1:A:523:LEU:HD23	1:A:527:LEU:HB3	1.96	0.48
1:A:828:GLN:NE2	1:A:829:PRO:HD2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:LEU:HD12	2:B:46:LEU:HG	1.94	0.48
2:B:230:PHE:HE2	2:B:262:GLN:HE21	1.61	0.48
1:C:123:LEU:O	1:C:127:VAL:HG23	2.14	0.48
1:C:979:THR:O	8:C:1104:CLR:H41	2.14	0.48
1:A:306:LEU:HD12	1:A:880:ARG:HH12	1.78	0.47
2:B:108:PHE:HA	2:B:111:LYS:HE3	1.94	0.47
1:C:818:GLU:OE2	1:C:931:LYS:HG2	2.13	0.47
8:A:1109:CLR:H162	8:A:1109:CLR:H222	1.53	0.47
1:C:229:PRO:O	1:C:232:THR:HG22	2.14	0.47
2:D:183:VAL:HB	2:D:186:PHE:CB	2.44	0.47
2:B:117:GLN:HA	2:B:123:PHE:CD2	2.49	0.47
2:D:64:PHE:CE2	2:D:140:ASN:HA	2.49	0.47
1:A:154:PHE:HE1	1:A:341:ALA:HB1	1.78	0.47
1:A:221:SER:N	1:A:233:ARG:O	2.45	0.47
1:A:823:ASP:HB2	1:A:934:ARG:HD2	1.96	0.47
1:C:160:GLN:NE2	1:C:733:ASP:OD2	2.47	0.47
2:D:114:ASP:N	2:D:114:ASP:OD1	2.44	0.47
1:A:799:THR:O	1:A:803:ILE:HG13	2.14	0.47
1:C:375:THR:HA	1:C:588:PRO:HA	1.96	0.47
2:D:130:PRO:HB2	2:D:207:TYR:HB2	1.97	0.47
1:C:857:GLY:O	1:C:861:THR:HG23	2.15	0.47
2:D:214:THR:OG1	2:D:215:GLY:N	2.48	0.47
1:C:657:VAL:HA	1:C:682:VAL:O	2.15	0.47
1:C:669:GLU:N	1:C:669:GLU:OE1	2.47	0.47
1:A:220:ARG:NH1	1:A:235:ILE:O	2.47	0.47
3:G:49:ARG:HB2	3:E:28:ASN:ND2	2.30	0.47
1:C:918:SER:HB3	1:C:984:ALA:HB2	1.97	0.47
2:D:196:LEU:HG	2:D:199:TYR:CE2	2.50	0.47
1:C:565:ASP:H	1:C:570:ASN:HD22	1.61	0.46
2:D:35:ILE:HD12	8:D:401:CLR:H21	1.97	0.46
9:A:1110:PC1:H261	1:C:982:PHE:CZ	2.49	0.46
2:D:91:ARG:HA	2:D:302:LYS:O	2.14	0.46
1:A:184:VAL:HG11	1:A:193:PRO:HG2	1.97	0.46
1:A:277:ILE:HD11	1:A:765:LEU:HD13	1.96	0.46
9:A:1107:PC1:H2B2	9:A:1107:PC1:H281	1.43	0.46
1:A:893:ASP:OD2	1:A:897:GLN:NE2	2.46	0.46
1:C:909:PHE:CE2	1:C:972:ARG:HD2	2.51	0.46
1:A:663:LEU:HB3	1:A:690:GLN:HE22	1.80	0.46
1:C:858:GLY:HA3	1:C:915:PHE:CE1	2.51	0.46
1:A:612:ASP:OD1	1:A:613:HIS:N	2.44	0.46
2:B:91:ARG:HD3	2:B:94:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:TYR:O	3:E:27:ARG:HG3	2.16	0.46
2:D:209:LEU:O	2:D:237:GLY:HA3	2.16	0.46
1:C:482:GLN:NE2	1:C:501:LYS:HE2	2.29	0.46
1:C:1009:TRP:CZ2	2:D:34:LYS:HB3	2.51	0.46
1:A:479:ASN:OD1	1:A:479:ASN:N	2.49	0.46
1:A:691:LYS:O	1:A:695:VAL:HG23	2.16	0.46
1:A:803:ILE:HG12	1:A:916:PHE:CD1	2.51	0.46
9:A:1105:PC1:H2B1	9:A:1105:PC1:H3D2	1.97	0.46
10:A:1114:PCW:H171	10:A:1114:PCW:H372	1.98	0.46
1:C:558:PHE:CZ	1:C:571:PHE:HA	2.51	0.46
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.97	0.46
2:D:79:GLN:HE21	2:D:79:GLN:N	2.14	0.46
2:B:81:PRO:HD3	2:B:105:ILE:HD11	1.98	0.45
1:A:159:PRO:O	1:A:161:GLN:NE2	2.50	0.45
9:A:1110:PC1:H231	12:E:102:DMU:H12	1.98	0.45
2:B:214:THR:OG1	2:B:215:GLY:N	2.49	0.45
1:C:471:VAL:HG21	1:C:564:PHE:HB2	1.97	0.45
1:A:498:LEU:O	1:A:550:HIS:HA	2.16	0.45
1:A:929:ILE:HB	1:A:995:ASP:OD2	2.16	0.45
1:C:310:TRP:H	1:C:310:TRP:CD1	2.33	0.45
1:A:427:GLN:H	1:A:430:GLN:HE22	1.63	0.45
1:C:322:VAL:HG11	1:C:801:LEU:HD13	1.97	0.45
1:A:365:THR:HA	1:A:605:LYS:O	2.17	0.45
1:C:386:PHE:CZ	1:C:411:TRP:HB2	2.52	0.45
1:A:989:LEU:HD13	1:A:989:LEU:HA	1.85	0.45
2:B:273:ARG:HG2	2:B:298:LYS:HG2	1.99	0.45
1:C:154:PHE:HE1	1:C:341:ALA:HB1	1.81	0.45
1:C:590:ALA:O	1:C:593:PRO:HD2	2.17	0.45
2:D:52:GLY:O	2:D:56:VAL:HG23	2.17	0.45
2:D:132:GLU:CD	2:D:133:LEU:H	2.25	0.45
1:A:659:HIS:CD2	1:A:661:SER:H	2.34	0.45
1:C:56:LEU:HD11	1:C:182:ASP:CG	2.42	0.45
1:A:516:ILE:O	1:A:519:LYS:HG2	2.17	0.45
2:B:18:ASN:OD1	2:B:23:GLU:HB2	2.17	0.45
2:B:239:PRO:HG2	2:B:242:TYR:CD1	2.52	0.45
1:C:96:LEU:HD21	1:C:318:ILE:HA	1.98	0.45
1:C:454:GLU:OE2	1:C:459:SER:HA	2.17	0.45
2:D:187:LYS:HE2	2:D:244:PRO:HG3	1.99	0.45
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.99	0.45
1:A:553:LEU:HD12	1:A:553:LEU:H	1.82	0.44
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:MET:HG2	1:C:350:LEU:HD11	2.00	0.44
1:C:241:ASN:ND2	1:C:737:GLN:HE22	2.16	0.44
1:C:870:GLY:O	1:C:893:ASP:HB2	2.17	0.44
1:C:902:GLU:HB2	2:D:289:ASP:CG	2.42	0.44
1:A:638:ALA:HB1	1:A:643:ILE:O	2.18	0.44
1:A:977:LYS:HD2	1:A:980:TRP:CH2	2.52	0.44
3:G:49:ARG:HB3	3:E:24:GLU:CD	2.42	0.44
8:E:101:CLR:H162	8:E:101:CLR:H222	1.56	0.44
1:A:332:THR:HG21	1:A:768:SER:OG	2.17	0.44
1:A:559:PRO:HD2	1:A:562:PHE:HD1	1.82	0.44
10:B:401:PCW:H62	10:B:401:PCW:H41	1.71	0.44
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.76	0.44
1:A:553:LEU:HD23	1:A:572:PRO:HD2	1.99	0.44
1:A:861:THR:HG22	1:A:983:CYS:CB	2.48	0.44
1:A:889:ASN:HD22	1:A:901:TYR:H	1.66	0.44
2:B:136:ARG:NH2	2:B:147:LYS:O	2.50	0.44
2:B:179:LYS:HB3	2:B:179:LYS:HE3	1.77	0.44
1:C:365:THR:HA	1:C:605:LYS:O	2.17	0.44
1:A:996:GLU:CB	9:A:1107:PC1:H292	2.46	0.44
9:A:1107:PC1:H3B2	9:A:1107:PC1:H382	1.54	0.44
1:A:482:GLN:HE21	1:A:482:GLN:HB2	1.51	0.44
1:C:665:ASP:OD1	1:C:665:ASP:N	2.51	0.44
1:C:795:LEU:HD13	1:C:915:PHE:HB3	2.00	0.44
1:C:906:ILE:HD12	1:C:974:TYR:CZ	2.53	0.44
1:A:649:ASN:HD22	1:A:650:PRO:CD	2.30	0.44
9:A:1110:PC1:H2A1	9:A:1110:PC1:H2D1	1.83	0.44
2:B:90:PHE:HE2	2:B:169:TYR:O	2.01	0.44
2:B:153:LEU:H	2:B:153:LEU:HG	1.62	0.44
2:B:186:PHE:HD1	3:G:19:PHE:CE2	2.36	0.44
1:C:103:LEU:HD13	1:C:314:VAL:HG11	2.00	0.44
1:A:937:VAL:HG13	1:A:996:GLU:OE2	2.17	0.43
1:C:860:PHE:O	1:C:864:VAL:HG23	2.18	0.43
1:A:229:PRO:O	1:A:232:THR:HG22	2.18	0.43
1:A:514:ILE:HD12	1:A:523:LEU:HD21	2.00	0.43
2:B:121:MET:HG3	2:B:122:ILE:HD13	1.99	0.43
1:C:688:PRO:HB2	1:C:713:ASN:HB2	1.99	0.43
1:C:799:THR:O	1:C:803:ILE:HG13	2.18	0.43
2:B:96:GLN:HA	2:B:99:GLU:HG3	2.00	0.43
1:C:81:GLU:HB3	1:C:141:TYR:OH	2.18	0.43
1:C:656:CYS:HB3	1:C:678:HIS:CD2	2.52	0.43
1:A:451:LYS:O	1:A:455:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:PHE:O	1:A:864:VAL:HG23	2.19	0.43
1:A:978:PRO:C	1:A:980:TRP:H	2.26	0.43
2:B:74:PRO:HG2	2:B:284:GLY:H	1.83	0.43
1:C:329:LEU:HD12	1:C:329:LEU:HA	1.73	0.43
1:C:413:ALA:O	1:C:417:ILE:HG23	2.19	0.43
1:C:695:VAL:HG22	1:C:707:VAL:HG21	1.99	0.43
2:D:200:PRO:HG2	2:D:212:HIS:CE1	2.53	0.43
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.80	0.43
1:A:440:VAL:HG12	1:A:441:ALA:H	1.84	0.43
1:C:237:PHE:O	1:C:240:THR:HG23	2.18	0.43
1:C:301:ILE:HG13	1:C:302:LEU:N	2.34	0.43
1:A:395:THR:OG1	1:A:400:SER:HB3	2.17	0.43
1:A:778:PRO:HB2	1:A:919:ILE:HD11	2.00	0.43
2:B:88:ILE:HG23	2:B:101:TYR:CE2	2.54	0.43
2:B:152:ARG:H	2:B:155:TRP:HZ3	1.64	0.43
1:C:450:LEU:HD21	1:C:460:VAL:HG21	2.01	0.43
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.99	0.43
2:D:239:PRO:HG2	2:D:242:TYR:CD1	2.53	0.43
1:A:482:GLN:O	1:A:500:MET:HB2	2.19	0.43
1:A:966:GLY:HA3	10:A:1114:PCW:H332	2.01	0.43
1:A:1003:ARG:O	10:A:1111:PCW:H82	2.19	0.43
1:C:874:ILE:H	1:C:874:ILE:HG13	1.48	0.43
2:B:166:THR:HG21	2:B:170:LYS:CB	2.48	0.43
2:B:220:ASP:O	2:B:224:VAL:HG23	2.19	0.43
1:A:565:ASP:HB3	1:A:568:ASP:O	2.19	0.43
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.54	0.43
1:A:479:ASN:HB3	1:A:481:TYR:CZ	2.54	0.42
1:A:488:ASN:HB3	1:A:493:GLU:CD	2.43	0.42
1:A:821:GLU:CD	1:A:932:THR:HG22	2.44	0.42
2:B:196:LEU:HA	2:B:199:TYR:CE2	2.54	0.42
1:C:352:LYS:HD3	1:C:739:ALA:O	2.19	0.42
1:C:453:ILE:HG13	1:C:454:GLU:N	2.33	0.42
1:A:938:PHE:CG	9:A:1107:PC1:H342	2.55	0.42
1:C:270:LEU:HD23	1:C:270:LEU:H	1.84	0.42
1:A:865:ILE:HG12	1:A:980:TRP:CE2	2.54	0.42
1:C:39:LEU:HB3	1:C:43:GLU:HB2	2.00	0.42
1:C:84:LYS:HD2	1:C:84:LYS:HA	1.74	0.42
1:C:972:ARG:HA	1:C:972:ARG:HD3	1.63	0.42
9:A:1110:PC1:H261	1:C:982:PHE:HZ	1.84	0.42
2:B:87:GLU:HG2	2:B:298:LYS:HD2	2.00	0.42
2:B:270:THR:C	2:B:300:GLU:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ASN:OD1	1:C:429:ASN:N	2.52	0.42
1:C:803:ILE:HG12	1:C:916:PHE:CD1	2.54	0.42
2:D:155:TRP:CE3	2:D:232:LEU:HA	2.55	0.42
8:E:101:CLR:H211	8:E:101:CLR:H232	1.87	0.42
2:B:77:LEU:HB3	2:B:295:PHE:HD2	1.85	0.42
1:C:31:GLU:HG3	1:C:32:VAL:H	1.85	0.42
1:C:93:PHE:CE2	1:C:322:VAL:HG22	2.55	0.42
1:A:285:ILE:HA	1:A:288:ILE:HG22	2.01	0.42
1:C:924:TRP:O	1:C:928:VAL:HG23	2.19	0.42
2:D:64:PHE:HD1	2:D:249:LEU:HD12	1.85	0.42
2:B:157:GLY:HA3	2:B:230:PHE:CE1	2.55	0.42
3:G:36:LEU:HD23	3:G:36:LEU:HA	1.83	0.42
10:C:1111:PCW:H63	10:C:1111:PCW:H42	1.75	0.42
2:D:179:LYS:HE2	2:D:179:LYS:HB3	1.80	0.42
1:A:743:LEU:HD12	1:A:743:LEU:HA	1.86	0.42
1:C:116:GLU:HG2	1:C:117:GLU:H	1.85	0.42
1:C:319:GLY:HA3	1:C:797:THR:HG23	2.02	0.42
1:C:514:ILE:O	1:C:520:GLU:HA	2.19	0.42
2:D:17:TRP:CD1	2:D:17:TRP:C	2.98	0.42
2:D:77:LEU:HB3	2:D:295:PHE:HD2	1.85	0.42
1:A:37:HIS:HB3	1:A:235:ILE:HD11	2.00	0.42
1:A:101:ALA:O	1:A:105:PHE:HD2	2.02	0.42
1:A:208:ASN:HD22	1:A:240:THR:HG21	1.83	0.42
1:A:461:LYS:HB2	1:A:461:LYS:HE2	1.82	0.42
1:A:584:MET:HE3	1:A:584:MET:HB2	1.91	0.42
1:A:695:VAL:HG22	1:A:707:VAL:HG21	2.00	0.42
1:A:857:GLY:O	1:A:861:THR:HG23	2.20	0.42
1:C:818:GLU:CD	1:C:931:LYS:HG2	2.45	0.42
1:C:898:GLN:NE2	2:D:181:ASN:OD1	2.45	0.42
1:C:312:GLU:O	1:C:316:PHE:HD1	2.03	0.41
1:C:964:CYS:HB3	1:C:967:MET:HG3	2.02	0.41
1:A:277:ILE:HG21	1:A:337:LEU:HD21	2.01	0.41
1:A:346:ARG:HD3	1:A:346:ARG:HA	1.90	0.41
1:A:613:HIS:CD2	1:A:615:ILE:H	2.36	0.41
1:C:25:MET:HA	1:C:29:LYS:NZ	2.35	0.41
1:C:443:ASP:OD1	1:C:443:ASP:N	2.51	0.41
1:C:808:ASP:HA	1:C:811:PRO:HD2	2.01	0.41
2:D:125:ASP:OD1	2:D:150:ARG:HD2	2.19	0.41
1:A:667:THR:HG23	1:A:670:GLN:H	1.86	0.41
2:B:77:LEU:HD12	2:B:77:LEU:HA	1.82	0.41
1:C:514:ILE:HG22	1:C:516:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:VAL:HG23	1:A:734:VAL:HG11	2.02	0.41
1:C:893:ASP:OD1	1:C:897:GLN:N	2.51	0.41
1:C:918:SER:O	1:C:922:VAL:HG22	2.20	0.41
1:A:422:ASN:HD21	1:A:446:GLU:HA	1.85	0.41
1:A:632:GLU:HB3	1:A:636:ASP:HB2	2.01	0.41
1:A:938:PHE:HB3	9:A:1107:PC1:H321	2.01	0.41
3:E:33:PHE:CD2	8:E:101:CLR:H71	2.55	0.41
10:A:1112:PCW:H73	10:A:1112:PCW:H42	1.76	0.41
2:B:91:ARG:HG2	2:B:94:ASP:H	1.86	0.41
2:B:188:PRO:HA	2:B:282:ASN:HD21	1.84	0.41
1:C:516:ILE:HD13	1:C:516:ILE:HA	1.86	0.41
10:C:1105:PCW:H73	10:C:1105:PCW:H42	1.87	0.41
2:D:149:CYS:HB3	2:D:242:TYR:CE2	2.55	0.41
2:B:74:PRO:HD2	2:B:292:GLN:OE1	2.21	0.41
3:G:47:SER:CB	3:G:50:LEU:HB2	2.47	0.41
1:C:277:ILE:HD11	1:C:837:LEU:HD13	2.03	0.41
1:C:284:PHE:CE1	1:C:838:VAL:HG11	2.56	0.41
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.86	0.41
1:C:371:THR:HA	1:C:375:THR:OG1	2.21	0.41
1:C:402:VAL:HG21	1:C:404:PHE:CZ	2.56	0.41
3:E:17:ASP:HB2	3:E:18:PRO:HD3	2.01	0.41
1:A:237:PHE:O	1:A:240:THR:OG1	2.36	0.41
1:A:672:ASP:O	1:A:676:LYS:HB2	2.20	0.41
1:A:725:VAL:HG13	1:A:741:MET:HE3	2.02	0.41
1:A:872:LEU:H	1:A:894:SER:HB2	1.85	0.41
1:A:938:PHE:CE1	9:A:1107:PC1:H362	2.55	0.41
2:B:230:PHE:HE2	2:B:262:GLN:NE2	2.19	0.41
3:G:32:ILE:HD13	3:G:32:ILE:HA	1.90	0.41
1:C:255:GLY:O	1:C:258:THR:HG23	2.20	0.41
1:C:332:THR:O	1:C:336:CYS:HB2	2.21	0.41
1:C:729:ILE:HB	1:C:746:ASP:OD1	2.21	0.41
1:C:964:CYS:HA	3:E:31:LEU:HD21	2.01	0.41
10:C:1107:PCW:H42	10:C:1107:PCW:H63	1.65	0.41
2:D:27:ARG:NH1	8:D:401:CLR:O1	2.54	0.41
1:A:519:LYS:HG2	1:A:519:LYS:H	1.77	0.41
2:B:186:PHE:CZ	2:B:282:ASN:HB2	2.56	0.41
1:C:770:ALA:O	1:C:774:THR:HG23	2.21	0.41
1:C:781:THR:N	1:C:782:PRO:HD2	2.36	0.41
1:C:786:PHE:CE1	1:C:880:ARG:HD2	2.55	0.41
2:D:193:ASN:HB3	2:D:204:TYR:CE2	2.56	0.41
5:H:1:NAG:H61	5:H:2:NAG:O5	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:PRO:HB2	1:A:553:LEU:O	2.21	0.40
1:A:649:ASN:HB3	1:A:652:ASP:CG	2.46	0.40
1:C:402:VAL:HG21	1:C:404:PHE:CE1	2.56	0.40
1:C:861:THR:HG23	1:C:861:THR:H	1.60	0.40
2:D:129:VAL:O	2:D:241:GLN:NE2	2.54	0.40
1:A:285:ILE:HA	1:A:285:ILE:HD13	1.81	0.40
1:A:674:ILE:O	1:A:678:HIS:HB2	2.21	0.40
1:C:621:ALA:HB1	1:C:627:ILE:HG13	2.03	0.40
1:C:765:LEU:HD23	1:C:765:LEU:HA	1.92	0.40
10:C:1109:PCW:H62	10:C:1109:PCW:H41	1.83	0.40
2:B:196:LEU:HA	2:B:199:TYR:CZ	2.56	0.40
2:B:232:LEU:HD22	2:B:239:PRO:HG3	2.04	0.40
2:B:269:ASP:CG	2:B:302:LYS:HA	2.47	0.40
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.91	0.40
2:B:189:LYS:HD3	2:B:189:LYS:HA	1.93	0.40
1:C:480:LYS:HD2	1:C:506:ARG:CZ	2.52	0.40
2:D:210:PRO:HG2	2:D:279:TYR:HB2	2.04	0.40
1:C:1000:LEU:HD11	1:C:1004:ARG:HD2	2.04	0.40
2:D:299:ILE:H	2:D:299:ILE:HG12	1.70	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	993/1021 (97%)	948 (96%)	45 (4%)	0	100	100
1	C	993/1021 (97%)	947 (95%)	46 (5%)	0	100	100
2	B	289/303 (95%)	276 (96%)	13 (4%)	0	100	100
2	D	289/303 (95%)	274 (95%)	15 (5%)	0	100	100
3	E	31/65 (48%)	30 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	33/65 (51%)	31 (94%)	2 (6%)	0	100	100
All	All	2628/2778 (95%)	2506 (95%)	122 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/864 (98%)	765 (90%)	80 (10%)	8	26
1	C	845/864 (98%)	752 (89%)	93 (11%)	6	20
2	B	261/269 (97%)	232 (89%)	29 (11%)	6	20
2	D	261/269 (97%)	236 (90%)	25 (10%)	8	26
3	E	27/52 (52%)	25 (93%)	2 (7%)	13	38
3	G	29/52 (56%)	28 (97%)	1 (3%)	32	66
All	All	2268/2370 (96%)	2038 (90%)	230 (10%)	7	24

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	44	LEU
1	A	56	LEU
1	A	60	ARG
1	A	89	LEU
1	A	148	SER
1	A	158	VAL
1	A	161	GLN
1	A	165	ILE
1	A	170	LYS
1	A	182	ASP
1	A	190	ASP
1	A	214	GLU

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Mol	Chain	Res	Type
1	A	221	SER
1	A	262	ARG
1	A	275	THR
1	A	285	ILE
1	A	286	HIS
1	A	302	LEU
1	A	304	LEU
1	A	306	LEU
1	A	314	VAL
1	A	318	ILE
1	A	324	ASN
1	A	327	GLU
1	A	329	LEU
1	A	339	LEU
1	A	340	THR
1	A	357	VAL
1	A	371	THR
1	A	396	THR
1	A	397	GLU
1	A	431	GLU
1	A	435	ILE
1	A	440	VAL
1	A	450	LEU
1	A	455	LEU
1	A	456	CYS
1	A	460	VAL
1	A	468	THR
1	A	471	VAL
1	A	476	ASN
1	A	479	ASN
1	A	482	GLN
1	A	493	GLU
1	A	495	ARG
1	A	498	LEU
1	A	508	LEU
1	A	514	ILE
1	A	527	LEU
1	A	541	LEU
1	A	566	THR
1	A	584	MET
1	A	585	ILE
1	A	589	ARG

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Mol	Chain	Res	Type
1	A	592	VAL
1	A	599	CYS
1	A	610	THR
1	A	663	LEU
1	A	671	LEU
1	A	701	GLN
1	A	713	ASN
1	A	761	ILE
1	A	763	ASP
1	A	774	THR
1	A	787	ILE
1	A	821	GLU
1	A	852	MET
1	A	865	ILE
1	A	874	ILE
1	A	904	ARG
1	A	918	SER
1	A	932	THR
1	A	951	LEU
1	A	953	GLU
1	A	957	LEU
1	A	976	LEU
1	A	989	LEU
1	A	991	ILE
1	A	1002	ILE
2	B	18	ASN
2	B	32	TRP
2	B	34	LYS
2	B	40	VAL
2	B	64	PHE
2	B	72	VAL
2	B	79	GLN
2	B	103	VAL
2	B	104	SER
2	B	133	LEU
2	B	153	LEU
2	B	160	SER
2	B	166	THR
2	B	171	ASP
2	B	175	CYS
2	B	180	LEU
2	B	199	TYR

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Mol	Chain	Res	Type
2	B	202	MET
2	B	208	VAL
2	B	214	THR
2	B	217	ARG
2	B	227	MET
2	B	249	LEU
2	B	265	ASN
2	B	266	LEU
2	B	274	ILE
2	B	282	ASN
2	B	299	ILE
2	B	301	VAL
3	G	42	LEU
1	C	24	ASP
1	C	29	LYS
1	C	36	ASP
1	C	56	LEU
1	C	60	ARG
1	C	73	LEU
1	C	83	VAL
1	C	125	LEU
1	C	144	GLU
1	C	146	LYS
1	C	161	GLN
1	C	169	GLU
1	C	179	VAL
1	C	180	VAL
1	C	219	THR
1	C	220	ARG
1	C	241	ASN
1	C	258	THR
1	C	260	MET
1	C	262	ARG
1	C	265	THR
1	C	275	THR
1	C	286	HIS
1	C	287	ILE
1	C	288	ILE
1	C	302	LEU
1	C	304	LEU
1	C	305	ILE
1	C	306	LEU

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Mol	Chain	Res	Type
1	C	317	LEU
1	C	327	GLU
1	C	329	LEU
1	C	336	CYS
1	C	339	LEU
1	C	350	LEU
1	C	351	VAL
1	C	357	VAL
1	C	360	LEU
1	C	368	SER
1	C	412	LEU
1	C	425	VAL
1	C	429	ASN
1	C	433	LEU
1	C	440	VAL
1	C	443	ASP
1	C	450	LEU
1	C	455	LEU
1	C	491	THR
1	C	495	ARG
1	C	498	LEU
1	C	508	LEU
1	C	515	LEU
1	C	520	GLU
1	C	521	GLN
1	C	523	LEU
1	C	525	GLU
1	C	545	VAL
1	C	566	THR
1	C	567	ASP
1	C	568	ASP
1	C	589	ARG
1	C	634	VAL
1	C	645	VAL
1	C	646	SER
1	C	649	ASN
1	C	665	ASP
1	C	671	LEU
1	C	673	ASP
1	C	689	GLN
1	C	701	GLN
1	C	723	ILE

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Mol	Chain	Res	Type
1	C	753	THR
1	C	756	GLU
1	C	761	ILE
1	C	784	LEU
1	C	791	ILE
1	C	798	VAL
1	C	810	VAL
1	C	815	LEU
1	C	837	LEU
1	C	852	MET
1	C	861	THR
1	C	869	ASN
1	C	874	ILE
1	C	880	ARG
1	C	881	VAL
1	C	919	ILE
1	C	932	THR
1	C	934	ARG
1	C	957	LEU
1	C	971	LEU
1	C	976	LEU
1	C	1005	ARG
2	D	25	LEU
2	D	27	ARG
2	D	28	THR
2	D	32	TRP
2	D	45	CYS
2	D	57	MET
2	D	64	PHE
2	D	67	THR
2	D	72	VAL
2	D	78	THR
2	D	79	GLN
2	D	114	ASP
2	D	132	GLU
2	D	141	ASN
2	D	149	CYS
2	D	159	CYS
2	D	177	ILE
2	D	180	LEU
2	D	183	VAL
2	D	196	LEU

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Mol	Chain	Res	Type
2	D	222	GLU
2	D	256	GLN
2	D	266	LEU
2	D	282	ASN
2	D	299	ILE
3	E	26	VAL
3	E	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	122	ASN
1	A	161	GLN
1	A	208	ASN
1	A	241	ASN
1	A	324	ASN
1	A	377	ASN
1	A	383	HIS
1	A	389	GLN
1	A	398	ASN
1	A	399	GLN
1	A	427	GLN
1	A	430	GLN
1	A	432	ASN
1	A	476	ASN
1	A	482	GLN
1	A	517	HIS
1	A	521	GLN
1	A	533	ASN
1	A	550	HIS
1	A	613	HIS
1	A	649	ASN
1	A	659	HIS
1	A	690	GLN
1	A	776	ASN
1	A	828	GLN
1	A	854	GLN
1	A	889	ASN
1	A	897	GLN
1	A	903	GLN
1	A	939	GLN

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Mol	Chain	Res	Type
2	B	79	GLN
2	B	82	GLN
2	B	128	ASN
2	B	140	ASN
2	B	251	GLN
2	B	262	GLN
1	C	119	GLN
1	C	161	GLN
1	C	167	ASN
1	C	226	ASN
1	C	376	GLN
1	C	432	ASN
1	C	482	GLN
1	C	533	ASN
1	C	570	ASN
1	C	613	HIS
1	C	631	ASN
1	C	659	HIS
1	C	690	GLN
1	C	737	GLN
1	C	776	ASN
1	C	849	GLN
1	C	869	ASN
2	D	18	ASN
2	D	79	GLN
2	D	82	GLN
2	D	96	GLN
2	D	282	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 ⓘ

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	F	1	4,2	14,14,15	0.70	1 (7%)	17,19,21	0.78	0
4	NAG	F	2	4	14,14,15	0.29	0	17,19,21	0.58	0
4	BMA	F	3	4	11,11,12	0.82	0	15,15,17	0.77	0
4	MAN	F	4	4	11,11,12	1.20	1 (9%)	15,15,17	1.20	1 (6%)
4	MAN	F	5	4	11,11,12	1.30	2 (18%)	15,15,17	1.56	2 (13%)
4	MAN	F	6	4	11,11,12	0.86	1 (9%)	15,15,17	0.97	2 (13%)
5	NAG	H	1	2,5	14,14,15	0.31	0	17,19,21	0.70	0
5	NAG	H	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.79	1 (5%)
5	BMA	H	3	5	11,11,12	1.51	2 (18%)	15,15,17	1.00	2 (13%)
5	MAN	H	4	5	11,11,12	1.16	2 (18%)	15,15,17	1.18	2 (13%)
5	MAN	H	5	5	11,11,12	0.98	1 (9%)	15,15,17	1.24	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
6	NAG	I	2	6	14,14,15	0.48	0	17,19,21	0.75	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	4,2	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	1/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	MAN	H	5	5	-	2/2/19/22	0/1/1/1

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	MAN	C1-C2	2.96	1.59	1.52
5	H	3	BMA	C1-C2	2.79	1.58	1.52
5	H	5	MAN	C1-C2	2.74	1.58	1.52
5	H	4	MAN	C2-C3	2.64	1.56	1.52
5	H	3	BMA	C4-C5	2.53	1.58	1.53
5	H	4	MAN	C1-C2	2.51	1.58	1.52
4	F	4	MAN	O5-C5	2.49	1.48	1.43
4	F	1	NAG	O5-C1	-2.42	1.39	1.43
4	F	5	MAN	O5-C1	2.24	1.47	1.43
6	I	1	NAG	C1-C2	2.22	1.55	1.52
5	H	2	NAG	O5-C1	2.09	1.47	1.43
4	F	6	MAN	C1-C2	2.09	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5	MAN	C1-O5-C5	4.72	118.51	112.19
4	F	4	MAN	C1-O5-C5	3.73	117.19	112.19
5	H	5	MAN	C1-O5-C5	3.34	116.66	112.19
4	F	6	MAN	O2-C2-C3	-2.30	105.39	110.15
5	H	4	MAN	C1-C2-C3	2.18	112.82	109.64
5	H	4	MAN	C1-O5-C5	2.18	115.11	112.19
5	H	2	NAG	C1-O5-C5	2.15	115.07	112.19
5	H	5	MAN	O2-C2-C3	-2.12	105.76	110.15
5	H	3	BMA	O3-C3-C2	2.06	114.25	110.05
5	H	3	BMA	O2-C2-C3	-2.04	105.92	110.15
4	F	6	MAN	C1-O5-C5	2.01	114.87	112.19
4	F	5	MAN	O2-C2-C3	-2.01	106.00	110.15

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	3	BMA	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6

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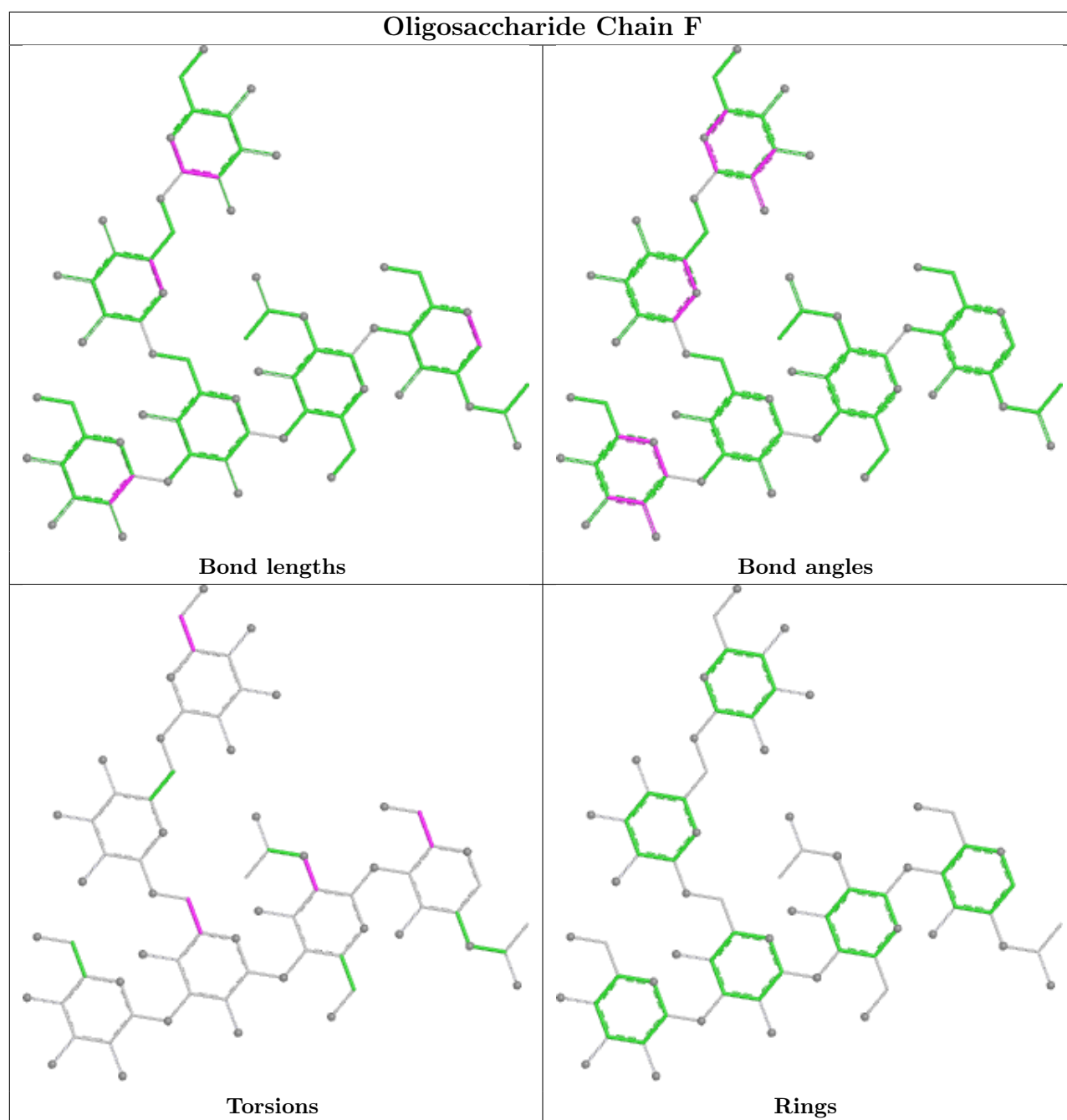
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
5	H	5	MAN	C4-C5-C6-O6
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	H	4	MAN	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6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

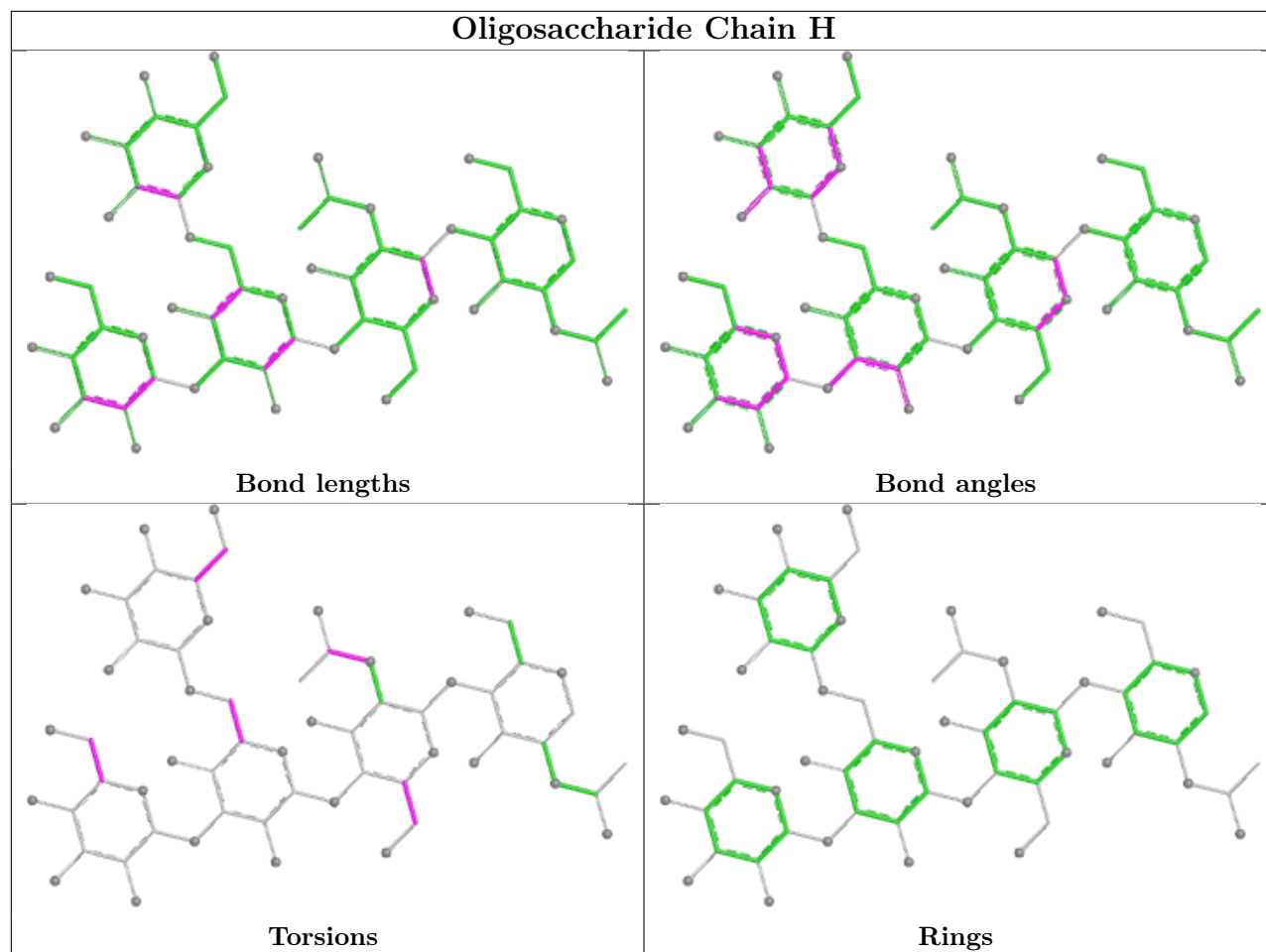
There are no ring outliers.

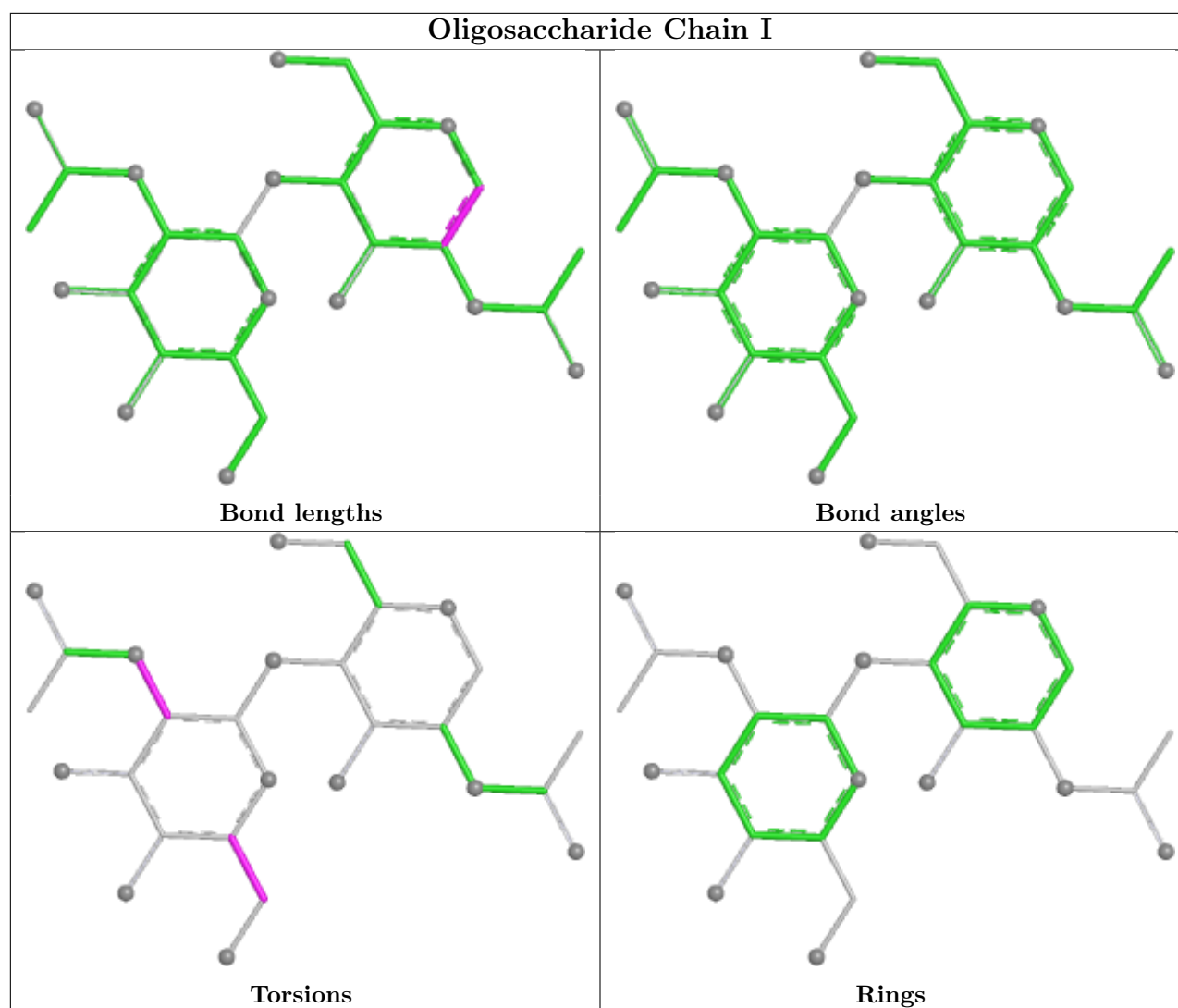
2 monomers are involved in 1 short contact:

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

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







5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	PCW	C	1107	-	21,21,53	0.92	0	27,29,61	1.15	3 (11%)
10	PCW	B	401	-	21,21,53	0.99	0	27,29,61	0.95	1 (3%)
11	NAG	D	402	2	14,14,15	0.46	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	A	1105	-	53,53,53	0.65	0	59,61,61	0.85	1 (1%)
10	PCW	A	1114	-	53,53,53	1.02	2 (3%)	59,61,61	0.85	0
10	PCW	A	1108	-	21,21,53	0.94	0	27,29,61	0.91	2 (7%)
10	PCW	A	1113	-	21,21,53	1.01	0	27,29,61	0.97	2 (7%)
10	PCW	A	1111	-	21,21,53	0.95	0	27,29,61	1.01	2 (7%)
10	PCW	C	1111	-	21,21,53	0.97	0	27,29,61	0.99	1 (3%)
10	PCW	C	1108	-	21,21,53	0.95	0	27,29,61	0.91	2 (7%)
8	CLR	E	101	-	31,31,31	1.14	2 (6%)	48,48,48	1.42	8 (16%)
9	PC1	A	1107	-	53,53,53	0.67	0	59,61,61	1.04	3 (5%)
10	PCW	C	1105	-	21,21,53	0.93	0	27,29,61	1.07	3 (11%)
8	CLR	A	1104	-	31,31,31	1.27	3 (9%)	48,48,48	1.47	11 (22%)
8	CLR	A	1109	-	31,31,31	1.21	2 (6%)	48,48,48	1.39	7 (14%)
10	PCW	A	1106	-	21,21,53	0.92	0	27,29,61	1.21	3 (11%)
10	PCW	A	1112	-	21,21,53	0.93	0	27,29,61	1.06	2 (7%)
8	CLR	D	401	-	31,31,31	1.24	2 (6%)	48,48,48	1.40	8 (16%)
12	DMU	E	102	-	34,34,34	0.65	0	45,45,45	1.23	4 (8%)
10	PCW	C	1106	-	21,21,53	0.98	0	27,29,61	0.84	1 (3%)
9	PC1	A	1110	-	53,53,53	0.65	0	59,61,61	1.01	3 (5%)
10	PCW	C	1109	-	21,21,53	0.91	0	27,29,61	0.90	2 (7%)
8	CLR	C	1104	-	31,31,31	1.16	1 (3%)	48,48,48	1.41	11 (22%)
8	CLR	G	101	-	31,31,31	1.19	2 (6%)	48,48,48	1.38	7 (14%)
10	PCW	C	1110	-	21,21,53	0.90	0	27,29,61	1.10	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	C	1107	-	-	8/23/23/57	-
10	PCW	B	401	-	-	10/23/23/57	-
11	NAG	D	402	2	-	0/6/23/26	0/1/1/1
9	PC1	A	1105	-	-	6/57/57/57	-
10	PCW	A	1114	-	-	22/57/57/57	-
10	PCW	A	1108	-	-	8/23/23/57	-
10	PCW	A	1113	-	-	10/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	A	1111	-	-	11/23/23/57	-
10	PCW	C	1111	-	-	5/23/23/57	-
10	PCW	C	1108	-	-	5/23/23/57	-
8	CLR	E	101	-	-	7/10/68/68	0/4/4/4
9	PC1	A	1107	-	-	11/57/57/57	-
10	PCW	C	1105	-	-	4/23/23/57	-
8	CLR	A	1104	-	-	0/10/68/68	0/4/4/4
8	CLR	A	1109	-	-	6/10/68/68	0/4/4/4
10	PCW	A	1106	-	-	8/23/23/57	-
10	PCW	A	1112	-	-	8/23/23/57	-
8	CLR	D	401	-	-	2/10/68/68	0/4/4/4
12	DMU	E	102	-	-	4/19/59/59	0/2/2/2
10	PCW	C	1106	-	-	10/23/23/57	-
9	PC1	A	1110	-	-	11/57/57/57	-
10	PCW	C	1109	-	-	3/23/23/57	-
8	CLR	C	1104	-	-	3/10/68/68	0/4/4/4
8	CLR	G	101	-	-	6/10/68/68	0/4/4/4
10	PCW	C	1110	-	-	8/23/23/57	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1114	PCW	C20-C19	4.06	1.54	1.31
10	A	1114	PCW	C40-C39	3.91	1.53	1.31
8	A	1104	CLR	C16-C17	3.08	1.60	1.54
8	D	401	CLR	C16-C17	3.07	1.60	1.54
8	G	101	CLR	C16-C17	2.97	1.60	1.54
8	E	101	CLR	C16-C17	2.86	1.60	1.54
8	C	1104	CLR	C16-C17	2.83	1.60	1.54
8	A	1109	CLR	C16-C17	2.68	1.59	1.54
8	A	1104	CLR	C12-C13	2.53	1.58	1.54
8	G	101	CLR	C16-C15	2.17	1.60	1.54
8	E	101	CLR	C16-C15	2.17	1.59	1.54
8	A	1109	CLR	C16-C15	2.14	1.59	1.54
8	A	1104	CLR	C13-C17	2.08	1.58	1.55
8	D	401	CLR	C7-C6	2.04	1.54	1.50

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1106	PCW	C2-O2-C31	-3.91	110.94	117.85
10	A	1112	PCW	C2-O2-C31	-3.60	111.49	117.85
9	A	1107	PC1	C3-O31-C31	-3.39	104.72	117.12
12	E	102	DMU	O1-C9-C11	3.27	114.55	106.44
10	A	1111	PCW	C2-O2-C31	-3.27	112.07	117.85
10	C	1110	PCW	C2-O2-C31	-3.25	112.10	117.85
10	C	1107	PCW	C3-O3-C11	-3.20	109.19	117.08
8	A	1104	CLR	C22-C20-C17	-3.13	103.84	110.33
10	C	1107	PCW	C2-O2-C31	-3.12	112.33	117.85
8	D	401	CLR	C22-C20-C17	-3.00	104.11	110.33
10	A	1113	PCW	C2-O2-C31	-2.95	112.63	117.85
8	E	101	CLR	C22-C20-C17	-2.94	104.24	110.33
12	E	102	DMU	O16-C18-C19	2.91	119.23	109.37
8	C	1104	CLR	C22-C20-C17	-2.89	104.34	110.33
10	B	401	PCW	C2-O2-C31	-2.85	112.81	117.85
10	C	1105	PCW	C3-O3-C11	-2.85	110.06	117.08
8	A	1109	CLR	C22-C20-C17	-2.78	104.56	110.33
8	G	101	CLR	C22-C20-C17	-2.78	104.56	110.33
9	A	1107	PC1	C2-O21-C21	2.77	124.44	117.80
10	C	1105	PCW	C2-O2-C31	-2.76	112.96	117.85
12	E	102	DMU	C18-O16-C6	-2.75	108.98	113.68
10	A	1108	PCW	C2-O2-C31	-2.71	113.06	117.85
10	C	1108	PCW	C2-O2-C31	-2.71	113.06	117.85
8	A	1104	CLR	C15-C14-C13	2.71	107.02	103.84
10	C	1110	PCW	C3-O3-C11	-2.60	110.66	117.08
9	A	1110	PC1	C2-O21-C21	2.55	123.89	117.80
9	A	1110	PC1	C34-C33-C32	-2.55	103.77	113.13
8	A	1104	CLR	C18-C13-C12	2.46	114.22	110.61
10	C	1111	PCW	C3-O3-C11	-2.45	111.03	117.08
9	A	1105	PC1	C3-C2-C1	-2.44	106.09	111.78
8	A	1104	CLR	C16-C17-C20	-2.41	108.53	112.18
8	A	1109	CLR	C19-C10-C9	-2.40	108.97	111.66
9	A	1107	PC1	C36-C35-C34	-2.40	102.26	114.37
8	E	101	CLR	C7-C8-C14	-2.39	107.54	110.93
8	G	101	CLR	C7-C8-C14	-2.38	107.56	110.93
8	A	1104	CLR	C7-C8-C14	-2.37	107.57	110.93
8	C	1104	CLR	C7-C8-C14	-2.37	107.58	110.93
8	D	401	CLR	C7-C8-C14	-2.37	107.58	110.93
8	A	1109	CLR	C7-C8-C14	-2.37	107.58	110.93
8	A	1109	CLR	C18-C13-C12	2.34	114.06	110.61
8	E	101	CLR	C18-C13-C12	2.34	114.05	110.61
9	A	1110	PC1	C3-O31-C31	-2.34	108.58	117.12
12	E	102	DMU	C25-C22-C19	-2.33	102.58	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	CLR	C18-C13-C12	2.33	114.04	110.61
8	A	1104	CLR	C21-C20-C17	2.33	116.38	112.88
8	G	101	CLR	C18-C13-C12	2.30	113.99	110.61
8	E	101	CLR	C19-C10-C9	-2.29	109.09	111.66
8	C	1104	CLR	C18-C13-C12	2.28	113.97	110.61
8	D	401	CLR	C15-C14-C13	2.27	106.51	103.84
10	A	1106	PCW	C3-O3-C11	-2.27	111.49	117.08
10	A	1113	PCW	O2-C31-C32	2.24	115.08	111.09
10	A	1112	PCW	C3-O3-C11	-2.21	111.64	117.08
10	C	1109	PCW	C2-O2-C31	-2.20	113.95	117.85
8	A	1104	CLR	C3-C4-C5	2.20	115.56	112.05
8	D	401	CLR	C16-C17-C20	-2.20	108.86	112.18
8	C	1104	CLR	C16-C17-C20	-2.19	108.86	112.18
8	C	1104	CLR	C15-C14-C13	2.19	106.42	103.84
8	E	101	CLR	C13-C17-C20	-2.19	116.12	119.50
8	D	401	CLR	C21-C20-C17	2.19	116.17	112.88
8	G	101	CLR	C11-C12-C13	-2.18	109.06	112.74
10	A	1106	PCW	O2-C31-C32	2.17	114.96	111.09
10	A	1111	PCW	O2-C31-C32	2.17	114.95	111.09
8	C	1104	CLR	C21-C20-C17	2.16	116.13	112.88
8	A	1104	CLR	C2-C3-C4	-2.15	107.26	110.29
10	C	1106	PCW	O2-C31-C32	2.15	114.93	111.09
8	G	101	CLR	C19-C10-C9	-2.15	109.24	111.66
8	A	1109	CLR	C13-C17-C20	-2.13	116.20	119.50
10	C	1107	PCW	O2-C31-C32	2.13	114.89	111.09
8	E	101	CLR	C10-C5-C6	2.12	126.03	122.93
8	A	1104	CLR	C24-C23-C22	-2.12	103.80	113.28
8	D	401	CLR	C24-C23-C22	-2.11	103.83	113.28
8	G	101	CLR	C3-C4-C5	2.10	115.40	112.05
8	A	1109	CLR	C11-C12-C13	-2.10	109.20	112.74
8	C	1104	CLR	C3-C4-C5	2.10	115.39	112.05
8	D	401	CLR	C3-C4-C5	2.09	115.38	112.05
10	C	1109	PCW	O2-C31-C32	2.09	114.81	111.09
8	C	1104	CLR	C24-C23-C22	-2.09	103.92	113.28
8	G	101	CLR	C24-C23-C22	-2.09	103.93	113.28
8	E	101	CLR	C17-C13-C14	-2.08	97.71	100.10
8	A	1104	CLR	C19-C10-C9	-2.06	109.34	111.66
10	C	1105	PCW	O2-C31-C32	2.05	114.75	111.09
8	E	101	CLR	C24-C23-C22	-2.04	104.14	113.28
10	C	1110	PCW	O2-C31-C32	2.04	114.72	111.09
8	C	1104	CLR	C19-C10-C9	-2.03	109.38	111.66
8	A	1109	CLR	C24-C23-C22	-2.03	104.16	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1104	CLR	C13-C17-C20	-2.03	116.36	119.50
8	C	1104	CLR	C10-C5-C6	2.02	125.88	122.93
10	A	1108	PCW	O2-C31-C32	2.02	114.69	111.09
10	C	1108	PCW	O2-C31-C32	2.02	114.68	111.09
8	A	1104	CLR	C10-C5-C6	2.00	125.86	122.93

There are no chirality outliers.

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	101	CLR	C13-C17-C20-C21
9	A	1105	PC1	C11-O13-P-O14
9	A	1107	PC1	C1-O11-P-O12
9	A	1110	PC1	C11-O13-P-O14
10	A	1106	PCW	O4P-C4-C5-N
10	A	1106	PCW	C1-O3P-P-O2P
10	A	1106	PCW	C1-O3P-P-O4P
10	A	1106	PCW	C4-O4P-P-O3P
10	A	1111	PCW	C5-C4-O4P-P
10	A	1111	PCW	C1-O3P-P-O1P
10	A	1111	PCW	C1-O3P-P-O4P
10	A	1111	PCW	C4-O4P-P-O3P
10	A	1112	PCW	O4P-C4-C5-N
10	A	1112	PCW	C1-O3P-P-O2P
10	A	1112	PCW	C4-O4P-P-O1P
10	A	1112	PCW	C4-O4P-P-O3P
10	A	1113	PCW	C4-O4P-P-O2P
10	A	1113	PCW	C4-O4P-P-O3P
10	A	1114	PCW	O4P-C4-C5-N
10	A	1114	PCW	C1-O3P-P-O2P
10	A	1114	PCW	C1-O3P-P-O4P
10	A	1114	PCW	C4-O4P-P-O1P
10	A	1114	PCW	C4-O4P-P-O2P
10	A	1114	PCW	C4-O4P-P-O3P
10	B	401	PCW	O4P-C4-C5-N
10	B	401	PCW	C4-O4P-P-O3P
10	C	1105	PCW	C1-O3P-P-O2P
10	C	1106	PCW	C32-C31-O2-C2
10	C	1106	PCW	C4-O4P-P-O1P
10	C	1106	PCW	C4-O4P-P-O3P
10	C	1107	PCW	O4P-C4-C5-N
10	C	1107	PCW	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
10	C	1107	PCW	C4-O4P-P-O2P
10	C	1107	PCW	C4-O4P-P-O3P
10	C	1108	PCW	C1-O3P-P-O4P
10	C	1108	PCW	C4-O4P-P-O1P
10	C	1108	PCW	C4-O4P-P-O3P
10	C	1109	PCW	C1-O3P-P-O4P
10	C	1110	PCW	C4-O4P-P-O2P
10	C	1110	PCW	C4-O4P-P-O3P
10	C	1111	PCW	C1-O3P-P-O2P
10	C	1111	PCW	C1-O3P-P-O4P
10	A	1112	PCW	C32-C31-O2-C2
10	C	1105	PCW	C32-C31-O2-C2
10	C	1106	PCW	O31-C31-O2-C2
8	A	1109	CLR	C13-C17-C20-C21
8	A	1109	CLR	C13-C17-C20-C22
10	A	1108	PCW	C32-C31-O2-C2
10	A	1108	PCW	C12-C11-O3-C3
10	A	1113	PCW	C32-C31-O2-C2
10	C	1107	PCW	C32-C31-O2-C2
8	A	1109	CLR	C16-C17-C20-C21
8	E	101	CLR	C16-C17-C20-C21
8	E	101	CLR	C13-C17-C20-C22
9	A	1107	PC1	C28-C29-C2A-C2B
9	A	1107	PC1	C38-C39-C3A-C3B
9	A	1110	PC1	C38-C39-C3A-C3B
10	C	1105	PCW	O31-C31-O2-C2
9	A	1110	PC1	C28-C29-C2A-C2B
10	A	1112	PCW	O31-C31-O2-C2
10	A	1108	PCW	O11-C11-O3-C3
8	E	101	CLR	C16-C17-C20-C22
8	G	101	CLR	C21-C20-C22-C23
10	A	1108	PCW	O31-C31-O2-C2
10	C	1107	PCW	O31-C31-O2-C2
10	A	1113	PCW	O31-C31-O2-C2
8	G	101	CLR	C17-C20-C22-C23
10	B	401	PCW	C32-C31-O2-C2
8	G	101	CLR	C22-C23-C24-C25
9	A	1105	PC1	C37-C38-C39-C3A
8	D	401	CLR	C20-C22-C23-C24
8	D	401	CLR	C22-C23-C24-C25
10	A	1112	PCW	C12-C11-O3-C3
8	C	1104	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
10	A	1111	PCW	C12-C11-O3-C3
8	A	1109	CLR	C23-C24-C25-C26
8	G	101	CLR	C23-C24-C25-C27
9	A	1107	PC1	C27-C28-C29-C2A
10	A	1114	PCW	C32-C31-O2-C2
10	C	1106	PCW	C12-C11-O3-C3
8	A	1109	CLR	C23-C24-C25-C27
8	G	101	CLR	C23-C24-C25-C26
9	A	1110	PC1	C37-C38-C39-C3A
9	A	1105	PC1	C39-C3A-C3B-C3C
10	A	1114	PCW	C31-C32-C33-C34
10	A	1114	PCW	O31-C31-O2-C2
9	A	1110	PC1	C39-C3A-C3B-C3C
10	A	1112	PCW	O11-C11-O3-C3
12	E	102	DMU	O6-C11-C9-O1
10	A	1114	PCW	C12-C13-C14-C15
12	E	102	DMU	C4-C3-O7-C10
9	A	1107	PC1	C37-C38-C39-C3A
8	A	1109	CLR	C16-C17-C20-C22
10	A	1108	PCW	O3P-C1-C2-C3
10	A	1113	PCW	O3P-C1-C2-C3
10	C	1107	PCW	O3P-C1-C2-C3
10	A	1111	PCW	O11-C11-O3-C3
10	A	1113	PCW	C12-C11-O3-C3
12	E	102	DMU	C2-C3-O7-C10
10	C	1106	PCW	C3-C2-O2-C31
10	A	1106	PCW	O3P-C1-C2-O2
10	B	401	PCW	O31-C31-O2-C2
9	A	1110	PC1	C29-C2A-C2B-C2C
10	A	1114	PCW	O2-C2-C3-O3
10	C	1106	PCW	O11-C11-O3-C3
8	E	101	CLR	C20-C22-C23-C24
10	A	1114	PCW	C1-C2-C3-O3
10	C	1110	PCW	C1-C2-C3-O3
8	E	101	CLR	C23-C24-C25-C26
10	A	1113	PCW	O3P-C1-C2-O2
10	C	1107	PCW	O3P-C1-C2-O2
10	C	1110	PCW	C2-C1-O3P-P
9	A	1107	PC1	C29-C2A-C2B-C2C
10	A	1114	PCW	C14-C15-C16-C17
9	A	1107	PC1	C39-C3A-C3B-C3C
10	C	1106	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	A	1114	PCW	C35-C36-C37-C38
10	B	401	PCW	O3P-C1-C2-O2
10	B	401	PCW	C5-C4-O4P-P
9	A	1105	PC1	O13-C11-C12-N
9	A	1107	PC1	O13-C11-C12-N
9	A	1110	PC1	O13-C11-C12-N
10	A	1108	PCW	O4P-C4-C5-N
10	A	1111	PCW	O4P-C4-C5-N
10	A	1113	PCW	O4P-C4-C5-N
10	C	1105	PCW	O4P-C4-C5-N
10	C	1106	PCW	O4P-C4-C5-N
10	C	1108	PCW	O4P-C4-C5-N
10	C	1109	PCW	O4P-C4-C5-N
10	C	1110	PCW	O4P-C4-C5-N
10	C	1111	PCW	O4P-C4-C5-N
8	G	101	CLR	C20-C22-C23-C24
10	B	401	PCW	C12-C11-O3-C3
8	E	101	CLR	C23-C24-C25-C27
10	C	1106	PCW	O3P-C1-C2-O2
10	A	1114	PCW	C22-C23-C24-C25
10	C	1110	PCW	O2-C2-C3-O3
9	A	1105	PC1	C27-C28-C29-C2A
10	A	1113	PCW	O11-C11-O3-C3
9	A	1107	PC1	C11-O13-P-O14
10	A	1106	PCW	C1-O3P-P-O1P
10	A	1106	PCW	C4-O4P-P-O2P
10	A	1108	PCW	C4-O4P-P-O2P
10	A	1111	PCW	C1-O3P-P-O2P
10	A	1111	PCW	C4-O4P-P-O2P
10	A	1113	PCW	C4-O4P-P-O1P
10	A	1114	PCW	C1-O3P-P-O1P
10	B	401	PCW	C4-O4P-P-O2P
10	C	1108	PCW	C1-O3P-P-O2P
10	C	1109	PCW	C1-O3P-P-O2P
10	C	1110	PCW	C1-O3P-P-O2P
10	C	1110	PCW	C4-O4P-P-O1P
10	C	1111	PCW	C1-O3P-P-O1P
10	C	1111	PCW	C4-O4P-P-O2P
10	A	1114	PCW	O3P-C1-C2-C3
10	A	1108	PCW	O3P-C1-C2-O2
10	A	1114	PCW	C37-C38-C39-C40
10	A	1114	PCW	O11-C11-O3-C3

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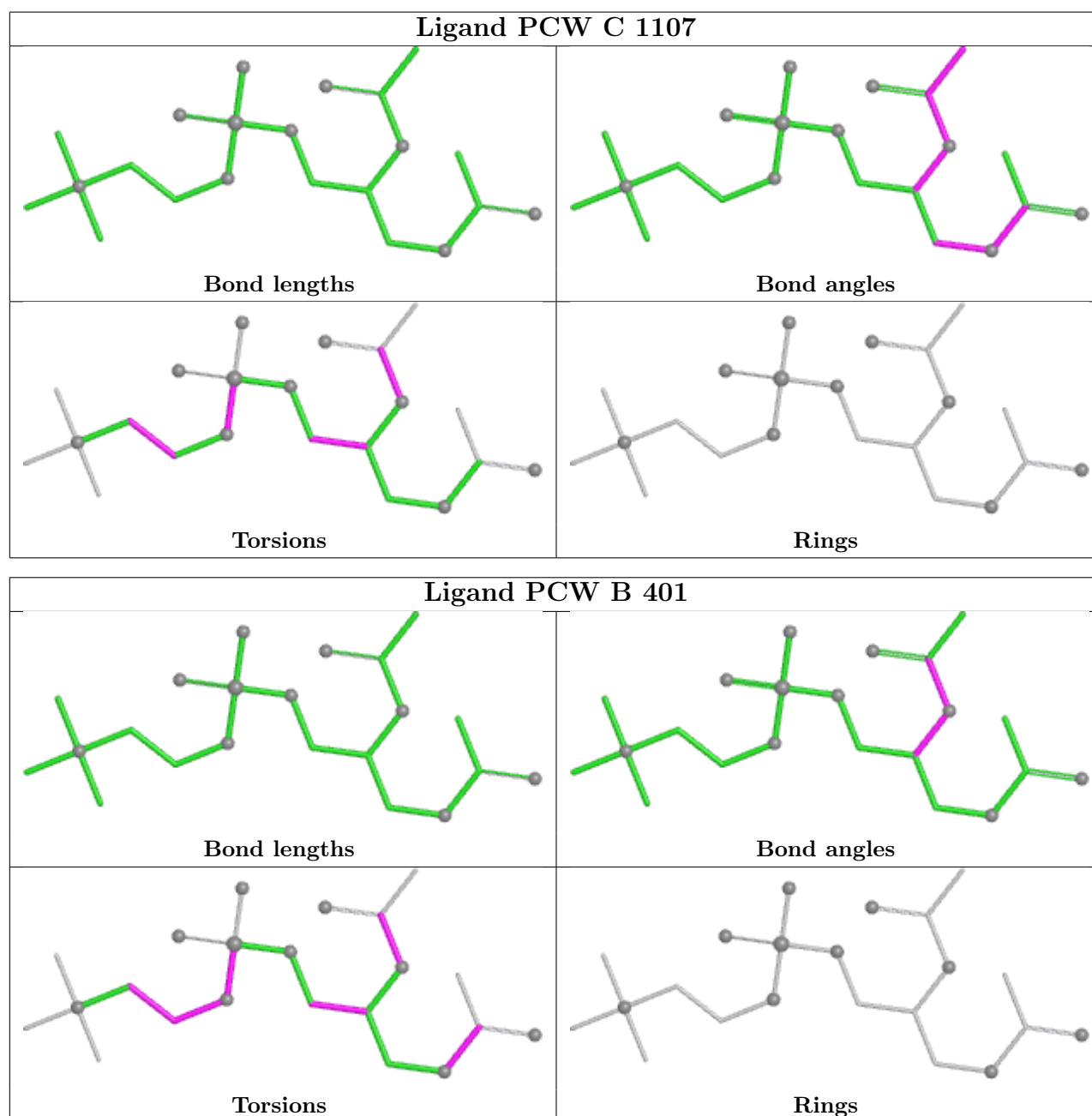
Mol	Chain	Res	Type	Atoms
10	A	1111	PCW	O3P-C1-C2-O2
9	A	1110	PC1	C2-C1-O11-P
8	C	1104	CLR	C22-C23-C24-C25
10	B	401	PCW	O11-C11-O3-C3
9	A	1107	PC1	O31-C31-C32-C33
10	A	1114	PCW	O2-C31-C32-C33
10	A	1106	PCW	O3P-C1-C2-C3
10	A	1114	PCW	C12-C11-O3-C3
9	A	1107	PC1	C3-C2-O21-C21
9	A	1110	PC1	C3-C2-O21-C21
9	A	1105	PC1	O31-C31-C32-C33
10	A	1111	PCW	O3P-C1-C2-C3
10	B	401	PCW	O3P-C1-C2-C3
8	C	1104	CLR	C23-C24-C25-C26
9	A	1110	PC1	O31-C31-C32-C33
12	E	102	DMU	C5-C10-O7-C3
9	A	1110	PC1	O32-C31-C32-C33
10	A	1114	PCW	O3-C11-C12-C13

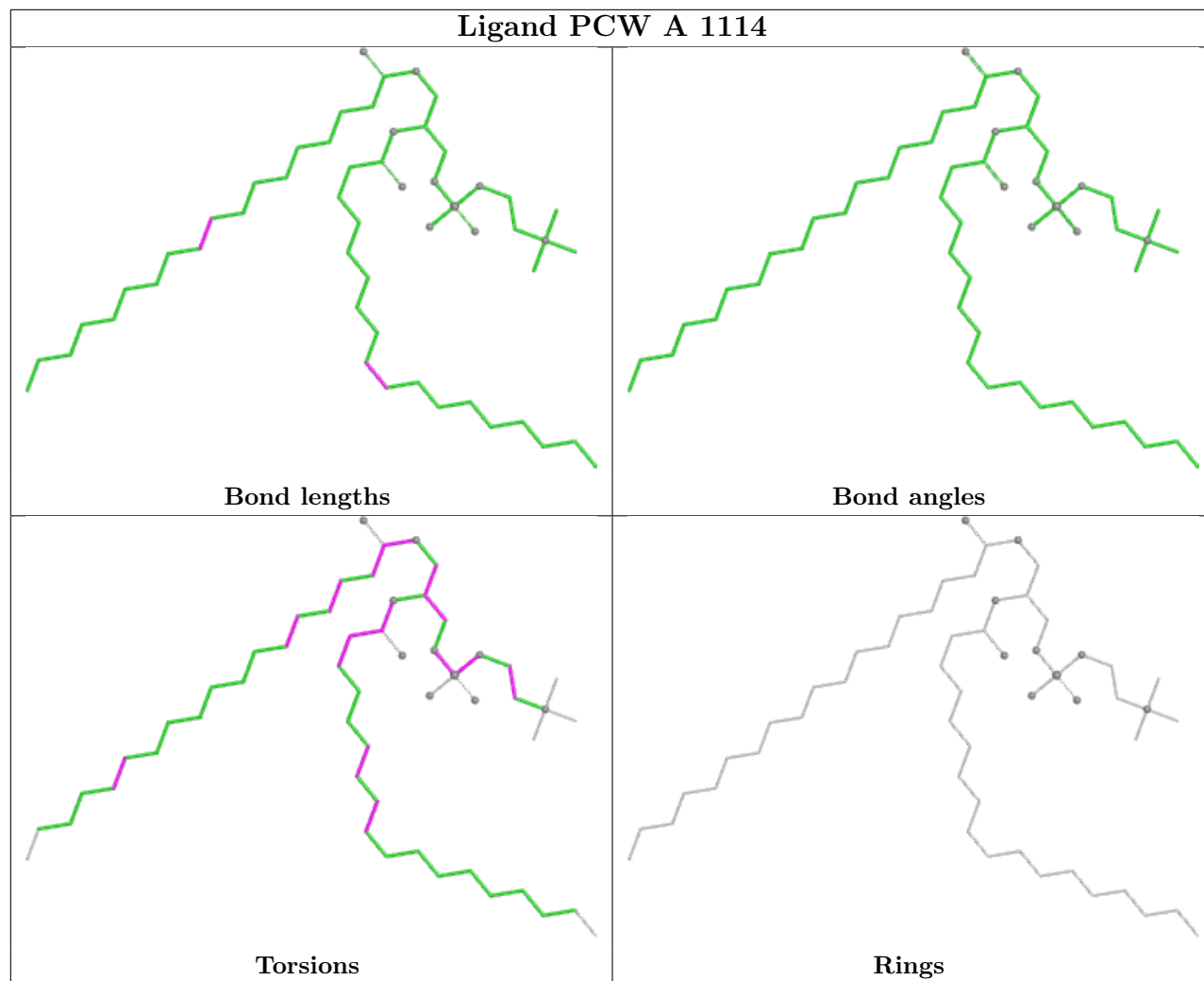
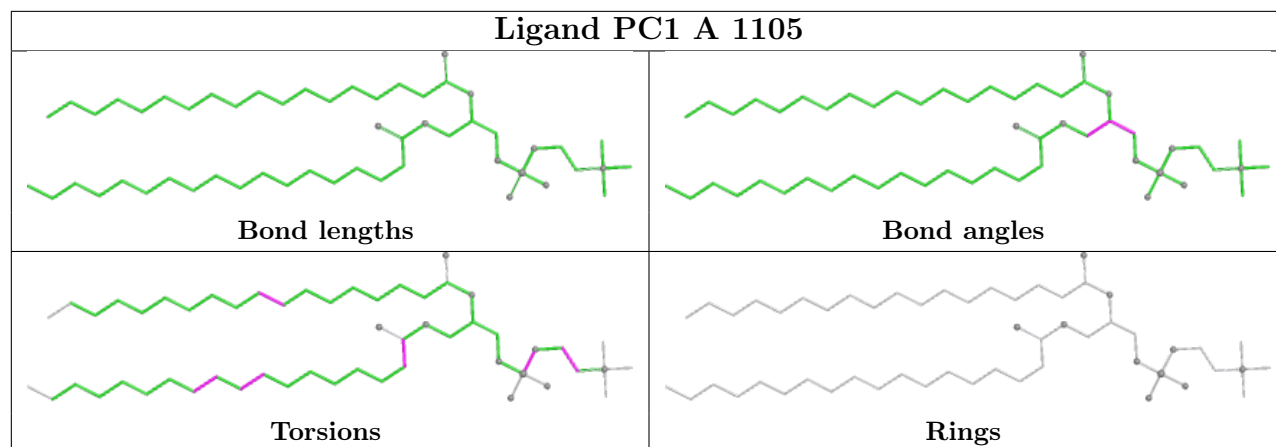
There are no ring outliers.

18 monomers are involved in 49 short contacts:

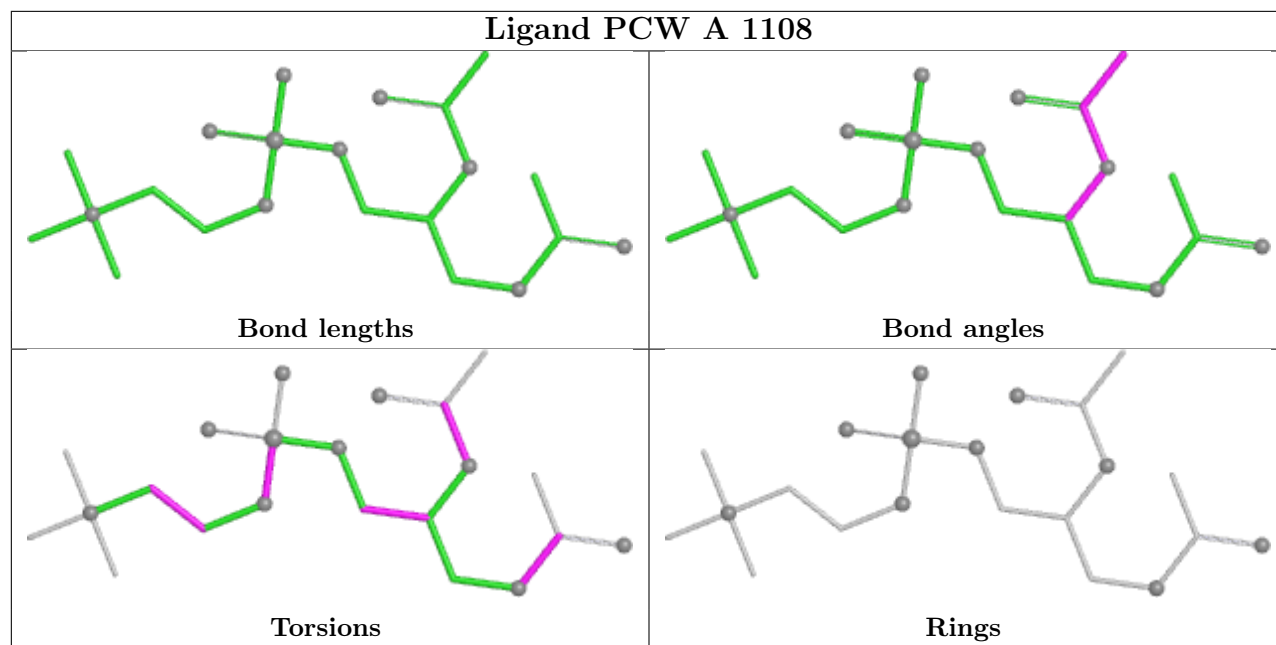
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1107	PCW	2	0
10	B	401	PCW	2	0
9	A	1105	PC1	1	0
10	A	1114	PCW	4	0
10	A	1111	PCW	2	0
10	C	1111	PCW	1	0
8	E	101	CLR	3	0
9	A	1107	PC1	13	0
10	C	1105	PCW	1	0
8	A	1104	CLR	1	0
8	A	1109	CLR	1	0
10	A	1112	PCW	2	0
8	D	401	CLR	3	0
12	E	102	DMU	3	0
9	A	1110	PC1	8	0
10	C	1109	PCW	2	0
8	C	1104	CLR	2	0
8	G	101	CLR	3	0

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

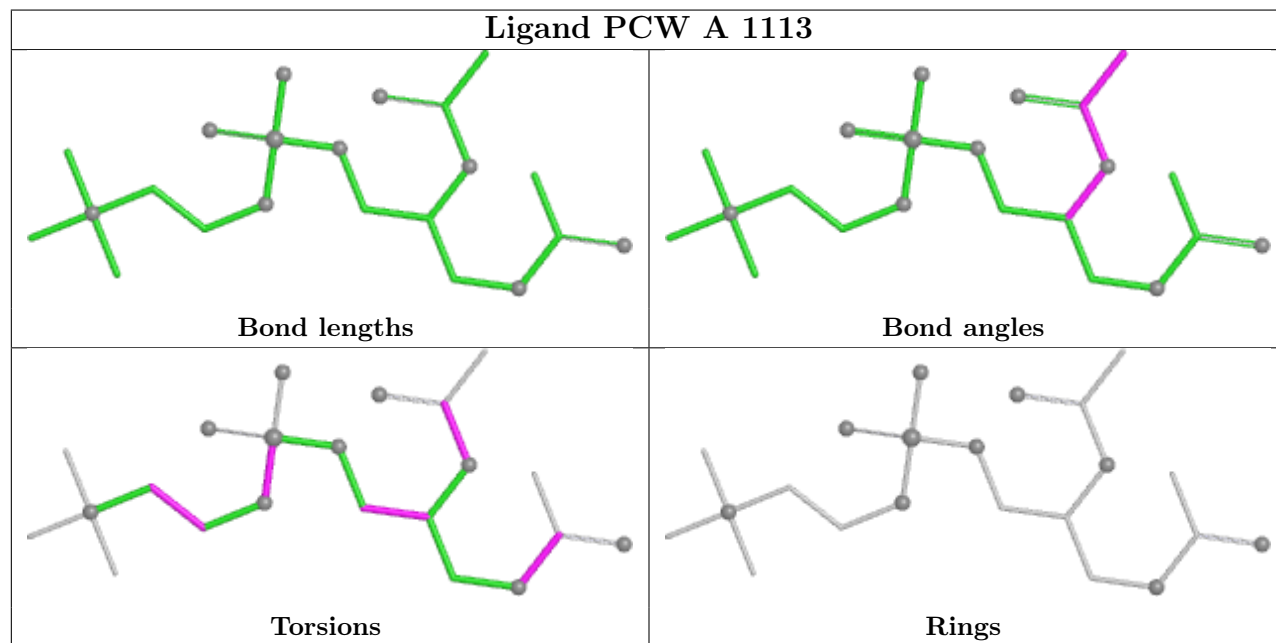


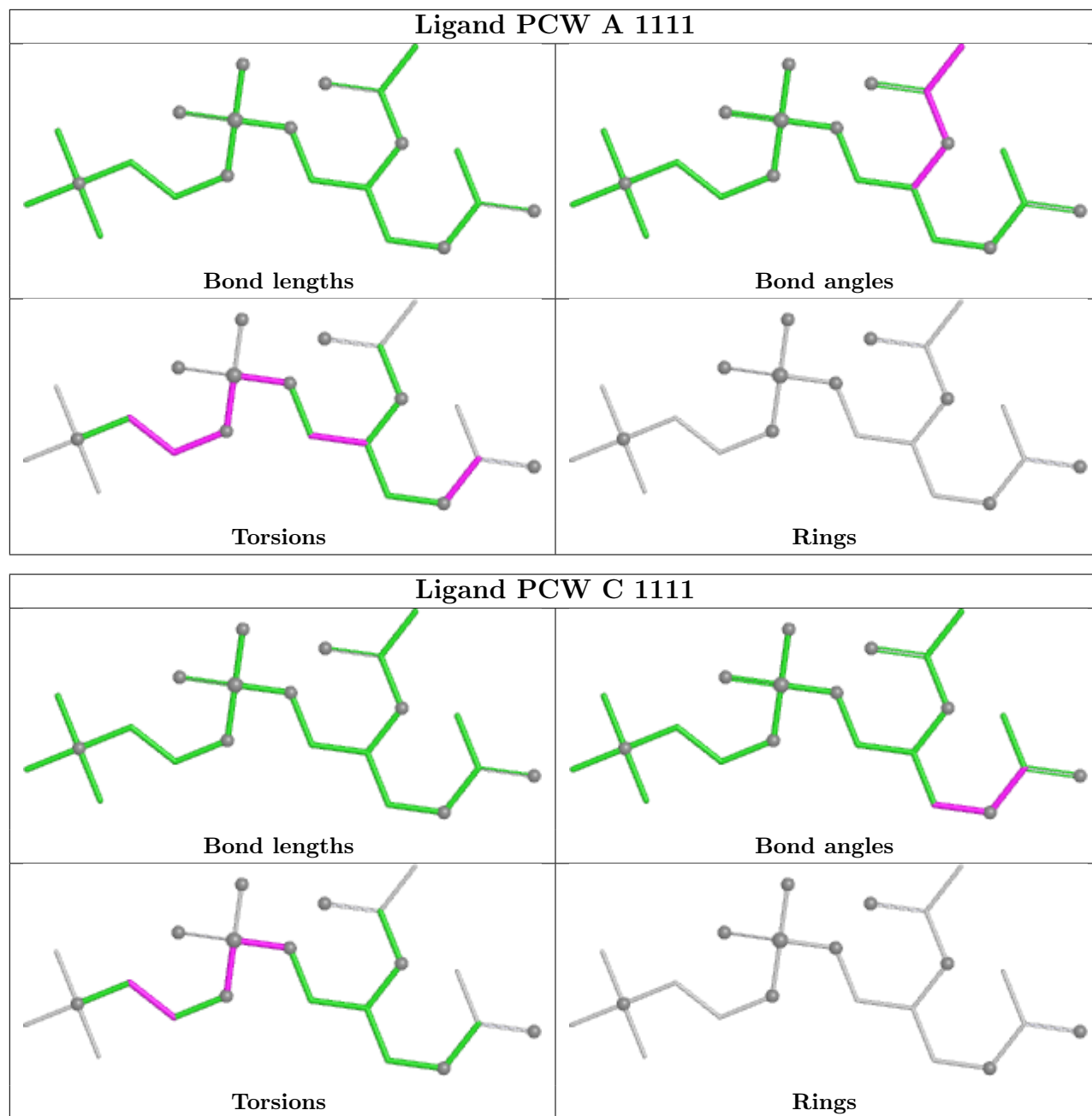


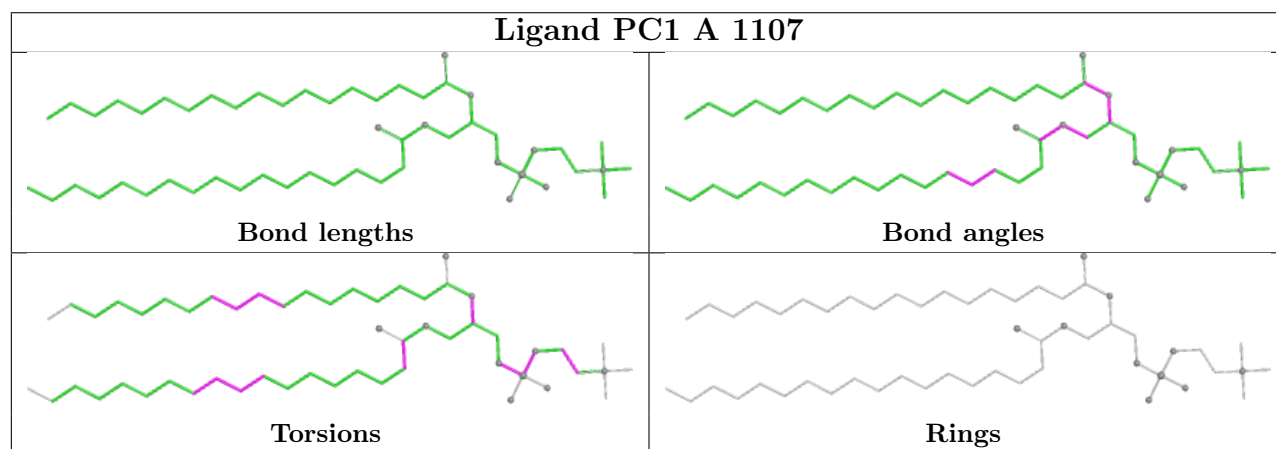
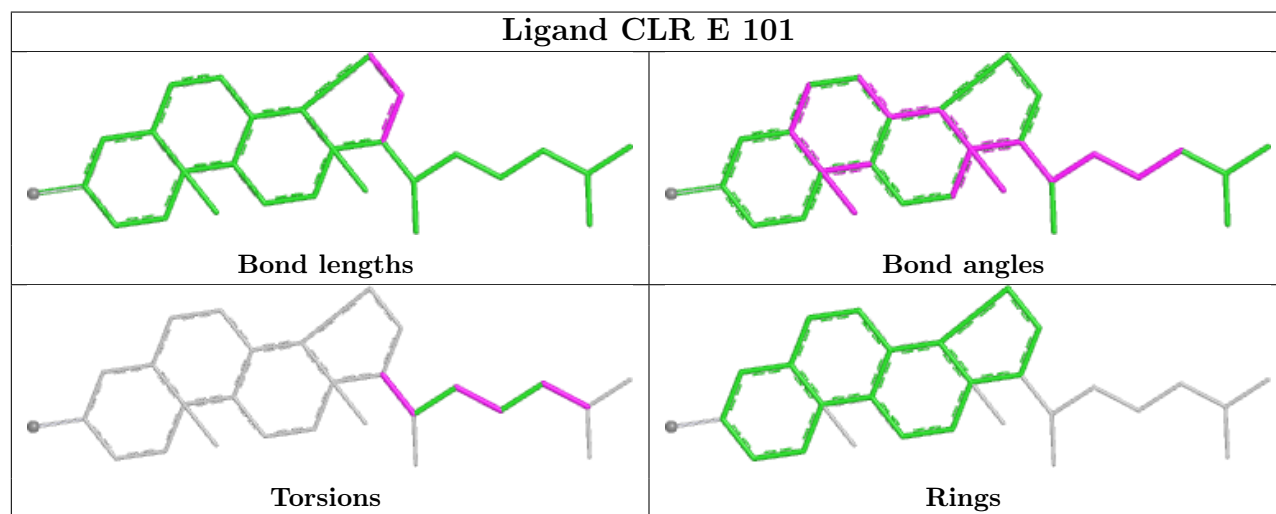
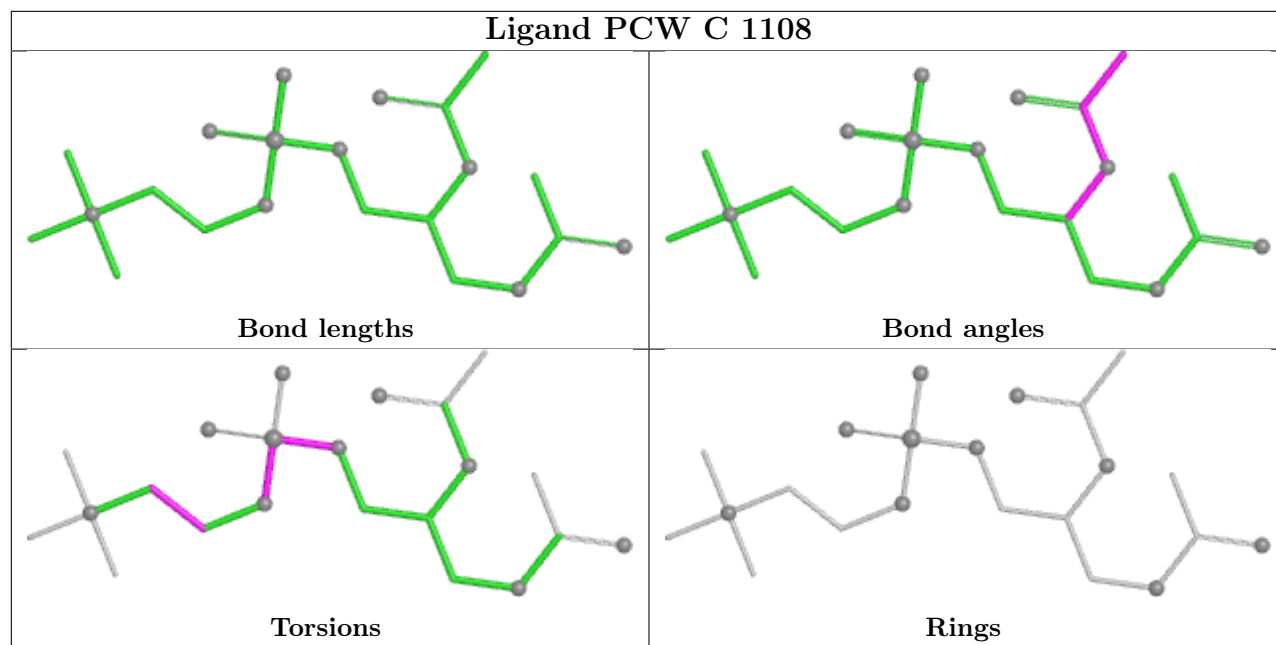
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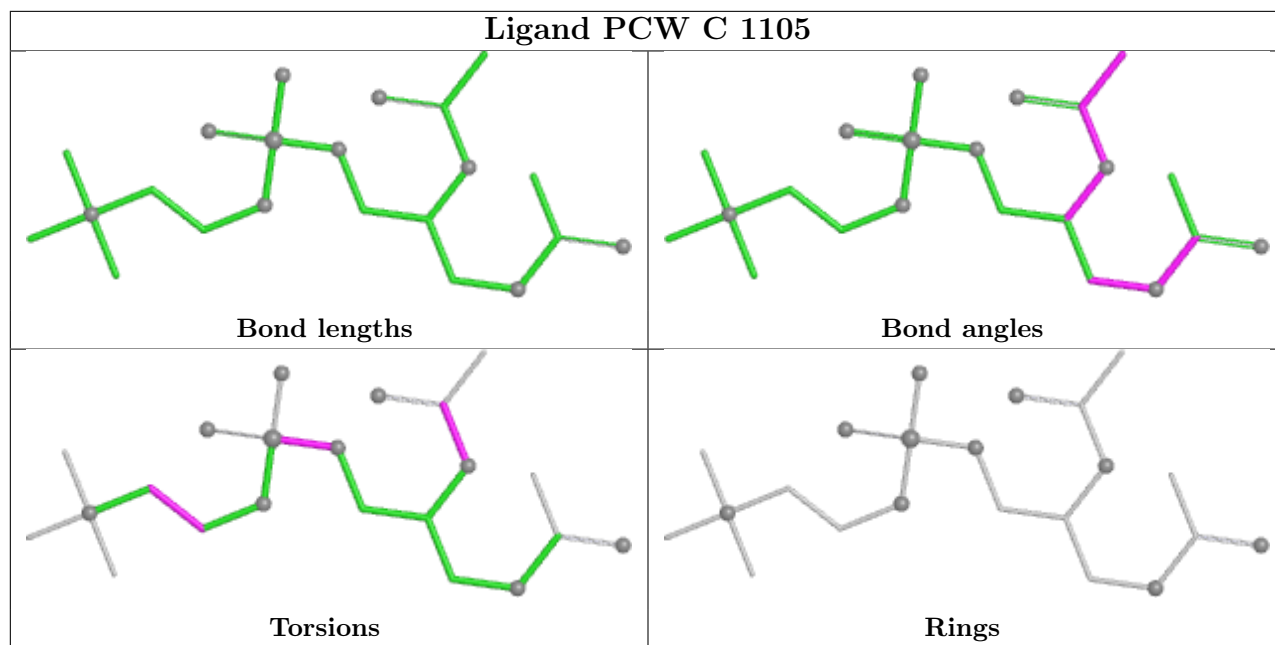
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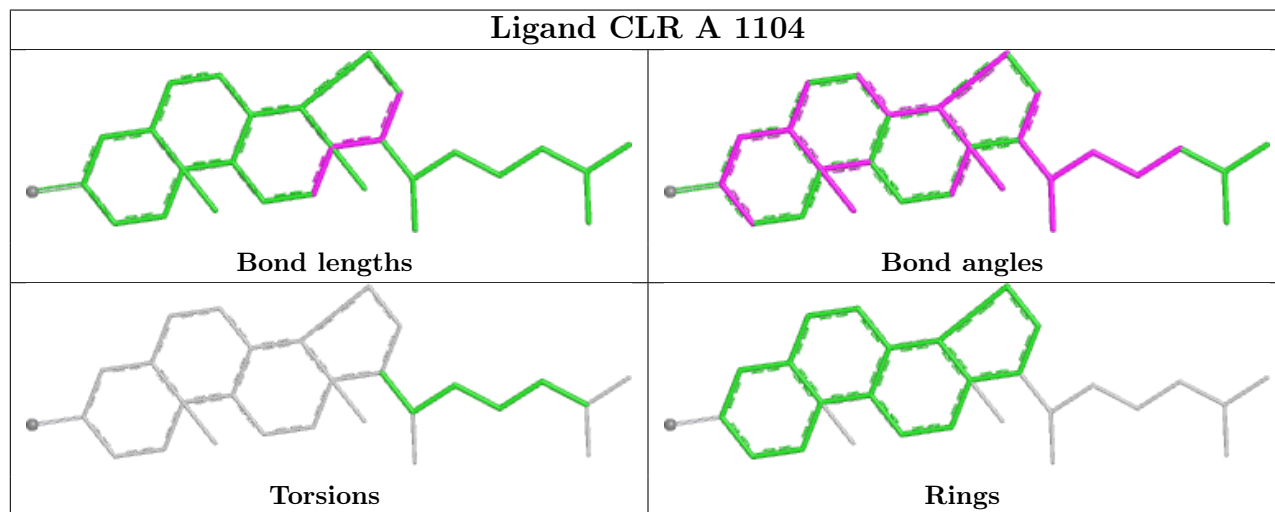




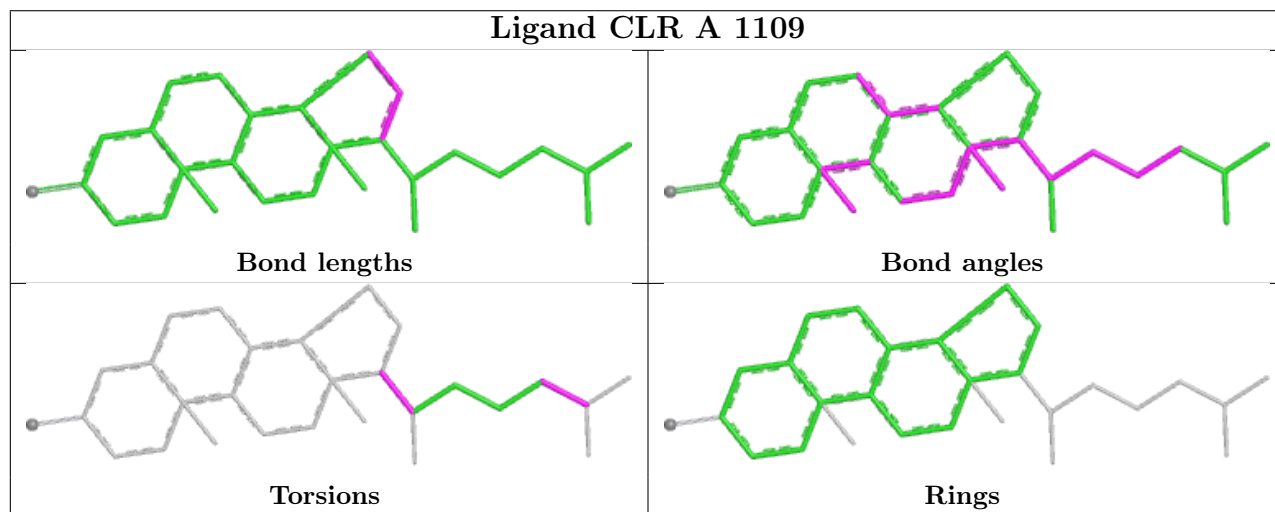
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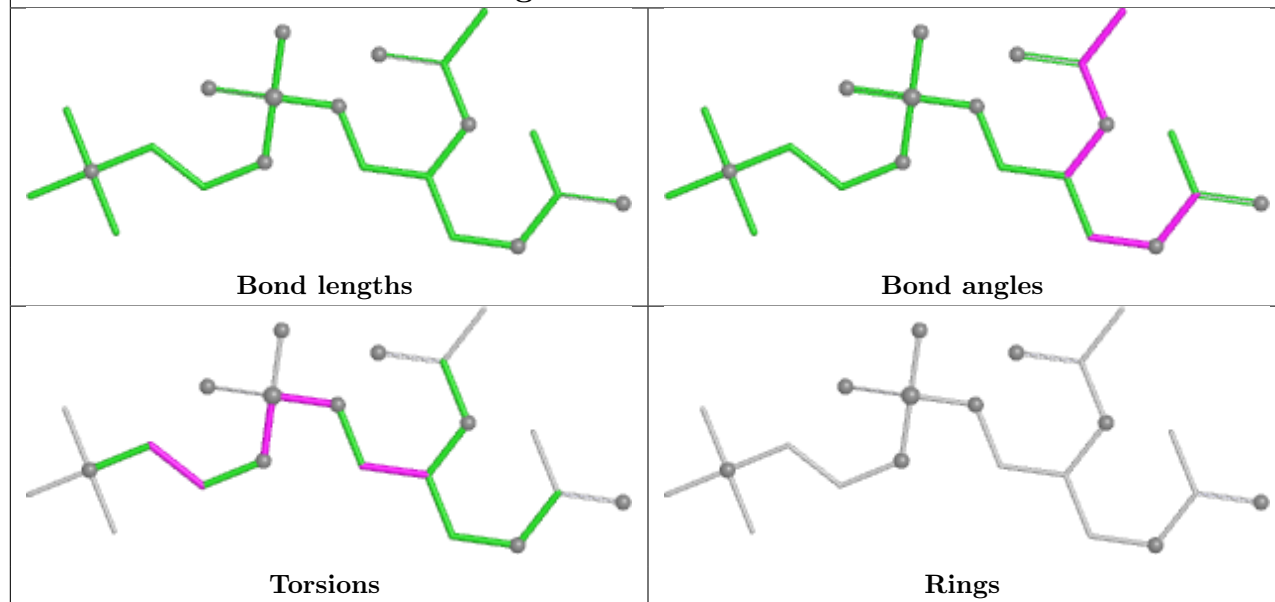
Ligand CLR A 1104



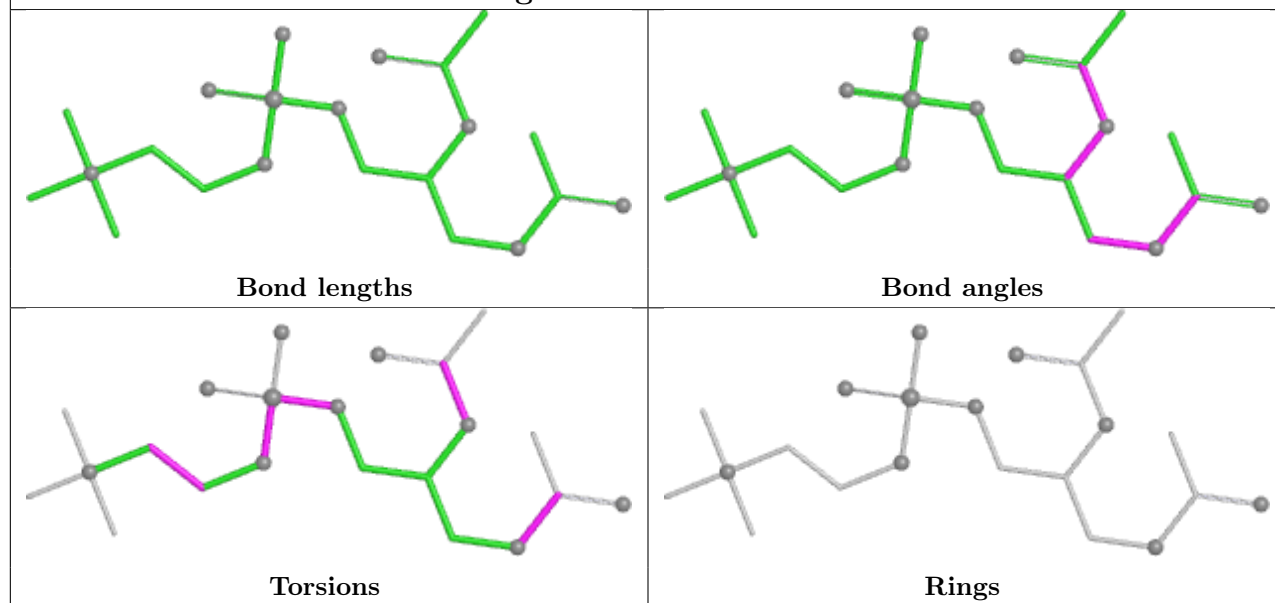
Ligand CLR A 1109

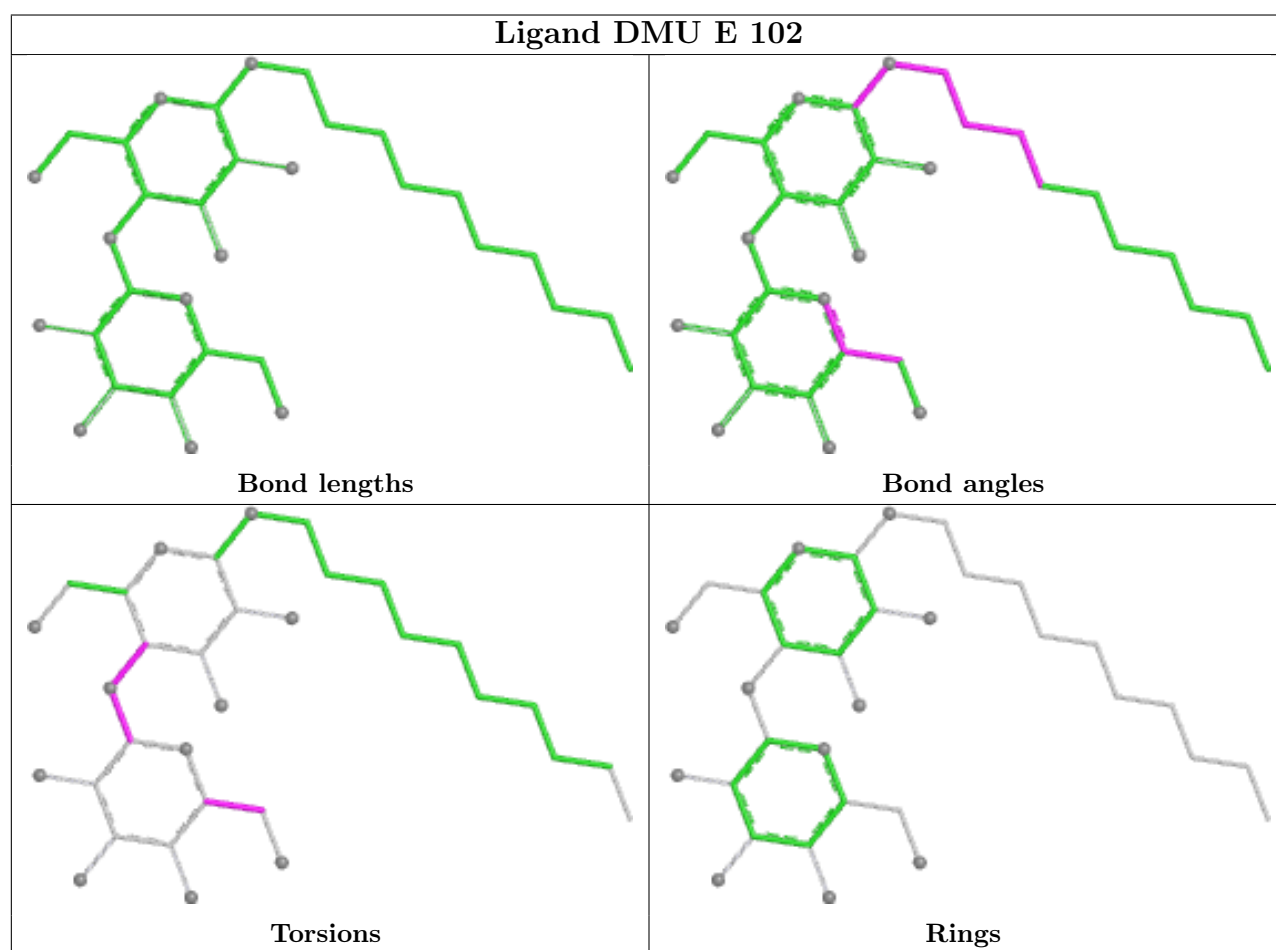
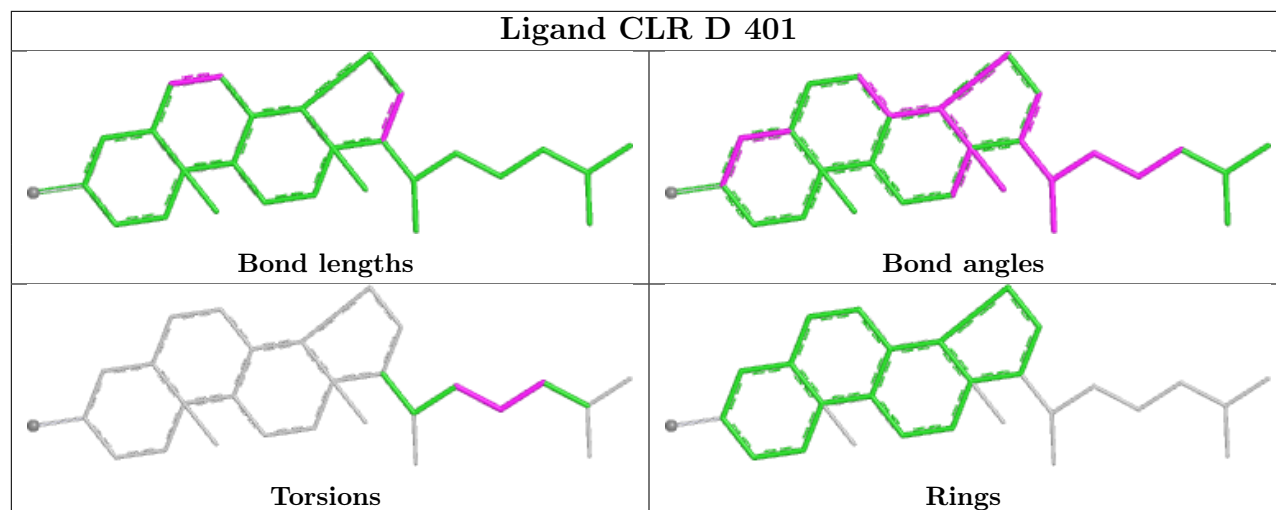


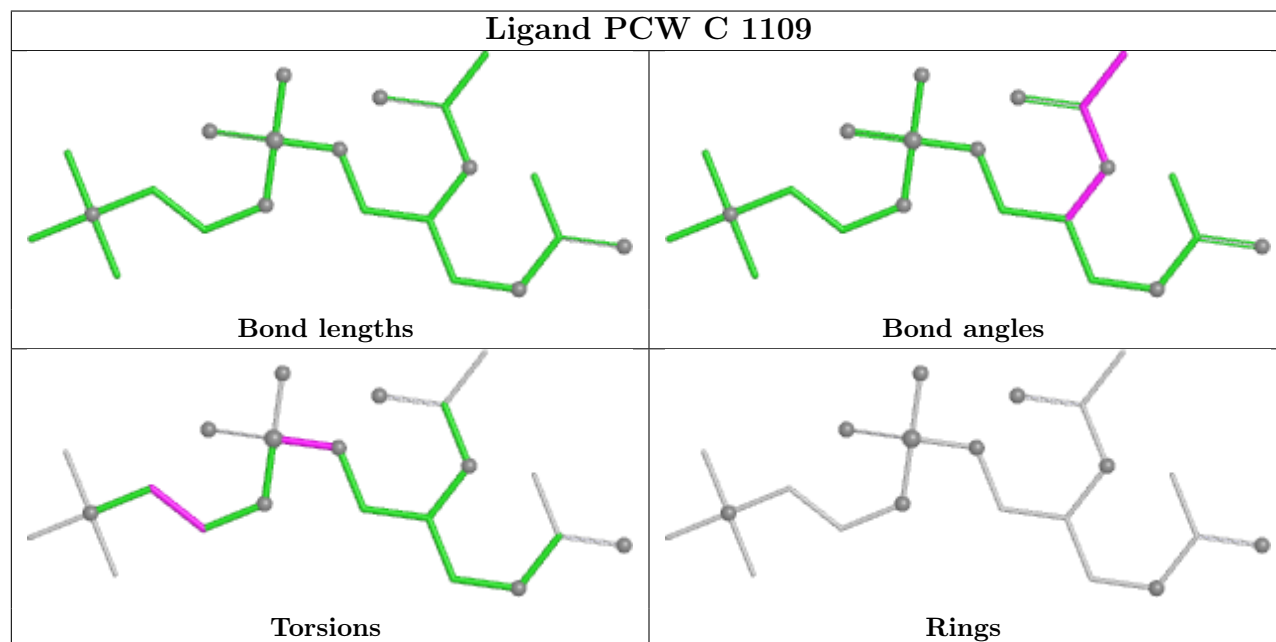
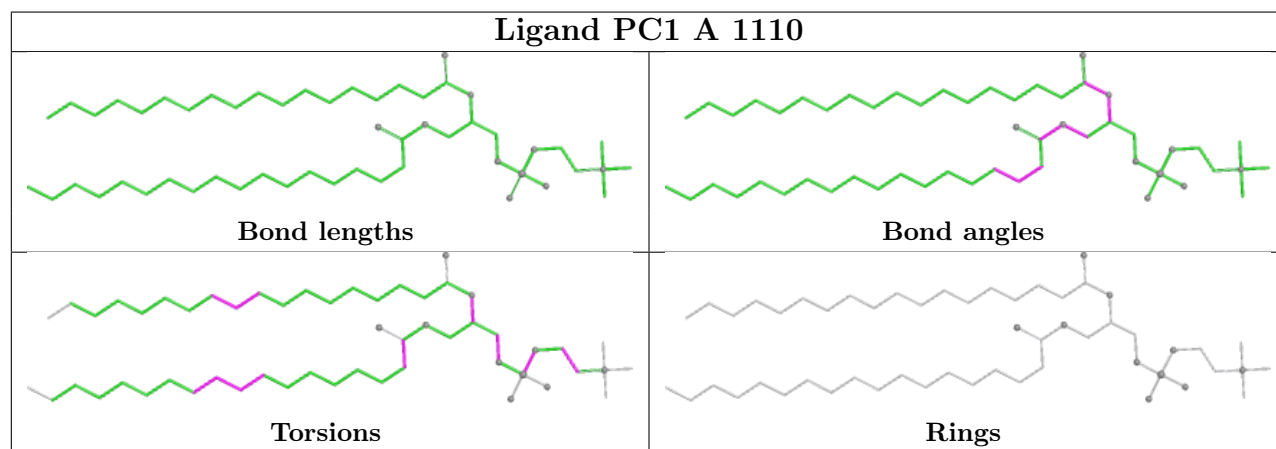
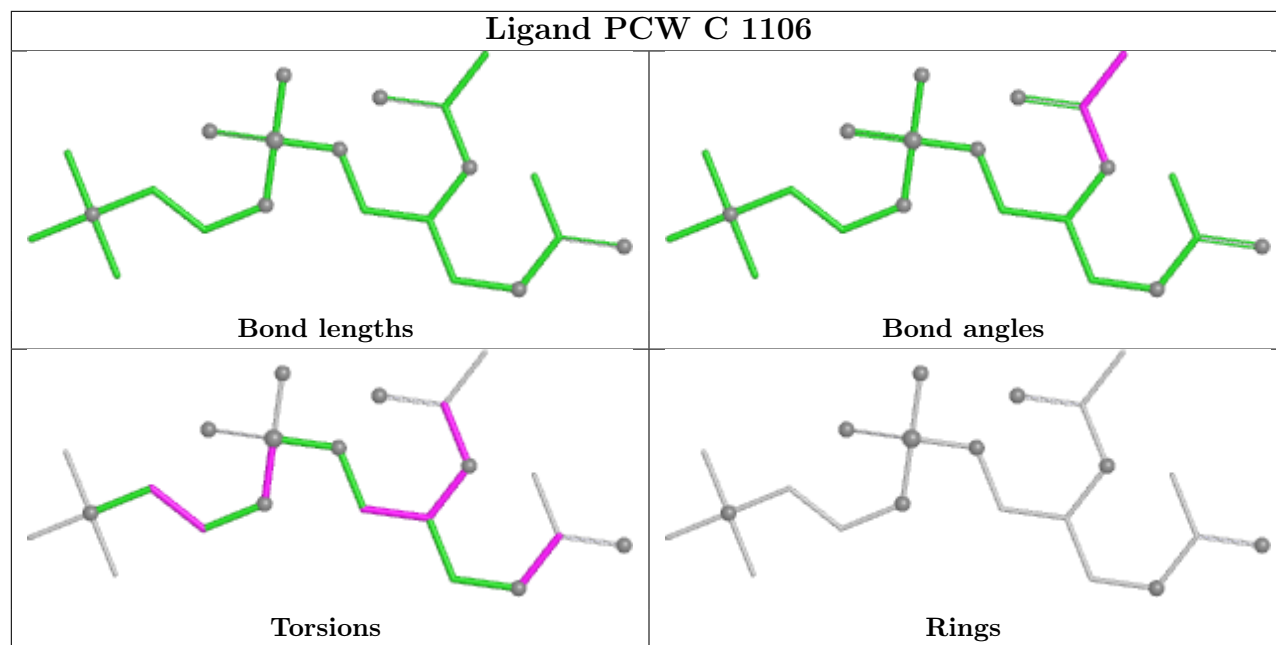
Ligand PCW A 1106

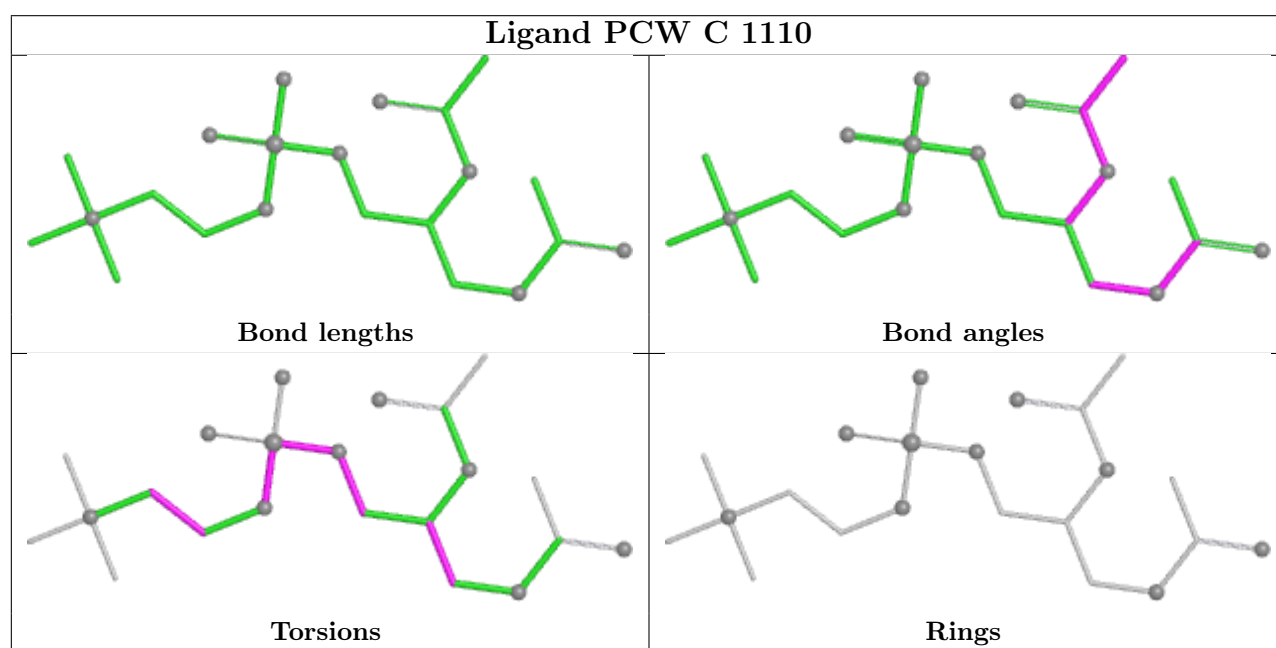
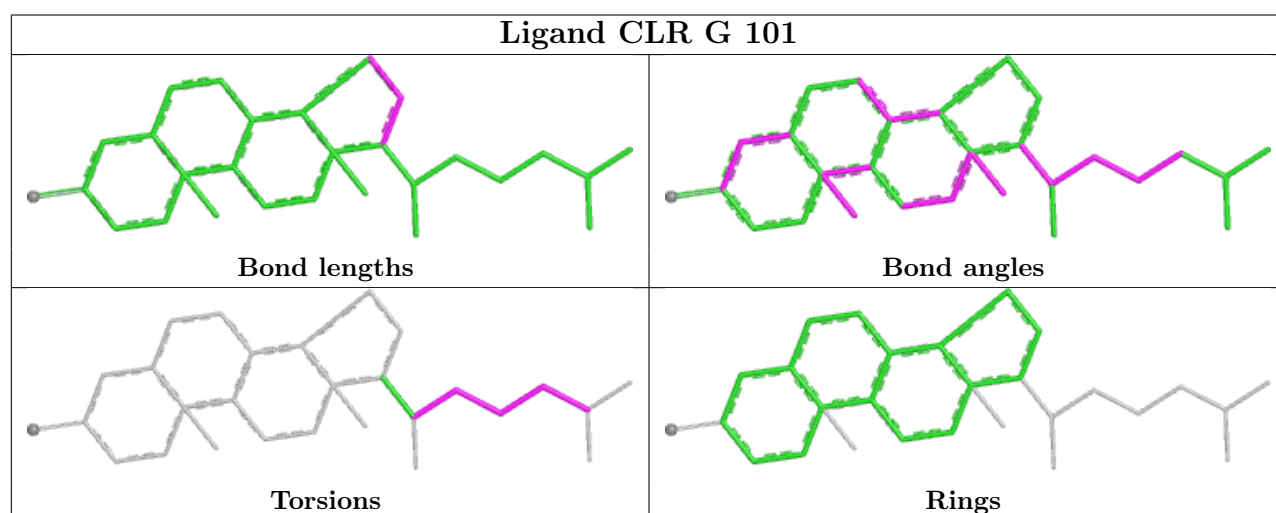
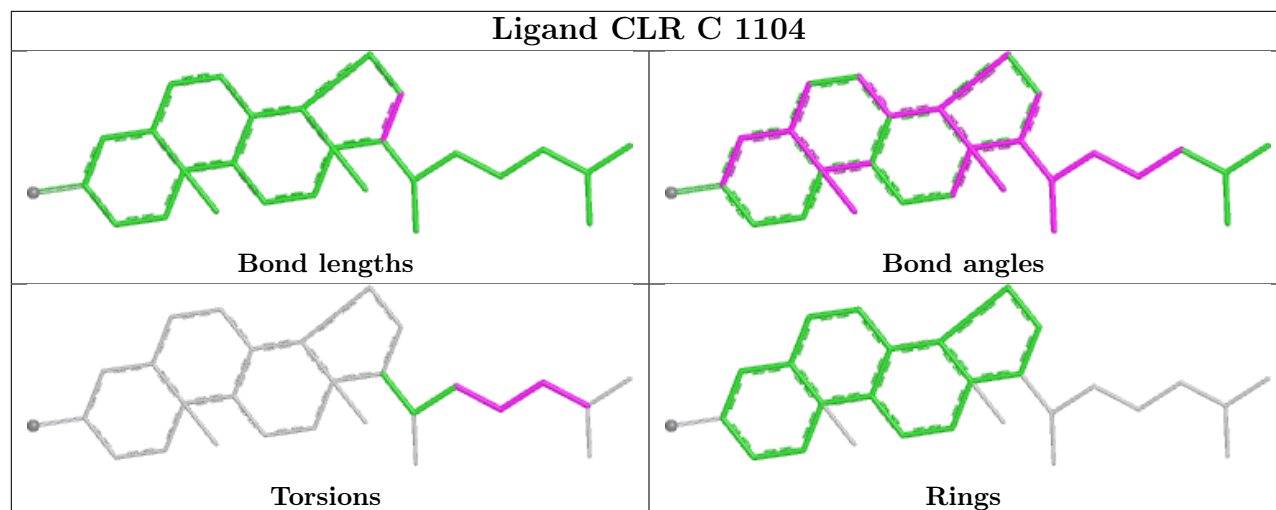


Ligand PCW A 1112









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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	995/1021 (97%)	-0.34	3 (0%) 90 87	25, 68, 144, 191	0
1	C	995/1021 (97%)	-0.38	4 (0%) 88 85	34, 76, 134, 190	0
2	B	291/303 (96%)	-0.20	3 (1%) 79 73	59, 93, 143, 172	0
2	D	291/303 (96%)	0.00	4 (1%) 73 65	67, 128, 168, 212	0
3	E	33/65 (50%)	-0.31	0 100 100	44, 56, 108, 138	0
3	G	35/65 (53%)	-0.30	0 100 100	37, 59, 105, 106	0
All	All	2640/2778 (95%)	-0.30	14 (0%) 87 83	25, 78, 150, 212	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	23	GLU	3.1
2	B	18	ASN	3.0
1	A	31	GLU	2.8
1	A	492	ALA	2.7
2	B	172	GLY	2.4
1	A	570	ASN	2.4
2	D	95	PRO	2.4
2	D	106	VAL	2.3
2	D	15	PHE	2.3
1	C	491	THR	2.3
1	C	400	SER	2.2
1	C	432	ASN	2.1
2	D	121	MET	2.0
1	C	431	GLU	2.0

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

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

6.3 Carbohydrates

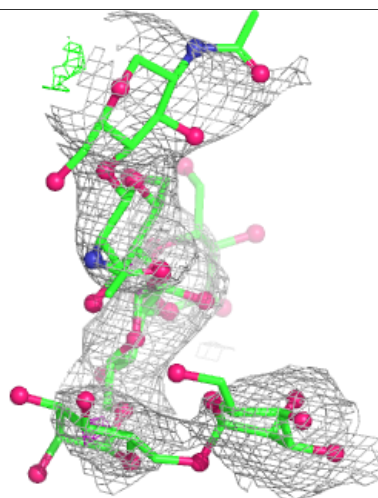
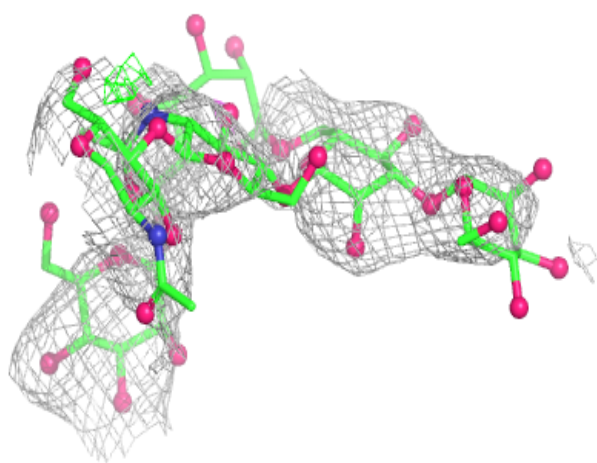
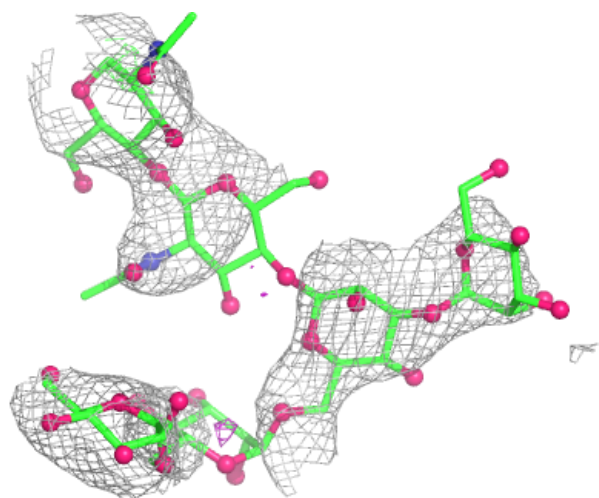
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	1	14/15	-	-	114,140,147,148	0
4	NAG	F	2	14/15	-	-	107,136,148,151	0
4	BMA	F	3	11/12	-	-	108,121,134,137	0
4	MAN	F	4	11/12	-	-	118,149,154,155	0
4	MAN	F	5	11/12	-	-	113,133,144,147	0
4	MAN	F	6	11/12	-	-	137,145,153,153	0
6	NAG	I	1	14/15	0.35	0.12	137,148,170,174	0
5	MAN	H	4	11/12	0.42	0.13	164,185,190,193	0
5	BMA	H	3	11/12	0.45	0.11	186,189,193,195	0
5	NAG	H	2	14/15	0.53	0.19	168,200,209,210	0
5	MAN	H	5	11/12	0.58	0.12	167,180,190,192	0
6	NAG	I	2	14/15	0.61	0.14	132,155,166,168	0
5	NAG	H	1	14/15	0.78	0.12	161,178,195,206	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

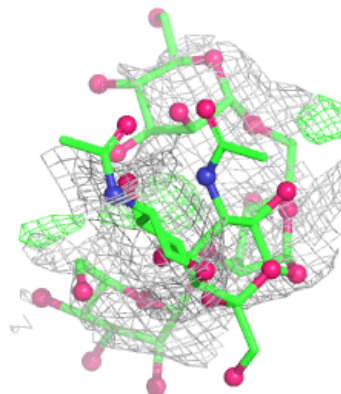
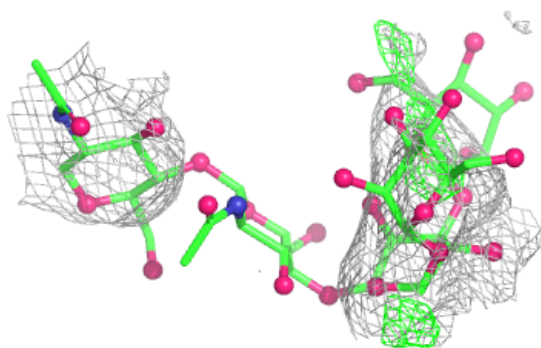
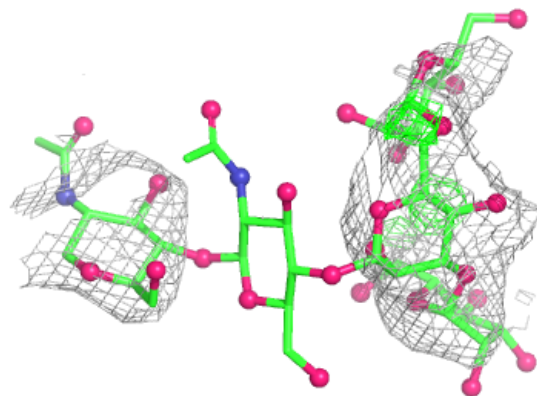
Electron density around Chain F:

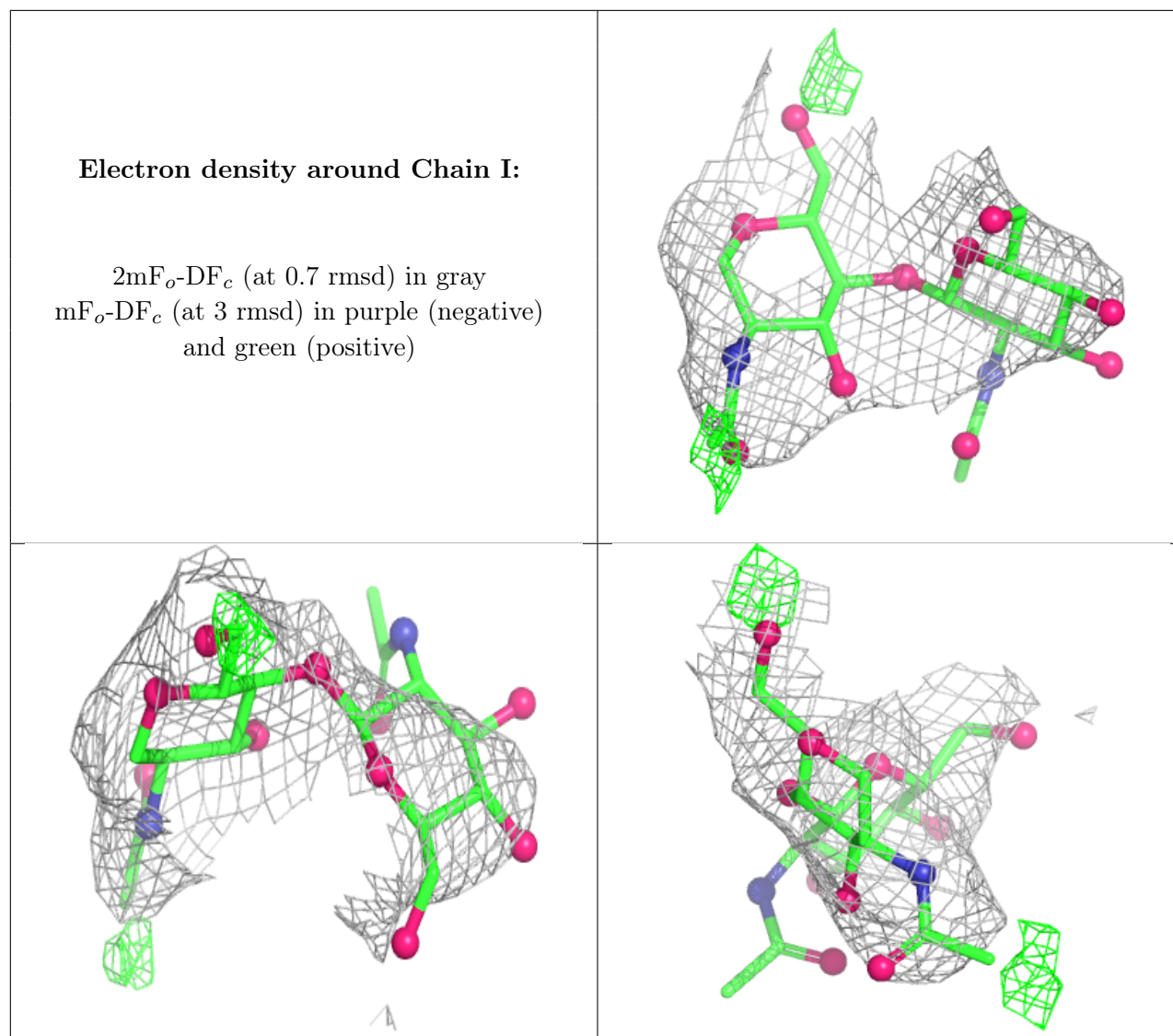
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PCW	C	1108	22/54	0.51	0.12	86,124,177,183	0
10	PCW	C	1107	22/54	0.53	0.14	90,122,165,173	0
10	PCW	A	1108	22/54	0.58	0.13	80,125,155,161	0
10	PCW	A	1113	22/54	0.64	0.13	102,130,158,164	0
10	PCW	C	1111	22/54	0.67	0.13	87,118,153,159	0
10	PCW	C	1110	22/54	0.69	0.13	105,126,137,144	0
9	PC1	A	1105	54/54	0.70	0.11	69,115,161,175	0

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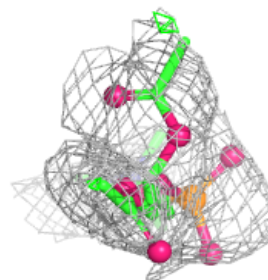
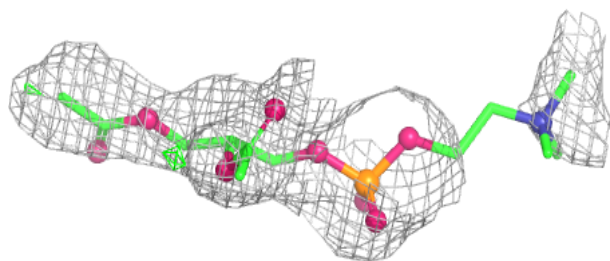
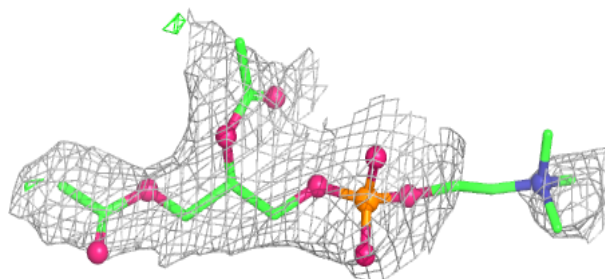
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	PCW	A	1112	22/54	0.71	0.11	88,128,140,144	0
10	PCW	C	1109	22/54	0.71	0.11	119,153,167,170	0
10	PCW	C	1105	22/54	0.72	0.11	92,113,161,172	0
10	PCW	A	1106	22/54	0.73	0.12	90,121,142,146	0
10	PCW	A	1114	54/54	0.73	0.11	64,87,156,173	0
11	NAG	D	402	14/15	0.74	0.10	156,170,184,184	0
10	PCW	B	401	22/54	0.75	0.13	76,114,145,152	0
8	CLR	A	1109	28/28	0.76	0.10	94,115,130,134	0
10	PCW	A	1111	22/54	0.77	0.11	67,109,117,126	0
10	PCW	C	1106	22/54	0.78	0.10	101,134,145,148	0
9	PC1	A	1110	54/54	0.85	0.12	48,88,132,137	0
8	CLR	A	1104	28/28	0.85	0.10	59,91,107,110	0
12	DMU	E	102	33/33	0.86	0.11	37,71,89,94	0
9	PC1	A	1107	54/54	0.87	0.11	50,91,122,137	0
8	CLR	D	401	28/28	0.87	0.09	81,107,112,117	0
7	MN	A	1101	1/1	0.89	0.06	77,77,77,77	0
8	CLR	G	101	28/28	0.93	0.11	33,50,107,113	0
7	MN	C	1102	1/1	0.95	0.03	68,68,68,68	0
8	CLR	C	1104	28/28	0.95	0.09	37,43,102,111	0
8	CLR	E	101	28/28	0.96	0.07	31,45,67,74	0
7	MN	C	1103	1/1	0.96	0.07	72,72,72,72	0
7	MN	A	1103	1/1	0.98	0.08	54,54,54,54	0
7	MN	A	1102	1/1	0.98	0.02	69,69,69,69	0
7	MN	C	1101	1/1	0.99	0.03	80,80,80,80	0

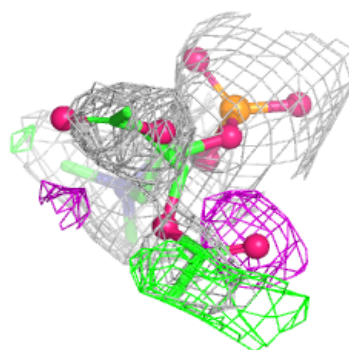
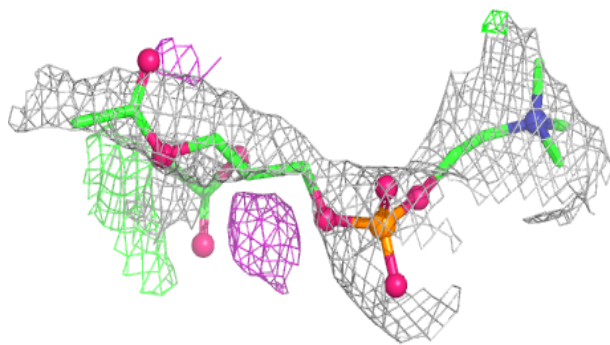
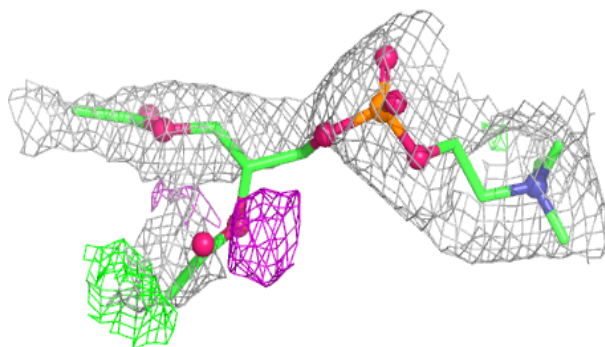
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PCW C 1108:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

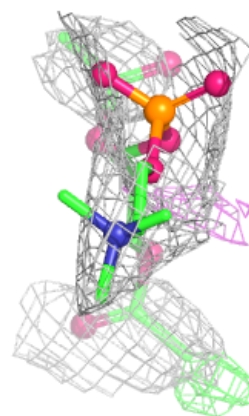
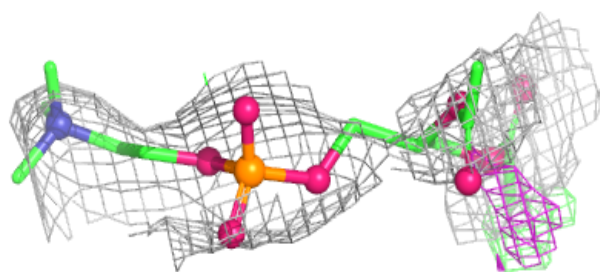
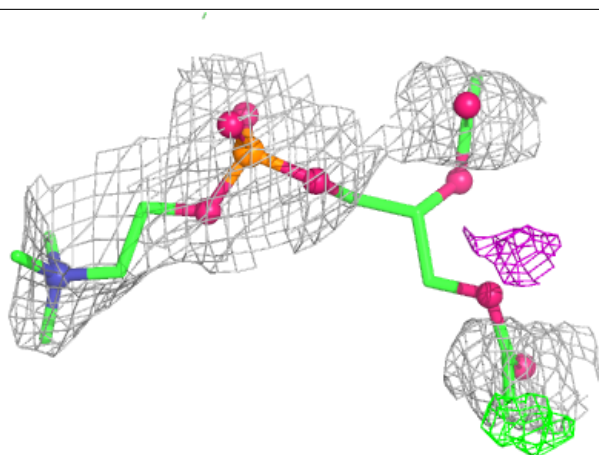
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and green (positive)

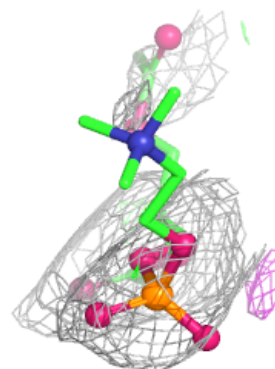
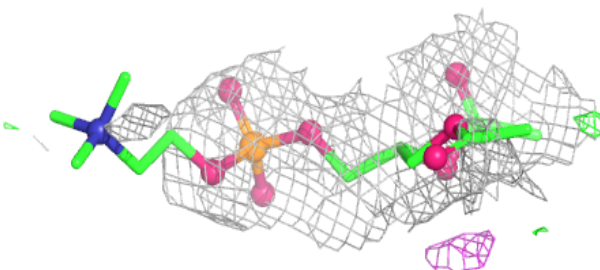
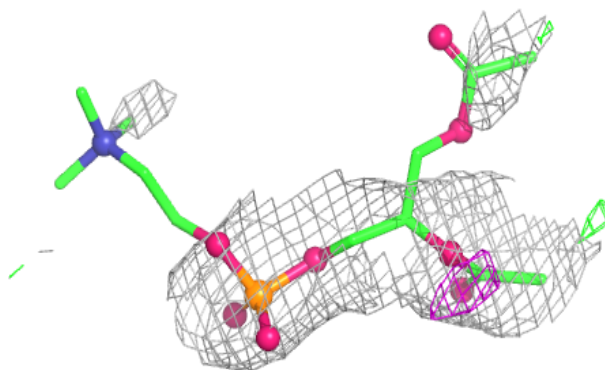


Electron density around PCW A 1108:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

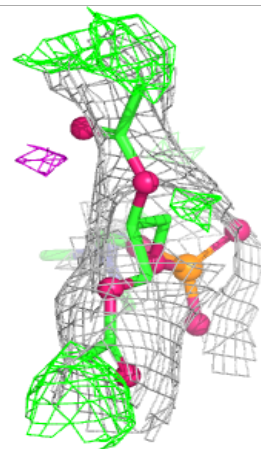
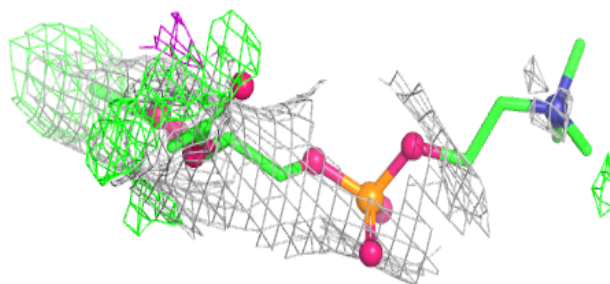
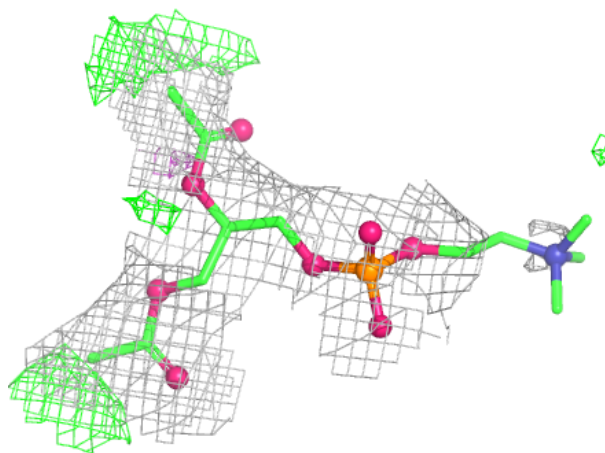
**Electron density around PCW A 1113:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



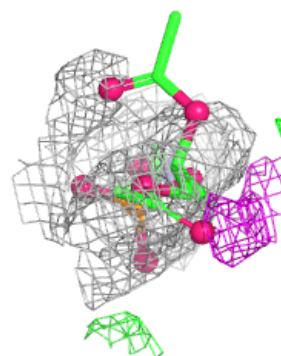
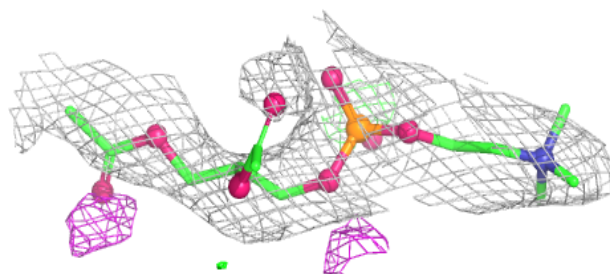
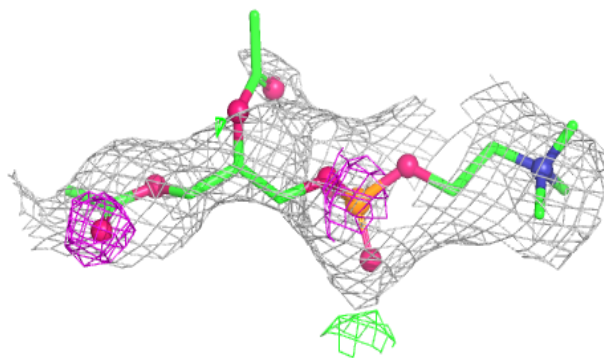
Electron density around PCW C 1111:

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and green (positive)

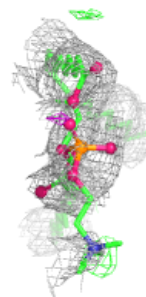
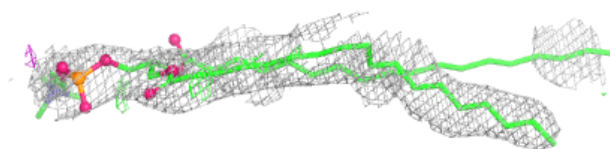
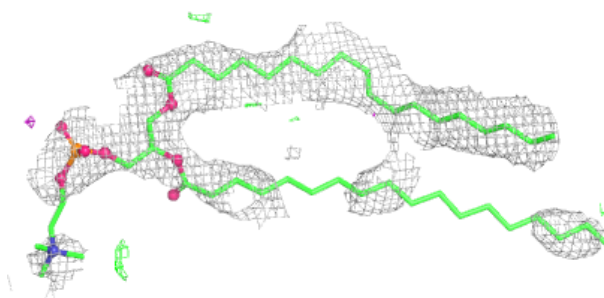


Electron density around PCW C 1110:

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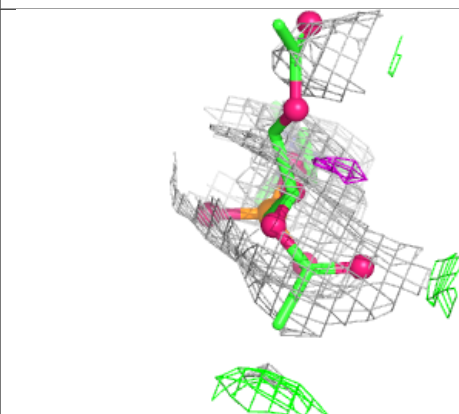
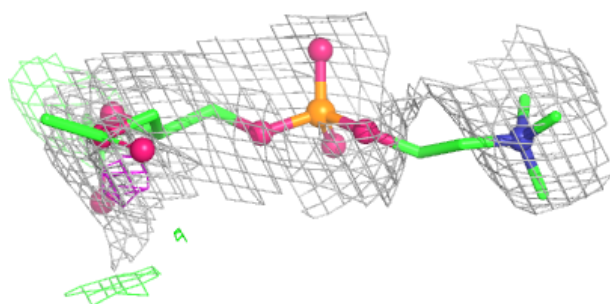
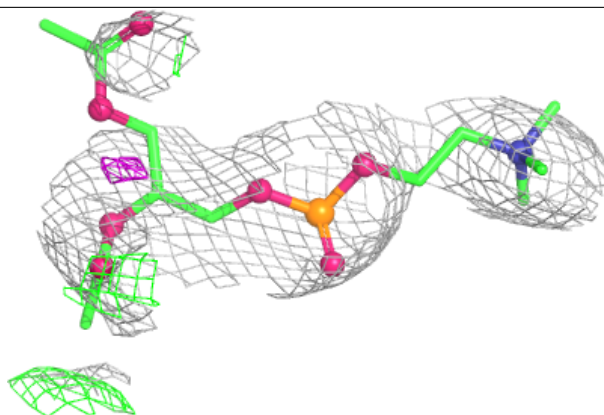
**Electron density around PC1 A 1105:**

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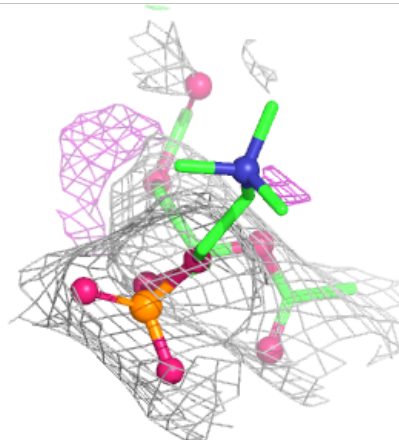
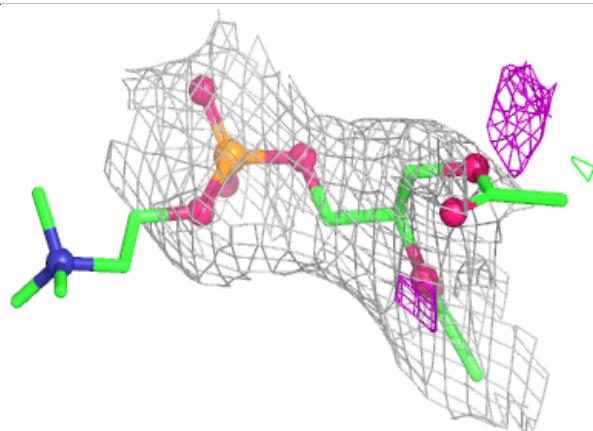
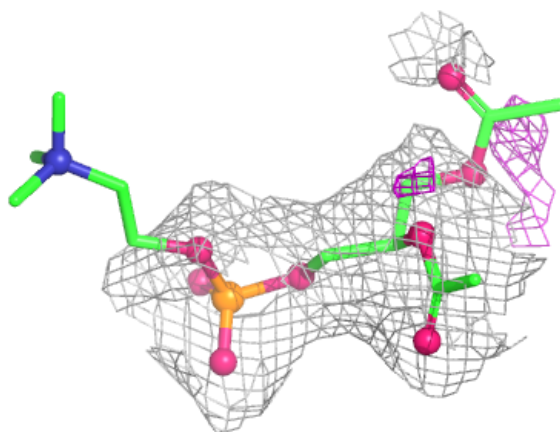


Electron density around PCW A 1112:

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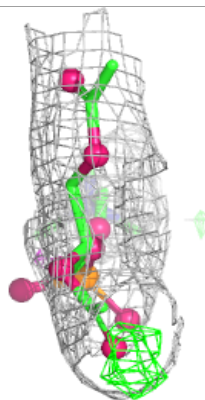
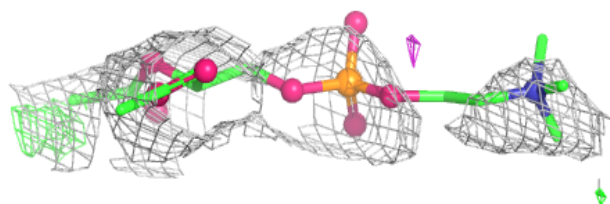
**Electron density around PCW C 1109:**

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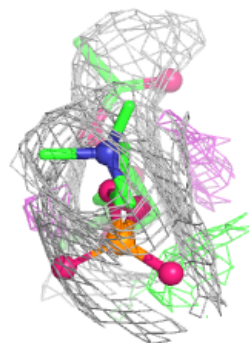
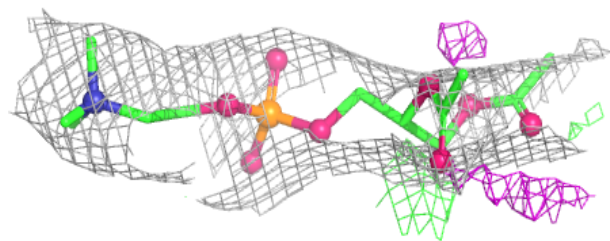
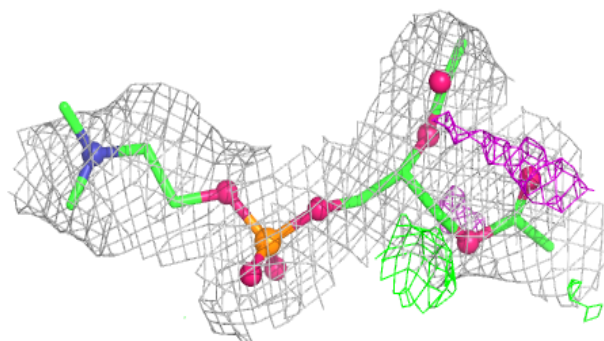


Electron density around PCW C 1105:

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and green (positive)

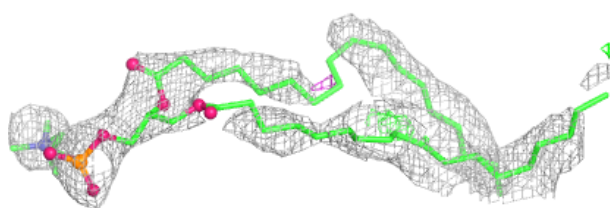
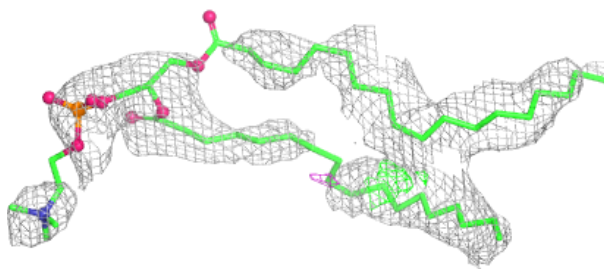
**Electron density around PCW A 1106:**

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and green (positive)



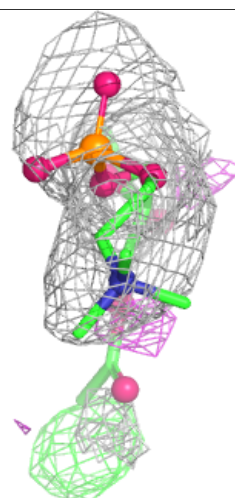
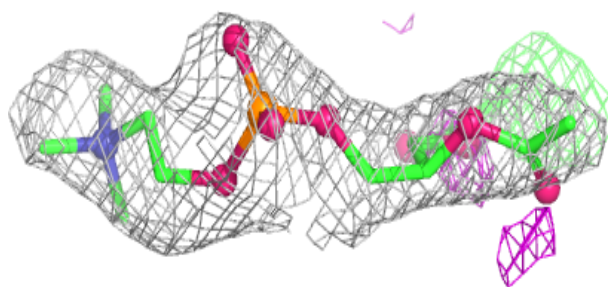
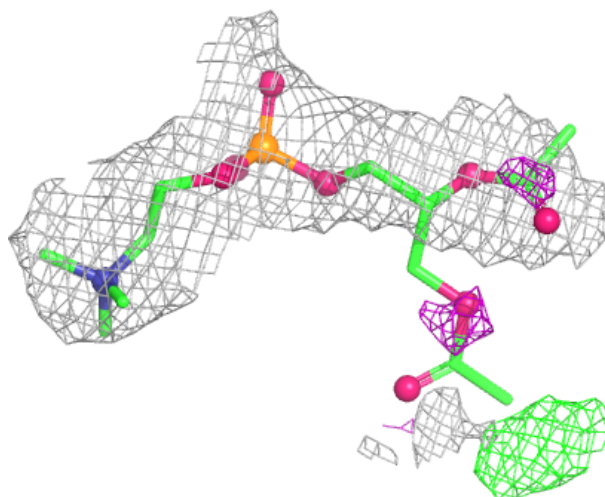
Electron density around PCW A 1114:

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and green (positive)



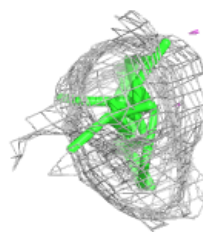
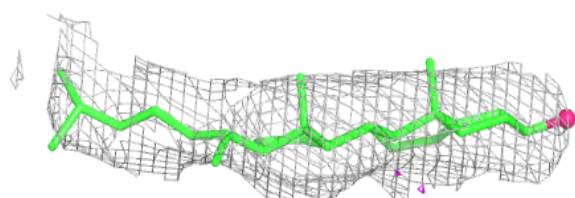
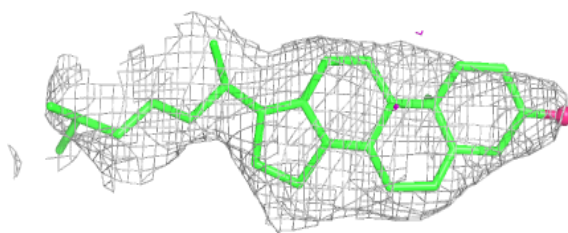
Electron density around PCW B 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

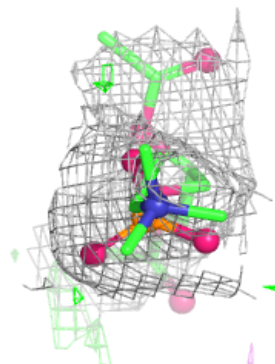
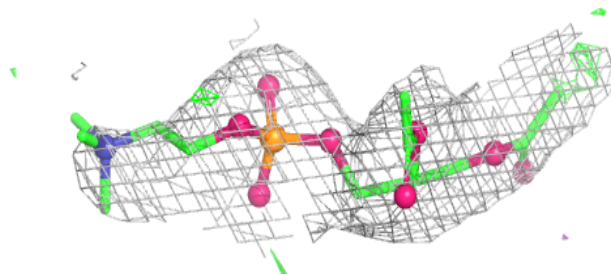
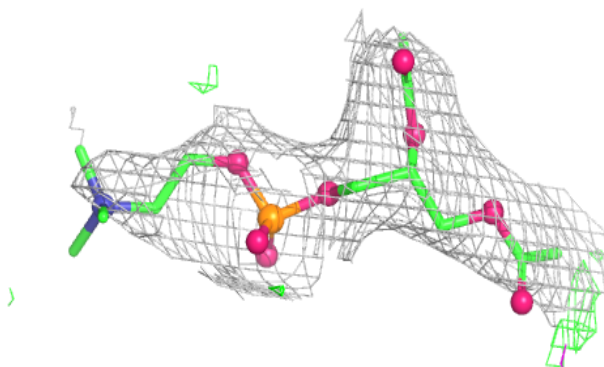


Electron density around CLR A 1109:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

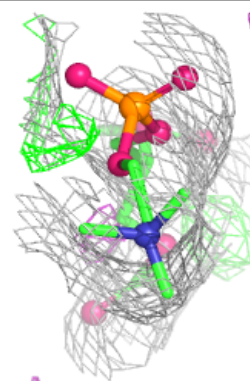
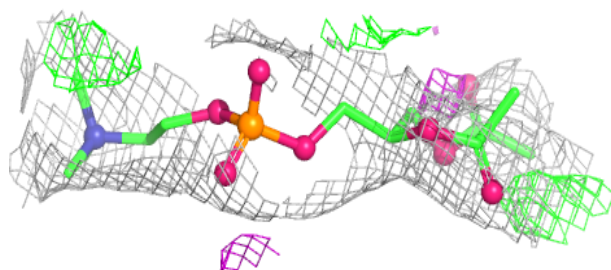
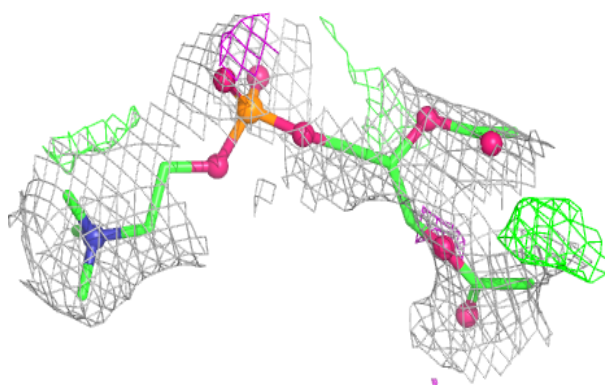
**Electron density around PCW A 1111:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

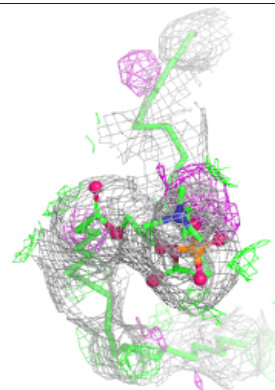
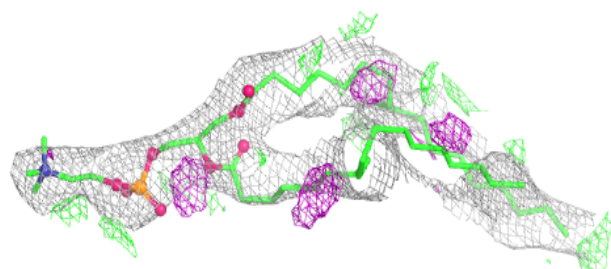
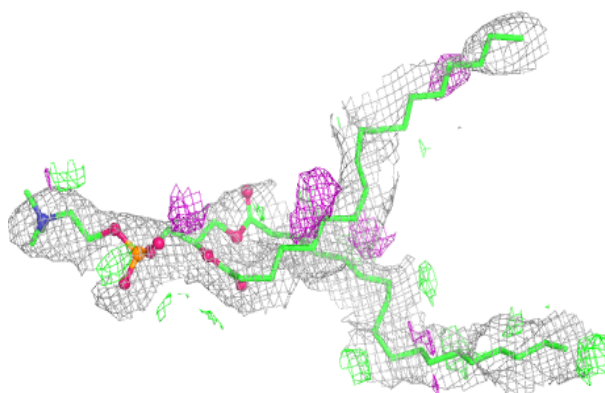


Electron density around PCW C 1106:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

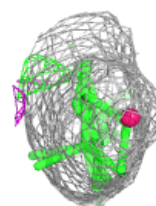
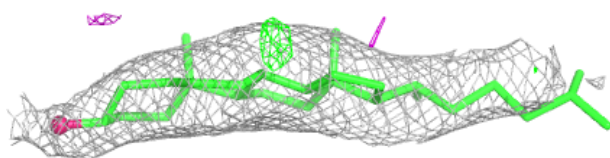
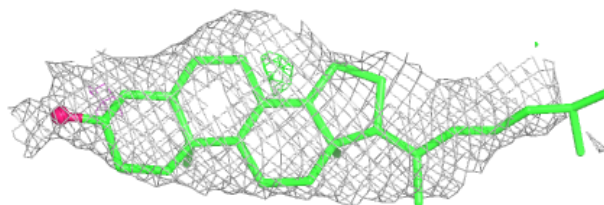
**Electron density around PC1 A 1110:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

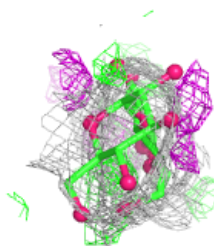
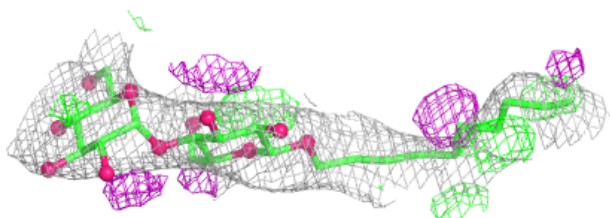
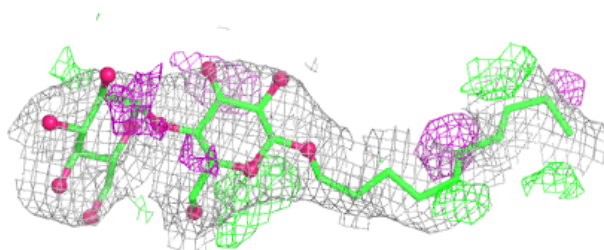


Electron density around CLR A 1104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

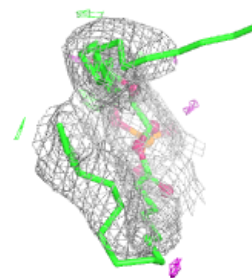
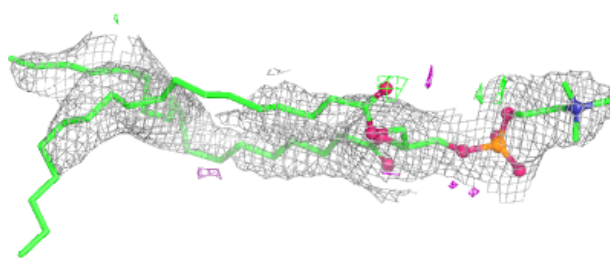
**Electron density around DMU E 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

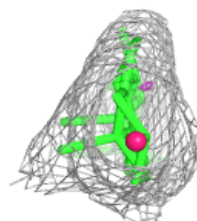
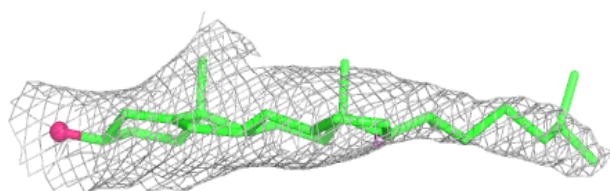
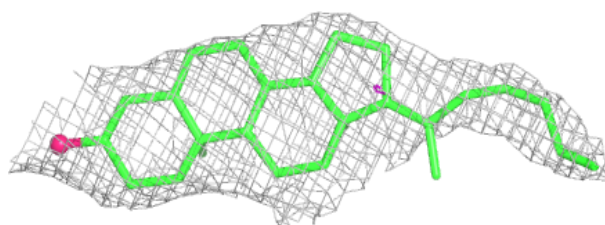


Electron density around PC1 A 1107:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

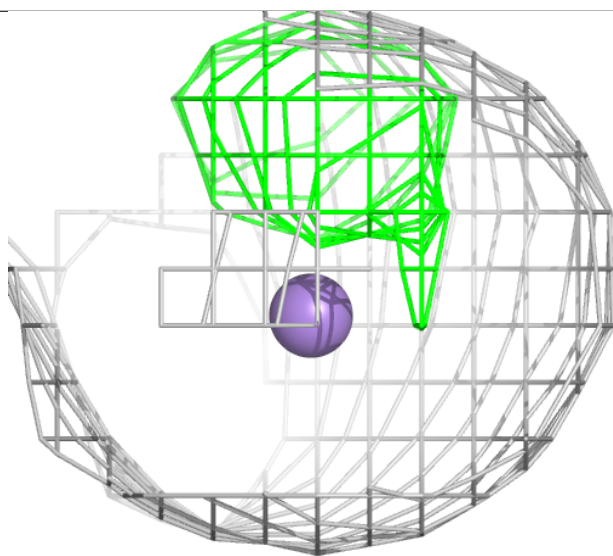
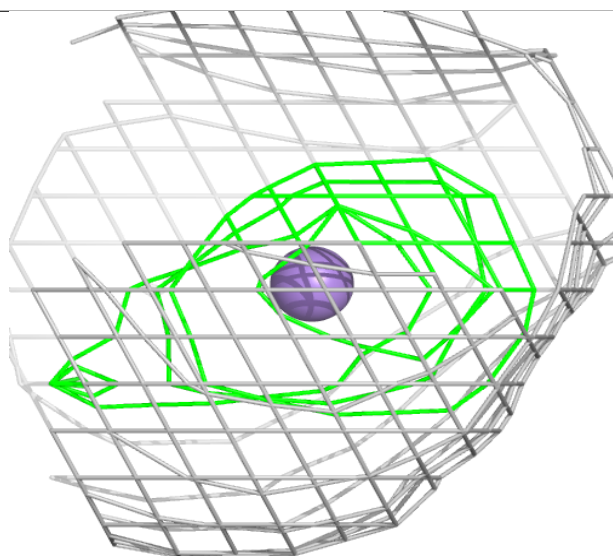
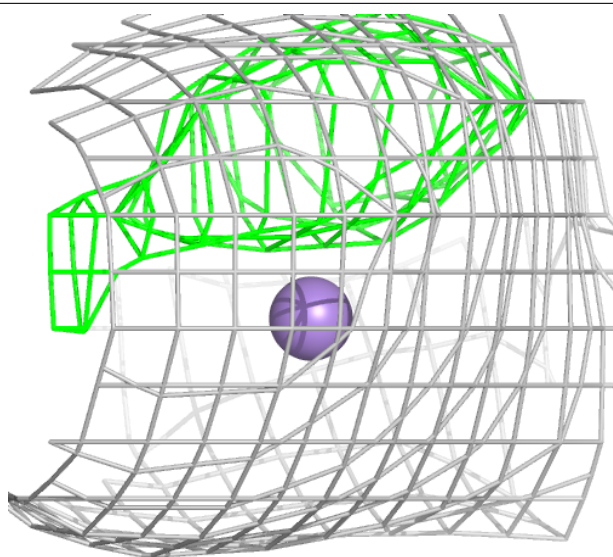
**Electron density around CLR D 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



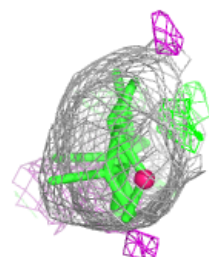
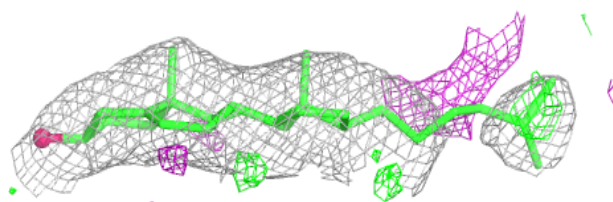
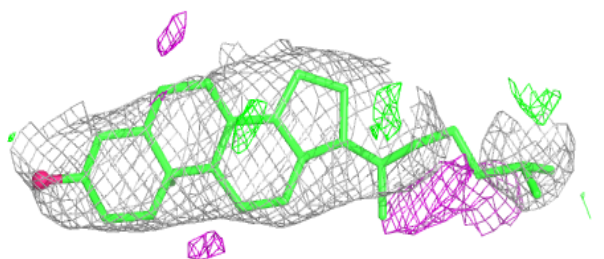
Electron density around MN A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



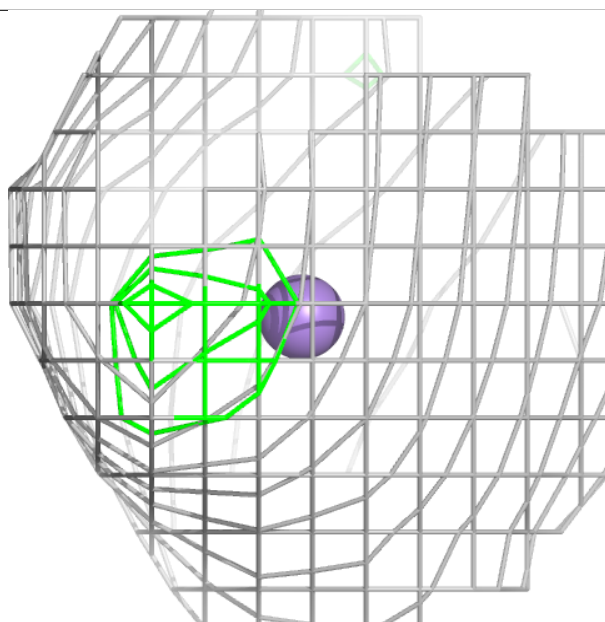
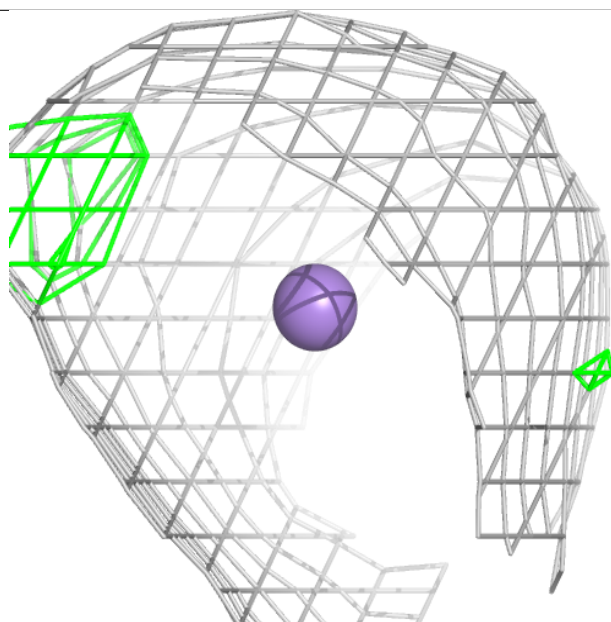
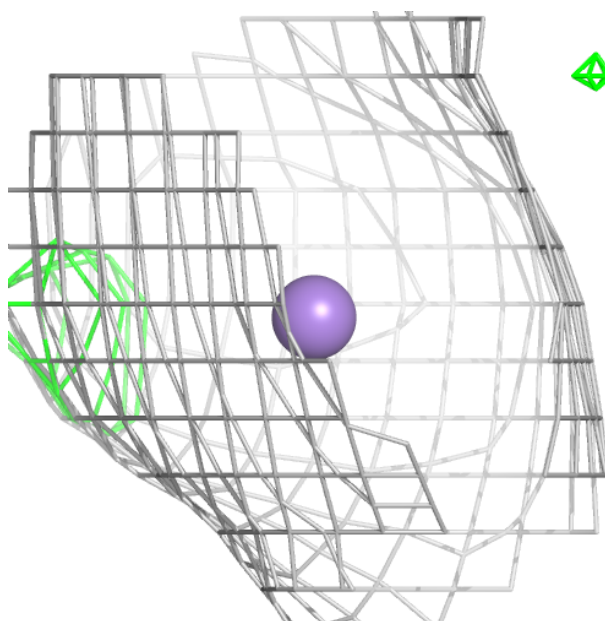
Electron density around CLR G 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



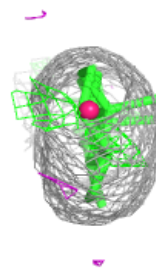
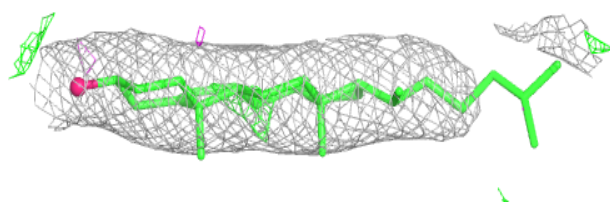
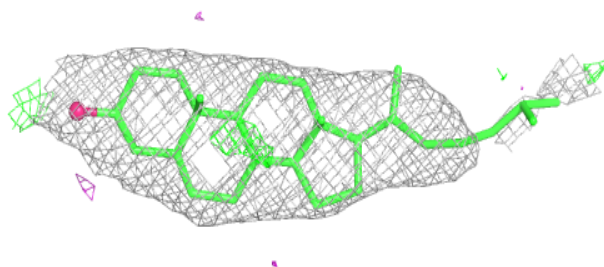
Electron density around MN C 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

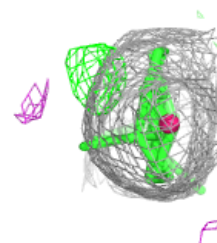
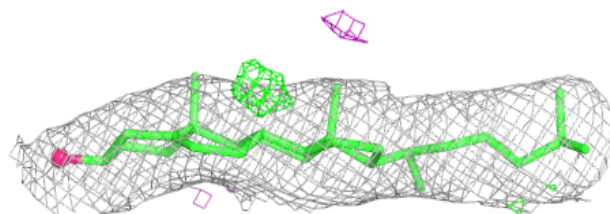
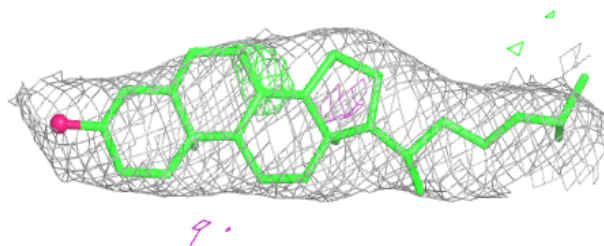


Electron density around CLR C 1104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

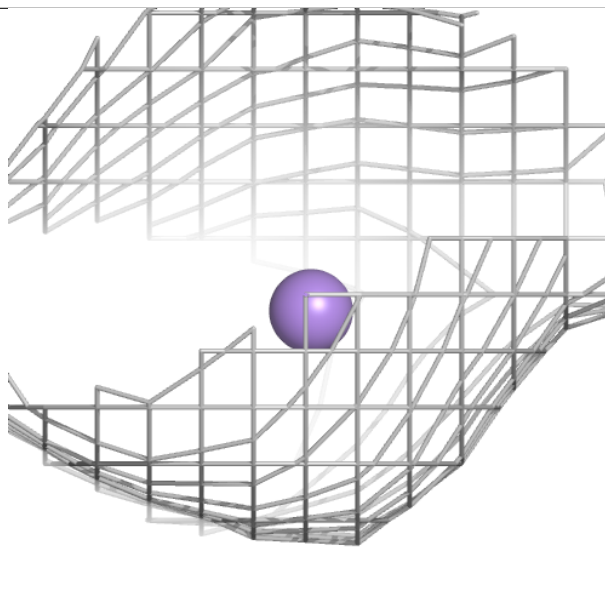
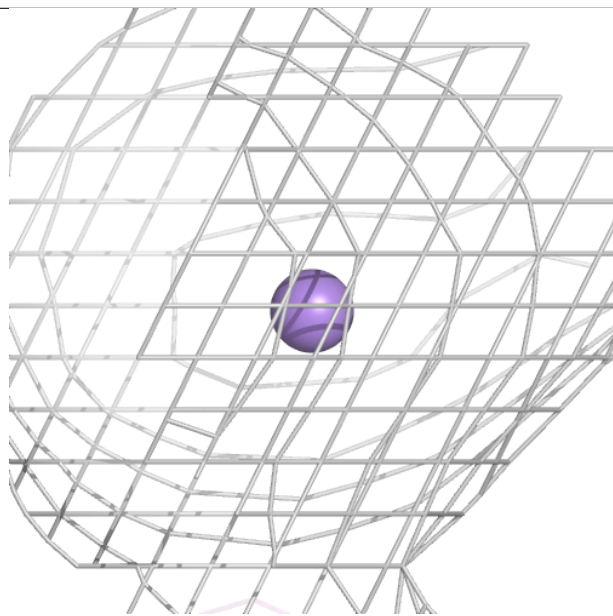
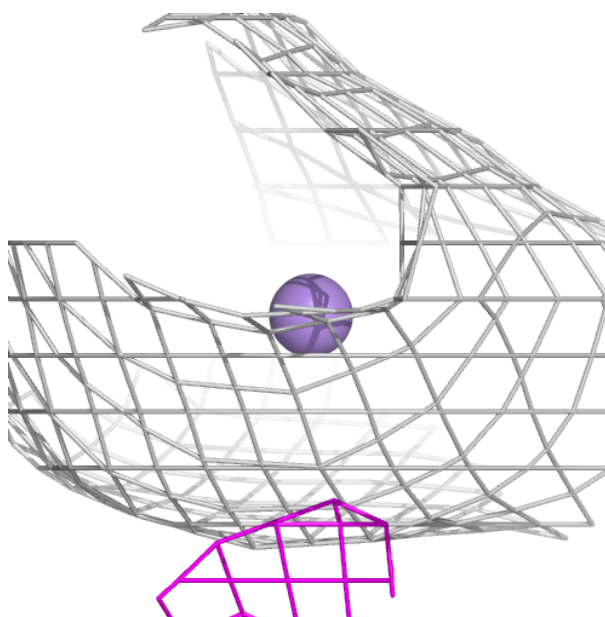
**Electron density around CLR E 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



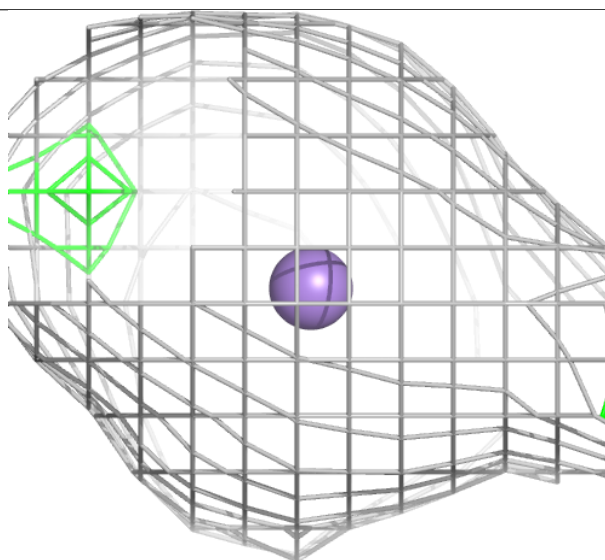
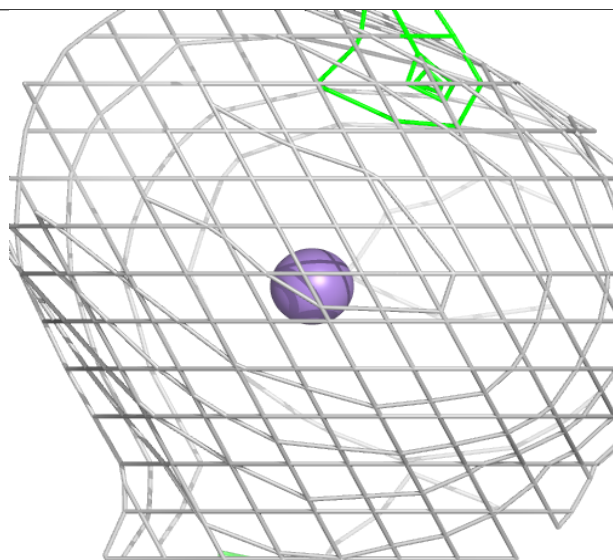
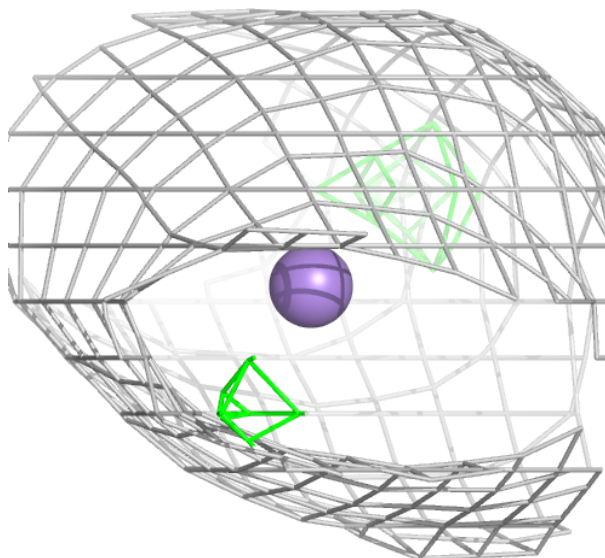
Electron density around MN C 1103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



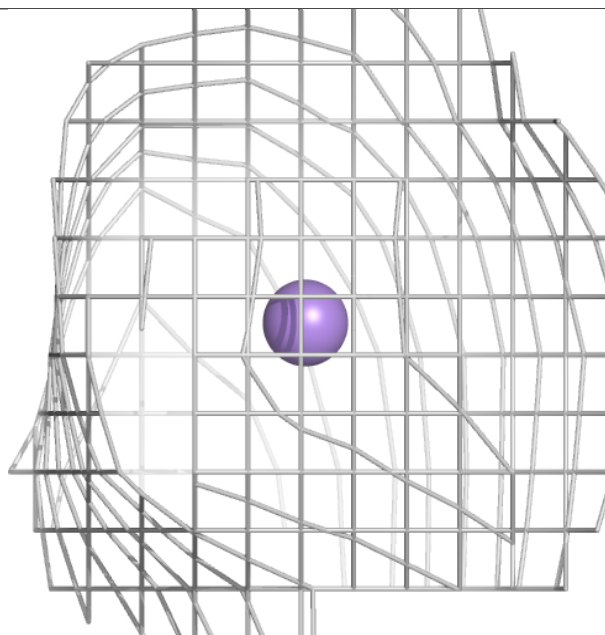
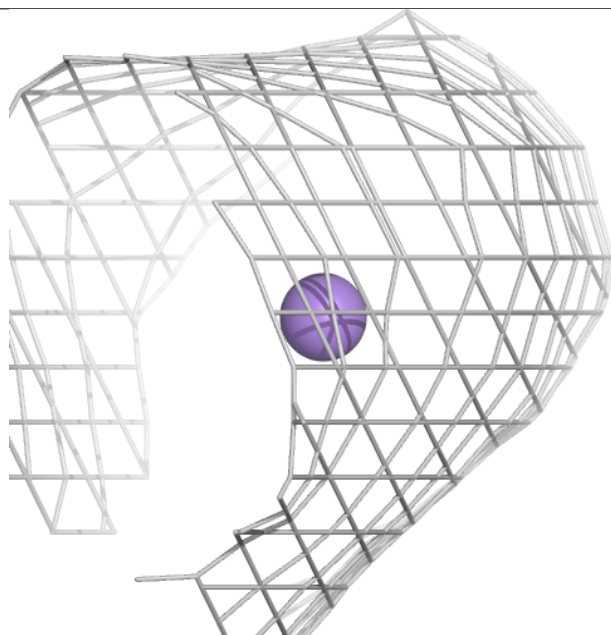
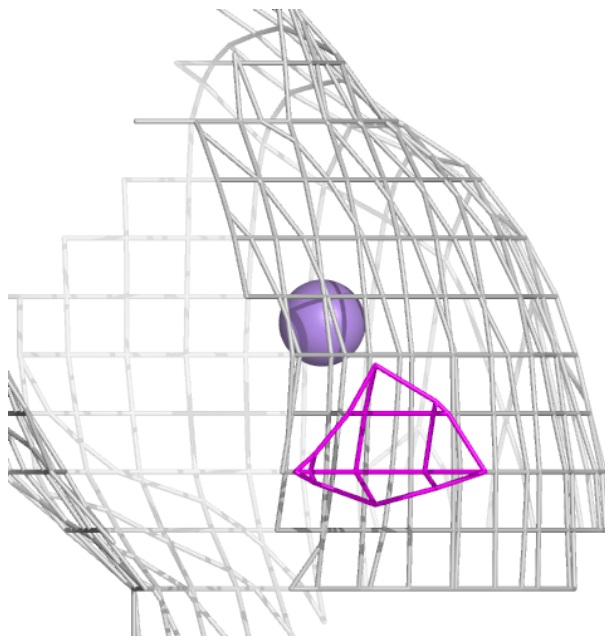
Electron density around MN A 1103:

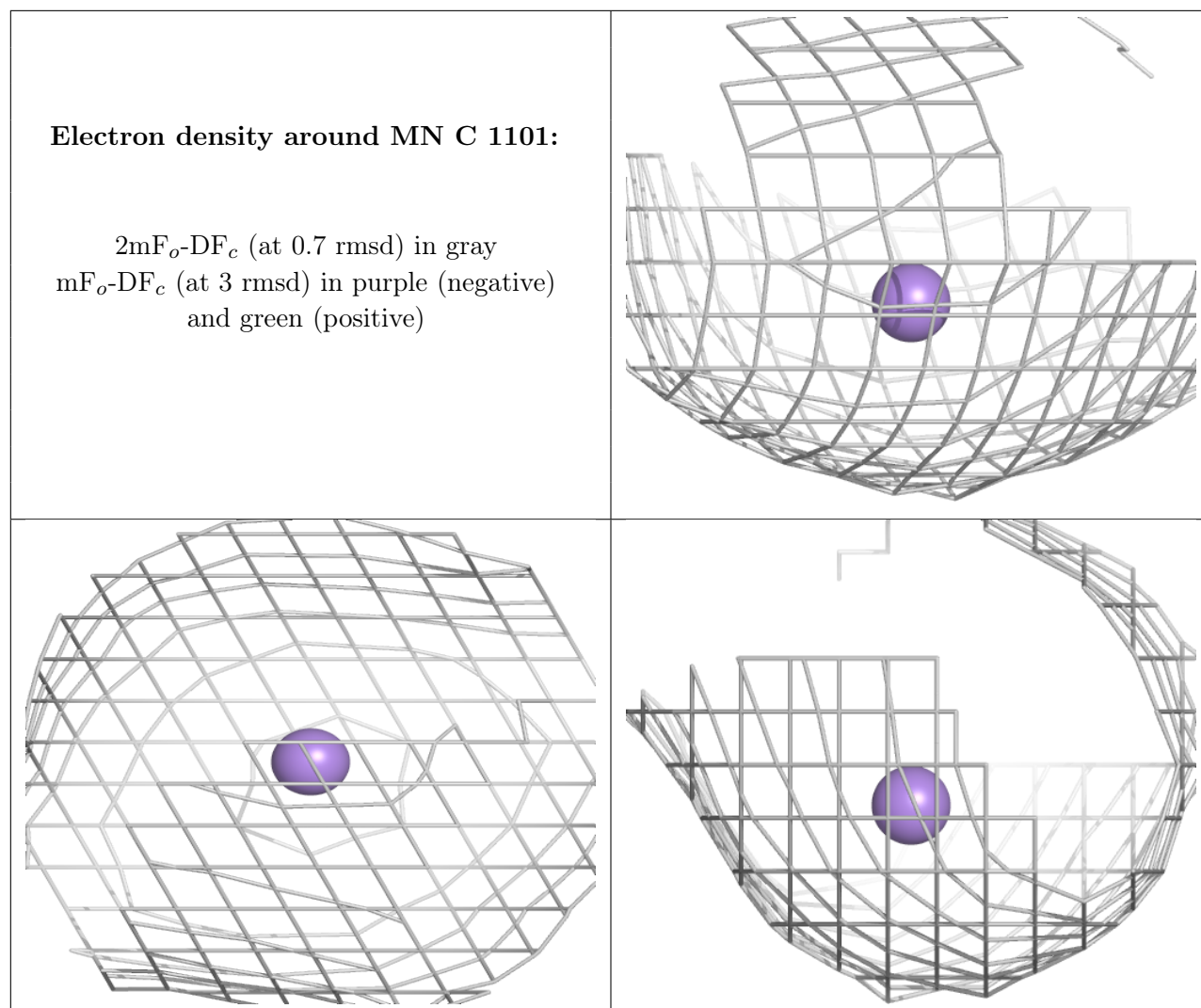
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.