Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 12:17 PM JST

PDB ID	:	8JBL
Title	:	Crystal structure of Na+,K+-ATPase in the E1.Mg2+ state
Authors	:	Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on	:	2023-05-09
Resolution	:	3.00 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:

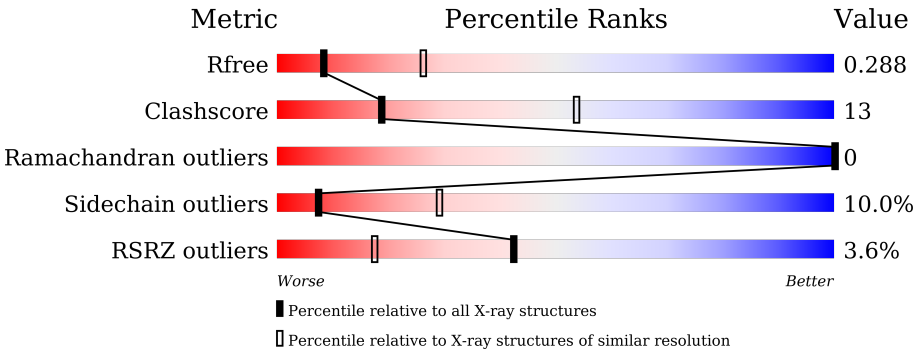
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	4% 64% 31%
1	C	1021	3% 64% 29%
2	B	303	3% 59% 33% 5%
2	D	303	7% 64% 29%
3	E	65	38% 11% 49%
3	G	65	2% 42% 12% 46%

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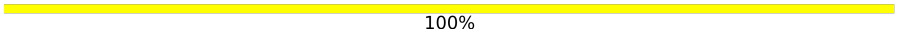
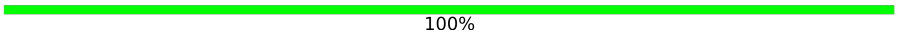
Mol	Chain	Length	Quality of chain
4	F	6	
5	H	5	
6	I	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PCW	A	1113	-	-	-	X
10	PCW	C	1110	-	-	-	X
11	NAG	D	401	-	-	-	X
4	NAG	F	1	-	-	-	X
4	MAN	F	5	-	-	-	X
4	MAN	F	6	-	-	-	X
5	NAG	H	2	-	-	-	X
5	MAN	H	4	-	-	-	X
5	MAN	H	5	-	-	-	X
6	NAG	I	1	-	-	-	X
9	PC1	A	1106	-	-	-	X

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			

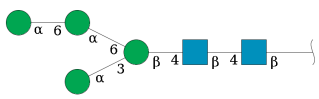
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

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.

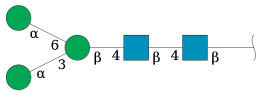
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	35	Total	C	N	O	0	0	0
			285	192	46	47			
3	E	33	Total	C	N	O	0	0	0
			262	179	38	45			

- 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
			Total	C	N	O			
5	H	5	61	34	2	25	0	0	0

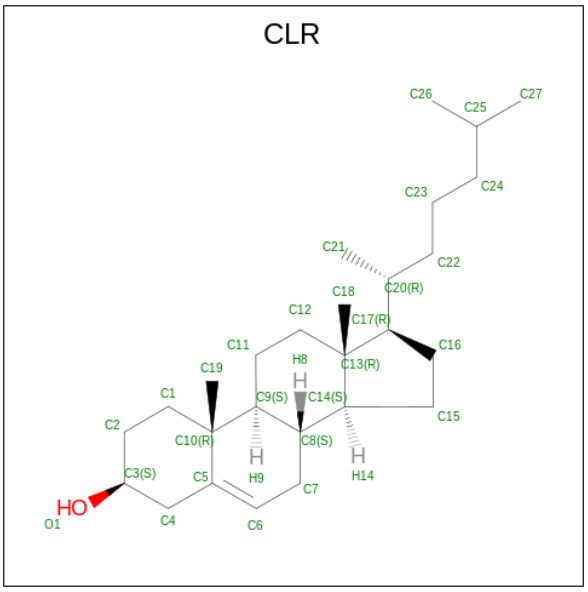
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

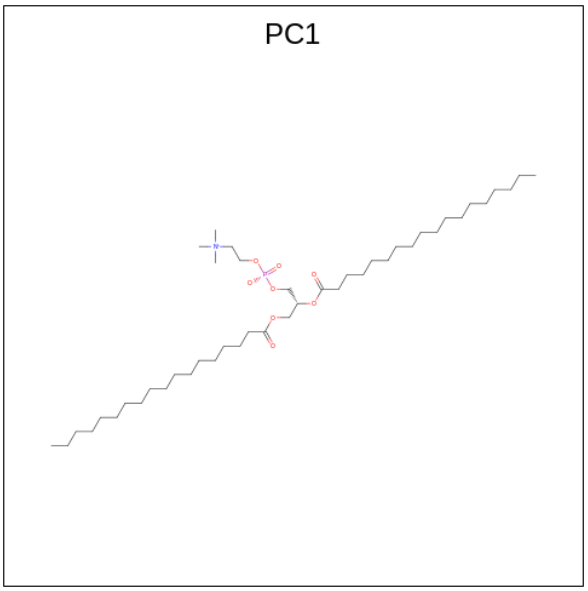
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	A	3	3	3	0	0
7	C	3	Total	Mg	0	0
			3	3		

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



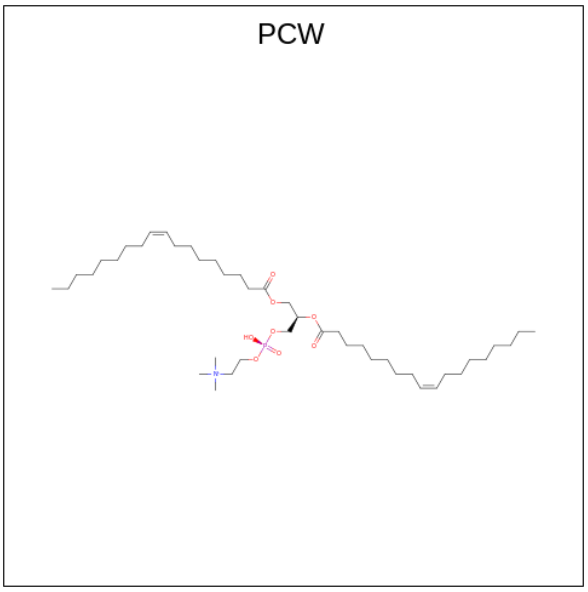
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 28 27 1	0	0
8	A	1	Total C O 28 27 1	0	0
8	A	1	Total C O 28 27 1	0	0
8	C	1	Total C O 28 27 1	0	0
8	C	1	Total C O 28 27 1	0	0
8	E	1	Total C O 28 27 1	0	0

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



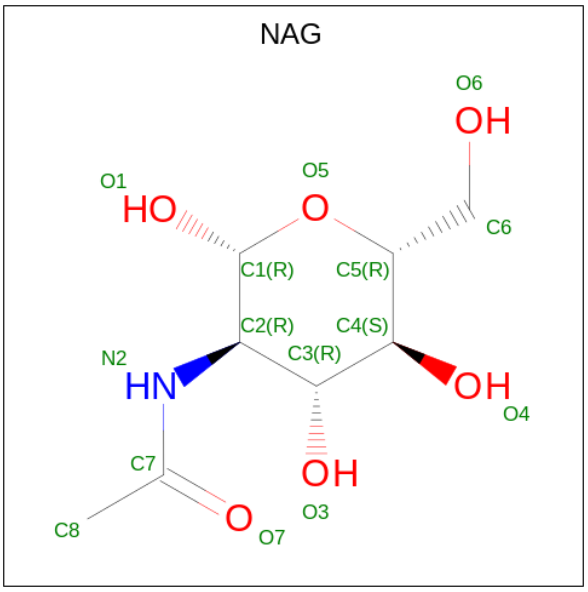
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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



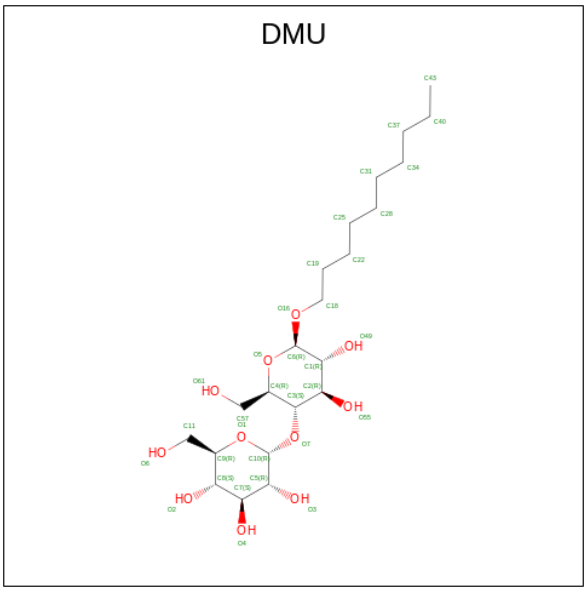
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O P 22 12 1 8 1	0	0
10	A	1	Total C N O P 22 12 1 8 1	0	0
10	A	1	Total C N O P 22 12 1 8 1	0	0
10	A	1	Total C N O P 22 12 1 8 1	0	0
10	A	1	Total C N O P 22 12 1 8 1	0	0
10	A	1	Total C N O P 22 12 1 8 1	0	0
10	A	1	Total C N O P 54 44 1 8 1	0	0
10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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: 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.

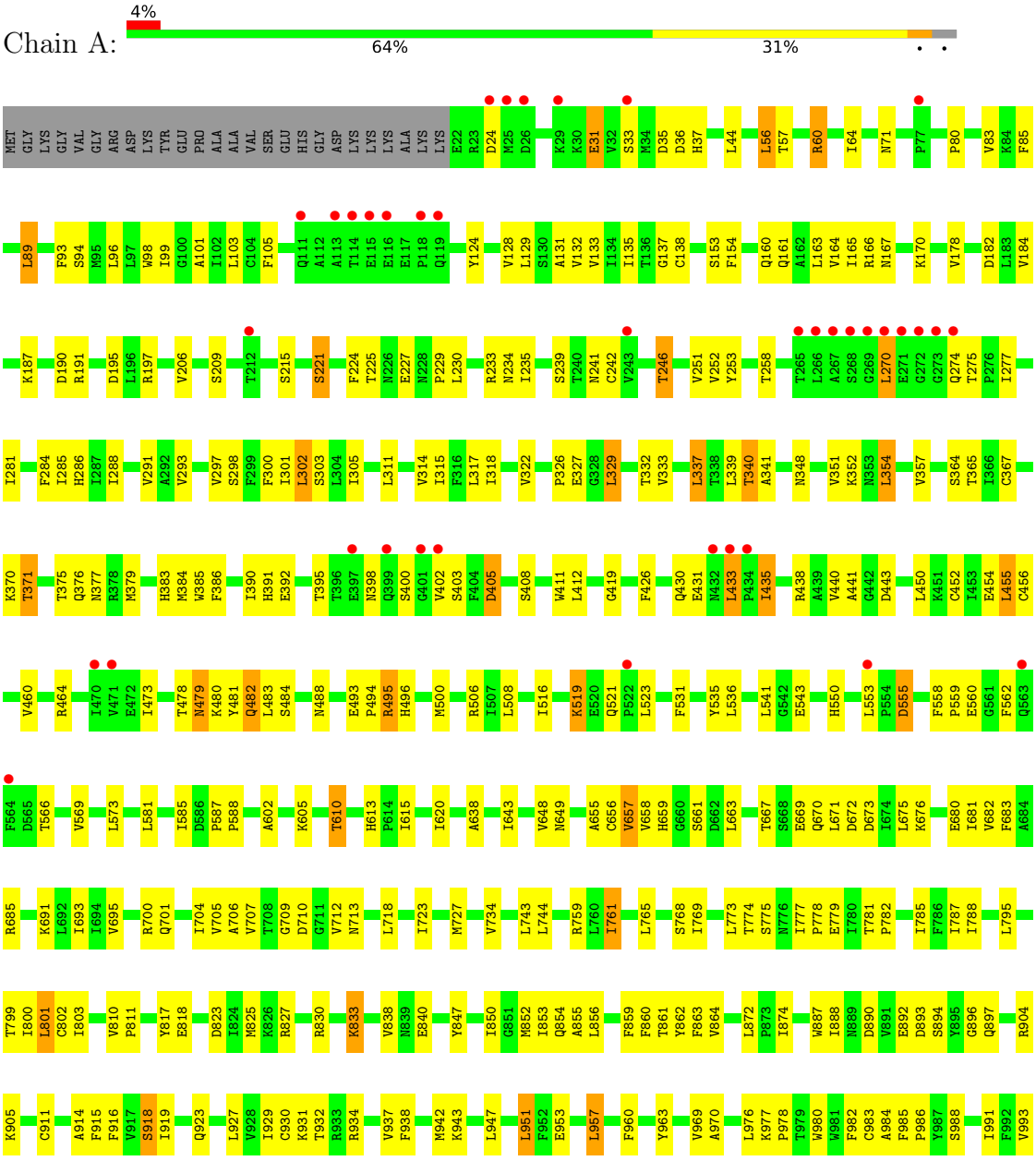
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	19	Total O 19 19	0	0
13	C	12	Total O 12 12	0	0
13	D	2	Total O 2 2	0	0

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 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.

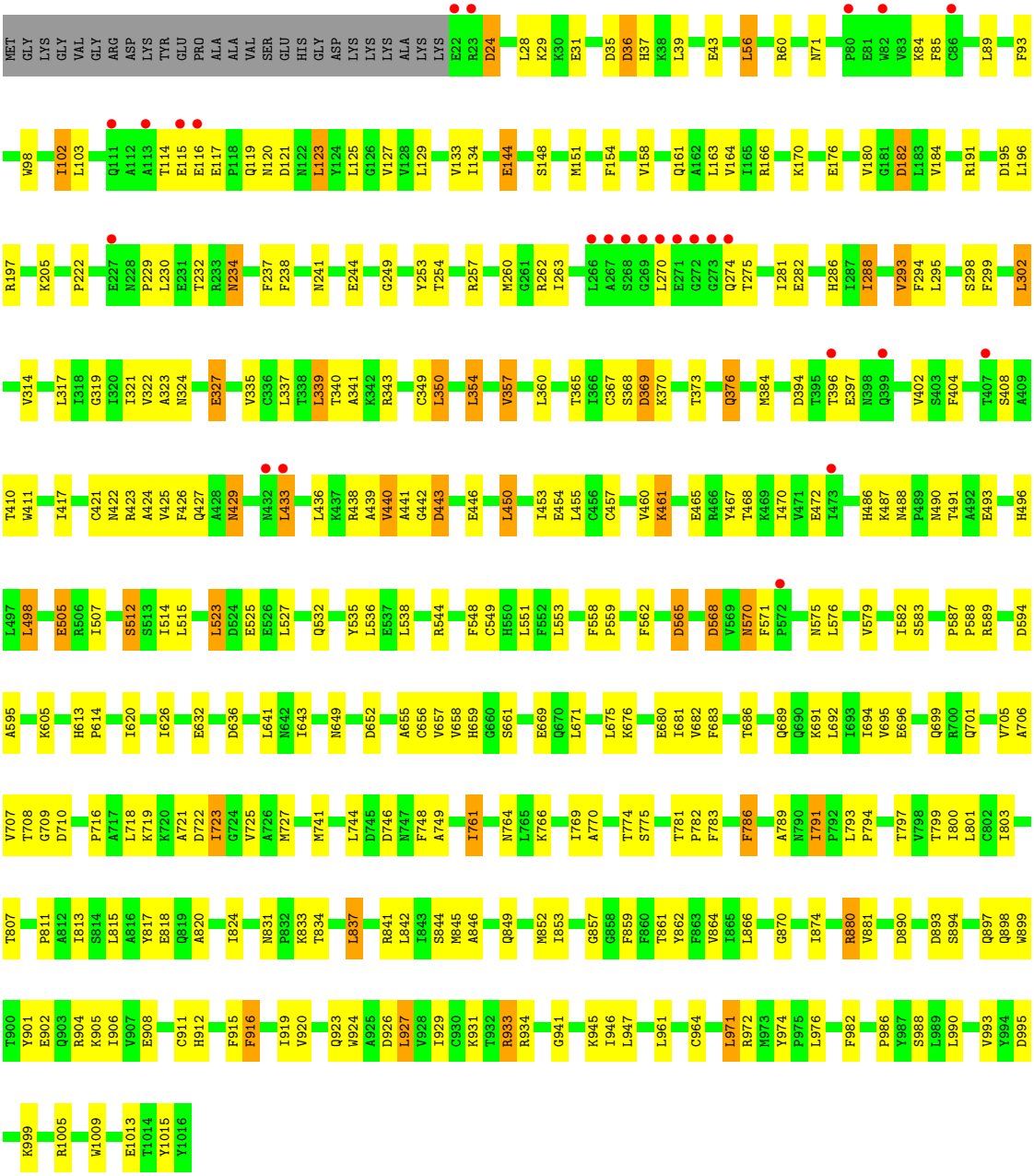
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

Chain A:



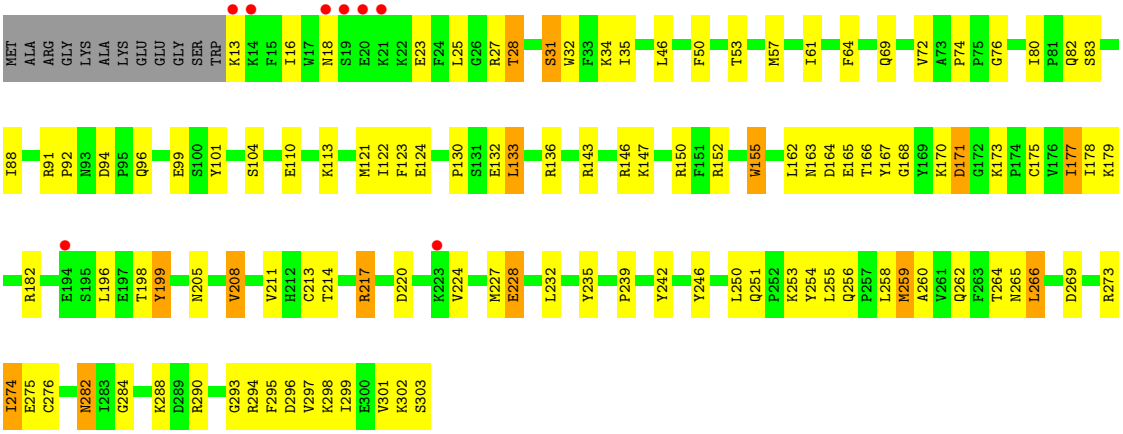
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

Chain C:



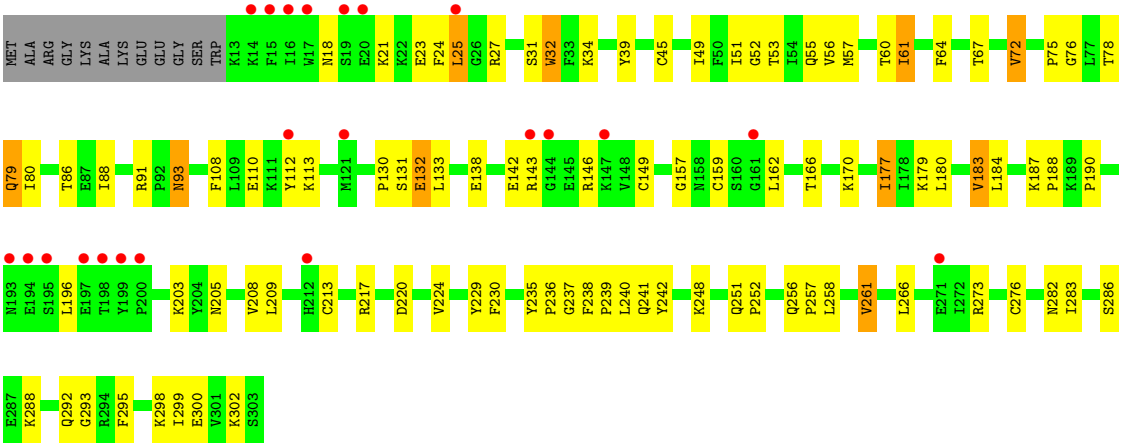
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



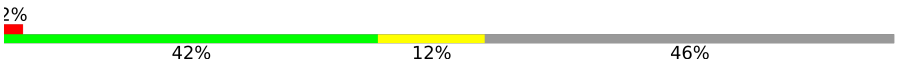
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



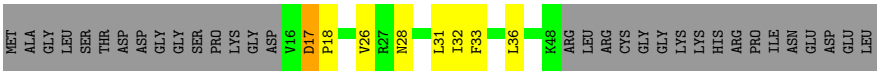
• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:



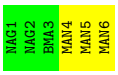
• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:



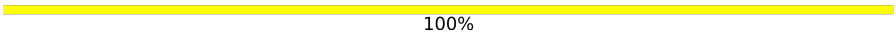
• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



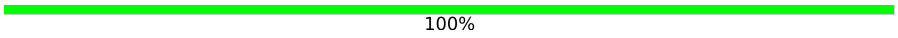
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	196.80Å 74.32Å 163.55Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	11.99 – 3.00 29.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	53.0 (11.99-3.00) 53.8 (29.98-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.233 , 0.282 0.237 , 0.288	Depositor DCC
R_{free} test set	2311 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	82.7	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21682	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/7873	0.53	0/10683
1	C	0.28	0/7873	0.53	0/10683
2	B	0.27	0/2449	0.53	0/3301
2	D	0.28	0/2449	0.54	0/3301
3	E	0.30	0/268	0.46	0/364
3	G	0.27	0/291	0.52	0/393
All	All	0.28	0/21203	0.53	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

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	207	0
1	C	7723	0	7775	213	0
2	B	2386	0	2362	68	0
2	D	2386	0	2362	60	0
3	E	262	0	268	9	0
3	G	285	0	296	11	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	84	0	138	7	0
8	C	56	0	92	5	0
8	E	28	0	46	2	0
9	A	162	0	264	23	0
10	A	186	0	192	11	0
10	C	154	0	126	4	0
11	D	14	0	13	0	0
12	E	33	0	42	7	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	568	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 13.

All (568) 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:C:1009:TRP:HE1	2:D:34:LYS:HD3	1.37	0.87
1:A:340:THR:HG21	1:A:761:ILE:HG12	1.62	0.80
1:C:565:ASP:HB2	1:C:570:ASN:HD22	1.44	0.80
9:A:1108:PC1:H372	8:C:1104:CLR:H71	1.64	0.80
9:A:1108:PC1:H2E2	9:A:1108:PC1:H392	1.65	0.79
1:A:195:ASP:OD2	1:A:258:THR:HA	1.82	0.79
1:C:775:SER:HB3	1:C:923:GLN:HE22	1.47	0.78
1:A:986:PRO:HG2	8:A:1104:CLR:H181	1.64	0.76
1:C:467:TYR:HB3	1:C:486:HIS:HB3	1.67	0.76
1:A:365:THR:HB	1:A:705:VAL:HG12	1.69	0.75
2:B:171:ASP:OD1	2:B:171:ASP:N	2.20	0.74
1:C:24:ASP:HA	1:C:28:LEU:HD13	1.70	0.73
1:A:209:SER:HB3	1:A:215:SER:HA	1.71	0.72
2:B:282:ASN:OD1	2:B:282:ASN:N	2.21	0.72
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.71	0.72
1:C:340:THR:HG21	1:C:761:ILE:HG12	1.72	0.72
1:C:659:HIS:HD2	1:C:661:SER:H	1.38	0.71
1:A:473:ILE:HB	1:A:483:LEU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ARG:HB3	10:A:1112:PCW:H52	1.73	0.71
1:C:512:SER:HB2	1:C:575:ASN:HA	1.72	0.70
3:G:49:ARG:HB2	3:E:28:ASN:HD21	1.56	0.70
2:B:96:GLN:HA	2:B:99:GLU:HG3	1.73	0.69
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.75	0.68
1:A:856:LEU:HD12	2:B:46:LEU:HG	1.76	0.68
1:C:114:THR:HG22	1:C:115:GLU:H	1.58	0.67
2:D:273:ARG:HG2	2:D:298:LYS:HB3	1.76	0.67
9:A:1111:PC1:H231	12:E:102:DMU:H8	1.77	0.66
1:A:33:SER:HB3	1:A:229:PRO:HG3	1.77	0.66
1:A:942:MET:HB2	12:E:102:DMU:H6	1.77	0.66
9:A:1106:PC1:H3D2	9:A:1106:PC1:H2B1	1.77	0.66
1:A:778:PRO:HG3	1:A:854:GLN:HE21	1.61	0.66
1:A:224:PHE:HZ	1:A:227:GLU:HG2	1.60	0.66
1:A:35:ASP:OD2	1:A:235:ILE:HD13	1.96	0.65
1:C:811:PRO:HB3	1:C:927:LEU:HD13	1.78	0.65
1:A:302:LEU:HD13	1:A:787:ILE:HG12	1.78	0.65
1:A:132:VAL:HG11	1:A:801:LEU:HD23	1.77	0.65
1:C:281:ILE:HD11	1:C:837:LEU:HD22	1.79	0.65
1:A:165:ILE:HD13	1:A:170:LYS:HB3	1.77	0.65
2:D:75:PRO:HG3	2:D:183:VAL:HG21	1.79	0.65
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	1.79	0.65
8:A:1105:CLR:H151	3:G:33:PHE:CZ	2.32	0.64
1:C:945:LYS:HG3	1:C:946:ILE:HD12	1.79	0.64
2:B:91:ARG:HD3	2:B:94:ASP:HB2	1.79	0.64
1:A:840:GLU:OE2	9:A:1106:PC1:H142	1.98	0.64
2:B:166:THR:HG21	2:B:170:LYS:HB3	1.80	0.64
1:C:831:ASN:HD21	1:C:834:THR:HB	1.63	0.64
1:C:559:PRO:HD2	1:C:562:PHE:HB2	1.81	0.63
1:A:602:ALA:HB1	1:A:759:ARG:HH12	1.64	0.63
8:A:1105:CLR:H17	9:A:1111:PC1:H3G1	1.80	0.63
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.80	0.63
1:A:559:PRO:HD2	1:A:562:PHE:HD1	1.63	0.63
1:A:493:GLU:OE2	1:A:495:ARG:HA	1.99	0.62
1:A:281:ILE:HG23	1:A:329:LEU:HD23	1.81	0.62
1:C:370:LYS:HE2	1:C:620:ILE:HG13	1.82	0.62
1:A:536:LEU:HD22	1:A:615:ILE:HG13	1.82	0.62
1:A:803:ILE:HD13	1:A:919:ILE:HG21	1.82	0.62
1:A:951:LEU:HD22	9:A:1111:PC1:H391	1.82	0.62
2:B:155:TRP:CD1	2:B:232:LEU:HA	2.34	0.61
1:C:538:LEU:HD13	1:C:583:SER:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:HIS:HB3	1:C:553:LEU:HD12	1.82	0.61
1:C:919:ILE:O	1:C:923:GLN:HG2	1.99	0.61
1:C:880:ARG:HH11	1:C:880:ARG:HB3	1.66	0.60
2:B:124:GLU:HB3	2:B:147:LYS:HB3	1.83	0.60
2:B:166:THR:HG23	2:B:168:GLY:H	1.67	0.60
1:C:335:VAL:HG11	1:C:813:ILE:HG23	1.83	0.60
1:C:470:ILE:HD11	1:C:487:LYS:HG3	1.84	0.60
1:C:337:LEU:HD23	1:C:354:LEU:HD22	1.84	0.60
1:C:454:GLU:OE2	1:C:460:VAL:HG22	2.02	0.60
1:C:657:VAL:HA	1:C:682:VAL:O	2.01	0.60
1:A:759:ARG:NH1	1:A:825:MET:SD	2.75	0.59
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.83	0.59
1:C:691:LYS:O	1:C:695:VAL:HG23	2.02	0.59
1:A:775:SER:HB3	1:A:923:GLN:HE22	1.68	0.59
1:A:270:LEU:HD23	1:A:270:LEU:H	1.66	0.59
1:A:281:ILE:HG13	1:A:333:VAL:HG21	1.85	0.59
1:A:569:VAL:HG11	1:A:573:LEU:HD11	1.85	0.59
1:C:995:ASP:OD2	1:C:999:LYS:HE2	2.03	0.59
2:D:177:ILE:HD11	2:D:258:LEU:HD22	1.84	0.59
9:A:1108:PC1:H3H2	8:C:1104:CLR:H242	1.84	0.59
1:C:422:ASN:HA	1:C:446:GLU:OE2	2.02	0.59
1:A:454:GLU:HG2	1:A:460:VAL:HG23	1.84	0.59
2:D:76:GLY:HA2	2:D:293:GLY:H	1.68	0.59
2:B:76:GLY:HA2	2:B:293:GLY:H	1.68	0.59
3:G:47:SER:HB2	3:G:50:LEU:HB2	1.85	0.59
1:C:505:GLU:HG3	1:C:535:TYR:HE1	1.68	0.59
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.37	0.59
2:D:133:LEU:HD13	2:D:187:LYS:HD3	1.85	0.59
1:A:480:LYS:HD3	1:A:506:ARG:CZ	2.33	0.58
3:E:33:PHE:HD1	12:E:102:DMU:H23	1.68	0.58
1:C:658:VAL:HB	1:C:683:PHE:HD2	1.67	0.58
1:C:766:LYS:HD2	1:C:933:ARG:HH22	1.69	0.58
1:A:371:THR:HG22	1:A:377:ASN:HD22	1.69	0.58
9:A:1108:PC1:H32	2:D:60:THR:HG23	1.85	0.58
2:D:166:THR:HG21	2:D:170:LYS:HB2	1.86	0.58
10:A:1116:PCW:H431	10:A:1116:PCW:H20	1.85	0.57
1:A:785:ILE:HG13	1:A:859:PHE:CE1	2.39	0.57
1:C:558:PHE:HZ	1:C:571:PHE:HA	1.68	0.57
1:A:440:VAL:HG12	1:A:441:ALA:H	1.69	0.57
1:A:405:ASP:OD1	1:A:405:ASP:N	2.29	0.57
2:B:28:THR:HG23	2:B:31:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASN:OD1	1:A:479:ASN:N	2.37	0.57
1:C:769:ILE:HD12	1:C:837:LEU:HD23	1.87	0.57
1:C:408:SER:HB3	1:C:411:TRP:HB3	1.86	0.57
1:A:938:PHE:HA	9:A:1111:PC1:H12	1.87	0.57
2:B:266:LEU:HD13	2:B:301:VAL:HG21	1.86	0.57
1:A:379:MET:HA	1:A:585:ILE:O	2.05	0.57
1:C:426:PHE:CE2	1:C:438:ARG:HD2	2.39	0.57
2:D:110:GLU:HG2	2:D:113:LYS:HE3	1.86	0.57
2:D:27:ARG:HH21	2:D:31:SER:HG	1.52	0.56
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.85	0.56
2:D:27:ARG:HG3	2:D:32:TRP:HD1	1.70	0.56
1:A:803:ILE:HG12	1:A:916:PHE:CD1	2.41	0.56
1:A:938:PHE:CE1	9:A:1108:PC1:H362	2.40	0.56
1:C:710:ASP:HB3	1:C:727:MET:HG3	1.87	0.56
2:D:51:ILE:O	2:D:55:GLN:HG2	2.06	0.56
2:B:23:GLU:HA	2:B:28:THR:HA	1.87	0.56
2:D:130:PRO:HB3	2:D:208:VAL:HG23	1.86	0.56
1:C:927:LEU:HD21	1:C:947:LEU:HG	1.86	0.56
2:D:131:SER:HB2	2:D:241:GLN:HB3	1.87	0.56
2:D:80:ILE:HG21	2:D:108:PHE:CD2	2.41	0.55
1:A:164:VAL:HG12	1:A:184:VAL:HG22	1.89	0.55
1:C:373:THR:HG22	1:C:748:PHE:HB2	1.87	0.55
1:A:799:THR:O	1:A:803:ILE:HG13	2.06	0.55
1:C:24:ASP:OD2	1:C:28:LEU:HD22	2.06	0.55
1:C:164:VAL:HG12	1:C:184:VAL:HG22	1.88	0.55
1:C:294:PHE:HD2	1:C:295:LEU:HD23	1.71	0.55
2:D:138:GLU:HG3	2:D:143:ARG:HH21	1.71	0.55
1:A:191:ARG:HA	1:A:241:ASN:HD22	1.72	0.55
1:A:778:PRO:HG3	1:A:854:GLN:NE2	2.21	0.55
1:A:1009:TRP:HB2	10:A:1113:PCW:H73	1.89	0.55
1:C:1009:TRP:NE1	2:D:34:LYS:HD3	2.16	0.55
1:C:337:LEU:HG	1:C:357:VAL:HG11	1.87	0.54
2:D:132:GLU:OE2	2:D:133:LEU:HG	2.08	0.54
1:C:197:ARG:O	1:C:249:GLY:HA2	2.07	0.54
1:A:57:THR:HG23	1:A:167:ASN:HD22	1.73	0.54
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.88	0.54
2:B:178:ILE:HB	2:B:259:MET:HE3	1.89	0.54
1:A:252:VAL:HG23	1:A:253:TYR:HD2	1.73	0.54
1:A:938:PHE:HB3	9:A:1108:PC1:H321	1.89	0.54
1:C:410:THR:HG23	1:C:515:LEU:HD22	1.90	0.54
1:C:695:VAL:HG22	1:C:707:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:THR:HG22	1:C:725:VAL:HB	1.90	0.54
9:A:1108:PC1:H3H1	1:C:986:PRO:HB3	1.90	0.54
1:C:453:ILE:HG13	1:C:454:GLU:N	2.23	0.54
1:A:982:PHE:HA	1:A:985:PHE:HD1	1.71	0.53
1:A:914:ALA:HB2	1:A:976:LEU:HD11	1.90	0.53
1:A:531:PHE:HE2	1:A:581:LEU:HD21	1.73	0.53
1:A:982:PHE:HA	1:A:985:PHE:CD1	2.44	0.53
1:C:933:ARG:HB2	1:C:1015:TYR:HE1	1.74	0.53
1:A:284:PHE:CD1	1:A:838:VAL:HG11	2.44	0.53
1:A:398:ASN:HD21	1:A:400:SER:HB2	1.74	0.53
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.24	0.53
2:D:239:PRO:HB2	2:D:241:GLN:HG2	1.91	0.53
1:A:970:ALA:HB1	10:A:1116:PCW:H39	1.91	0.53
1:C:897:GLN:OE1	2:D:184:LEU:N	2.40	0.53
1:A:375:THR:HA	1:A:588:PRO:HA	1.91	0.52
1:C:197:ARG:NH2	1:C:222:PRO:O	2.42	0.52
1:C:946:ILE:HD12	1:C:946:ILE:H	1.73	0.52
2:D:79:GLN:OE1	2:D:86:THR:HG22	2.09	0.52
1:A:376:GLN:NE2	1:A:587:PRO:HG2	2.24	0.52
1:A:101:ALA:O	1:A:105:PHE:HD2	1.93	0.52
1:A:281:ILE:HD11	1:A:769:ILE:HD11	1.91	0.52
1:A:80:PRO:HD2	1:A:83:VAL:HG21	1.91	0.52
1:A:370:LYS:HE2	1:A:620:ILE:HD12	1.91	0.52
1:C:443:ASP:OD1	1:C:443:ASP:N	2.42	0.52
1:A:960:PHE:HZ	10:A:1116:PCW:H171	1.73	0.52
1:C:709:GLY:HA3	1:C:718:LEU:HD11	1.91	0.52
1:A:937:VAL:HG22	1:A:996:GLU:OE2	2.10	0.52
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.73	0.52
1:A:638:ALA:HB2	1:A:648:VAL:HG21	1.91	0.52
1:A:221:SER:N	1:A:233:ARG:O	2.40	0.52
1:A:775:SER:HB3	1:A:923:GLN:NE2	2.23	0.52
10:A:1116:PCW:H361	10:A:1116:PCW:H141	1.92	0.51
1:A:709:GLY:HA3	1:A:718:LEU:HD21	1.93	0.51
1:A:1007:GLY:H	1:A:1011:GLU:CD	2.12	0.51
1:C:649:ASN:HB3	1:C:652:ASP:OD2	2.10	0.51
2:D:217:ARG:HH12	2:D:273:ARG:HH21	1.58	0.51
3:E:17:ASP:HB2	3:E:18:PRO:HD3	1.91	0.51
1:C:961:LEU:HD22	1:C:971:LEU:HD11	1.92	0.51
1:A:488:ASN:HB3	1:A:493:GLU:OE2	2.10	0.51
1:A:862:TYR:HD2	1:A:911:CYS:HB3	1.75	0.51
1:C:369:ASP:N	1:C:369:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:LYS:H	1:A:833:LYS:HD2	1.76	0.51
2:B:143:ARG:HB3	2:B:146:ARG:NH1	2.25	0.51
1:C:426:PHE:CZ	1:C:450:LEU:HD22	2.46	0.51
2:D:300:GLU:OE1	2:D:302:LYS:HB2	2.11	0.51
1:C:514:ILE:HG13	1:C:523:LEU:HG	1.93	0.51
1:A:386:PHE:CZ	1:A:411:TRP:HB2	2.46	0.51
1:A:893:ASP:OD2	1:A:897:GLN:HB2	2.11	0.51
1:A:93:PHE:HZ	1:A:322:VAL:HA	1.75	0.50
1:A:659:HIS:HD2	1:A:661:SER:H	1.59	0.50
2:B:177:ILE:HA	2:B:260:ALA:HA	1.93	0.50
1:C:323:ALA:HB2	1:C:800:ILE:HG21	1.92	0.50
1:C:866:LEU:HG	1:C:911:CYS:SG	2.51	0.50
1:A:435:ILE:HG13	1:A:455:LEU:HG	1.93	0.50
8:A:1105:CLR:H222	9:A:1111:PC1:H3E1	1.94	0.50
1:A:225:THR:HG21	1:A:233:ARG:HD2	1.92	0.50
1:A:131:ALA:O	1:A:135:ILE:HG12	2.10	0.50
1:C:205:LYS:HD2	1:C:244:GLU:OE2	2.12	0.50
1:C:789:ALA:HB3	1:C:791:ILE:HD12	1.92	0.50
1:A:496:HIS:NE2	1:A:558:PHE:O	2.40	0.50
1:C:450:LEU:HD23	1:C:454:GLU:HG3	1.93	0.50
1:C:532:GLN:O	1:C:536:LEU:HG	2.11	0.50
2:B:275:GLU:OE2	2:B:294:ARG:HD2	2.11	0.50
1:C:905:LYS:NZ	1:C:908:GLU:OE1	2.44	0.50
5:H:1:NAG:H4	5:H:2:NAG:H83	1.93	0.50
1:C:93:PHE:HZ	1:C:322:VAL:HA	1.77	0.49
1:C:365:THR:HB	1:C:705:VAL:HG12	1.94	0.49
1:C:870:GLY:O	1:C:893:ASP:HB2	2.12	0.49
2:D:217:ARG:NH1	2:D:273:ARG:HH21	2.09	0.49
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.93	0.49
1:A:98:TRP:NE1	1:A:133:VAL:HG11	2.27	0.49
8:A:1105:CLR:H122	9:A:1111:PC1:H3I2	1.94	0.49
3:G:40:VAL:HG21	3:E:36:LEU:HD11	1.94	0.49
1:A:96:LEU:HG	1:A:318:ILE:HG12	1.95	0.49
3:G:47:SER:CB	3:G:50:LEU:HB2	2.42	0.49
1:C:116:GLU:HG2	1:C:117:GLU:H	1.78	0.49
2:D:229:TYR:HD2	2:D:236:PRO:HB3	1.77	0.49
1:C:89:LEU:HD21	1:C:134:ILE:HA	1.95	0.49
1:C:461:LYS:O	1:C:465:GLU:HB2	2.12	0.49
1:C:1009:TRP:HZ2	2:D:34:LYS:HB3	1.76	0.49
2:D:91:ARG:HA	2:D:302:LYS:O	2.10	0.49
1:A:370:LYS:HB3	1:A:610:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:GLU:HB3	9:A:1108:PC1:H292	1.94	0.49
1:A:89:LEU:HD22	1:A:137:GLY:HA3	1.94	0.49
1:A:494:PRO:HB3	1:A:555:ASP:HB2	1.93	0.49
2:B:110:GLU:HG2	2:B:113:LYS:HE3	1.94	0.49
1:A:99:ILE:O	1:A:103:LEU:HG	2.12	0.49
1:A:890:ASP:OD1	1:A:890:ASP:N	2.46	0.49
2:B:290:ARG:HD2	2:B:296:ASP:OD2	2.13	0.49
1:A:433:LEU:O	1:A:438:ARG:NH2	2.41	0.48
1:A:823:ASP:HB2	1:A:934:ARG:HD2	1.94	0.48
1:A:1005:ARG:HH22	10:A:1113:PCW:H72	1.78	0.48
9:A:1111:PC1:H261	1:C:982:PHE:CZ	2.48	0.48
1:A:887:TRP:O	2:B:82:GLN:NE2	2.42	0.48
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.96	0.48
1:A:479:ASN:HB3	1:A:481:TYR:CZ	2.49	0.48
2:B:269:ASP:HA	2:B:302:LYS:HG3	1.95	0.48
1:C:565:ASP:HB2	1:C:570:ASN:ND2	2.22	0.48
1:A:129:LEU:O	1:A:133:VAL:HG23	2.13	0.48
2:D:286:SER:HB2	2:D:292:GLN:HB3	1.94	0.48
1:C:902:GLU:O	1:C:906:ILE:HG12	2.14	0.48
2:B:213:CYS:HA	2:B:276:CYS:HA	1.94	0.48
1:C:234:ASN:OD1	1:C:234:ASN:N	2.46	0.48
1:A:365:THR:HA	1:A:605:LYS:O	2.12	0.48
1:A:430:GLN:O	1:A:438:ARG:CZ	2.62	0.48
1:A:613:HIS:HD2	1:A:615:ILE:H	1.59	0.48
1:A:669:GLU:N	1:A:669:GLU:OE1	2.47	0.48
2:B:27:ARG:NH1	2:B:35:ILE:HG21	2.29	0.48
1:A:853:ILE:HG21	1:A:991:ILE:HG13	1.95	0.48
1:C:37:HIS:HB2	1:C:234:ASN:ND2	2.29	0.48
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.95	0.48
1:A:60:ARG:O	1:A:64:ILE:HG13	2.13	0.48
1:C:589:ARG:NH1	1:C:746:ASP:O	2.47	0.48
1:A:667:THR:HG23	1:A:670:GLN:H	1.79	0.48
1:C:119:GLN:OE1	2:D:288:LYS:NZ	2.47	0.48
1:A:85:PHE:HE1	1:A:138:CYS:HG	1.61	0.47
1:A:293:VAL:O	1:A:297:VAL:HG22	2.14	0.47
2:B:13:LYS:HA	2:B:16:ILE:HD12	1.97	0.47
1:C:699:GLN:HE22	1:C:721:ALA:HA	1.77	0.47
1:A:419:GLY:O	1:A:464:ARG:NH2	2.47	0.47
1:C:783:PHE:CD2	1:C:793:LEU:HD11	2.49	0.47
1:C:658:VAL:HB	1:C:683:PHE:CD2	2.48	0.47
1:C:695:VAL:CG2	1:C:707:VAL:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.97	0.47
1:A:779:GLU:O	1:A:800:ILE:HD11	2.15	0.47
9:A:1108:PC1:H281	9:A:1108:PC1:H2B2	1.56	0.47
1:C:337:LEU:HB3	1:C:354:LEU:HD21	1.97	0.47
1:C:339:LEU:HD22	1:C:343:ARG:HE	1.79	0.47
2:D:49:ILE:O	2:D:53:THR:HG23	2.15	0.47
9:A:1111:PC1:H3G2	3:G:33:PHE:HE1	1.80	0.47
1:A:408:SER:HB3	1:A:411:TRP:HB3	1.96	0.47
1:A:778:PRO:HB2	1:A:919:ILE:HD11	1.97	0.47
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.97	0.47
2:B:132:GLU:HG3	2:B:133:LEU:HD12	1.97	0.47
1:C:890:ASP:OD1	1:C:898:GLN:NE2	2.47	0.47
2:D:18:ASN:HD21	2:D:23:GLU:HB2	1.80	0.47
2:D:21:LYS:HD2	2:D:21:LYS:HA	1.67	0.47
1:A:288:ILE:HA	1:A:291:VAL:HG22	1.95	0.47
1:A:978:PRO:HG3	8:A:1105:CLR:H22	1.95	0.47
2:B:262:GLN:HG2	2:B:264:THR:HG23	1.96	0.47
1:A:553:LEU:HD12	1:A:553:LEU:H	1.80	0.47
1:A:706:ALA:HA	1:A:723:ILE:O	2.14	0.47
1:A:785:ILE:HG13	1:A:859:PHE:HE1	1.80	0.47
1:C:93:PHE:CZ	1:C:322:VAL:HG22	2.50	0.47
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.50	0.47
2:D:248:LYS:HG2	2:D:252:PRO:HA	1.96	0.47
1:A:691:LYS:O	1:A:695:VAL:HG23	2.15	0.47
1:A:860:PHE:CZ	2:B:53:THR:HB	2.50	0.47
2:B:274:ILE:HD13	2:B:297:VAL:O	2.14	0.47
1:C:163:LEU:HD11	1:C:170:LYS:HB2	1.97	0.47
1:C:587:PRO:HA	1:C:588:PRO:HD3	1.85	0.47
1:A:333:VAL:HA	1:A:765:LEU:HD21	1.97	0.46
1:C:121:ASP:N	1:C:121:ASP:OD1	2.48	0.46
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.97	0.46
1:C:1009:TRP:CZ2	2:D:34:LYS:HB3	2.51	0.46
2:D:138:GLU:O	2:D:146:ARG:NH2	2.48	0.46
1:A:818:GLU:OE2	1:A:931:LYS:NZ	2.39	0.46
10:A:1116:PCW:H42	10:A:1116:PCW:H83	1.66	0.46
2:B:217:ARG:H	2:B:220:ASP:HB2	1.80	0.46
1:C:397:GLU:HA	1:C:455:LEU:HD11	1.97	0.46
1:A:348:ASN:HA	1:A:744:LEU:HB2	1.97	0.46
2:B:246:TYR:HB3	2:B:250:LEU:HB2	1.98	0.46
1:A:197:ARG:HD2	1:A:234:ASN:O	2.16	0.46
1:A:827:ARG:HE	1:A:934:ARG:HE	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:GLU:OE1	1:C:669:GLU:N	2.43	0.46
1:C:845:MET:HA	1:C:849:GLN:NE2	2.29	0.46
1:A:56:LEU:HD12	1:A:166:ARG:HG2	1.98	0.46
1:A:896:GLY:O	2:B:182:ARG:NH2	2.49	0.46
8:A:1105:CLR:H6	3:G:30:GLY:HA2	1.96	0.46
1:C:402:VAL:HG21	1:C:404:PHE:CE1	2.51	0.46
2:D:146:ARG:HB2	2:D:251:GLN:HE21	1.80	0.46
1:C:786:PHE:HA	1:C:791:ILE:HD13	1.97	0.46
1:C:906:ILE:HD12	1:C:974:TYR:CZ	2.50	0.46
1:C:924:TRP:CZ3	8:E:101:CLR:H242	2.51	0.46
1:C:945:LYS:HE3	1:C:946:ILE:HD11	1.96	0.46
1:C:84:LYS:HD2	1:C:84:LYS:HA	1.66	0.46
1:C:553:LEU:HB3	1:C:558:PHE:CD2	2.50	0.46
1:C:659:HIS:CD2	1:C:661:SER:H	2.26	0.46
1:A:385:TRP:HD1	1:A:390:ILE:HG12	1.81	0.46
1:A:781:THR:N	1:A:782:PRO:HD2	2.30	0.46
1:C:803:ILE:HD13	1:C:919:ILE:HG21	1.96	0.46
1:C:901:TYR:HD1	1:C:904:ARG:HH12	1.64	0.46
1:A:897:GLN:OE1	2:B:69:GLN:NE2	2.45	0.46
1:A:1003:ARG:O	10:A:1112:PCW:H82	2.15	0.46
1:C:56:LEU:HD11	1:C:182:ASP:CG	2.36	0.46
1:C:692:LEU:HD22	1:C:716:PRO:HB2	1.99	0.46
1:C:964:CYS:HA	3:E:31:LEU:HD21	1.98	0.46
1:A:993:VAL:HG23	9:A:1108:PC1:H2A1	1.98	0.45
1:C:764:ASN:HD21	1:C:818:GLU:N	2.14	0.45
1:C:857:GLY:O	1:C:861:THR:HG23	2.16	0.45
1:C:154:PHE:HE1	1:C:341:ALA:HB1	1.81	0.45
1:A:395:THR:OG1	1:A:400:SER:HB3	2.17	0.45
1:A:743:LEU:HD12	1:A:743:LEU:HA	1.86	0.45
2:B:239:PRO:HG2	2:B:242:TYR:CD1	2.51	0.45
1:C:781:THR:N	1:C:782:PRO:HD2	2.32	0.45
2:D:112:TYR:CZ	2:D:258:LEU:HD11	2.52	0.45
1:A:693:ILE:HD13	1:A:693:ILE:HA	1.83	0.45
1:C:426:PHE:CE1	1:C:450:LEU:HD22	2.51	0.45
1:C:551:LEU:HD13	1:C:576:LEU:HD23	1.97	0.45
1:C:632:GLU:HB3	1:C:636:ASP:HB2	1.98	0.45
1:C:905:LYS:HD3	1:C:905:LYS:HA	1.78	0.45
1:A:277:ILE:HG21	1:A:337:LEU:HD21	1.99	0.45
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.52	0.45
1:A:332:THR:HG21	1:A:768:SER:OG	2.17	0.45
1:A:695:VAL:HG22	1:A:707:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:VAL:HG23	1:A:734:VAL:HG11	1.99	0.45
2:B:110:GLU:HA	2:B:113:LYS:HE3	1.99	0.45
1:C:103:LEU:HD13	1:C:314:VAL:HG21	1.97	0.45
1:C:675:LEU:HD12	1:C:681:ILE:HD13	1.98	0.45
1:C:818:GLU:OE2	1:C:931:LYS:HG2	2.17	0.45
2:D:205:ASN:HB2	2:D:235:TYR:CE2	2.52	0.45
1:A:71:ASN:HB2	1:A:178:VAL:O	2.17	0.45
1:A:638:ALA:HB1	1:A:643:ILE:O	2.17	0.45
1:A:710:ASP:HB3	1:A:727:MET:HG3	1.99	0.45
1:C:424:ALA:HB2	1:C:442:GLY:HA3	1.98	0.45
2:D:190:PRO:HD3	2:D:240:LEU:HD21	1.99	0.45
1:A:888:ILE:O	1:A:904:ARG:NH2	2.50	0.45
1:C:595:ALA:HB2	1:C:749:ALA:HA	1.98	0.45
3:E:26:VAL:HG22	12:E:102:DMU:H36	1.99	0.45
1:A:872:LEU:H	1:A:894:SER:HB2	1.82	0.44
2:B:92:PRO:HD2	2:B:303:SER:HB2	1.99	0.44
1:C:426:PHE:HD1	1:C:440:VAL:HG13	1.82	0.44
1:A:495:ARG:HG2	1:A:560:GLU:HB2	1.98	0.44
1:A:672:ASP:O	1:A:676:LYS:HB2	2.16	0.44
1:C:327:GLU:H	1:C:327:GLU:HG3	1.47	0.44
1:A:124:TYR:O	1:A:128:VAL:HG23	2.17	0.44
1:A:364:SER:OG	1:A:704:ILE:N	2.49	0.44
1:A:375:THR:HG22	1:A:588:PRO:HA	1.99	0.44
1:A:376:GLN:HE21	1:A:587:PRO:HG2	1.82	0.44
2:B:220:ASP:O	2:B:224:VAL:HG23	2.18	0.44
1:C:36:ASP:HB2	1:C:39:LEU:HG	1.99	0.44
1:C:433:LEU:HD11	1:C:438:ARG:HA	1.98	0.44
2:B:123:PHE:HB3	2:B:150:ARG:CG	2.46	0.44
2:B:262:GLN:HE21	2:B:262:GLN:HB2	1.56	0.44
3:G:49:ARG:HB2	3:E:28:ASN:ND2	2.28	0.44
1:C:148:SER:HA	1:C:151:MET:HE2	1.99	0.44
1:C:498:LEU:HD22	1:C:551:LEU:HB3	2.00	0.44
1:C:915:PHE:O	1:C:919:ILE:HG12	2.18	0.44
1:A:206:VAL:HA	1:A:242:CYS:HA	2.00	0.44
1:A:426:PHE:CD1	1:A:440:VAL:HG13	2.52	0.44
1:A:963:TYR:HE1	3:G:26:VAL:HG12	1.82	0.44
1:C:422:ASN:OD1	1:C:423:ARG:N	2.51	0.44
1:C:429:ASN:OD1	1:C:429:ASN:N	2.50	0.44
1:C:166:ARG:NH2	1:C:182:ASP:OD1	2.43	0.44
1:C:656:CYS:SG	1:C:681:ILE:HG23	2.57	0.44
10:C:1110:PCW:H62	10:C:1110:PCW:H41	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.81	0.44
1:A:672:ASP:OD1	1:A:700:ARG:NE	2.45	0.44
1:A:788:ILE:HD12	9:A:1106:PC1:H2H1	1.99	0.44
2:B:136:ARG:HB2	2:B:246:TYR:CE2	2.53	0.44
2:B:196:LEU:HA	2:B:199:TYR:CZ	2.53	0.44
1:C:339:LEU:HD11	1:C:817:TYR:CD1	2.53	0.44
1:C:774:THR:HG22	1:C:846:ALA:HA	1.98	0.44
1:A:300:PHE:CD1	1:A:317:LEU:HD12	2.53	0.43
1:A:803:ILE:HG12	1:A:916:PHE:CE1	2.53	0.43
1:C:831:ASN:ND2	1:C:834:THR:HB	2.31	0.43
1:C:931:LYS:NZ	1:C:941:GLY:O	2.51	0.43
1:A:777:ILE:HG13	1:A:847:TYR:HA	1.99	0.43
1:C:436:LEU:HD12	1:C:436:LEU:H	1.82	0.43
1:C:565:ASP:HB3	1:C:568:ASP:O	2.17	0.43
1:C:349:CYS:HA	1:C:741:MET:HE3	1.99	0.43
1:C:384:MET:HG2	1:C:582:ILE:HG12	2.00	0.43
1:C:676:LYS:HB2	1:C:701:GLN:CD	2.39	0.43
1:C:1009:TRP:HB3	10:C:1110:PCW:H32	2.01	0.43
1:A:160:GLN:NE2	1:A:191:ARG:HB3	2.33	0.43
1:A:163:LEU:HD11	1:A:170:LYS:HB2	2.00	0.43
1:A:326:PRO:HG3	1:A:773:LEU:HD21	2.01	0.43
1:A:943:LYS:HG3	12:E:102:DMU:H29	2.00	0.43
2:B:205:ASN:HB2	2:B:235:TYR:CE2	2.53	0.43
1:C:507:ILE:HD13	1:C:507:ILE:HA	1.79	0.43
10:A:1107:PCW:H73	10:A:1107:PCW:H42	1.78	0.43
8:C:1104:CLR:H211	8:C:1104:CLR:H232	1.81	0.43
1:A:195:ASP:OD2	1:A:258:THR:CA	2.61	0.43
1:A:927:LEU:HD21	1:A:947:LEU:HG	2.00	0.43
1:C:719:LYS:HD2	1:C:719:LYS:HA	1.76	0.43
1:C:766:LYS:HD2	1:C:933:ARG:NH2	2.33	0.43
1:C:849:GLN:O	1:C:853:ILE:HG13	2.18	0.43
2:D:52:GLY:O	2:D:56:VAL:HG23	2.18	0.43
1:A:685:ARG:HD3	1:A:685:ARG:HA	1.79	0.43
1:A:803:ILE:HG12	1:A:916:PHE:HD1	1.83	0.43
1:A:905:LYS:HA	1:A:905:LYS:HD3	1.76	0.43
1:C:708:THR:HA	1:C:725:VAL:O	2.19	0.43
1:A:339:LEU:HG	1:A:817:TYR:CE1	2.53	0.43
2:B:152:ARG:H	2:B:155:TRP:HZ3	1.67	0.43
1:C:123:LEU:O	1:C:127:VAL:HG23	2.19	0.43
1:C:180:VAL:HG22	1:C:254:THR:HB	2.00	0.43
1:C:350:LEU:HD12	1:C:744:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1109:PCW:H73	10:C:1109:PCW:H42	1.78	0.43
9:A:1111:PC1:H2D1	9:A:1111:PC1:H2A1	1.74	0.43
1:A:383:HIS:ND1	1:A:543:GLU:OE2	2.52	0.43
1:A:482:GLN:HE21	1:A:482:GLN:HB2	1.56	0.43
1:A:488:ASN:HB3	1:A:493:GLU:CD	2.39	0.43
1:A:656:CYS:SG	1:A:681:ILE:HG23	2.59	0.43
1:A:861:THR:HG22	1:A:983:CYS:CB	2.49	0.43
2:B:88:ILE:O	2:B:299:ILE:HA	2.19	0.43
1:C:293:VAL:HG23	1:C:321:ILE:HD11	2.00	0.43
1:C:376:GLN:HE21	1:C:376:GLN:HB2	1.63	0.43
1:C:427:GLN:HE22	1:C:441:ALA:HB2	1.83	0.43
1:C:692:LEU:O	1:C:696:GLU:HG3	2.19	0.43
2:D:203:LYS:HB3	2:D:236:PRO:HD2	2.01	0.43
1:A:516:ILE:HD12	1:A:521:GLN:NE2	2.34	0.42
1:A:658:VAL:HB	1:A:683:PHE:CD2	2.54	0.42
2:B:164:ASP:OD2	2:B:167:TYR:N	2.52	0.42
1:C:990:LEU:HA	1:C:993:VAL:HG12	2.01	0.42
1:A:861:THR:HG22	1:A:983:CYS:HB2	2.01	0.42
1:C:195:ASP:OD1	1:C:238:PHE:N	2.53	0.42
1:C:683:PHE:HB3	1:C:686:THR:OG1	2.19	0.42
1:A:479:ASN:HB3	1:A:481:TYR:CE1	2.53	0.42
1:A:810:VAL:HB	1:A:811:PRO:HD3	2.00	0.42
2:B:168:GLY:HA3	2:B:173:LYS:O	2.20	0.42
2:B:276:CYS:HB2	2:B:295:PHE:CE2	2.54	0.42
1:C:120:ASN:HB3	1:C:123:LEU:HD23	2.01	0.42
1:C:196:LEU:HB3	1:C:249:GLY:HA3	2.01	0.42
1:C:467:TYR:HB3	1:C:486:HIS:CB	2.44	0.42
1:C:972:ARG:NH2	1:C:974:TYR:OH	2.53	0.42
1:A:892:GLU:HA	1:A:897:GLN:O	2.19	0.42
1:A:918:SER:HB3	1:A:984:ALA:HB2	2.01	0.42
1:C:450:LEU:CD2	1:C:454:GLU:HG3	2.50	0.42
1:C:899:TRP:CH2	2:D:72:VAL:HG22	2.54	0.42
2:D:24:PHE:CZ	2:D:25:LEU:HD23	2.54	0.42
2:B:74:PRO:HG2	2:B:284:GLY:H	1.85	0.42
2:B:80:ILE:HB	2:B:177:ILE:HG23	2.01	0.42
2:B:178:ILE:N	2:B:259:MET:O	2.41	0.42
1:C:288:ILE:HD12	1:C:288:ILE:HA	1.75	0.42
1:C:427:GLN:HG2	1:C:439:ALA:O	2.20	0.42
1:C:676:LYS:HB2	1:C:701:GLN:OE1	2.19	0.42
1:C:786:PHE:HB2	1:C:794:PRO:HD3	2.01	0.42
1:C:820:ALA:HB1	1:C:824:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:TYR:CD2	2:D:236:PRO:HB3	2.55	0.42
1:A:376:GLN:H	1:A:376:GLN:HG2	1.65	0.42
1:A:957:LEU:HD22	1:A:957:LEU:HA	1.82	0.42
1:C:417:ILE:CD1	1:C:548:PHE:HB3	2.50	0.42
1:C:926:ASP:O	1:C:929:ILE:HG12	2.19	0.42
2:D:209:LEU:O	2:D:237:GLY:HA3	2.18	0.42
1:A:31:GLU:H	1:A:31:GLU:HG3	1.74	0.42
1:A:301:ILE:O	1:A:305:ILE:HG12	2.20	0.42
2:B:88:ILE:HA	2:B:101:TYR:CE2	2.55	0.42
2:B:273:ARG:HG2	2:B:298:LYS:HG2	2.00	0.42
1:C:655:ALA:HA	1:C:680:GLU:O	2.19	0.42
1:C:841:ARG:HG2	1:C:1013:GLU:O	2.19	0.42
2:D:241:GLN:HG3	2:D:242:TYR:CD1	2.55	0.42
1:A:154:PHE:HE1	1:A:341:ALA:HB1	1.85	0.42
1:A:977:LYS:HD2	1:A:980:TRP:CH2	2.55	0.42
1:C:319:GLY:HA3	1:C:797:THR:HG23	2.02	0.42
1:C:488:ASN:CG	1:C:493:GLU:HG3	2.40	0.42
1:C:558:PHE:CZ	1:C:571:PHE:HA	2.52	0.42
1:C:833:LYS:HB2	1:C:833:LYS:HE3	1.87	0.42
1:A:850:ILE:O	1:A:854:GLN:HG3	2.20	0.42
1:C:874:ILE:HG21	10:C:1111:PCW:O1P	2.20	0.42
2:D:157:GLY:H	2:D:230:PHE:HB3	1.85	0.42
2:B:211:VAL:HG11	2:B:259:MET:HE1	2.02	0.42
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.54	0.42
1:C:274:GLN:NE2	1:C:282:GLU:OE1	2.51	0.42
1:C:770:ALA:HA	1:C:842:LEU:HD21	2.01	0.42
2:D:209:LEU:HD11	2:D:283:ILE:HD13	2.02	0.42
1:A:430:GLN:O	1:A:438:ARG:NH2	2.53	0.41
1:A:856:LEU:HD13	2:B:50:PHE:HB2	2.02	0.41
1:A:942:MET:HB2	12:E:102:DMU:C18	2.47	0.41
1:A:1009:TRP:CH2	1:A:1013:GLU:HG2	2.55	0.41
10:A:1114:PCW:H41	10:A:1114:PCW:H73	1.74	0.41
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.55	0.41
1:C:859:PHE:HD2	1:C:915:PHE:HE2	1.67	0.41
1:C:253:TYR:HD1	1:C:257:ARG:HB3	1.84	0.41
1:C:683:PHE:CD1	1:C:694:ILE:HD13	2.54	0.41
1:A:929:ILE:HB	1:A:995:ASP:OD2	2.20	0.41
1:A:56:LEU:H	1:A:56:LEU:HG	1.62	0.41
1:A:695:VAL:HG13	1:A:705:VAL:HG21	2.01	0.41
1:A:996:GLU:CB	9:A:1108:PC1:H292	2.50	0.41
1:C:24:ASP:O	1:C:28:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:SER:O	1:C:302:LEU:HB2	2.20	0.41
1:C:803:ILE:O	1:C:807:THR:HB	2.20	0.41
1:C:864:VAL:HA	2:D:57:MET:SD	2.60	0.41
2:D:220:ASP:O	2:D:224:VAL:HG23	2.20	0.41
1:A:288:ILE:HG21	1:A:326:PRO:HD2	2.02	0.41
2:B:143:ARG:HB3	2:B:146:ARG:HH12	1.86	0.41
2:B:179:LYS:HD2	2:B:256:GLN:OE1	2.21	0.41
1:A:1001:ILE:HG21	1:A:1010:VAL:HG21	2.01	0.41
1:C:706:ALA:HA	1:C:723:ILE:O	2.20	0.41
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.84	0.41
2:B:196:LEU:HA	2:B:199:TYR:CE2	2.56	0.41
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.79	0.41
2:D:213:CYS:HA	2:D:276:CYS:HA	2.03	0.41
2:B:18:ASN:OD1	2:B:23:GLU:HB2	2.21	0.41
1:C:613:HIS:CG	1:C:614:PRO:HD2	2.56	0.41
1:C:844:SER:OG	8:C:1107:CLR:H42	2.21	0.41
1:C:916:PHE:O	1:C:920:VAL:HG23	2.21	0.41
1:A:187:LYS:HA	1:A:246:THR:HA	2.02	0.41
1:A:657:VAL:HA	1:A:682:VAL:O	2.21	0.41
2:B:121:MET:HG3	2:B:122:ILE:HD13	2.02	0.41
2:B:122:ILE:HG21	2:B:253:LYS:HE2	2.03	0.41
2:B:255:LEU:HD23	2:B:255:LEU:HA	1.90	0.41
3:G:40:VAL:O	3:G:44:ILE:HG12	2.21	0.41
1:C:71:ASN:HB3	1:C:176:GLU:HA	2.03	0.41
1:C:468:THR:O	1:C:486:HIS:HA	2.21	0.41
1:C:514:ILE:HD12	1:C:527:LEU:HD13	2.01	0.41
1:C:626:ILE:HD13	1:C:626:ILE:HA	1.96	0.41
1:C:641:LEU:O	1:C:643:ILE:HG23	2.21	0.41
1:C:710:ASP:HB3	1:C:727:MET:CG	2.51	0.41
2:D:61:ILE:HG23	2:D:67:THR:HG23	2.02	0.41
3:E:33:PHE:CD2	8:E:101:CLR:H71	2.56	0.41
1:A:182:ASP:O	1:A:251:VAL:HG23	2.21	0.41
1:A:230:LEU:H	1:A:230:LEU:HG	1.73	0.41
1:A:778:PRO:HA	1:A:855:ALA:HB2	2.03	0.41
2:B:91:ARG:HG3	2:B:303:SER:HA	2.03	0.41
1:C:56:LEU:H	1:C:56:LEU:HG	1.63	0.41
1:C:84:LYS:HE3	1:C:144:GLU:OE2	2.20	0.41
2:D:276:CYS:HB2	2:D:295:PHE:CE2	2.56	0.41
3:E:28:ASN:O	3:E:32:ILE:HG12	2.21	0.41
12:E:102:DMU:H36	12:E:102:DMU:O55	2.21	0.41
1:A:311:LEU:O	1:A:315:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LYS:H	1:A:519:LYS:HG2	1.55	0.40
1:A:655:ALA:HA	1:A:680:GLU:O	2.20	0.40
1:A:352:LYS:HB3	1:A:352:LYS:HE2	1.88	0.40
2:B:297:VAL:HG12	2:B:299:ILE:HG23	2.03	0.40
1:C:39:LEU:HB3	1:C:43:GLU:HB3	2.03	0.40
1:C:116:GLU:HG2	1:C:117:GLU:N	2.35	0.40
1:C:775:SER:HB3	1:C:923:GLN:NE2	2.23	0.40
8:C:1107:CLR:H211	8:C:1107:CLR:H232	1.88	0.40
2:B:130:PRO:HB3	2:B:208:VAL:HG23	2.03	0.40
2:B:228:GLU:HB3	2:B:262:GLN:HB3	2.02	0.40
1:C:365:THR:HA	1:C:605:LYS:O	2.22	0.40
2:D:93:ASN:ND2	2:D:93:ASN:H	2.19	0.40
1:A:354:LEU:HA	1:A:354:LEU:HD23	1.79	0.40
2:B:177:ILE:HD11	2:B:258:LEU:HD13	2.03	0.40
1:C:229:PRO:O	1:C:232:THR:HG22	2.21	0.40
1:C:874:ILE:H	1:C:874:ILE:HG13	1.55	0.40
2:D:179:LYS:HD2	2:D:256:GLN:CD	2.41	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%)	963 (97%)	30 (3%)	0	100	100
1	C	993/1021 (97%)	942 (95%)	51 (5%)	0	100	100
2	B	289/303 (95%)	276 (96%)	13 (4%)	0	100	100
2	D	289/303 (95%)	269 (93%)	20 (7%)	0	100	100
3	E	31/65 (48%)	29 (94%)	2 (6%)	0	100	100
3	G	33/65 (51%)	31 (94%)	2 (6%)	0	100	100
All	All	2628/2778 (95%)	2510 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	759 (90%)	86 (10%)	7 28
1	C	845/864 (98%)	759 (90%)	86 (10%)	7 28
2	B	261/269 (97%)	230 (88%)	31 (12%)	5 22
2	D	261/269 (97%)	239 (92%)	22 (8%)	11 38
3	E	27/52 (52%)	26 (96%)	1 (4%)	34 70
3	G	29/52 (56%)	29 (100%)	0	100 100
All	All	2268/2370 (96%)	2042 (90%)	226 (10%)	7 29

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	31	GLU
1	A	36	ASP
1	A	44	LEU
1	A	56	LEU
1	A	60	ARG
1	A	89	LEU
1	A	94	SER
1	A	153	SER
1	A	161	GLN
1	A	190	ASP
1	A	221	SER
1	A	239	SER
1	A	246	THR
1	A	270	LEU
1	A	274	GLN
1	A	275	THR
1	A	286	HIS
1	A	298	SER

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Mol	Chain	Res	Type
1	A	302	LEU
1	A	303	SER
1	A	314	VAL
1	A	327	GLU
1	A	329	LEU
1	A	337	LEU
1	A	340	THR
1	A	351	VAL
1	A	354	LEU
1	A	357	VAL
1	A	371	THR
1	A	384	MET
1	A	391	HIS
1	A	392	GLU
1	A	402	VAL
1	A	403	SER
1	A	405	ASP
1	A	412	LEU
1	A	431	GLU
1	A	433	LEU
1	A	435	ILE
1	A	443	ASP
1	A	450	LEU
1	A	452	CYS
1	A	455	LEU
1	A	456	CYS
1	A	478	THR
1	A	479	ASN
1	A	482	GLN
1	A	484	SER
1	A	495	ARG
1	A	500	MET
1	A	508	LEU
1	A	519	LYS
1	A	523	LEU
1	A	535	TYR
1	A	541	LEU
1	A	550	HIS
1	A	555	ASP
1	A	566	THR
1	A	610	THR
1	A	649	ASN

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Mol	Chain	Res	Type
1	A	657	VAL
1	A	663	LEU
1	A	671	LEU
1	A	673	ASP
1	A	675	LEU
1	A	701	GLN
1	A	713	ASN
1	A	761	ILE
1	A	774	THR
1	A	801	LEU
1	A	802	CYS
1	A	830	ARG
1	A	833	LYS
1	A	852	MET
1	A	863	PHE
1	A	874	ILE
1	A	918	SER
1	A	930	CYS
1	A	932	THR
1	A	951	LEU
1	A	953	GLU
1	A	957	LEU
1	A	969	VAL
1	A	988	SER
1	A	995	ASP
2	B	25	LEU
2	B	28	THR
2	B	31	SER
2	B	32	TRP
2	B	34	LYS
2	B	61	ILE
2	B	64	PHE
2	B	72	VAL
2	B	83	SER
2	B	104	SER
2	B	133	LEU
2	B	155	TRP
2	B	162	LEU
2	B	163	ASN
2	B	165	GLU
2	B	171	ASP
2	B	175	CYS

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Mol	Chain	Res	Type
2	B	177	ILE
2	B	198	THR
2	B	199	TYR
2	B	208	VAL
2	B	214	THR
2	B	217	ARG
2	B	227	MET
2	B	228	GLU
2	B	259	MET
2	B	265	ASN
2	B	266	LEU
2	B	274	ILE
2	B	282	ASN
2	B	288	LYS
1	C	24	ASP
1	C	29	LYS
1	C	31	GLU
1	C	35	ASP
1	C	36	ASP
1	C	56	LEU
1	C	60	ARG
1	C	85	PHE
1	C	102	ILE
1	C	123	LEU
1	C	125	LEU
1	C	144	GLU
1	C	158	VAL
1	C	161	GLN
1	C	182	ASP
1	C	191	ARG
1	C	234	ASN
1	C	241	ASN
1	C	260	MET
1	C	262	ARG
1	C	263	ILE
1	C	270	LEU
1	C	275	THR
1	C	286	HIS
1	C	288	ILE
1	C	293	VAL
1	C	299	PHE
1	C	302	LEU

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Mol	Chain	Res	Type
1	C	317	LEU
1	C	324	ASN
1	C	327	GLU
1	C	339	LEU
1	C	350	LEU
1	C	354	LEU
1	C	357	VAL
1	C	360	LEU
1	C	368	SER
1	C	369	ASP
1	C	376	GLN
1	C	394	ASP
1	C	396	THR
1	C	421	CYS
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	457	CYS
1	C	461	LYS
1	C	472	GLU
1	C	490	ASN
1	C	491	THR
1	C	498	LEU
1	C	505	GLU
1	C	512	SER
1	C	523	LEU
1	C	525	GLU
1	C	544	ARG
1	C	565	ASP
1	C	568	ASP
1	C	570	ASN
1	C	594	ASP
1	C	671	LEU
1	C	689	GLN
1	C	722	ASP
1	C	723	ILE
1	C	761	ILE
1	C	786	PHE
1	C	791	ILE

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Mol	Chain	Res	Type
1	C	801	LEU
1	C	815	LEU
1	C	837	LEU
1	C	852	MET
1	C	862	TYR
1	C	880	ARG
1	C	881	VAL
1	C	894	SER
1	C	916	PHE
1	C	927	LEU
1	C	933	ARG
1	C	934	ARG
1	C	971	LEU
1	C	976	LEU
1	C	988	SER
1	C	1005	ARG
2	D	25	LEU
2	D	32	TRP
2	D	39	TYR
2	D	45	CYS
2	D	61	ILE
2	D	64	PHE
2	D	72	VAL
2	D	78	THR
2	D	79	GLN
2	D	93	ASN
2	D	132	GLU
2	D	142	GLU
2	D	149	CYS
2	D	159	CYS
2	D	162	LEU
2	D	177	ILE
2	D	180	LEU
2	D	183	VAL
2	D	196	LEU
2	D	261	VAL
2	D	266	LEU
2	D	282	ASN
3	E	17	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	120	ASN
1	A	122	ASN
1	A	167	ASN
1	A	241	ASN
1	A	376	GLN
1	A	377	ASN
1	A	389	GLN
1	A	398	ASN
1	A	399	GLN
1	A	476	ASN
1	A	482	GLN
1	A	490	ASN
1	A	521	GLN
1	A	613	HIS
1	A	649	ASN
1	A	659	HIS
1	A	776	ASN
1	A	854	GLN
1	A	939	GLN
2	B	262	GLN
1	C	376	GLN
1	C	482	GLN
1	C	521	GLN
1	C	533	ASN
1	C	550	HIS
1	C	570	ASN
1	C	659	HIS
1	C	689	GLN
1	C	776	ASN
1	C	854	GLN
1	C	898	GLN
1	C	903	GLN
1	C	923	GLN
2	D	82	GLN
2	D	212	HIS
2	D	256	GLN
2	D	292	GLN
3	E	28	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	2,4	14,14,15	0.32	0	17,19,21	0.55	0
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.59	0
4	BMA	F	3	4	11,11,12	0.80	0	15,15,17	0.82	0
4	MAN	F	4	4	11,11,12	0.88	0	15,15,17	1.19	1 (6%)
4	MAN	F	5	4	11,11,12	1.38	3 (27%)	15,15,17	1.85	2 (13%)
4	MAN	F	6	4	11,11,12	0.88	1 (9%)	15,15,17	1.21	2 (13%)
5	NAG	H	1	2,5	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	H	2	5	14,14,15	0.74	0	17,19,21	0.73	0
5	BMA	H	3	5	11,11,12	1.62	2 (18%)	15,15,17	1.11	1 (6%)
5	MAN	H	4	5	11,11,12	1.04	2 (18%)	15,15,17	1.13	2 (13%)
5	MAN	H	5	5	11,11,12	1.03	1 (9%)	15,15,17	1.09	1 (6%)
6	NAG	I	1	2,6	14,14,15	0.42	0	17,19,21	0.54	0
6	NAG	I	2	6	14,14,15	0.34	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	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	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	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	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	MAN	H	5	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	3.22	1.59	1.52
5	H	3	BMA	C4-C5	3.01	1.59	1.53
4	F	5	MAN	O5-C5	2.63	1.48	1.43
4	F	5	MAN	O5-C1	2.62	1.47	1.43
4	F	5	MAN	C1-C2	2.57	1.58	1.52
5	H	5	MAN	C1-C2	2.56	1.58	1.52
4	F	6	MAN	C1-C2	2.36	1.57	1.52
5	H	4	MAN	C1-C2	2.10	1.57	1.52
5	H	4	MAN	C2-C3	2.08	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5	MAN	C1-O5-C5	5.81	120.06	112.19
4	F	4	MAN	C1-O5-C5	3.19	116.51	112.19
4	F	6	MAN	C1-O5-C5	3.05	116.33	112.19
5	H	4	MAN	C1-O5-C5	2.59	115.70	112.19
5	H	3	BMA	O5-C1-C2	-2.37	107.11	110.77
4	F	5	MAN	O2-C2-C3	-2.31	105.52	110.14
5	H	5	MAN	C1-O5-C5	2.26	115.25	112.19
4	F	6	MAN	O2-C2-C3	-2.21	105.72	110.14
5	H	4	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

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

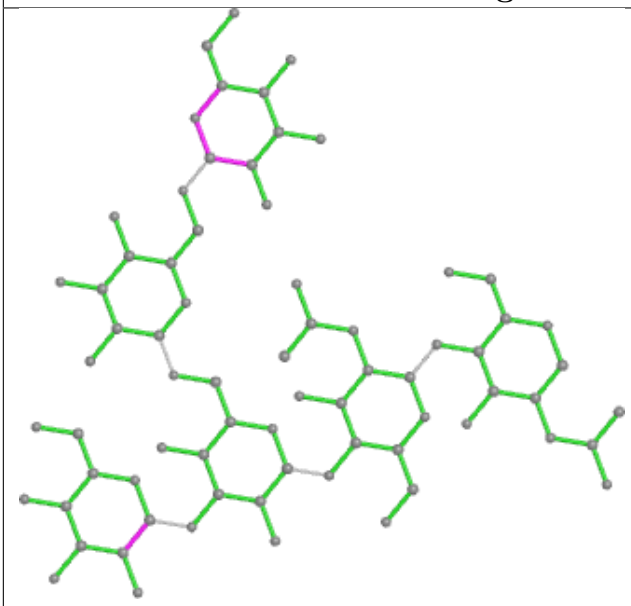
There are no ring outliers.

2 monomers are involved in 1 short contact:

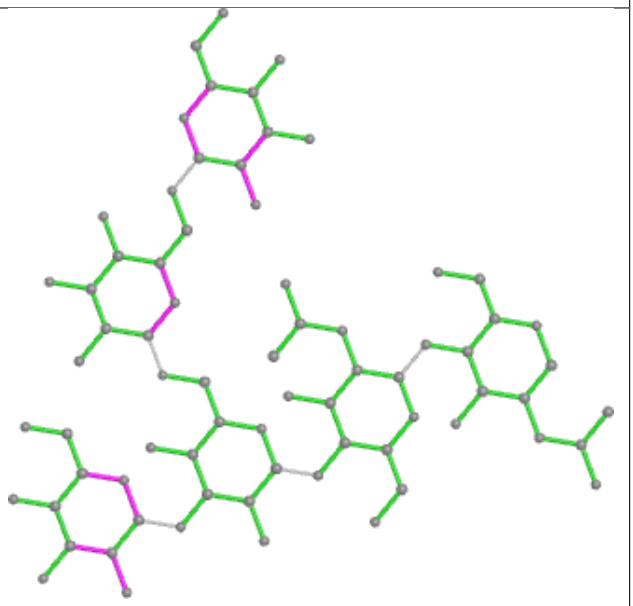
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
5	H	2	NAG	1	0

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

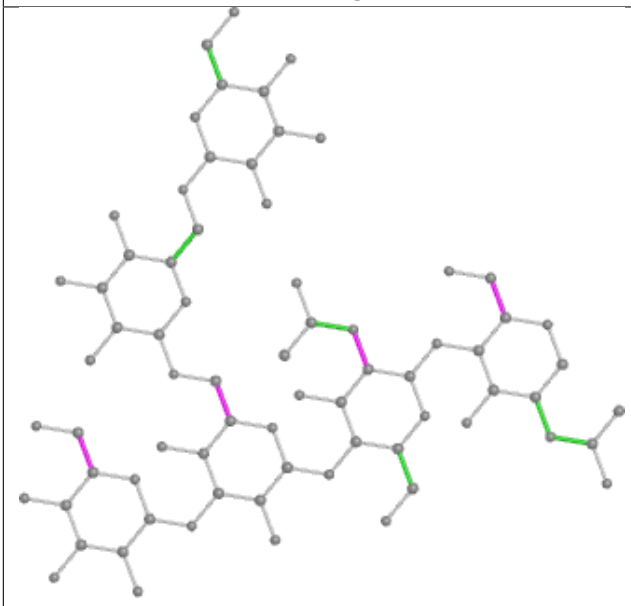
Oligosaccharide Chain F



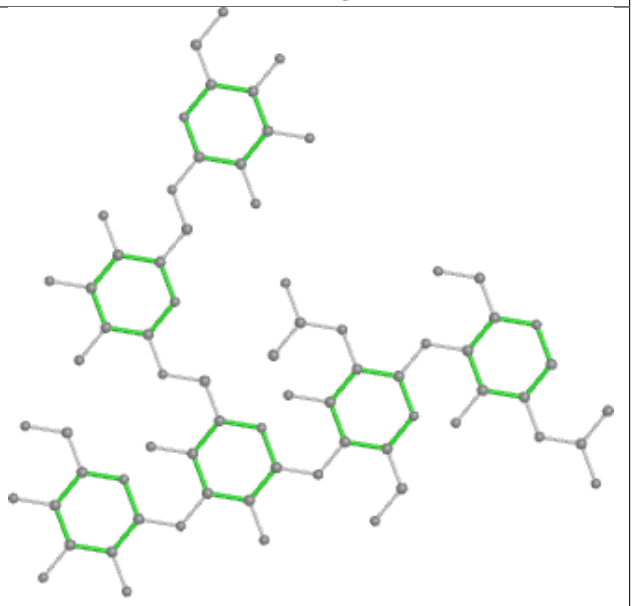
Bond lengths



Bond angles

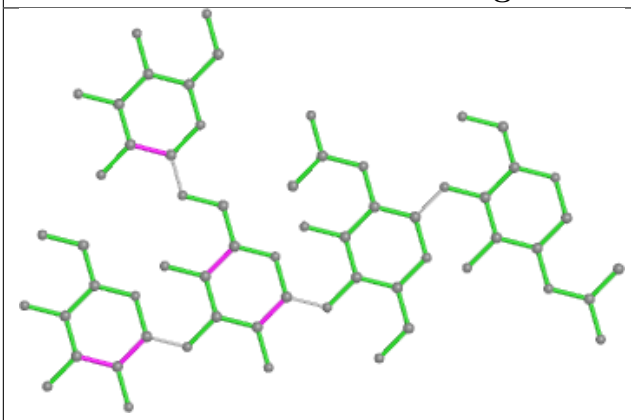


Torsions

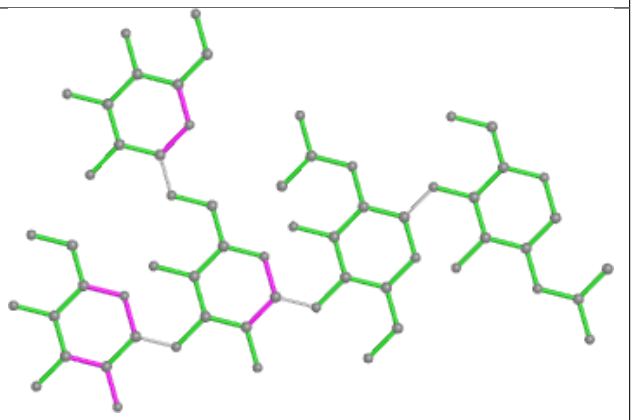


Rings

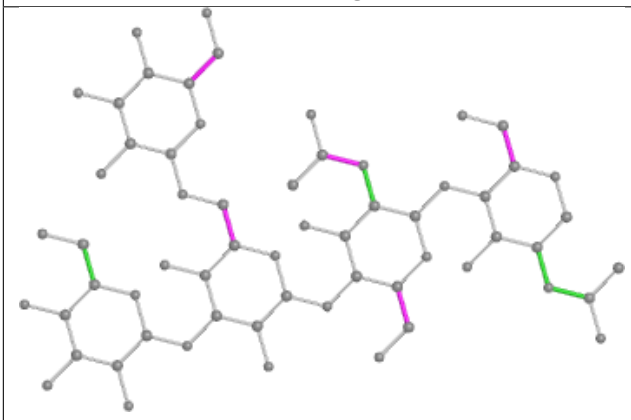
Oligosaccharide Chain H



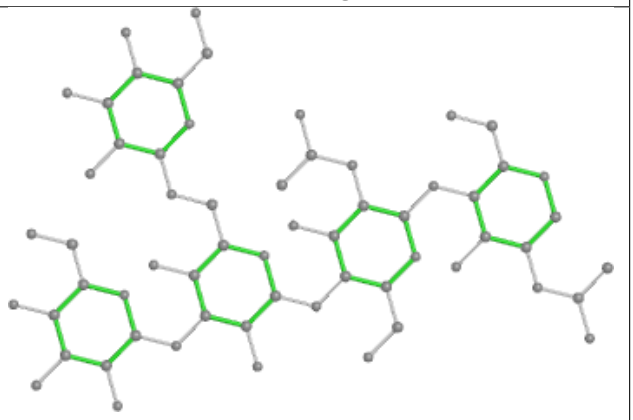
Bond lengths



Bond angles

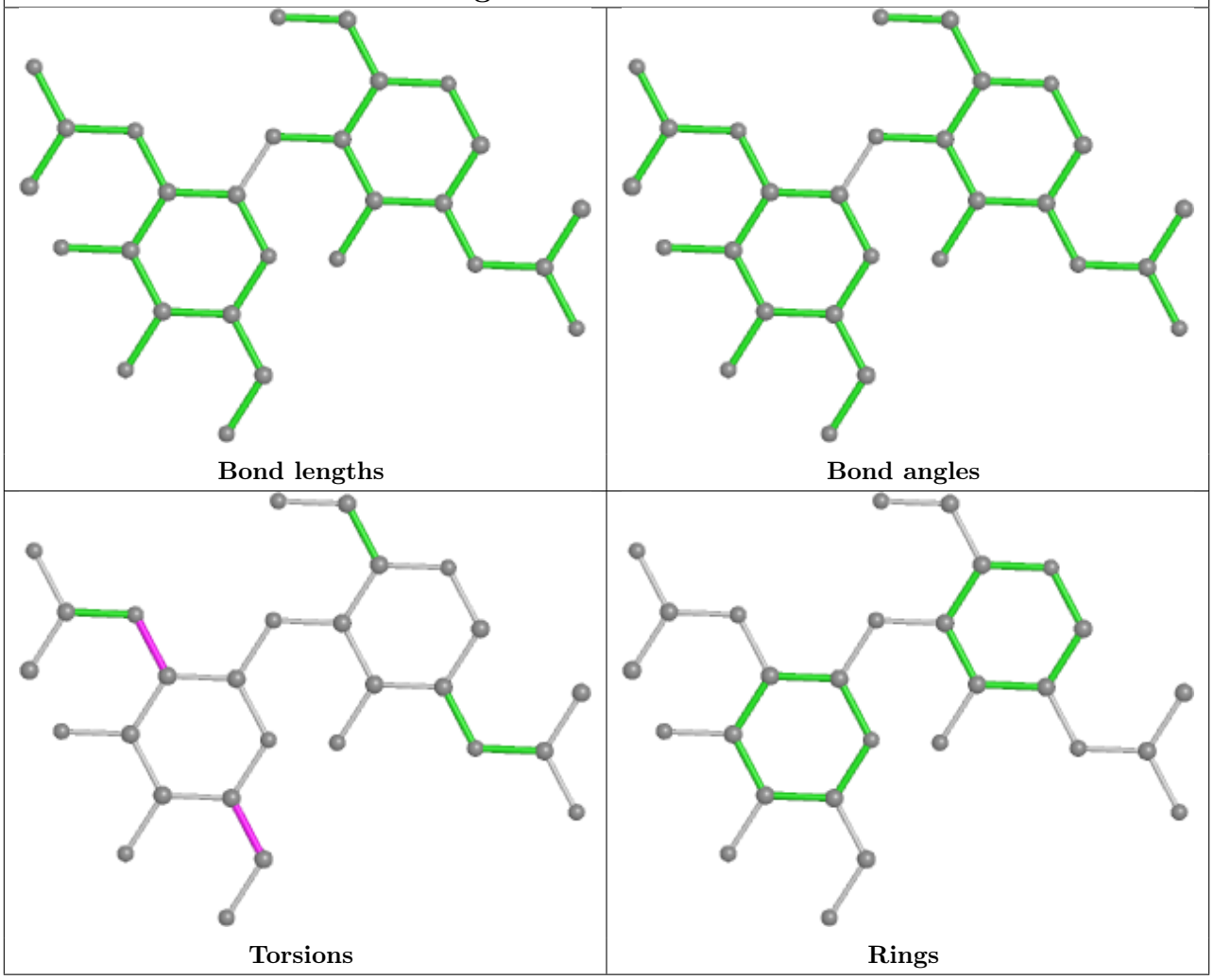


Torsions



Rings

Oligosaccharide Chain I



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	A	1107	-	21,21,53	0.91	0	27,29,61	1.10	3 (11%)
10	PCW	C	1109	-	21,21,53	0.87	0	27,29,61	1.29	3 (11%)
10	PCW	A	1113	-	21,21,53	0.90	0	27,29,61	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CLR	E	101	-	31,31,31	1.17	2 (6%)	48,48,48	1.36	7 (14%)
8	CLR	C	1104	-	31,31,31	1.16	2 (6%)	48,48,48	1.40	8 (16%)
9	PC1	A	1111	-	53,53,53	0.69	0	59,61,61	0.86	1 (1%)
8	CLR	C	1107	-	31,31,31	1.19	1 (3%)	48,48,48	1.35	7 (14%)
10	PCW	C	1105	-	21,21,53	0.89	0	27,29,61	1.05	2 (7%)
9	PC1	A	1106	-	53,53,53	0.62	0	59,61,61	0.85	1 (1%)
10	PCW	A	1112	-	21,21,53	0.91	0	27,29,61	1.02	2 (7%)
12	DMU	E	102	-	34,34,34	0.69	1 (2%)	45,45,45	1.09	4 (8%)
8	CLR	A	1105	-	31,31,31	1.14	1 (3%)	48,48,48	1.37	7 (14%)
10	PCW	A	1109	-	21,21,53	0.94	0	27,29,61	1.02	2 (7%)
10	PCW	A	1114	-	21,21,53	0.87	0	27,29,61	1.17	3 (11%)
10	PCW	A	1115	-	21,21,53	0.99	0	27,29,61	0.78	1 (3%)
11	NAG	D	401	2	14,14,15	0.41	0	17,19,21	0.37	0
8	CLR	A	1110	-	31,31,31	1.20	2 (6%)	48,48,48	1.34	4 (8%)
9	PC1	A	1108	-	53,53,53	0.61	0	59,61,61	1.08	2 (3%)
10	PCW	C	1112	-	21,21,53	0.88	0	27,29,61	0.99	1 (3%)
8	CLR	A	1104	-	31,31,31	1.19	1 (3%)	48,48,48	1.42	9 (18%)
10	PCW	A	1116	-	53,53,53	1.01	2 (3%)	59,61,61	0.75	0
10	PCW	C	1106	-	21,21,53	0.99	0	27,29,61	0.88	2 (7%)
10	PCW	C	1110	-	21,21,53	0.90	0	27,29,61	0.95	3 (11%)
10	PCW	C	1111	-	21,21,53	0.91	0	27,29,61	1.27	3 (11%)
10	PCW	C	1108	-	21,21,53	0.95	0	27,29,61	1.00	2 (7%)

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	A	1107	-	-	4/23/23/57	-
10	PCW	C	1109	-	-	5/23/23/57	-
10	PCW	A	1113	-	-	5/23/23/57	-
8	CLR	E	101	-	-	1/10/68/68	0/4/4/4
8	CLR	C	1104	-	-	3/10/68/68	0/4/4/4
9	PC1	A	1111	-	-	10/57/57/57	-
8	CLR	C	1107	-	-	4/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	C	1105	-	-	7/23/23/57	-
9	PC1	A	1106	-	-	5/57/57/57	-
10	PCW	A	1112	-	-	10/23/23/57	-
12	DMU	E	102	-	-	3/19/59/59	0/2/2/2
8	CLR	A	1105	-	-	2/10/68/68	0/4/4/4
10	PCW	A	1109	-	-	8/23/23/57	-
10	PCW	A	1114	-	-	7/23/23/57	-
10	PCW	A	1115	-	-	9/23/23/57	-
11	NAG	D	401	2	-	0/6/23/26	0/1/1/1
8	CLR	A	1110	-	-	3/10/68/68	0/4/4/4
9	PC1	A	1108	-	-	16/57/57/57	-
10	PCW	C	1112	-	-	10/23/23/57	-
8	CLR	A	1104	-	-	3/10/68/68	0/4/4/4
10	PCW	A	1116	-	-	19/57/57/57	-
10	PCW	C	1106	-	-	10/23/23/57	-
10	PCW	C	1110	-	-	3/23/23/57	-
10	PCW	C	1111	-	-	8/23/23/57	-
10	PCW	C	1108	-	-	9/23/23/57	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1116	PCW	C20-C19	3.83	1.54	1.31
10	A	1116	PCW	C40-C39	3.79	1.53	1.31
8	A	1104	CLR	C16-C17	3.01	1.60	1.54
8	A	1110	CLR	C16-C17	2.98	1.60	1.54
8	C	1104	CLR	C16-C17	2.96	1.60	1.54
8	E	101	CLR	C16-C17	2.91	1.60	1.54
8	C	1107	CLR	C16-C17	2.89	1.60	1.54
8	A	1105	CLR	C16-C17	2.79	1.60	1.54
12	E	102	DMU	O16-C6	2.21	1.44	1.40
8	A	1110	CLR	C16-C15	2.04	1.59	1.54
8	C	1104	CLR	C7-C6	2.03	1.54	1.50
8	E	101	CLR	C16-C15	2.02	1.59	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1109	PCW	C2-O2-C31	-4.97	108.64	117.90
10	C	1111	PCW	C2-O2-C31	-4.55	109.41	117.90
9	A	1108	PC1	C3-O31-C31	-3.78	103.11	117.12
10	A	1107	PCW	C2-O2-C31	-3.57	111.24	117.90
10	C	1105	PCW	C3-O3-C11	-3.30	108.81	117.10
8	A	1104	CLR	C22-C20-C17	-3.26	103.54	110.28
10	A	1113	PCW	C2-O2-C31	-3.26	111.83	117.90
10	A	1114	PCW	C3-O3-C11	-3.20	109.07	117.10
10	A	1109	PCW	C3-O3-C11	-3.18	109.10	117.10
8	E	101	CLR	C22-C20-C17	-3.14	103.80	110.28
8	C	1107	CLR	C22-C20-C17	-2.96	104.18	110.28
10	A	1112	PCW	C2-O2-C31	-2.96	112.39	117.90
9	A	1108	PC1	C2-O21-C21	2.89	124.92	117.79
8	A	1110	CLR	C22-C20-C17	-2.88	104.34	110.28
12	E	102	DMU	C18-O16-C6	-2.83	109.15	113.84
10	A	1114	PCW	C2-O2-C31	-2.78	112.71	117.90
10	C	1108	PCW	C3-O3-C11	-2.75	110.20	117.10
8	C	1104	CLR	C22-C20-C17	-2.75	104.61	110.28
10	C	1108	PCW	O2-C31-C32	2.68	116.02	111.09
8	C	1104	CLR	C13-C17-C20	-2.65	115.33	119.49
10	A	1107	PCW	C3-O3-C11	-2.62	110.51	117.10
10	C	1111	PCW	C3-O3-C11	-2.61	110.54	117.10
10	C	1112	PCW	C3-O3-C11	-2.58	110.63	117.10
8	A	1105	CLR	C22-C20-C17	-2.57	104.97	110.28
8	A	1104	CLR	C15-C14-C13	2.48	106.83	103.84
9	A	1106	PC1	C3-C2-C1	-2.45	106.00	111.79
10	C	1111	PCW	O2-C31-C32	2.39	115.49	111.09
10	C	1109	PCW	C3-O3-C11	-2.39	111.10	117.10
9	A	1111	PC1	C34-C33-C32	-2.38	104.63	113.19
10	A	1112	PCW	C3-O3-C11	-2.38	111.13	117.10
10	C	1106	PCW	C3-O3-C11	-2.36	111.16	117.10
8	A	1104	CLR	C7-C8-C14	-2.35	107.50	110.91
8	A	1105	CLR	C7-C8-C14	-2.35	107.51	110.91
8	E	101	CLR	C7-C8-C14	-2.35	107.51	110.91
8	A	1110	CLR	C7-C8-C14	-2.34	107.52	110.91
8	C	1107	CLR	C7-C8-C14	-2.31	107.55	110.91
8	C	1104	CLR	C7-C8-C14	-2.31	107.56	110.91
8	A	1104	CLR	C16-C17-C20	-2.28	108.61	112.15
10	C	1110	PCW	C3-O3-C11	-2.26	111.43	117.10
12	E	102	DMU	O16-C18-C19	2.25	117.45	109.56
8	A	1105	CLR	C19-C10-C9	-2.25	109.00	111.68
8	A	1104	CLR	C21-C20-C17	2.24	116.35	112.92
8	A	1110	CLR	C18-C13-C12	2.22	114.09	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1107	CLR	C18-C13-C12	2.22	114.09	110.59
8	A	1105	CLR	C18-C13-C12	2.19	114.05	110.59
8	A	1104	CLR	C18-C13-C12	2.19	114.05	110.59
8	C	1104	CLR	C18-C13-C12	2.19	114.05	110.59
10	A	1107	PCW	O2-C31-C32	2.18	115.10	111.09
8	A	1104	CLR	C3-C4-C5	2.17	115.71	112.03
10	A	1113	PCW	O2-C31-C32	2.17	115.08	111.09
8	C	1104	CLR	C19-C10-C9	-2.15	109.12	111.68
8	C	1104	CLR	C11-C12-C13	-2.15	109.10	112.78
8	A	1105	CLR	C21-C20-C17	2.14	116.20	112.92
8	A	1105	CLR	C13-C17-C20	-2.14	116.14	119.49
10	C	1109	PCW	O2-C31-C32	2.14	115.02	111.09
10	A	1115	PCW	O2-C31-C32	2.13	115.01	111.09
8	C	1107	CLR	C19-C10-C9	-2.12	109.15	111.68
8	A	1110	CLR	C10-C5-C6	2.11	126.14	122.90
8	E	101	CLR	C18-C13-C12	2.11	113.92	110.59
10	C	1110	PCW	O2-C31-C32	2.11	114.97	111.09
8	A	1105	CLR	C11-C12-C13	-2.10	109.19	112.78
12	E	102	DMU	O1-C9-C11	2.10	111.65	106.44
8	A	1104	CLR	C24-C23-C22	-2.09	103.65	113.24
10	C	1110	PCW	C2-O2-C31	-2.06	114.06	117.90
8	C	1104	CLR	C24-C23-C22	-2.06	103.79	113.24
8	A	1104	CLR	C10-C5-C6	2.05	126.04	122.90
10	A	1109	PCW	O2-C31-C32	2.04	114.84	111.09
10	A	1114	PCW	O2-C31-C32	2.04	114.84	111.09
8	E	101	CLR	C3-C4-C5	2.03	115.47	112.03
8	C	1107	CLR	C21-C20-C17	2.03	116.03	112.92
8	C	1107	CLR	C3-C4-C5	2.02	115.46	112.03
10	C	1106	PCW	O2-C31-C32	2.02	114.81	111.09
8	E	101	CLR	C10-C5-C6	2.02	126.00	122.90
8	E	101	CLR	C24-C23-C22	-2.02	103.96	113.24
8	E	101	CLR	C2-C3-C4	-2.02	107.54	110.31
8	C	1104	CLR	C21-C20-C17	2.01	116.00	112.92
8	C	1107	CLR	C24-C23-C22	-2.01	104.00	113.24
12	E	102	DMU	C25-C22-C19	-2.01	104.24	114.42
10	C	1105	PCW	O2-C31-C32	2.00	114.77	111.09

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1108	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
9	A	1108	PC1	C1-O11-P-O12
9	A	1111	PC1	C11-O13-P-O14
10	A	1109	PCW	C4-O4P-P-O3P
10	A	1112	PCW	C5-C4-O4P-P
10	A	1112	PCW	C1-O3P-P-O1P
10	A	1113	PCW	C1-O3P-P-O2P
10	A	1113	PCW	C1-O3P-P-O4P
10	A	1114	PCW	O4P-C4-C5-N
10	A	1114	PCW	C1-O3P-P-O2P
10	A	1115	PCW	C1-O3P-P-O1P
10	A	1115	PCW	C1-O3P-P-O2P
10	A	1115	PCW	C4-O4P-P-O2P
10	A	1115	PCW	C4-O4P-P-O3P
10	A	1116	PCW	O4P-C4-C5-N
10	A	1116	PCW	C4-O4P-P-O3P
10	C	1105	PCW	C4-O4P-P-O2P
10	C	1106	PCW	C4-O4P-P-O1P
10	C	1108	PCW	C32-C31-O2-C2
10	C	1108	PCW	O31-C31-O2-C2
10	C	1108	PCW	C4-O4P-P-O1P
10	C	1109	PCW	O4P-C4-C5-N
10	C	1109	PCW	C4-O4P-P-O1P
10	C	1110	PCW	O4P-C4-C5-N
10	C	1110	PCW	C4-O4P-P-O2P
10	C	1110	PCW	C4-O4P-P-O3P
10	C	1111	PCW	O4P-C4-C5-N
10	C	1111	PCW	C4-O4P-P-O2P
10	C	1112	PCW	O4P-C4-C5-N
10	C	1112	PCW	C1-O3P-P-O2P
10	C	1106	PCW	C32-C31-O2-C2
10	C	1111	PCW	C12-C11-O3-C3
10	C	1105	PCW	C32-C31-O2-C2
10	C	1112	PCW	C12-C11-O3-C3
10	C	1106	PCW	O31-C31-O2-C2
9	A	1108	PC1	C28-C29-C2A-C2B
9	A	1108	PC1	C38-C39-C3A-C3B
9	A	1111	PC1	C28-C29-C2A-C2B
9	A	1111	PC1	C38-C39-C3A-C3B
10	A	1109	PCW	O11-C11-O3-C3
9	A	1106	PC1	C37-C38-C39-C3A
10	A	1109	PCW	C12-C11-O3-C3
10	C	1111	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
10	C	1112	PCW	O11-C11-O3-C3
8	C	1107	CLR	C22-C23-C24-C25
10	C	1105	PCW	O31-C31-O2-C2
8	A	1105	CLR	C20-C22-C23-C24
10	A	1112	PCW	C12-C11-O3-C3
10	A	1112	PCW	C4-O4P-P-O3P
10	A	1113	PCW	C4-O4P-P-O3P
10	A	1114	PCW	C4-O4P-P-O3P
10	A	1115	PCW	C1-O3P-P-O4P
10	C	1106	PCW	C4-O4P-P-O3P
10	C	1108	PCW	C4-O4P-P-O3P
10	C	1109	PCW	C1-O3P-P-O4P
10	C	1109	PCW	C4-O4P-P-O3P
10	C	1111	PCW	C4-O4P-P-O3P
9	A	1108	PC1	C27-C28-C29-C2A
9	A	1108	PC1	C37-C38-C39-C3A
10	A	1116	PCW	C14-C15-C16-C17
10	A	1112	PCW	O11-C11-O3-C3
12	E	102	DMU	O6-C11-C9-O1
9	A	1111	PC1	C39-C3A-C3B-C3C
9	A	1111	PC1	C29-C2A-C2B-C2C
8	C	1107	CLR	C20-C22-C23-C24
10	C	1106	PCW	O3P-C1-C2-C3
10	A	1116	PCW	C31-C32-C33-C34
12	E	102	DMU	C4-C3-O7-C10
10	C	1112	PCW	C1-C2-C3-O3
8	A	1110	CLR	C23-C24-C25-C26
12	E	102	DMU	C2-C3-O7-C10
10	A	1107	PCW	O3P-C1-C2-C3
10	A	1116	PCW	O3P-C1-C2-C3
10	C	1108	PCW	O3P-C1-C2-C3
10	C	1108	PCW	C1-C2-C3-O3
10	C	1105	PCW	C4-O4P-P-O3P
10	C	1111	PCW	C1-O3P-P-O4P
8	C	1104	CLR	C23-C24-C25-C26
10	A	1109	PCW	O2-C2-C3-O3
10	A	1116	PCW	O2-C2-C3-O3
10	A	1116	PCW	C33-C34-C35-C36
9	A	1111	PC1	C2-C1-O11-P
8	C	1107	CLR	C23-C24-C25-C26
10	A	1114	PCW	O3P-C1-C2-C3
10	C	1112	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	A	1104	CLR	C17-C20-C22-C23
10	A	1116	PCW	C16-C17-C18-C19
10	A	1116	PCW	C44-C45-C46-C47
8	A	1110	CLR	C13-C17-C20-C21
10	A	1107	PCW	O3P-C1-C2-O2
10	A	1116	PCW	O3P-C1-C2-O2
10	C	1108	PCW	O3P-C1-C2-O2
10	C	1108	PCW	O2-C2-C3-O3
10	C	1112	PCW	O2-C2-C3-O3
8	A	1105	CLR	C22-C23-C24-C25
8	A	1104	CLR	C21-C20-C22-C23
9	A	1108	PC1	C11-O13-P-O11
10	C	1105	PCW	C1-O3P-P-O4P
10	C	1112	PCW	C1-O3P-P-O4P
9	A	1108	PC1	C11-O13-P-O12
10	A	1109	PCW	C4-O4P-P-O1P
10	A	1112	PCW	C4-O4P-P-O2P
10	A	1113	PCW	C4-O4P-P-O1P
10	A	1114	PCW	C4-O4P-P-O2P
10	A	1116	PCW	C4-O4P-P-O1P
10	C	1109	PCW	C1-O3P-P-O2P
10	C	1111	PCW	C1-O3P-P-O1P
10	C	1111	PCW	C4-O4P-P-O1P
10	A	1114	PCW	C5-C4-O4P-P
10	A	1114	PCW	O3P-C1-C2-O2
10	C	1106	PCW	O3P-C1-C2-O2
9	A	1108	PC1	O31-C31-C32-C33
9	A	1106	PC1	O13-C11-C12-N
9	A	1108	PC1	O13-C11-C12-N
9	A	1111	PC1	O13-C11-C12-N
10	A	1107	PCW	O4P-C4-C5-N
10	A	1109	PCW	O4P-C4-C5-N
10	A	1112	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
9	A	1108	PC1	O32-C31-O31-C3
10	A	1116	PCW	O2-C31-C32-C33
10	A	1107	PCW	C4-O4P-P-O3P
10	C	1112	PCW	C4-O4P-P-O3P
10	A	1109	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	A	1110	CLR	C23-C24-C25-C27
9	A	1108	PC1	C32-C31-O31-C3
8	E	101	CLR	C20-C22-C23-C24
8	C	1104	CLR	C21-C20-C22-C23
9	A	1108	PC1	C3-C2-O21-C21
8	C	1104	CLR	C23-C24-C25-C27
10	A	1116	PCW	C35-C36-C37-C38
10	A	1116	PCW	C11-C12-C13-C14
8	C	1107	CLR	C23-C24-C25-C27
10	A	1116	PCW	C22-C23-C24-C25
10	C	1112	PCW	O3P-C1-C2-O2
10	A	1115	PCW	C4-C5-N-C7
9	A	1108	PC1	C29-C2A-C2B-C2C
10	A	1116	PCW	C37-C38-C39-C40
10	A	1116	PCW	C1-C2-C3-O3
10	A	1112	PCW	O31-C31-O2-C2
9	A	1106	PC1	O31-C31-C32-C33
10	A	1112	PCW	O2-C2-C3-O3
10	A	1115	PCW	C4-C5-N-C6
9	A	1111	PC1	O31-C31-C32-C33
10	A	1116	PCW	C23-C24-C25-C26
8	A	1104	CLR	C23-C24-C25-C27
9	A	1108	PC1	C1-O11-P-O14
10	A	1112	PCW	C1-O3P-P-O2P
10	A	1115	PCW	C4-C5-N-C8
10	C	1106	PCW	C1-O3P-P-O1P
10	C	1106	PCW	C1-O3P-P-O2P
10	C	1106	PCW	C4-O4P-P-O2P
10	A	1109	PCW	O3P-C1-C2-C3
10	A	1115	PCW	O3P-C1-C2-C3
9	A	1106	PC1	O21-C21-C22-C23
10	A	1116	PCW	O3-C11-C12-C13
9	A	1108	PC1	C12-C11-O13-P
9	A	1111	PC1	C3-C2-O21-C21
9	A	1111	PC1	O32-C31-C32-C33
10	C	1105	PCW	C12-C11-O3-C3
9	A	1106	PC1	O22-C21-C22-C23

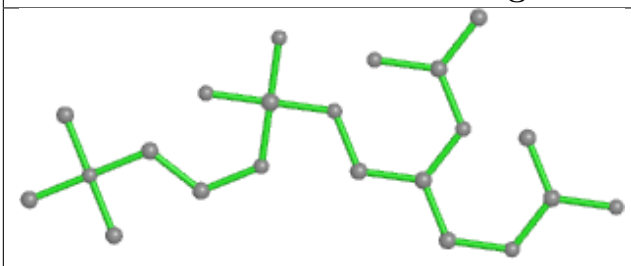
There are no ring outliers.

17 monomers are involved in 53 short contacts:

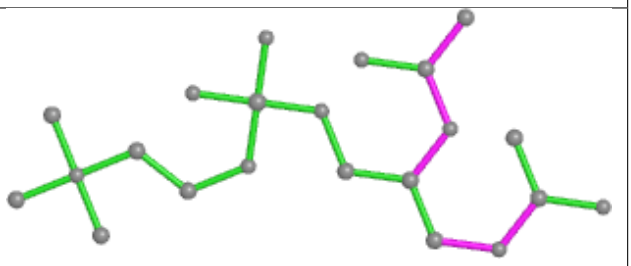
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1107	PCW	1	0
10	C	1109	PCW	1	0
10	A	1113	PCW	2	0
8	E	101	CLR	2	0
8	C	1104	CLR	3	0
9	A	1111	PC1	9	0
8	C	1107	CLR	2	0
9	A	1106	PC1	3	0
10	A	1112	PCW	2	0
12	E	102	DMU	7	0
8	A	1105	CLR	6	0
10	A	1114	PCW	1	0
9	A	1108	PC1	11	0
8	A	1104	CLR	1	0
10	A	1116	PCW	5	0
10	C	1110	PCW	2	0
10	C	1111	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.

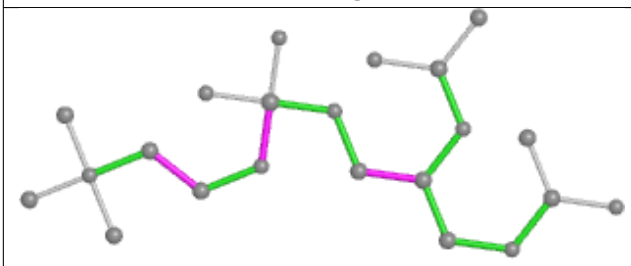
Ligand PCW A 1107



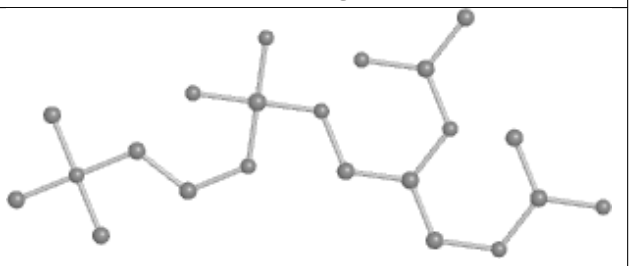
Bond lengths



Bond angles

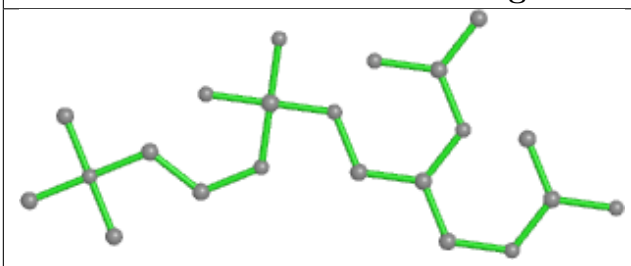


Torsions

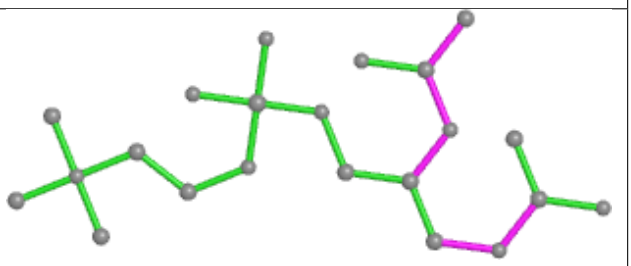


Rings

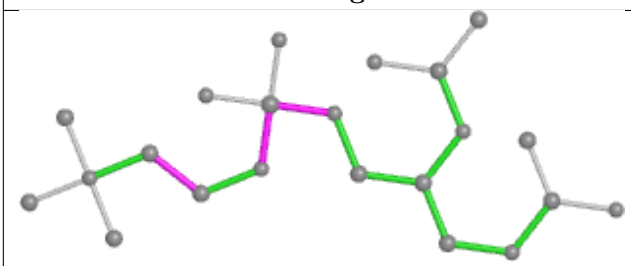
Ligand PCW C 1109



Bond lengths



Bond angles



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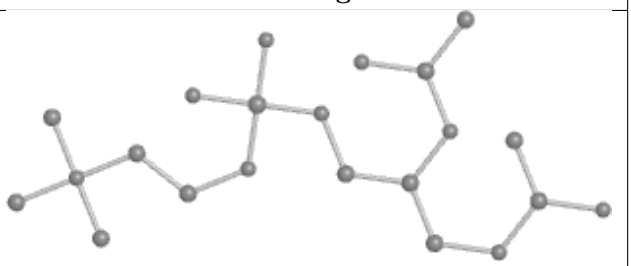
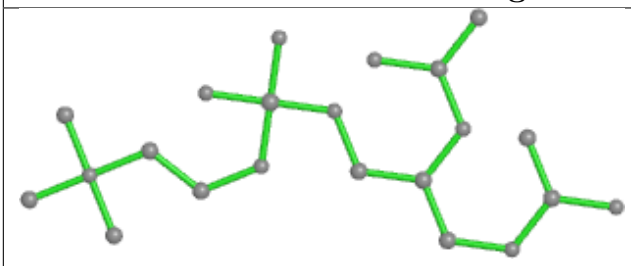
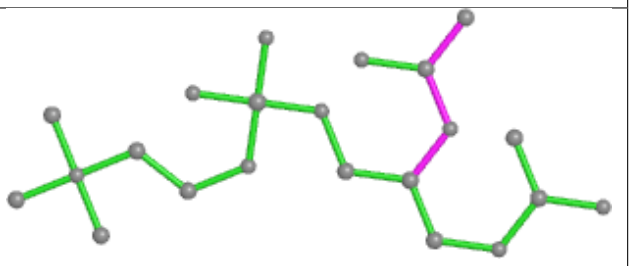


Rings

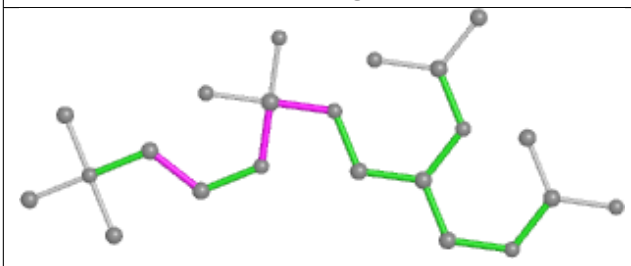
Ligand PCW A 1113



Bond lengths



Bond angles



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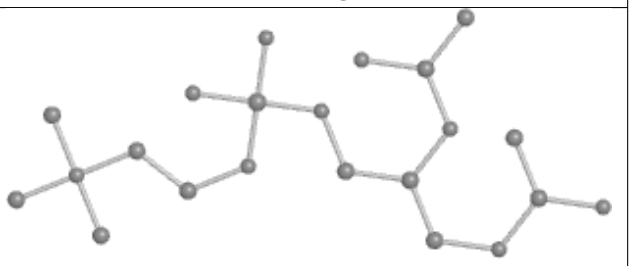
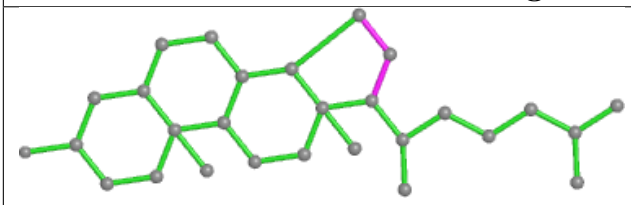
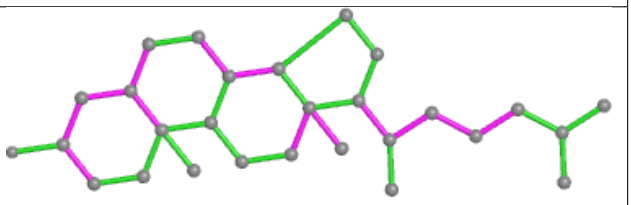


Rings

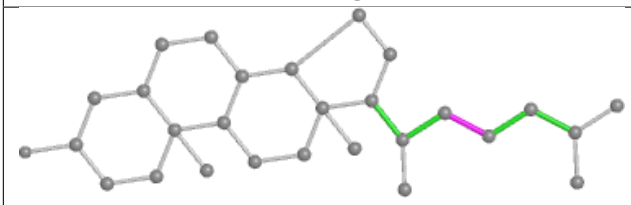
Ligand CLR E 101



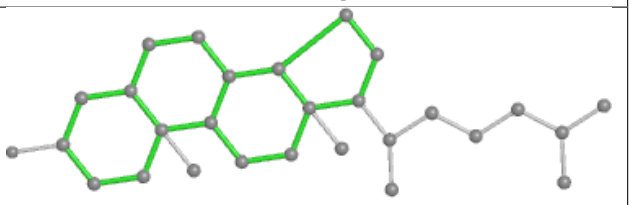
Bond lengths



Bond angles

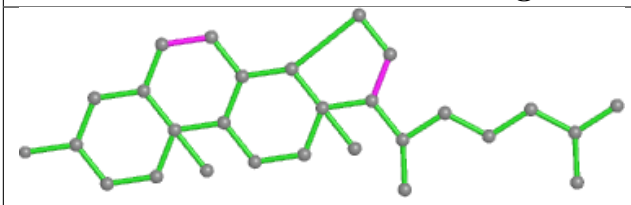


Torsions

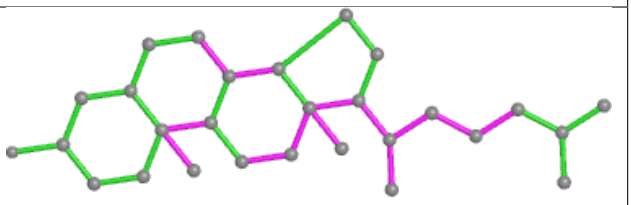


Rings

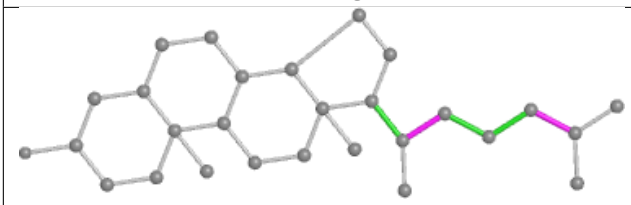
Ligand CLR C 1104



Bond lengths



Bond angles



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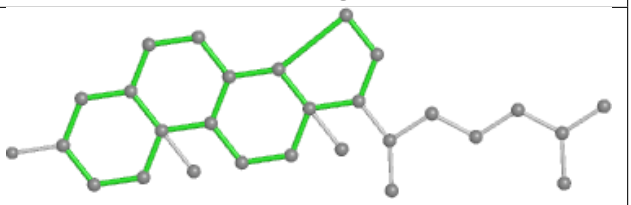
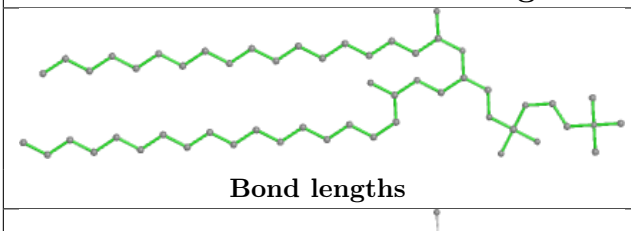


Rings

Ligand PC1 A 1111



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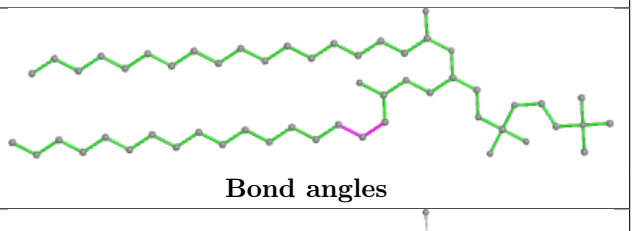

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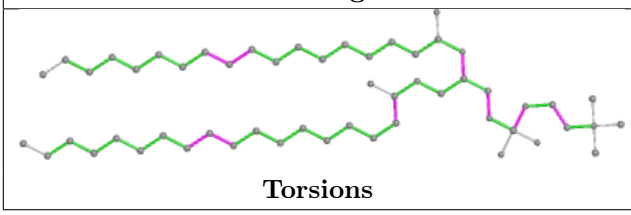

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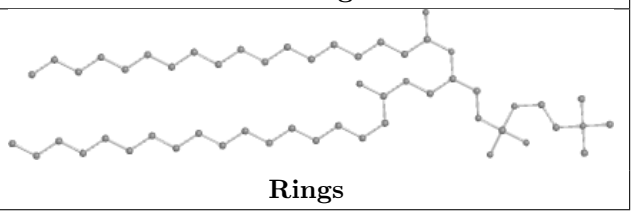
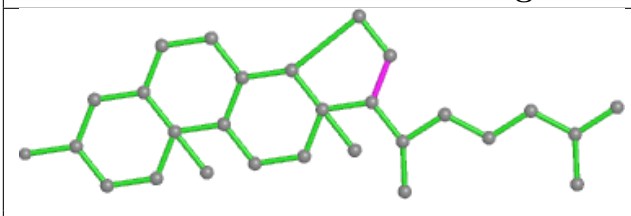
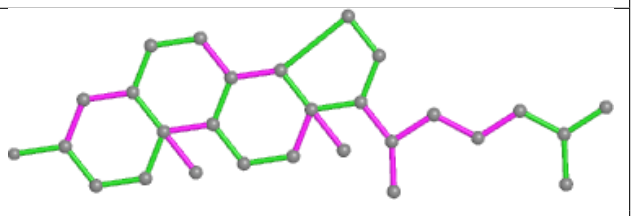


Rings

Ligand CLR C 1107



Bond lengths



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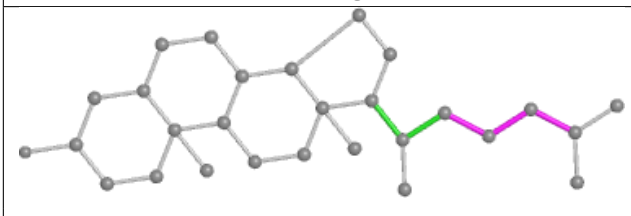

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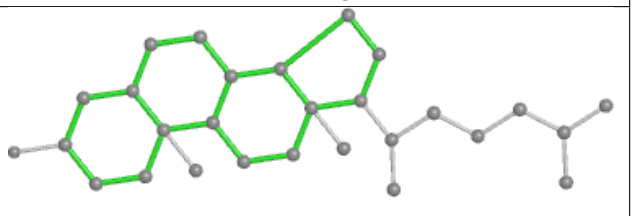
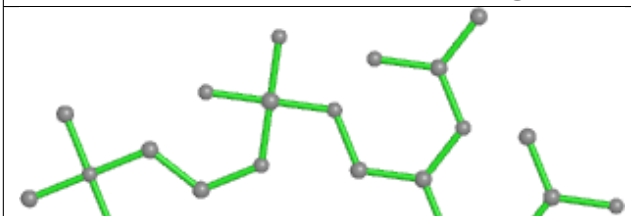
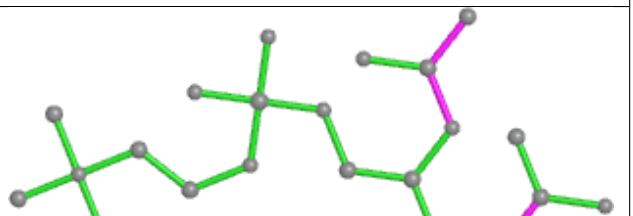


Rings

Ligand PCW C 1105



Bond lengths



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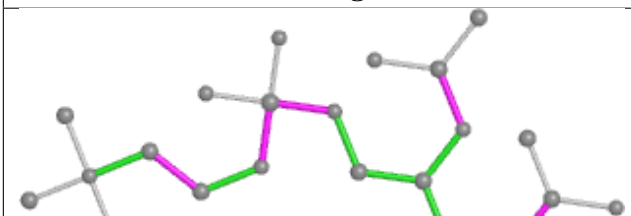
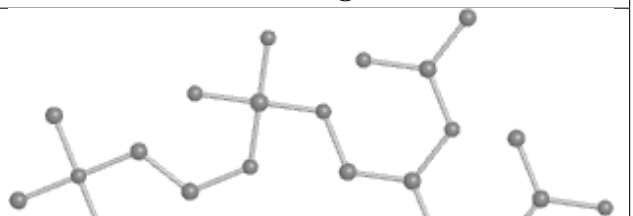
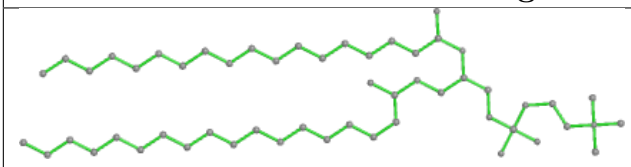


Torsions

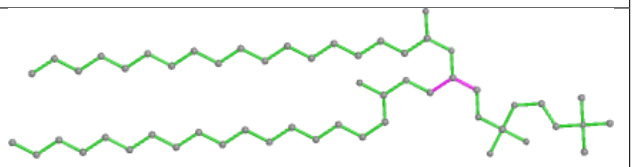


Rings

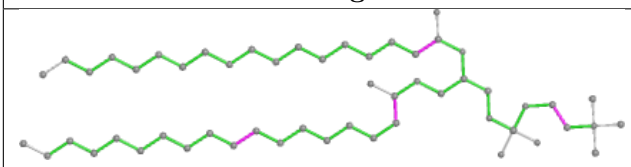
Ligand PC1 A 1106



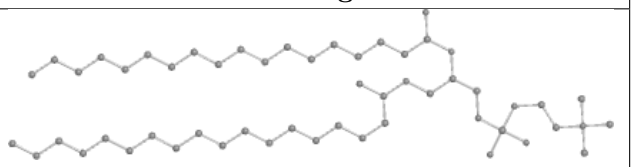
Bond lengths



Bond angles

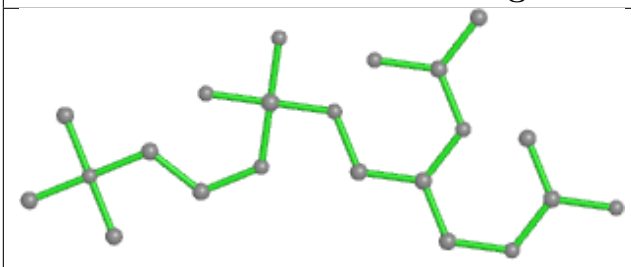


Torsions



Rings

Ligand PCW A 1112



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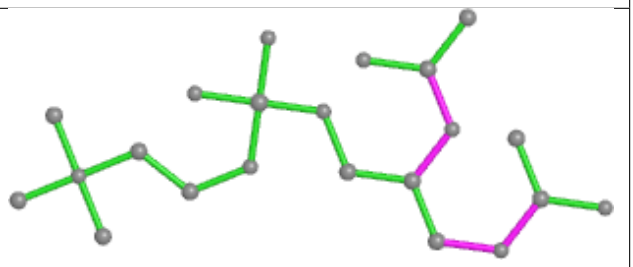
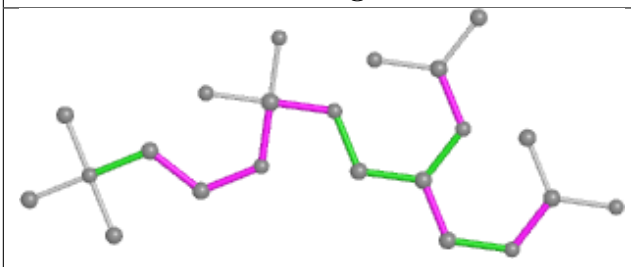
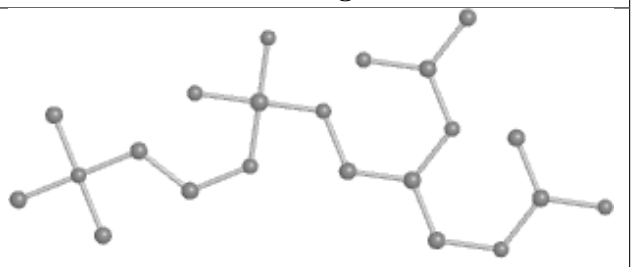


Bond angles

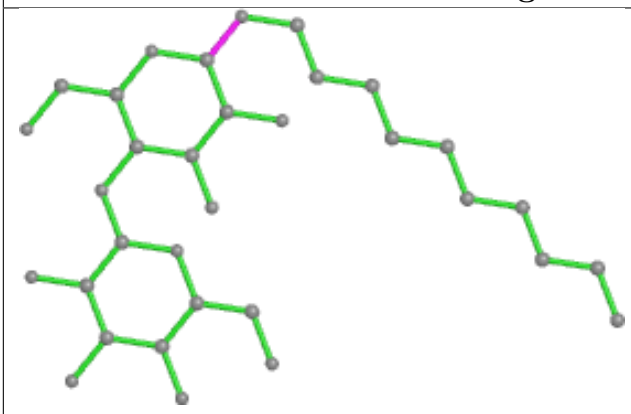


Torsions

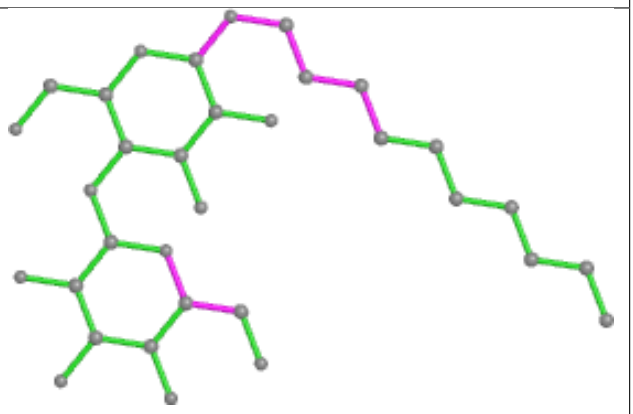


Rings

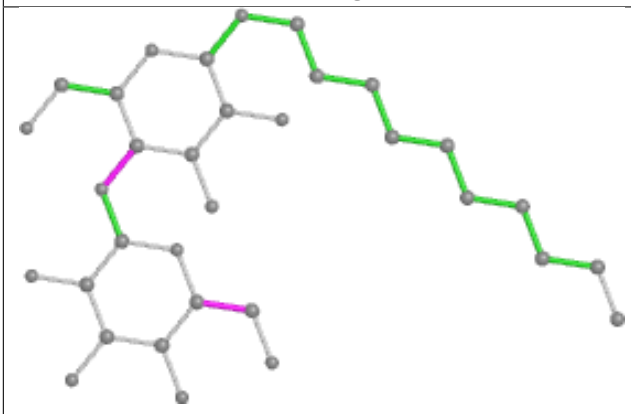
Ligand DMU E 102



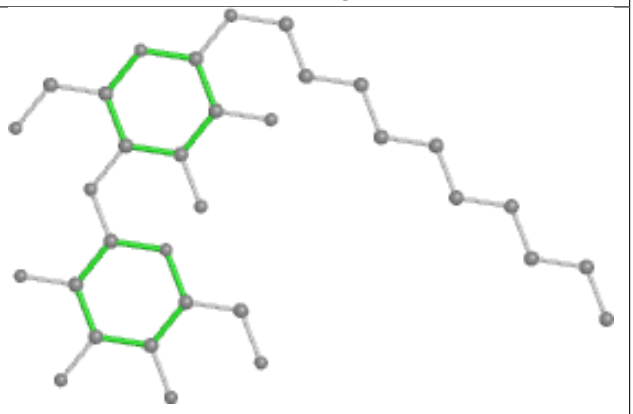
Bond lengths



Bond angles

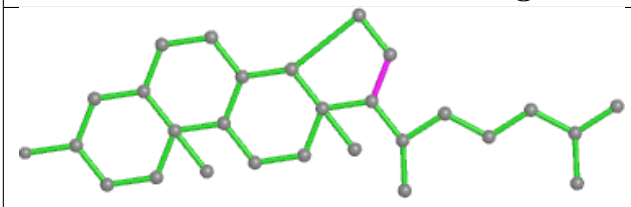


Torsions



Rings

Ligand CLR A 1105



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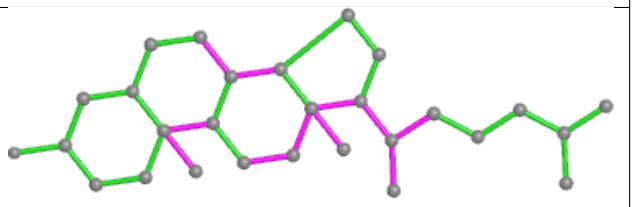
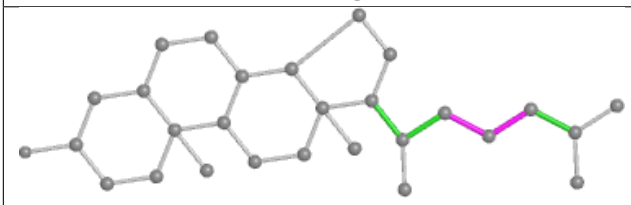
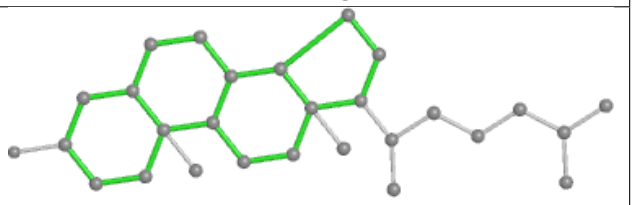


Bond angles

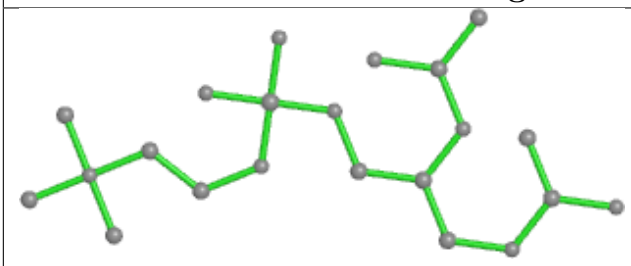


Torsions



Rings

Ligand PCW A 1109



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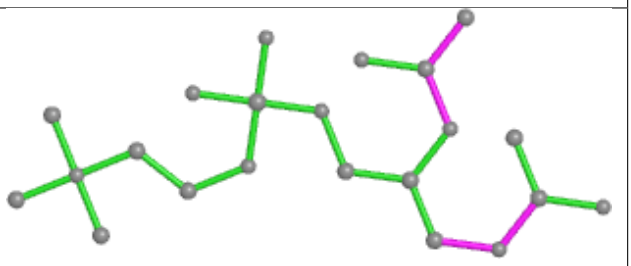
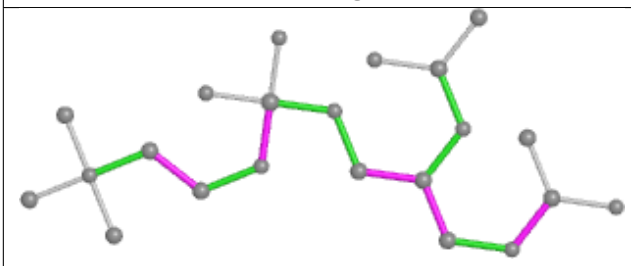
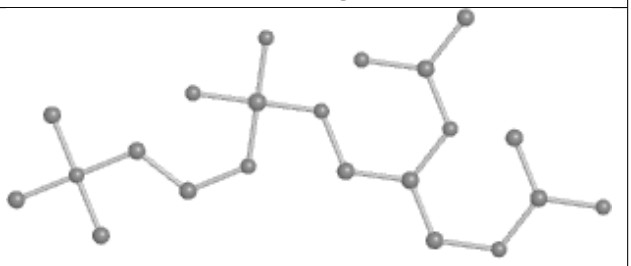


Bond angles

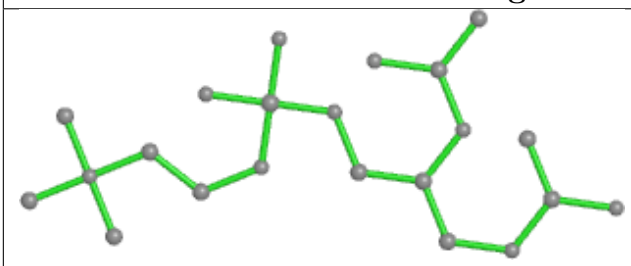


Torsions

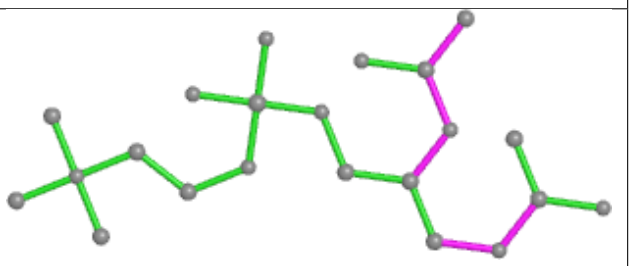


Rings

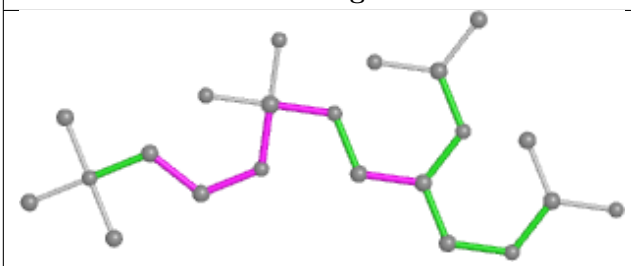
Ligand PCW A 1114



Bond lengths



Bond angles



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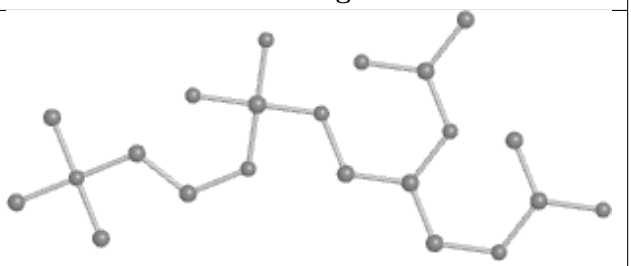
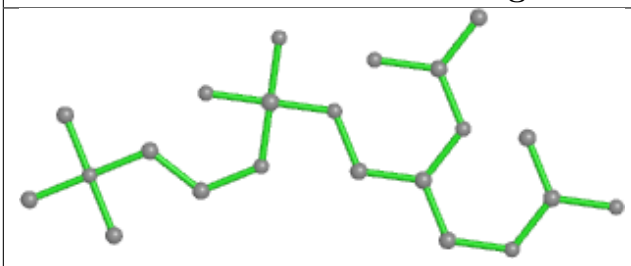


Rings

Ligand PCW A 1115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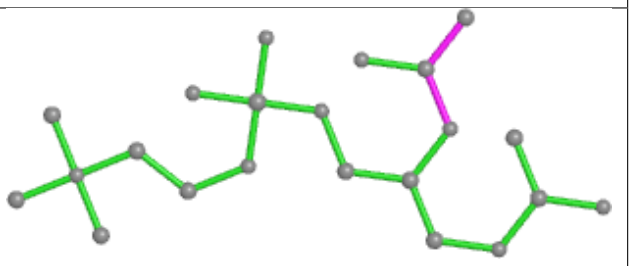
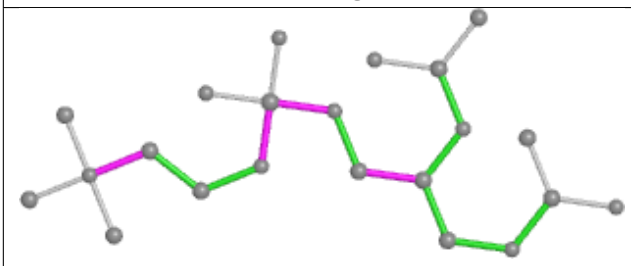
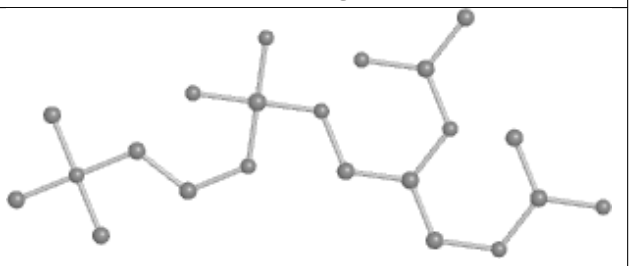
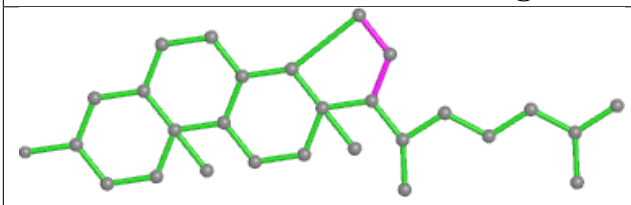

Bond angles


Torsions


Rings

Ligand CLR A 1110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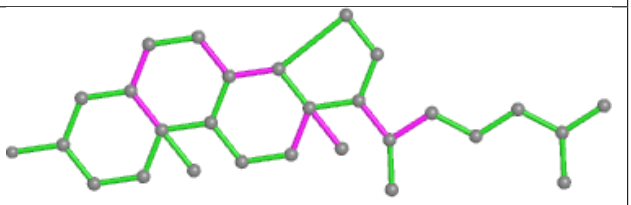
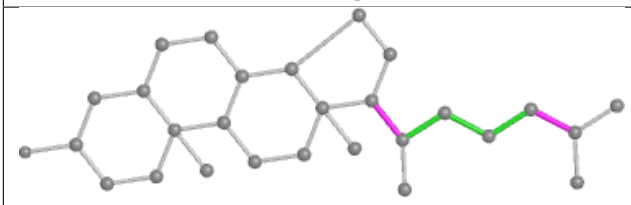

Bond angles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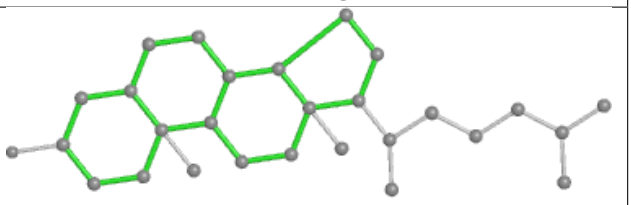
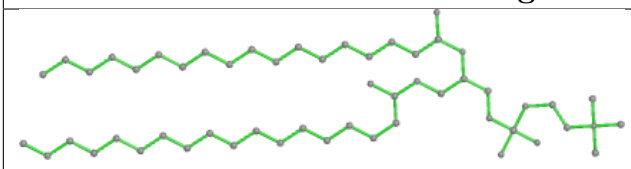

Rings

Ligand PC1 A 1108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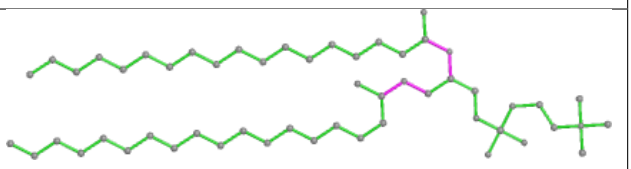
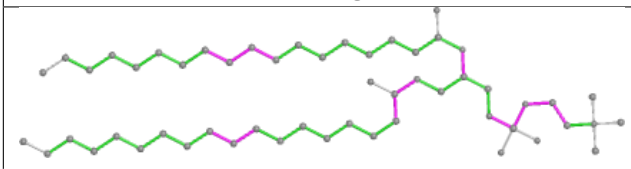
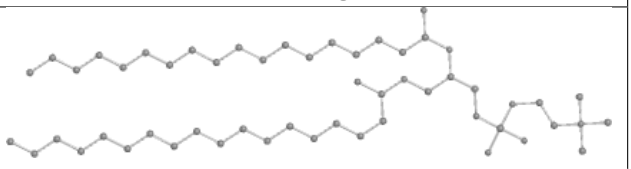
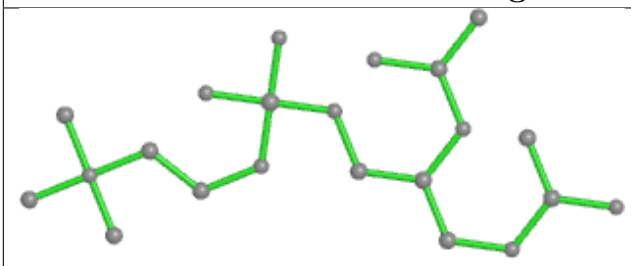

Bond angles

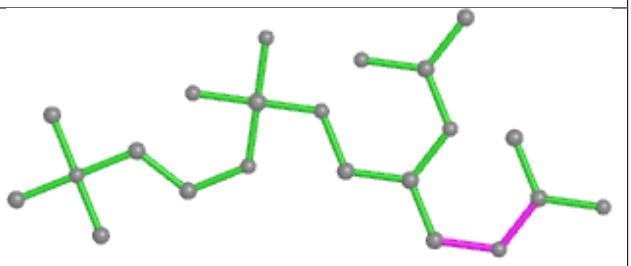

Torsions


Rings

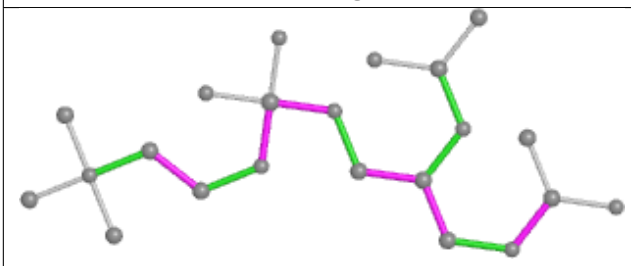
Ligand PCW C 1112



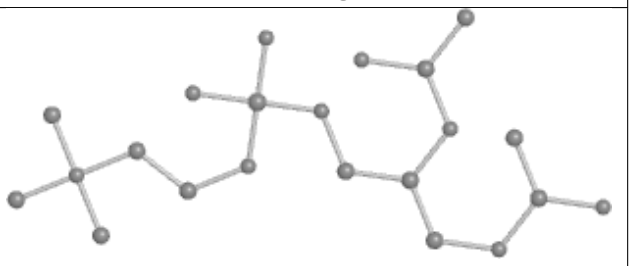
Bond lengths



Bond angles

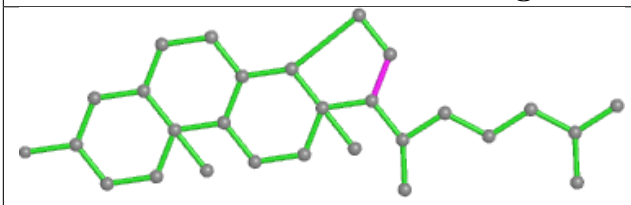


Torsions



Rings

Ligand CLR A 1104



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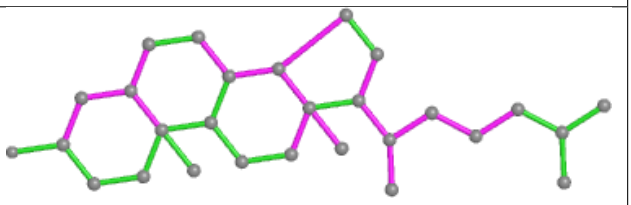
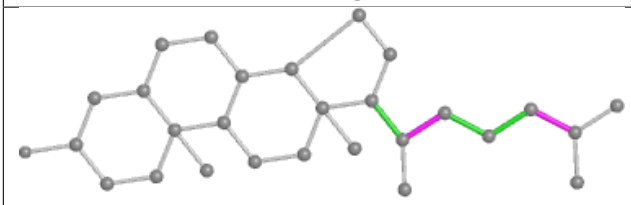
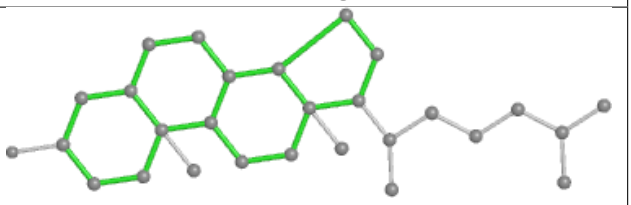


Bond angles

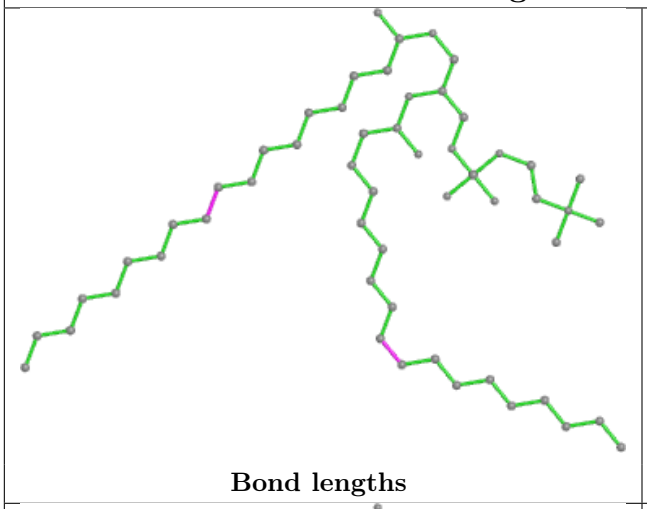


Torsions



Rings

Ligand PCW A 1116



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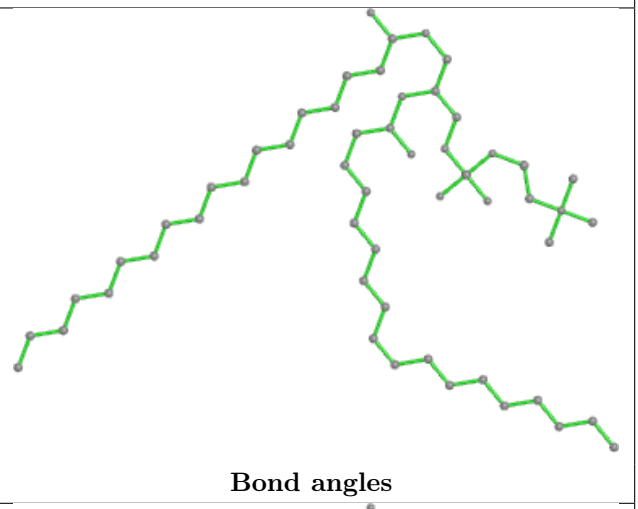
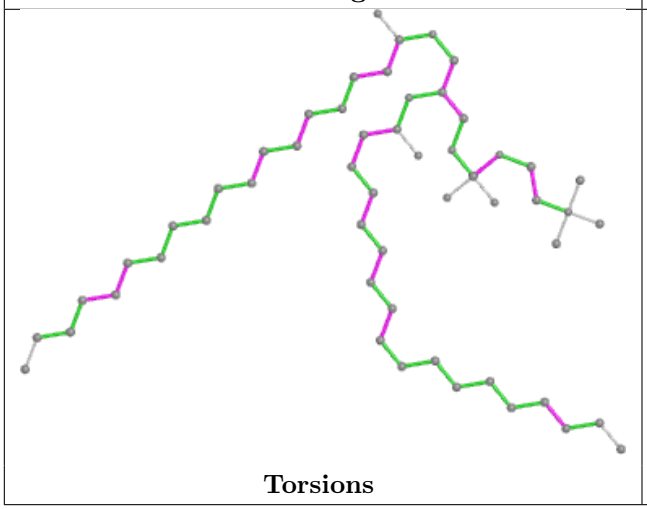
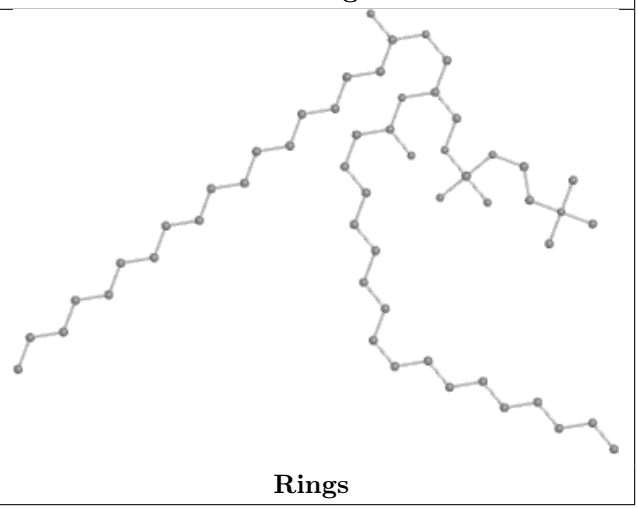


Bond angles

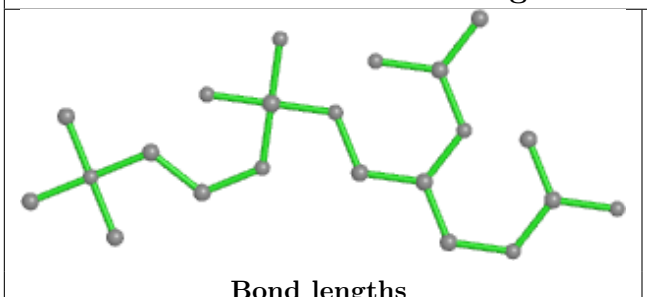


Torsions



Rings

Ligand PCW C 1106



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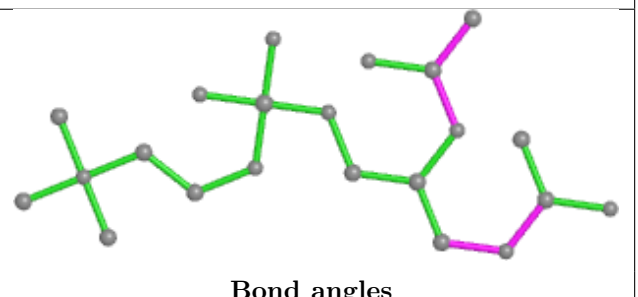
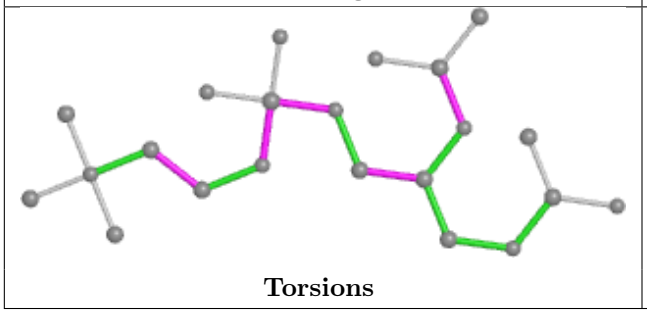
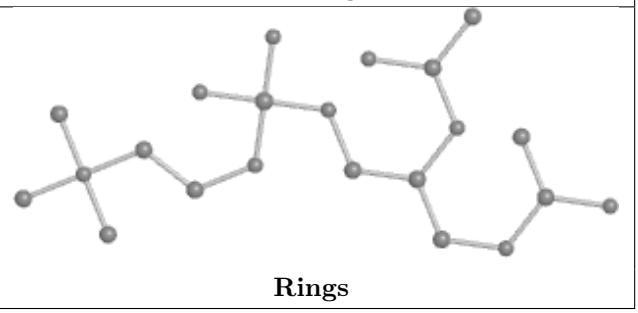


Bond angles

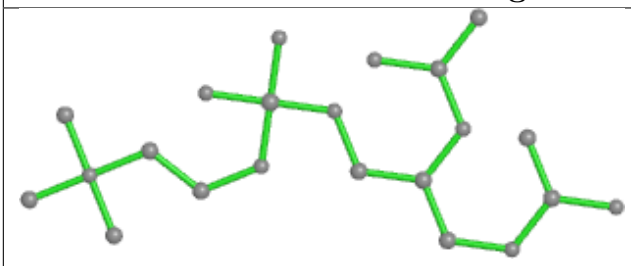


Torsions



Rings

Ligand PCW C 1110



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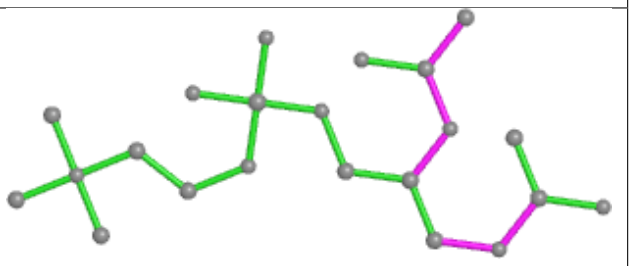
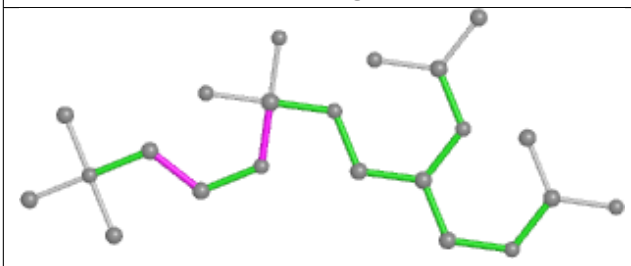
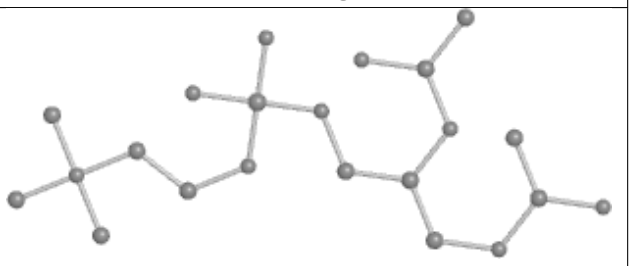


Bond angles

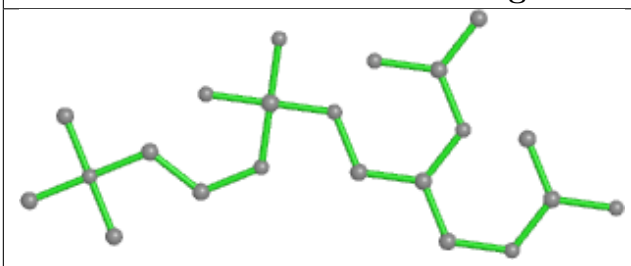


Torsions



Rings

Ligand PCW C 1111



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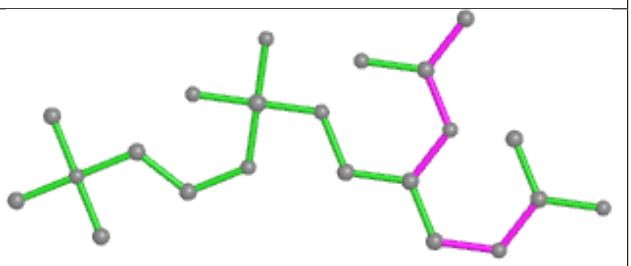
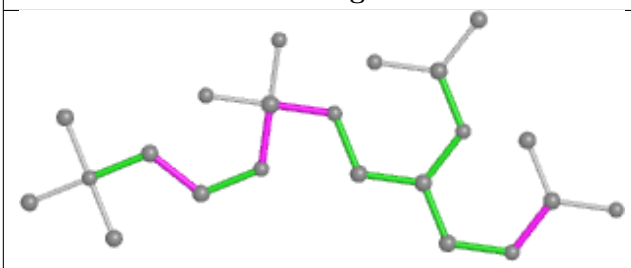
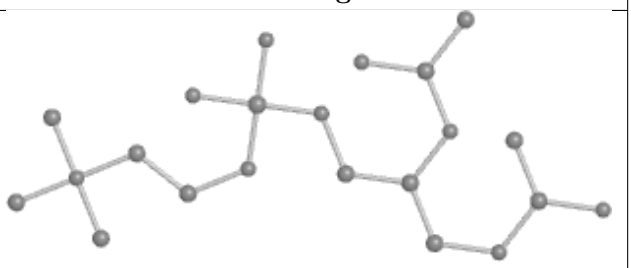


Bond angles

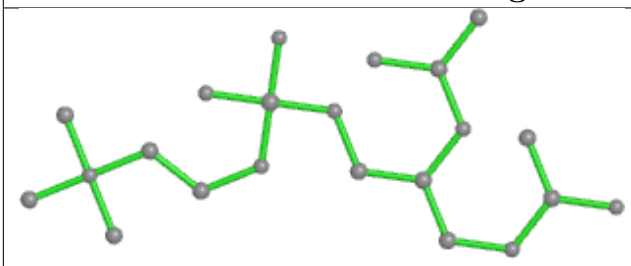


Torsions

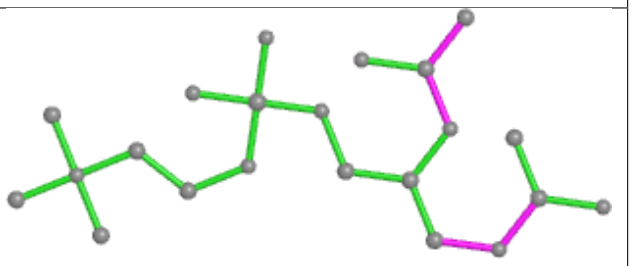


Rings

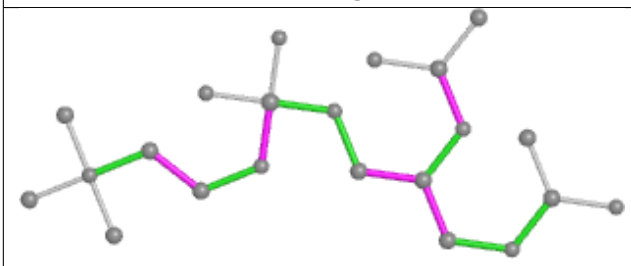
Ligand PCW C 1108



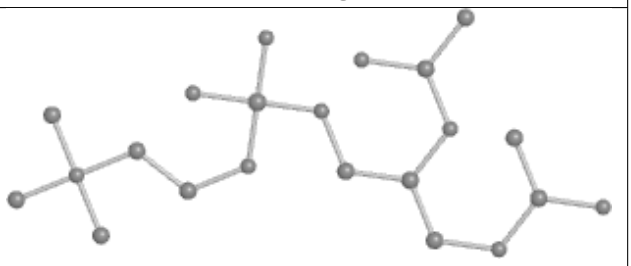
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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, 95^{th} 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%)	-0.16	38 (3%) 40 16	25, 70, 147, 184	0
1	C	995/1021 (97%)	-0.20	26 (2%) 56 27	37, 80, 138, 197	0
2	B	291/303 (96%)	-0.17	8 (2%) 54 26	54, 94, 146, 183	0
2	D	291/303 (96%)	0.19	22 (7%) 13 4	58, 134, 171, 212	0
3	E	33/65 (50%)	-0.37	0 100 100	41, 57, 116, 130	0
3	G	35/65 (53%)	-0.38	1 (2%) 51 23	44, 60, 98, 116	0
All	All	2640/2778 (95%)	-0.14	95 (3%) 42 17	25, 81, 153, 212	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	200	PRO	6.9
1	C	268	SER	6.6
1	C	267	ALA	5.7
1	A	267	ALA	5.3
1	C	269	GLY	5.2
1	C	432	ASN	5.1
1	A	271	GLU	4.9
1	C	23	ARG	4.8
1	A	268	SER	4.4
1	A	272	GLY	4.2
2	D	199	TYR	4.1
1	C	115	GLU	4.0
1	A	26	ASP	4.0
2	D	197	GLU	3.9
2	D	198	THR	3.9
1	C	271	GLU	3.9
1	A	29	LYS	3.8
2	D	15	PHE	3.8
1	A	269	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	116	GLU	3.7
1	A	266	LEU	3.7
1	C	270	LEU	3.6
1	A	433	LEU	3.5
1	A	470	ILE	3.4
1	A	401	GLY	3.4
1	A	113	ALA	3.2
1	A	114	THR	3.2
2	B	13	LYS	3.2
1	C	80	PRO	3.2
1	C	399	GLN	3.2
2	D	112	TYR	3.2
1	A	399	GLN	3.1
2	D	271	GLU	3.1
1	A	115	GLU	3.1
2	D	20	GLU	3.1
2	D	19	SER	3.0
1	C	266	LEU	3.0
1	C	473	ILE	2.9
1	A	25	MET	2.9
1	C	274	GLN	2.9
1	C	116	GLU	2.9
1	A	564	PHE	2.8
1	C	407	THR	2.8
1	C	22	GLU	2.8
2	B	20	GLU	2.8
1	A	397	GLU	2.8
3	G	17	ASP	2.8
1	A	77	PRO	2.7
2	D	193	ASN	2.7
2	B	19	SER	2.7
1	C	227	GLU	2.7
1	A	432	ASN	2.6
1	A	402	VAL	2.6
1	A	118	PRO	2.6
2	B	18	ASN	2.6
1	A	434	PRO	2.6
2	B	194	GLU	2.6
1	A	273	GLY	2.6
1	A	471	VAL	2.5
1	A	111	GLN	2.5
2	D	121	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	17	TRP	2.4
2	D	212	HIS	2.4
1	A	24	ASP	2.3
1	A	33	SER	2.3
1	C	111	GLN	2.3
1	C	433	LEU	2.3
2	D	147	LYS	2.3
2	B	223	LYS	2.3
1	C	82	TRP	2.3
1	A	212	THR	2.3
1	C	272	GLY	2.3
1	A	553	LEU	2.2
2	B	14	LYS	2.2
2	D	161	GLY	2.2
1	C	572	PRO	2.2
1	A	274	GLN	2.2
2	B	21	LYS	2.2
1	C	396	THR	2.2
2	D	14	LYS	2.2
1	C	113	ALA	2.2
1	C	273	GLY	2.1
2	D	25	LEU	2.1
2	D	143	ARG	2.1
1	A	265	THR	2.1
1	A	522	PRO	2.1
1	A	270	LEU	2.1
1	A	243	VAL	2.1
2	D	144	GLY	2.1
1	A	563	GLN	2.1
2	D	16	ILE	2.1
1	C	86	CYS	2.0
2	D	195	SER	2.0
1	A	119	GLN	2.0
2	D	194	GLU	2.0

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

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

6.3 Carbohydrates (i)

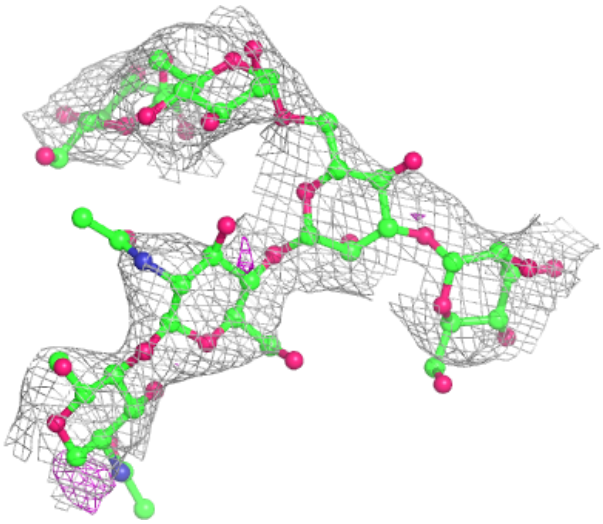
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

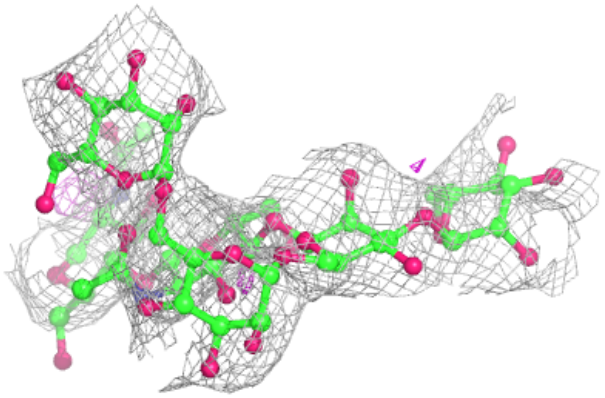
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	2	14/15	0.47	0.75	149,186,195,199	0
6	NAG	I	1	14/15	0.59	0.54	143,156,178,186	0
4	MAN	F	5	11/12	0.64	0.49	124,139,150,159	0
5	MAN	H	4	11/12	0.65	0.66	164,183,197,201	0
5	MAN	H	5	11/12	0.66	0.44	143,162,174,178	0
5	BMA	H	3	11/12	0.66	0.34	168,171,186,195	0
4	MAN	F	4	11/12	0.71	0.39	127,139,145,149	0
4	MAN	F	6	11/12	0.74	0.56	155,157,164,165	0
5	NAG	H	1	14/15	0.76	0.23	127,137,163,184	0
4	NAG	F	1	14/15	0.76	0.59	119,135,146,148	0
4	BMA	F	3	11/12	0.83	0.45	127,140,149,155	0
4	NAG	F	2	14/15	0.86	0.66	132,151,163,169	0
6	NAG	I	2	14/15	0.86	0.52	127,150,160,164	0

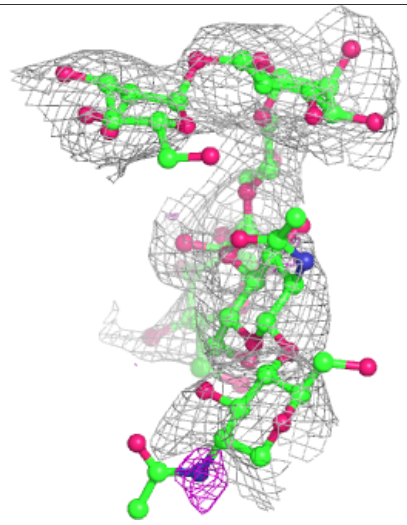
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

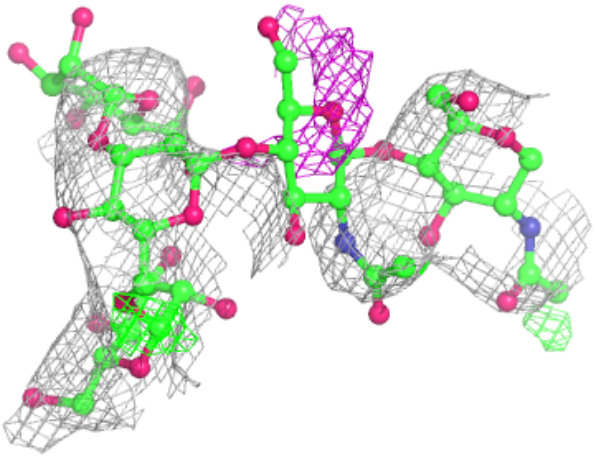


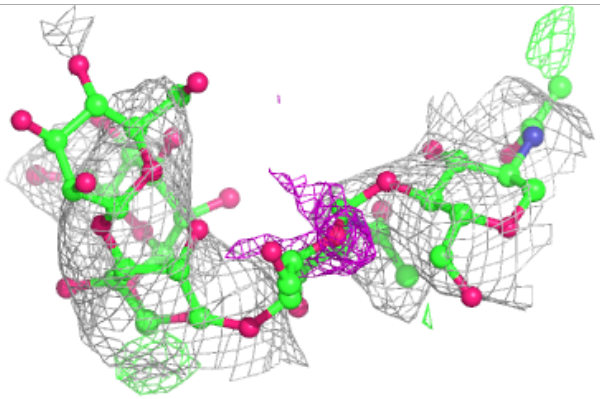


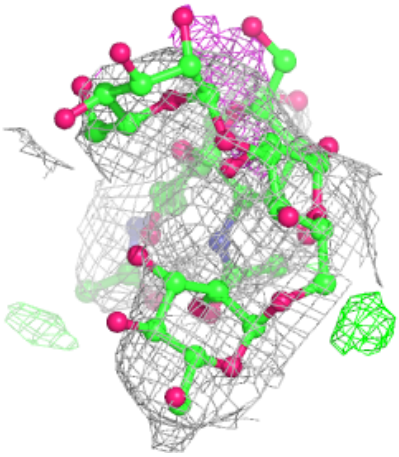


Electron density around Chain H:

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

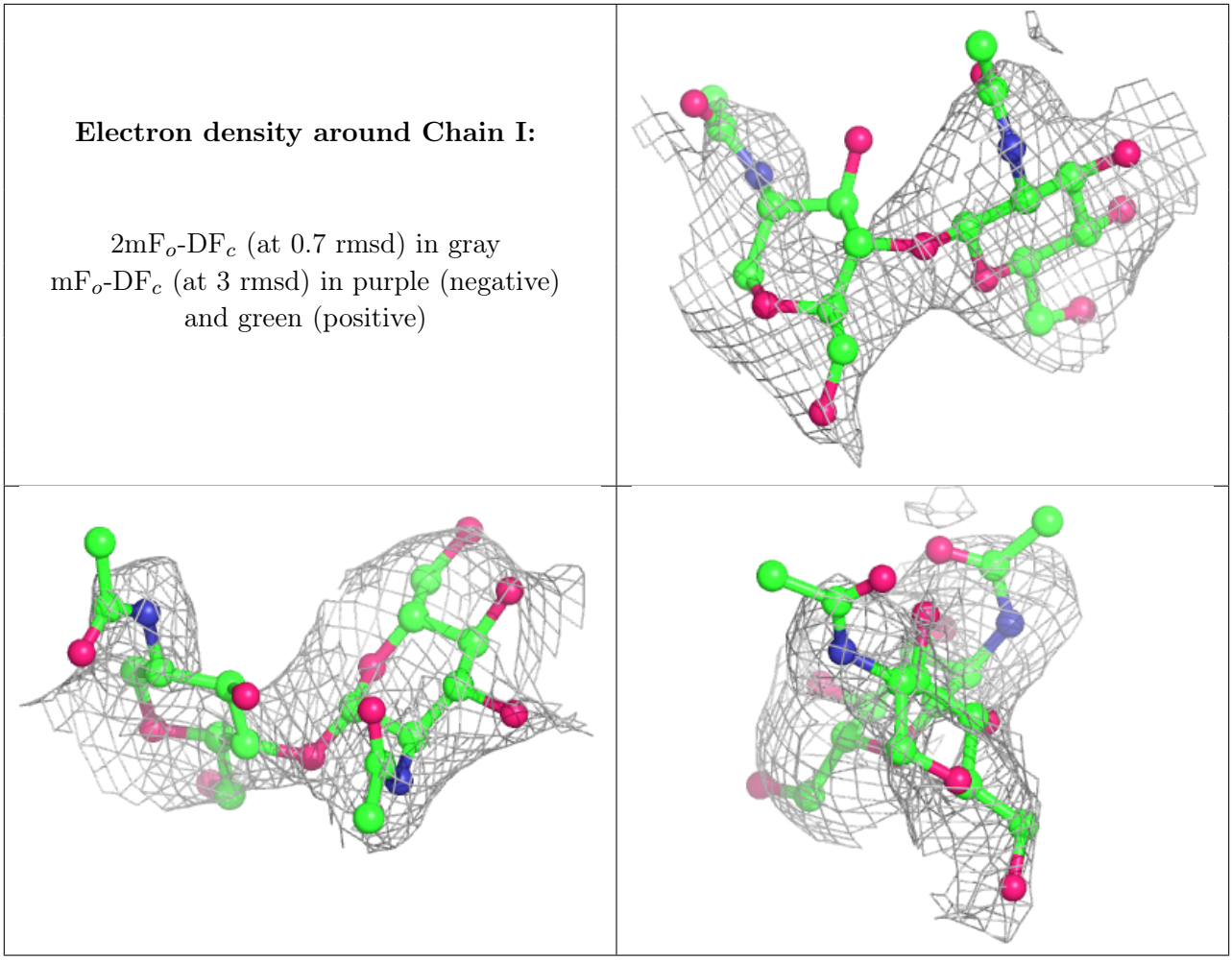






Electron density around Chain I:

$2mF_o$-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, 95^{th} 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
9	PC1	A	1106	54/54	0.66	0.49	77,109,142,152	0
11	NAG	D	401	14/15	0.66	0.41	152,167,170,172	0
10	PCW	A	1109	22/54	0.67	0.33	99,133,167,168	0
10	PCW	A	1113	22/54	0.69	0.53	99,143,149,156	0
10	PCW	C	1105	22/54	0.70	0.34	84,117,184,198	0
10	PCW	C	1112	22/54	0.72	0.34	78,124,156,168	0
8	CLR	A	1110	28/28	0.73	0.37	103,117,133,137	0
10	PCW	C	1109	22/54	0.74	0.37	90,125,155,158	0
10	PCW	C	1108	22/54	0.79	0.25	86,115,141,152	0
10	PCW	C	1110	22/54	0.79	0.52	102,140,160,161	0

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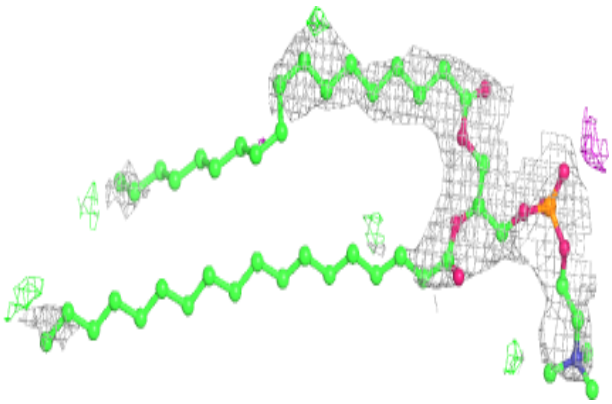
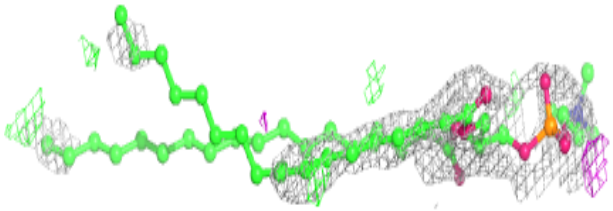
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	1102	1/1	0.81	0.26	89,89,89,89	0
10	PCW	A	1107	22/54	0.81	0.33	102,121,151,156	0
10	PCW	A	1115	22/54	0.81	0.57	94,128,152,155	0
10	PCW	C	1106	22/54	0.82	0.49	85,127,136,141	0
10	PCW	A	1114	22/54	0.82	0.21	88,125,139,145	0
8	CLR	C	1107	28/28	0.83	0.45	92,110,124,125	0
10	PCW	A	1116	54/54	0.84	0.60	60,88,136,146	0
9	PC1	A	1108	54/54	0.85	0.37	52,87,109,122	0
10	PCW	C	1111	22/54	0.85	0.43	78,111,130,136	0
8	CLR	A	1104	28/28	0.87	0.35	72,97,107,111	0
10	PCW	A	1112	22/54	0.87	0.36	68,119,130,139	0
9	PC1	A	1111	54/54	0.89	0.34	44,83,119,128	0
8	CLR	C	1104	28/28	0.90	0.25	39,46,84,104	0
7	MG	A	1101	1/1	0.91	0.10	66,66,66,66	0
12	DMU	E	102	33/33	0.93	0.23	42,67,85,110	0
7	MG	C	1102	1/1	0.94	0.22	64,64,64,64	0
7	MG	C	1101	1/1	0.95	0.12	95,95,95,95	0
8	CLR	E	101	28/28	0.95	0.22	31,40,61,83	0
8	CLR	A	1105	28/28	0.95	0.26	33,53,90,93	0
7	MG	A	1103	1/1	0.96	0.15	34,34,34,34	0
7	MG	C	1103	1/1	0.98	0.08	44,44,44,44	0

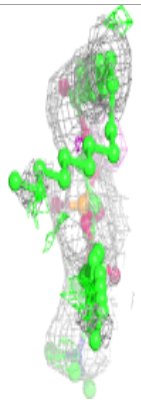
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 A 1106:

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

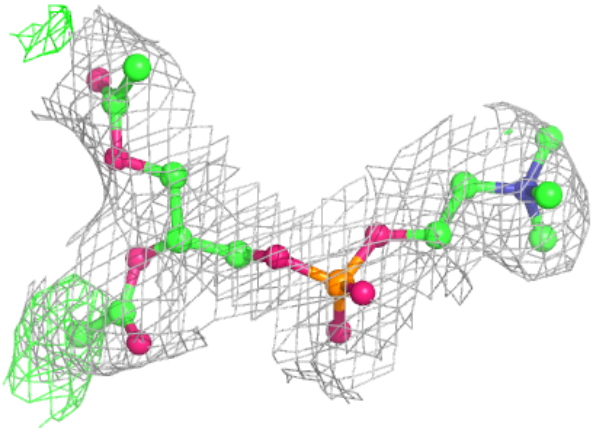


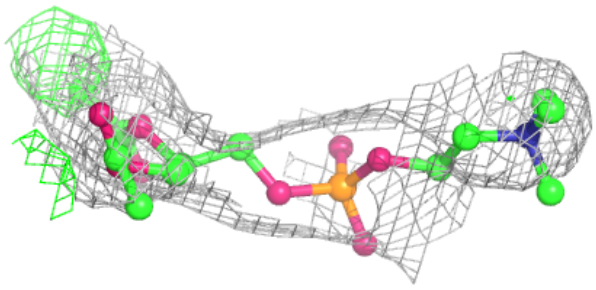


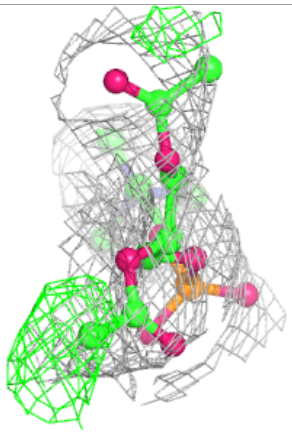


Electron density around PCW A 1109:

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

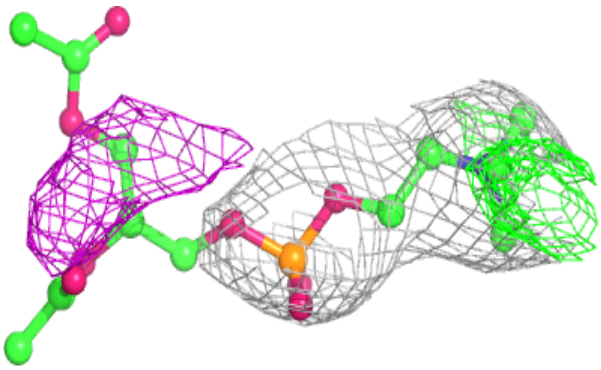


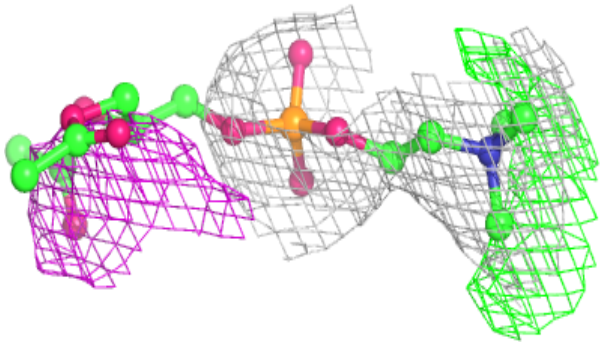


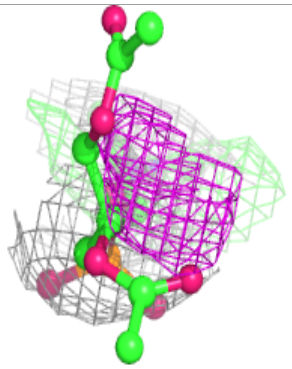


Electron density around PCW A 1113:

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

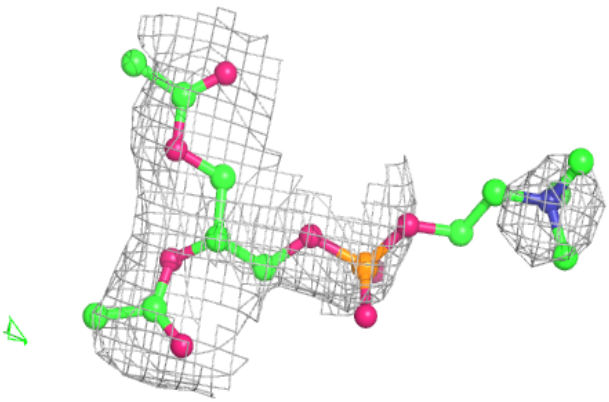


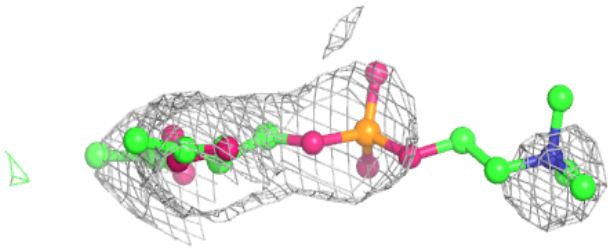


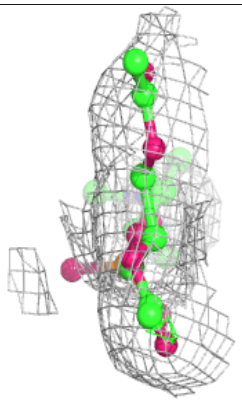


Electron density around PCW C 1105:

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

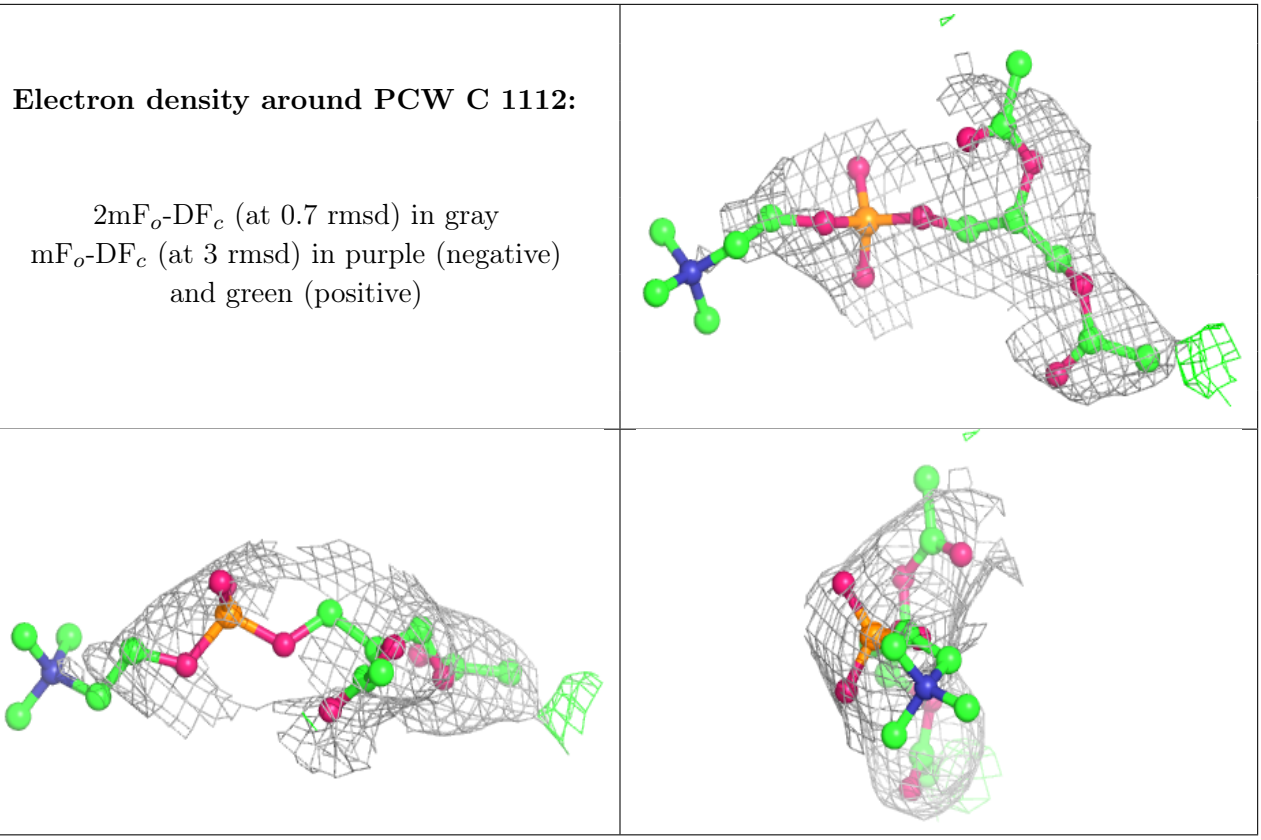






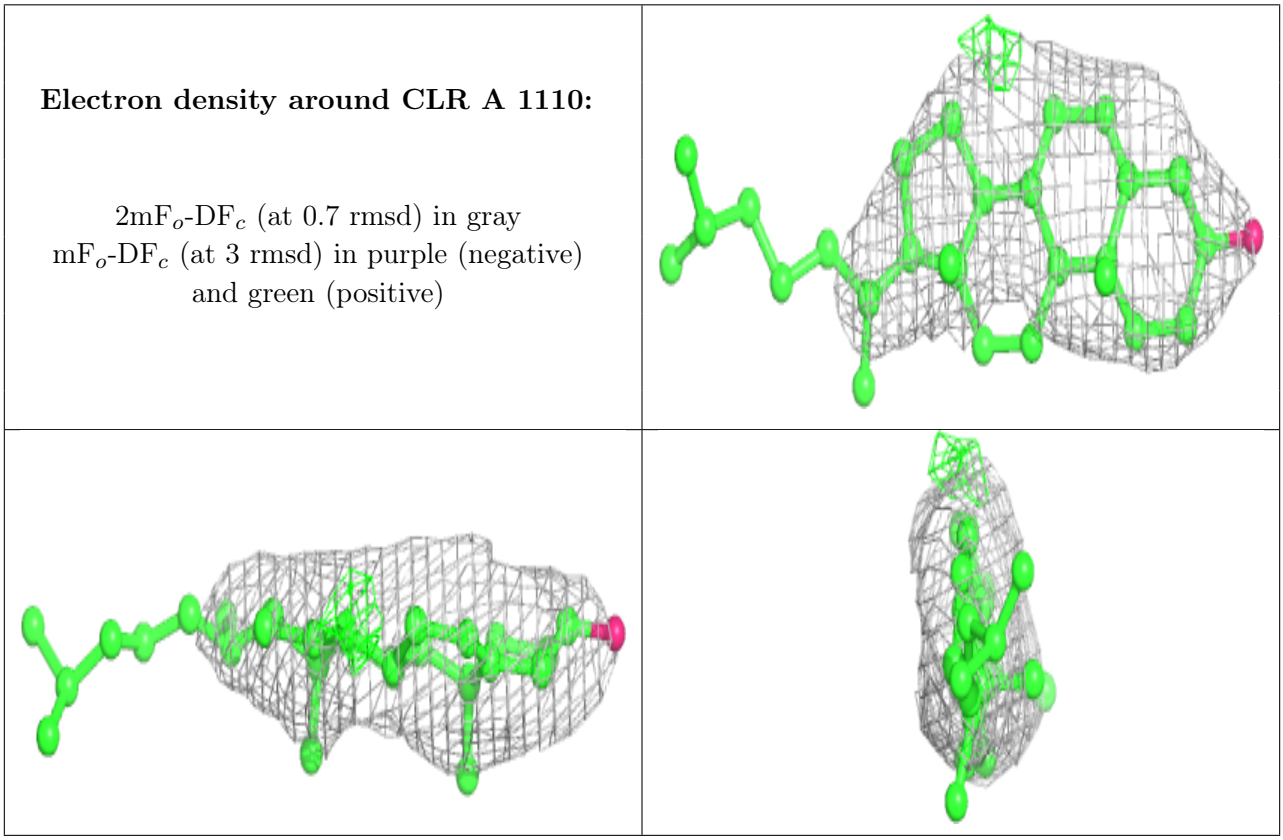
Electron density around PCW C 1112:

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



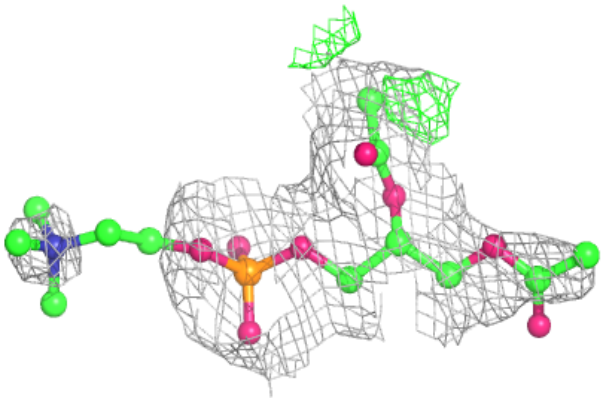
Electron density around CLR A 1110:

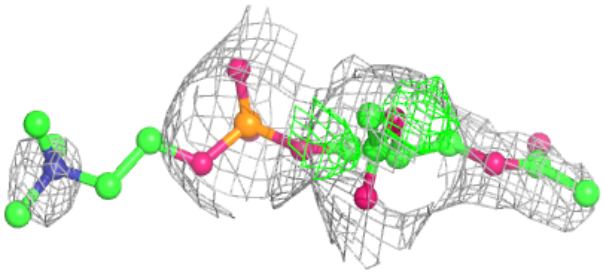
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

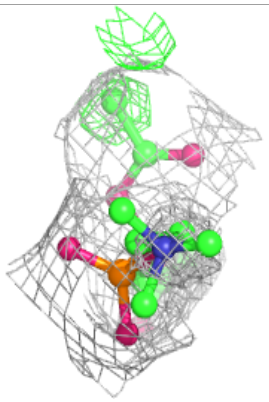


Electron density around PCW C 1109:

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

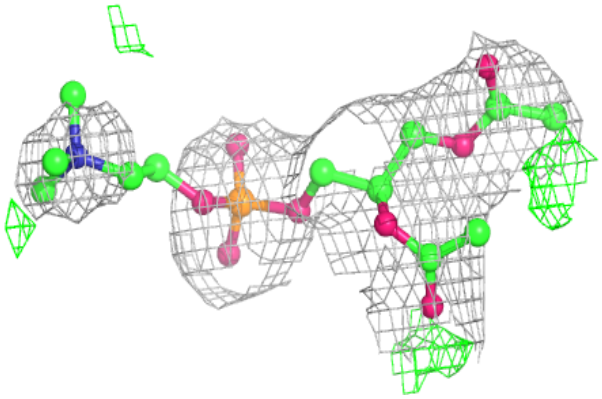


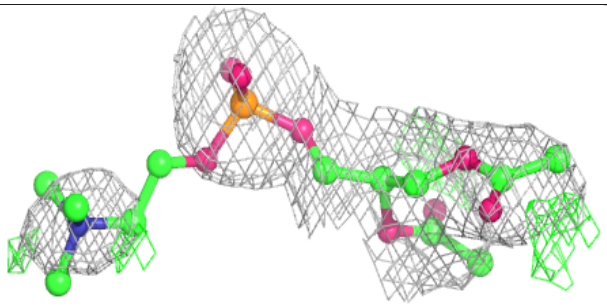


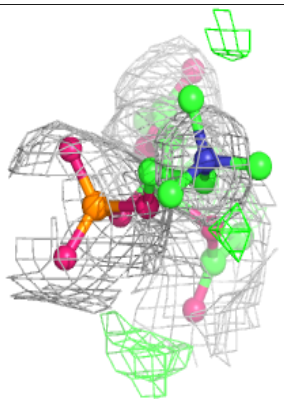


Electron density around PCW C 1108:

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

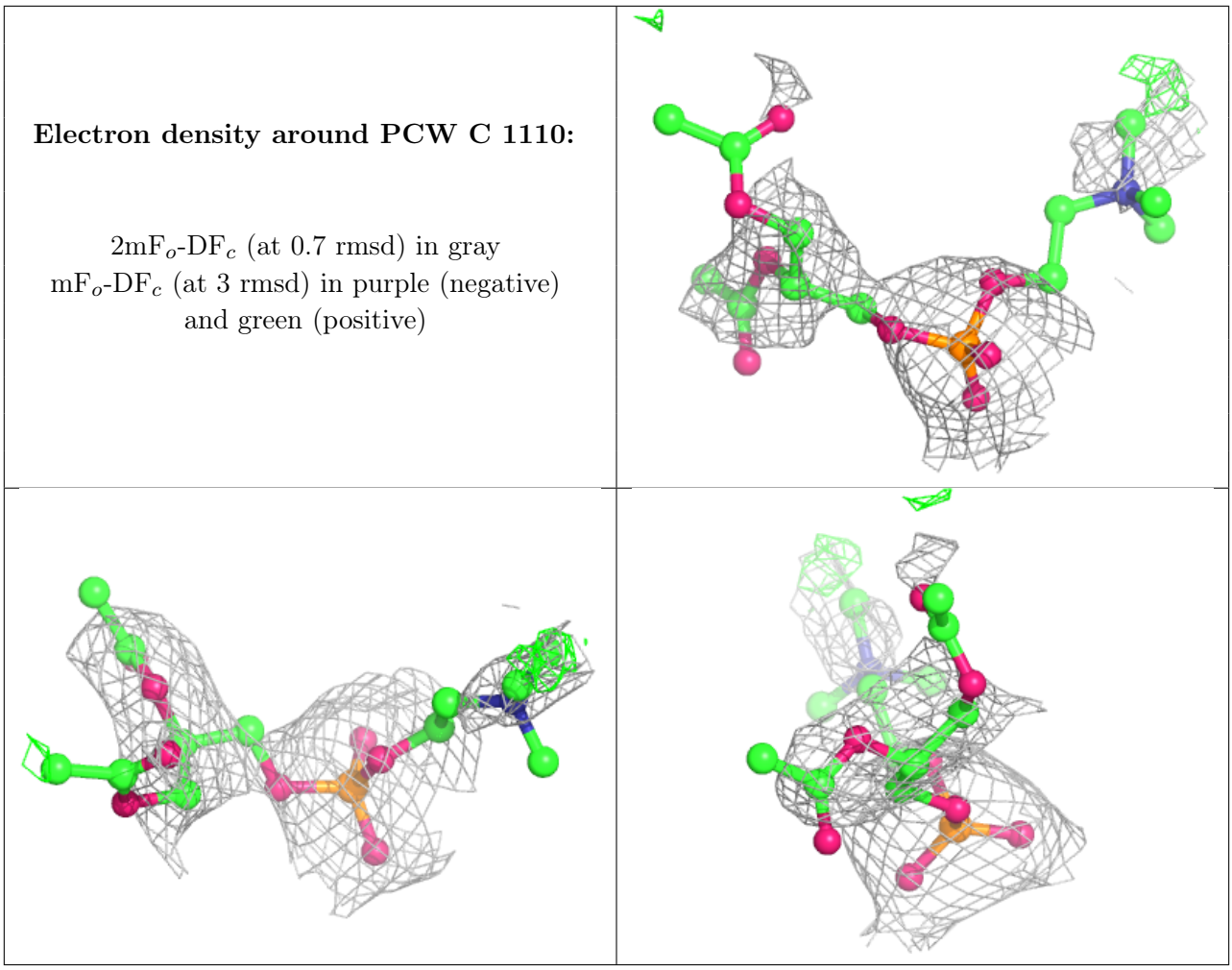






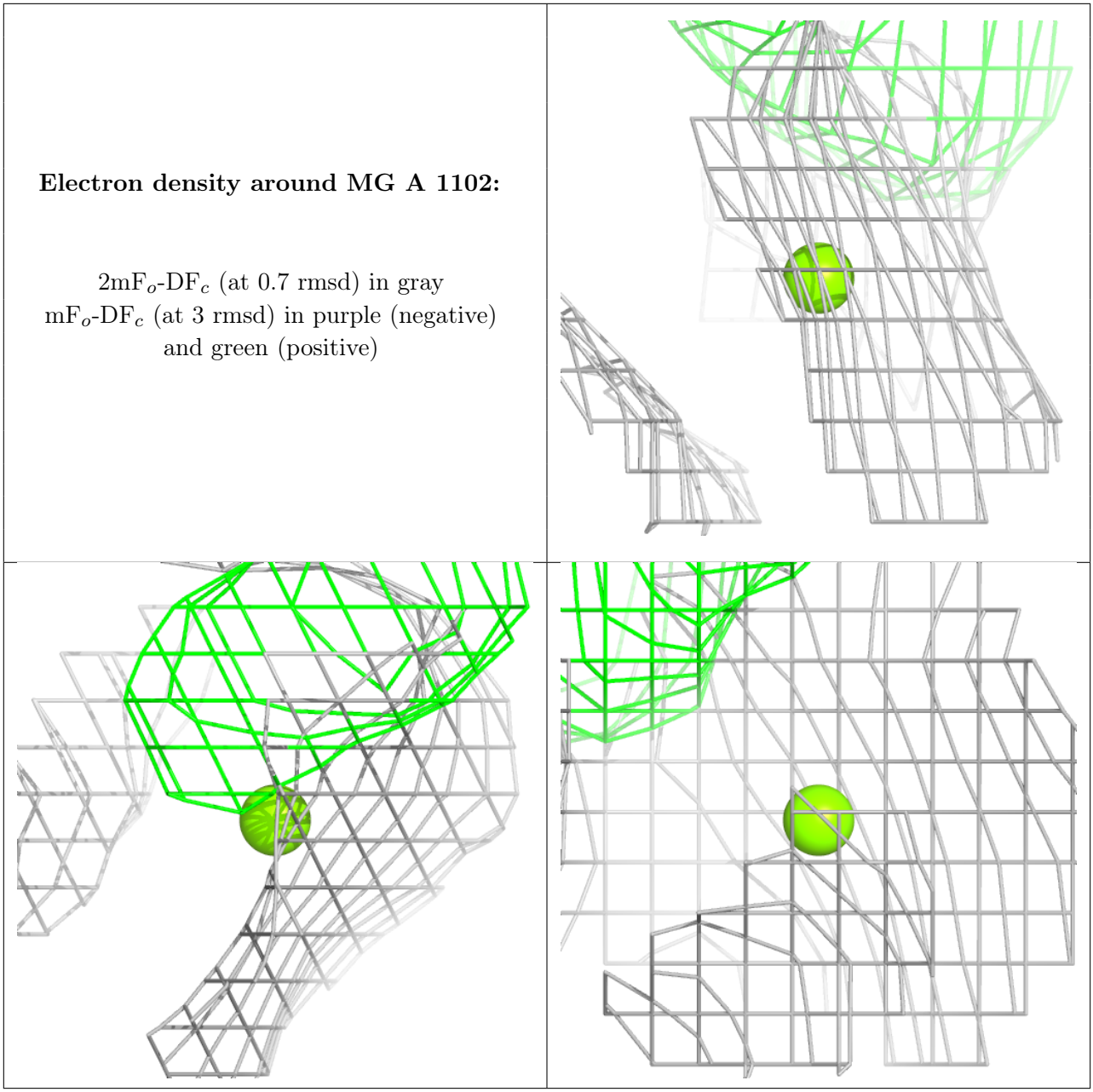
Electron density around PCW C 1110:

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



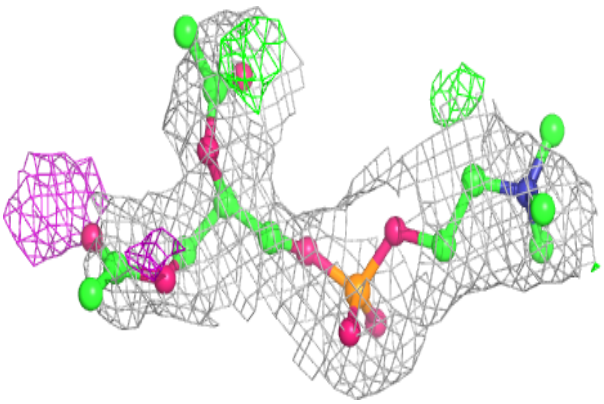
Electron density around MG A 1102:

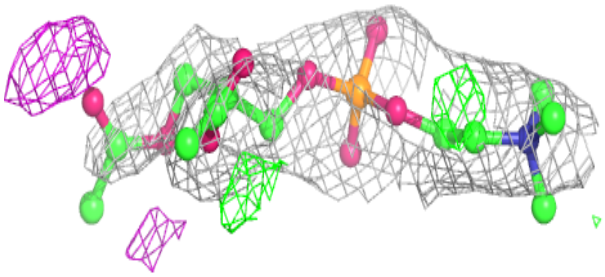
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

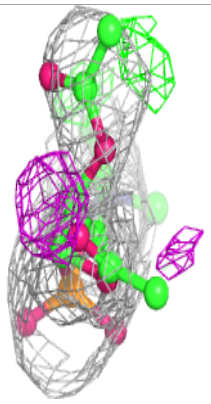


Electron density around PCW A 1107:

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

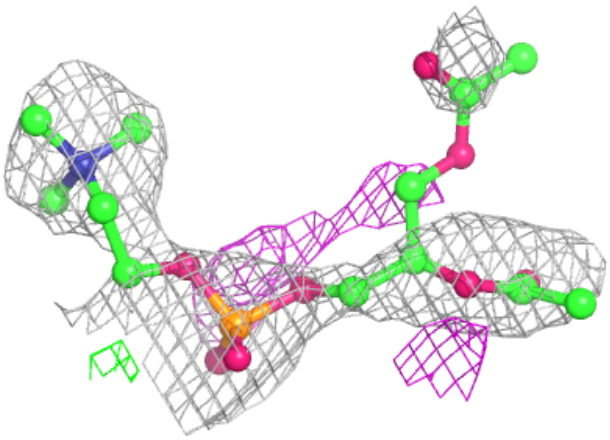


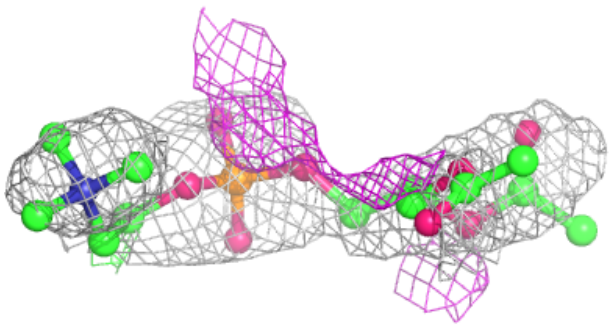


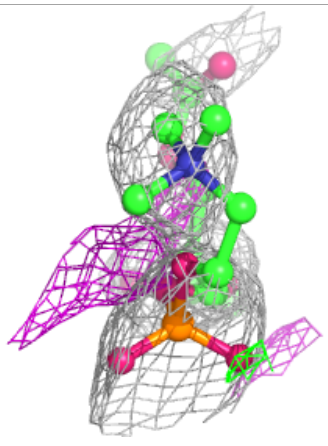


Electron density around PCW A 1115:

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

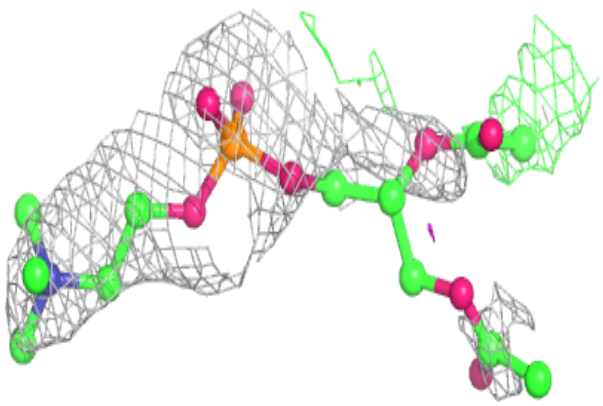


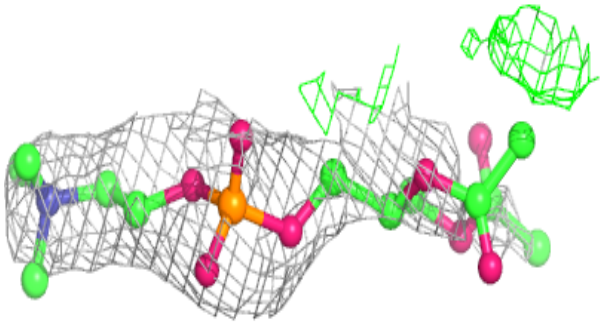


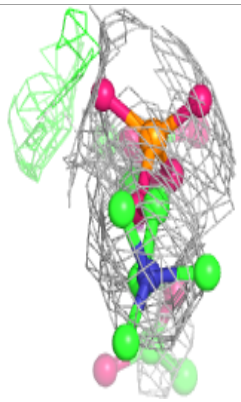


Electron density around PCW C 1106:

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

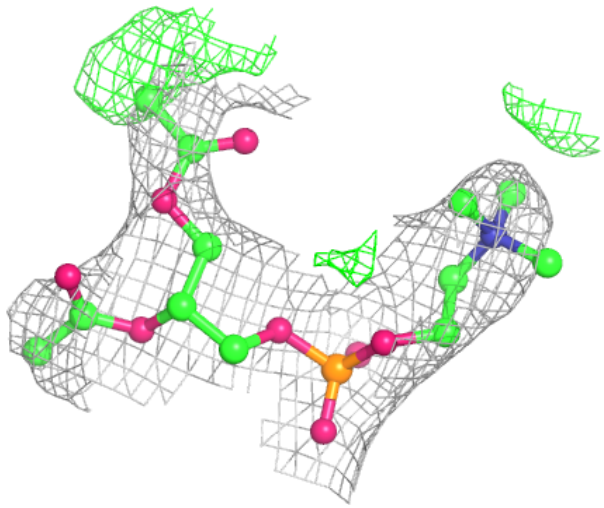


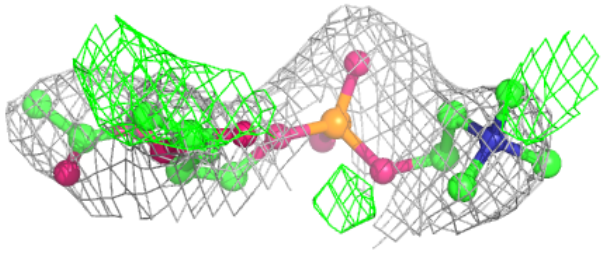


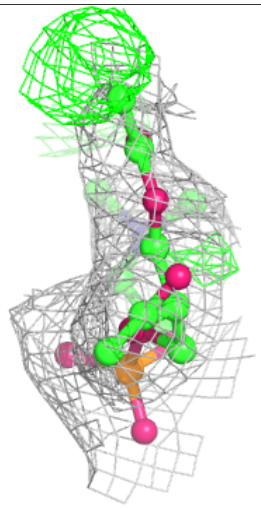


Electron density around PCW A 1114:

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

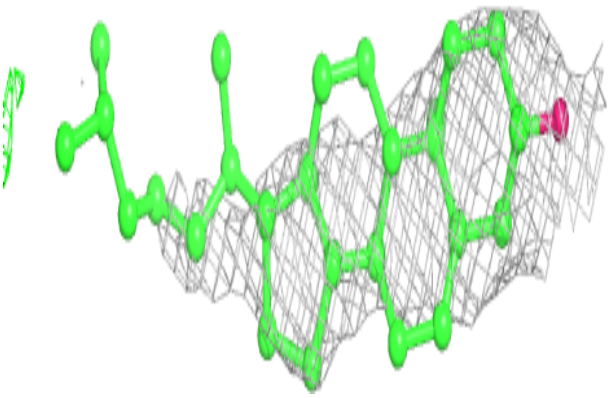


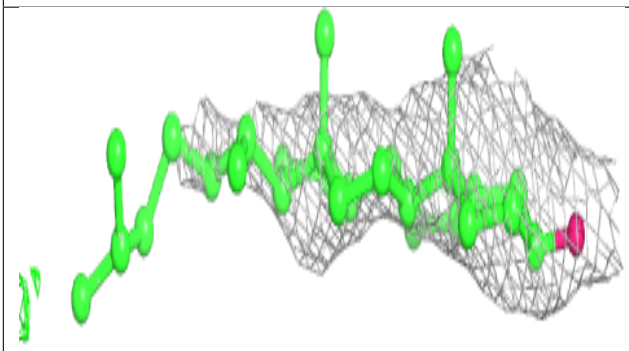


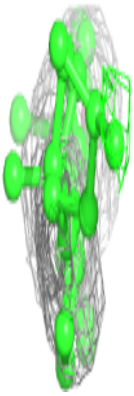


Electron density around CLR C 1107:

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

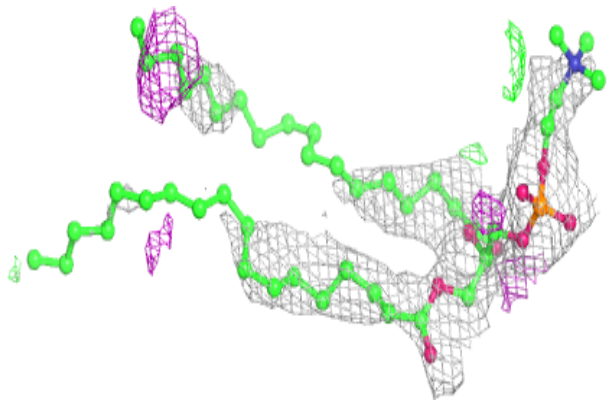


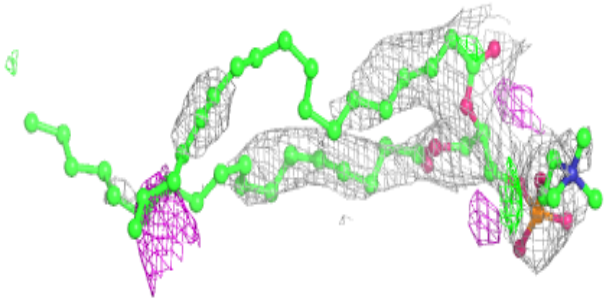


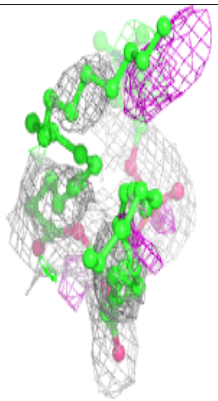


Electron density around PCW A 1116:

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

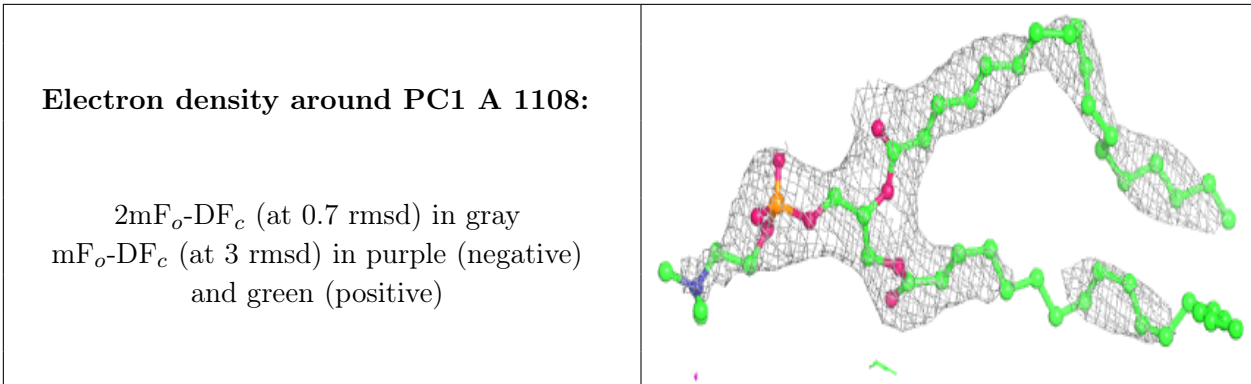






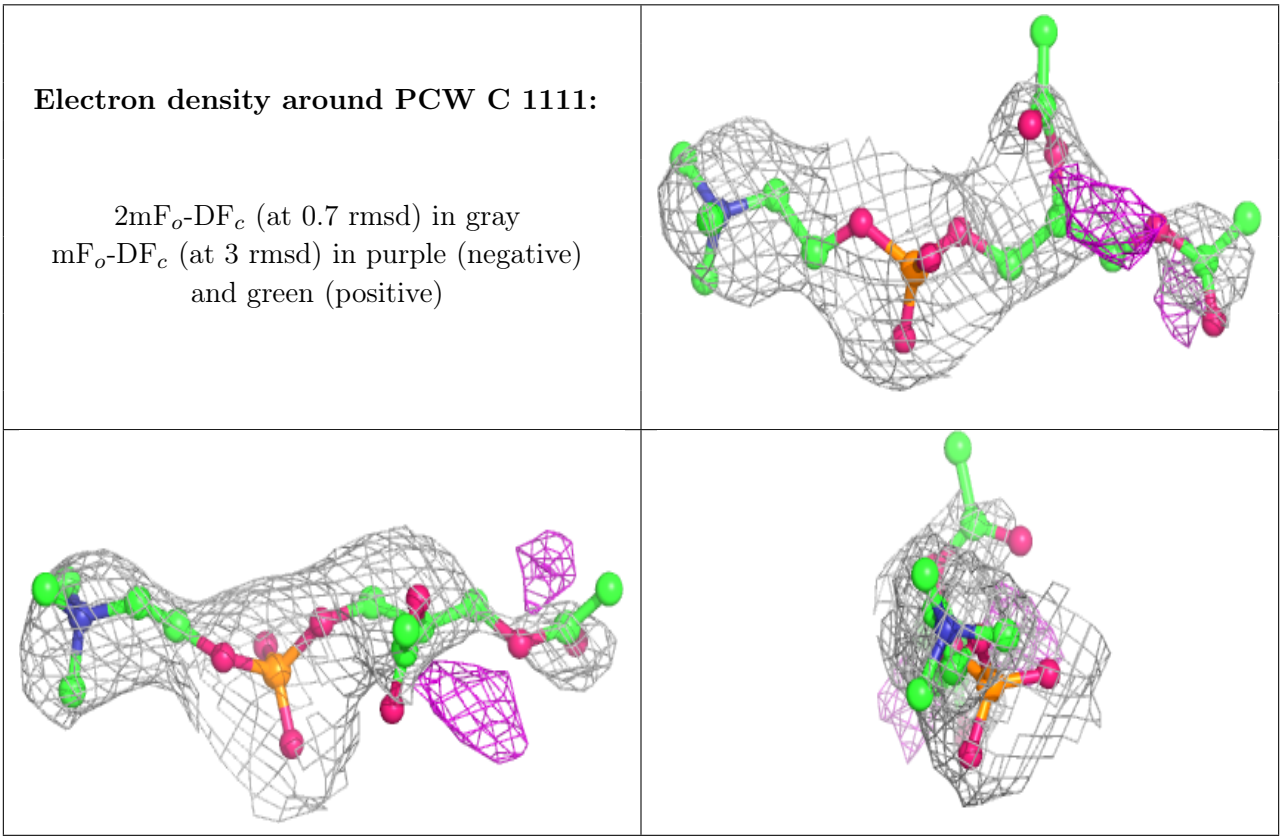
Electron density around PC1 A 1108:

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



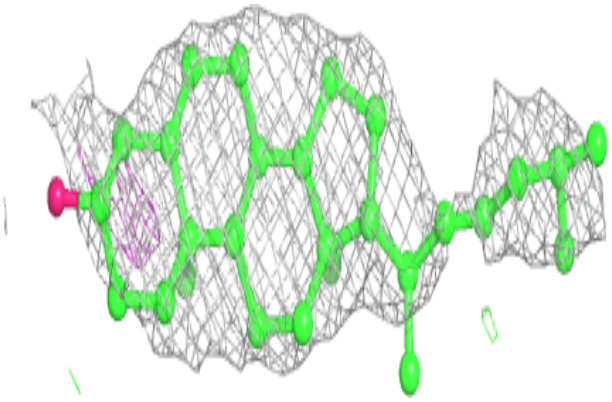
Electron density around PCW C 1111:

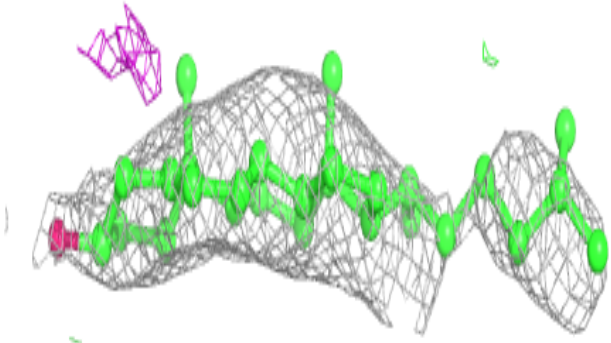
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

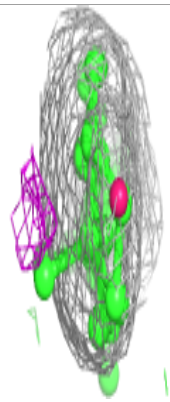


Electron density around CLR A 1104:

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

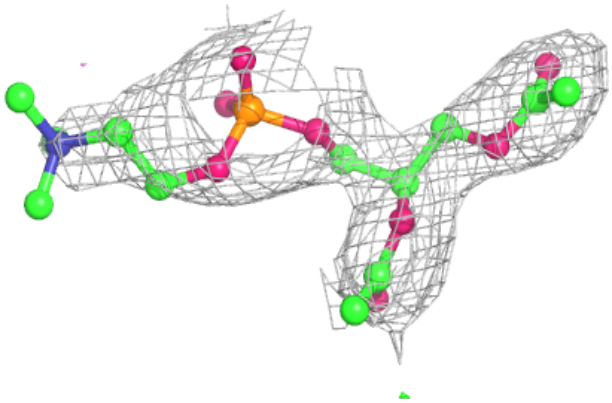


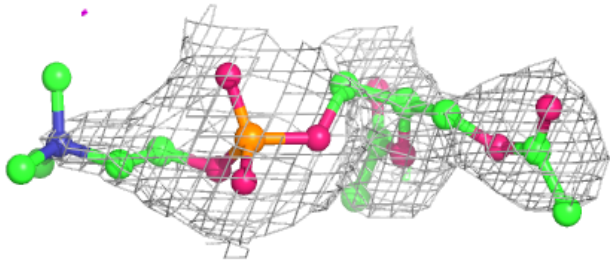


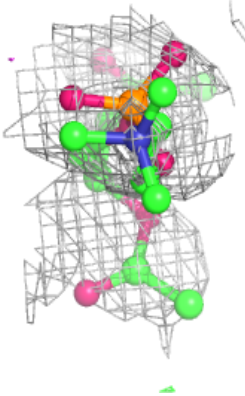


Electron density around PCW A 1112:

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

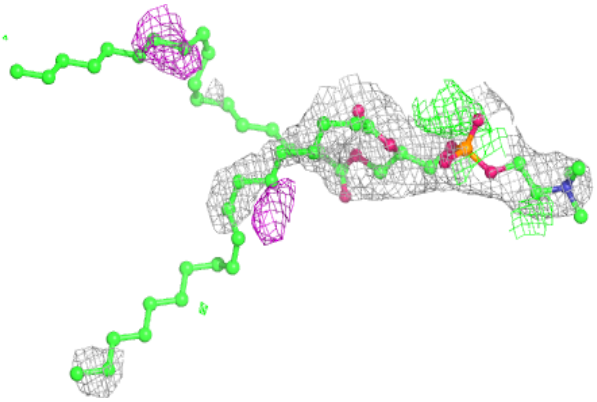


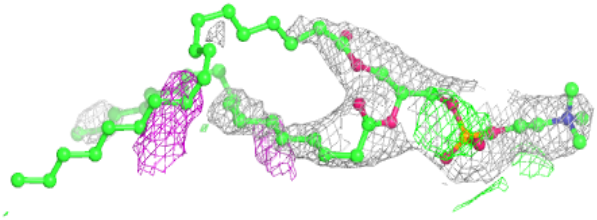


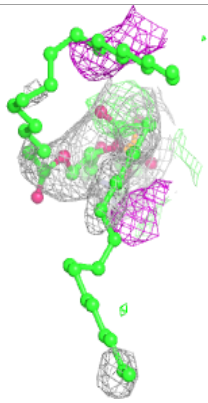


Electron density around PC1 A 1111:

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

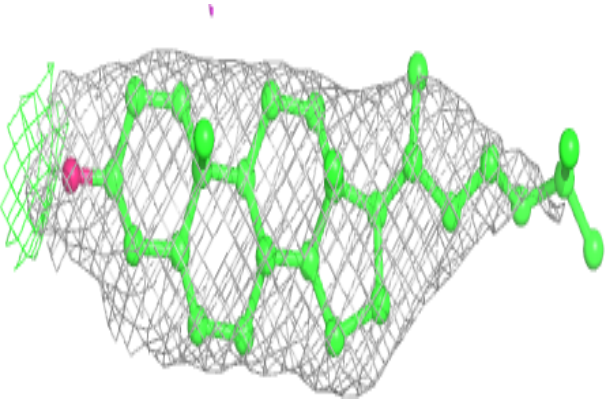


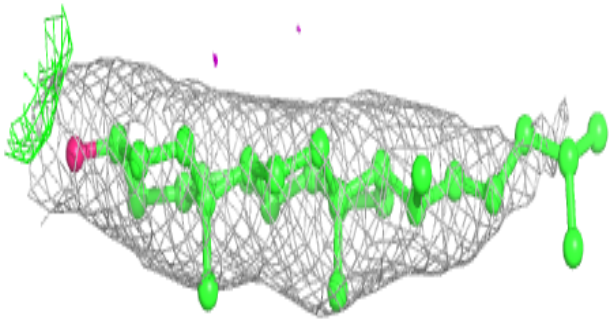


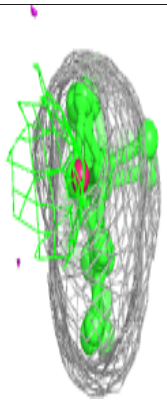


Electron density around CLR C 1104:

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

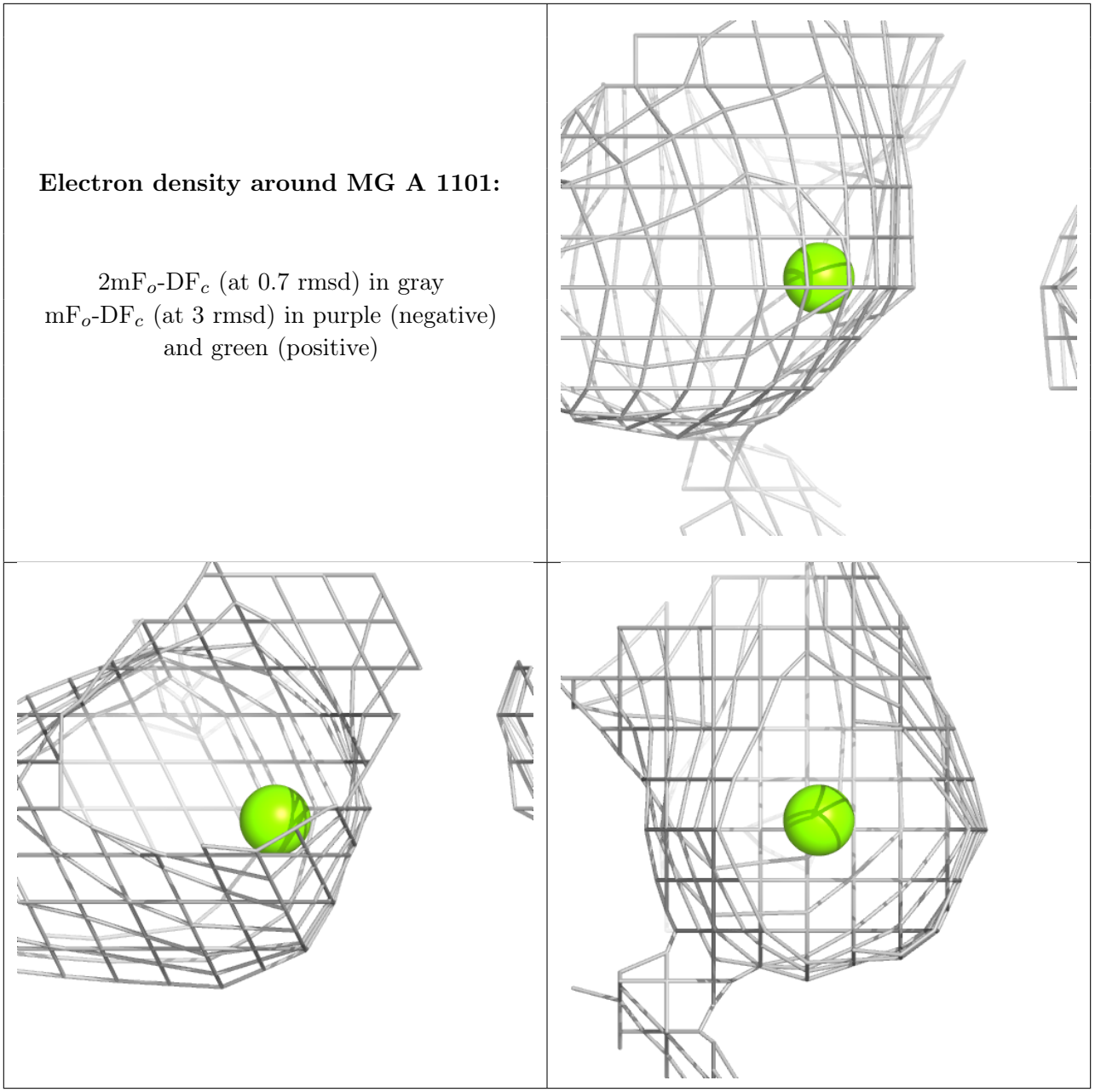






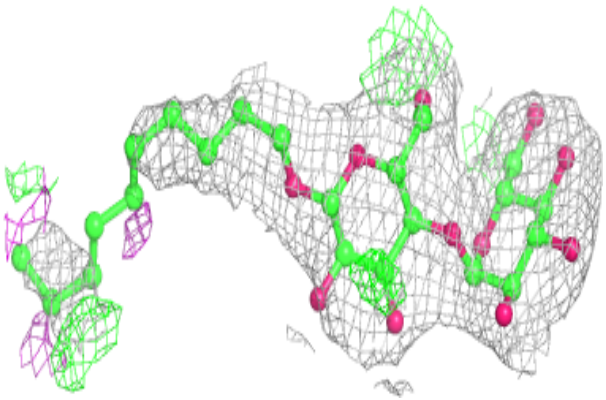
Electron density around MG A 1101:

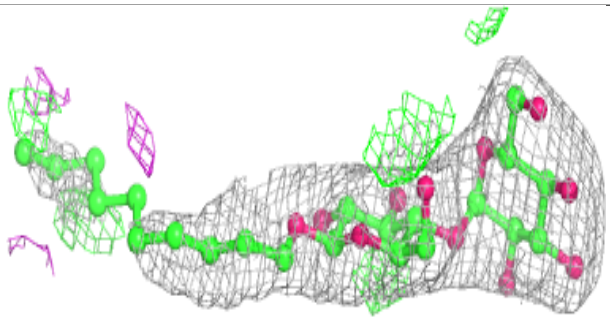
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

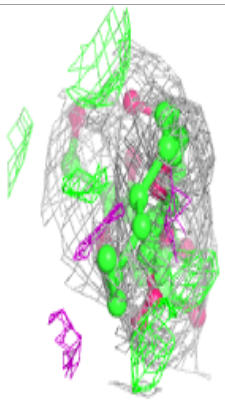


Electron density around DMU E 102:

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

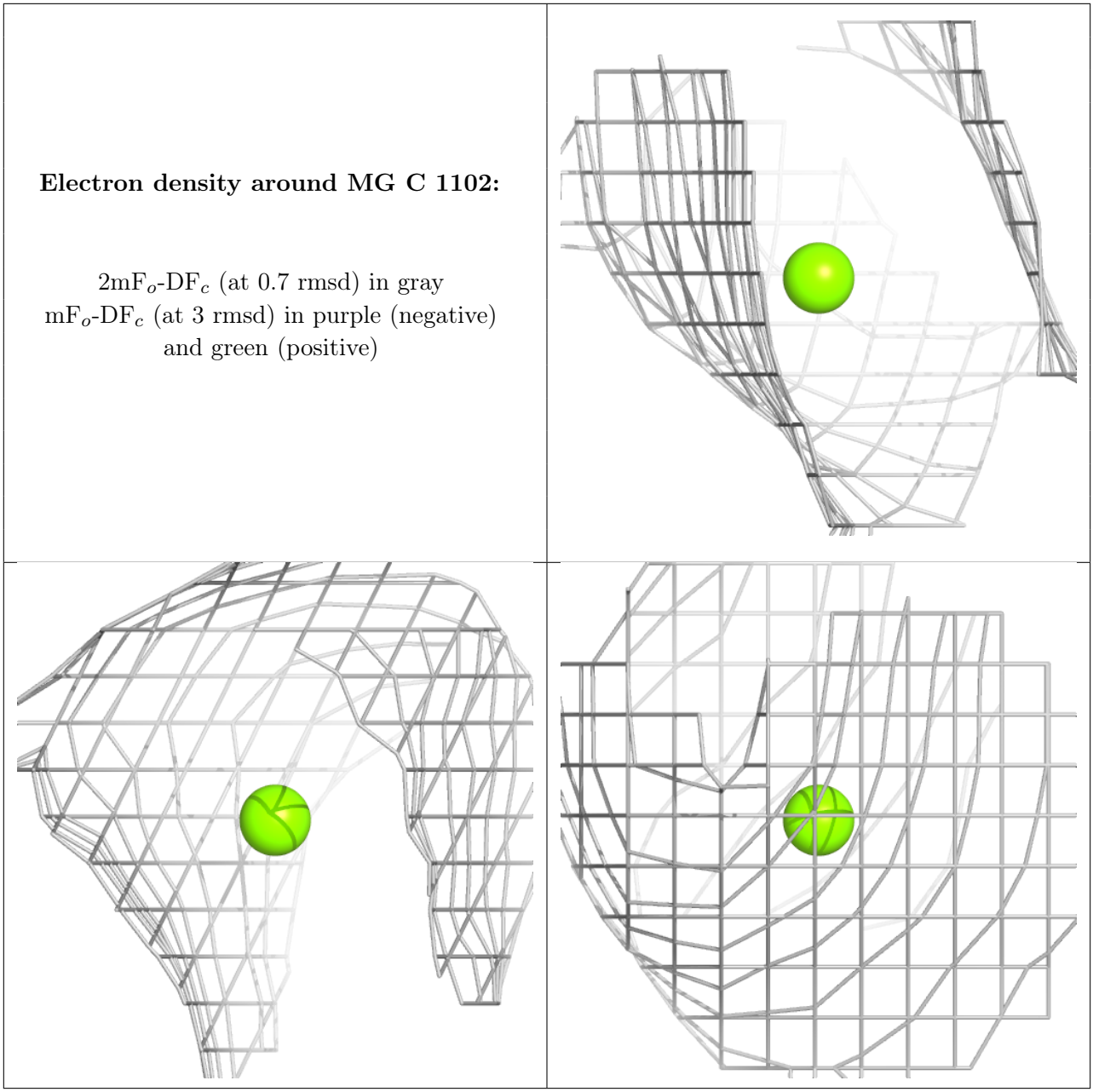






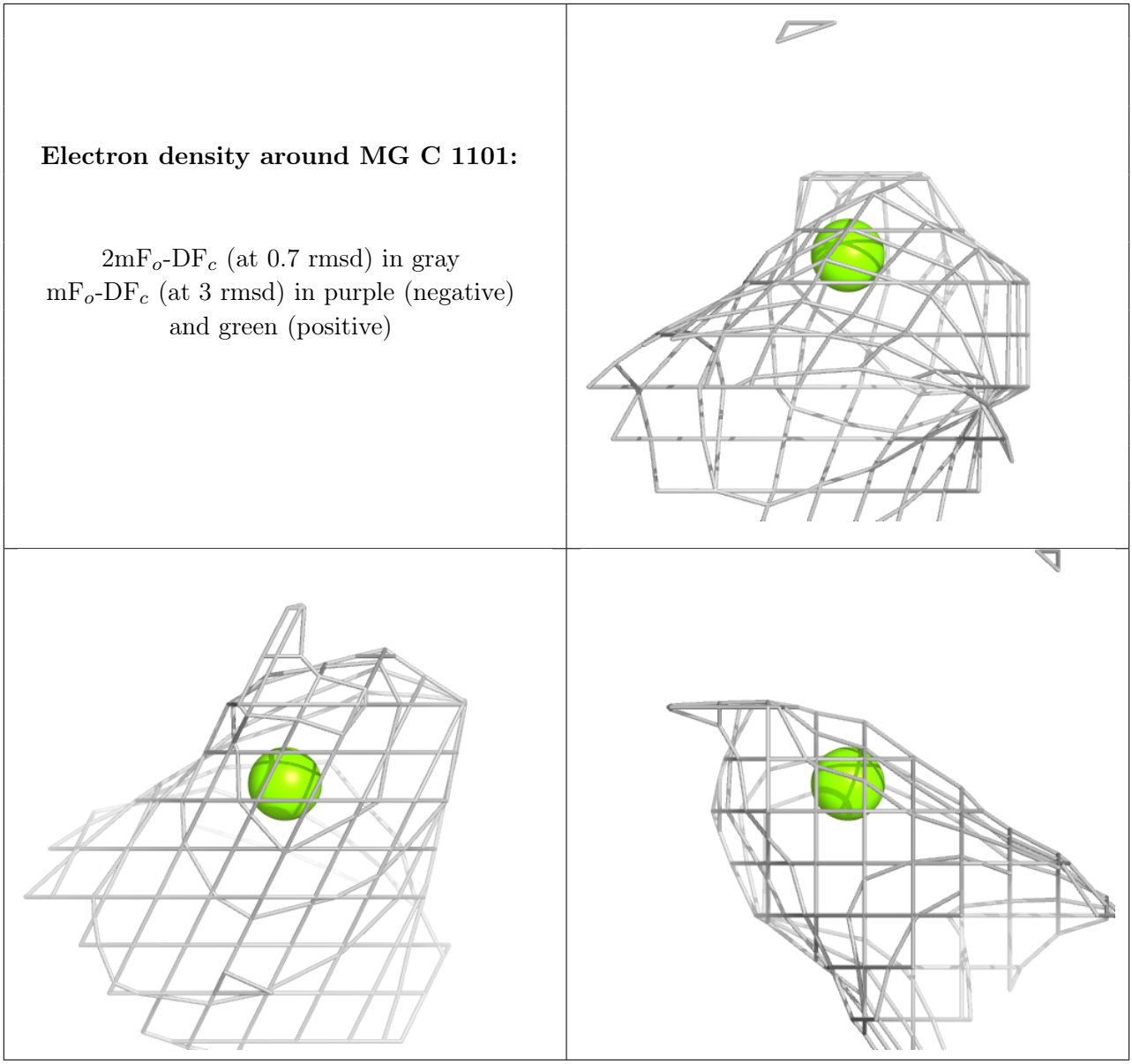
Electron density around MG C 1102:

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



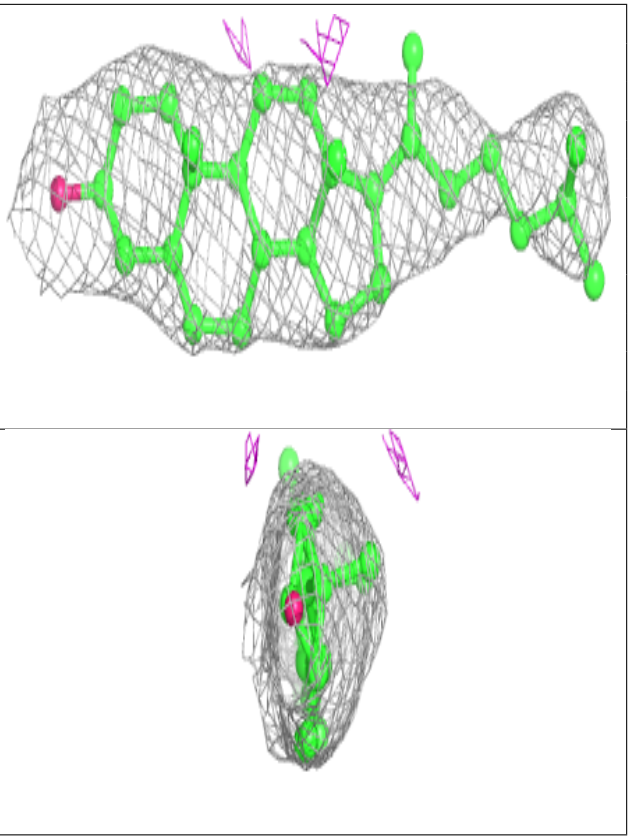
Electron density around MG C 1101:

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



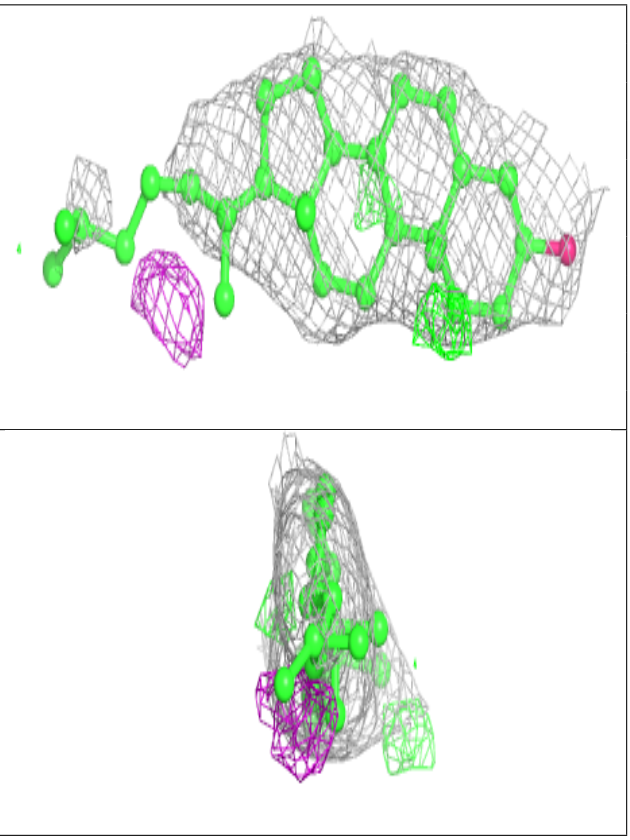
Electron density around CLR E 101:

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



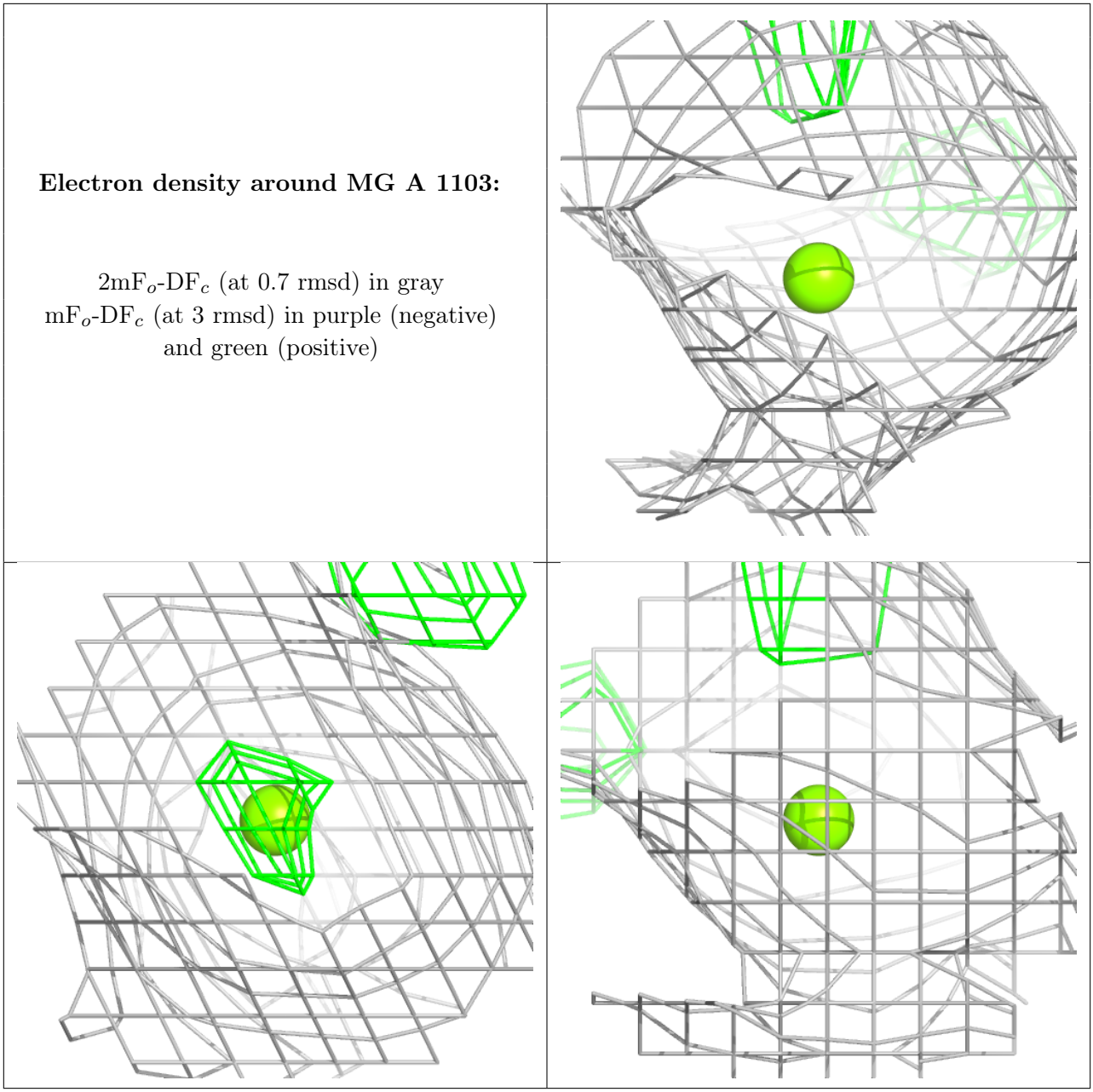
Electron density around CLR A 1105:

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



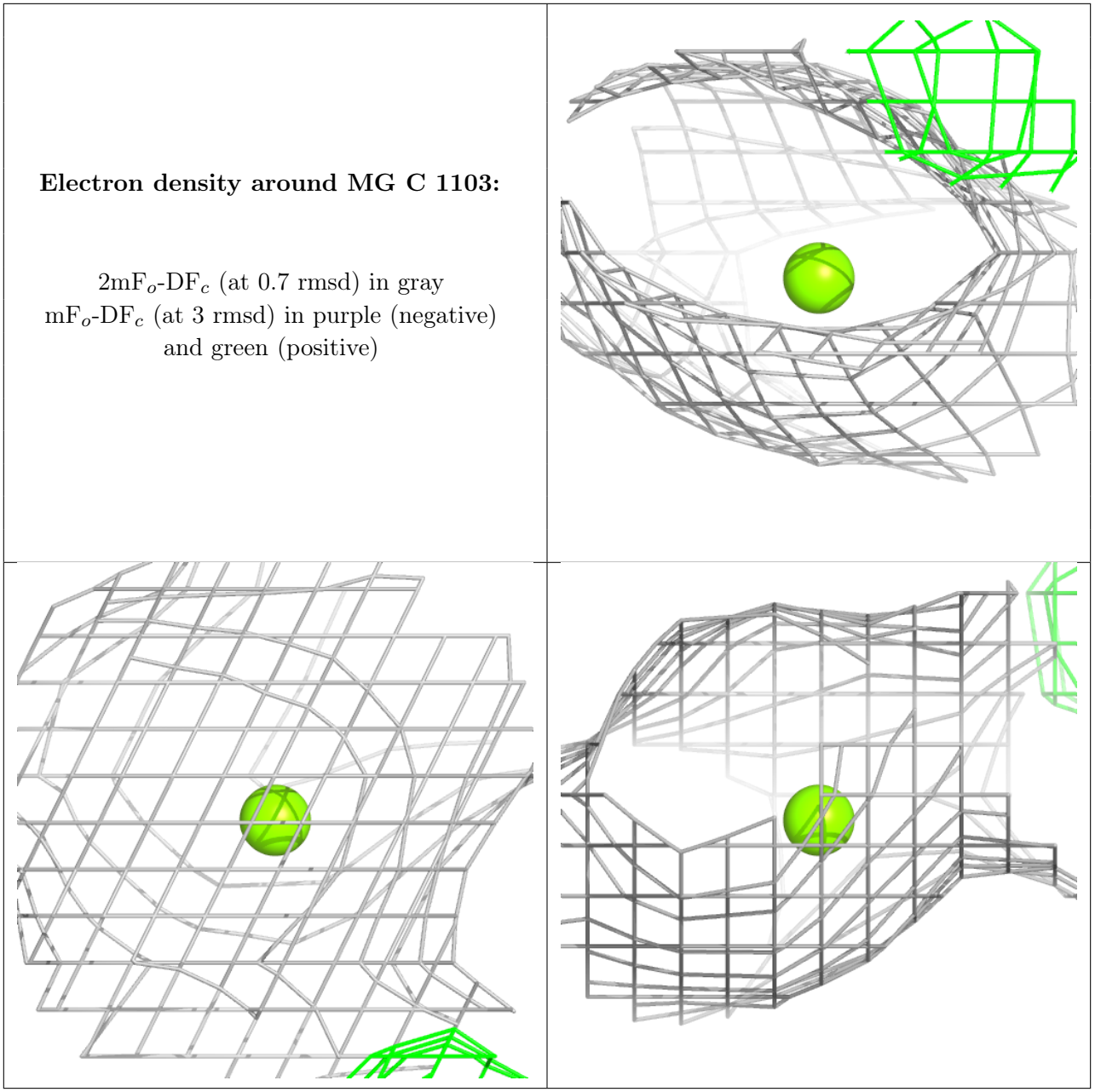
Electron density around MG A 1103:

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



Electron density around MG 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)



6.5 Other polymers (i)

There are no such residues in this entry.