Full wwPDB X-ray Structure Validation Report (i)

Mar 12, 2026 – 09:16 PM UTC

PDB ID	:	8JBK / pdb_00008jbk
Title	:	Crystal structure of Na+,K+-ATPase in the E1.3Na+ state
Authors	:	Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on	:	2023-05-09
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

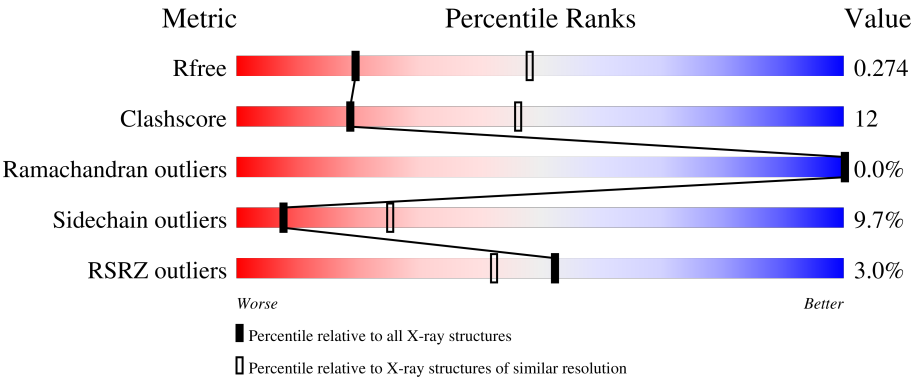
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	3% 67% 27%
1	C	1021	3% 68% 26%
2	B	303	5% 60% 33%
2	D	303	4% 61% 32%
3	E	65	40% 11% 49%

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Mol	Chain	Length	Quality of chain
3	G	65	38% 17% 45%
4	F	6	33% 67%
5	H	5	40% 60%
6	I	2	50% 50%

2 Entry composition (i)

There are 14 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			

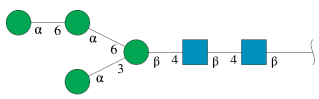
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

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.

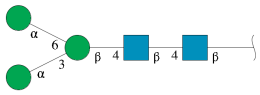
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	36	Total	C	N	O	0	0	0
			292	197	47	48			
3	E	33	Total	C	N	O	0	0	0
			262	179	38	45			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	5	Total C N O 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
6	I	2	Total C N O 28 16 2 10	0	0	0

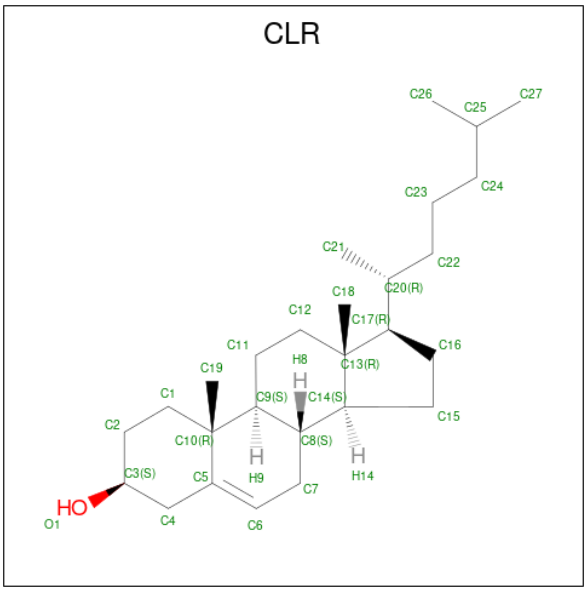
- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mn 1 1	0	0
7	C	1	Total Mn 1 1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

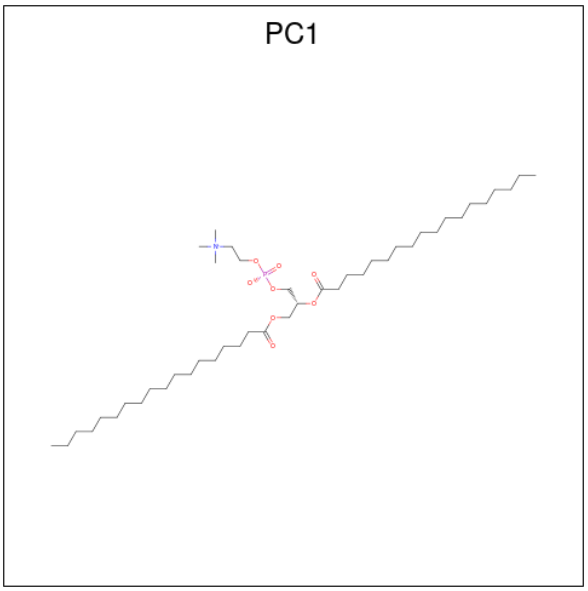
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total Na 4 4	0	0
8	C	4	Total Na 4 4	0	0

- Molecule 9 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



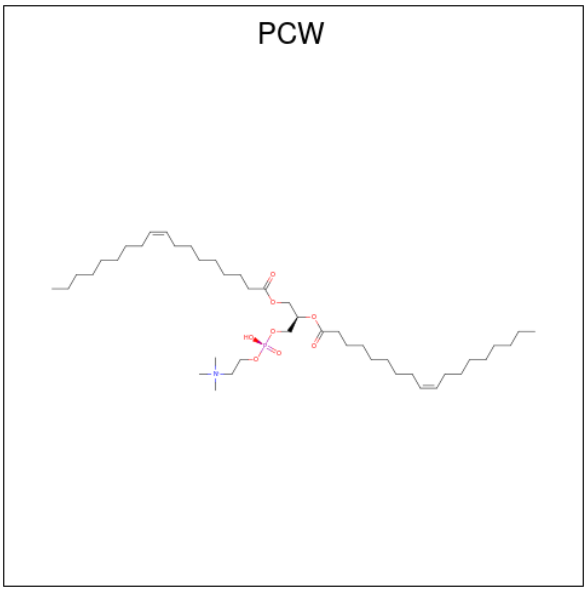
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 28 27 1	0	0
9	A	1	Total C O 28 27 1	0	0
9	B	1	Total C O 28 27 1	0	0
9	C	1	Total C O 28 27 1	0	0
9	D	1	Total C O 28 27 1	0	0
9	E	1	Total C O 28 27 1	0	0

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



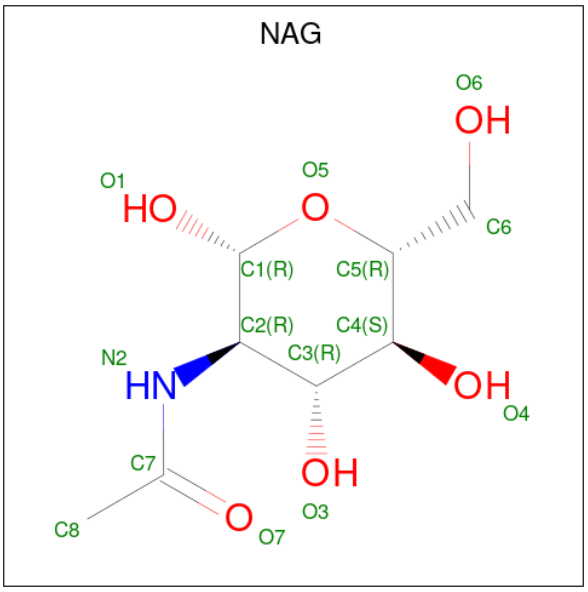
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



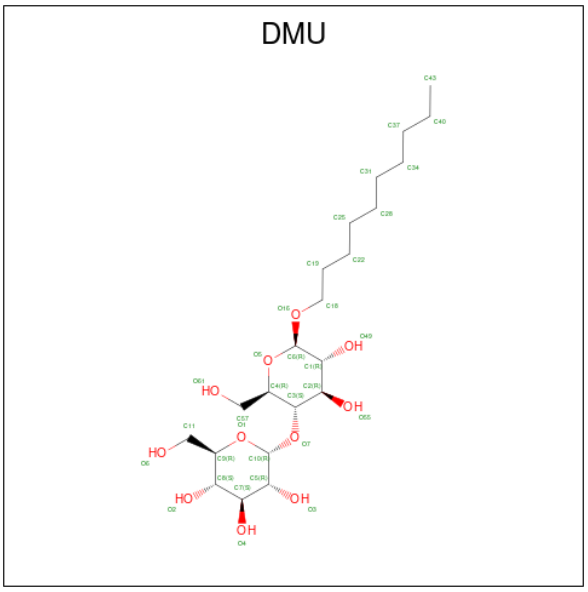
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	B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

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 13 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	15	Total O 15 15	0	0
14	C	14	Total O 14 14	0	0
14	D	3	Total O 3 3	0	0

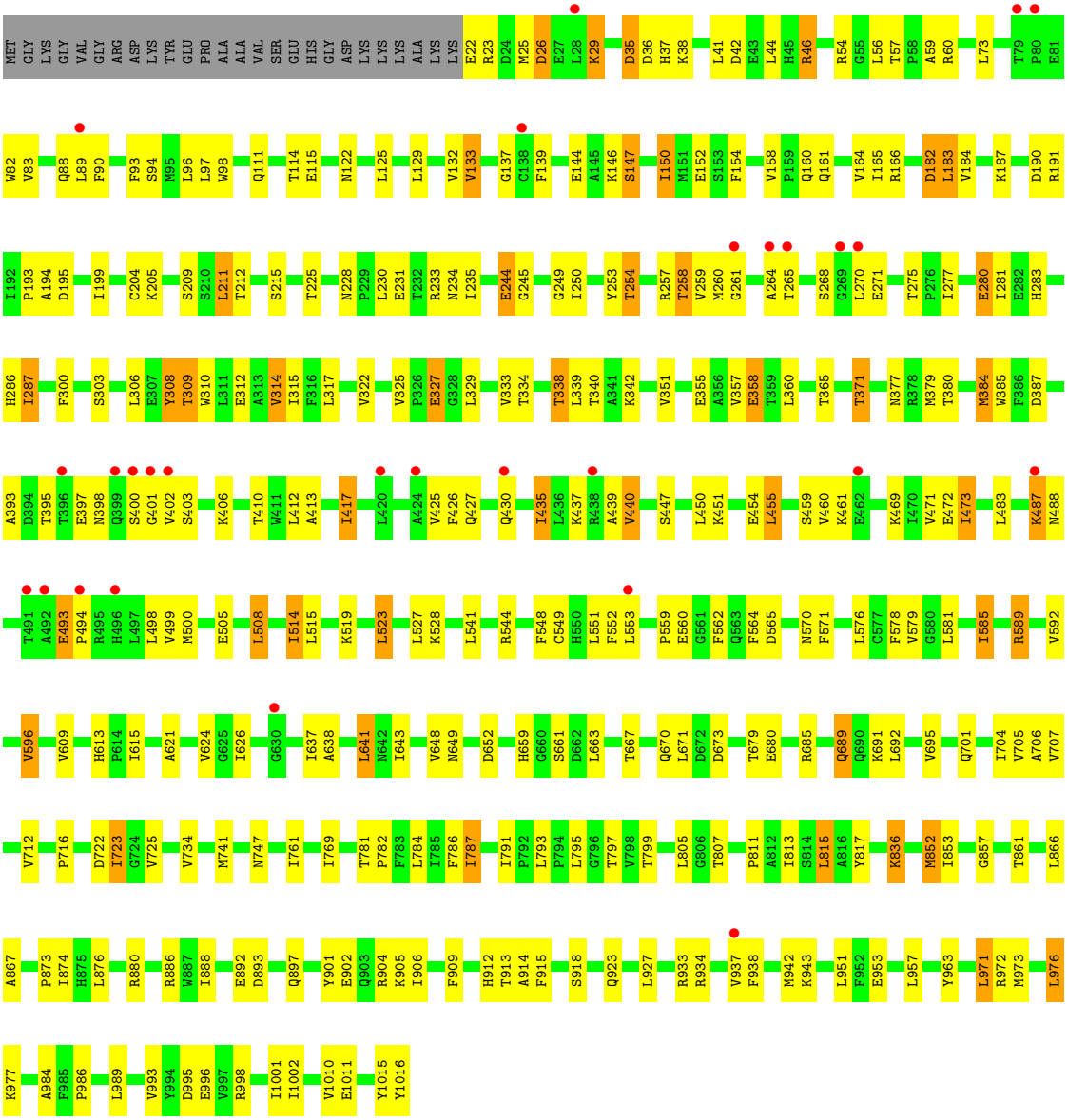
3 Residue-property plots (i)

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

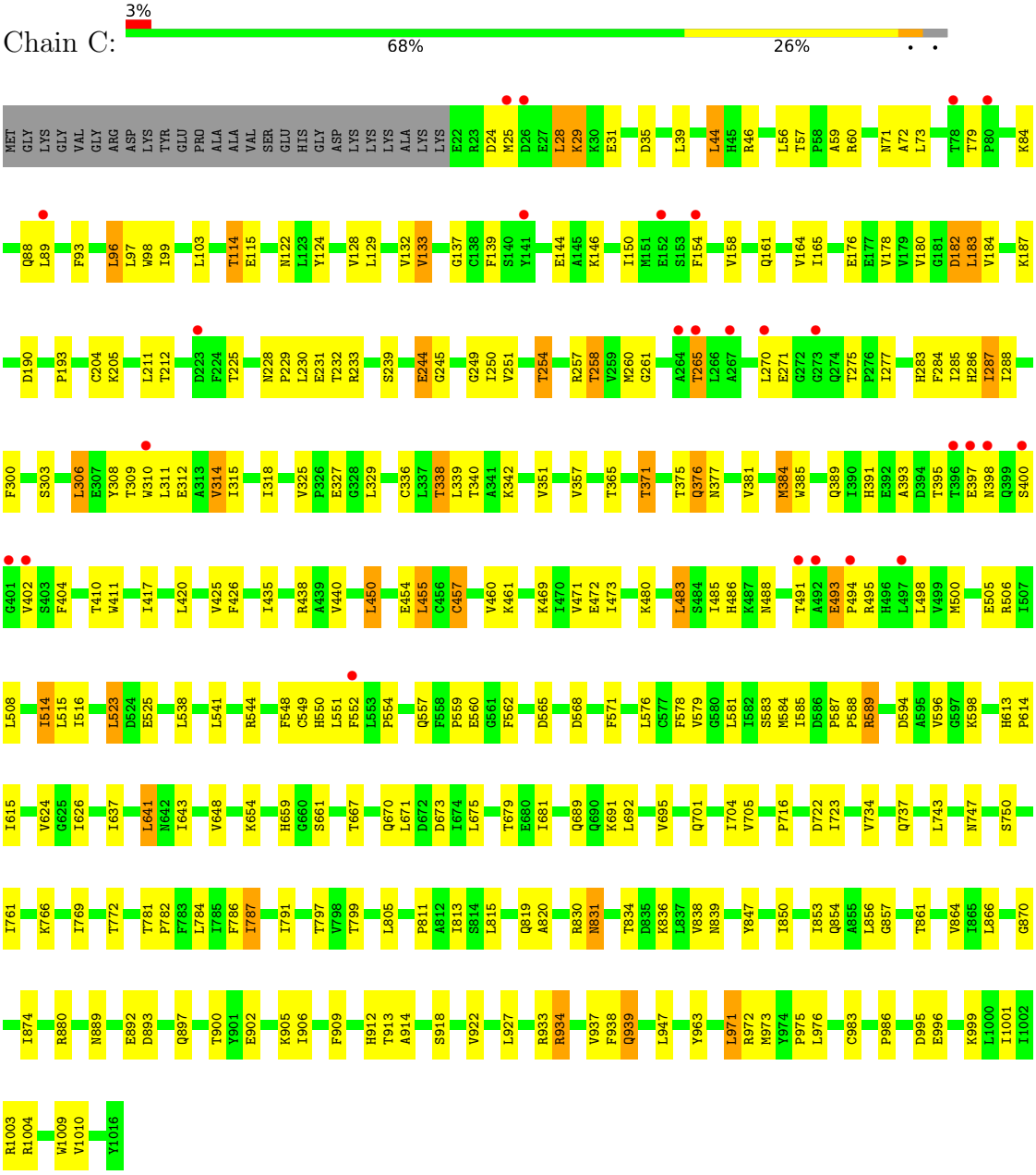
Chain A:





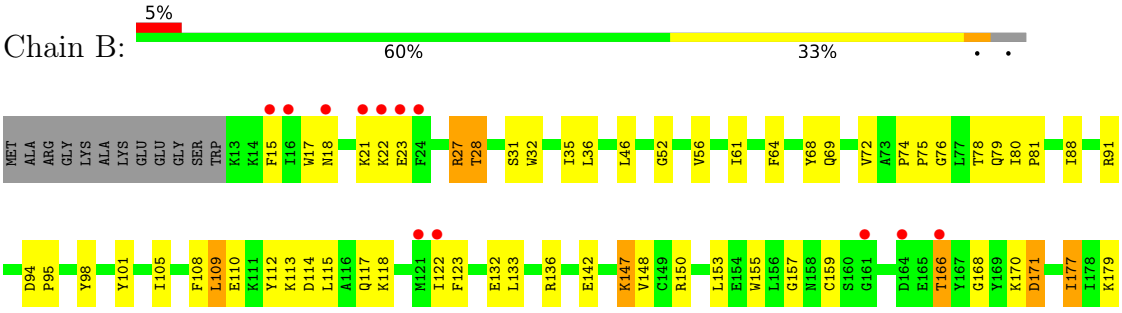
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

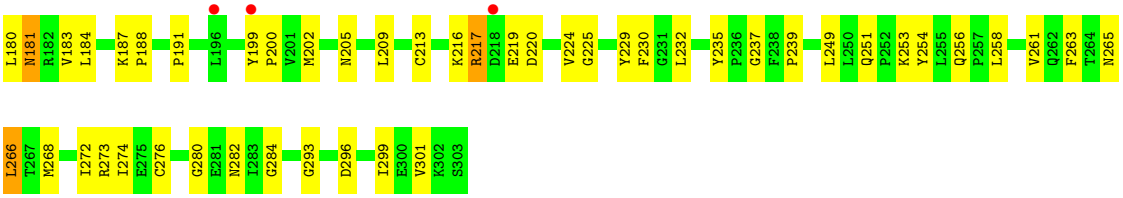
Chain C:



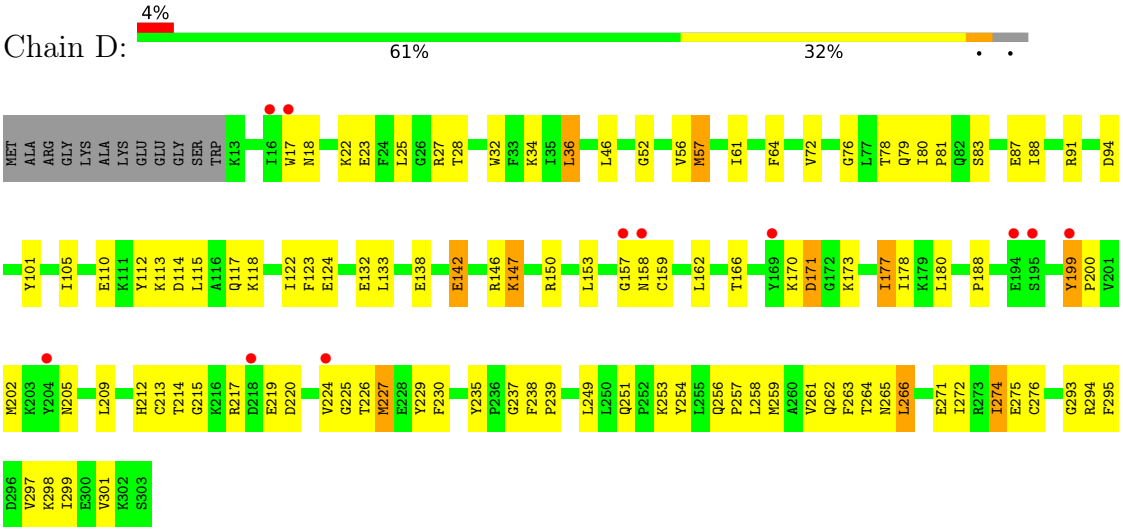
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:

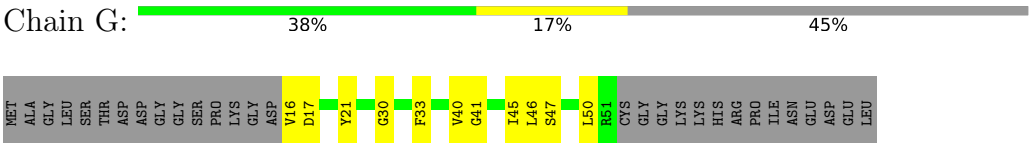




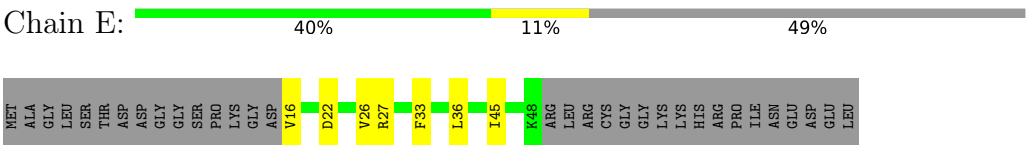
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: FXYD domain-containing ion transport regulator



• Molecule 3: FXYD domain-containing ion transport regulator



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



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

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	193.74Å 74.49Å 162.56Å 90.00° 115.72° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	64.6 (15.00-2.80) 64.1 (15.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.270 0.235 , 0.274	Depositor DCC
R_{free} test set	3358 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21682	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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, CLR, PCW, PC1, BMA, NA, MN, DMU, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.16	0/7873	0.38	0/10683
1	C	0.16	0/7873	0.37	0/10683
2	B	0.14	0/2449	0.38	0/3301
2	D	0.15	0/2449	0.35	0/3301
3	E	0.15	0/268	0.31	0/364
3	G	0.14	0/298	0.28	0/403
All	All	0.16	0/21210	0.37	0/28735

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	7774	194	0
1	C	7723	0	7774	168	0
2	B	2386	0	2362	73	0
2	D	2386	0	2362	62	0
3	E	262	0	268	6	0
3	G	292	0	305	9	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	2	0
6	I	28	0	25	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
9	A	56	0	92	7	0
9	B	28	0	46	4	0
9	C	28	0	46	4	0
9	D	28	0	46	2	0
9	E	28	0	46	1	0
10	A	162	0	264	16	0
11	A	132	0	108	2	0
11	B	22	0	18	2	0
11	C	176	0	144	7	0
12	D	14	0	13	0	0
13	E	33	0	42	3	0
14	A	15	0	0	0	0
14	C	14	0	0	0	0
14	D	3	0	0	0	0
All	All	21682	0	21848	517	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 12.

All (517) 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:494:PRO:HG2	1:C:552:PHE:HB3	1.55	0.87
1:A:417:ILE:HD11	1:A:548:PHE:HB3	1.56	0.86
1:A:993:VAL:HG23	10:A:1110:PC1:H291	1.60	0.82
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.61	0.81
10:A:1110:PC1:H372	9:C:1106:CLR:H71	1.64	0.80
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.62	0.79
2:B:266:LEU:HD13	2:B:301:VAL:HG21	1.62	0.79
9:A:1107:CLR:H261	10:A:1111:PC1:H271	1.63	0.79
1:A:306:LEU:HD12	1:A:880:ARG:HH12	1.46	0.79
2:D:266:LEU:HD13	2:D:301:VAL:HG21	1.64	0.78
1:A:340:THR:HG21	1:A:761:ILE:HG12	1.66	0.77
2:B:166:THR:HG22	2:B:168:GLY:H	1.50	0.76
1:C:986:PRO:HG3	9:C:1106:CLR:H162	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HZ	1:A:342:LYS:HA	1.50	0.75
2:D:91:ARG:HE	2:D:94:ASP:HB2	1.50	0.75
10:A:1111:PC1:H332	10:A:1111:PC1:H231	1.70	0.74
1:A:26:ASP:HA	1:A:29:LYS:HD3	1.69	0.74
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.69	0.73
1:A:89:LEU:HD23	1:A:137:GLY:HA3	1.72	0.71
1:A:454:GLU:HG2	1:A:460:VAL:HG23	1.73	0.71
1:A:379:MET:HE1	1:A:544:ARG:HH11	1.56	0.70
2:B:122:ILE:HG21	2:B:253:LYS:HE2	1.73	0.69
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.75	0.68
1:A:942:MET:HB2	13:E:102:DMU:H6	1.75	0.67
1:A:114:THR:HG22	1:A:115:GLU:H	1.61	0.66
1:A:977:LYS:HG2	3:G:21:TYR:HE2	1.60	0.66
1:A:184:VAL:HG11	1:A:193:PRO:HG2	1.78	0.66
1:C:913:THR:HG23	1:C:973:MET:HE2	1.77	0.65
1:C:340:THR:HG21	1:C:761:ILE:HG12	1.78	0.65
2:B:157:GLY:H	2:B:230:PHE:HB3	1.62	0.65
1:C:551:LEU:HD12	1:C:576:LEU:HA	1.79	0.65
1:C:914:ALA:HA	1:C:976:LEU:HD21	1.79	0.65
1:A:309:THR:HG23	1:A:312:GLU:HB2	1.78	0.65
1:C:184:VAL:HG11	1:C:193:PRO:HG2	1.78	0.64
2:D:122:ILE:HG21	2:D:253:LYS:HE2	1.79	0.64
1:A:211:LEU:HD23	1:A:212:THR:HG23	1.79	0.64
10:A:1110:PC1:H121	10:A:1111:PC1:H151	1.78	0.64
1:A:264:ALA:O	1:A:268:SER:HB2	1.98	0.63
1:A:986:PRO:HG3	9:A:1106:CLR:H162	1.81	0.63
2:D:157:GLY:H	2:D:230:PHE:HB3	1.64	0.63
1:A:211:LEU:HD21	1:A:230:LEU:HD23	1.81	0.63
1:C:559:PRO:HD2	1:C:562:PHE:HD1	1.64	0.62
1:C:514:ILE:HG13	1:C:523:LEU:HG	1.82	0.62
1:C:784:LEU:HD13	9:D:401:CLR:H273	1.82	0.62
1:A:951:LEU:HD13	10:A:1111:PC1:H291	1.81	0.61
2:D:251:GLN:HB3	2:D:254:TYR:HB2	1.82	0.61
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.81	0.61
1:A:205:LYS:HB2	1:A:244:GLU:HG3	1.83	0.61
1:C:469:LYS:HD2	1:C:472:GLU:HB3	1.82	0.61
2:B:166:THR:HG21	2:B:170:LYS:H	1.65	0.61
5:H:1:NAG:H62	5:H:2:NAG:H2	1.83	0.61
1:A:371:THR:HG22	1:A:377:ASN:HD22	1.66	0.60
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.82	0.60
1:A:469:LYS:HD2	1:A:472:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.82	0.60
1:C:384:MET:HE1	1:C:393:ALA:HB3	1.82	0.60
2:B:91:ARG:HE	2:B:94:ASP:HB2	1.65	0.60
1:A:254:THR:HG22	1:A:257:ARG:HH21	1.67	0.60
2:D:110:GLU:HG2	2:D:113:LYS:HE3	1.83	0.59
1:A:934:ARG:HG2	1:A:1015:TYR:HE1	1.65	0.59
1:A:613:HIS:HD2	1:A:615:ILE:H	1.51	0.59
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.82	0.59
1:C:73:LEU:HB3	1:C:265:THR:HG21	1.83	0.59
1:C:308:TYR:HD1	1:C:312:GLU:HG3	1.67	0.59
1:C:211:LEU:HD23	1:C:212:THR:HG23	1.84	0.59
1:C:283:HIS:O	1:C:287:ILE:HG12	2.02	0.59
2:B:216:LYS:HD2	2:B:296:ASP:OD2	2.03	0.59
1:C:613:HIS:HD2	1:C:615:ILE:H	1.49	0.59
1:A:551:LEU:HD12	1:A:576:LEU:HA	1.85	0.59
2:B:220:ASP:O	2:B:224:VAL:HG23	2.03	0.58
1:C:187:LYS:HG2	1:C:190:ASP:OD2	2.03	0.58
1:A:139:PHE:HZ	1:A:813:ILE:HG13	1.67	0.58
1:A:893:ASP:OD2	1:A:897:GLN:HB2	2.03	0.58
1:A:643:ILE:HD11	1:A:648:VAL:HG22	1.85	0.58
1:C:554:PRO:HG2	1:C:557:GLN:HB3	1.84	0.58
1:C:165:ILE:HB	1:C:183:LEU:HD21	1.84	0.58
1:C:154:PHE:CZ	1:C:342:LYS:HA	2.38	0.58
9:B:402:CLR:H212	9:B:402:CLR:H183	1.86	0.58
1:C:129:LEU:O	1:C:133:VAL:HG23	2.04	0.58
1:C:435:ILE:HD12	1:C:455:LEU:HG	1.86	0.57
1:C:831:ASN:HD21	1:C:834:THR:HB	1.69	0.57
2:D:91:ARG:NE	2:D:94:ASP:HB2	2.18	0.57
1:A:902:GLU:O	1:A:906:ILE:HG12	2.04	0.57
1:C:180:VAL:HG22	1:C:254:THR:HB	1.86	0.57
1:C:488:ASN:HB3	1:C:493:GLU:HG3	1.85	0.57
1:A:36:ASP:OD2	1:A:36:ASP:N	2.38	0.57
1:A:667:THR:HG23	1:A:670:GLN:H	1.68	0.57
1:C:659:HIS:CD2	1:C:661:SER:H	2.23	0.57
1:C:667:THR:HG23	1:C:670:GLN:H	1.70	0.57
1:A:514:ILE:HG13	1:A:523:LEU:HG	1.87	0.56
2:D:220:ASP:O	2:D:224:VAL:HG23	2.05	0.56
1:A:132:VAL:HG13	1:A:805:LEU:HD11	1.87	0.56
2:B:232:LEU:HD13	2:B:239:PRO:HG3	1.87	0.56
1:A:165:ILE:HB	1:A:183:LEU:HD21	1.86	0.56
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:ASN:HD21	2:D:23:GLU:HB2	1.70	0.56
1:C:122:ASN:HD22	1:C:311:LEU:HD23	1.70	0.56
1:C:306:LEU:HD12	1:C:880:ARG:HH12	1.70	0.56
1:C:986:PRO:HG3	9:C:1106:CLR:C16	2.36	0.56
1:A:473:ILE:HG13	1:A:483:LEU:HD23	1.88	0.56
1:A:913:THR:HG23	1:A:973:MET:HE2	1.86	0.56
1:C:902:GLU:O	1:C:906:ILE:HG12	2.06	0.56
2:B:81:PRO:HD3	2:B:105:ILE:HD11	1.87	0.56
1:C:329:LEU:HD11	1:C:769:ILE:HG12	1.87	0.56
1:C:371:THR:HG22	1:C:377:ASN:HD22	1.71	0.55
2:B:110:GLU:HG2	2:B:113:LYS:HE3	1.86	0.55
1:C:893:ASP:OD2	1:C:897:GLN:HB2	2.06	0.55
1:A:146:LYS:NZ	11:A:1109:PCW:H41	2.21	0.55
1:C:122:ASN:ND2	1:C:311:LEU:HD23	2.20	0.55
1:A:989:LEU:HD13	10:A:1111:PC1:H3E1	1.89	0.55
1:A:187:LYS:HG2	1:A:190:ASP:OD2	2.06	0.55
1:C:114:THR:HG22	1:C:115:GLU:H	1.72	0.55
1:A:384:MET:HE1	1:A:393:ALA:HB3	1.88	0.54
1:A:692:LEU:HD13	1:A:716:PRO:HB2	1.88	0.54
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.89	0.54
2:D:132:GLU:OE2	2:D:133:LEU:HG	2.07	0.54
1:A:365:THR:HB	1:A:705:VAL:HG12	1.90	0.54
1:C:300:PHE:HE1	1:C:314:VAL:HG12	1.72	0.54
2:D:199:TYR:O	2:D:200:PRO:C	2.50	0.54
1:A:280:GLU:OE2	1:A:836:LYS:HA	2.07	0.54
1:C:786:PHE:HD2	1:C:787:ILE:HD12	1.72	0.54
2:B:266:LEU:H	2:B:266:LEU:HD12	1.73	0.54
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.90	0.54
1:C:315:ILE:HG22	1:C:797:THR:HG21	1.90	0.54
11:C:1108:PCW:H73	3:E:45:ILE:HD11	1.89	0.54
1:A:129:LEU:O	1:A:133:VAL:HG23	2.07	0.53
1:A:483:LEU:HD21	1:A:571:PHE:HE2	1.73	0.53
1:A:712:VAL:HG23	1:A:734:VAL:HG11	1.91	0.53
3:G:40:VAL:HG21	3:E:36:LEU:HD11	1.89	0.53
1:C:139:PHE:CZ	1:C:813:ILE:HG13	2.43	0.53
10:A:1111:PC1:H2G1	3:G:33:PHE:HE1	1.73	0.53
1:C:365:THR:HB	1:C:705:VAL:HG12	1.90	0.53
1:A:398:ASN:HD21	1:A:400:SER:HB2	1.73	0.53
2:D:178:ILE:HB	2:D:259:MET:HE2	1.89	0.53
1:A:508:LEU:HD11	1:A:528:LYS:HG2	1.90	0.53
1:A:649:ASN:HB3	1:A:652:ASP:OD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:PRO:O	2:D:202:MET:HG3	2.09	0.53
1:A:42:ASP:OD2	1:A:46:ARG:NH1	2.41	0.53
1:A:300:PHE:HE1	1:A:314:VAL:HG12	1.73	0.53
2:D:23:GLU:HG2	2:D:28:THR:HG22	1.91	0.53
1:C:25:MET:O	1:C:29:LYS:HB2	2.09	0.53
1:A:277:ILE:HG22	1:A:358:GLU:OE2	2.09	0.52
3:G:47:SER:HB2	3:G:50:LEU:HB2	1.92	0.52
1:C:613:HIS:CD2	1:C:615:ILE:H	2.27	0.52
1:C:589:ARG:HG2	1:C:747:ASN:ND2	2.25	0.52
1:C:937:VAL:HG13	1:C:996:GLU:OE2	2.10	0.52
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.75	0.52
1:A:786:PHE:HD2	1:A:787:ILE:HD12	1.74	0.52
2:B:171:ASP:OD1	2:B:171:ASP:N	2.43	0.52
1:C:847:TYR:HB3	9:D:401:CLR:H152	1.92	0.52
2:D:177:ILE:HD11	2:D:258:LEU:HD22	1.92	0.52
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.44	0.52
1:A:111:GLN:NE2	1:A:122:ASN:OD1	2.42	0.52
1:C:139:PHE:HZ	1:C:813:ILE:HG13	1.75	0.52
1:C:857:GLY:O	1:C:861:THR:HG23	2.08	0.52
2:D:81:PRO:HG3	2:D:101:TYR:HB3	1.91	0.52
2:D:117:GLN:HB3	2:D:150:ARG:HD3	1.92	0.52
1:A:430:GLN:NE2	1:A:439:ALA:O	2.43	0.52
1:A:549:CYS:HA	1:A:579:VAL:HG23	1.91	0.52
1:A:888:ILE:O	1:A:904:ARG:NH2	2.42	0.52
1:C:594:ASP:OD1	1:C:598:LYS:NZ	2.44	0.52
1:C:675:LEU:HD12	1:C:681:ILE:HD13	1.92	0.52
1:C:839:ASN:HA	11:C:1107:PCW:O2P	2.10	0.51
1:C:309:THR:HB	1:C:312:GLU:HG2	1.91	0.51
1:C:150:ILE:HG21	1:C:338:THR:HG23	1.91	0.51
1:A:609:VAL:HG11	1:A:691:LYS:HG3	1.92	0.51
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.45	0.51
2:B:177:ILE:HD11	2:B:258:LEU:HD22	1.91	0.51
2:B:217:ARG:HH11	2:B:273:ARG:HE	1.57	0.51
1:C:861:THR:HG22	1:C:983:CYS:HB2	1.92	0.51
1:A:146:LYS:HZ1	11:A:1109:PCW:H41	1.75	0.51
1:C:781:THR:HA	1:C:784:LEU:HD12	1.92	0.51
1:A:488:ASN:HB3	1:A:493:GLU:HG3	1.93	0.51
2:B:155:TRP:CD1	2:B:232:LEU:HA	2.45	0.51
1:C:918:SER:O	1:C:922:VAL:HG22	2.11	0.51
1:C:963:TYR:O	3:E:27:ARG:HG3	2.10	0.51
1:A:853:ILE:HG12	2:B:46:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1108:PC1:H2B1	9:B:402:CLR:H222	1.93	0.51
2:B:166:THR:HG21	2:B:170:LYS:N	2.25	0.51
1:C:766:LYS:HD2	1:C:933:ARG:NH2	2.26	0.51
1:A:454:GLU:OE2	1:A:459:SER:HA	2.10	0.51
1:A:22:GLU:HB2	1:A:25:MET:HE2	1.93	0.51
2:B:132:GLU:OE2	2:B:133:LEU:HG	2.11	0.51
3:G:47:SER:CB	3:G:50:LEU:HB2	2.41	0.51
1:C:225:THR:HG21	1:C:233:ARG:HD3	1.92	0.51
2:D:213:CYS:HA	2:D:276:CYS:HA	1.93	0.51
1:A:413:ALA:O	1:A:417:ILE:HG23	2.11	0.51
1:A:225:THR:HG21	1:A:233:ARG:HD3	1.93	0.50
1:A:613:HIS:CD2	1:A:615:ILE:H	2.27	0.50
1:A:781:THR:HA	1:A:784:LEU:HD12	1.93	0.50
1:C:500:MET:HG2	1:C:549:CYS:SG	2.51	0.50
1:A:275:THR:HB	1:A:358:GLU:OE2	2.11	0.50
2:B:91:ARG:NE	2:B:94:ASP:HB2	2.26	0.50
2:D:239:PRO:HD2	2:D:257:PRO:HB3	1.93	0.50
2:D:217:ARG:NH1	2:D:220:ASP:OD2	2.45	0.50
1:A:892:GLU:HA	1:A:897:GLN:O	2.12	0.50
1:A:691:LYS:O	1:A:695:VAL:HG23	2.12	0.50
9:A:1107:CLR:H151	3:G:33:PHE:CZ	2.46	0.50
2:B:115:LEU:O	2:B:118:LYS:HG3	2.12	0.50
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.94	0.50
1:A:514:ILE:HG12	1:A:578:PHE:HB3	1.94	0.50
1:A:971:LEU:HB2	1:A:973:MET:HG3	1.94	0.50
1:A:914:ALA:HA	1:A:976:LEU:HD21	1.94	0.49
2:D:202:MET:SD	2:D:212:HIS:HB2	2.51	0.49
2:B:112:TYR:OH	2:B:256:GLN:HG2	2.13	0.49
1:C:204:CYS:HA	1:C:245:GLY:HA3	1.94	0.49
1:C:84:LYS:HE2	1:C:144:GLU:HG3	1.94	0.49
1:A:725:VAL:HG22	1:A:741:MET:HE2	1.93	0.49
1:A:1001:ILE:HG21	1:A:1010:VAL:HG21	1.94	0.49
1:C:258:THR:HG23	1:C:261:GLY:HA3	1.94	0.49
1:A:228:ASN:HB3	1:A:231:GLU:HG3	1.95	0.49
2:D:18:ASN:ND2	2:D:23:GLU:HB2	2.27	0.49
9:A:1107:CLR:H231	10:A:1111:PC1:H2D2	1.94	0.49
1:C:381:VAL:HG22	1:C:584:MET:HG2	1.94	0.49
1:A:559:PRO:HD2	1:A:562:PHE:HD1	1.77	0.49
1:C:1001:ILE:HG21	1:C:1010:VAL:HG21	1.95	0.49
1:C:303:SER:O	1:C:308:TYR:HB2	2.12	0.49
1:C:393:ALA:HB1	1:C:402:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:ASP:OD2	1:C:568:ASP:HB2	2.13	0.49
1:A:150:ILE:HD12	1:A:338:THR:HG23	1.94	0.48
1:A:281:ILE:HG13	1:A:333:VAL:HG21	1.93	0.48
1:A:398:ASN:ND2	1:A:400:SER:HB2	2.28	0.48
1:C:228:ASN:HB3	1:C:231:GLU:HG3	1.95	0.48
11:C:1107:PCW:H52	11:C:1110:PCW:H73	1.95	0.48
1:C:892:GLU:HA	1:C:897:GLN:O	2.13	0.48
2:B:220:ASP:OD1	2:B:272:ILE:HA	2.12	0.48
1:C:211:LEU:HD21	1:C:230:LEU:HD22	1.94	0.48
1:C:303:SER:HB2	1:C:308:TYR:CG	2.48	0.48
2:B:155:TRP:CE2	2:B:232:LEU:HG	2.48	0.48
1:C:165:ILE:HB	1:C:183:LEU:CD2	2.44	0.48
2:B:69:GLN:HE22	2:B:184:LEU:HB3	1.79	0.48
2:D:171:ASP:OD1	2:D:171:ASP:N	2.47	0.48
2:D:112:TYR:OH	2:D:256:GLN:HG2	2.13	0.48
2:B:217:ARG:NE	2:B:220:ASP:OD2	2.47	0.48
1:C:39:LEU:HB2	1:C:44:LEU:HD23	1.96	0.48
1:C:154:PHE:HZ	1:C:342:LYS:HA	1.78	0.48
1:A:93:PHE:CZ	1:A:325:VAL:HG11	2.49	0.48
1:A:160:GLN:NE2	1:A:191:ARG:HB3	2.28	0.48
1:A:695:VAL:HG22	1:A:707:VAL:HG21	1.96	0.48
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.96	0.48
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.96	0.48
1:A:303:SER:O	1:A:308:TYR:HB2	2.13	0.48
1:A:379:MET:HA	1:A:585:ILE:O	2.13	0.48
1:A:385:TRP:HB3	1:A:581:LEU:HB2	1.96	0.48
1:A:943:LYS:HE3	13:E:102:DMU:H33	1.94	0.48
1:C:483:LEU:HD21	1:C:571:PHE:HE2	1.79	0.48
2:B:17:TRP:HH2	2:B:22:LYS:HE2	1.79	0.47
2:D:138:GLU:O	2:D:146:ARG:NH2	2.47	0.47
1:A:35:ASP:OD2	1:A:235:ILE:HD13	2.14	0.47
1:C:691:LYS:O	1:C:695:VAL:HG23	2.14	0.47
3:E:33:PHE:CD2	9:E:101:CLR:H71	2.50	0.47
1:A:435:ILE:HB	1:A:455:LEU:HG	1.95	0.47
1:A:781:THR:HG21	1:A:852:MET:HE1	1.95	0.47
1:C:205:LYS:HB2	1:C:244:GLU:HG3	1.97	0.47
2:B:213:CYS:HA	2:B:276:CYS:HA	1.96	0.47
1:C:454:GLU:OE2	1:C:460:VAL:HG22	2.14	0.47
1:C:637:ILE:HG22	1:C:641:LEU:HD11	1.96	0.47
2:D:76:GLY:HA2	2:D:293:GLY:H	1.80	0.47
1:A:97:LEU:HB3	1:A:133:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:VAL:HG22	1:C:971:LEU:HD22	1.97	0.47
1:A:393:ALA:HB1	1:A:402:VAL:HG12	1.95	0.47
1:C:71:ASN:HB2	1:C:178:VAL:O	2.15	0.47
1:C:96:LEU:HG	1:C:318:ILE:HD12	1.95	0.47
3:E:22:ASP:HB3	13:E:102:DMU:O3	2.15	0.47
1:A:329:LEU:HD11	1:A:769:ILE:HG12	1.95	0.47
1:A:417:ILE:HB	1:A:499:VAL:HB	1.97	0.47
1:C:146:LYS:HZ1	11:C:1108:PCW:H52	1.80	0.47
1:A:689:GLN:HE22	1:A:716:PRO:HG3	1.79	0.47
1:C:254:THR:HG22	1:C:257:ARG:HH21	1.80	0.47
1:C:934:ARG:HD3	1:C:1003:ARG:HG2	1.96	0.47
2:B:95:PRO:HA	2:B:98:TYR:CE1	2.50	0.47
1:A:427:GLN:HB2	1:A:430:GLN:OE1	2.15	0.46
3:G:45:ILE:HG23	3:G:46:LEU:HG	1.97	0.46
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.97	0.46
2:B:15:PHE:CE1	11:B:401:PCW:H11	2.50	0.46
1:A:659:HIS:HD2	1:A:661:SER:HB2	1.81	0.46
1:C:410:THR:HG23	1:C:515:LEU:HD22	1.97	0.46
1:C:514:ILE:HG12	1:C:578:PHE:HB3	1.97	0.46
2:D:173:LYS:HG2	2:D:264:THR:HA	1.97	0.46
1:A:234:ASN:OD1	1:A:234:ASN:N	2.48	0.46
1:A:795:LEU:HD13	1:A:915:PHE:CD1	2.51	0.46
1:A:283:HIS:O	1:A:287:ILE:HG12	2.16	0.46
1:C:495:ARG:HD3	1:C:560:GLU:OE1	2.15	0.46
1:A:679:THR:HG23	1:A:680:GLU:HG3	1.98	0.46
1:A:977:LYS:HD3	2:B:68:TYR:CZ	2.50	0.46
1:C:376:GLN:HE21	1:C:587:PRO:HG2	1.80	0.46
2:D:52:GLY:O	2:D:56:VAL:HG23	2.15	0.46
1:A:857:GLY:O	1:A:861:THR:HG23	2.15	0.46
1:C:975:PRO:HG2	3:E:27:ARG:HH21	1.80	0.46
2:D:220:ASP:HA	2:D:272:ILE:HD12	1.98	0.46
1:A:624:VAL:HG23	1:A:626:ILE:HG12	1.97	0.46
2:B:263:PHE:O	2:B:266:LEU:HG	2.15	0.46
1:C:314:VAL:O	1:C:318:ILE:HG12	2.15	0.46
1:C:389:GLN:HB3	1:C:391:HIS:CE1	2.51	0.46
1:A:315:ILE:HG22	1:A:797:THR:HG21	1.98	0.46
2:B:18:ASN:HD21	2:B:23:GLU:HB2	1.81	0.46
2:B:81:PRO:HG3	2:B:101:TYR:HB3	1.97	0.46
1:C:704:ILE:HA	1:C:722:ASP:OD2	2.16	0.46
2:D:266:LEU:HD12	2:D:266:LEU:H	1.80	0.46
1:A:621:ALA:HB1	1:A:626:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:THR:HG22	1:C:59:ALA:H	1.80	0.46
1:C:781:THR:N	1:C:782:PRO:HD2	2.31	0.46
1:A:57:THR:HG22	1:A:59:ALA:H	1.81	0.45
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.97	0.45
2:D:166:THR:HG21	2:D:170:LYS:HB2	1.98	0.45
1:A:565:ASP:H	1:A:570:ASN:HB2	1.82	0.45
2:B:95:PRO:HA	2:B:98:TYR:CZ	2.51	0.45
1:C:927:LEU:HD21	1:C:947:LEU:HG	1.98	0.45
2:D:17:TRP:HH2	2:D:22:LYS:HE2	1.81	0.45
9:A:1107:CLR:H262	10:A:1111:PC1:H361	1.99	0.45
2:B:117:GLN:HB3	2:B:150:ARG:HG2	1.98	0.45
2:B:123:PHE:HB3	2:B:150:ARG:HG3	1.98	0.45
1:C:93:PHE:CZ	1:C:325:VAL:HG11	2.52	0.45
1:C:786:PHE:CD2	1:C:787:ILE:HD12	2.51	0.45
2:D:124:GLU:OE1	2:D:147:LYS:HG3	2.16	0.45
2:B:268:MET:HA	2:B:301:VAL:HG23	1.99	0.45
1:A:258:THR:HG23	1:A:261:GLY:HA3	1.97	0.45
1:A:706:ALA:HA	1:A:723:ILE:O	2.17	0.45
1:C:587:PRO:HA	1:C:588:PRO:HD3	1.89	0.45
2:D:275:GLU:OE2	2:D:294:ARG:HD2	2.17	0.45
1:A:144:GLU:HA	1:A:147:SER:OG	2.16	0.45
1:A:527:LEU:HD23	1:A:527:LEU:HA	1.88	0.45
1:A:589:ARG:HG2	1:A:747:ASN:ND2	2.32	0.45
1:C:495:ARG:HG2	1:C:560:GLU:HA	1.98	0.45
9:A:1106:CLR:H272	9:A:1106:CLR:H231	1.57	0.45
1:C:692:LEU:HD13	1:C:716:PRO:HB2	1.98	0.45
1:A:613:HIS:CD2	1:A:615:ILE:HG12	2.52	0.44
1:A:886:ARG:HG2	1:A:901:TYR:CZ	2.52	0.44
1:A:685:ARG:HD3	1:A:685:ARG:HA	1.86	0.44
1:C:624:VAL:HG23	1:C:626:ILE:HG12	2.00	0.44
1:A:160:GLN:HE22	1:A:191:ARG:HB3	1.83	0.44
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.98	0.44
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.99	0.44
2:B:31:SER:O	2:B:35:ILE:HG12	2.17	0.44
1:A:483:LEU:HD21	1:A:571:PHE:CE2	2.52	0.44
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.86	0.44
1:A:937:VAL:HG22	1:A:996:GLU:OE2	2.17	0.44
2:B:136:ARG:HD2	2:B:147:LYS:HG2	1.98	0.44
2:B:177:ILE:HD11	2:B:258:LEU:HD13	2.00	0.44
2:B:205:ASN:HB2	2:B:235:TYR:CE2	2.53	0.44
2:B:229:TYR:CD1	2:B:261:VAL:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:THR:HA	1:C:588:PRO:HA	2.00	0.44
1:C:971:LEU:HB2	1:C:973:MET:HG3	1.98	0.44
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.86	0.44
1:A:426:PHE:HE2	1:A:454:GLU:HG3	1.81	0.44
2:B:27:ARG:HD3	9:B:402:CLR:O1	2.18	0.44
2:B:52:GLY:O	2:B:56:VAL:HG23	2.18	0.44
2:D:147:LYS:H	2:D:147:LYS:HD3	1.82	0.44
1:A:165:ILE:HB	1:A:183:LEU:CD2	2.48	0.44
1:A:592:VAL:O	1:A:596:VAL:HG13	2.17	0.44
2:B:23:GLU:HG2	2:B:28:THR:HG22	2.00	0.44
1:C:836:LYS:HD2	11:C:1107:PCW:H51	2.00	0.44
2:D:263:PHE:CE2	2:D:274:ILE:HD12	2.53	0.44
1:A:303:SER:HB2	1:A:308:TYR:CG	2.53	0.44
1:C:99:ILE:O	1:C:103:LEU:HG	2.18	0.44
1:C:132:VAL:HG13	1:C:805:LEU:HD11	1.98	0.44
2:D:81:PRO:HD3	2:D:105:ILE:HD11	1.98	0.44
2:D:226:THR:HB	2:D:264:THR:HG23	2.00	0.44
1:A:89:LEU:O	1:A:94:SER:HB3	2.18	0.44
1:A:483:LEU:HD13	1:A:500:MET:HB3	2.00	0.44
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.53	0.44
2:D:115:LEU:O	2:D:118:LYS:HG3	2.17	0.44
2:D:123:PHE:HB3	2:D:150:ARG:HG3	1.99	0.44
1:A:166:ARG:NH2	1:A:182:ASP:OD1	2.40	0.43
1:A:209:SER:HB3	1:A:215:SER:HA	1.98	0.43
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	2.00	0.43
1:A:306:LEU:HD12	1:A:880:ARG:NH1	2.23	0.43
1:A:401:GLY:HA3	1:A:406:LYS:NZ	2.33	0.43
1:A:933:ARG:NH2	1:A:1016:TYR:O	2.51	0.43
1:C:229:PRO:O	1:C:232:THR:HG22	2.18	0.43
1:C:285:ILE:HA	1:C:288:ILE:HG22	2.00	0.43
1:C:743:LEU:HD11	1:C:750:SER:HB2	2.00	0.43
1:A:97:LEU:CB	1:A:133:VAL:HG22	2.48	0.43
2:B:76:GLY:HA2	2:B:293:GLY:H	1.82	0.43
1:C:154:PHE:CE1	1:C:342:LYS:HA	2.53	0.43
1:C:889:ASN:HD22	1:C:900:THR:HB	1.83	0.43
1:A:938:PHE:O	10:A:1111:PC1:H112	2.19	0.43
1:A:866:LEU:HD23	1:A:866:LEU:HA	1.83	0.43
1:A:963:TYR:OH	1:A:976:LEU:O	2.35	0.43
10:A:1108:PC1:H2C2	10:A:1108:PC1:H3E1	1.99	0.43
2:B:179:LYS:HE2	2:B:179:LYS:HB3	1.74	0.43
1:C:909:PHE:HB3	1:C:972:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ASN:HB2	2:D:262:GLN:HE22	1.82	0.43
2:D:225:GLY:HA3	2:D:265:ASN:O	2.18	0.43
1:A:73:LEU:HD13	1:A:265:THR:HG23	2.01	0.43
1:A:793:LEU:O	1:A:912:HIS:NE2	2.46	0.43
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.99	0.43
1:A:125:LEU:HD21	1:A:315:ILE:HG21	2.01	0.43
1:A:355:GLU:O	1:A:358:GLU:HG3	2.19	0.43
2:B:74:PRO:HG2	2:B:284:GLY:H	1.84	0.43
1:C:435:ILE:O	1:C:438:ARG:HG2	2.19	0.43
1:A:90:PHE:HD1	1:A:98:TRP:NE1	2.17	0.43
1:A:97:LEU:HD21	1:A:322:VAL:HG21	2.01	0.43
1:A:986:PRO:HG2	9:A:1106:CLR:H181	2.00	0.43
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.52	0.43
1:C:164:VAL:HG12	1:C:184:VAL:HG22	2.00	0.43
1:C:483:LEU:HD21	1:C:571:PHE:CE2	2.53	0.43
1:A:54:ARG:HE	1:A:54:ARG:HB3	1.55	0.43
1:A:410:THR:HG23	1:A:515:LEU:HD22	2.00	0.43
1:C:254:THR:O	1:C:257:ARG:NH2	2.52	0.43
1:C:505:GLU:CD	1:C:505:GLU:H	2.26	0.43
1:C:514:ILE:HG22	1:C:516:ILE:HG12	2.01	0.43
2:B:209:LEU:O	2:B:237:GLY:HA3	2.19	0.43
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.54	0.43
1:A:440:VAL:HG21	1:A:447:SER:OG	2.19	0.42
1:A:781:THR:N	1:A:782:PRO:HD2	2.34	0.42
1:C:97:LEU:CB	1:C:133:VAL:HG22	2.49	0.42
1:C:426:PHE:CZ	1:C:450:LEU:HD22	2.54	0.42
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.86	0.42
10:A:1108:PC1:H221	11:B:401:PCW:O3	2.19	0.42
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.87	0.42
2:B:22:LYS:O	2:B:28:THR:HA	2.19	0.42
1:C:402:VAL:HG21	1:C:404:PHE:CE1	2.54	0.42
1:C:550:HIS:C	1:C:550:HIS:CD2	2.96	0.42
1:C:734:VAL:O	1:C:737:GLN:HG2	2.19	0.42
1:C:1009:TRP:NE1	2:D:34:LYS:HD3	2.33	0.42
2:D:227:MET:HE2	2:D:227:MET:HB2	1.96	0.42
5:H:2:NAG:H5	5:H:3:BMA:O2	2.18	0.42
1:A:487:LYS:HE2	1:A:487:LYS:HB3	1.85	0.42
1:A:565:ASP:H	1:A:570:ASN:CB	2.31	0.42
1:A:918:SER:HB3	1:A:984:ALA:HB2	2.00	0.42
1:C:97:LEU:HB3	1:C:133:VAL:HG22	2.00	0.42
1:C:183:LEU:HA	1:C:249:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LEU:HD12	1:C:880:ARG:NH1	2.33	0.42
1:C:480:LYS:HD3	1:C:506:ARG:NE	2.35	0.42
2:D:188:PRO:HB3	2:D:209:LEU:HD22	2.01	0.42
1:C:538:LEU:HD13	1:C:583:SER:HB3	2.01	0.42
1:A:164:VAL:HG12	1:A:184:VAL:HG22	2.02	0.42
1:C:24:ASP:O	1:C:28:LEU:HB2	2.20	0.42
1:C:89:LEU:HD23	1:C:137:GLY:HA3	2.02	0.42
1:C:856:LEU:HD23	1:C:856:LEU:HA	1.82	0.42
1:A:73:LEU:HB3	1:A:265:THR:HG21	2.01	0.42
1:A:514:ILE:HD12	1:A:527:LEU:HD13	2.01	0.42
2:B:108:PHE:CZ	2:B:179:LYS:HD3	2.54	0.42
2:B:157:GLY:H	2:B:230:PHE:CB	2.29	0.42
1:C:398:ASN:HD21	1:C:400:SER:HB2	1.84	0.42
1:C:853:ILE:HG12	2:D:46:LEU:HD11	2.01	0.42
2:D:229:TYR:HD1	2:D:261:VAL:HG12	1.83	0.42
1:A:387:ASP:OD1	1:A:387:ASP:N	2.53	0.42
1:A:451:LYS:O	1:A:455:LEU:HB2	2.20	0.42
1:C:995:ASP:OD2	1:C:999:LYS:HE2	2.20	0.42
1:A:427:GLN:H	1:A:430:GLN:HE22	1.68	0.42
1:A:551:LEU:HD22	1:A:553:LEU:HD23	2.02	0.42
2:B:75:PRO:HG3	2:B:183:VAL:HG21	2.02	0.42
2:B:191:PRO:HG3	2:B:280:GLY:HA2	2.02	0.42
2:D:87:GLU:HA	2:D:298:LYS:O	2.20	0.42
1:A:37:HIS:HB3	1:A:235:ILE:HD11	2.01	0.42
10:A:1110:PC1:H2B2	10:A:1110:PC1:H281	1.52	0.42
2:B:109:LEU:HD12	2:B:153:LEU:HD11	2.02	0.42
2:B:200:PRO:O	2:B:202:MET:HG3	2.20	0.42
1:C:284:PHE:CE1	1:C:838:VAL:HG11	2.55	0.42
1:A:325:VAL:O	1:A:327:GLU:HG3	2.20	0.41
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.90	0.41
2:B:166:THR:HG21	2:B:170:LYS:HB2	2.02	0.41
1:C:28:LEU:O	1:C:31:GLU:HG2	2.20	0.41
1:C:654:LYS:HB3	1:C:679:THR:HG22	2.02	0.41
2:D:271:GLU:OE2	2:D:298:LYS:HD2	2.20	0.41
1:A:339:LEU:HD11	1:A:817:TYR:CE1	2.56	0.41
1:C:182:ASP:O	1:C:251:VAL:HG23	2.20	0.41
1:A:194:ALA:HB1	1:A:253:TYR:O	2.20	0.41
1:A:306:LEU:HD13	1:A:306:LEU:HA	1.87	0.41
1:A:704:ILE:HA	1:A:722:ASP:OD2	2.20	0.41
1:A:807:THR:HB	1:A:923:GLN:HE21	1.85	0.41
1:A:909:PHE:HB3	1:A:972:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:GLU:OE2	3:G:41:GLY:HA3	2.20	0.41
1:C:905:LYS:HA	1:C:905:LYS:HD3	1.79	0.41
1:A:204:CYS:HA	1:A:245:GLY:HA3	2.02	0.41
1:A:564:PHE:HB3	1:A:571:PHE:HD1	1.86	0.41
1:C:283:HIS:CE1	1:C:287:ILE:HD11	2.55	0.41
2:D:276:CYS:HB2	2:D:295:PHE:CE2	2.56	0.41
1:A:942:MET:HE3	1:A:942:MET:HB3	1.88	0.41
1:C:98:TRP:CD1	1:C:133:VAL:HG11	2.55	0.41
2:B:18:ASN:ND2	2:B:23:GLU:HB2	2.35	0.41
2:B:187:LYS:O	2:B:282:ASN:ND2	2.53	0.41
1:C:411:TRP:NE1	1:C:457:CYS:SG	2.94	0.41
1:C:819:GLN:HG3	1:C:820:ALA:H	1.84	0.41
1:C:938:PHE:CD1	11:C:1109:PCW:H32	2.56	0.41
2:D:205:ASN:HB2	2:D:235:TYR:CE2	2.56	0.41
1:A:287:ILE:HG12	1:A:287:ILE:H	1.54	0.41
1:C:495:ARG:HA	1:C:495:ARG:HE	1.86	0.41
1:C:864:VAL:HA	2:D:57:MET:SD	2.59	0.41
1:C:870:GLY:O	1:C:893:ASP:HB2	2.20	0.41
1:C:874:ILE:HD12	1:C:874:ILE:H	1.85	0.41
1:A:874:ILE:HD12	1:A:874:ILE:H	1.85	0.41
1:C:799:THR:HG22	1:C:973:MET:HE3	2.01	0.41
1:C:850:ILE:O	1:C:854:GLN:HG3	2.21	0.41
2:D:274:ILE:HG12	2:D:297:VAL:O	2.21	0.41
1:A:559:PRO:HD2	1:A:562:PHE:CD1	2.55	0.41
1:A:784:LEU:HD13	9:B:402:CLR:H271	2.02	0.41
2:B:181:ASN:HD22	2:B:181:ASN:HA	1.64	0.41
1:C:308:TYR:CD1	1:C:312:GLU:HG3	2.53	0.41
1:C:667:THR:HG22	1:C:670:GLN:OE1	2.21	0.41
2:D:142:GLU:H	2:D:142:GLU:HG2	1.65	0.41
1:A:41:LEU:HD22	1:A:199:ILE:HD12	2.03	0.41
2:B:225:GLY:HA3	2:B:265:ASN:O	2.21	0.41
2:B:282:ASN:OD1	2:B:282:ASN:N	2.53	0.41
1:A:905:LYS:HD3	1:A:905:LYS:HA	1.87	0.40
10:A:1110:PC1:C37	9:C:1106:CLR:H71	2.42	0.40
2:B:122:ILE:O	2:B:148:VAL:N	2.55	0.40
2:B:157:GLY:HA3	2:B:230:PHE:CD1	2.56	0.40
1:A:98:TRP:NE1	1:A:133:VAL:HG11	2.37	0.40
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.75	0.40
1:A:379:MET:HE1	1:A:544:ARG:NH1	2.32	0.40
1:A:761:ILE:H	1:A:761:ILE:HG13	1.64	0.40
1:C:124:TYR:O	1:C:128:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:GLN:HG2	11:C:1109:PCW:H83	2.04	0.40
1:A:183:LEU:HA	1:A:249:GLY:O	2.22	0.40
1:A:195:ASP:OD2	1:A:259:VAL:HG23	2.22	0.40
1:A:637:ILE:HG22	1:A:641:LEU:HD11	2.03	0.40
2:B:28:THR:O	2:B:32:TRP:HD1	2.04	0.40
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.92	0.40
1:C:613:HIS:CG	1:C:614:PRO:HD2	2.57	0.40
2:D:214:THR:OG1	2:D:215:GLY:N	2.54	0.40
1:A:638:ALA:HB1	1:A:643:ILE:O	2.22	0.40
2:B:109:LEU:HD13	2:B:109:LEU:HA	1.84	0.40
2:D:32:TRP:O	2:D:36:LEU:HB2	2.21	0.40
2:D:209:LEU:O	2:D:237:GLY:HA3	2.20	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%)	951 (96%)	41 (4%)	1 (0%)	48 77
1	C	993/1021 (97%)	959 (97%)	34 (3%)	0	100 100
2	B	289/303 (95%)	276 (96%)	13 (4%)	0	100 100
2	D	289/303 (95%)	273 (94%)	16 (6%)	0	100 100
3	E	31/65 (48%)	30 (97%)	1 (3%)	0	100 100
3	G	34/65 (52%)	32 (94%)	2 (6%)	0	100 100
All	All	2629/2778 (95%)	2521 (96%)	107 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	758 (90%)	87 (10%)	7 23
1	C	845/864 (98%)	764 (90%)	81 (10%)	8 26
2	B	261/269 (97%)	237 (91%)	24 (9%)	8 27
2	D	261/269 (97%)	237 (91%)	24 (9%)	8 27
3	E	27/52 (52%)	25 (93%)	2 (7%)	13 37
3	G	30/52 (58%)	28 (93%)	2 (7%)	15 42
All	All	2269/2370 (96%)	2049 (90%)	220 (10%)	8 25

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	29	LYS
1	A	35	ASP
1	A	38	LYS
1	A	44	LEU
1	A	46	ARG
1	A	56	LEU
1	A	60	ARG
1	A	82	TRP
1	A	83	VAL
1	A	88	GLN
1	A	96	LEU
1	A	133	VAL
1	A	147	SER
1	A	150	ILE
1	A	152	GLU
1	A	158	VAL
1	A	161	GLN
1	A	182	ASP
1	A	183	LEU
1	A	211	LEU
1	A	244	GLU

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Mol	Chain	Res	Type
1	A	250	ILE
1	A	254	THR
1	A	258	THR
1	A	260	MET
1	A	270	LEU
1	A	271	GLU
1	A	280	GLU
1	A	286	HIS
1	A	287	ILE
1	A	308	TYR
1	A	309	THR
1	A	310	TRP
1	A	314	VAL
1	A	317	LEU
1	A	327	GLU
1	A	334	THR
1	A	338	THR
1	A	351	VAL
1	A	357	VAL
1	A	358	GLU
1	A	371	THR
1	A	380	THR
1	A	384	MET
1	A	395	THR
1	A	397	GLU
1	A	403	SER
1	A	412	LEU
1	A	417	ILE
1	A	425	VAL
1	A	435	ILE
1	A	437	LYS
1	A	440	VAL
1	A	450	LEU
1	A	455	LEU
1	A	461	LYS
1	A	471	VAL
1	A	473	ILE
1	A	487	LYS
1	A	493	GLU
1	A	498	LEU
1	A	505	GLU
1	A	508	LEU

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Mol	Chain	Res	Type
1	A	514	ILE
1	A	519	LYS
1	A	523	LEU
1	A	541	LEU
1	A	560	GLU
1	A	585	ILE
1	A	589	ARG
1	A	596	VAL
1	A	641	LEU
1	A	663	LEU
1	A	671	LEU
1	A	673	ASP
1	A	689	GLN
1	A	701	GLN
1	A	723	ILE
1	A	787	ILE
1	A	791	ILE
1	A	815	LEU
1	A	836	LYS
1	A	852	MET
1	A	957	LEU
1	A	971	LEU
1	A	976	LEU
2	B	27	ARG
2	B	28	THR
2	B	36	LEU
2	B	61	ILE
2	B	64	PHE
2	B	72	VAL
2	B	78	THR
2	B	79	GLN
2	B	109	LEU
2	B	114	ASP
2	B	142	GLU
2	B	147	LYS
2	B	159	CYS
2	B	166	THR
2	B	171	ASP
2	B	177	ILE
2	B	180	LEU
2	B	181	ASN
2	B	199	TYR

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Mol	Chain	Res	Type
2	B	217	ARG
2	B	219	GLU
2	B	249	LEU
2	B	266	LEU
2	B	274	ILE
3	G	16	VAL
3	G	17	ASP
1	C	28	LEU
1	C	29	LYS
1	C	35	ASP
1	C	44	LEU
1	C	46	ARG
1	C	56	LEU
1	C	60	ARG
1	C	79	THR
1	C	88	GLN
1	C	96	LEU
1	C	114	THR
1	C	133	VAL
1	C	158	VAL
1	C	161	GLN
1	C	182	ASP
1	C	183	LEU
1	C	239	SER
1	C	244	GLU
1	C	250	ILE
1	C	254	THR
1	C	258	THR
1	C	260	MET
1	C	265	THR
1	C	270	LEU
1	C	271	GLU
1	C	275	THR
1	C	277	ILE
1	C	286	HIS
1	C	287	ILE
1	C	306	LEU
1	C	310	TRP
1	C	314	VAL
1	C	327	GLU
1	C	336	CYS
1	C	338	THR

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Mol	Chain	Res	Type
1	C	339	LEU
1	C	351	VAL
1	C	357	VAL
1	C	371	THR
1	C	376	GLN
1	C	384	MET
1	C	395	THR
1	C	397	GLU
1	C	425	VAL
1	C	440	VAL
1	C	450	LEU
1	C	455	LEU
1	C	457	CYS
1	C	461	LYS
1	C	471	VAL
1	C	473	ILE
1	C	483	LEU
1	C	485	ILE
1	C	491	THR
1	C	493	GLU
1	C	498	LEU
1	C	508	LEU
1	C	514	ILE
1	C	523	LEU
1	C	525	GLU
1	C	541	LEU
1	C	544	ARG
1	C	585	ILE
1	C	589	ARG
1	C	596	VAL
1	C	641	LEU
1	C	671	LEU
1	C	673	ASP
1	C	689	GLN
1	C	701	GLN
1	C	723	ILE
1	C	772	THR
1	C	787	ILE
1	C	791	ILE
1	C	815	LEU
1	C	830	ARG
1	C	831	ASN

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Mol	Chain	Res	Type
1	C	934	ARG
1	C	939	GLN
1	C	971	LEU
1	C	1004	ARG
2	D	25	LEU
2	D	27	ARG
2	D	36	LEU
2	D	57	MET
2	D	61	ILE
2	D	64	PHE
2	D	72	VAL
2	D	78	THR
2	D	79	GLN
2	D	83	SER
2	D	114	ASP
2	D	142	GLU
2	D	147	LYS
2	D	159	CYS
2	D	162	LEU
2	D	171	ASP
2	D	177	ILE
2	D	180	LEU
2	D	199	TYR
2	D	219	GLU
2	D	227	MET
2	D	249	LEU
2	D	266	LEU
2	D	274	ILE
3	E	16	VAL
3	E	26	VAL

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

Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	GLN
1	A	122	ASN
1	A	156	ASN
1	A	160	GLN
1	A	161	GLN
1	A	202	ASN
1	A	377	ASN

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Mol	Chain	Res	Type
1	A	399	GLN
1	A	432	ASN
1	A	476	ASN
1	A	613	HIS
1	A	649	ASN
1	A	659	HIS
1	A	689	GLN
1	A	764	ASN
1	A	854	GLN
1	A	897	GLN
1	A	898	GLN
2	B	18	ASN
2	B	69	GLN
2	B	79	GLN
2	B	82	GLN
2	B	140	ASN
2	B	181	ASN
2	B	256	GLN
2	B	262	GLN
2	B	292	GLN
1	C	119	GLN
1	C	120	ASN
1	C	160	GLN
1	C	202	ASN
1	C	283	HIS
1	C	376	GLN
1	C	377	ASN
1	C	399	GLN
1	C	432	ASN
1	C	476	ASN
1	C	486	HIS
1	C	533	ASN
1	C	550	HIS
1	C	613	HIS
1	C	649	ASN
1	C	659	HIS
1	C	854	GLN
1	C	882	ASN
1	C	889	ASN
1	C	897	GLN
1	C	903	GLN
2	D	18	ASN

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Mol	Chain	Res	Type
2	D	69	GLN
2	D	79	GLN
2	D	82	GLN
2	D	93	ASN
2	D	140	ASN
2	D	262	GLN
2	D	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	2,4	14,14,15	0.58	0	17,19,21	0.63	0
4	NAG	F	2	4	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
4	BMA	F	3	4	11,11,12	1.19	1 (9%)	15,15,17	1.33	1 (6%)
4	MAN	F	4	4	11,11,12	0.92	0	15,15,17	0.89	1 (6%)
4	MAN	F	5	4	11,11,12	0.73	0	15,15,17	0.99	2 (13%)
4	MAN	F	6	4	11,11,12	0.91	0	15,15,17	0.89	0
5	NAG	H	1	2,5	14,14,15	1.10	1 (7%)	17,19,21	1.34	3 (17%)
5	NAG	H	2	5	14,14,15	0.82	1 (7%)	17,19,21	1.05	1 (5%)
5	BMA	H	3	5	11,11,12	1.49	2 (18%)	15,15,17	0.95	1 (6%)
5	MAN	H	4	5	11,11,12	1.13	1 (9%)	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	H	5	5	11,11,12	1.24	1 (9%)	15,15,17	1.52	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.47	0	17,19,21	0.69	0
6	NAG	I	2	6	14,14,15	0.37	0	17,19,21	0.79	1 (5%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-3.78	1.37	1.43
5	H	5	MAN	C1-C2	3.12	1.59	1.52
5	H	3	BMA	C1-C2	3.02	1.59	1.52
4	F	3	BMA	C1-C2	2.89	1.59	1.52
5	H	4	MAN	C1-C2	2.81	1.58	1.52
5	H	2	NAG	O5-C1	2.63	1.48	1.43
5	H	3	BMA	C4-C5	2.28	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	5	MAN	C1-O5-C5	4.49	118.20	112.19
4	F	2	NAG	C1-O5-C5	3.49	116.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	4	MAN	C1-O5-C5	3.31	116.63	112.19
5	H	2	NAG	C1-O5-C5	3.15	116.40	112.19
5	H	1	NAG	C1-O5-C5	3.08	116.32	112.19
5	H	1	NAG	C3-C4-C5	2.78	115.27	110.23
4	F	5	MAN	C1-O5-C5	2.55	115.60	112.19
4	F	2	NAG	O4-C4-C3	2.44	116.12	110.38
6	I	2	NAG	C1-O5-C5	2.35	115.33	112.19
5	H	3	BMA	O2-C2-C3	-2.30	105.39	110.15
5	H	1	NAG	O4-C4-C3	-2.27	105.02	110.38
4	F	3	BMA	C3-C4-C5	-2.23	106.20	110.23
4	F	5	MAN	O2-C2-C3	-2.22	105.55	110.15
4	F	4	MAN	C1-O5-C5	2.14	115.06	112.19
5	H	4	MAN	C1-C2-C3	2.13	112.75	109.64
5	H	5	MAN	C1-C2-C3	2.05	112.63	109.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

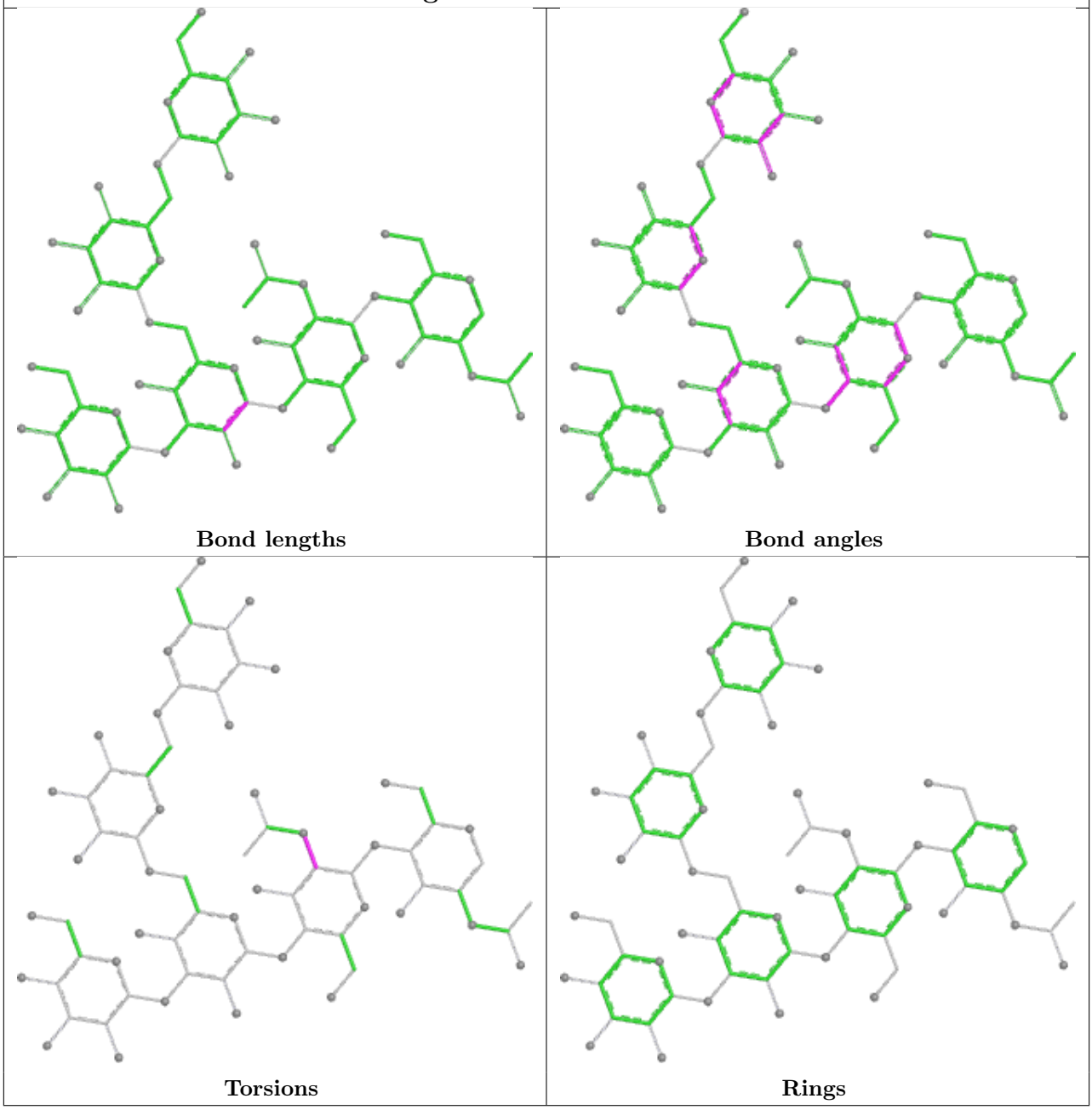
There are no ring outliers.

3 monomers are involved in 2 short contacts:

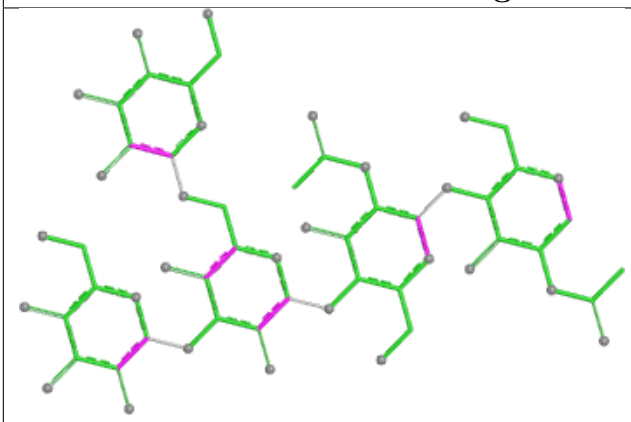
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
5	H	3	BMA	1	0
5	H	2	NAG	2	0

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

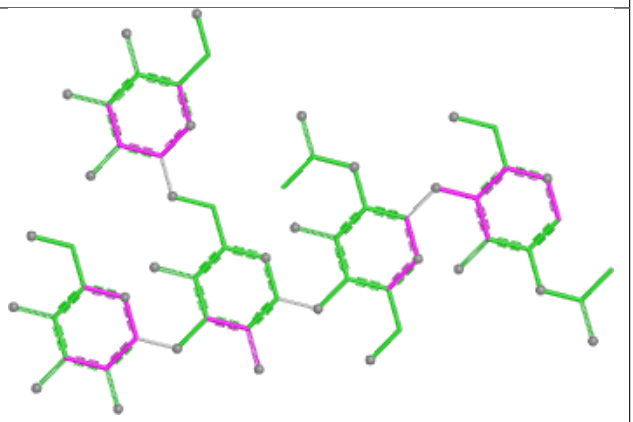
Oligosaccharide Chain F



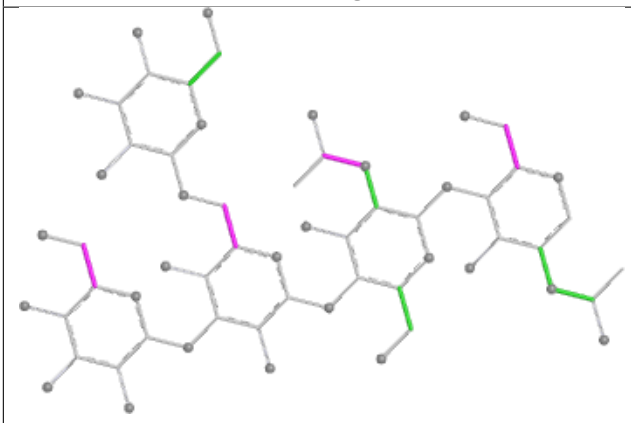
Oligosaccharide Chain H



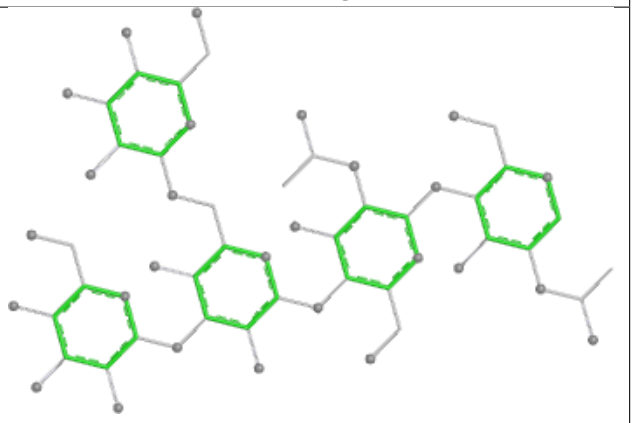
Bond lengths



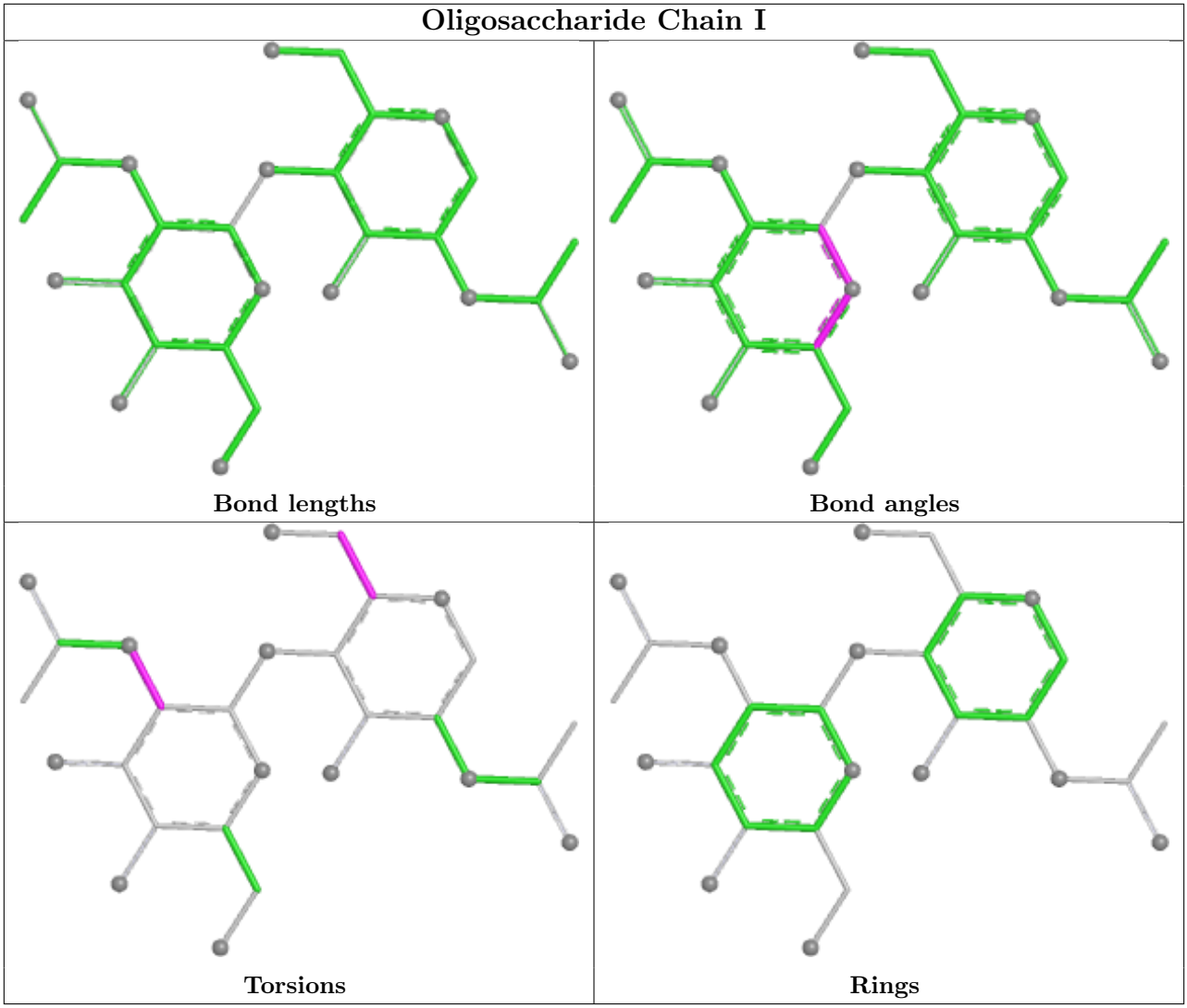
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
11	PCW	C	1114	-	21,21,53	0.86	0	27,29,61	0.93	1 (3%)
9	CLR	D	401	-	31,31,31	1.57	7 (22%)	48,48,48	1.45	10 (20%)
11	PCW	C	1112	-	21,21,53	0.86	0	27,29,61	1.12	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PC1	A	1110	-	53,53,53	0.76	0	59,61,61	1.19	5 (8%)
11	PCW	A	1116	-	21,21,53	0.85	0	27,29,61	1.04	2 (7%)
11	PCW	C	1107	-	21,21,53	0.85	0	27,29,61	1.03	2 (7%)
11	PCW	C	1113	-	21,21,53	0.86	0	27,29,61	0.89	1 (3%)
9	CLR	E	101	-	31,31,31	1.54	7 (22%)	48,48,48	1.49	10 (20%)
9	CLR	B	402	-	31,31,31	1.52	7 (22%)	48,48,48	1.43	10 (20%)
9	CLR	A	1107	-	31,31,31	1.55	7 (22%)	48,48,48	1.46	11 (22%)
11	PCW	A	1115	-	21,21,53	0.85	0	27,29,61	1.16	3 (11%)
9	CLR	C	1106	-	31,31,31	1.49	6 (19%)	48,48,48	1.45	11 (22%)
11	PCW	B	401	-	21,21,53	0.86	0	27,29,61	1.08	3 (11%)
13	DMU	E	102	-	34,34,34	0.88	2 (5%)	45,45,45	1.38	5 (11%)
11	PCW	A	1113	-	21,21,53	0.86	0	27,29,61	1.05	2 (7%)
11	PCW	C	1109	-	21,21,53	0.86	0	27,29,61	1.02	2 (7%)
11	PCW	C	1108	-	21,21,53	0.86	0	27,29,61	0.92	1 (3%)
11	PCW	C	1110	-	21,21,53	0.87	0	27,29,61	0.90	1 (3%)
11	PCW	A	1112	-	21,21,53	0.85	0	27,29,61	1.09	2 (7%)
11	PCW	A	1114	-	21,21,53	0.85	0	27,29,61	1.03	3 (11%)
11	PCW	C	1111	-	21,21,53	0.85	0	27,29,61	1.00	2 (7%)
10	PC1	A	1108	-	53,53,53	0.64	0	59,61,61	0.94	1 (1%)
11	PCW	A	1109	-	21,21,53	0.86	0	27,29,61	1.19	3 (11%)
9	CLR	A	1106	-	31,31,31	1.52	6 (19%)	48,48,48	1.46	12 (25%)
12	NAG	D	402	2	14,14,15	0.33	0	17,19,21	0.49	0
10	PC1	A	1111	-	53,53,53	0.71	0	59,61,61	0.87	2 (3%)

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
11	PCW	C	1114	-	-	5/23/23/57	-
9	CLR	D	401	-	-	4/10/68/68	0/4/4/4
11	PCW	C	1112	-	-	4/23/23/57	-
10	PC1	A	1110	-	-	15/57/57/57	-
11	PCW	A	1116	-	-	7/23/23/57	-
11	PCW	C	1107	-	-	7/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PCW	C	1113	-	-	8/23/23/57	-
9	CLR	E	101	-	-	1/10/68/68	0/4/4/4
9	CLR	B	402	-	-	8/10/68/68	0/4/4/4
9	CLR	A	1107	-	-	5/10/68/68	0/4/4/4
11	PCW	A	1115	-	-	7/23/23/57	-
9	CLR	C	1106	-	-	1/10/68/68	0/4/4/4
11	PCW	B	401	-	-	1/23/23/57	-
13	DMU	E	102	-	-	2/19/59/59	0/2/2/2
11	PCW	A	1113	-	-	4/23/23/57	-
11	PCW	C	1109	-	-	7/23/23/57	-
11	PCW	C	1108	-	-	5/23/23/57	-
11	PCW	C	1110	-	-	8/23/23/57	-
11	PCW	A	1112	-	-	7/23/23/57	-
11	PCW	A	1114	-	-	7/23/23/57	-
11	PCW	C	1111	-	-	7/23/23/57	-
10	PC1	A	1108	-	-	9/57/57/57	-
11	PCW	A	1109	-	-	2/23/23/57	-
9	CLR	A	1106	-	-	3/10/68/68	0/4/4/4
12	NAG	D	402	2	-	2/6/23/26	0/1/1/1
10	PC1	A	1111	-	-	15/57/57/57	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	401	CLR	C4-C3	3.42	1.58	1.52
9	E	101	CLR	C4-C3	3.23	1.57	1.52
9	A	1107	CLR	C4-C3	3.22	1.57	1.52
9	A	1106	CLR	C4-C3	3.13	1.57	1.52
13	E	102	DMU	O16-C6	3.10	1.45	1.40
9	B	402	CLR	C16-C17	3.01	1.60	1.54
9	C	1106	CLR	C4-C3	3.01	1.57	1.52
9	A	1107	CLR	C16-C17	2.90	1.60	1.54
9	D	401	CLR	C16-C17	2.89	1.60	1.54
9	A	1106	CLR	C16-C17	2.86	1.60	1.54
9	B	402	CLR	C4-C3	2.86	1.57	1.52
9	E	101	CLR	C16-C17	2.80	1.60	1.54
9	C	1106	CLR	C16-C17	2.79	1.60	1.54
9	A	1107	CLR	C10-C9	-2.68	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	101	CLR	C10-C9	-2.65	1.51	1.56
9	D	401	CLR	C13-C14	2.59	1.59	1.55
9	A	1107	CLR	C16-C15	2.54	1.60	1.54
9	B	402	CLR	C16-C15	2.52	1.60	1.54
9	A	1106	CLR	C10-C9	-2.50	1.52	1.56
9	A	1106	CLR	C13-C14	2.50	1.59	1.55
9	E	101	CLR	C7-C6	2.49	1.55	1.50
9	A	1107	CLR	C13-C14	2.49	1.59	1.55
9	D	401	CLR	C10-C9	-2.48	1.52	1.56
9	D	401	CLR	C16-C15	2.48	1.60	1.54
9	B	402	CLR	C13-C14	2.46	1.59	1.55
9	E	101	CLR	C16-C15	2.45	1.60	1.54
9	A	1106	CLR	C16-C15	2.43	1.60	1.54
9	D	401	CLR	C7-C6	2.42	1.55	1.50
9	C	1106	CLR	C13-C14	2.40	1.59	1.55
9	C	1106	CLR	C16-C15	2.38	1.60	1.54
9	A	1107	CLR	C7-C6	2.38	1.55	1.50
9	E	101	CLR	C13-C14	2.36	1.59	1.55
9	A	1106	CLR	C7-C6	2.28	1.54	1.50
9	C	1106	CLR	C10-C9	-2.24	1.52	1.56
9	B	402	CLR	C7-C6	2.15	1.54	1.50
9	C	1106	CLR	C7-C6	2.15	1.54	1.50
9	D	401	CLR	C4-C5	2.11	1.55	1.51
9	B	402	CLR	C10-C9	-2.06	1.52	1.56
9	A	1107	CLR	C4-C5	2.03	1.55	1.51
9	B	402	CLR	C10-C5	2.02	1.56	1.52
9	E	101	CLR	C4-C5	2.02	1.55	1.51
13	E	102	DMU	O7-C3	2.01	1.49	1.43

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1110	PC1	C2-O21-C21	4.40	128.32	117.80
13	E	102	DMU	O16-C18-C19	4.19	123.58	109.37
11	A	1109	PCW	C2-O2-C31	-3.95	110.87	117.85
11	C	1112	PCW	C2-O2-C31	-3.70	111.31	117.85
9	C	1106	CLR	C22-C20-C17	-3.30	103.49	110.33
9	A	1106	CLR	C22-C20-C17	-3.16	103.77	110.33
11	A	1112	PCW	C3-O3-C11	-3.13	109.37	117.08
11	A	1115	PCW	C3-O3-C11	-3.08	109.48	117.08
11	C	1111	PCW	C2-O2-C31	-3.07	112.42	117.85
9	E	101	CLR	C22-C20-C17	-3.07	103.97	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	401	CLR	C22-C20-C17	-3.07	103.97	110.33
11	C	1109	PCW	C2-O2-C31	-3.03	112.49	117.85
9	A	1107	CLR	C22-C20-C17	-3.01	104.09	110.33
11	A	1113	PCW	C2-O2-C31	-3.01	112.53	117.85
11	A	1116	PCW	C3-O3-C11	-2.96	109.77	117.08
9	B	402	CLR	C22-C20-C17	-2.96	104.19	110.33
10	A	1110	PC1	C3-O31-C31	-2.93	106.40	117.12
11	A	1109	PCW	C3-O3-C11	-2.90	109.93	117.08
11	B	401	PCW	C2-O2-C31	-2.86	112.79	117.85
11	C	1107	PCW	C3-O3-C11	-2.86	110.03	117.08
11	C	1114	PCW	C3-O3-C11	-2.81	110.14	117.08
11	B	401	PCW	C3-O3-C11	-2.79	110.21	117.08
13	E	102	DMU	C25-C22-C19	-2.79	100.29	114.37
13	E	102	DMU	C18-O16-C6	-2.78	108.92	113.68
10	A	1110	PC1	C24-C23-C22	-2.78	102.91	113.13
11	C	1109	PCW	C3-O3-C11	-2.78	110.23	117.08
11	A	1113	PCW	C3-O3-C11	-2.76	110.26	117.08
11	C	1112	PCW	C3-O3-C11	-2.75	110.31	117.08
11	C	1110	PCW	C3-O3-C11	-2.71	110.40	117.08
11	C	1107	PCW	C2-O2-C31	-2.71	113.07	117.85
11	A	1114	PCW	C3-O3-C11	-2.68	110.46	117.08
11	A	1115	PCW	C3-C2-C1	-2.67	105.57	111.78
10	A	1108	PC1	O31-C3-C2	-2.66	100.73	108.40
13	E	102	DMU	O1-C9-C11	2.63	112.95	106.44
11	A	1115	PCW	C2-O2-C31	-2.60	113.26	117.85
11	C	1108	PCW	C3-O3-C11	-2.55	110.79	117.08
11	C	1113	PCW	C3-O3-C11	-2.51	110.89	117.08
11	C	1111	PCW	C3-O3-C11	-2.51	110.89	117.08
9	A	1107	CLR	C19-C10-C9	-2.50	108.85	111.66
9	E	101	CLR	C19-C10-C9	-2.49	108.86	111.66
9	D	401	CLR	C3-C4-C5	2.46	115.97	112.05
9	A	1107	CLR	C3-C4-C5	2.43	115.93	112.05
10	A	1110	PC1	O21-C2-C3	-2.43	99.61	108.34
9	E	101	CLR	C3-C4-C5	2.43	115.93	112.05
9	A	1106	CLR	C19-C10-C9	-2.43	108.94	111.66
11	A	1114	PCW	C2-O2-C31	-2.42	113.58	117.85
9	D	401	CLR	C19-C10-C9	-2.41	108.96	111.66
9	B	402	CLR	C7-C8-C14	-2.41	107.53	110.93
9	A	1106	CLR	C3-C4-C5	2.40	115.88	112.05
9	C	1106	CLR	C7-C8-C14	-2.39	107.54	110.93
9	A	1106	CLR	C7-C8-C14	-2.39	107.56	110.93
9	E	101	CLR	C11-C12-C13	-2.37	108.73	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1107	CLR	C7-C8-C14	-2.37	107.58	110.93
9	D	401	CLR	C7-C8-C14	-2.37	107.58	110.93
9	E	101	CLR	C7-C8-C14	-2.36	107.59	110.93
10	A	1111	PC1	O31-C3-C2	2.34	115.14	108.40
9	C	1106	CLR	C3-C4-C5	2.34	115.78	112.05
9	A	1107	CLR	C11-C12-C13	-2.32	108.82	112.74
9	B	402	CLR	C3-C4-C5	2.31	115.73	112.05
11	A	1116	PCW	C2-O2-C31	-2.30	113.78	117.85
9	C	1106	CLR	C18-C13-C12	2.29	113.98	110.61
9	C	1106	CLR	C19-C10-C9	-2.29	109.09	111.66
9	B	402	CLR	C18-C13-C12	2.29	113.98	110.61
9	D	401	CLR	C11-C12-C13	-2.28	108.90	112.74
9	B	402	CLR	C19-C10-C9	-2.27	109.11	111.66
11	A	1112	PCW	C2-O2-C31	-2.27	113.83	117.85
9	C	1106	CLR	C24-C23-C22	-2.22	103.31	113.28
9	A	1106	CLR	C11-C12-C13	-2.21	109.00	112.74
9	A	1106	CLR	C18-C13-C12	2.20	113.85	110.61
13	E	102	DMU	C11-C9-C8	-2.20	107.61	113.02
9	A	1107	CLR	C18-C13-C12	2.19	113.84	110.61
9	E	101	CLR	C18-C13-C12	2.19	113.83	110.61
9	D	401	CLR	C18-C13-C12	2.19	113.83	110.61
9	B	402	CLR	C21-C20-C17	2.18	116.15	112.88
9	C	1106	CLR	C16-C17-C20	-2.18	108.89	112.18
9	D	401	CLR	C21-C20-C17	2.15	116.11	112.88
9	E	101	CLR	C24-C23-C22	-2.15	103.65	113.28
9	A	1106	CLR	C16-C17-C20	-2.15	108.93	112.18
10	A	1110	PC1	O31-C31-C32	2.14	118.35	111.83
9	E	101	CLR	C16-C17-C20	-2.13	108.95	112.18
9	A	1106	CLR	C21-C20-C17	2.12	116.07	112.88
9	A	1106	CLR	O1-C3-C4	2.12	114.49	109.71
9	A	1107	CLR	O1-C3-C4	2.12	114.49	109.71
9	B	402	CLR	O1-C3-C4	2.12	114.49	109.71
9	E	101	CLR	C21-C20-C17	2.11	116.05	112.88
9	C	1106	CLR	O1-C3-C4	2.11	114.47	109.71
9	A	1107	CLR	C21-C20-C17	2.11	116.05	112.88
9	B	402	CLR	C2-C3-C4	-2.11	107.33	110.29
9	B	402	CLR	C24-C23-C22	-2.10	103.86	113.28
9	D	401	CLR	C16-C17-C20	-2.10	109.00	112.18
9	D	401	CLR	O1-C3-C4	2.10	114.44	109.71
9	C	1106	CLR	C21-C20-C17	2.10	116.03	112.88
9	E	101	CLR	O1-C3-C4	2.09	114.43	109.71
9	A	1107	CLR	C1-C10-C5	2.09	112.34	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	402	CLR	C11-C12-C13	-2.07	109.24	112.74
9	A	1106	CLR	C24-C23-C22	-2.07	103.99	113.28
9	D	401	CLR	C24-C23-C22	-2.07	104.01	113.28
9	A	1107	CLR	C24-C23-C22	-2.06	104.04	113.28
9	C	1106	CLR	C2-C3-C4	-2.04	107.42	110.29
11	A	1109	PCW	O2-C31-C32	2.03	114.71	111.09
9	A	1106	CLR	C1-C10-C5	2.02	112.23	108.74
11	B	401	PCW	C3-C2-C1	-2.02	107.07	111.78
9	A	1106	CLR	C2-C3-C4	-2.02	107.45	110.29
9	C	1106	CLR	C11-C12-C13	-2.01	109.34	112.74
9	A	1107	CLR	C2-C3-C4	-2.01	107.47	110.29
10	A	1111	PC1	C3-O31-C31	-2.00	109.80	117.12
11	A	1114	PCW	O2-C31-C32	2.00	114.66	111.09

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1108	PC1	C11-O13-P-O14
10	A	1110	PC1	C11-O13-P-O12
10	A	1110	PC1	C11-O13-P-O14
10	A	1110	PC1	C11-O13-P-O11
10	A	1110	PC1	C1-O11-P-O12
10	A	1110	PC1	C1-O11-P-O13
10	A	1111	PC1	C11-O13-P-O14
10	A	1111	PC1	C11-O13-P-O11
10	A	1111	PC1	C1-O11-P-O14
10	A	1111	PC1	C1-O11-P-O13
11	A	1112	PCW	C1-O3P-P-O2P
11	A	1112	PCW	C1-O3P-P-O4P
11	A	1112	PCW	C4-O4P-P-O1P
11	A	1112	PCW	C4-O4P-P-O2P
11	A	1112	PCW	C4-O4P-P-O3P
11	A	1113	PCW	C4-O4P-P-O1P
11	A	1113	PCW	C4-O4P-P-O2P
11	A	1113	PCW	C4-O4P-P-O3P
11	A	1114	PCW	C1-O3P-P-O1P
11	A	1114	PCW	C4-O4P-P-O1P
11	A	1114	PCW	C4-O4P-P-O2P
11	A	1114	PCW	C4-O4P-P-O3P
11	A	1115	PCW	C1-O3P-P-O1P
11	A	1115	PCW	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
11	A	1115	PCW	C1-O3P-P-O4P
11	A	1115	PCW	C4-O4P-P-O1P
11	A	1115	PCW	C4-O4P-P-O2P
11	A	1115	PCW	C4-O4P-P-O3P
11	A	1116	PCW	C1-O3P-P-O2P
11	A	1116	PCW	C1-O3P-P-O4P
11	A	1116	PCW	C4-O4P-P-O1P
11	A	1116	PCW	C4-O4P-P-O3P
11	C	1107	PCW	C1-O3P-P-O2P
11	C	1107	PCW	C1-O3P-P-O4P
11	C	1107	PCW	C4-O4P-P-O1P
11	C	1107	PCW	C4-O4P-P-O2P
11	C	1107	PCW	C4-O4P-P-O3P
11	C	1108	PCW	C4-O4P-P-O2P
11	C	1108	PCW	C4-O4P-P-O3P
11	C	1109	PCW	C1-O3P-P-O2P
11	C	1109	PCW	C1-O3P-P-O4P
11	C	1109	PCW	C4-O4P-P-O2P
11	C	1109	PCW	C4-O4P-P-O3P
11	C	1110	PCW	C1-O3P-P-O1P
11	C	1110	PCW	C1-O3P-P-O2P
11	C	1110	PCW	C1-O3P-P-O4P
11	C	1110	PCW	C4-O4P-P-O2P
11	C	1110	PCW	C4-O4P-P-O3P
11	C	1111	PCW	C1-O3P-P-O2P
11	C	1111	PCW	C4-O4P-P-O2P
11	C	1111	PCW	C4-O4P-P-O3P
11	C	1112	PCW	C1-O3P-P-O1P
11	C	1112	PCW	C1-O3P-P-O2P
11	C	1112	PCW	C1-O3P-P-O4P
11	C	1113	PCW	C1-O3P-P-O2P
11	C	1113	PCW	C1-O3P-P-O4P
11	C	1113	PCW	C4-O4P-P-O2P
11	C	1113	PCW	C4-O4P-P-O3P
11	C	1114	PCW	C4-O4P-P-O1P
11	C	1114	PCW	C4-O4P-P-O2P
11	C	1114	PCW	C4-O4P-P-O3P
10	A	1110	PC1	C38-C39-C3A-C3B
10	A	1111	PC1	C28-C29-C2A-C2B
10	A	1110	PC1	C28-C29-C2A-C2B
10	A	1111	PC1	C38-C39-C3A-C3B
9	B	402	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
9	A	1107	CLR	C17-C20-C22-C23
9	B	402	CLR	C17-C20-C22-C23
12	D	402	NAG	C4-C5-C6-O6
9	A	1107	CLR	C21-C20-C22-C23
9	B	402	CLR	C21-C20-C22-C23
12	D	402	NAG	O5-C5-C6-O6
9	A	1106	CLR	C22-C23-C24-C25
9	A	1107	CLR	C20-C22-C23-C24
9	D	401	CLR	C20-C22-C23-C24
9	A	1107	CLR	C23-C24-C25-C26
9	A	1107	CLR	C23-C24-C25-C27
10	A	1110	PC1	C27-C28-C29-C2A
10	A	1110	PC1	C37-C38-C39-C3A
10	A	1111	PC1	C39-C3A-C3B-C3C
10	A	1111	PC1	C22-C21-O21-C2
10	A	1110	PC1	C29-C2A-C2B-C2C
10	A	1111	PC1	O22-C21-O21-C2
13	E	102	DMU	C4-C3-O7-C10
13	E	102	DMU	C2-C3-O7-C10
10	A	1111	PC1	C27-C28-C29-C2A
9	D	401	CLR	C23-C24-C25-C26
9	B	402	CLR	C16-C17-C20-C21
9	E	101	CLR	C23-C24-C25-C26
10	A	1108	PC1	O13-C11-C12-N
10	A	1110	PC1	O13-C11-C12-N
10	A	1111	PC1	O13-C11-C12-N
11	A	1109	PCW	O4P-C4-C5-N
11	A	1112	PCW	O4P-C4-C5-N
11	A	1113	PCW	O4P-C4-C5-N
11	A	1114	PCW	O4P-C4-C5-N
11	A	1115	PCW	O4P-C4-C5-N
11	A	1116	PCW	O4P-C4-C5-N
11	B	401	PCW	O4P-C4-C5-N
11	C	1107	PCW	O4P-C4-C5-N
11	C	1108	PCW	O4P-C4-C5-N
11	C	1109	PCW	O4P-C4-C5-N
11	C	1110	PCW	O4P-C4-C5-N
11	C	1111	PCW	O4P-C4-C5-N
11	C	1112	PCW	O4P-C4-C5-N
11	C	1113	PCW	O4P-C4-C5-N
11	C	1114	PCW	O4P-C4-C5-N
10	A	1108	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
10	A	1108	PC1	C39-C3A-C3B-C3C
10	A	1111	PC1	C37-C38-C39-C3A
10	A	1110	PC1	O31-C31-C32-C33
10	A	1108	PC1	C11-O13-P-O12
10	A	1108	PC1	C11-O13-P-O11
10	A	1110	PC1	C1-O11-P-O14
10	A	1111	PC1	C11-O13-P-O12
10	A	1111	PC1	C1-O11-P-O12
11	A	1109	PCW	C1-O3P-P-O2P
11	A	1112	PCW	C1-O3P-P-O1P
11	A	1114	PCW	C1-O3P-P-O2P
11	A	1114	PCW	C1-O3P-P-O4P
11	A	1116	PCW	C1-O3P-P-O1P
11	A	1116	PCW	C4-O4P-P-O2P
11	C	1107	PCW	C1-O3P-P-O1P
11	C	1108	PCW	C4-O4P-P-O1P
11	C	1109	PCW	C1-O3P-P-O1P
11	C	1109	PCW	C4-O4P-P-O1P
11	C	1110	PCW	C4-O4P-P-O1P
11	C	1111	PCW	C1-O3P-P-O1P
11	C	1111	PCW	C1-O3P-P-O4P
11	C	1111	PCW	C4-O4P-P-O1P
11	C	1113	PCW	C1-O3P-P-O1P
11	C	1113	PCW	C4-O4P-P-O1P
9	B	402	CLR	C13-C17-C20-C22
9	C	1106	CLR	C23-C24-C25-C26
9	B	402	CLR	C13-C17-C20-C21
9	A	1106	CLR	C20-C22-C23-C24
9	B	402	CLR	C22-C23-C24-C25
10	A	1110	PC1	C3-C2-O21-C21
11	C	1108	PCW	C3-C2-O2-C31
11	C	1110	PCW	C3-C2-O2-C31
11	C	1114	PCW	C3-C2-O2-C31
10	A	1111	PC1	O31-C31-C32-C33
9	A	1106	CLR	C23-C24-C25-C27
9	D	401	CLR	C23-C24-C25-C27
11	C	1113	PCW	C3-C2-O2-C31
9	D	401	CLR	C22-C23-C24-C25
10	A	1108	PC1	O31-C31-C32-C33
10	A	1110	PC1	O32-C31-C32-C33
10	A	1108	PC1	C37-C38-C39-C3A
9	B	402	CLR	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
10	A	1108	PC1	O32-C31-C32-C33

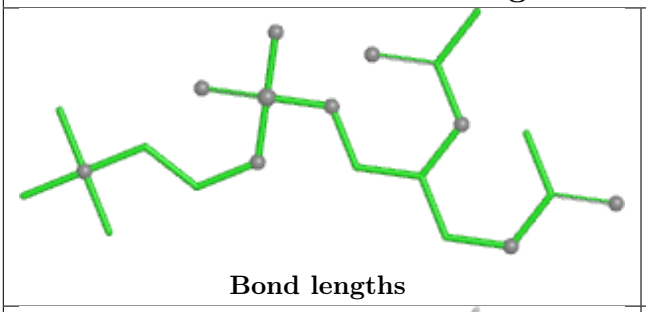
There are no ring outliers.

16 monomers are involved in 41 short contacts:

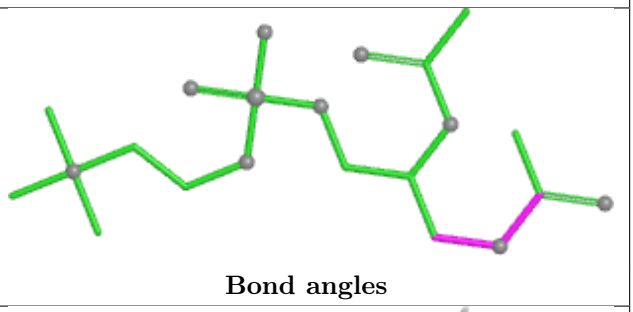
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	401	CLR	2	0
10	A	1110	PC1	5	0
11	C	1107	PCW	3	0
9	E	101	CLR	1	0
9	B	402	CLR	4	0
9	A	1107	CLR	4	0
9	C	1106	CLR	4	0
11	B	401	PCW	2	0
13	E	102	DMU	3	0
11	C	1109	PCW	2	0
11	C	1108	PCW	2	0
11	C	1110	PCW	1	0
10	A	1108	PC1	3	0
11	A	1109	PCW	2	0
9	A	1106	CLR	3	0
10	A	1111	PC1	9	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.

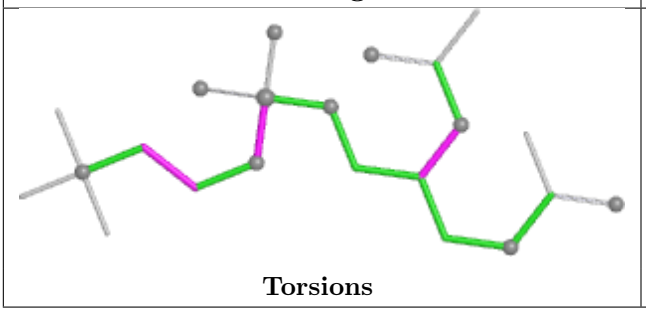
Ligand PCW C 1114



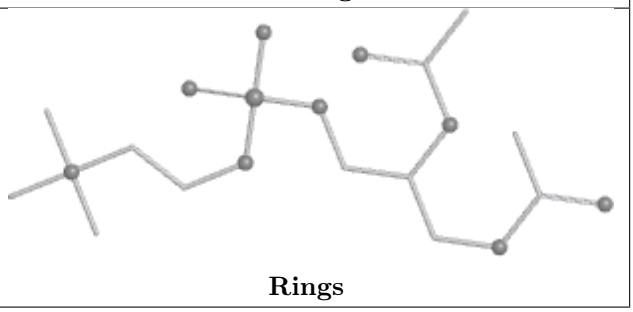
Bond lengths



Bond angles

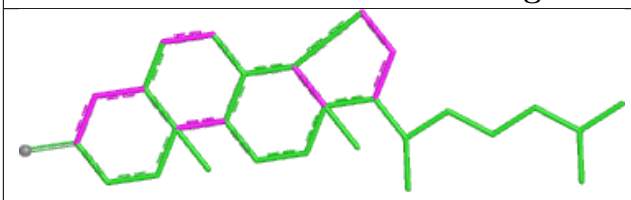


Torsions

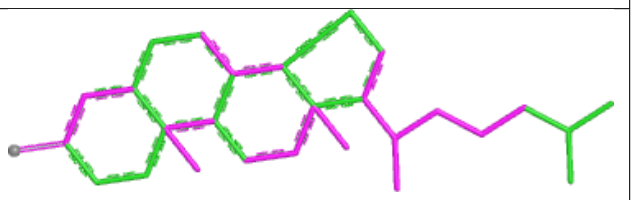


Rings

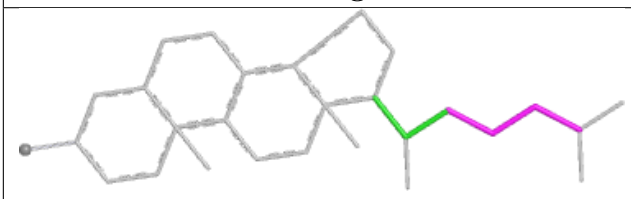
Ligand CLR D 401



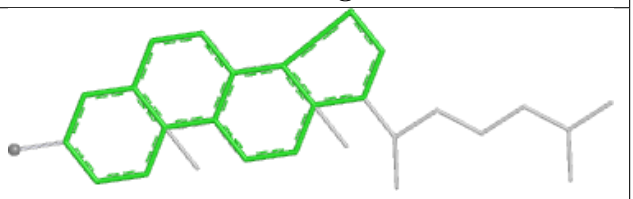
Bond lengths



Bond angles

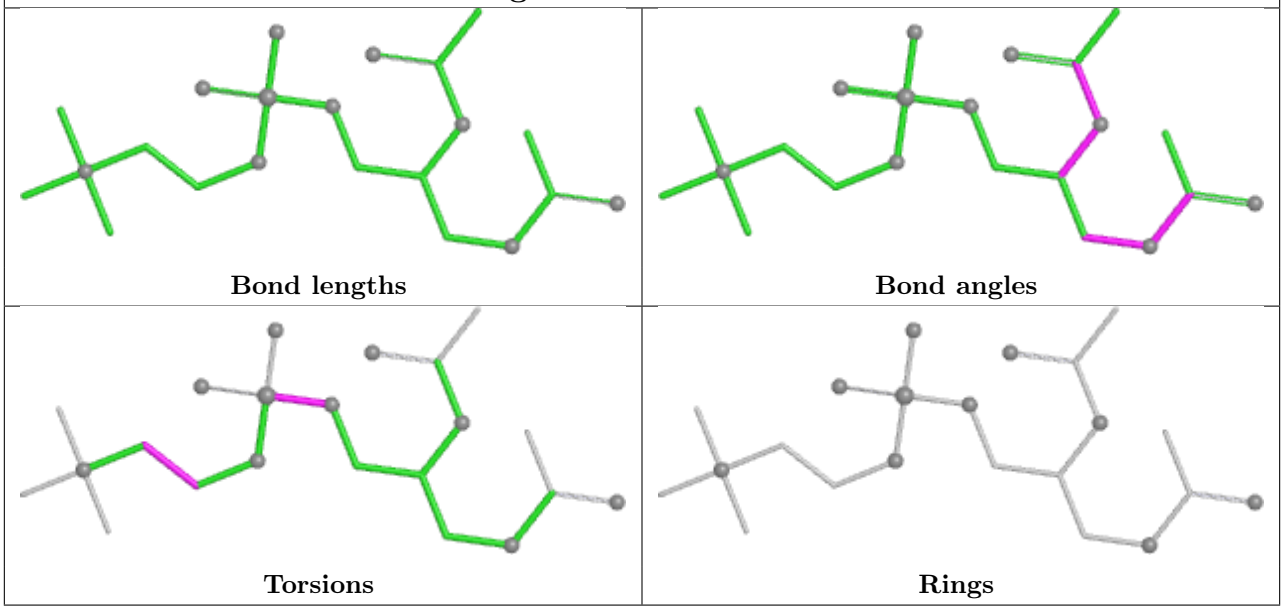


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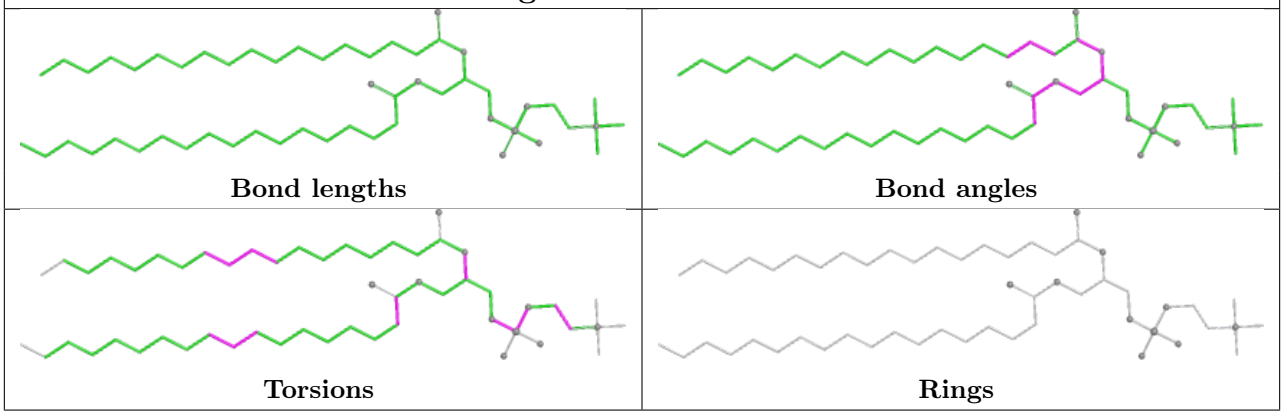


Rings

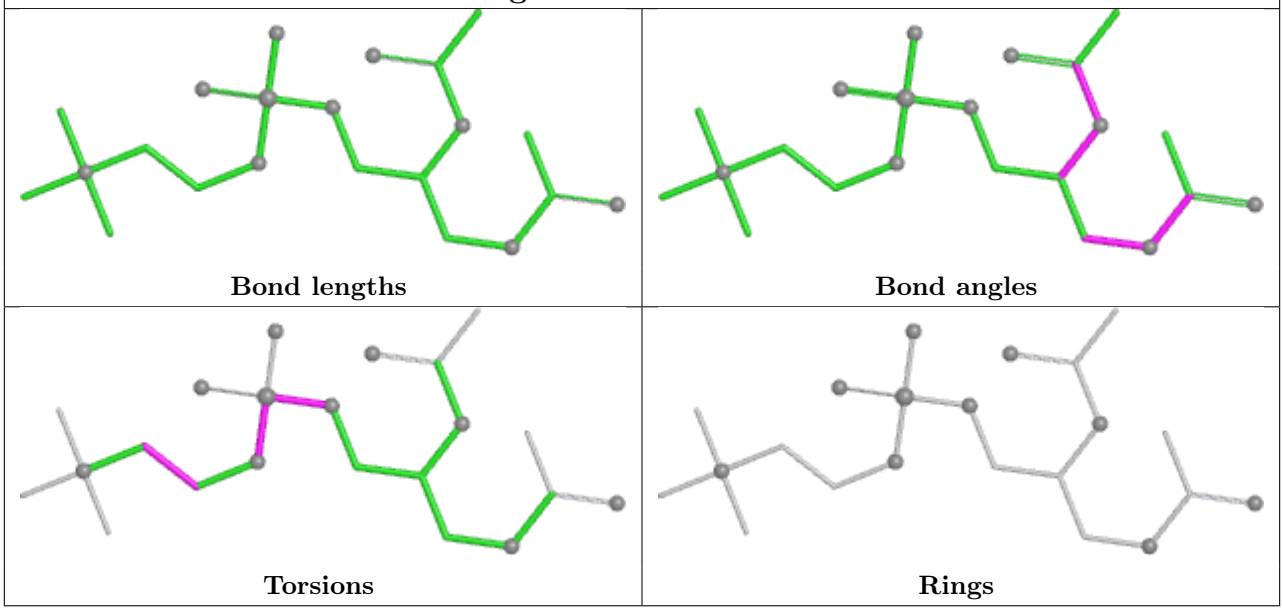
Ligand PCW C 1112



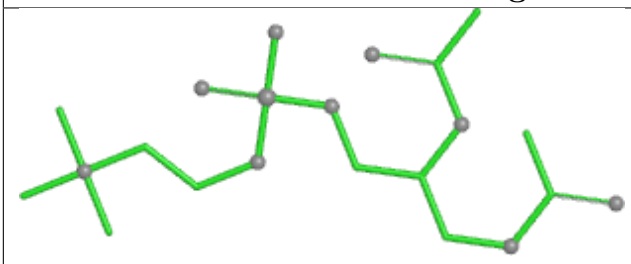
Ligand PC1 A 1110



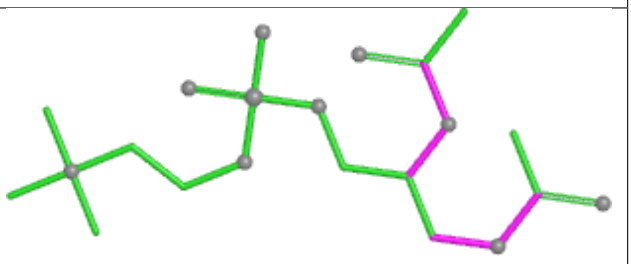
Ligand PCW A 1116



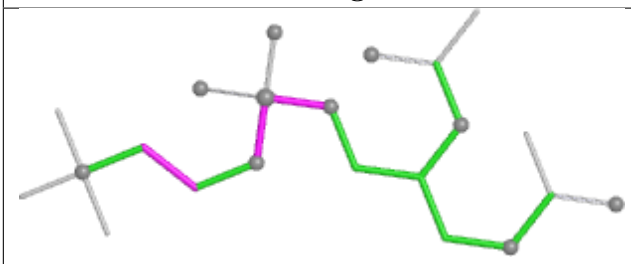
Ligand PCW C 1107



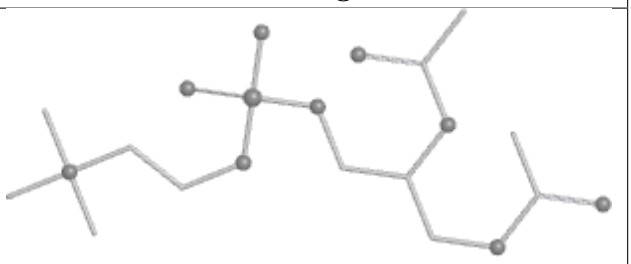
Bond lengths



Bond angles

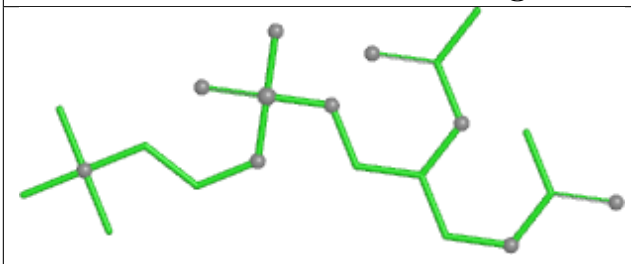


Torsions

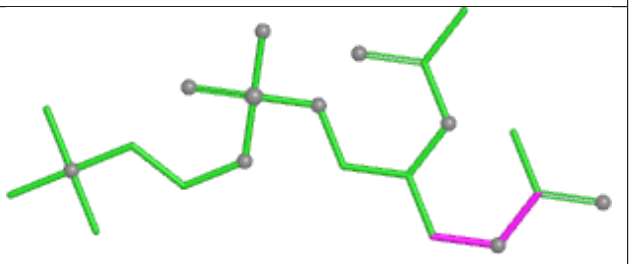


Rings

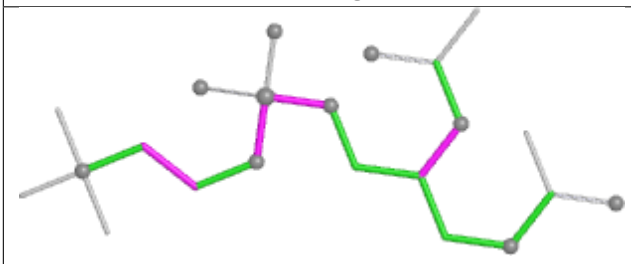
Ligand PCW C 1113



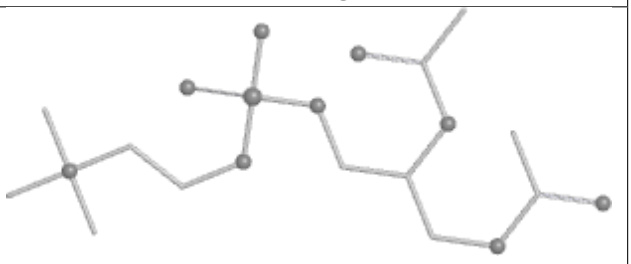
Bond lengths



Bond angles

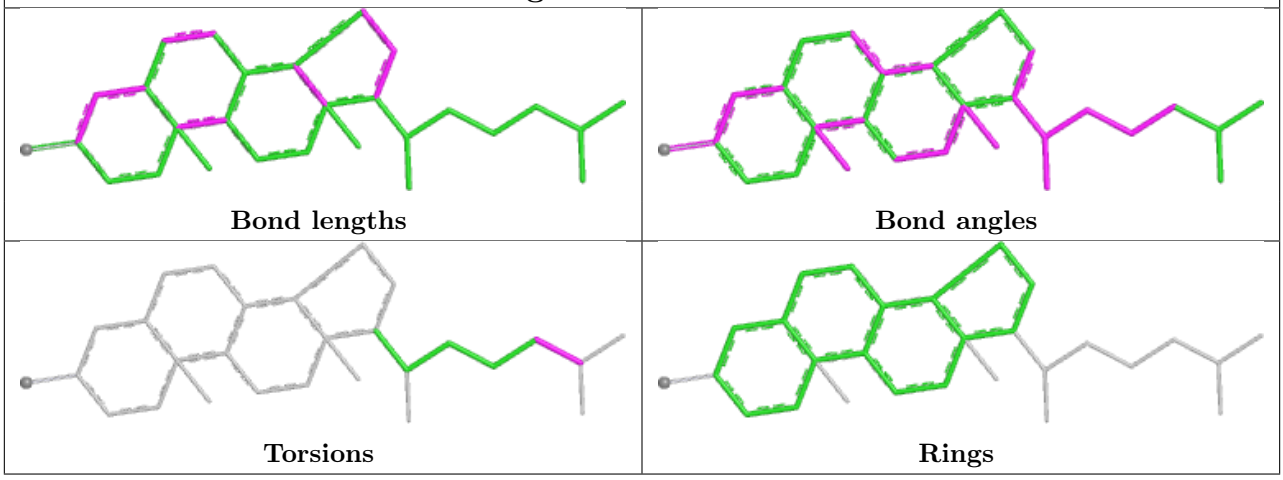


Torsions

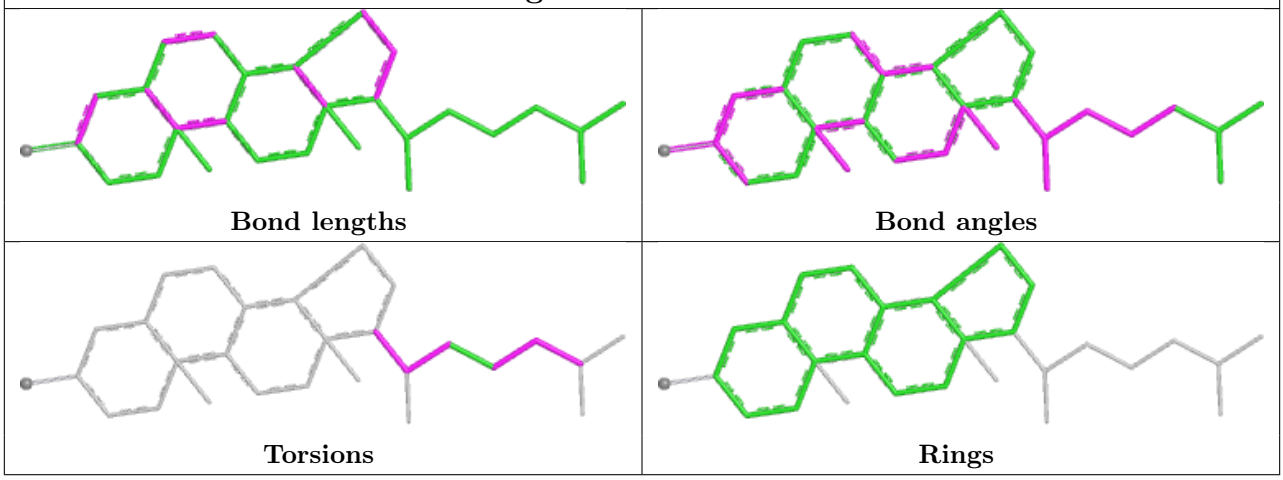


Rings

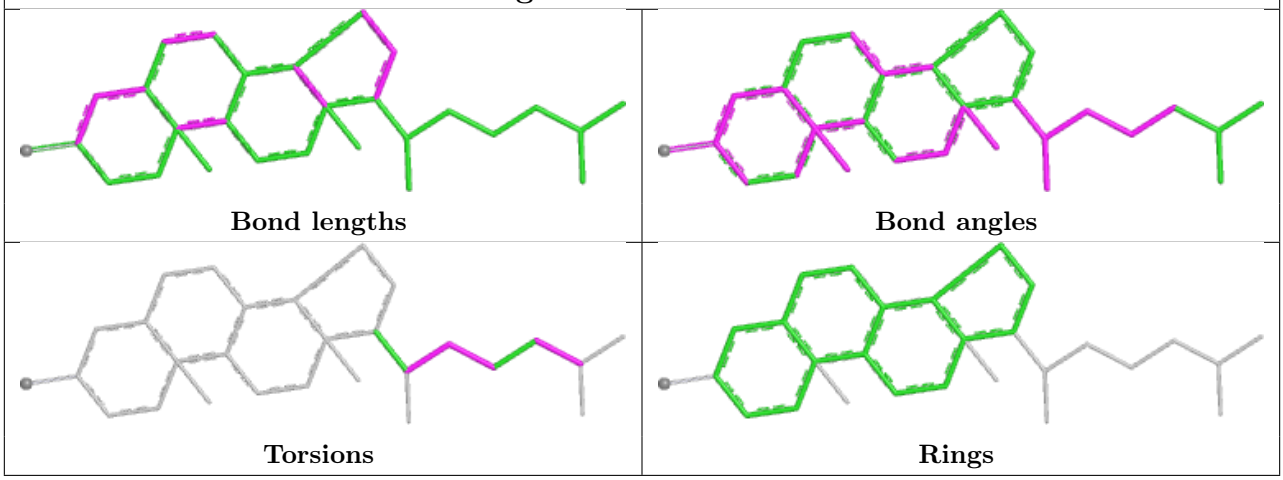
Ligand CLR E 101



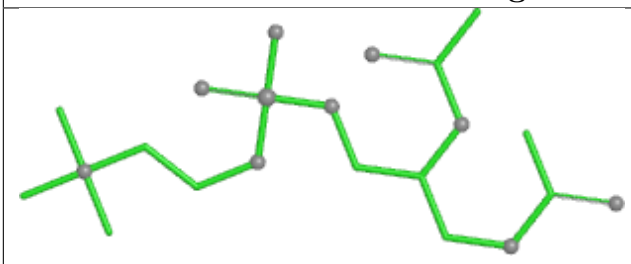
Ligand CLR B 402



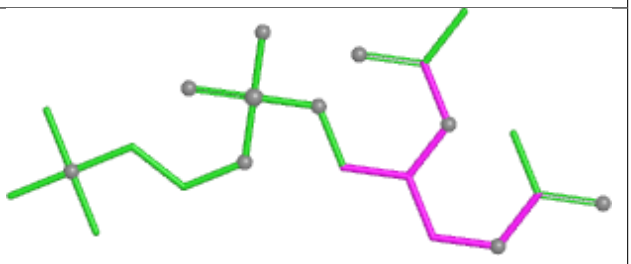
Ligand CLR A 1107



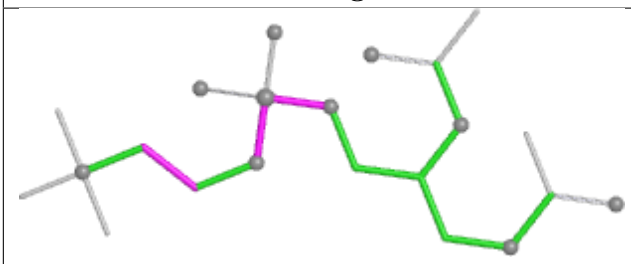
Ligand PCW A 1115



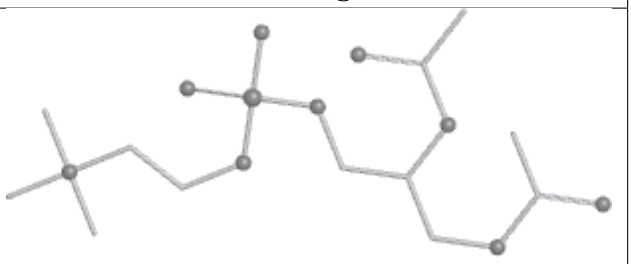
Bond lengths



Bond angles

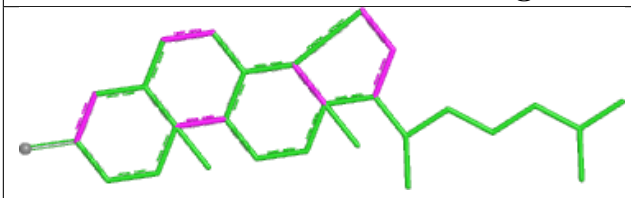


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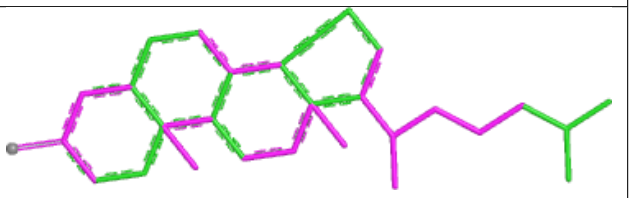


Rings

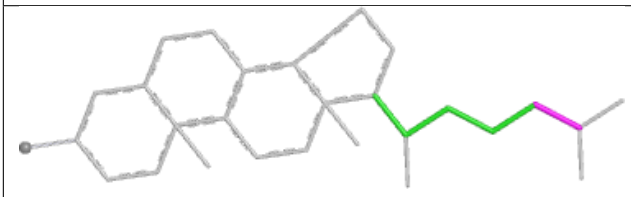
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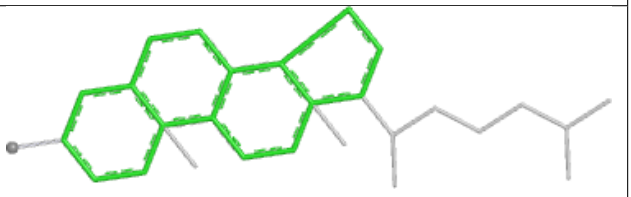
Bond lengths



Bond angles

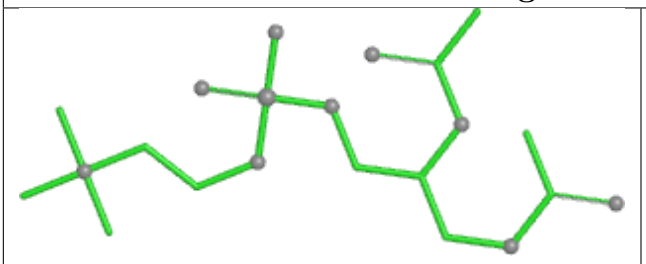


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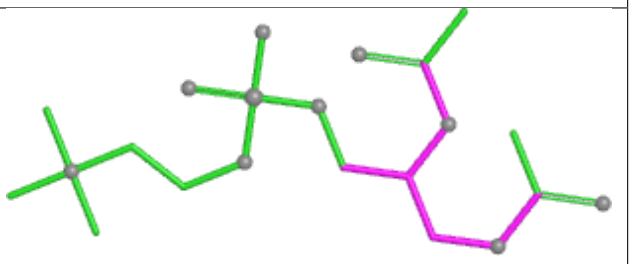


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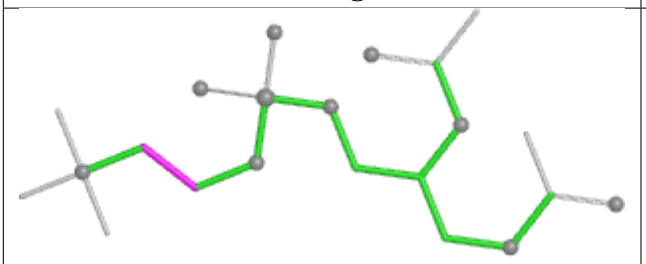
Ligand PCW B 401



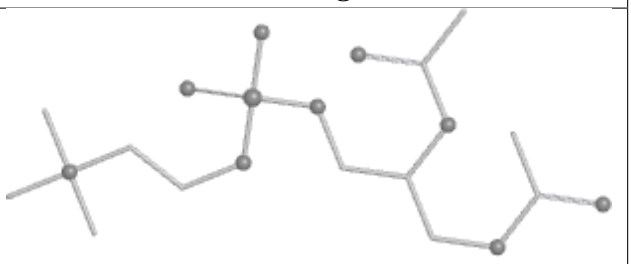
Bond lengths



Bond angles

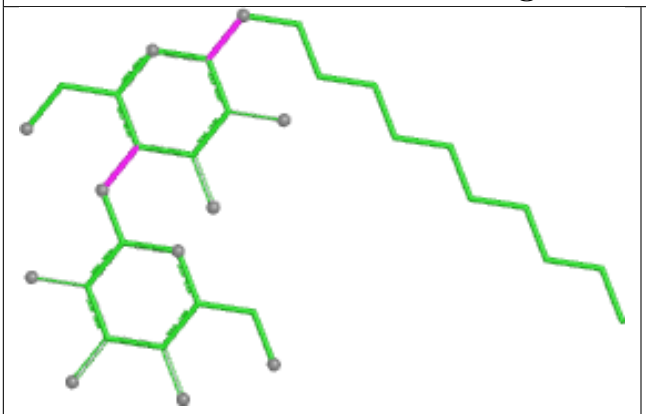


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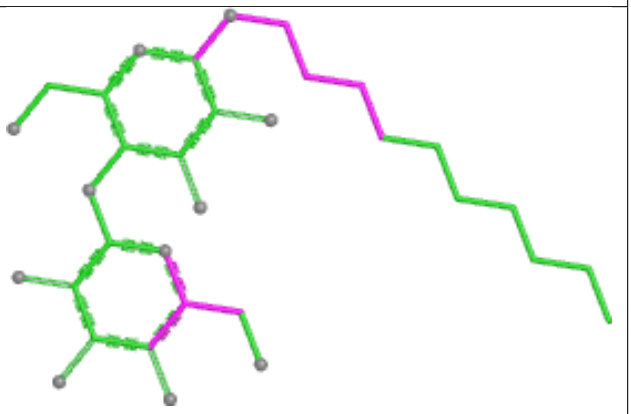


Rings

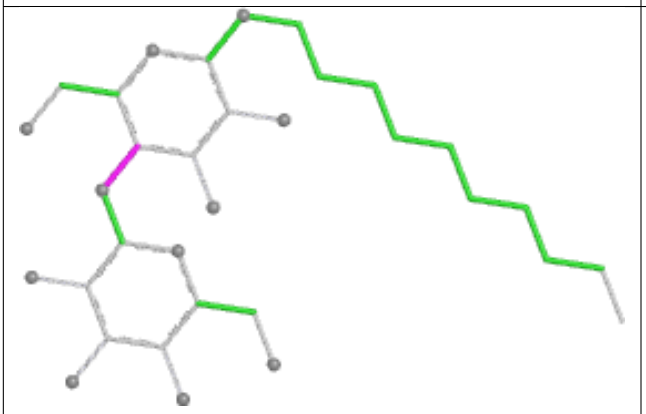
Ligand DMU E 102



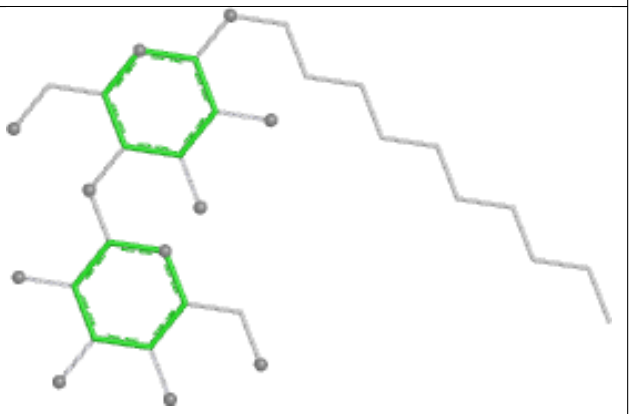
Bond lengths



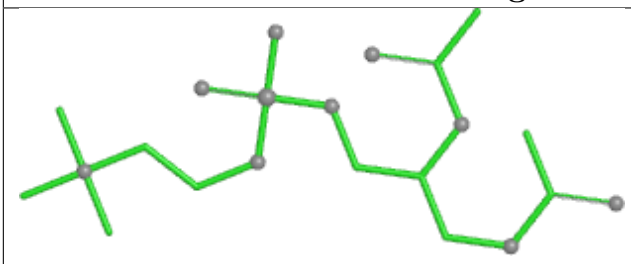
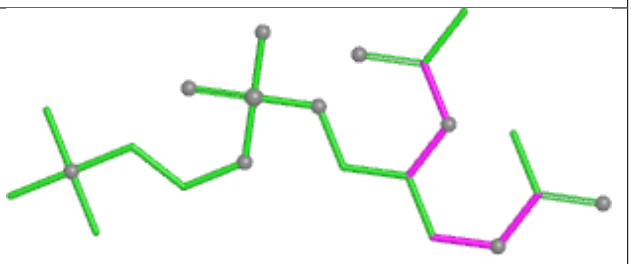
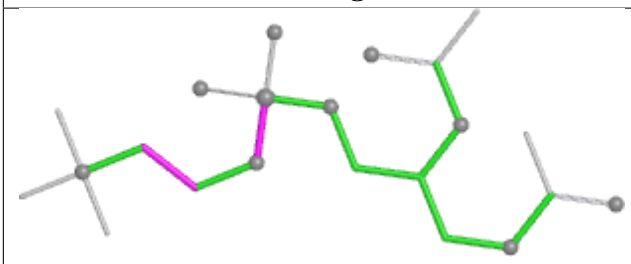
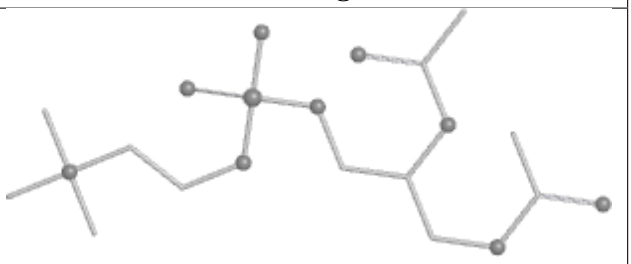
Bond angles

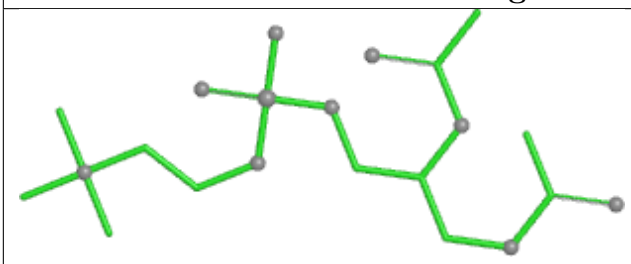
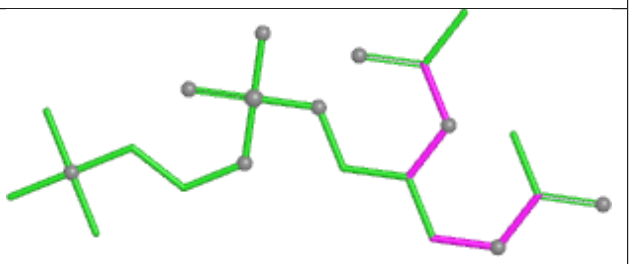
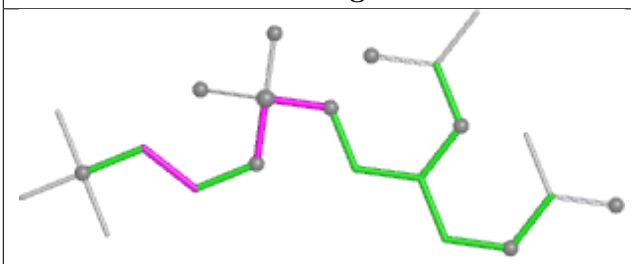
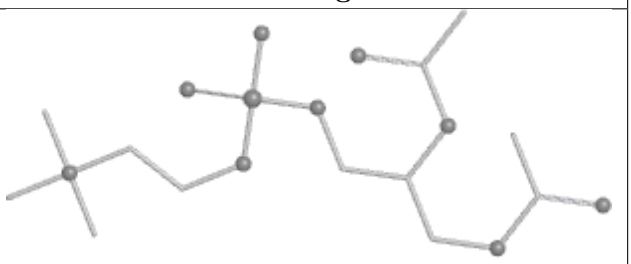


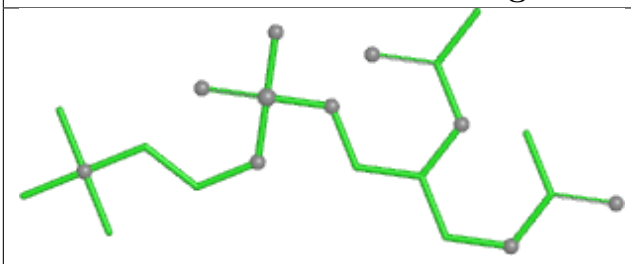
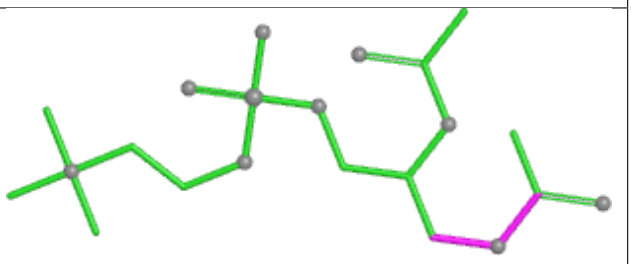
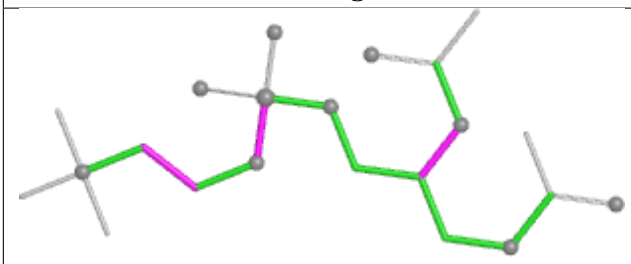
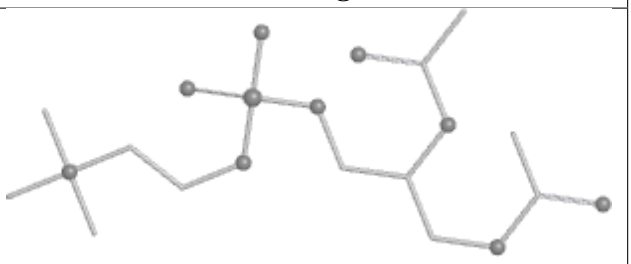
Torsions

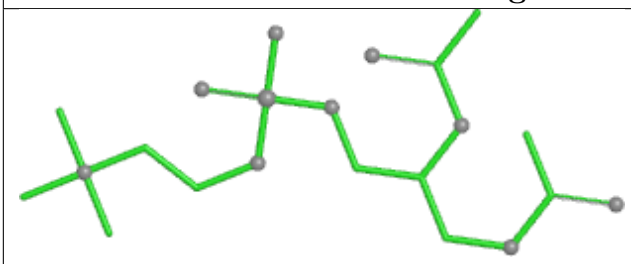
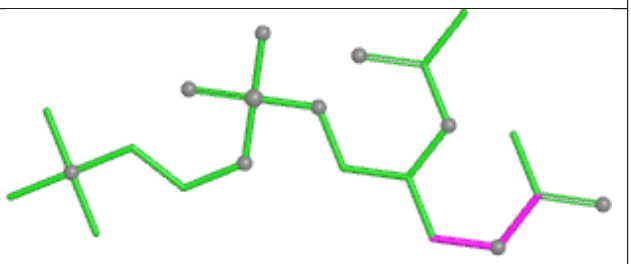
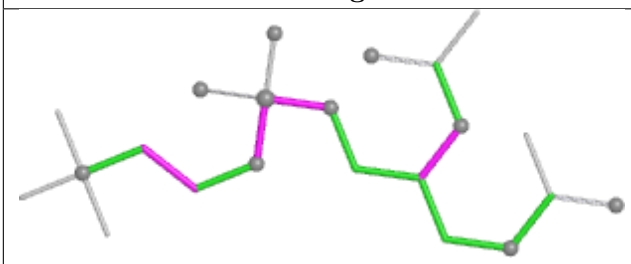
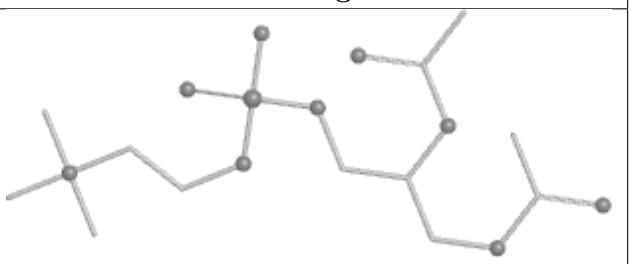


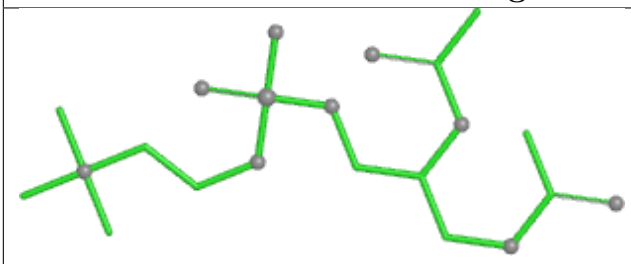
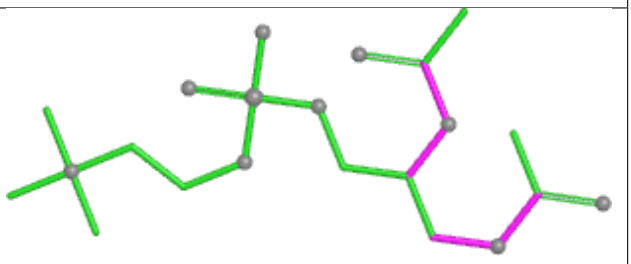
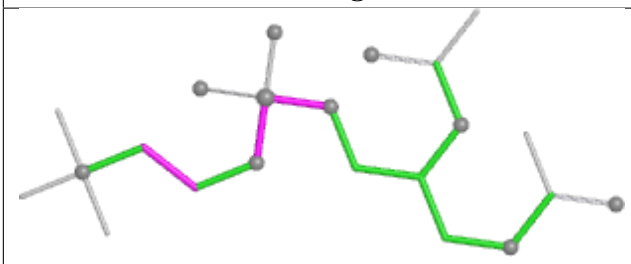
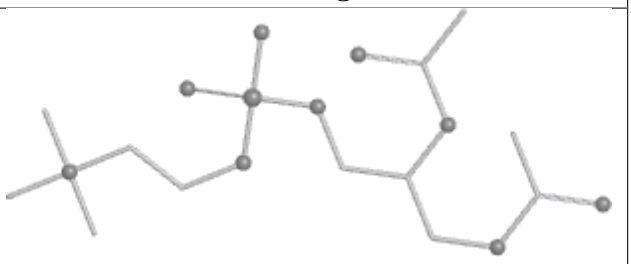
Rings

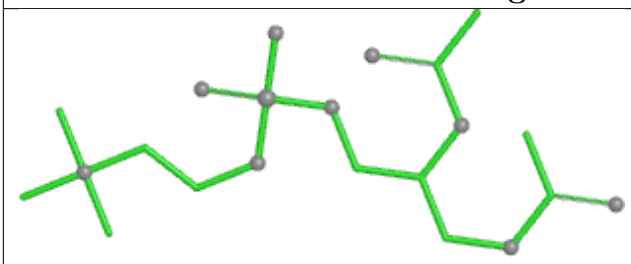
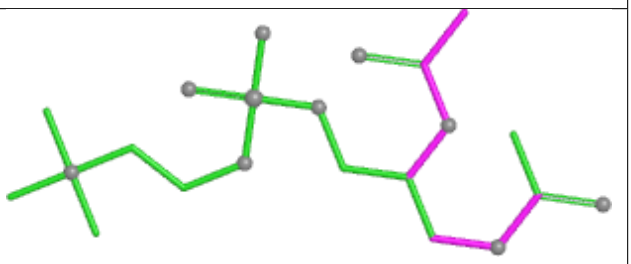
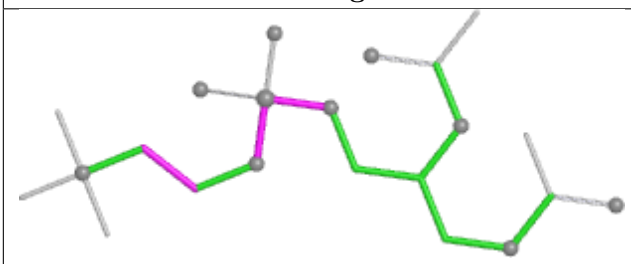
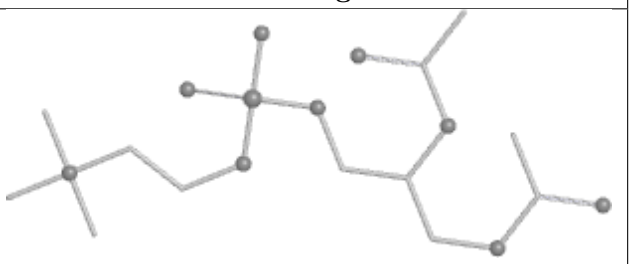
Ligand PCW A 1113	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW C 1109	
 Bond lengths	 Bond angles
 Torsions	 Rings

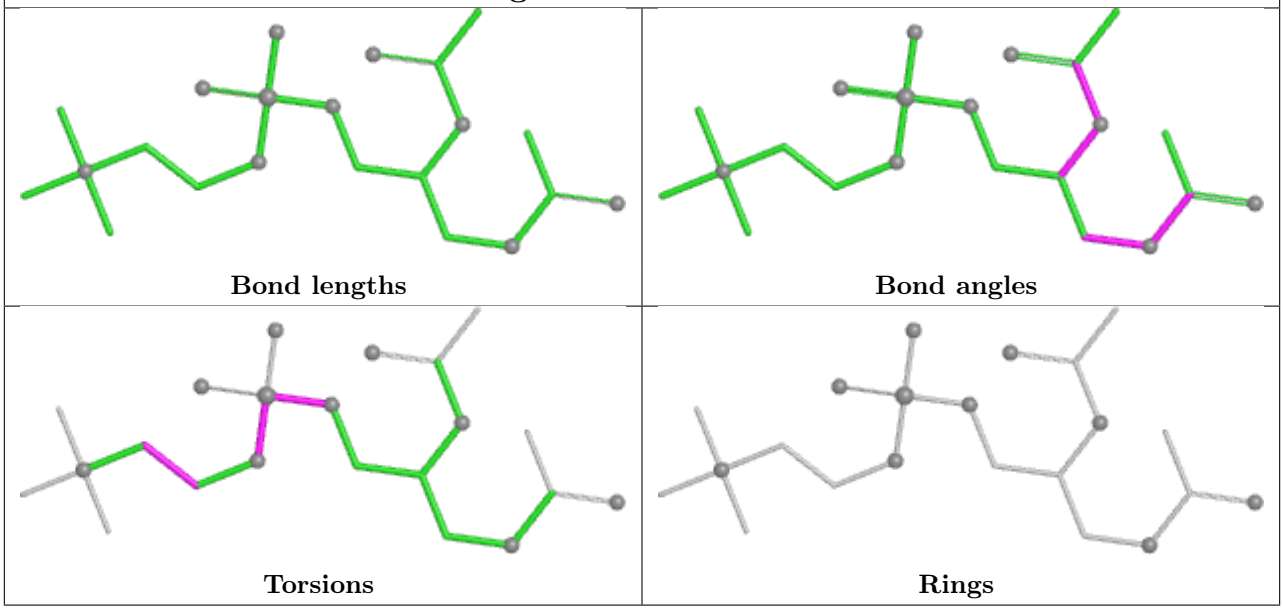
Ligand PCW C 1108	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW C 1110	
 Bond lengths	 Bond angles
 Torsions	 Rings

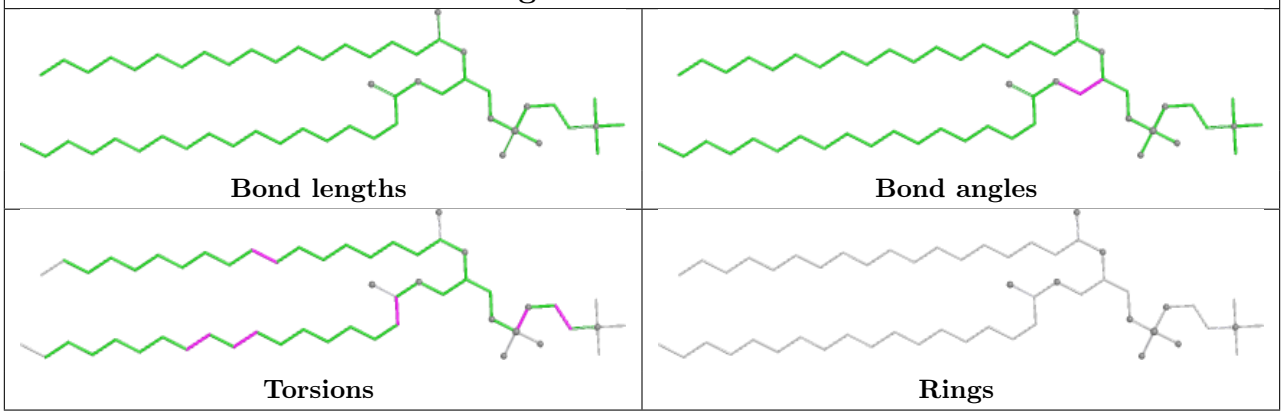
Ligand PCW A 1112	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW A 1114	
 Bond lengths	 Bond angles
 Torsions	 Rings

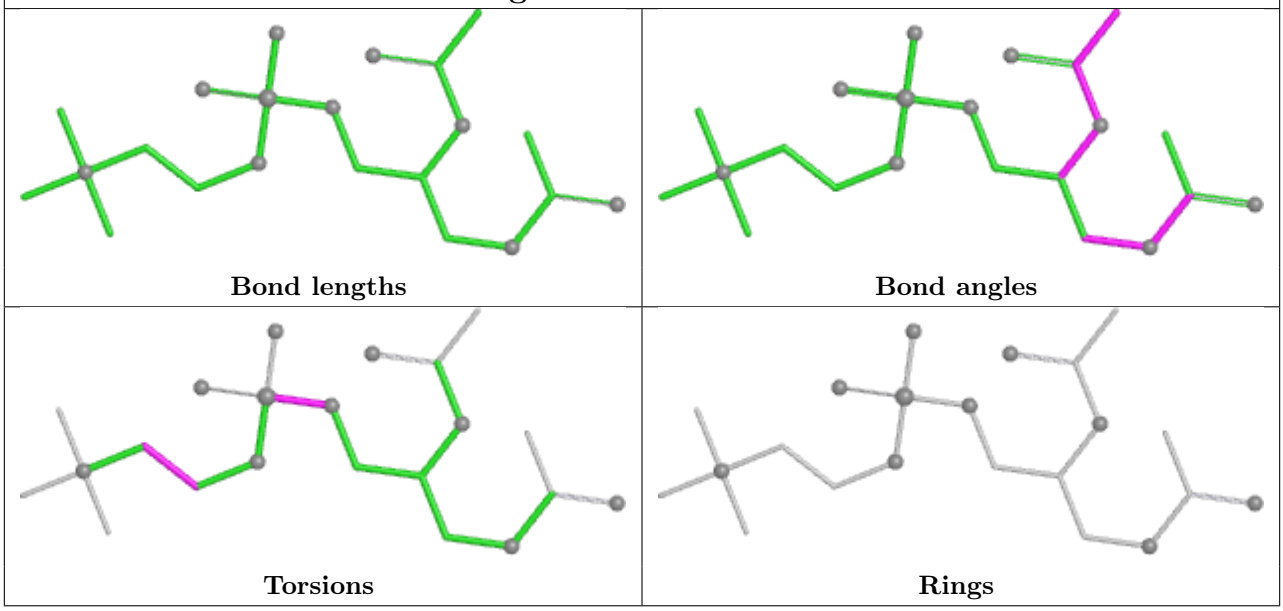
Ligand PCW C 1111

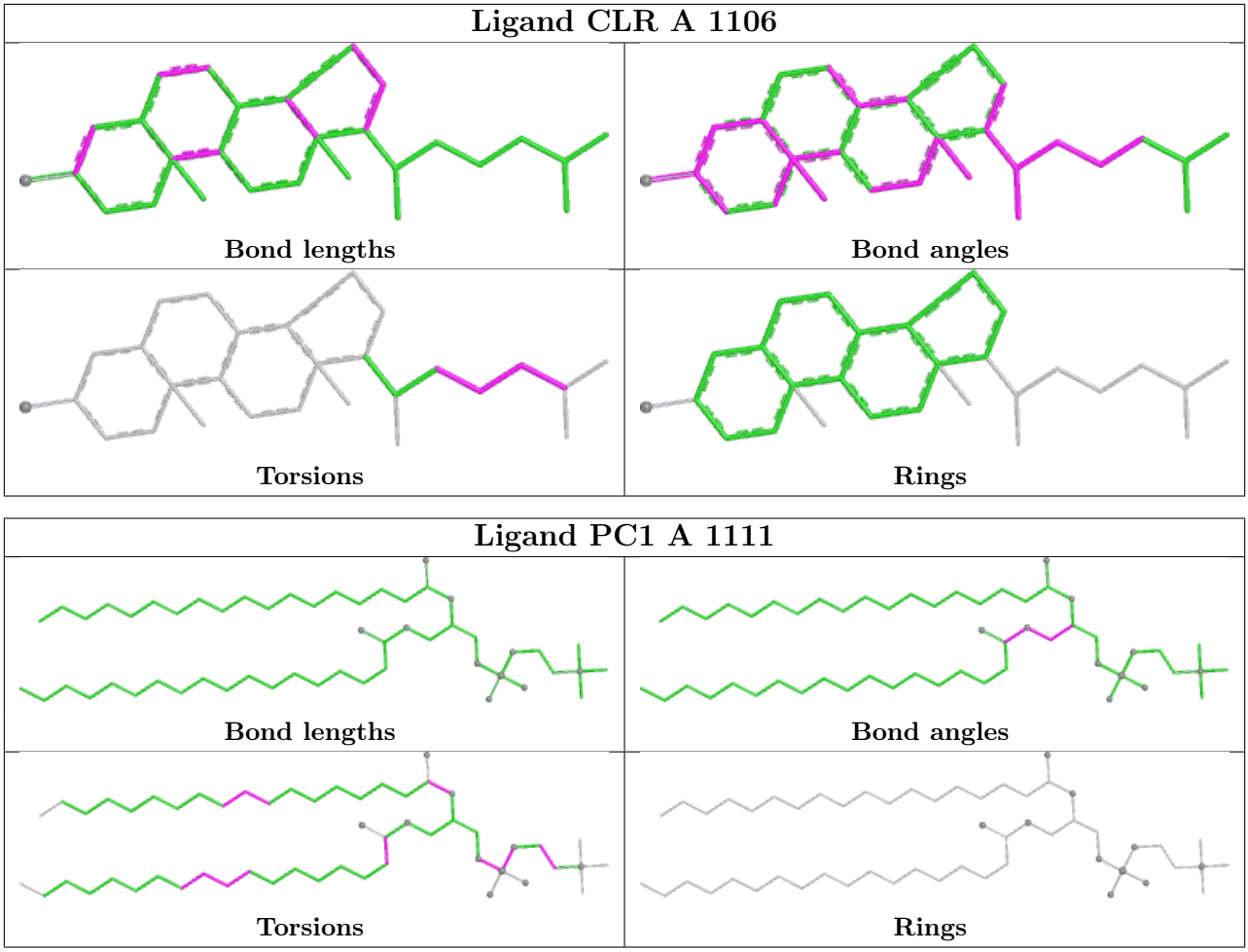


Ligand PC1 A 1108



Ligand PCW A 1109





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%)	-0.10	28 (2%) 55 45	18, 59, 151, 249	0
1	C	995/1021 (97%)	-0.02	26 (2%) 57 47	28, 67, 158, 303	0
2	B	291/303 (96%)	0.35	15 (5%) 33 25	52, 95, 162, 212	0
2	D	291/303 (96%)	0.40	11 (3%) 44 35	52, 105, 172, 228	0
3	E	33/65 (50%)	-0.33	0 100 100	36, 50, 100, 101	0
3	G	36/65 (55%)	-0.15	0 100 100	34, 58, 113, 140	0
All	All	2641/2778 (95%)	0.03	80 (3%) 52 42	18, 73, 158, 303	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	265	THR	4.5
1	A	401	GLY	4.1
2	B	122	ILE	3.6
1	A	138	CYS	3.6
1	A	487	LYS	3.5
1	A	264	ALA	3.3
2	B	22	LYS	3.3
1	C	494	PRO	3.3
1	C	264	ALA	3.2
1	A	261	GLY	3.2
1	A	491	THR	3.1
1	A	269	GLY	3.1
2	B	218	ASP	3.1
2	B	199	TYR	3.0
2	D	16	ILE	3.0
2	B	18	ASN	2.9
1	C	396	THR	2.9
1	C	401	GLY	2.9
1	A	420	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	402	VAL	2.8
1	A	402	VAL	2.8
2	B	196	LEU	2.8
2	B	16	ILE	2.7
1	C	400	SER	2.7
1	C	270	LEU	2.7
2	D	157	GLY	2.7
1	A	492	ALA	2.7
1	C	552	PHE	2.6
2	B	24	PHE	2.6
2	D	224	VAL	2.6
1	C	152	GLU	2.6
2	D	17	TRP	2.5
1	A	396	THR	2.5
2	D	199	TYR	2.5
2	D	218	ASP	2.5
1	A	494	PRO	2.5
1	A	400	SER	2.5
1	A	630	GLY	2.5
2	B	15	PHE	2.4
2	B	23	GLU	2.4
2	D	204	TYR	2.4
1	C	492	ALA	2.4
1	A	438	ARG	2.3
2	D	158	ASN	2.3
1	C	267	ALA	2.3
1	A	28	LEU	2.3
1	C	80	PRO	2.3
2	B	161	GLY	2.3
1	A	462	GLU	2.3
1	C	223	ASP	2.3
1	C	154	PHE	2.3
1	C	78	THR	2.3
2	D	194	GLU	2.3
1	A	265	THR	2.3
2	B	166	THR	2.3
1	A	79	THR	2.2
1	C	398	ASN	2.2
1	C	273	GLY	2.2
2	D	195	SER	2.2
1	A	399	GLN	2.2
1	A	496	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	491	THR	2.2
1	C	310	TRP	2.2
1	C	397	GLU	2.2
1	C	26	ASP	2.1
1	A	89	LEU	2.1
1	A	430	GLN	2.1
1	A	553	LEU	2.1
1	C	497	LEU	2.1
1	A	937	VAL	2.1
2	B	21	LYS	2.1
1	C	89	LEU	2.1
1	C	25	MET	2.0
1	A	80	PRO	2.0
1	C	141	TYR	2.0
1	A	270	LEU	2.0
1	A	424	ALA	2.0
2	B	164	ASP	2.0
2	B	121	MET	2.0
2	D	169	TYR	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
4	NAG	F	1	14/15	-	-	91,109,118,123	0
4	NAG	F	2	14/15	-	-	125,132,138,140	0
4	BMA	F	3	11/12	-	-	127,131,138,140	0
4	MAN	F	4	11/12	-	-	123,132,136,136	0
4	MAN	F	5	11/12	-	-	98,113,126,130	0
4	MAN	F	6	11/12	-	-	119,128,130,131	0
6	NAG	I	2	14/15	0.24	0.14	119,132,138,141	0
5	MAN	H	5	11/12	0.29	0.17	149,152,155,155	0
5	NAG	H	1	14/15	0.30	0.18	122,134,143,151	0

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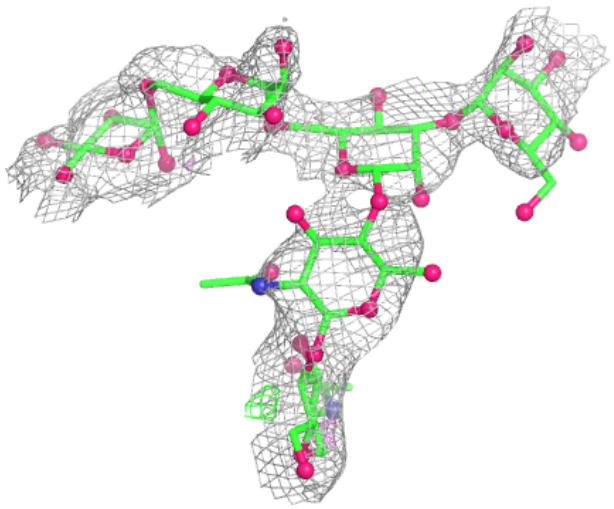
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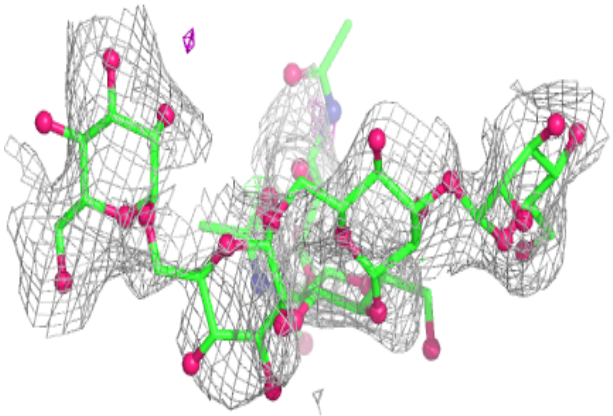
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	H	4	11/12	0.36	0.15	129,142,147,147	0
5	BMA	H	3	11/12	0.38	0.13	148,150,153,153	0
5	NAG	H	2	14/15	0.65	0.12	138,152,154,155	0
6	NAG	I	1	14/15	0.71	0.14	109,128,131,132	0

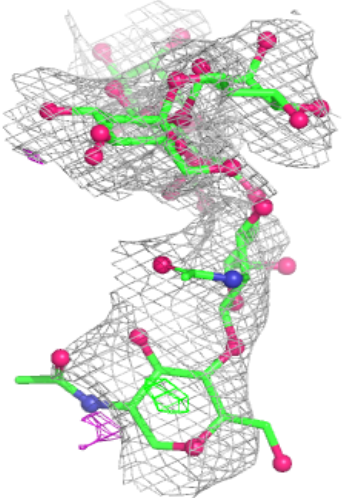
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

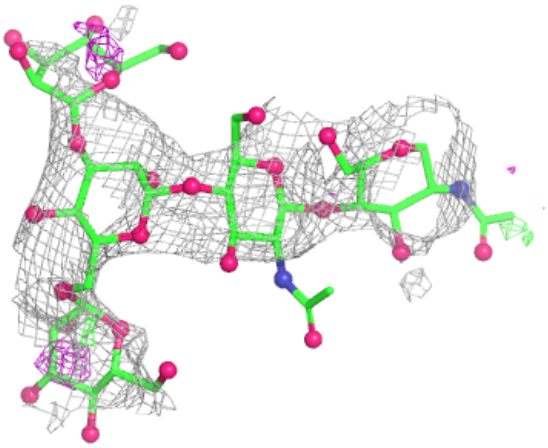


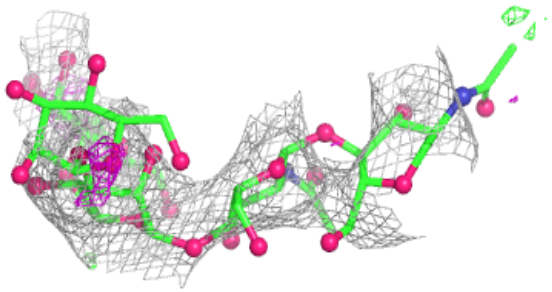


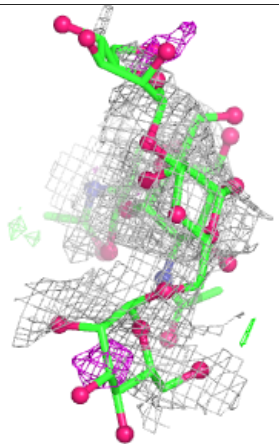


Electron density around Chain H:

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

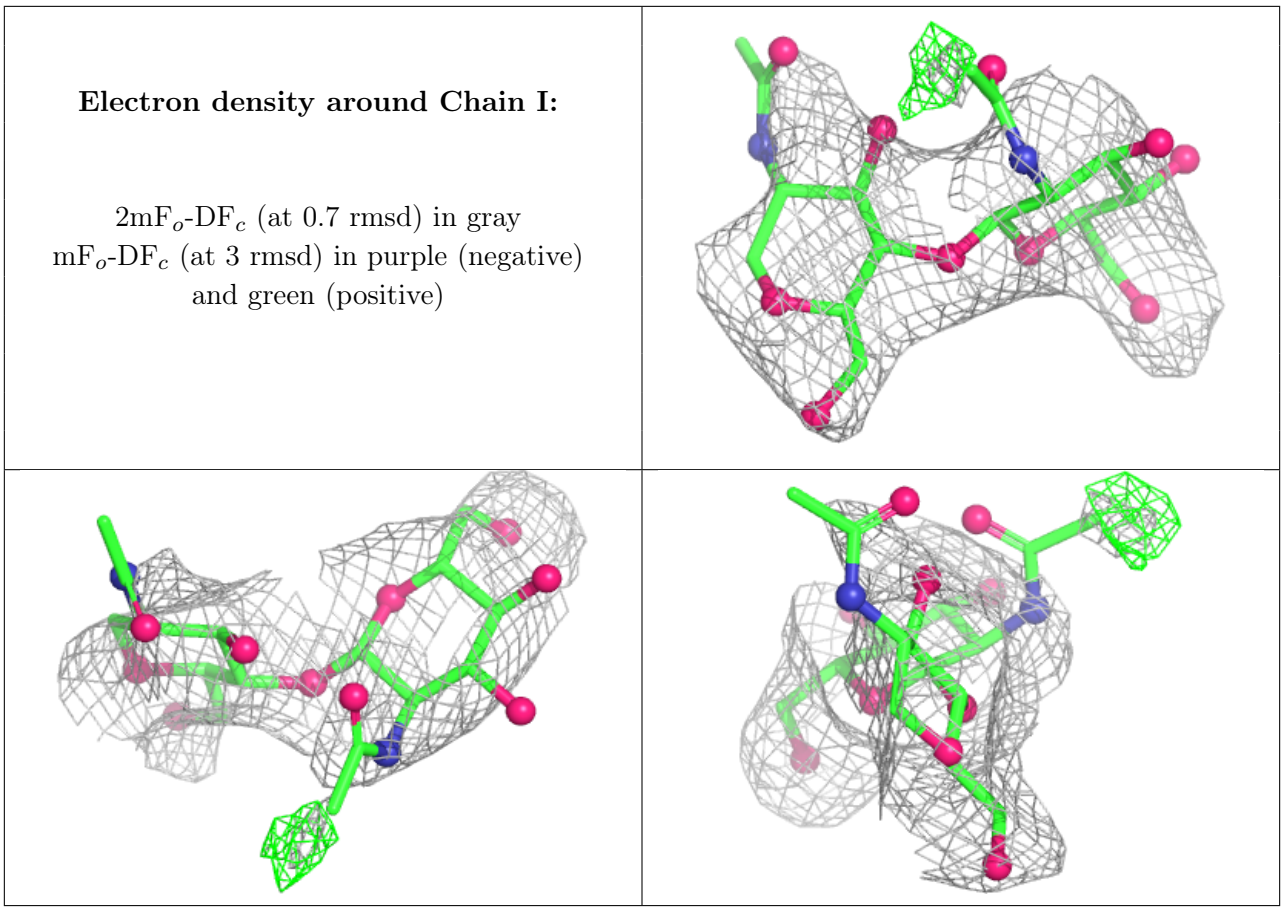






Electron density around Chain I:

$2mF_o$-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
11	PCW	C	1113	22/54	0.37	0.18	98,136,160,164	0
11	PCW	B	401	22/54	0.39	0.16	117,127,163,165	0
12	NAG	D	402	14/15	0.48	0.14	125,134,147,152	0
11	PCW	A	1116	22/54	0.50	0.19	119,151,157,160	0
11	PCW	C	1110	22/54	0.51	0.18	111,143,151,152	0
11	PCW	A	1115	22/54	0.53	0.19	112,135,148,153	0
11	PCW	C	1111	22/54	0.53	0.17	74,127,149,150	0
11	PCW	C	1112	22/54	0.59	0.21	84,120,138,145	0
11	PCW	A	1113	22/54	0.60	0.16	114,129,150,152	0
11	PCW	A	1109	22/54	0.61	0.18	115,135,151,154	0
11	PCW	C	1109	22/54	0.64	0.18	99,124,153,154	0
11	PCW	C	1107	22/54	0.66	0.18	84,111,146,149	0
11	PCW	C	1108	22/54	0.66	0.19	106,122,130,138	0

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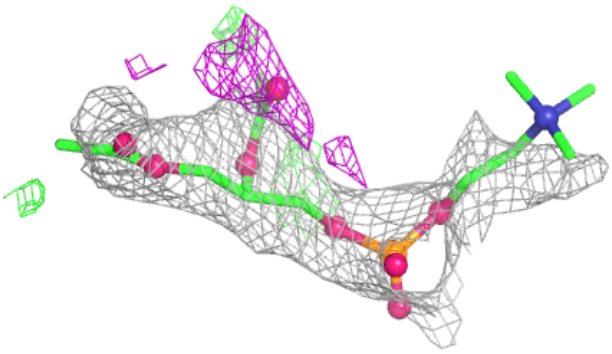
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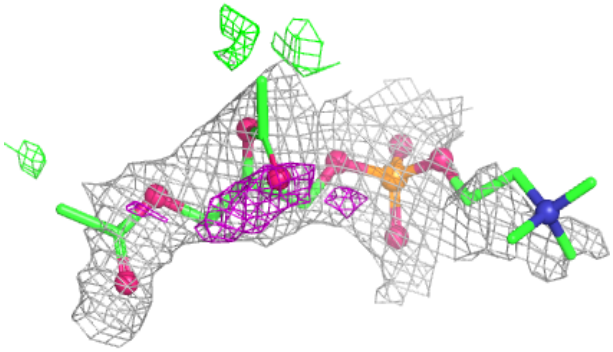
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	PCW	C	1114	22/54	0.67	0.17	95,130,146,151	0
11	PCW	A	1114	22/54	0.72	0.17	109,129,141,146	0
9	CLR	D	401	28/28	0.74	0.15	71,87,93,97	0
10	PC1	A	1108	54/54	0.76	0.13	72,96,122,127	0
10	PC1	A	1110	54/54	0.81	0.15	58,71,109,115	0
9	CLR	B	402	28/28	0.81	0.14	87,99,107,112	0
11	PCW	A	1112	22/54	0.83	0.16	72,117,123,126	0
8	NA	C	1103	1/1	0.84	0.12	88,88,88,88	0
8	NA	A	1103	1/1	0.86	0.10	73,73,73,73	0
10	PC1	A	1111	54/54	0.86	0.15	42,79,107,113	0
9	CLR	A	1106	28/28	0.88	0.12	65,77,87,95	0
13	DMU	E	102	33/33	0.88	0.13	28,55,78,85	0
8	NA	C	1102	1/1	0.89	0.09	76,76,76,76	0
8	NA	A	1102	1/1	0.90	0.06	61,61,61,61	0
9	CLR	A	1107	28/28	0.93	0.09	25,46,57,64	0
8	NA	C	1104	1/1	0.94	0.07	67,67,67,67	0
9	CLR	E	101	28/28	0.94	0.09	22,40,52,62	0
8	NA	C	1105	1/1	0.95	0.09	62,62,62,62	0
9	CLR	C	1106	28/28	0.95	0.10	25,33,84,91	0
7	MN	C	1101	1/1	0.97	0.04	69,69,69,69	0
8	NA	A	1105	1/1	0.97	0.07	47,47,47,47	0
7	MN	A	1101	1/1	0.98	0.02	58,58,58,58	0
8	NA	A	1104	1/1	0.99	0.04	49,49,49,49	0

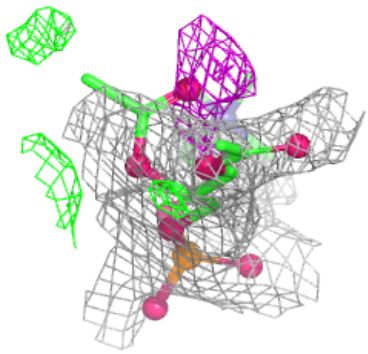
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCW C 1113:

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

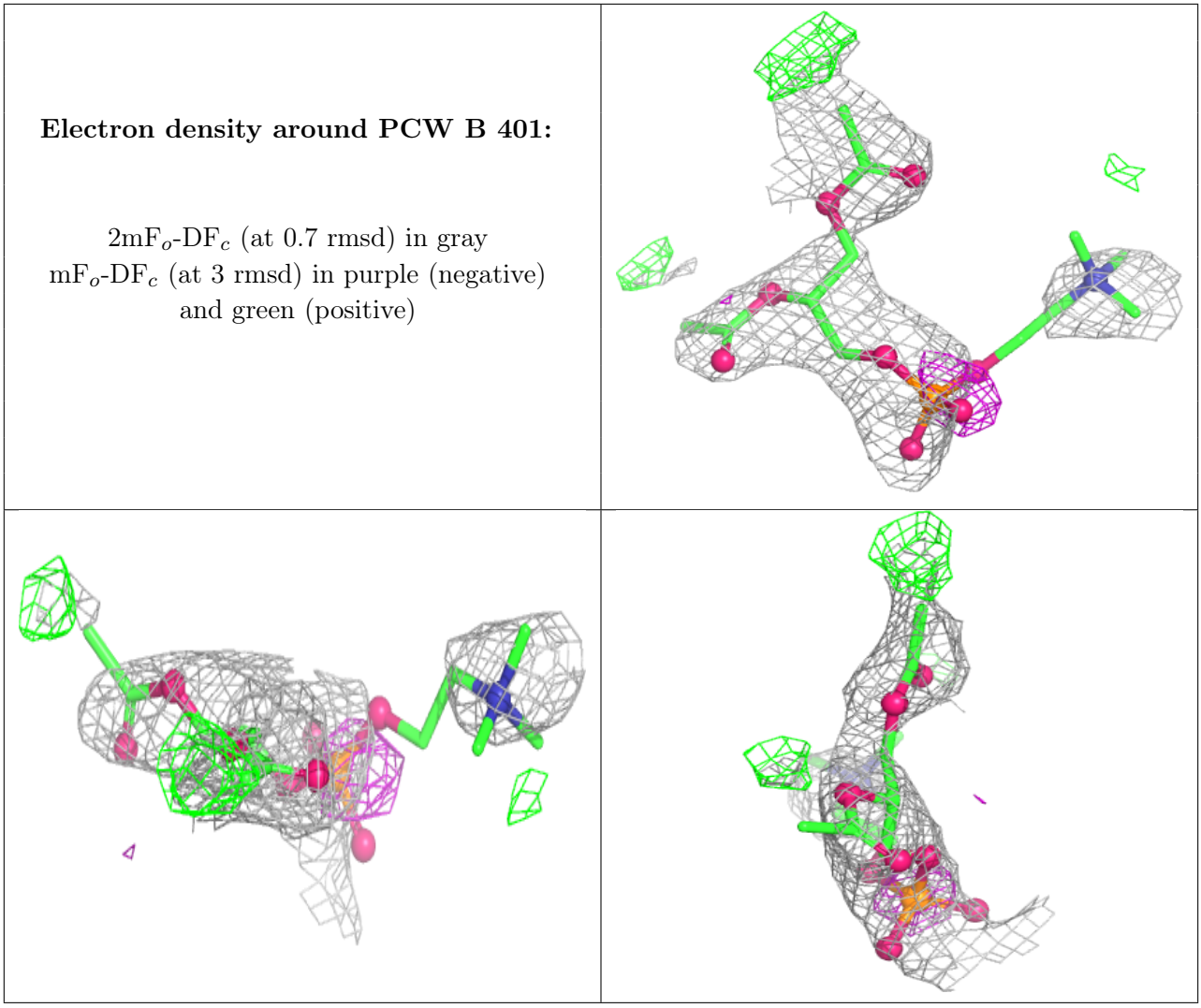






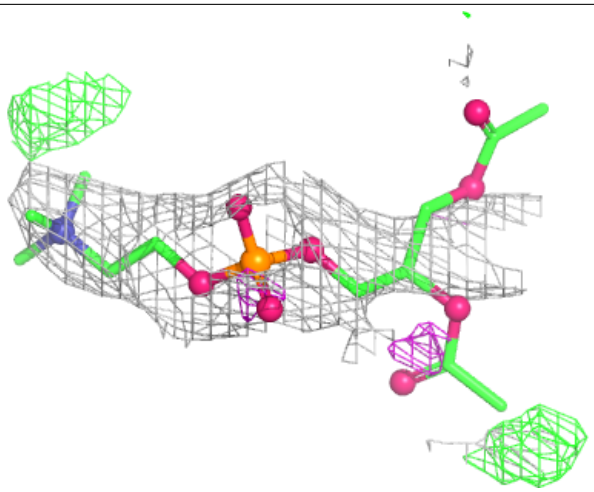
Electron density around PCW B 401:

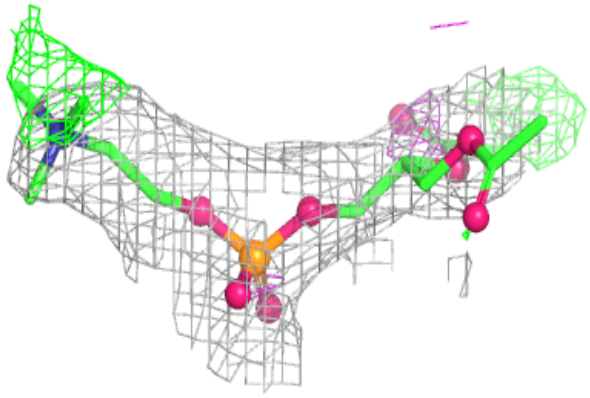
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

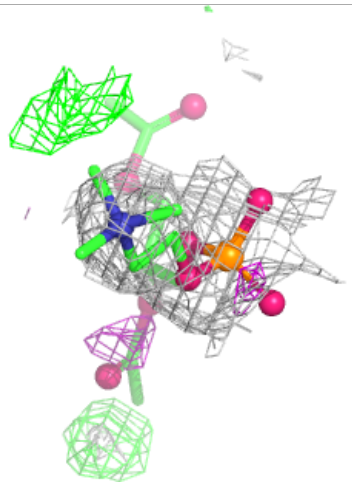


Electron density around PCW A 1116:

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

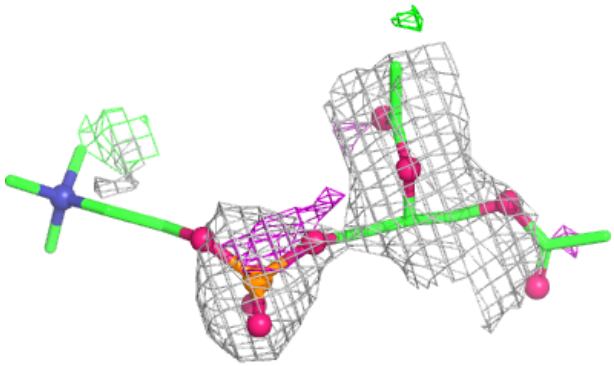


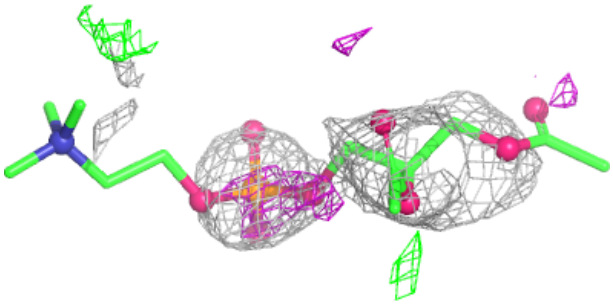


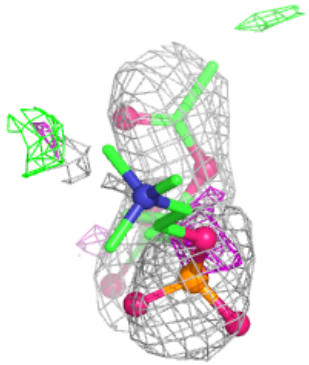


Electron density around PCW C 1110:

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

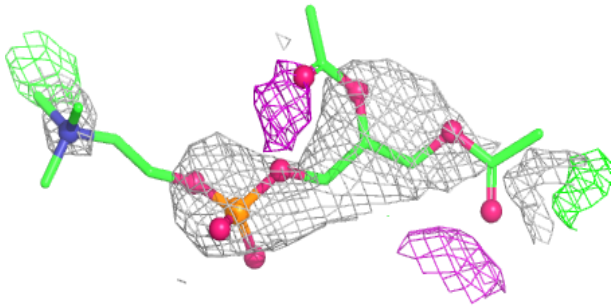


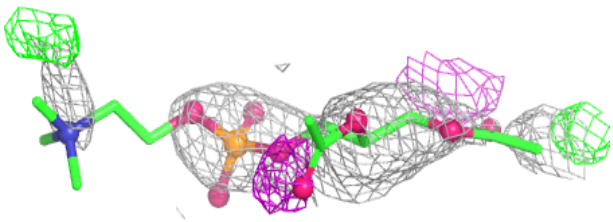


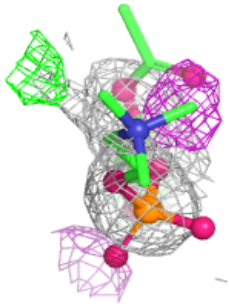


Electron density around PCW A 1115:

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

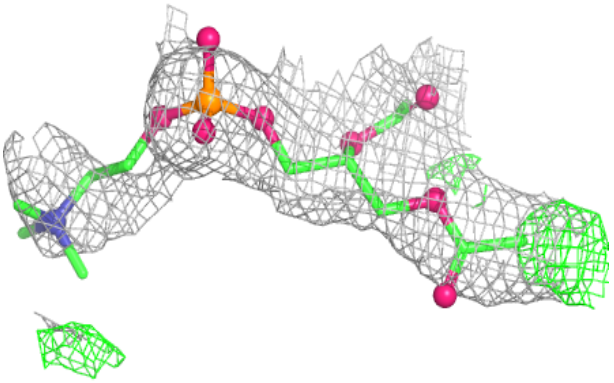


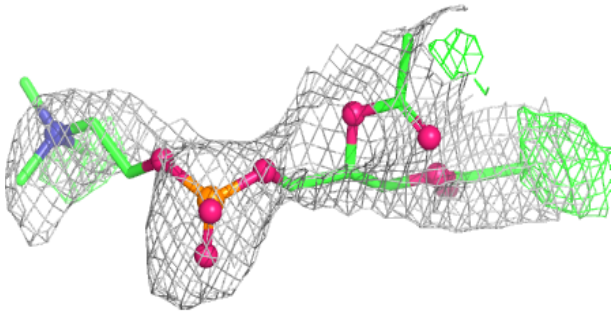


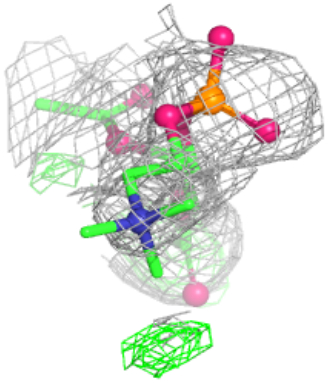


Electron density around PCW C 1111:

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

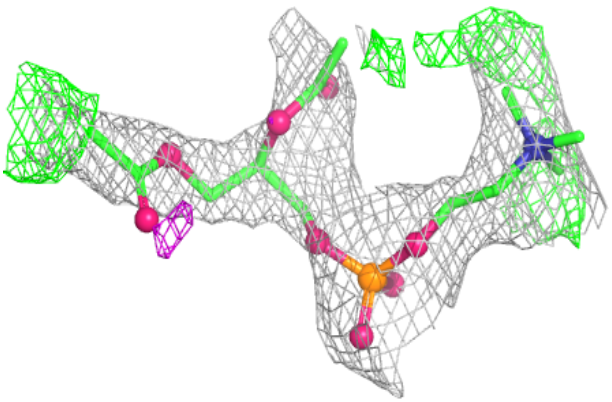


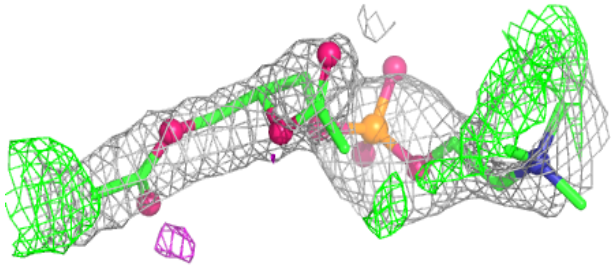


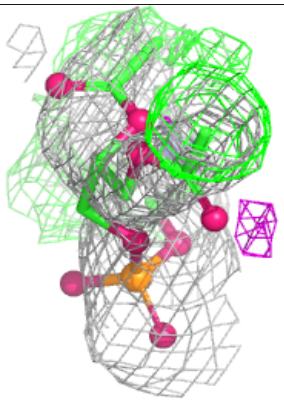


Electron density around PCW C 1112:

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

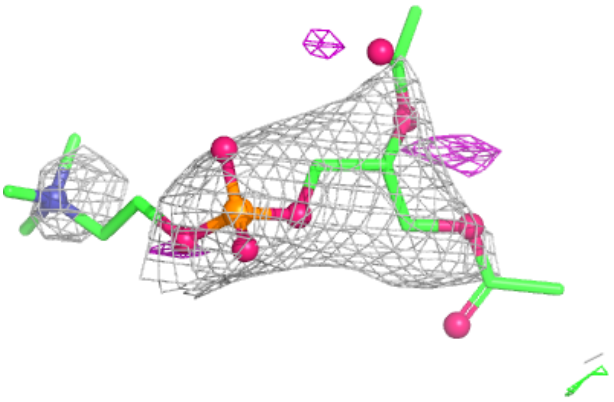


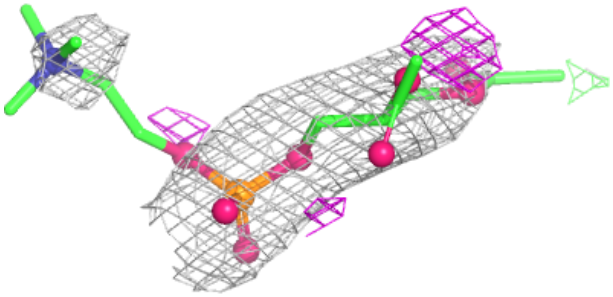


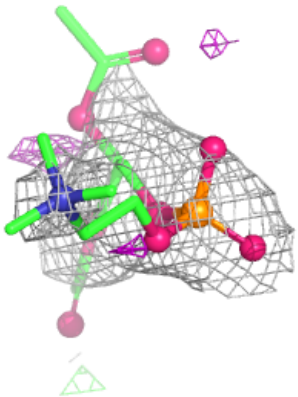


Electron density around PCW A 1113:

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

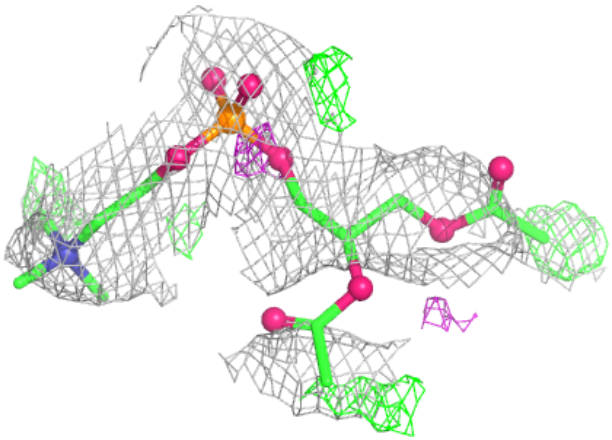


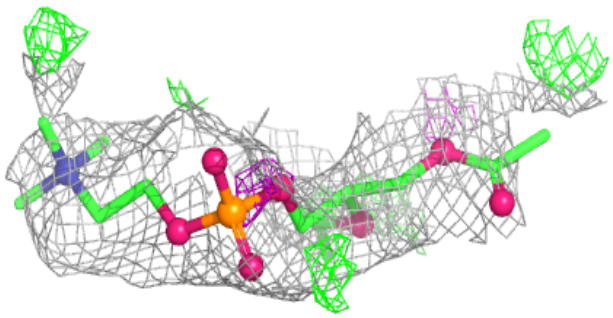


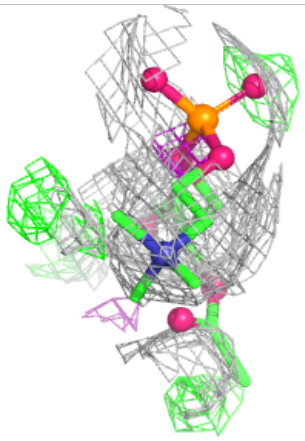


Electron density around PCW A 1109:

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

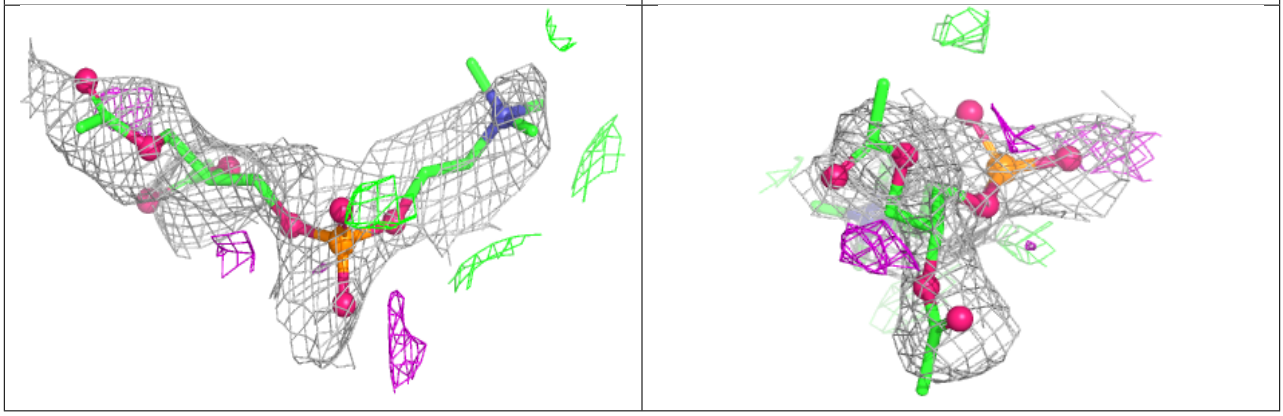






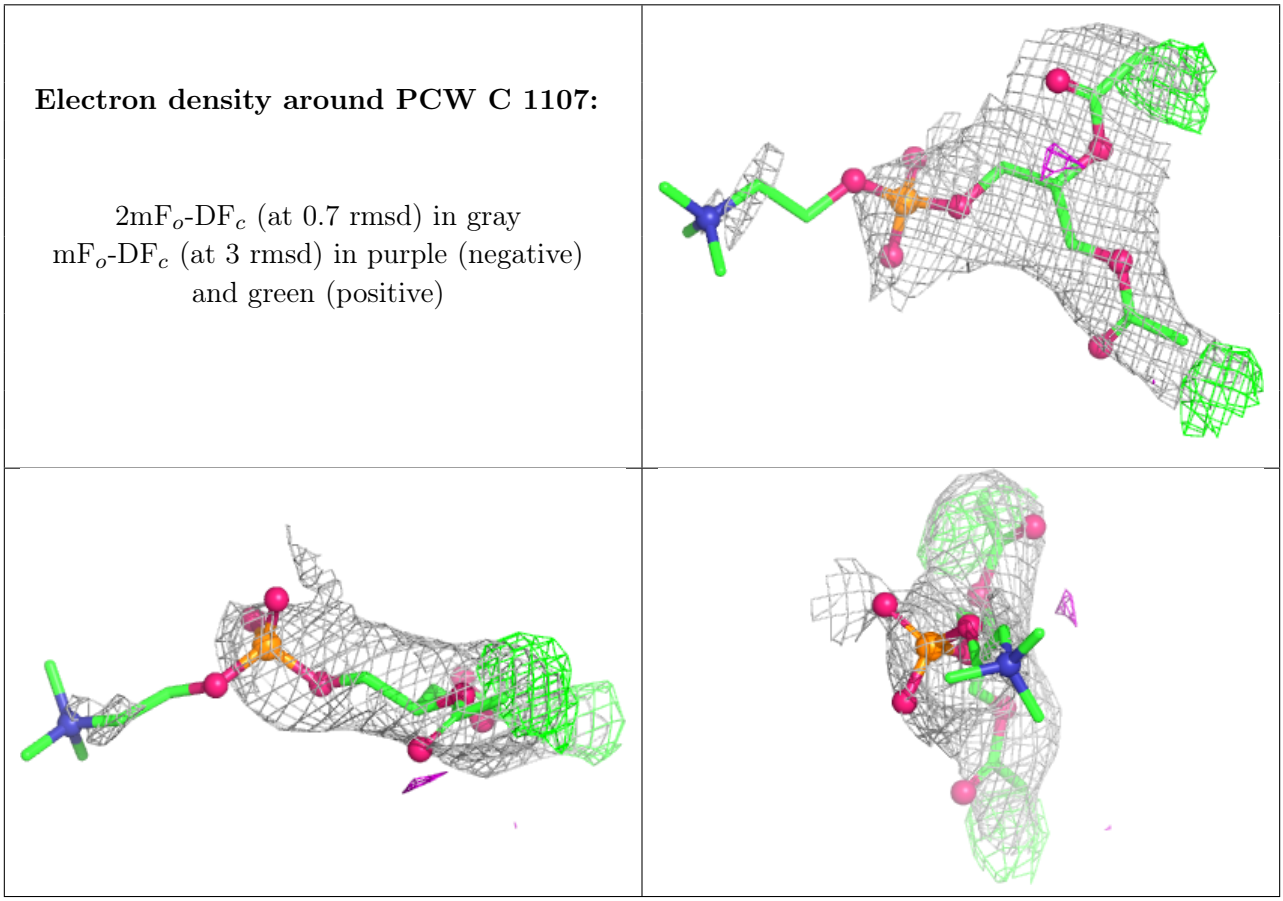
Electron density around PCW C 1109:

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



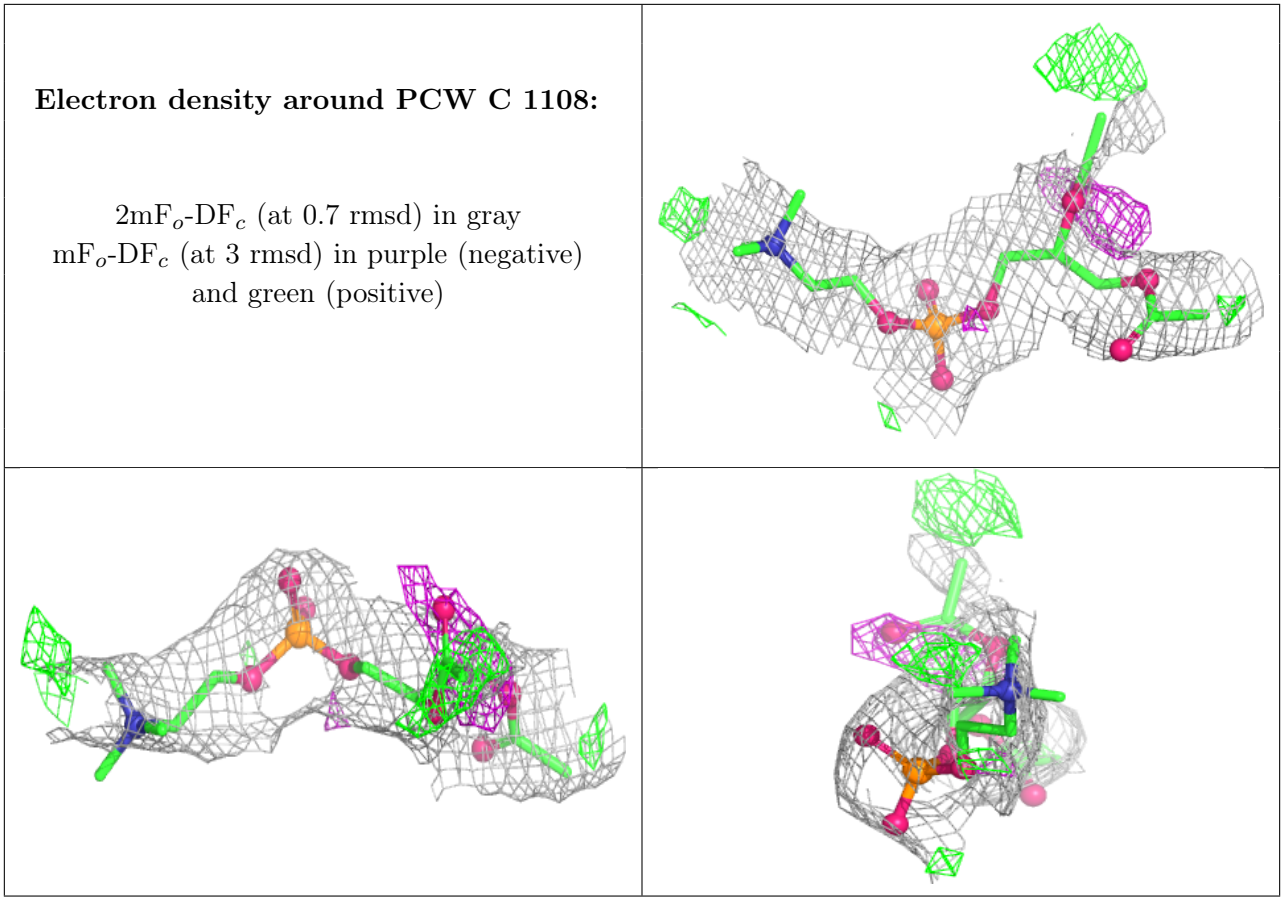
Electron density around PCW C 1107:

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



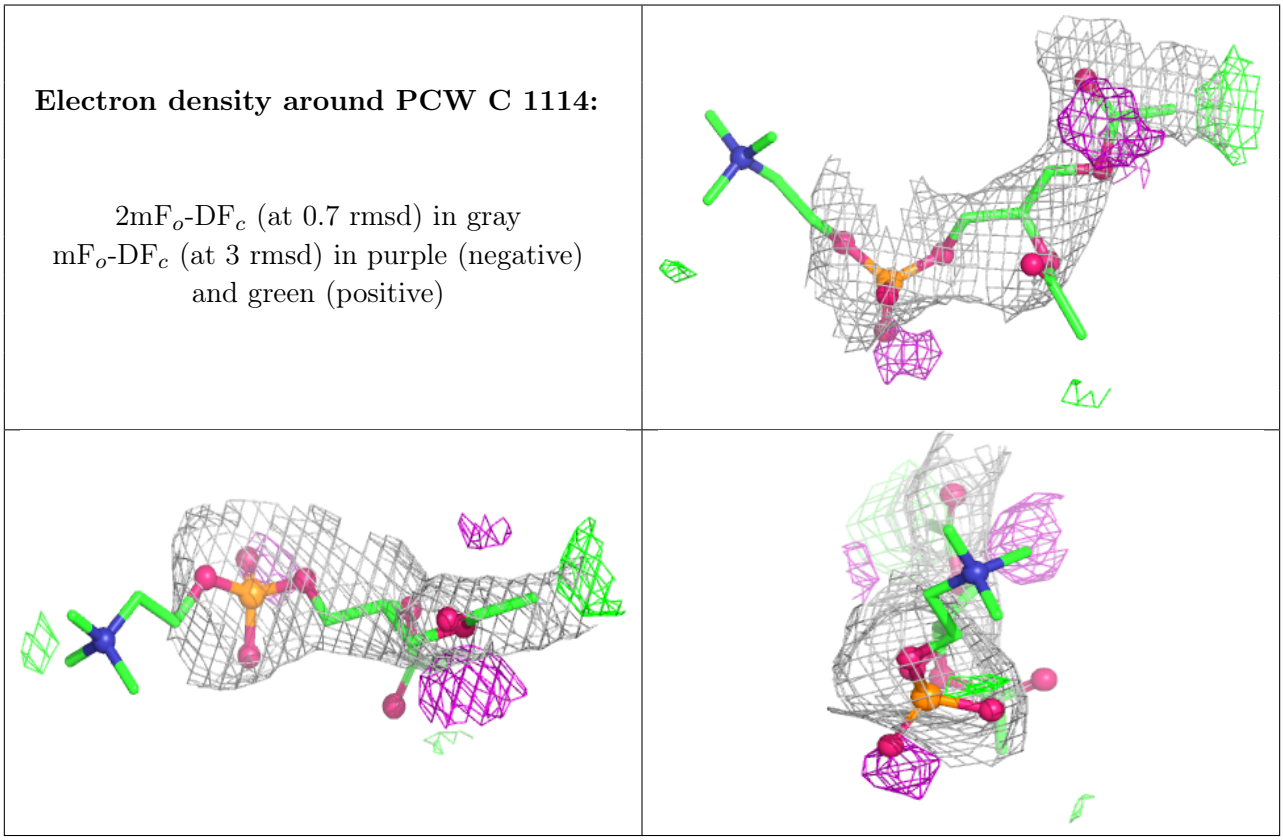
Electron density around PCW C 1108:

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



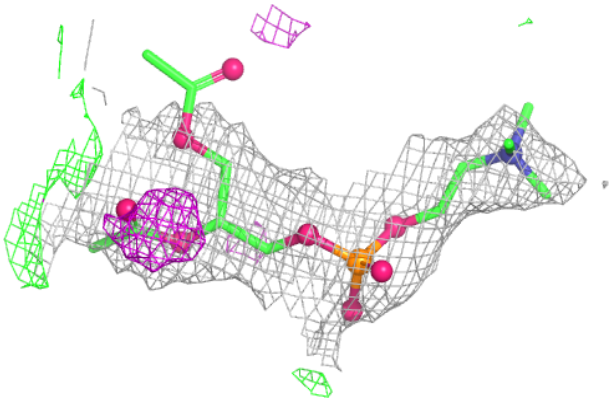
Electron density around PCW C 1114:

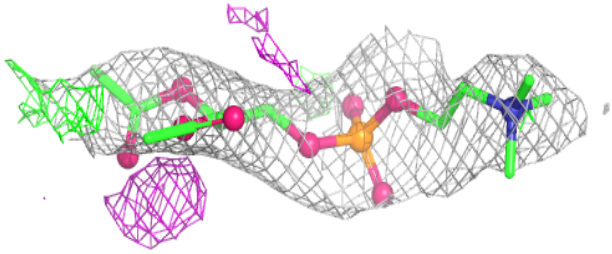
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

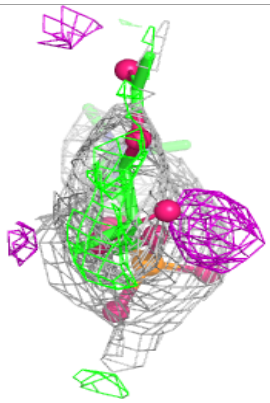


Electron density around PCW A 1114:

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

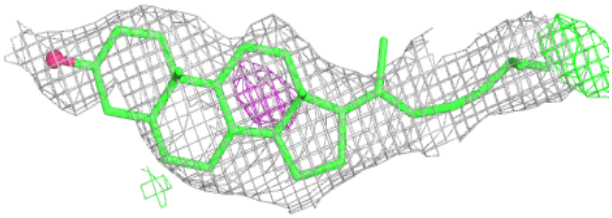


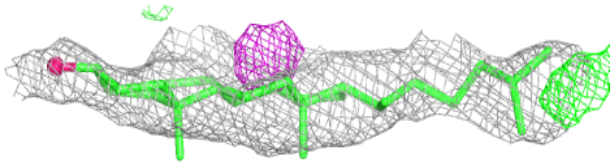


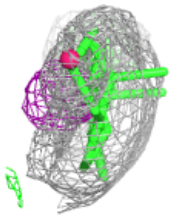


Electron density around CLR D 401:

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

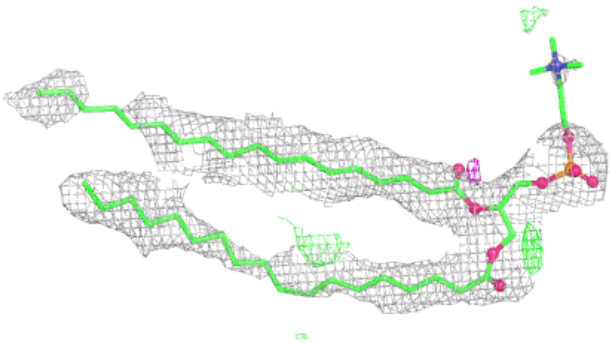


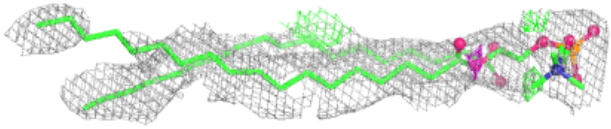


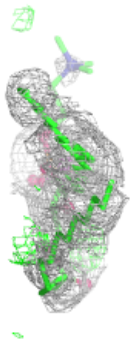


Electron density around PC1 A 1108:

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

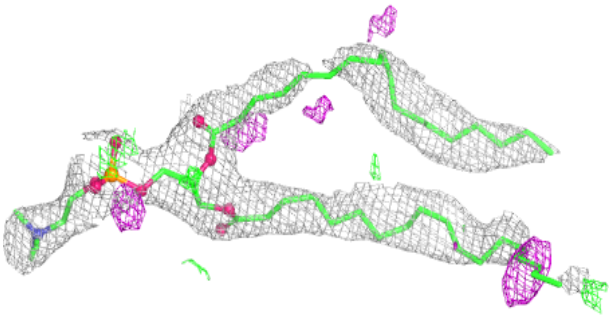


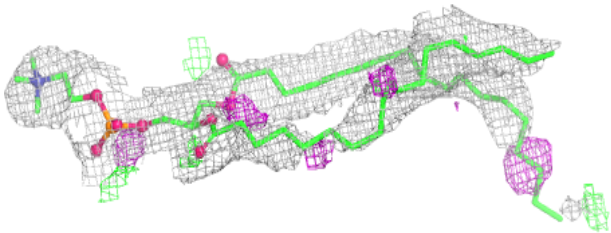


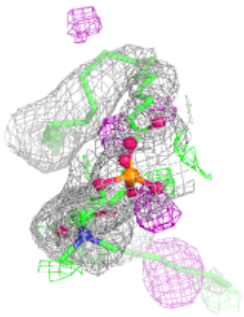


Electron density around PC1 A 1110:

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

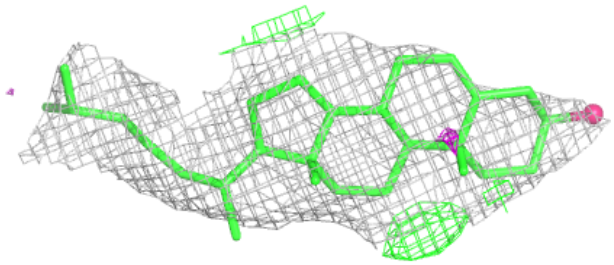


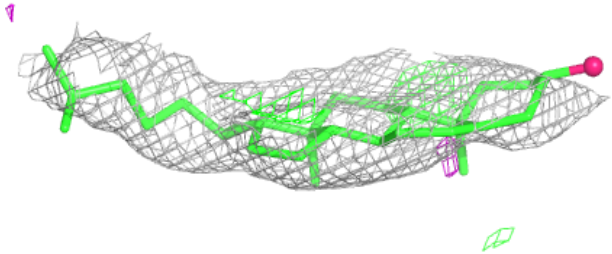


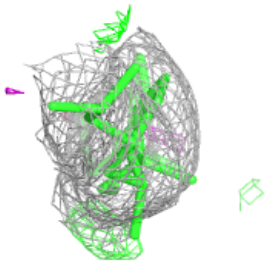


Electron density around CLR B 402:

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

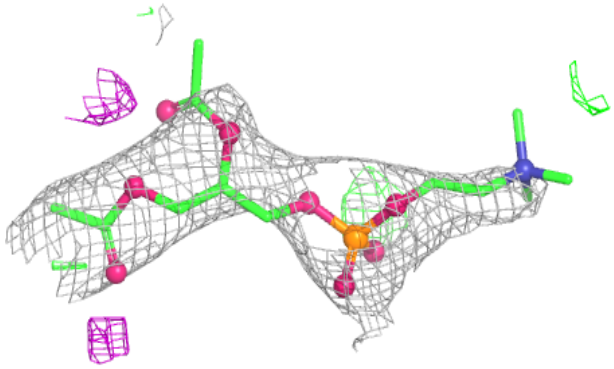


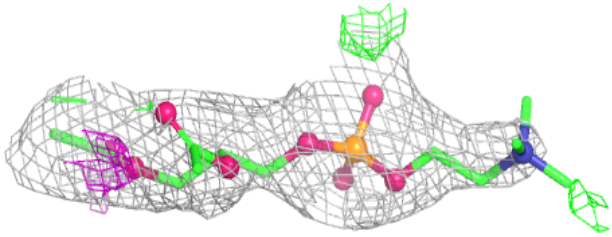


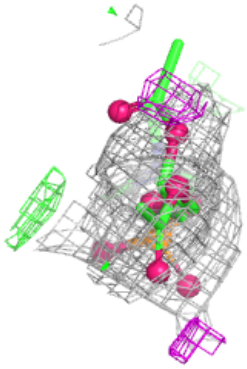


Electron density around PCW A 1112:

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

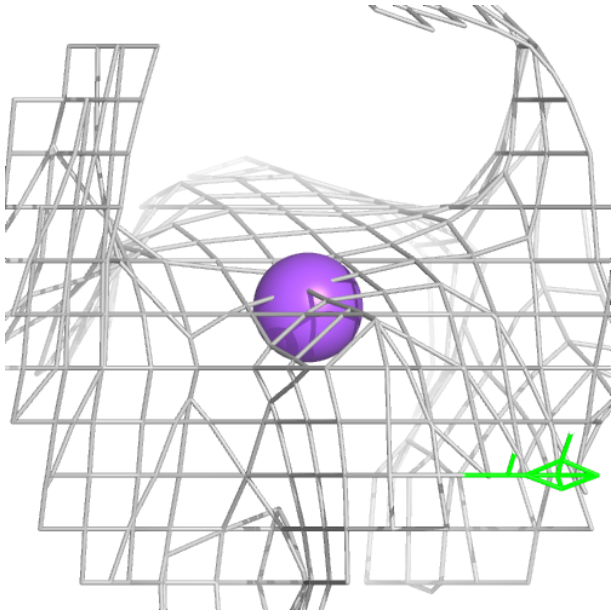


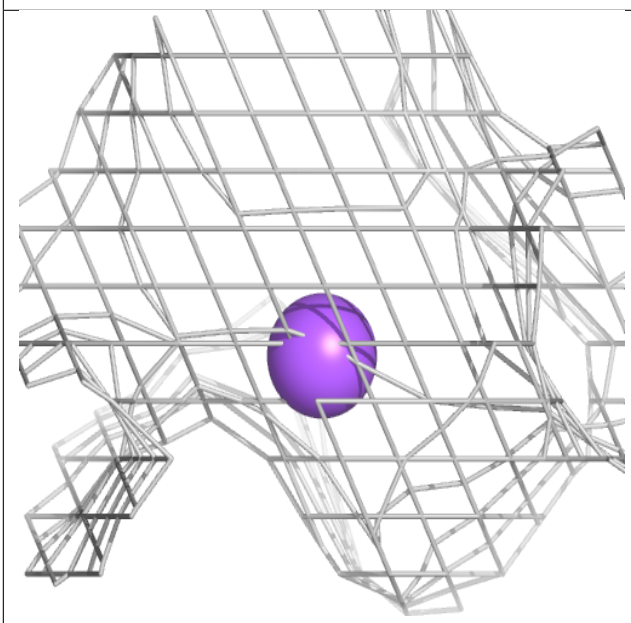


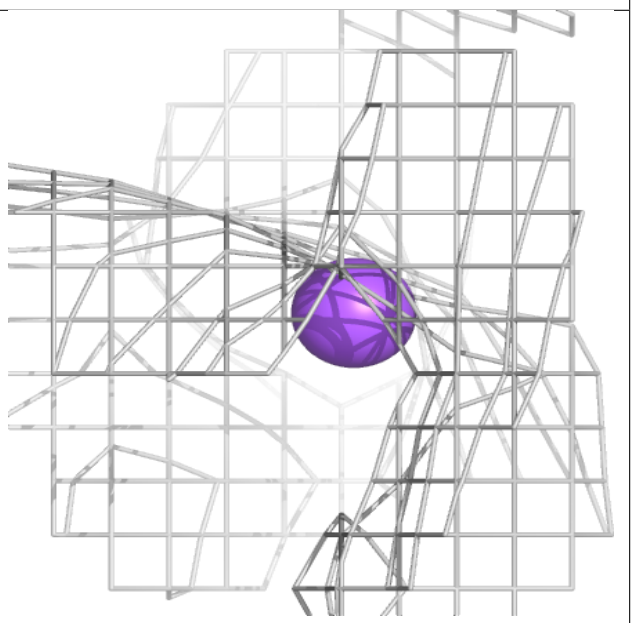


Electron density around NA C 1103:

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

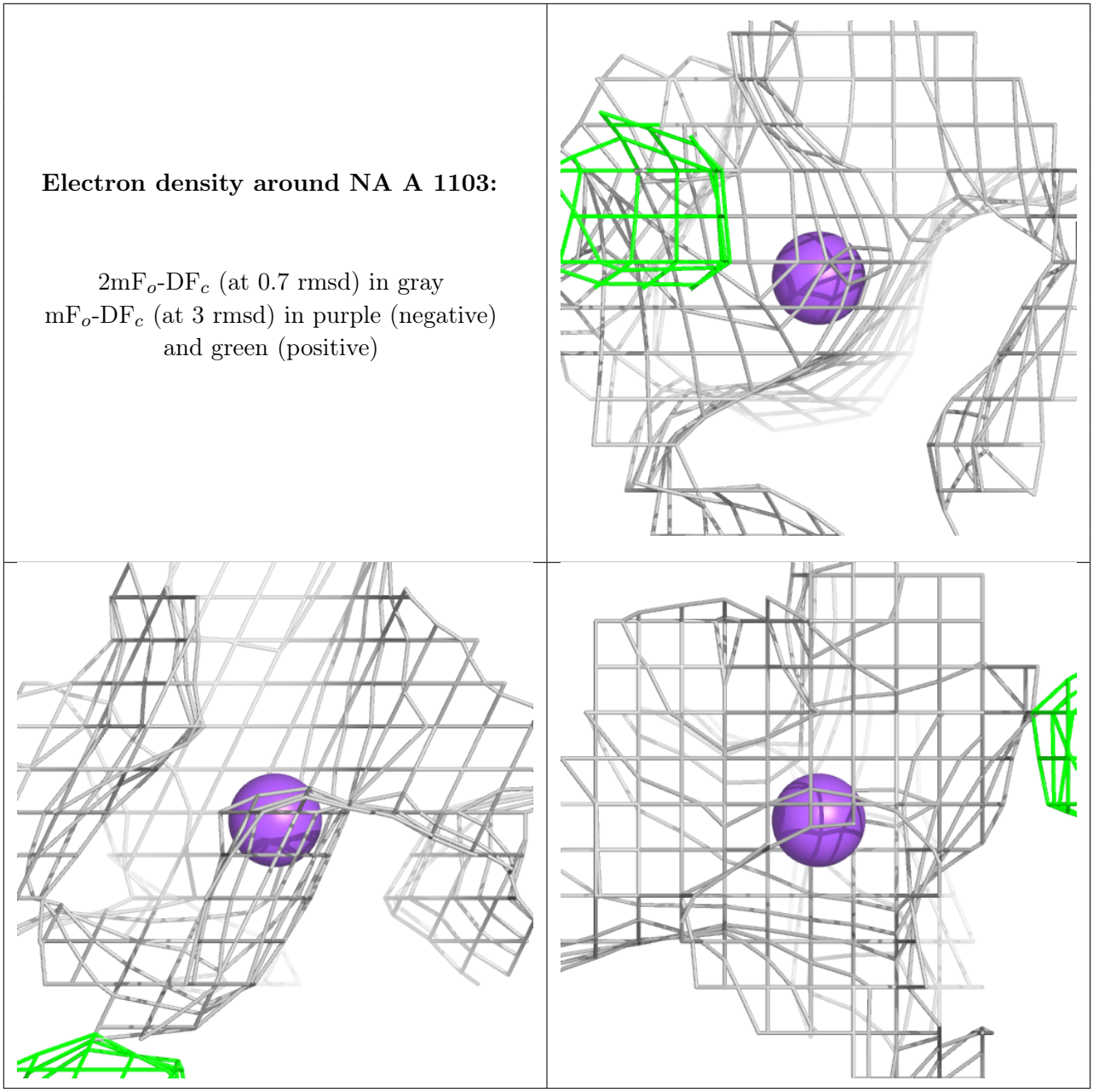






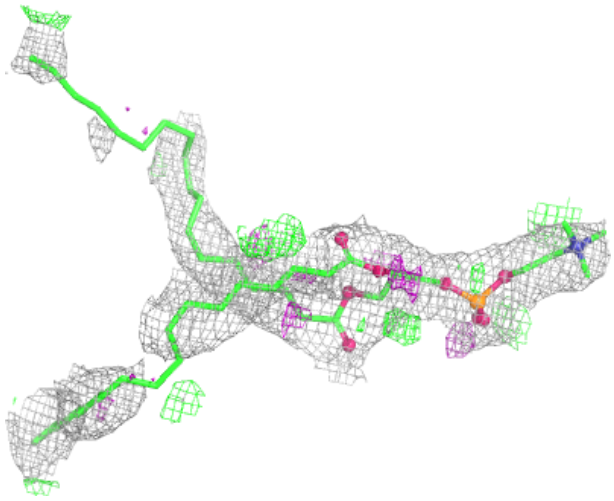
Electron density around NA A 1103:

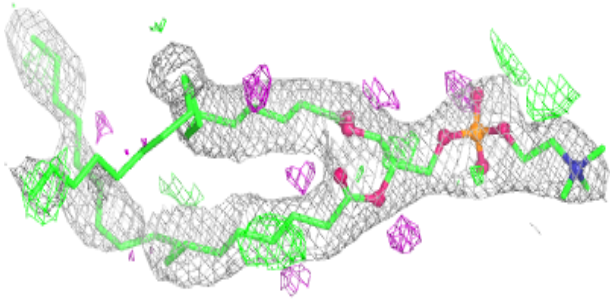
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

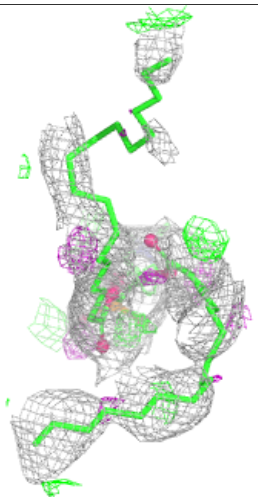


Electron density around PC1 A 1111:

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

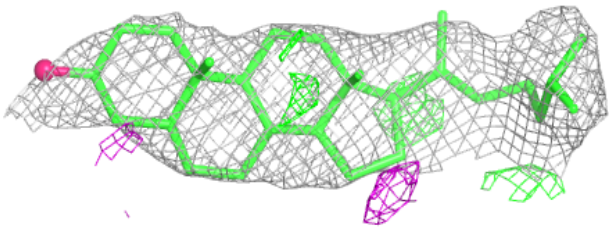


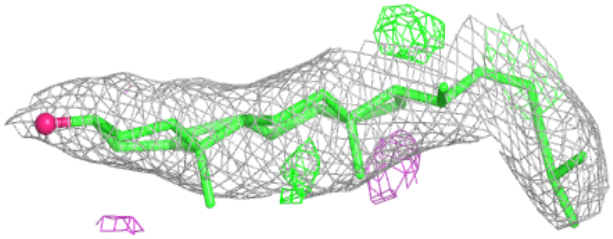


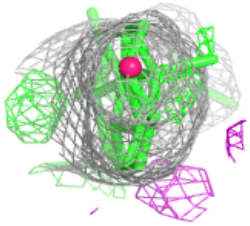


Electron density around CLR A 1106:

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

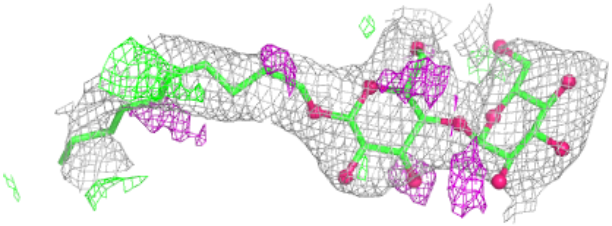


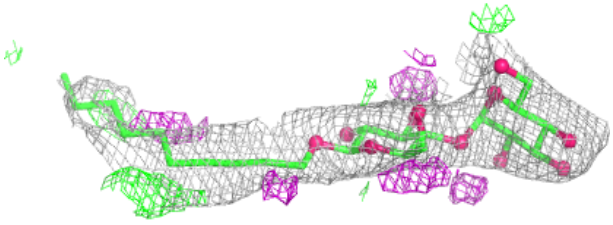


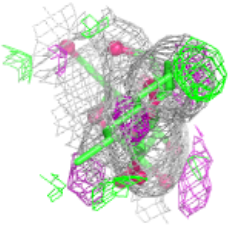


Electron density around DMU E 102:

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

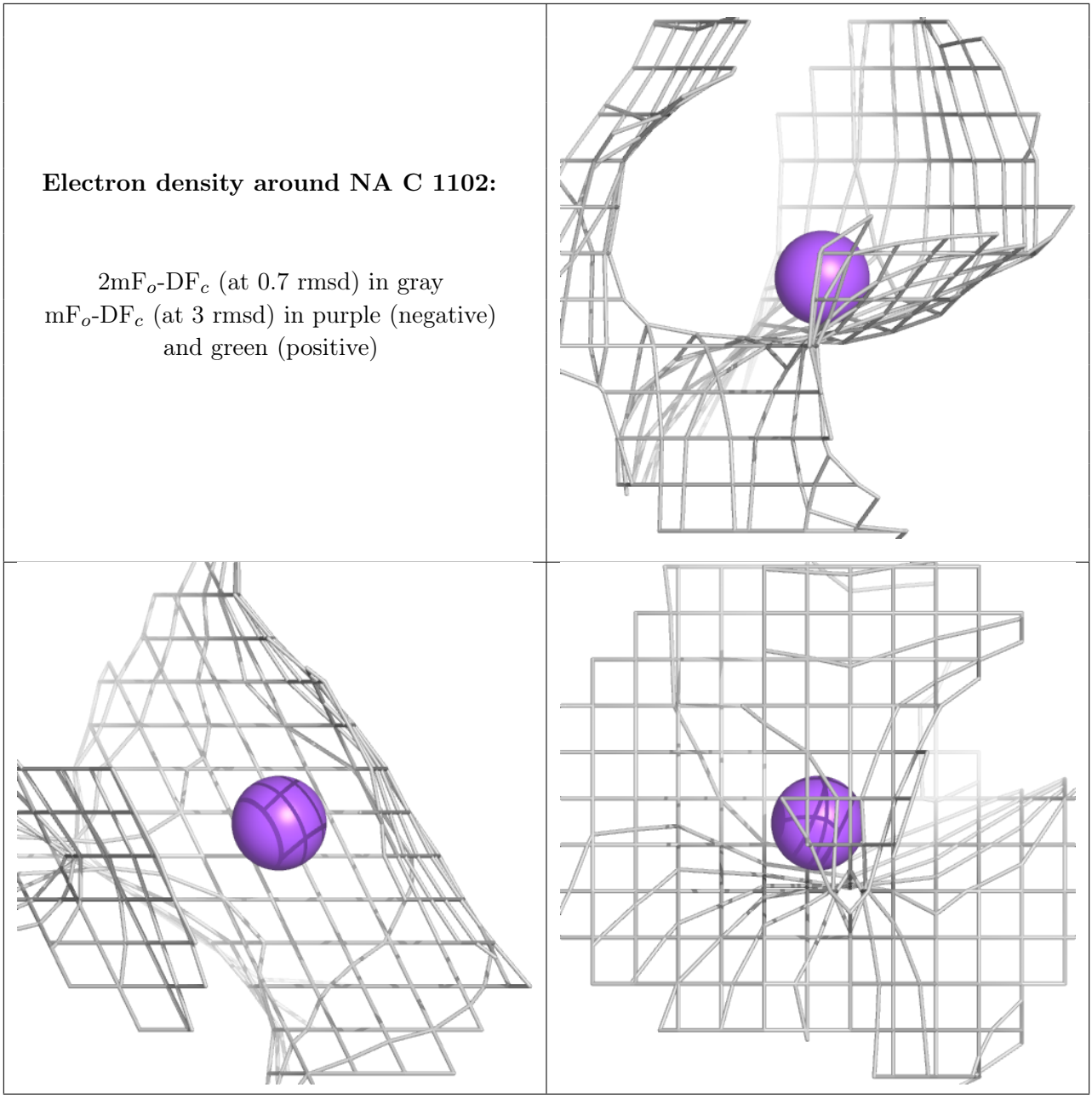






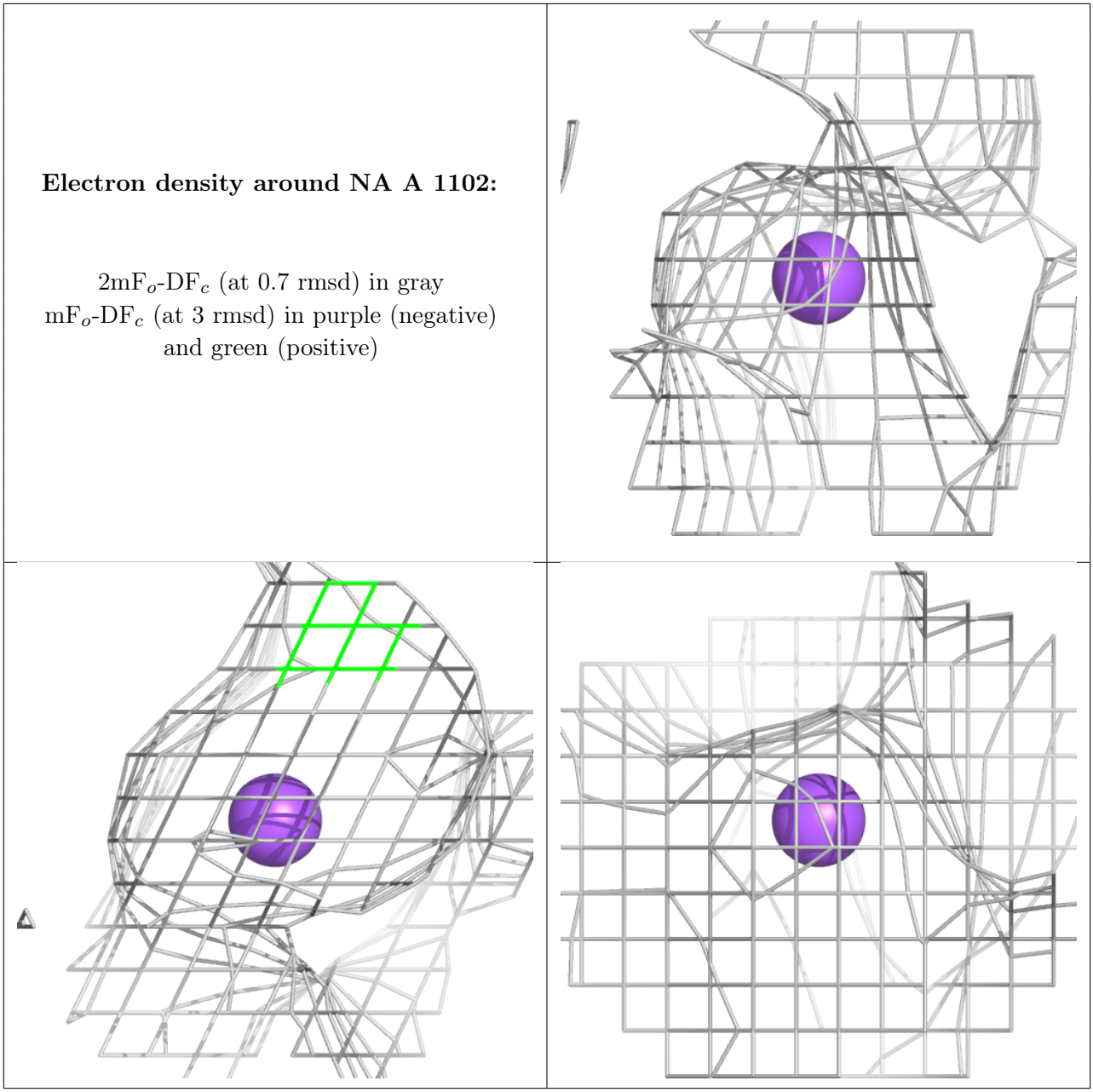
Electron density around NA C 1102:

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



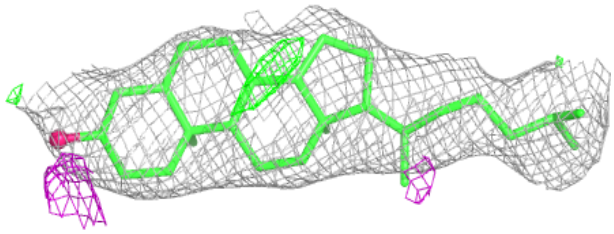
Electron density around NA A 1102:

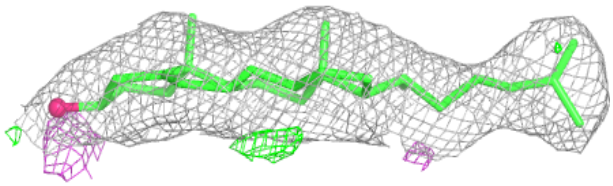
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

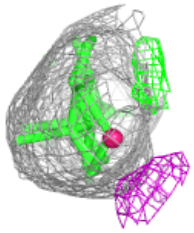


Electron density around CLR A 1107:

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

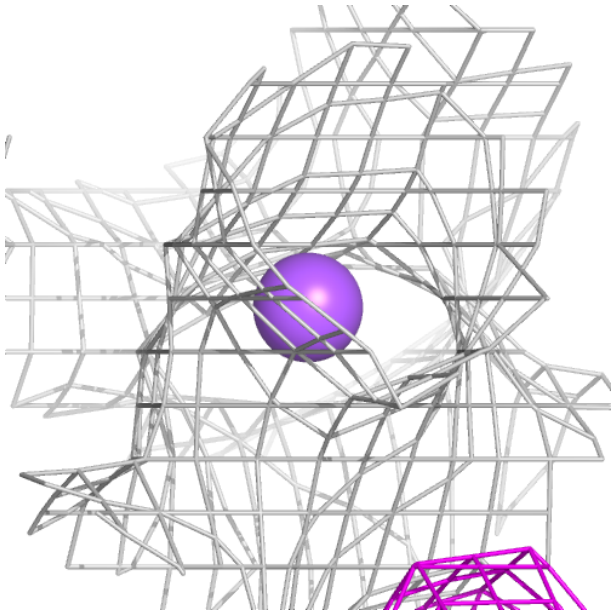


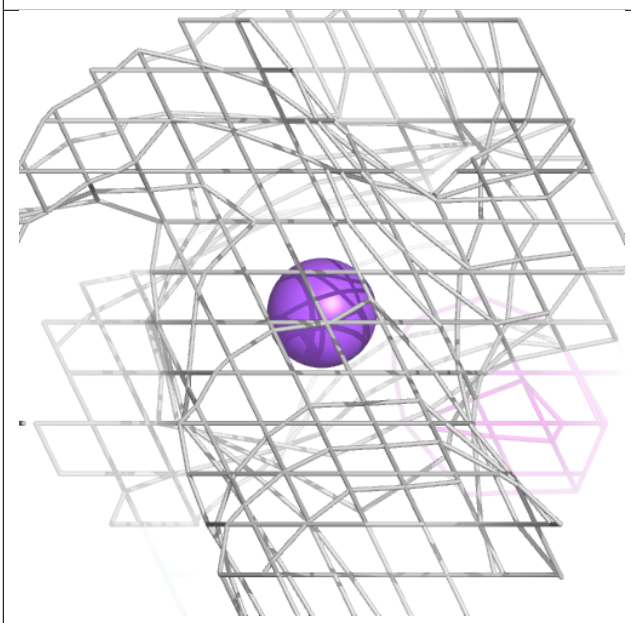


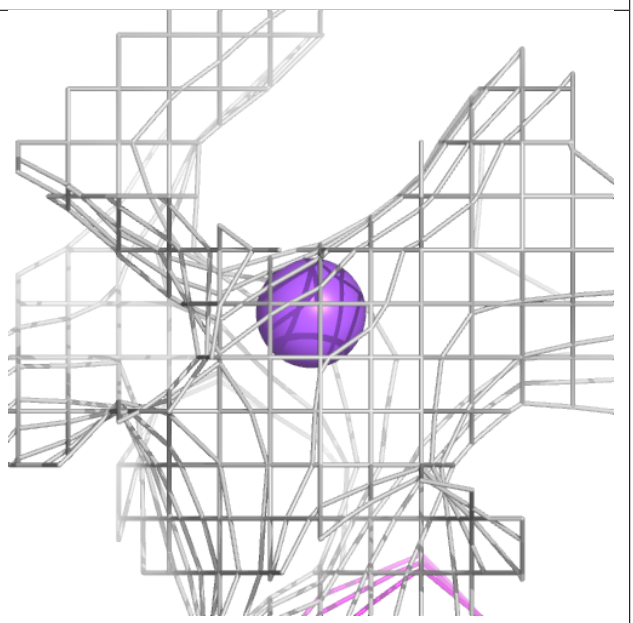


Electron density around NA C 1104:

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

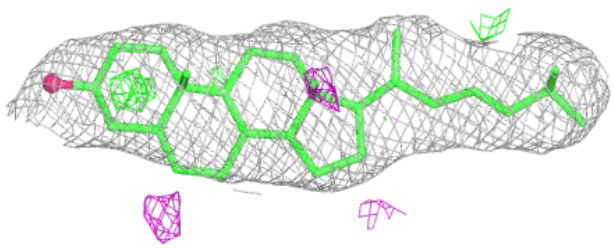


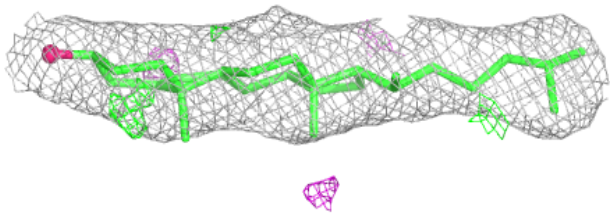


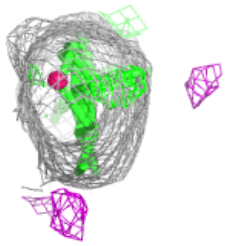


Electron density around CLR E 101:

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

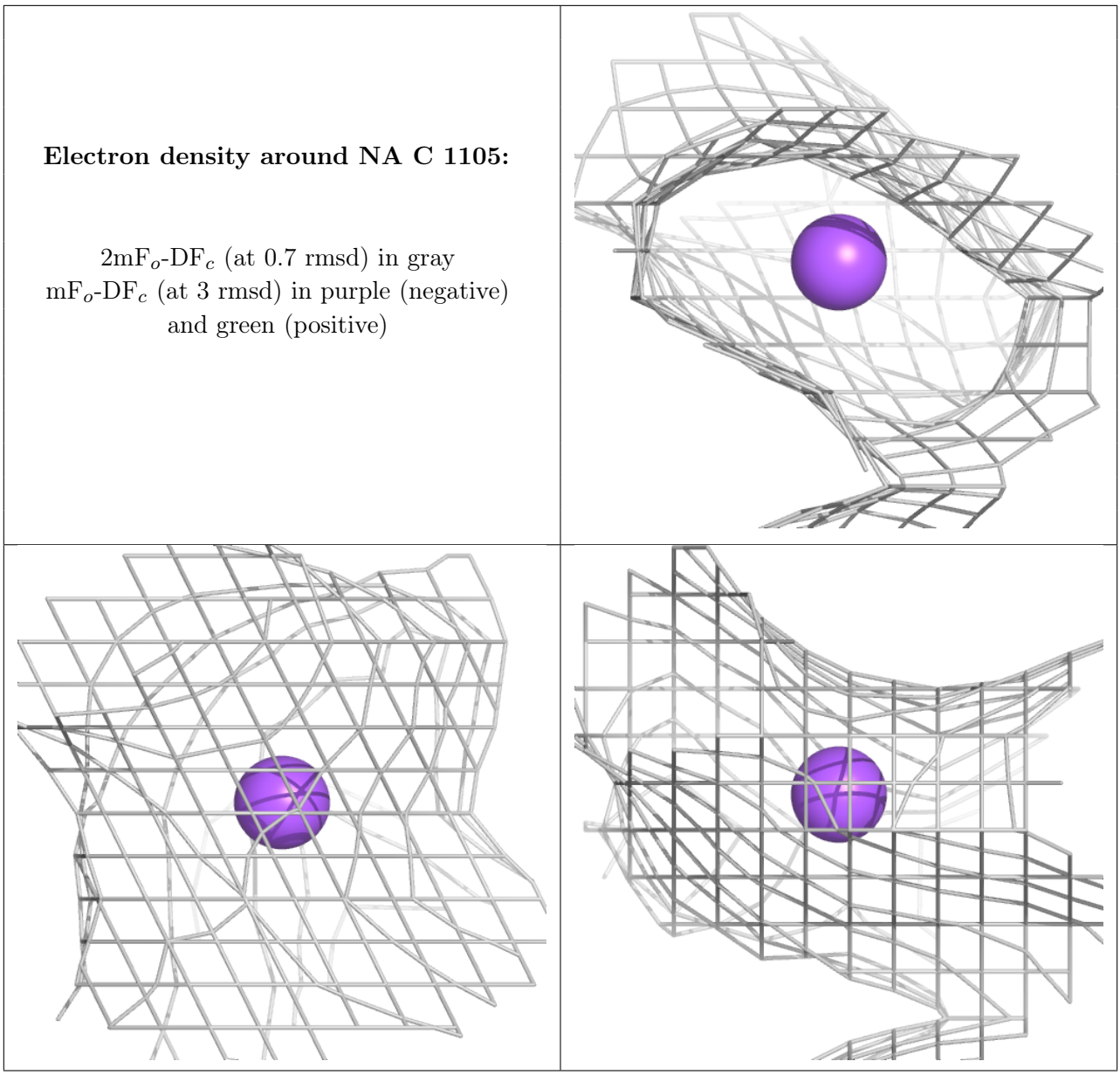






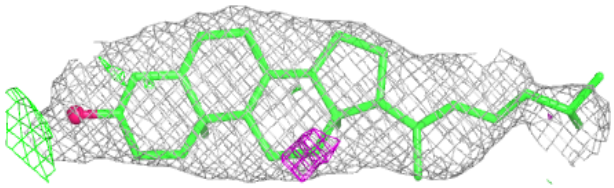
Electron density around NA C 1105:

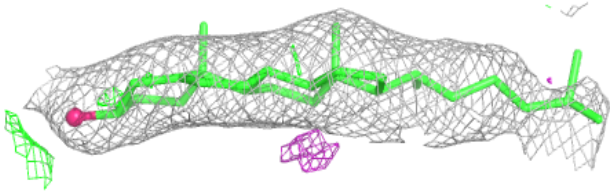
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

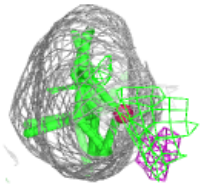


Electron density around CLR C 1106:

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

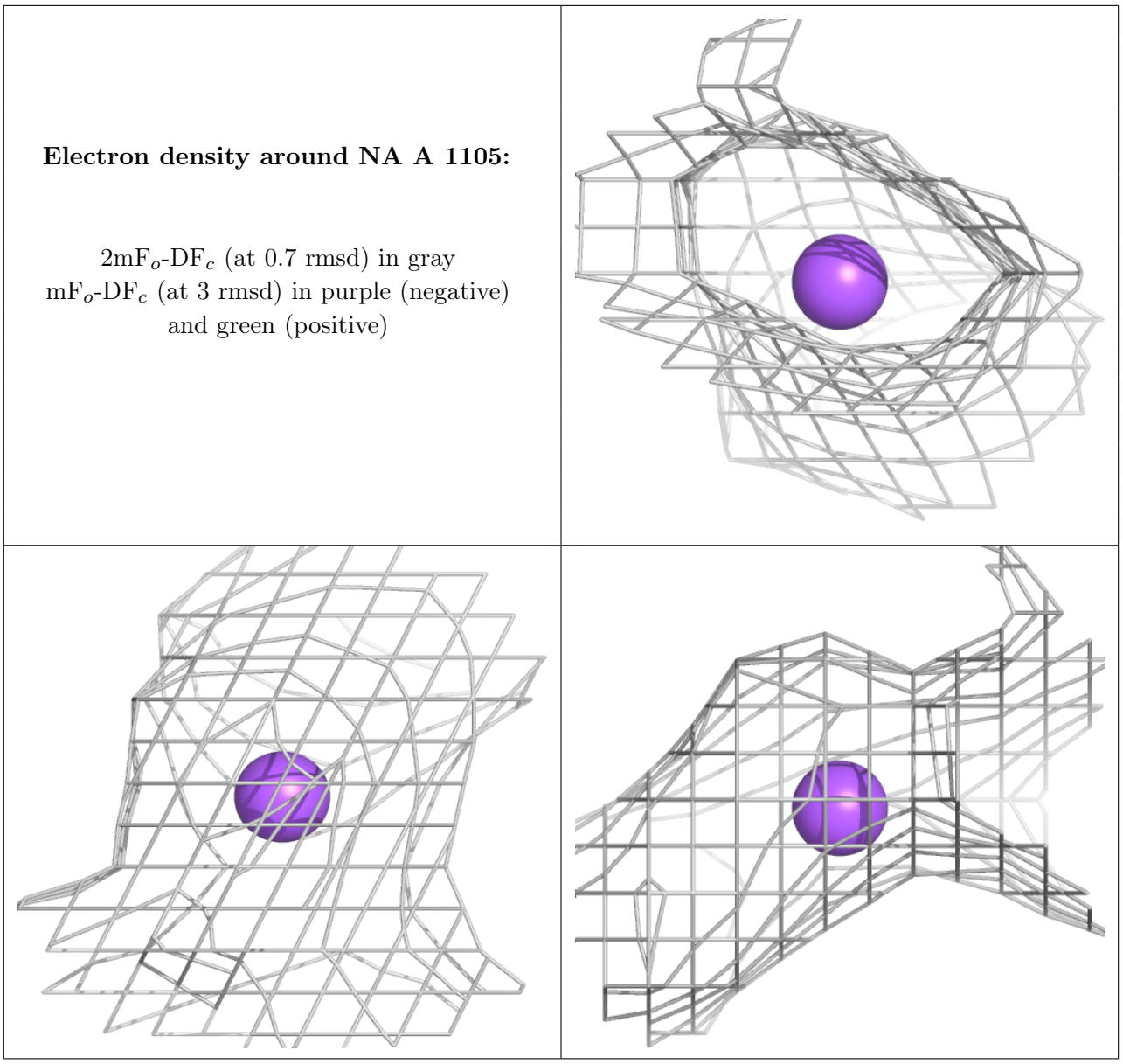






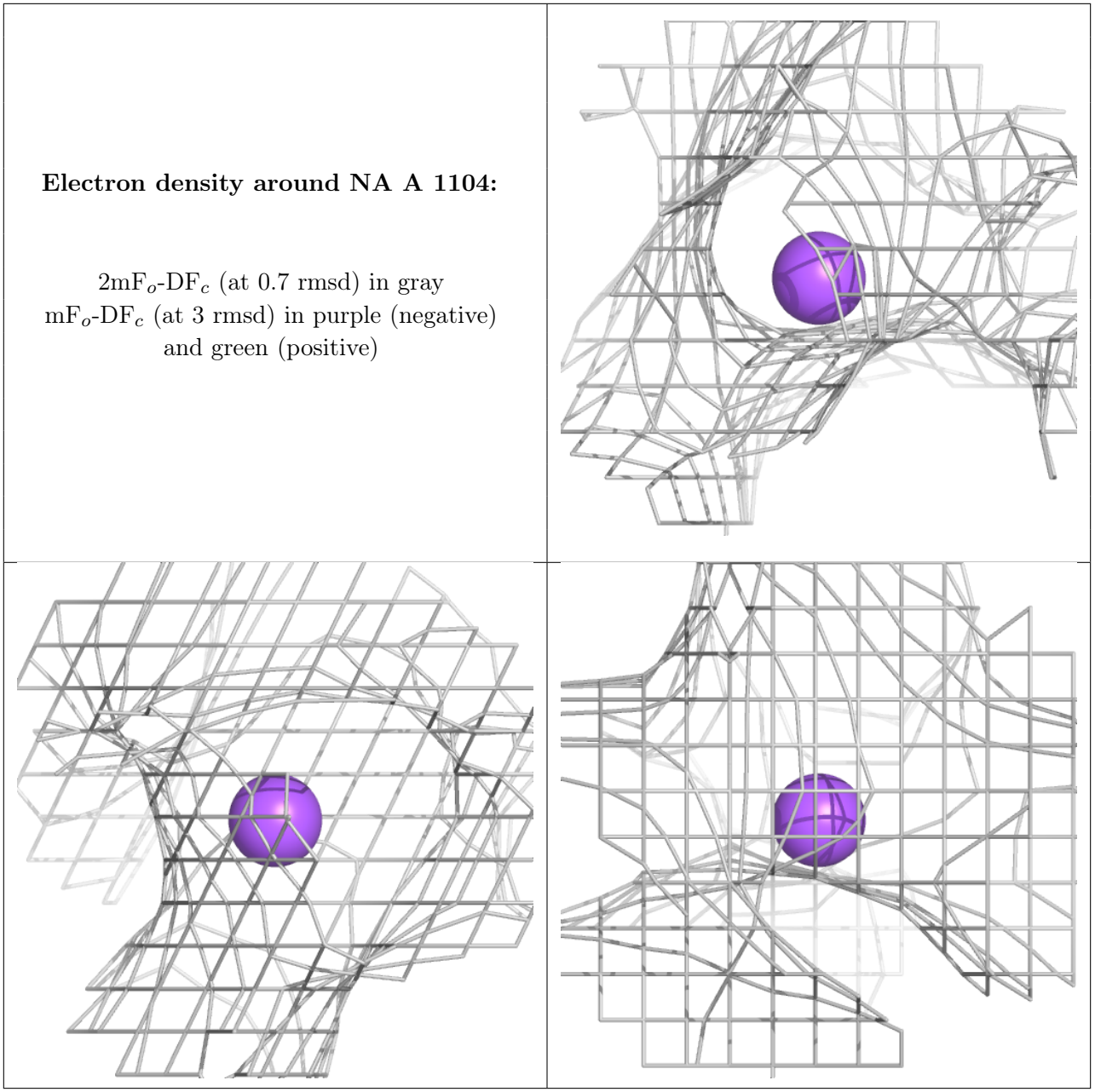
Electron density around NA A 1105:

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



Electron density around NA 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)



6.5 Other polymers (i)

There are no such residues in this entry.