



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 07:51 PM JST

PDB ID : 7DDH
Title : Crystal structures of Na⁺,K⁺-ATPase in complex with digoxin
Authors : Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.
Deposited on : 2020-10-29
Resolution : 3.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

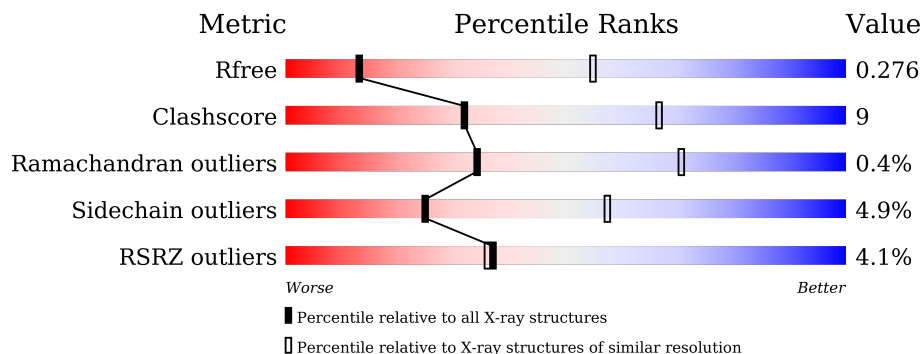
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 Å.

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



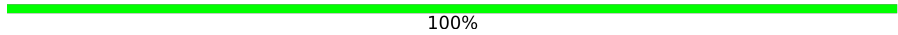



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1016	 4% (poor fit), 75% (0-1 outliers), 21% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
1	C	1016	 3% (poor fit), 75% (0-1 outliers), 21% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
2	B	303	 7% (poor fit), 69% (0-1 outliers), 25% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
2	D	303	 4% (poor fit), 64% (0-1 outliers), 28% (2-3 outliers), 6% (4+ outliers), 0% (not modelled)
3	E	65	 0% (poor fit), 40% (0-1 outliers), 9% (2-3 outliers), 51% (4+ outliers), 0% (not modelled)
3	G	65	 0% (poor fit), 48% (0-1 outliers), 0% (2-3 outliers), 51% (4+ outliers), 0% (not modelled)

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	H	2	 50% 50%
4	I	2	 50% 50%
4	J	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	H	2	-	-	-	X
8	PCW	A	1106	-	-	-	X
8	PCW	A	1107	-	-	-	X
8	PCW	A	1108	-	-	-	X
8	PCW	C	1105	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21344 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	996	7730	4922	1301	1459	1	47	0	0	0
1	C	996	7730	4922	1301	1459	1	47	0	0	0

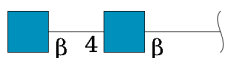
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	291	2386	1546	390	437	13	0	0	0
2	D	285	2334	1514	383	424	13	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	32	255	174	37	44	0	0	0
3	E	32	255	174	37	44	0	0	0

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



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

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

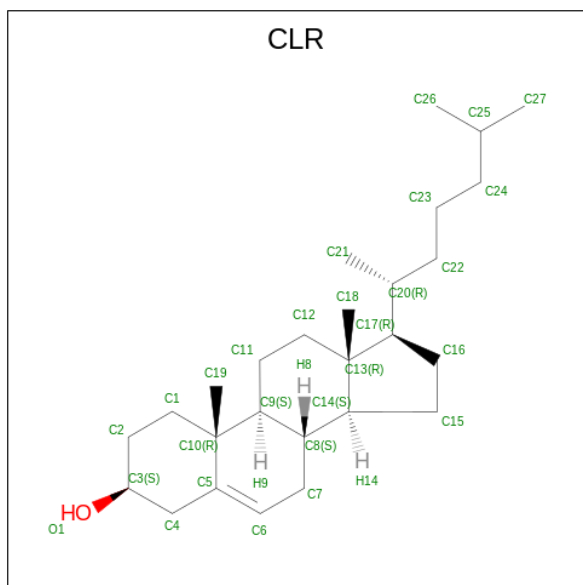
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

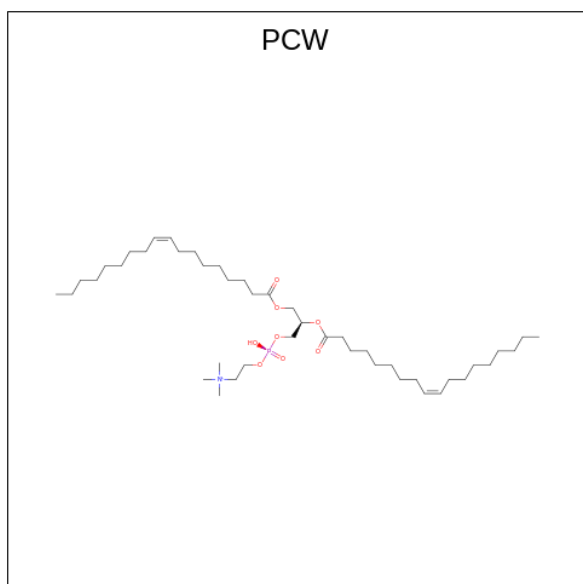
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



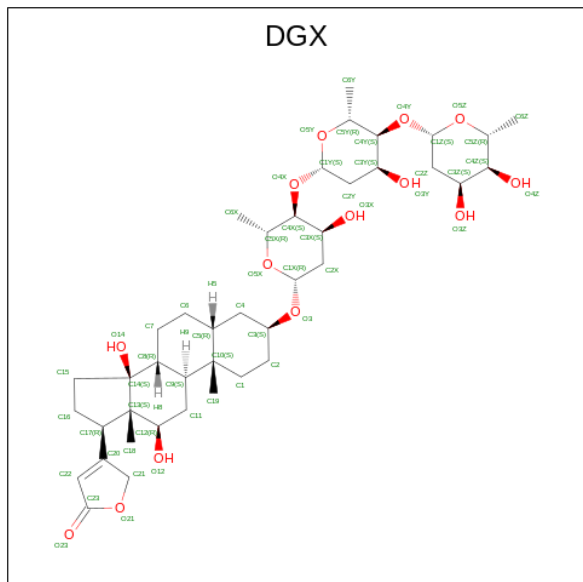
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

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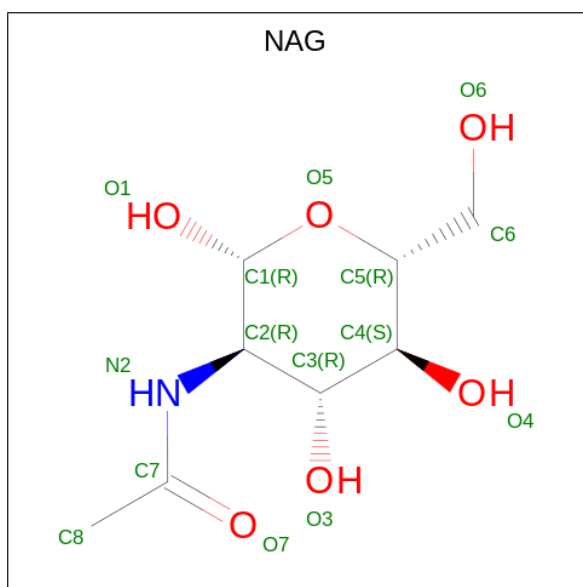
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
8	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 9 is DIGOXIN (three-letter code: DGX) (formula: C₄₁H₆₄O₁₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			55	41	14		
9	C	1	Total	C	O	0	0
			55	41	14		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

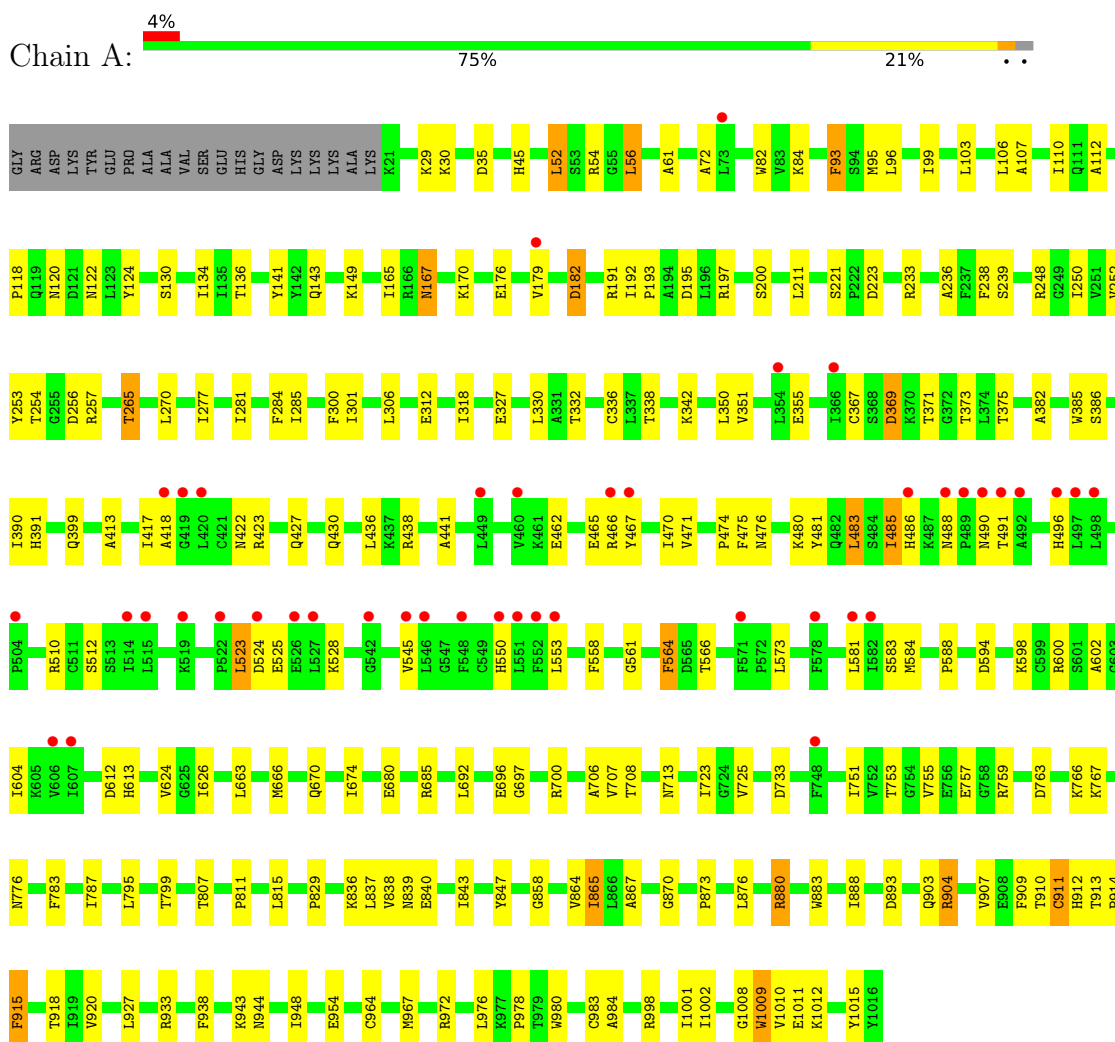
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	5	5	5	0	0
11	C	5	5	5	0	0

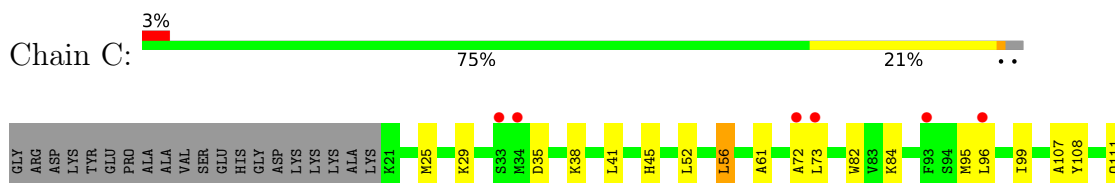
3 Residue-property plots i

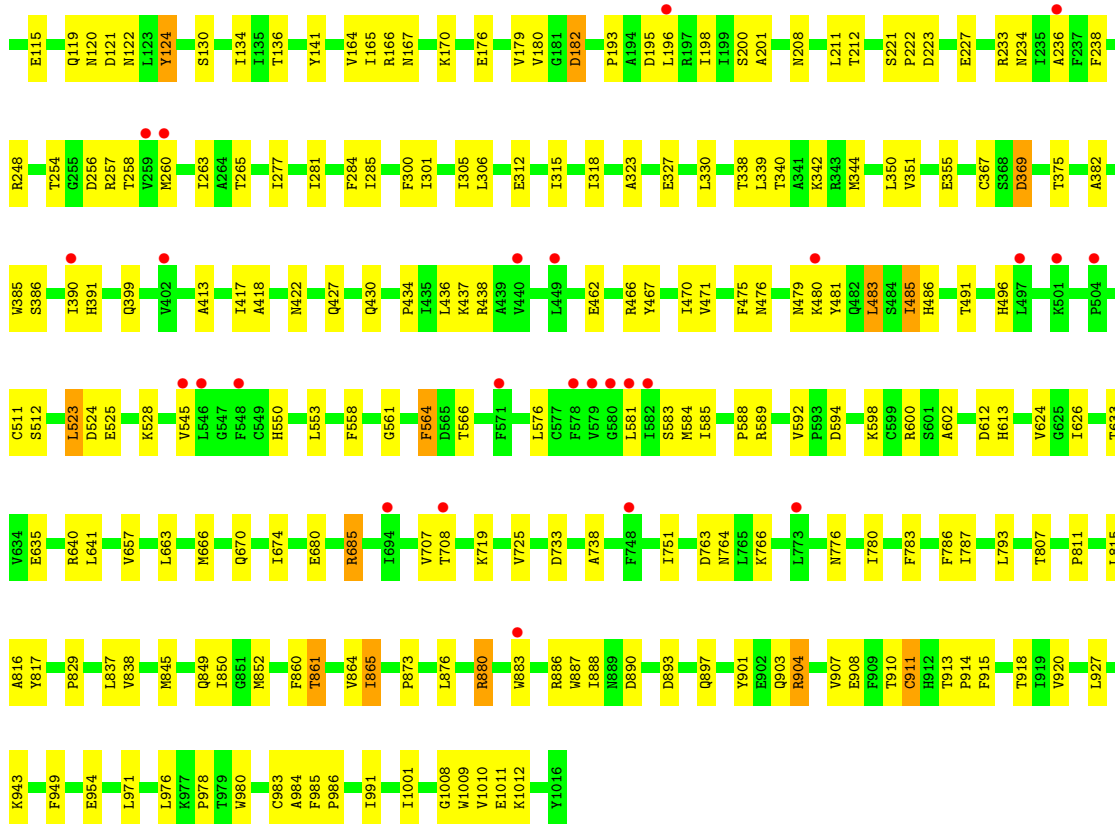
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

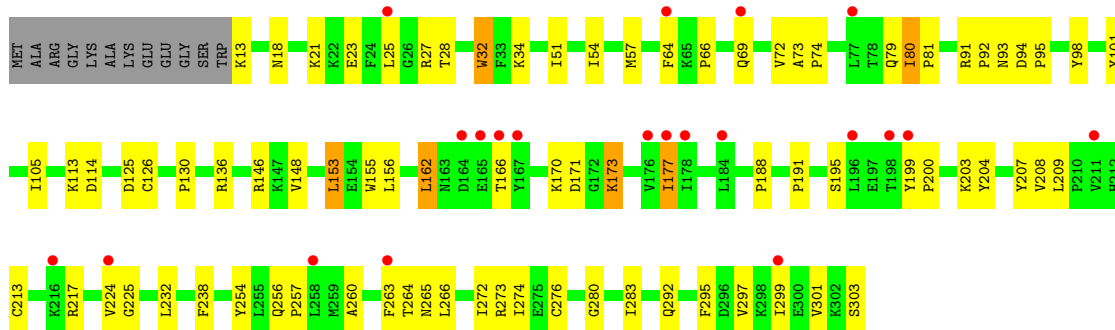


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

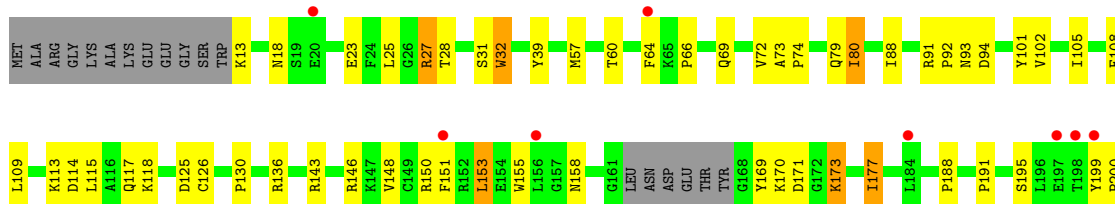


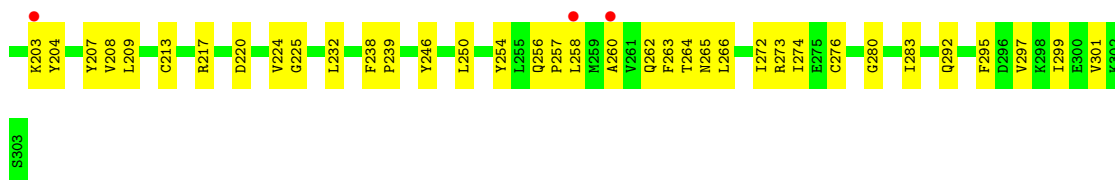


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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





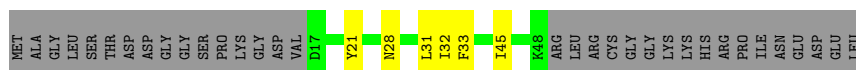
- Molecule 3: FXYD domain-containing ion transport regulator

Chain G: 48% 51%



- Molecule 3: FXYD domain-containing ion transport regulator

Chain E: 40% 9% 51%



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

Chain F: 100%



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

Chain H: 50% 50%



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

Chain I: 50% 50%



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

Chain J: 50% 50%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.97Å 118.49Å 495.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 3.46 49.72 – 3.46	Depositor EDS
% Data completeness (in resolution range)	55.1 (15.99-3.46) 55.5 (49.72-3.46)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.241 , 0.272 0.252 , 0.276	Depositor DCC
R_{free} test set	2477 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	108.1	Xtrriage
Anisotropy	0.321	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.068 for k,h,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21344	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PCW, CLR, DGX, NAG, PHD, NA

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	0.29	0/7867	0.50	0/10674
1	C	0.29	0/7867	0.51	0/10674
2	B	0.29	0/2449	0.54	0/3301
2	D	0.30	0/2395	0.54	0/3225
3	E	0.32	0/261	0.51	0/354
3	G	0.33	0/261	0.47	0/354
All	All	0.29	0/21100	0.51	0/28582

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7730	0	7777	137	0
1	C	7730	0	7777	135	0
2	B	2386	0	2361	49	0
2	D	2334	0	2317	55	0
3	E	255	0	259	6	0
3	G	255	0	259	0	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	28	0	46	2	0
7	B	28	0	46	0	0
7	C	28	0	46	3	0
7	D	28	0	46	1	0
7	E	28	0	46	6	0
7	G	28	0	46	1	0
8	A	110	0	90	9	0
8	B	22	0	18	2	0
8	C	88	0	72	4	0
9	A	55	0	64	1	0
9	C	55	0	64	2	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	5	0	0	0	0
11	C	5	0	0	0	0
All	All	21344	0	21460	380	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 9.

All (380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HG3	1:A:141:TYR:HE1	1.41	0.85
1:C:978:PRO:HB3	7:E:101:CLR:H192	1.62	0.82
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.63	0.81
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.65	0.78
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.66	0.78
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.66	0.78
1:A:375:THR:HA	1:A:588:PRO:HA	1.67	0.76
2:D:204:TYR:HE1	2:D:207:TYR:HB2	1.50	0.76
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.70	0.73
1:A:978:PRO:HB3	7:G:101:CLR:H192	1.70	0.73
1:C:375:THR:HA	1:C:588:PRO:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:H	1:A:233:ARG:HB3	1.54	0.72
1:C:1008:GLY:HA2	1:C:1011:GLU:HB3	1.72	0.72
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.73	0.71
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.70	0.71
1:A:807:THR:HB	1:A:954:GLU:HG3	1.73	0.71
1:A:488:ASN:HD21	1:A:490:ASN:HB2	1.56	0.70
1:A:72:ALA:HB2	1:A:176:GLU:HG2	1.74	0.69
1:C:807:THR:HB	1:C:954:GLU:HG3	1.75	0.68
1:A:496:HIS:HB2	1:A:553:LEU:HB2	1.75	0.68
2:B:13:LYS:HG3	8:B:403:PCW:H72	1.76	0.68
2:D:177:ILE:HA	2:D:260:ALA:HA	1.77	0.67
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.78	0.66
1:A:913:THR:HB	1:A:976:LEU:HD21	1.77	0.66
1:C:96:LEU:HD22	1:C:285:ILE:HG23	1.78	0.66
1:C:221:SER:H	1:C:233:ARG:HB3	1.60	0.65
1:A:978:PRO:HB2	8:C:1107:PCW:H31	1.79	0.65
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.78	0.65
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.78	0.65
1:A:843:ILE:HG23	1:A:847:TYR:HD2	1.62	0.64
2:B:13:LYS:HD2	8:B:403:PCW:H52	1.79	0.64
1:C:165:ILE:HG12	1:C:170:LYS:HG2	1.80	0.64
1:A:1008:GLY:HA2	1:A:1011:GLU:HB3	1.78	0.64
1:C:907:VAL:HA	1:C:910:THR:HG22	1.78	0.64
2:B:204:TYR:HE1	2:B:207:TYR:HB2	1.63	0.64
2:D:102:VAL:HG13	2:D:169:TYR:HD2	1.63	0.63
1:C:120:ASN:O	1:C:124:TYR:HB2	1.98	0.63
1:A:165:ILE:HG12	1:A:170:LYS:HG2	1.82	0.62
1:C:260:MET:HA	1:C:263:ILE:HD12	1.82	0.62
1:A:45:HIS:HB2	1:A:52:LEU:HD11	1.82	0.61
1:A:708:THR:HG22	1:A:725:VAL:HB	1.80	0.61
1:A:907:VAL:HA	1:A:910:THR:HG22	1.83	0.61
1:A:427:GLN:HB2	1:A:430:GLN:HE21	1.66	0.60
2:D:27:ARG:HG3	2:D:32:TRP:CD1	2.36	0.60
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.66	0.60
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.66	0.60
1:C:901:TYR:HA	1:C:904:ARG:HH21	1.66	0.60
1:C:766:LYS:HE2	1:C:837:LEU:HA	1.83	0.60
1:C:907:VAL:O	1:C:911:CYS:HB2	2.00	0.60
2:D:80:ILE:HD11	2:D:177:ILE:H	1.66	0.60
1:A:907:VAL:O	1:A:911:CYS:HB2	2.01	0.60
1:A:512:SER:HA	1:A:523:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:GLN:HB2	1:C:430:GLN:HE21	1.67	0.59
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.85	0.59
1:C:72:ALA:HB2	1:C:176:GLU:HG2	1.84	0.59
1:C:986:PRO:HB3	7:C:1104:CLR:H213	1.85	0.58
1:C:481:TYR:HE2	1:C:483:LEU:HD23	1.68	0.58
1:A:839:ASN:HA	8:A:1106:PCW:H52	1.86	0.58
2:D:191:PRO:HD3	2:D:280:GLY:HA2	1.85	0.58
1:A:385:TRP:HB3	1:A:581:LEU:H	1.69	0.57
1:A:920:VAL:HG13	1:A:954:GLU:HG2	1.84	0.57
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.85	0.57
1:A:56:LEU:HD11	1:A:182:ASP:HB3	1.87	0.57
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.87	0.56
1:A:312:GLU:HG2	9:A:1110:DGX:H6XB	1.86	0.56
2:B:80:ILE:HD11	2:B:177:ILE:H	1.69	0.56
1:A:976:LEU:HB3	1:A:980:TRP:HD1	1.71	0.56
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.86	0.56
1:A:481:TYR:HE2	1:A:483:LEU:HD23	1.70	0.56
2:D:173:LYS:HB3	2:D:262:GLN:HE21	1.71	0.56
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.88	0.56
2:B:225:GLY:HA3	2:B:265:ASN:HB3	1.87	0.55
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.42	0.55
2:B:217:ARG:HH12	2:B:273:ARG:HD2	1.70	0.55
3:E:33:PHE:CE2	7:E:101:CLR:H151	2.41	0.55
2:D:66:PRO:HG2	2:D:69:GLN:HG2	1.89	0.55
2:B:27:ARG:HG3	2:B:32:TRP:CD1	2.41	0.55
1:A:112:ALA:HA	1:A:118:PRO:HG2	1.89	0.55
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.89	0.55
2:D:91:ARG:HG2	2:D:93:ASN:H	1.72	0.54
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.89	0.54
2:B:177:ILE:HA	2:B:260:ALA:HA	1.89	0.54
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.73	0.54
1:C:45:HIS:HB2	1:C:52:LEU:HD11	1.89	0.54
1:C:277:ILE:HG21	1:C:355:GLU:HB2	1.90	0.54
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.91	0.53
1:C:107:ALA:HB2	1:C:318:ILE:HG21	1.90	0.53
1:C:633:THR:HG21	1:C:657:VAL:HG23	1.90	0.53
1:C:111:GLN:HG3	1:C:315:ILE:HD12	1.91	0.53
1:A:462:GLU:HA	1:A:465:GLU:HG2	1.91	0.53
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.90	0.53
1:C:978:PRO:HB3	7:E:101:CLR:C19	2.37	0.53
1:A:200:SER:HB3	1:A:248:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:ARG:O	2:D:146:ARG:NH1	2.42	0.53
1:A:983:CYS:SG	7:A:1104:CLR:H21	2.49	0.53
1:C:382:ALA:HB2	1:C:585:ILE:HG22	1.90	0.53
1:A:903:GLN:HG3	2:B:292:GLN:HE21	1.74	0.52
1:C:385:TRP:HB3	1:C:581:LEU:H	1.74	0.52
1:C:708:THR:HG22	1:C:725:VAL:HB	1.91	0.52
1:C:861:THR:HG23	1:C:983:CYS:HB2	1.92	0.52
2:B:66:PRO:HG2	2:B:69:GLN:HG2	1.91	0.52
1:C:512:SER:HA	1:C:523:LEU:HD23	1.90	0.52
1:C:640:ARG:HH21	1:C:641:LEU:HD11	1.74	0.52
1:C:385:TRP:HD1	1:C:390:ILE:HD13	1.73	0.52
1:C:594:ASP:O	1:C:598:LYS:HG2	2.09	0.52
2:D:130:PRO:HB3	2:D:239:PRO:HB3	1.91	0.52
2:D:225:GLY:HA3	2:D:265:ASN:HB3	1.91	0.52
1:A:93:PHE:HB3	1:A:330:LEU:HD13	1.92	0.52
1:A:300:PHE:HD2	1:A:301:ILE:HD12	1.75	0.52
1:C:470:ILE:HB	1:C:485:ILE:HG23	1.92	0.52
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.91	0.52
2:D:224:VAL:HG21	2:D:274:ILE:HD11	1.92	0.52
1:A:594:ASP:O	1:A:598:LYS:HG2	2.10	0.51
1:C:558:PHE:HB3	1:C:564:PHE:HE2	1.74	0.51
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.93	0.51
1:C:903:GLN:HG3	2:D:292:GLN:HE21	1.75	0.51
1:C:300:PHE:HD2	1:C:301:ILE:HD12	1.75	0.51
1:C:888:ILE:O	1:C:904:ARG:NH2	2.43	0.51
2:B:136:ARG:O	2:B:146:ARG:NH1	2.44	0.51
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.93	0.51
1:C:312:GLU:HG2	9:C:1121:DGX:H6XB	1.92	0.51
1:C:883:TRP:CE2	1:C:904:ARG:HG3	2.46	0.51
2:D:224:VAL:HG22	2:D:272:ILE:HD12	1.92	0.50
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.92	0.50
1:C:84:LYS:HG3	1:C:141:TYR:HE1	1.76	0.50
1:C:340:THR:O	1:C:344:MET:HG2	2.12	0.50
1:A:182:ASP:OD1	1:A:182:ASP:N	2.44	0.50
1:A:475:PHE:HB2	1:A:480:LYS:HG3	1.93	0.50
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.47	0.50
1:A:427:GLN:HE21	1:A:441:ALA:HB2	1.77	0.50
2:D:213:CYS:HA	2:D:276:CYS:HA	1.94	0.50
1:C:475:PHE:HB2	1:C:480:LYS:HG3	1.92	0.50
1:A:943:LYS:NZ	8:A:1109:PCW:H52	2.26	0.50
2:B:101:TYR:O	2:B:105:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:VAL:HG21	2:B:274:ILE:HD11	1.93	0.50
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.76	0.50
1:A:470:ILE:HB	1:A:485:ILE:HG23	1.93	0.50
1:A:783:PHE:O	1:A:787:ILE:HG12	2.12	0.50
1:A:413:ALA:O	1:A:417:ILE:HG12	2.12	0.49
1:A:670:GLN:O	1:A:674:ILE:HG13	2.13	0.49
1:A:766:LYS:HE2	1:A:837:LEU:HA	1.93	0.49
1:A:120:ASN:O	1:A:124:TYR:HB2	2.12	0.49
1:A:602:ALA:HB1	1:A:759:ARG:HH22	1.77	0.49
1:C:200:SER:HB3	1:C:248:ARG:HB2	1.93	0.49
1:C:418:ALA:O	1:C:422:ASN:ND2	2.45	0.49
1:C:182:ASP:N	1:C:182:ASP:OD1	2.45	0.49
1:A:143:GLN:NE2	8:A:1105:PCW:O1P	2.43	0.49
2:D:217:ARG:NH1	2:D:220:ASP:OD2	2.46	0.49
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.95	0.49
1:A:382:ALA:H	1:A:584:MET:HA	1.78	0.49
1:C:195:ASP:OD1	1:C:238:PHE:N	2.45	0.49
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.78	0.49
1:A:467:TYR:HB3	1:A:486:HIS:HB3	1.95	0.48
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.95	0.48
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.48	0.48
1:C:612:ASP:OD1	1:C:613:HIS:N	2.46	0.48
1:A:836:LYS:HB2	8:A:1106:PCW:H83	1.94	0.48
1:C:338:THR:O	1:C:342:LYS:HG2	2.14	0.48
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.95	0.48
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.95	0.48
1:A:918:THR:HG23	1:A:984:ALA:HB2	1.94	0.48
2:B:91:ARG:HG2	2:B:93:ASN:H	1.77	0.48
1:A:545:VAL:HA	1:A:583:SER:HA	1.95	0.48
2:D:280:GLY:HA3	2:D:283:ILE:HD13	1.94	0.48
1:C:976:LEU:HB3	1:C:980:TRP:HD1	1.79	0.48
2:D:217:ARG:HH12	2:D:273:ARG:HD2	1.78	0.48
1:A:369:PHD:OP1	1:A:371:THR:N	2.44	0.48
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.96	0.48
2:B:191:PRO:HD3	2:B:280:GLY:HA2	1.95	0.48
2:B:213:CYS:HA	2:B:276:CYS:HA	1.95	0.48
1:C:61:ALA:O	1:C:179:VAL:HG11	2.14	0.48
1:A:84:LYS:HG3	1:A:141:TYR:CE1	2.33	0.48
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.96	0.48
1:A:558:PHE:HB3	1:A:564:PHE:HE2	1.79	0.48
1:C:890:ASP:N	1:C:890:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.95	0.48
2:D:101:TYR:O	2:D:105:ILE:HG12	2.13	0.48
1:A:462:GLU:O	1:A:466:ARG:HB2	2.14	0.47
1:A:149:LYS:HB3	8:A:1108:PCW:H63	1.95	0.47
2:D:130:PRO:HD3	2:D:232:LEU:HD12	1.95	0.47
1:A:192:ILE:HG21	1:A:236:ALA:HB1	1.96	0.47
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.95	0.47
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.96	0.47
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.97	0.47
2:B:263:PHE:HB3	2:B:266:LEU:HD21	1.97	0.47
2:D:18:ASN:HA	2:D:23:GLU:O	2.14	0.47
1:C:382:ALA:H	1:C:584:MET:HA	1.80	0.47
1:C:670:GLN:O	1:C:674:ILE:HG13	2.15	0.47
1:C:786:PHE:CZ	1:C:880:ARG:HD2	2.50	0.47
2:D:27:ARG:NH1	2:D:31:SER:OG	2.48	0.47
1:A:836:LYS:HG3	8:A:1106:PCW:H72	1.97	0.47
2:B:80:ILE:HB	2:B:105:ILE:HD12	1.97	0.47
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.96	0.47
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.97	0.46
1:C:417:ILE:HD12	1:C:550:HIS:HB3	1.96	0.46
2:D:263:PHE:HB3	2:D:266:LEU:HD21	1.97	0.46
1:A:107:ALA:HB2	1:A:318:ILE:HG21	1.98	0.46
2:B:156:LEU:HD13	2:B:260:ALA:HB2	1.97	0.46
1:C:108:TYR:HA	1:C:111:GLN:HE21	1.80	0.46
2:D:266:LEU:HD22	2:D:272:ILE:HD11	1.97	0.46
1:A:61:ALA:O	1:A:179:VAL:HG11	2.16	0.46
1:A:130:SER:O	1:A:134:ILE:HG12	2.16	0.46
1:A:418:ALA:O	1:A:422:ASN:ND2	2.49	0.46
2:B:173:LYS:HG3	2:B:264:THR:O	2.16	0.46
1:C:130:SER:O	1:C:134:ILE:HG12	2.16	0.46
1:C:764:ASN:HB3	1:C:816:ALA:HA	1.98	0.46
1:A:254:THR:HG23	1:A:257:ARG:HH21	1.80	0.46
1:A:417:ILE:HD12	1:A:550:HIS:HB3	1.98	0.46
1:C:413:ALA:O	1:C:417:ILE:HG12	2.16	0.46
1:A:149:LYS:HD3	1:A:149:LYS:HA	1.79	0.46
1:A:338:THR:O	1:A:342:LYS:HG2	2.16	0.46
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.97	0.46
2:B:92:PRO:HD2	2:B:303:SER:HA	1.98	0.46
2:B:266:LEU:HD22	2:B:272:ILE:HD11	1.98	0.46
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.97	0.46
1:C:1008:GLY:O	1:C:1012:LYS:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG21	1:A:564:PHE:O	2.16	0.45
1:A:1002:ILE:HD13	1:A:1015:TYR:HB2	1.98	0.45
1:A:1009:TRP:HZ2	2:B:34:LYS:HB3	1.81	0.45
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.98	0.45
1:A:663:LEU:HA	1:A:666:MET:HG3	1.98	0.45
1:C:56:LEU:HD11	1:C:182:ASP:HB3	1.98	0.45
1:C:136:THR:HG21	1:C:330:LEU:HG	1.97	0.45
1:C:545:VAL:HG11	1:C:581:LEU:HD13	1.98	0.45
1:C:920:VAL:HG13	1:C:954:GLU:HG2	1.98	0.45
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.98	0.45
2:B:27:ARG:HG3	2:B:32:TRP:HD1	1.81	0.45
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.82	0.45
1:A:481:TYR:CE2	1:A:483:LEU:HD23	2.50	0.45
1:A:706:ALA:HA	1:A:723:ILE:O	2.17	0.45
1:C:254:THR:HG23	1:C:257:ARG:HH21	1.82	0.45
1:C:865:ILE:HD12	1:C:914:PRO:HG3	1.99	0.45
2:D:204:TYR:O	2:D:208:VAL:HG12	2.17	0.45
1:A:888:ILE:O	1:A:904:ARG:NH2	2.50	0.45
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.98	0.44
2:B:204:TYR:O	2:B:208:VAL:HG12	2.17	0.44
3:E:28:ASN:O	3:E:32:ILE:HG12	2.17	0.44
1:A:195:ASP:OD1	1:A:238:PHE:N	2.50	0.44
1:A:136:THR:HG21	1:A:330:LEU:HG	1.98	0.44
1:A:281:ILE:O	1:A:285:ILE:HG12	2.17	0.44
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.99	0.44
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.98	0.44
1:C:208:ASN:HB3	1:C:212:THR:HG22	1.99	0.44
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.82	0.44
2:D:173:LYS:HG3	2:D:264:THR:O	2.18	0.44
2:D:117:GLN:O	2:D:150:ARG:NH1	2.50	0.44
1:A:385:TRP:HD1	1:A:390:ILE:HD13	1.82	0.44
7:A:1104:CLR:H162	7:A:1104:CLR:H222	1.86	0.44
1:A:602:ALA:O	1:A:829:PRO:HD3	2.18	0.44
1:C:545:VAL:HA	1:C:583:SER:HA	2.00	0.44
1:A:52:LEU:HD12	1:A:250:ILE:HD11	2.00	0.44
1:C:481:TYR:CE2	1:C:483:LEU:HD23	2.50	0.44
1:C:95:MET:O	1:C:99:ILE:HG23	2.18	0.44
1:C:850:ILE:HD12	1:C:991:ILE:HG23	1.98	0.44
2:D:246:TYR:O	2:D:250:LEU:HB2	2.17	0.44
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.99	0.43
1:C:886:ARG:HD2	1:C:887:TRP:CZ2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:893:ASP:OD2	1:C:897:GLN:HB2	2.18	0.43
1:C:913:THR:HB	1:C:976:LEU:HD21	1.99	0.43
1:C:918:THR:HG23	1:C:984:ALA:HB2	2.00	0.43
1:C:323:ALA:HB1	1:C:780:ILE:HG12	2.00	0.43
1:C:524:ASP:OD1	1:C:524:ASP:N	2.51	0.43
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.98	0.43
1:C:783:PHE:O	1:C:787:ILE:HG13	2.17	0.43
3:E:33:PHE:CZ	7:E:101:CLR:H151	2.53	0.43
1:A:54:ARG:HH21	1:A:167:ASN:HD22	1.64	0.43
1:A:909:PHE:HB3	1:A:972:ARG:O	2.18	0.43
1:A:106:LEU:O	1:A:110:ILE:HG12	2.19	0.43
1:C:281:ILE:O	1:C:285:ILE:HG12	2.18	0.43
2:B:155:TRP:CD2	2:B:232:LEU:HD22	2.53	0.43
1:C:301:ILE:O	1:C:305:ILE:HG12	2.18	0.43
1:C:467:TYR:HB3	1:C:486:HIS:HB3	1.99	0.43
2:D:74:PRO:HG2	2:D:292:GLN:OE1	2.17	0.43
1:A:423:ARG:NH1	1:A:474:PRO:HB3	2.34	0.43
1:A:697:GLY:HA2	1:A:700:ARG:CZ	2.49	0.43
2:B:74:PRO:HG2	2:B:292:GLN:OE1	2.18	0.43
1:C:883:TRP:CZ2	1:C:904:ARG:HG3	2.53	0.43
1:C:369:PHD:OP3	1:C:369:PHD:OD2	2.36	0.43
2:D:115:LEU:HD13	2:D:118:LYS:HD2	2.01	0.43
1:A:197:ARG:HB2	1:A:252:VAL:HG23	2.00	0.43
1:C:277:ILE:CG2	1:C:355:GLU:HB2	2.49	0.43
2:D:108:PHE:HD1	2:D:109:LEU:HD12	1.83	0.43
1:A:485:ILE:HD11	1:A:496:HIS:HD2	1.84	0.43
1:A:938:PHE:CD2	7:C:1104:CLR:H191	2.54	0.43
2:B:162:LEU:HD22	2:B:162:LEU:HA	1.90	0.43
1:C:238:PHE:CD2	1:C:258:THR:HG21	2.54	0.43
2:B:51:ILE:O	2:B:54:ILE:HG22	2.18	0.43
1:C:198:ILE:HB	1:C:234:ASN:HA	2.01	0.43
1:C:613:HIS:CD2	1:C:685:ARG:HH21	2.37	0.43
1:C:663:LEU:HA	1:C:666:MET:HG3	2.01	0.43
1:C:971:LEU:HD23	8:C:1105:PCW:H31	2.01	0.43
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.92	0.42
1:C:943:LYS:NZ	8:C:1107:PCW:H52	2.34	0.42
1:C:386:SER:HB2	1:C:391:HIS:CD2	2.54	0.42
1:C:815:LEU:HD12	1:C:815:LEU:HA	1.85	0.42
1:A:277:ILE:HG21	1:A:355:GLU:HB2	2.00	0.42
1:C:84:LYS:HG3	1:C:141:TYR:CE1	2.55	0.42
2:D:158:ASN:OD1	4:I:1:NAG:N2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHD:O	1:A:373:THR:HB	2.19	0.42
2:B:18:ASN:HA	2:B:23:GLU:O	2.19	0.42
2:D:146:ARG:H	2:D:146:ARG:HG2	1.67	0.42
2:D:153:LEU:H	2:D:153:LEU:HD12	1.85	0.42
1:A:767:LYS:HE2	1:A:933:ARG:HG3	2.02	0.42
1:A:795:LEU:HD13	1:A:915:PHE:HB3	2.02	0.42
1:A:964:CYS:O	1:A:967:MET:HG2	2.19	0.42
1:C:600:ARG:NH2	1:C:680:GLU:HG2	2.35	0.42
1:A:1008:GLY:O	1:A:1012:LYS:N	2.48	0.42
1:C:25:MET:O	1:C:29:LYS:HG3	2.19	0.42
1:C:602:ALA:O	1:C:829:PRO:HD3	2.20	0.42
1:A:103:LEU:HD22	1:A:318:ILE:HD12	2.02	0.42
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.84	0.42
8:A:1105:PCW:H62	8:A:1105:PCW:H41	1.76	0.42
8:A:1108:PCW:H41	8:A:1108:PCW:H62	1.86	0.42
2:B:130:PRO:HD3	2:B:232:LEU:HD12	2.02	0.42
1:C:719:LYS:HD3	1:C:738:ALA:HB1	2.02	0.42
1:A:30:LYS:HE2	1:A:692:LEU:HD21	2.01	0.42
1:A:524:ASP:OD1	1:A:524:ASP:N	2.51	0.42
1:A:612:ASP:OD1	1:A:613:HIS:N	2.49	0.42
1:C:73:LEU:HD11	1:C:260:MET:SD	2.60	0.42
1:C:196:LEU:HB2	1:C:236:ALA:HB3	2.00	0.42
2:B:91:ARG:HD2	2:B:94:ASP:HB2	2.02	0.42
1:A:29:LYS:HE2	1:A:265:THR:HB	2.02	0.42
1:A:332:THR:O	1:A:336:CYS:HB2	2.20	0.42
1:A:911:CYS:C	1:A:914:PRO:HD2	2.41	0.41
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.55	0.41
2:D:151:PHE:HE2	2:D:258:LEU:HB2	1.85	0.41
1:A:386:SER:HB2	1:A:391:HIS:CD2	2.55	0.41
2:D:39:TYR:CZ	7:D:402:CLR:H191	2.55	0.41
1:C:201:ALA:HB3	1:C:222:PRO:HD3	2.02	0.41
1:C:949:PHE:HB2	3:E:45:ILE:HG23	2.02	0.41
1:A:545:VAL:HG11	1:A:581:LEU:HD13	2.01	0.41
1:A:708:THR:HA	1:A:725:VAL:O	2.20	0.41
1:C:119:GLN:HE22	9:C:1121:DGX:H2X	1.84	0.41
3:E:31:LEU:HD23	3:E:31:LEU:HA	1.90	0.41
1:C:164:VAL:HG12	1:C:166:ARG:HG3	2.02	0.41
1:C:511:CYS:SG	1:C:576:LEU:HB2	2.61	0.41
1:C:985:PHE:HZ	7:E:101:CLR:H20	1.86	0.41
3:E:33:PHE:CD2	7:E:101:CLR:H71	2.55	0.41
1:A:510:ARG:HD2	1:A:573:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.87	0.41
1:C:845:MET:SD	1:C:849:GLN:NE2	2.94	0.41
1:A:753:THR:O	1:A:757:GLU:HG2	2.21	0.41
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.79	0.41
1:C:852:MET:HB2	1:C:852:MET:HE2	1.95	0.41
2:D:80:ILE:HB	2:D:105:ILE:HD12	2.02	0.41
1:A:600:ARG:NH2	1:A:680:GLU:HG2	2.35	0.41
1:A:944:ASN:O	1:A:948:ILE:HG12	2.20	0.41
1:A:998:ARG:O	1:A:1002:ILE:HG13	2.21	0.41
1:C:111:GLN:O	1:C:115:GLU:HG2	2.20	0.41
1:C:708:THR:HA	1:C:725:VAL:O	2.20	0.41
1:A:95:MET:O	1:A:99:ILE:HG23	2.21	0.41
1:A:696:GLU:O	1:A:700:ARG:HG3	2.20	0.41
8:A:1106:PCW:H73	8:A:1106:PCW:H41	1.76	0.41
2:B:95:PRO:HA	2:B:98:TYR:CZ	2.56	0.41
1:C:38:LYS:NZ	1:C:227:GLU:OE1	2.49	0.41
2:D:88:ILE:HB	2:D:299:ILE:HG22	2.03	0.41
2:D:91:ARG:HD2	2:D:94:ASP:H	1.86	0.41
1:A:545:VAL:HG22	1:A:583:SER:HB3	2.03	0.41
1:A:858:GLY:HA3	1:A:915:PHE:CE1	2.56	0.41
1:C:462:GLU:O	1:C:466:ARG:HB2	2.21	0.41
1:C:635:GLU:OE1	1:C:635:GLU:N	2.54	0.41
1:C:725:VAL:HG11	1:C:751:ILE:HD11	2.02	0.41
2:D:143:ARG:HD2	2:D:146:ARG:NH1	2.36	0.41
2:B:156:LEU:HD22	2:B:260:ALA:H	1.86	0.40
1:C:793:LEU:HB3	1:C:908:GLU:OE2	2.21	0.40
1:A:713:ASN:OD1	1:A:713:ASN:N	2.54	0.40
1:C:124:TYR:CE1	8:C:1105:PCW:H2	2.56	0.40
1:A:870:GLY:O	1:A:893:ASP:HB2	2.22	0.40
1:A:938:PHE:CE2	7:C:1104:CLR:H191	2.56	0.40
2:B:80:ILE:HD12	2:B:81:PRO:HD3	2.02	0.40
1:C:471:VAL:HG21	1:C:564:PHE:O	2.20	0.40
1:C:860:PHE:O	1:C:864:VAL:HG23	2.21	0.40
2:D:102:VAL:HG13	2:D:169:TYR:CD2	2.51	0.40
1:A:865:ILE:HD12	1:A:914:PRO:HG3	2.02	0.40
1:C:339:LEU:HD13	1:C:817:TYR:CE1	2.56	0.40
1:A:191:ARG:HE	1:A:239:SER:HA	1.85	0.40
1:C:41:LEU:HD12	1:C:41:LEU:H	1.86	0.40
1:C:238:PHE:HD2	1:C:258:THR:HG21	1.86	0.40
1:C:479:ASN:O	1:C:481:TYR:HD1	2.05	0.40
2:D:155:TRP:CD2	2:D:232:LEU:HD22	2.57	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	993/1016 (98%)	907 (91%)	83 (8%)	3 (0%)	41	75
1	C	993/1016 (98%)	906 (91%)	84 (8%)	3 (0%)	41	75
2	B	289/303 (95%)	260 (90%)	27 (9%)	2 (1%)	22	60
2	D	281/303 (93%)	252 (90%)	27 (10%)	2 (1%)	22	60
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	26 (87%)	4 (13%)	0	100	100
All	All	2616/2768 (94%)	2379 (91%)	227 (9%)	10 (0%)	34	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
1	A	193	PRO
1	C	193	PRO
1	C	306	LEU
2	D	200	PRO
1	A	306	LEU
2	B	199	TYR
2	D	199	TYR
1	A	561	GLY
1	C	561	GLY

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	846/861 (98%)	813 (96%)	33 (4%)	32	64
1	C	846/861 (98%)	812 (96%)	34 (4%)	31	63
2	B	261/269 (97%)	240 (92%)	21 (8%)	12	40
2	D	255/269 (95%)	234 (92%)	21 (8%)	11	39
3	E	26/52 (50%)	25 (96%)	1 (4%)	33	64
3	G	26/52 (50%)	25 (96%)	1 (4%)	33	64
All	All	2260/2364 (96%)	2149 (95%)	111 (5%)	25	57

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	52	LEU
1	A	56	LEU
1	A	82	TRP
1	A	93	PHE
1	A	122	ASN
1	A	167	ASN
1	A	182	ASP
1	A	211	LEU
1	A	223	ASP
1	A	256	ASP
1	A	265	THR
1	A	327	GLU
1	A	350	LEU
1	A	351	VAL
1	A	476	ASN
1	A	483	LEU
1	A	485	ILE
1	A	491	THR
1	A	523	LEU
1	A	564	PHE
1	A	566	THR
1	A	685	ARG
1	A	733	ASP
1	A	763	ASP
1	A	776	ASN
1	A	840	GLU

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Mol	Chain	Res	Type
1	A	865	ILE
1	A	880	ARG
1	A	904	ARG
1	A	911	CYS
1	A	915	PHE
1	A	1009	TRP
2	B	25	LEU
2	B	28	THR
2	B	32	TRP
2	B	64	PHE
2	B	72	VAL
2	B	80	ILE
2	B	114	ASP
2	B	125	ASP
2	B	126	CYS
2	B	153	LEU
2	B	162	LEU
2	B	166	THR
2	B	170	LYS
2	B	171	ASP
2	B	173	LYS
2	B	177	ILE
2	B	195	SER
2	B	203	LYS
2	B	256	GLN
2	B	297	VAL
2	B	299	ILE
3	G	21	TYR
1	C	35	ASP
1	C	56	LEU
1	C	82	TRP
1	C	121	ASP
1	C	122	ASN
1	C	124	TYR
1	C	167	ASN
1	C	180	VAL
1	C	182	ASP
1	C	211	LEU
1	C	223	ASP
1	C	256	ASP
1	C	265	THR
1	C	327	GLU

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Mol	Chain	Res	Type
1	C	350	LEU
1	C	351	VAL
1	C	476	ASN
1	C	483	LEU
1	C	485	ILE
1	C	491	THR
1	C	523	LEU
1	C	564	PHE
1	C	566	THR
1	C	685	ARG
1	C	733	ASP
1	C	763	ASP
1	C	776	ASN
1	C	861	THR
1	C	865	ILE
1	C	880	ARG
1	C	904	ARG
1	C	911	CYS
1	C	915	PHE
1	C	1009	TRP
2	D	13	LYS
2	D	25	LEU
2	D	27	ARG
2	D	28	THR
2	D	32	TRP
2	D	60	THR
2	D	64	PHE
2	D	72	VAL
2	D	80	ILE
2	D	114	ASP
2	D	125	ASP
2	D	126	CYS
2	D	153	LEU
2	D	170	LYS
2	D	171	ASP
2	D	173	LYS
2	D	177	ILE
2	D	195	SER
2	D	203	LYS
2	D	256	GLN
2	D	297	VAL
3	E	21	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	122	ASN
1	A	324	ASN
1	A	377	ASN
1	A	399	GLN
1	A	427	GLN
1	A	430	GLN
1	A	488	ASN
1	A	897	GLN
1	A	935	ASN
1	C	111	GLN
1	C	234	ASN
1	C	283	HIS
1	C	324	ASN
1	C	399	GLN
1	C	430	GLN
1	C	482	GLN
1	C	897	GLN
1	C	898	GLN
2	D	262	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](#)

2 non-standard protein/DNA/RNA residues 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
1	PHD	A	369	1,5	9,11,12	0.93	0	10,15,17	1.47	2 (20%)
1	PHD	C	369	1,5	9,11,12	0.92	0	10,15,17	1.39	2 (20%)

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
1	PHD	A	369	1,5	-	0/8/11/13	-
1	PHD	C	369	1,5	-	0/8/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	CA-CB-CG	2.91	118.95	112.86
1	A	369	PHD	OD1-CG-CB	2.78	118.76	111.11
1	A	369	PHD	CA-CB-CG	2.71	118.54	112.86
1	C	369	PHD	OD1-CG-CB	2.38	117.66	111.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	369	PHD	2	0
1	C	369	PHD	1	0

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	4,2	14,14,15	0.35	0	17,19,21	0.43	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1	4,2	14,14,15	0.62	1 (7%)	17,19,21	0.70	0
4	NAG	H	2	4	14,14,15	0.32	0	17,19,21	0.36	0
4	NAG	I	1	4,2	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	I	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	J	1	4,2	14,14,15	0.61	1 (7%)	17,19,21	0.63	0
4	NAG	J	2	4	14,14,15	0.31	0	17,19,21	0.34	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.18	1.40	1.43
4	J	1	NAG	O5-C1	-2.09	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

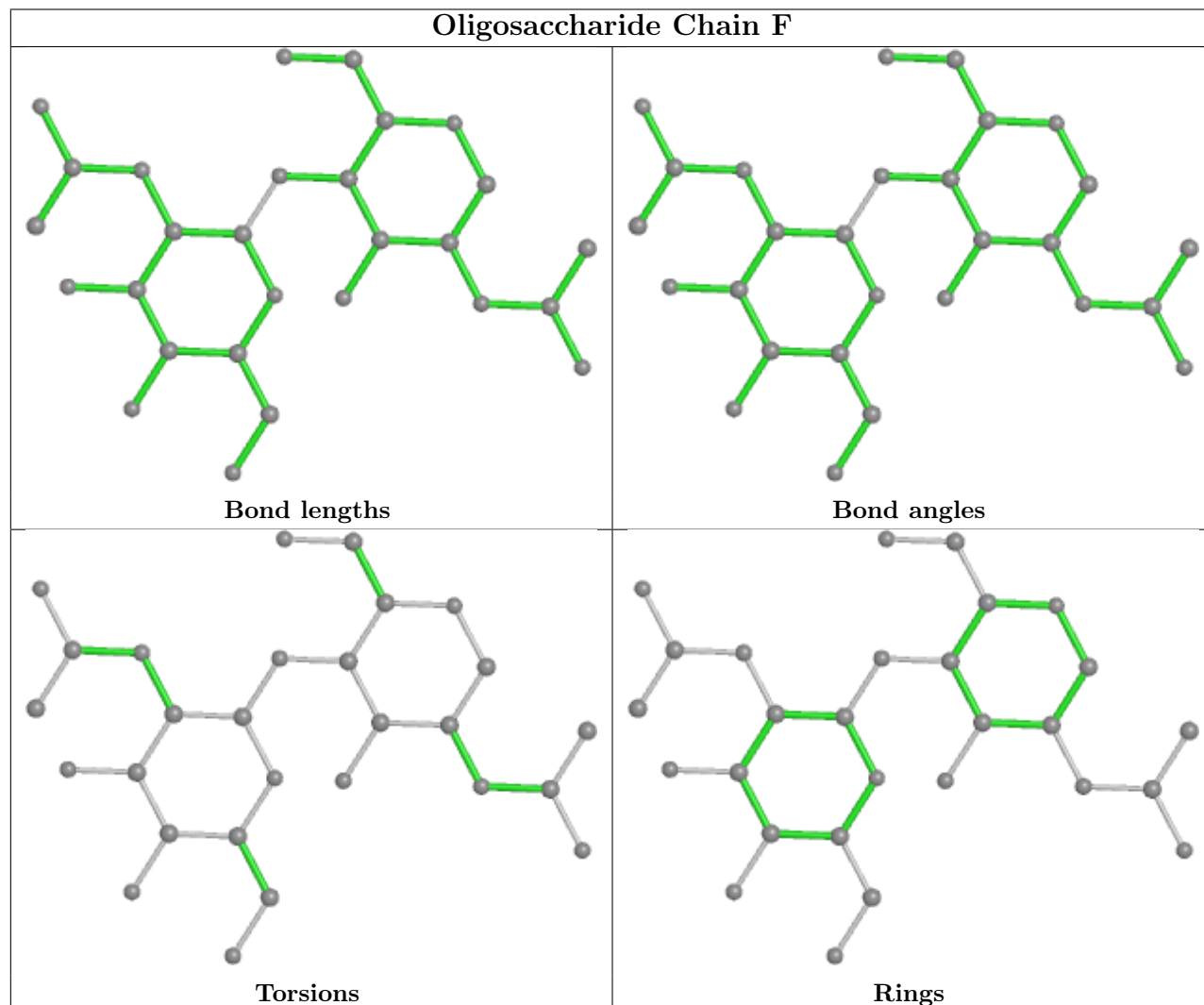
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

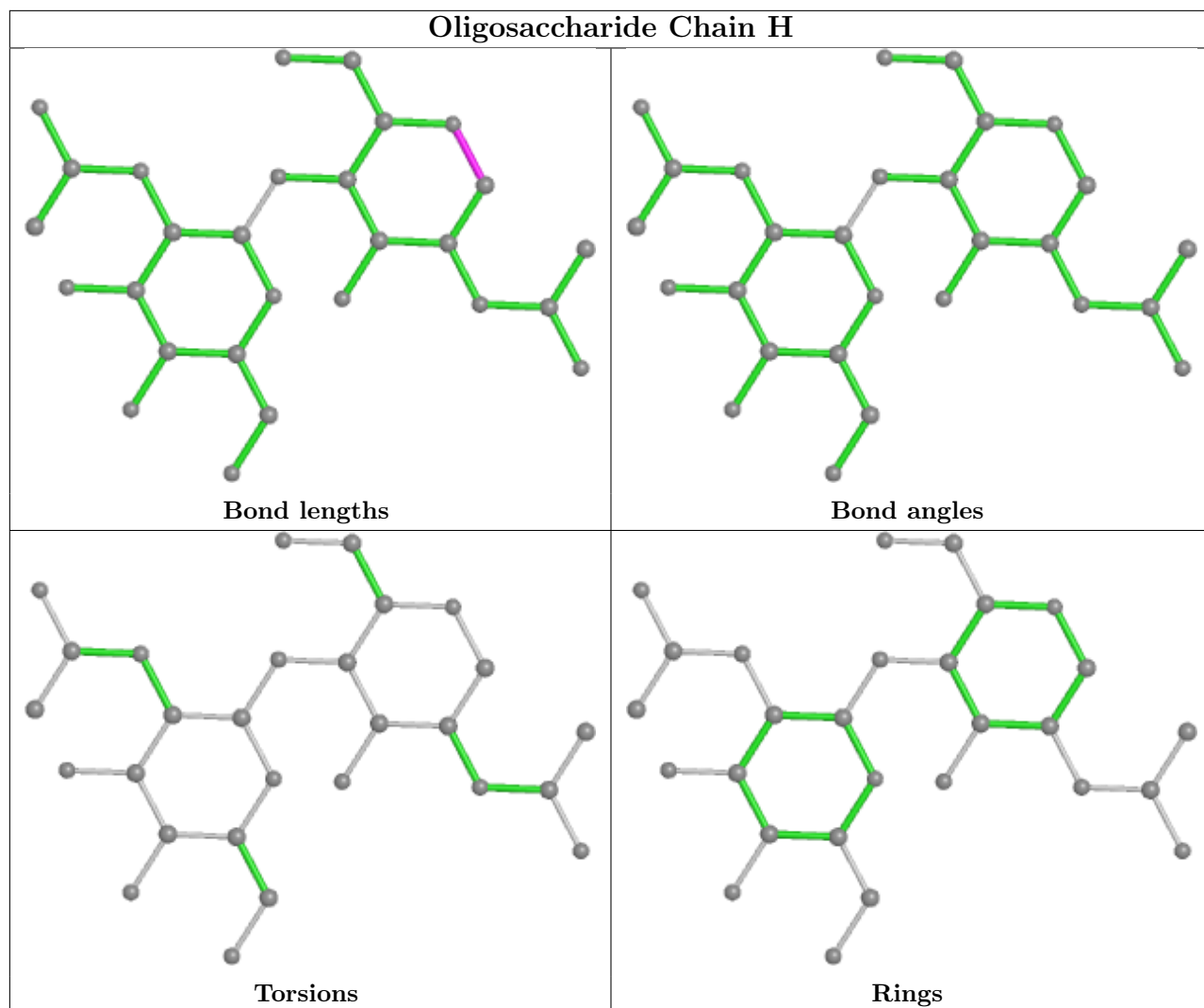
There are no ring outliers.

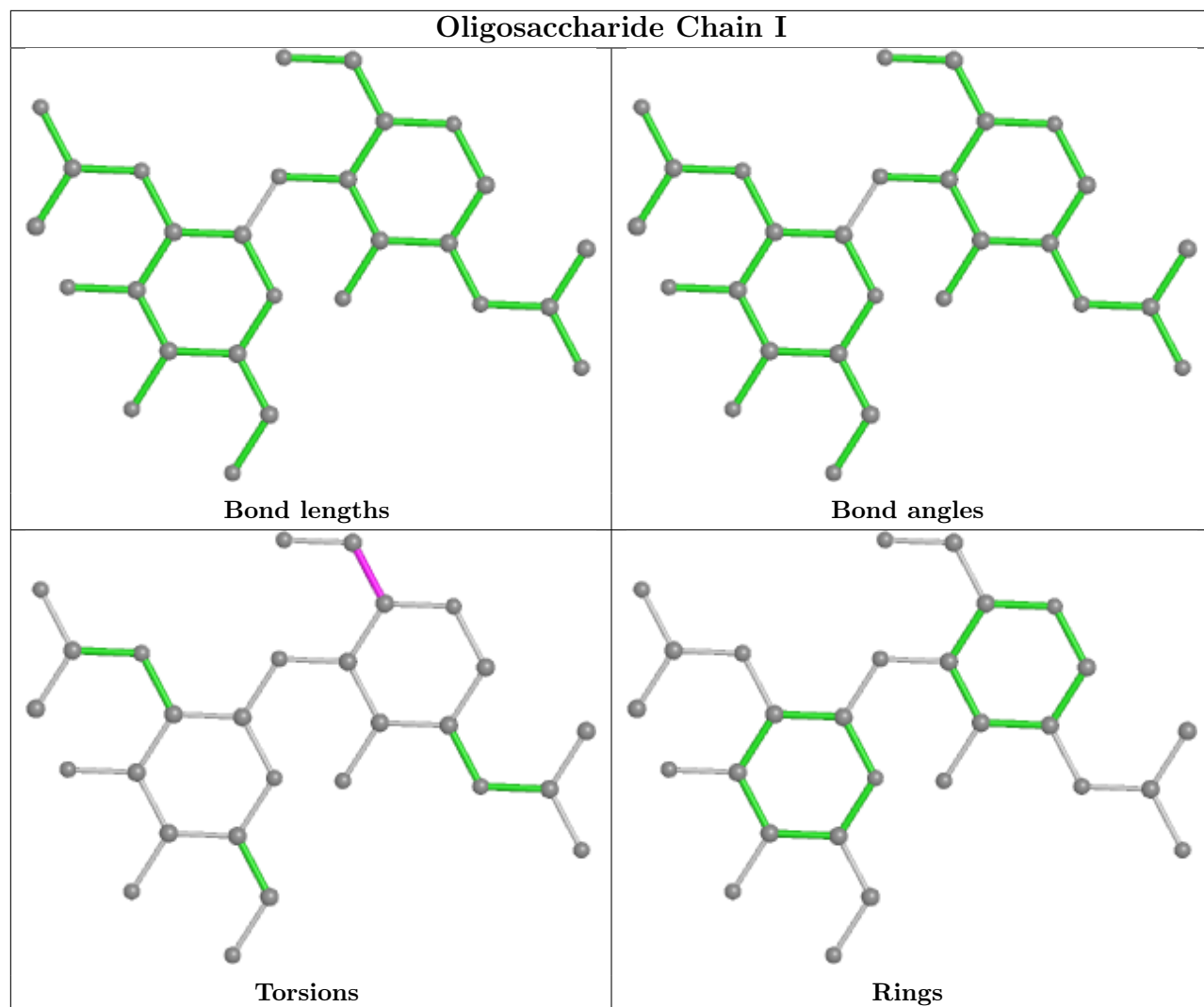
1 monomer is involved in 1 short contact:

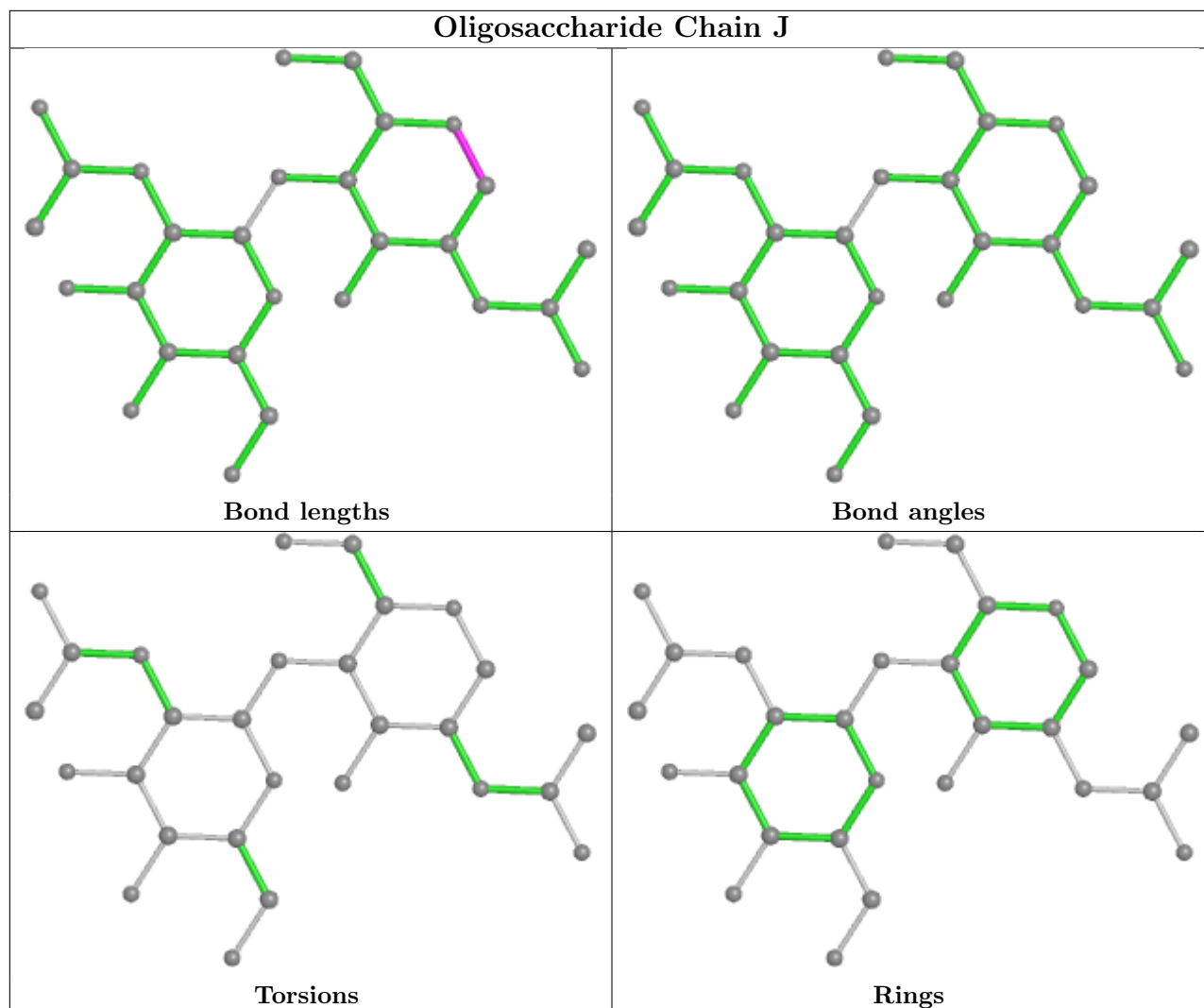
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	PCW	A	1108	-	21,21,53	1.68	5 (23%)	27,29,61	1.20	1 (3%)
9	DGX	A	1110	-	62,62,62	1.21	3 (4%)	89,98,98	1.29	7 (7%)
10	NAG	B	401	2	14,14,15	0.33	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PCW	A	1109	-	21,21,53	1.69	5 (23%)	27,29,61	1.35	2 (7%)
7	CLR	G	101	-	31,31,31	1.77	8 (25%)	48,48,48	1.62	12 (25%)
8	PCW	A	1107	-	21,21,53	1.68	6 (28%)	27,29,61	1.16	1 (3%)
7	CLR	E	101	-	31,31,31	1.74	9 (29%)	48,48,48	1.57	11 (22%)
10	NAG	D	401	2	14,14,15	0.31	0	17,19,21	0.53	0
8	PCW	C	1107	-	21,21,53	1.69	5 (23%)	27,29,61	1.45	3 (11%)
7	CLR	C	1104	-	31,31,31	1.92	9 (29%)	48,48,48	1.61	16 (33%)
9	DGX	C	1121	-	62,62,62	1.18	2 (3%)	89,98,98	1.24	8 (8%)
8	PCW	A	1106	-	21,21,53	1.67	4 (19%)	27,29,61	1.17	1 (3%)
8	PCW	A	1105	-	21,21,53	1.71	5 (23%)	27,29,61	1.33	1 (3%)
8	PCW	C	1105	-	21,21,53	1.72	4 (19%)	27,29,61	1.15	1 (3%)
8	PCW	B	403	-	21,21,53	1.69	5 (23%)	27,29,61	1.23	1 (3%)
7	CLR	A	1104	-	31,31,31	1.91	11 (35%)	48,48,48	1.57	10 (20%)
7	CLR	B	402	-	31,31,31	1.96	12 (38%)	48,48,48	1.63	13 (27%)
8	PCW	C	1106	-	21,21,53	1.68	6 (28%)	27,29,61	1.23	1 (3%)
8	PCW	C	1108	-	21,21,53	1.68	6 (28%)	27,29,61	1.20	1 (3%)
7	CLR	D	402	-	31,31,31	1.99	10 (32%)	48,48,48	1.55	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PCW	A	1108	-	-	10/23/23/57	-
9	DGX	A	1110	-	-	4/16/141/141	0/8/8/8
10	NAG	B	401	2	-	1/6/23/26	0/1/1/1
8	PCW	A	1109	-	-	14/23/23/57	-
7	CLR	G	101	-	-	3/10/68/68	0/4/4/4
8	PCW	A	1107	-	-	11/23/23/57	-
7	CLR	E	101	-	-	3/10/68/68	0/4/4/4
10	NAG	D	401	2	-	4/6/23/26	0/1/1/1
8	PCW	C	1107	-	-	10/23/23/57	-
7	CLR	C	1104	-	-	6/10/68/68	0/4/4/4
9	DGX	C	1121	-	-	4/16/141/141	0/8/8/8
8	PCW	A	1106	-	-	16/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PCW	A	1105	-	-	12/23/23/57	-
8	PCW	C	1105	-	-	11/23/23/57	-
8	PCW	B	403	-	-	11/23/23/57	-
7	CLR	A	1104	-	-	6/10/68/68	0/4/4/4
7	CLR	B	402	-	-	1/10/68/68	0/4/4/4
8	PCW	C	1106	-	-	9/23/23/57	-
8	PCW	C	1108	-	-	13/23/23/57	-
7	CLR	D	402	-	-	1/10/68/68	0/4/4/4

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	402	CLR	C10-C9	5.14	1.64	1.56
7	A	1104	CLR	C10-C9	4.90	1.64	1.56
7	D	402	CLR	C10-C9	4.77	1.64	1.56
7	C	1104	CLR	C10-C9	4.73	1.64	1.56
7	G	101	CLR	C10-C9	4.17	1.63	1.56
8	C	1105	PCW	O2-C31	3.89	1.44	1.35
7	E	101	CLR	C10-C9	3.87	1.62	1.56
8	A	1105	PCW	O2-C31	3.85	1.43	1.35
8	A	1106	PCW	O2-C31	3.76	1.43	1.35
8	A	1108	PCW	O2-C31	3.72	1.43	1.35
8	C	1106	PCW	O2-C31	3.67	1.43	1.35
8	A	1107	PCW	O2-C31	3.66	1.43	1.35
8	B	403	PCW	O2-C31	3.63	1.43	1.35
7	G	101	CLR	C13-C14	3.61	1.61	1.55
7	E	101	CLR	C13-C14	3.61	1.61	1.55
7	E	101	CLR	C16-C17	3.61	1.61	1.54
8	C	1107	PCW	O2-C31	3.61	1.43	1.35
8	C	1108	PCW	O2-C31	3.61	1.43	1.35
7	D	402	CLR	C13-C14	3.57	1.61	1.55
8	A	1109	PCW	O2-C31	3.56	1.43	1.35
7	G	101	CLR	C16-C17	3.53	1.61	1.54
7	C	1104	CLR	C11-C9	3.51	1.59	1.53
7	D	402	CLR	C4-C3	3.48	1.58	1.52
7	B	402	CLR	C12-C13	3.43	1.60	1.54
7	A	1104	CLR	C12-C11	3.31	1.60	1.53
7	B	402	CLR	C12-C11	3.26	1.60	1.53
7	G	101	CLR	C10-C5	3.23	1.59	1.52
7	B	402	CLR	C13-C14	3.22	1.61	1.55
7	C	1104	CLR	C12-C11	3.21	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1104	CLR	C13-C14	3.15	1.61	1.55
7	A	1104	CLR	C11-C9	3.14	1.59	1.53
7	B	402	CLR	C16-C17	3.09	1.60	1.54
7	A	1104	CLR	C13-C14	3.08	1.60	1.55
7	D	402	CLR	C16-C17	3.03	1.60	1.54
7	D	402	CLR	C12-C13	2.97	1.59	1.54
7	A	1104	CLR	C16-C17	2.96	1.60	1.54
7	D	402	CLR	C12-C11	2.92	1.59	1.53
7	C	1104	CLR	C4-C3	2.89	1.57	1.52
7	C	1104	CLR	C16-C17	2.87	1.60	1.54
7	D	402	CLR	C11-C9	2.83	1.58	1.53
7	D	402	CLR	C4-C5	2.82	1.57	1.51
7	E	101	CLR	C10-C5	2.81	1.58	1.52
7	C	1104	CLR	C4-C5	2.73	1.57	1.51
7	A	1104	CLR	C12-C13	2.72	1.59	1.54
8	A	1106	PCW	C6-N	-2.56	1.42	1.50
7	B	402	CLR	C11-C9	2.50	1.58	1.53
7	B	402	CLR	C13-C17	2.50	1.59	1.55
8	A	1109	PCW	C7-N	-2.49	1.42	1.50
8	B	403	PCW	C6-N	-2.49	1.42	1.50
8	C	1107	PCW	C6-N	-2.48	1.42	1.50
8	C	1107	PCW	C7-N	-2.46	1.42	1.50
8	C	1108	PCW	C6-N	-2.46	1.42	1.50
8	A	1109	PCW	C6-N	-2.46	1.42	1.50
8	A	1105	PCW	C7-N	-2.44	1.42	1.50
8	A	1108	PCW	C7-N	-2.44	1.42	1.50
8	A	1107	PCW	C7-N	-2.43	1.42	1.50
8	C	1106	PCW	C7-N	-2.43	1.42	1.50
8	A	1107	PCW	C6-N	-2.43	1.42	1.50
8	A	1105	PCW	C6-N	-2.43	1.42	1.50
8	C	1108	PCW	C7-N	-2.42	1.42	1.50
8	B	403	PCW	C7-N	-2.42	1.42	1.50
8	C	1105	PCW	C7-N	-2.42	1.42	1.50
8	C	1105	PCW	C6-N	-2.42	1.43	1.50
7	G	101	CLR	C12-C11	2.40	1.58	1.53
8	A	1108	PCW	C6-N	-2.40	1.43	1.50
8	C	1106	PCW	C6-N	-2.38	1.43	1.50
7	E	101	CLR	C12-C11	2.38	1.58	1.53
9	C	1121	DGX	C3Z-C4Z	2.38	1.56	1.52
7	D	402	CLR	C13-C17	2.36	1.59	1.55
7	B	402	CLR	C4-C5	2.35	1.56	1.51
7	B	402	CLR	C10-C5	2.33	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1104	CLR	C12-C13	2.33	1.58	1.54
7	D	402	CLR	C16-C15	2.32	1.60	1.54
8	A	1106	PCW	C7-N	-2.32	1.43	1.50
7	G	101	CLR	C12-C13	2.31	1.58	1.54
7	A	1104	CLR	C4-C3	2.30	1.56	1.52
7	A	1104	CLR	C4-C5	2.28	1.56	1.51
7	B	402	CLR	C4-C3	2.27	1.56	1.52
8	C	1107	PCW	O2-C2	-2.25	1.41	1.46
7	E	101	CLR	C12-C13	2.23	1.58	1.54
8	A	1105	PCW	P-O3P	2.21	1.68	1.59
8	B	403	PCW	P-O3P	2.20	1.68	1.59
8	C	1105	PCW	P-O3P	2.20	1.68	1.59
9	A	1110	DGX	C3Z-C4Z	2.19	1.55	1.52
9	C	1121	DGX	C2Z-C1Z	2.19	1.55	1.51
7	G	101	CLR	C13-C17	2.18	1.59	1.55
8	A	1109	PCW	O2-C2	-2.17	1.41	1.46
8	A	1106	PCW	C8-N	-2.17	1.43	1.50
7	A	1104	CLR	C10-C5	2.16	1.57	1.52
7	E	101	CLR	C13-C17	2.15	1.59	1.55
8	C	1108	PCW	O2-C2	-2.13	1.41	1.46
7	E	101	CLR	C4-C3	2.13	1.55	1.52
7	A	1104	CLR	C16-C15	2.12	1.59	1.54
7	C	1104	CLR	C16-C15	2.12	1.59	1.54
8	C	1106	PCW	P-O3P	2.12	1.67	1.59
8	A	1108	PCW	P-O3P	2.10	1.67	1.59
8	A	1109	PCW	P-O3P	2.09	1.67	1.59
8	A	1107	PCW	O2-C2	-2.08	1.41	1.46
7	G	101	CLR	C4-C3	2.08	1.55	1.52
8	B	403	PCW	O2-C2	-2.07	1.41	1.46
7	A	1104	CLR	C13-C17	2.06	1.58	1.55
9	A	1110	DGX	C2Z-C1Z	2.06	1.55	1.51
8	A	1107	PCW	P-O3P	2.05	1.67	1.59
9	A	1110	DGX	C2Y-C1Y	2.05	1.55	1.51
8	A	1105	PCW	C8-N	-2.04	1.44	1.50
8	C	1106	PCW	O2-C2	-2.04	1.41	1.46
8	C	1108	PCW	C8-N	-2.03	1.44	1.50
8	C	1108	PCW	P-O3P	2.03	1.67	1.59
7	B	402	CLR	C8-C14	-2.03	1.49	1.53
8	A	1107	PCW	C8-N	-2.03	1.44	1.50
7	B	402	CLR	C16-C15	2.02	1.59	1.54
8	A	1108	PCW	C8-N	-2.02	1.44	1.50
8	C	1107	PCW	P-O3P	2.01	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1106	PCW	C8-N	-2.01	1.44	1.50
7	E	101	CLR	C16-C15	2.00	1.59	1.54

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1110	DGX	O21-C23-C22	5.45	115.79	108.67
9	C	1121	DGX	O21-C23-C22	5.32	115.63	108.67
8	A	1105	PCW	O2-C31-C32	5.21	120.67	111.09
8	C	1107	PCW	O2-C31-C32	5.12	120.50	111.09
8	A	1109	PCW	O2-C31-C32	4.98	120.24	111.09
8	C	1106	PCW	O2-C31-C32	4.82	119.95	111.09
8	A	1106	PCW	O2-C31-C32	4.80	119.92	111.09
8	B	403	PCW	O2-C31-C32	4.77	119.87	111.09
8	A	1108	PCW	O2-C31-C32	4.72	119.78	111.09
8	C	1105	PCW	O2-C31-C32	4.68	119.71	111.09
8	A	1107	PCW	O2-C31-C32	4.60	119.55	111.09
8	C	1108	PCW	O2-C31-C32	4.56	119.47	111.09
9	A	1110	DGX	O23-C23-C22	-4.16	122.38	130.81
9	C	1121	DGX	O23-C23-C22	-4.11	122.49	130.81
7	G	101	CLR	C17-C13-C14	-3.92	95.43	100.07
7	E	101	CLR	C17-C13-C14	-3.73	95.65	100.07
7	C	1104	CLR	C8-C7-C6	-3.72	107.39	112.73
7	B	402	CLR	C4-C5-C6	-3.59	115.44	120.61
9	C	1121	DGX	C4-C3-C2	-3.44	107.10	111.54
9	A	1110	DGX	C4-C3-C2	-3.42	107.12	111.54
7	A	1104	CLR	C8-C7-C6	-3.33	107.95	112.73
7	G	101	CLR	C4-C5-C6	-3.17	116.04	120.61
9	A	1110	DGX	C16-C15-C14	-3.12	99.89	105.19
7	A	1104	CLR	C4-C5-C6	-3.09	116.16	120.61
8	C	1107	PCW	C2-O2-C31	-3.07	112.17	117.90
7	E	101	CLR	C4-C5-C6	-2.99	116.30	120.61
9	C	1121	DGX	C20-C22-C23	-2.99	102.64	108.84
9	A	1110	DGX	C20-C22-C23	-2.98	102.65	108.84
7	D	402	CLR	C8-C7-C6	-2.98	108.45	112.73
7	B	402	CLR	C2-C3-C4	-2.98	106.22	110.31
7	G	101	CLR	C2-C3-C4	-2.97	106.24	110.31
7	G	101	CLR	C22-C20-C17	-2.96	104.17	110.28
9	C	1121	DGX	C21-O21-C23	-2.85	105.40	108.85
9	A	1110	DGX	C21-O21-C23	-2.83	105.42	108.85
7	E	101	CLR	C2-C3-C4	-2.83	106.43	110.31
7	E	101	CLR	C22-C20-C17	-2.80	104.50	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	402	CLR	C4-C5-C6	-2.72	116.69	120.61
7	D	402	CLR	C4-C5-C10	-2.69	112.84	116.42
7	C	1104	CLR	C19-C10-C5	2.66	112.65	108.34
7	D	402	CLR	C19-C10-C5	2.66	112.65	108.34
8	A	1109	PCW	C2-O2-C31	-2.64	112.98	117.90
7	B	402	CLR	C8-C7-C6	-2.63	108.95	112.73
7	B	402	CLR	C19-C10-C5	2.63	112.59	108.34
7	B	402	CLR	C17-C13-C14	-2.63	96.96	100.07
7	C	1104	CLR	C4-C5-C10	-2.62	112.94	116.42
7	A	1104	CLR	C2-C3-C4	-2.60	106.74	110.31
7	B	402	CLR	C4-C5-C10	-2.59	112.98	116.42
7	B	402	CLR	C11-C9-C10	2.55	116.44	113.08
7	D	402	CLR	C2-C3-C4	-2.49	106.88	110.31
8	C	1107	PCW	C3-O3-C11	-2.49	110.85	117.10
7	C	1104	CLR	C4-C5-C6	-2.49	117.03	120.61
7	B	402	CLR	O1-C3-C2	2.49	116.49	110.16
9	C	1121	DGX	C16-C15-C14	-2.45	101.02	105.19
7	A	1104	CLR	C19-C10-C5	2.45	112.31	108.34
9	A	1110	DGX	O5Y-C1Y-C2Y	-2.44	107.19	110.87
7	A	1104	CLR	C4-C5-C10	-2.43	113.19	116.42
9	C	1121	DGX	O5Y-C1Y-C2Y	-2.41	107.23	110.87
7	G	101	CLR	O1-C3-C2	2.40	116.27	110.16
7	C	1104	CLR	C2-C3-C4	-2.38	107.04	110.31
7	A	1104	CLR	O1-C3-C2	2.35	116.14	110.16
7	E	101	CLR	C18-C13-C12	2.33	114.27	110.59
7	E	101	CLR	O1-C3-C2	2.32	116.08	110.16
7	B	402	CLR	C22-C20-C17	-2.32	105.49	110.28
7	G	101	CLR	C18-C13-C12	2.32	114.25	110.59
7	B	402	CLR	C18-C13-C12	2.32	114.25	110.59
7	G	101	CLR	C16-C17-C20	-2.29	108.60	112.15
7	C	1104	CLR	C7-C6-C5	-2.29	120.84	125.06
7	C	1104	CLR	C15-C14-C8	-2.28	115.32	119.08
7	G	101	CLR	C19-C10-C5	2.28	112.03	108.34
7	E	101	CLR	C8-C7-C6	-2.26	109.49	112.73
7	A	1104	CLR	C18-C13-C12	2.25	114.14	110.59
7	D	402	CLR	C22-C20-C17	-2.23	105.67	110.28
7	E	101	CLR	C19-C10-C5	2.23	111.95	108.34
7	D	402	CLR	C18-C13-C12	2.23	114.11	110.59
7	C	1104	CLR	C22-C20-C17	-2.21	105.72	110.28
7	D	402	CLR	O1-C3-C2	2.20	115.76	110.16
7	C	1104	CLR	C10-C5-C6	2.20	126.27	122.90
7	A	1104	CLR	C15-C14-C8	-2.19	115.48	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1104	CLR	C18-C13-C12	2.19	114.04	110.59
7	A	1104	CLR	C22-C20-C17	-2.18	105.78	110.28
7	C	1104	CLR	O1-C3-C2	2.18	115.70	110.16
7	B	402	CLR	C16-C17-C20	-2.18	108.78	112.15
7	A	1104	CLR	C7-C6-C5	-2.17	121.05	125.06
7	D	402	CLR	C3-C4-C5	2.17	115.71	112.03
7	E	101	CLR	C21-C20-C17	2.15	116.22	112.92
7	E	101	CLR	C16-C17-C20	-2.15	108.82	112.15
7	G	101	CLR	C21-C20-C17	2.13	116.18	112.92
7	D	402	CLR	C17-C13-C14	-2.13	97.55	100.07
7	C	1104	CLR	C16-C17-C20	-2.12	108.86	112.15
7	G	101	CLR	C11-C9-C10	2.12	115.87	113.08
7	C	1104	CLR	C21-C20-C17	2.12	116.16	112.92
7	E	101	CLR	O1-C3-C4	2.12	114.21	109.68
7	D	402	CLR	C21-C20-C17	2.11	116.15	112.92
9	C	1121	DGX	C11-C9-C10	-2.11	111.56	113.73
7	C	1104	CLR	C13-C17-C20	-2.10	116.19	119.49
7	C	1104	CLR	C15-C14-C13	2.08	106.35	103.84
7	G	101	CLR	O1-C3-C4	2.08	114.13	109.68
7	C	1104	CLR	C3-C4-C5	2.05	115.50	112.03
7	B	402	CLR	C21-C20-C17	2.03	116.03	112.92
7	G	101	CLR	C8-C7-C6	-2.03	109.82	112.73
7	D	402	CLR	C16-C17-C20	-2.02	109.03	112.15
7	B	402	CLR	C15-C14-C8	-2.00	115.78	119.08

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1105	PCW	C4-O4P-P-O1P
8	A	1106	PCW	O4P-C4-C5-N
8	A	1107	PCW	C1-O3P-P-O2P
8	A	1108	PCW	C4-O4P-P-O1P
8	A	1108	PCW	C4-O4P-P-O2P
8	A	1109	PCW	C1-O3P-P-O1P
8	A	1109	PCW	C1-O3P-P-O2P
8	C	1108	PCW	O4P-C4-C5-N
8	C	1108	PCW	C32-C31-O2-C2
8	C	1108	PCW	C1-O3P-P-O1P
8	C	1108	PCW	C1-O3P-P-O2P
8	C	1108	PCW	C1-O3P-P-O4P
8	C	1105	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
8	C	1105	PCW	C1-O3P-P-O2P
8	C	1105	PCW	C1-O3P-P-O4P
8	C	1105	PCW	C4-O4P-P-O1P
8	C	1105	PCW	C4-O4P-P-O2P
8	C	1107	PCW	C4-O4P-P-O2P
8	A	1105	PCW	C32-C31-O2-C2
8	A	1106	PCW	C32-C31-O2-C2
8	A	1109	PCW	C32-C31-O2-C2
8	C	1105	PCW	C32-C31-O2-C2
8	C	1107	PCW	C32-C31-O2-C2
8	A	1106	PCW	O31-C31-O2-C2
8	B	403	PCW	C32-C31-O2-C2
8	A	1105	PCW	O31-C31-O2-C2
8	A	1109	PCW	O31-C31-O2-C2
8	C	1106	PCW	C32-C31-O2-C2
8	A	1107	PCW	C32-C31-O2-C2
8	A	1105	PCW	O11-C11-O3-C3
8	C	1108	PCW	O31-C31-O2-C2
8	C	1105	PCW	O31-C31-O2-C2
8	A	1105	PCW	C12-C11-O3-C3
8	C	1106	PCW	C12-C11-O3-C3
8	A	1106	PCW	O11-C11-O3-C3
8	A	1109	PCW	O11-C11-O3-C3
8	C	1108	PCW	C12-C11-O3-C3
8	A	1108	PCW	C32-C31-O2-C2
8	B	403	PCW	C12-C11-O3-C3
10	D	401	NAG	O5-C5-C6-O6
8	C	1107	PCW	O11-C11-O3-C3
8	C	1107	PCW	O31-C31-O2-C2
7	G	101	CLR	C21-C20-C22-C23
8	C	1107	PCW	C12-C11-O3-C3
8	B	403	PCW	O31-C31-O2-C2
10	D	401	NAG	C8-C7-N2-C2
10	D	401	NAG	O7-C7-N2-C2
8	C	1106	PCW	O31-C31-O2-C2
10	D	401	NAG	C4-C5-C6-O6
7	E	101	CLR	C21-C20-C22-C23
8	A	1109	PCW	C12-C11-O3-C3
8	A	1106	PCW	C12-C11-O3-C3
8	C	1105	PCW	C12-C11-O3-C3
8	C	1108	PCW	O11-C11-O3-C3
7	C	1104	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	B	403	PCW	O11-C11-O3-C3
7	A	1104	CLR	C20-C22-C23-C24
8	C	1106	PCW	O11-C11-O3-C3
8	A	1105	PCW	C4-O4P-P-O3P
8	A	1108	PCW	C4-O4P-P-O3P
8	A	1109	PCW	C1-O3P-P-O4P
8	A	1109	PCW	C4-O4P-P-O3P
8	C	1105	PCW	C4-O4P-P-O3P
8	A	1107	PCW	O31-C31-O2-C2
8	A	1106	PCW	C4-C5-N-C6
8	A	1106	PCW	C4-C5-N-C7
8	A	1106	PCW	C4-C5-N-C8
7	E	101	CLR	C20-C22-C23-C24
7	C	1104	CLR	C23-C24-C25-C26
8	A	1108	PCW	O31-C31-O2-C2
7	B	402	CLR	C21-C20-C22-C23
8	A	1108	PCW	C1-C2-C3-O3
7	A	1104	CLR	C23-C24-C25-C26
8	C	1105	PCW	O11-C11-O3-C3
7	E	101	CLR	C22-C23-C24-C25
8	A	1107	PCW	O2-C2-C3-O3
7	G	101	CLR	C22-C23-C24-C25
8	A	1109	PCW	O3P-C1-C2-C3
8	C	1108	PCW	O3P-C1-C2-C3
8	C	1107	PCW	O3P-C1-C2-C3
8	A	1107	PCW	C12-C11-O3-C3
7	C	1104	CLR	C23-C24-C25-C27
7	G	101	CLR	C20-C22-C23-C24
9	C	1121	DGX	C5X-C4X-O4X-C1Y
8	C	1108	PCW	O2-C2-C3-O3
7	A	1104	CLR	C13-C17-C20-C21
7	C	1104	CLR	C13-C17-C20-C21
9	C	1121	DGX	C3X-C4X-O4X-C1Y
8	A	1106	PCW	O3P-C1-C2-C3
8	A	1107	PCW	C1-C2-C3-O3
8	B	403	PCW	C1-C2-C3-O3
8	C	1106	PCW	C1-C2-C3-O3
8	C	1107	PCW	C1-O3P-P-O4P
8	A	1105	PCW	O2-C2-C3-O3
7	A	1104	CLR	C23-C24-C25-C27
10	B	401	NAG	O5-C5-C6-O6
8	A	1105	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	A	1106	PCW	C3-C2-O2-C31
8	A	1109	PCW	C1-C2-C3-O3
8	A	1106	PCW	O3P-C1-C2-O2
8	C	1108	PCW	O3P-C1-C2-O2
8	B	403	PCW	O2-C2-C3-O3
9	A	1110	DGX	C5X-C4X-O4X-C1Y
9	A	1110	DGX	C3Y-C4Y-O4Y-C1Z
9	A	1110	DGX	C5Y-C4Y-O4Y-C1Z
8	A	1107	PCW	C1-O3P-P-O4P
8	C	1107	PCW	C4-O4P-P-O3P
8	A	1105	PCW	C4-O4P-P-O2P
8	A	1109	PCW	C4-O4P-P-O2P
9	A	1110	DGX	C3X-C4X-O4X-C1Y
9	C	1121	DGX	C5Y-C4Y-O4Y-C1Z
8	A	1105	PCW	O3P-C1-C2-O2
8	A	1109	PCW	O3P-C1-C2-O2
8	A	1107	PCW	O11-C11-O3-C3
8	A	1105	PCW	C1-C2-C3-O3
8	A	1105	PCW	O4P-C4-C5-N
8	A	1107	PCW	O4P-C4-C5-N
8	A	1108	PCW	O4P-C4-C5-N
8	A	1109	PCW	O4P-C4-C5-N
8	B	403	PCW	O4P-C4-C5-N
8	C	1108	PCW	C1-C2-C3-O3
8	C	1105	PCW	O4P-C4-C5-N
8	C	1106	PCW	O4P-C4-C5-N
8	C	1107	PCW	O4P-C4-C5-N
9	C	1121	DGX	C3Y-C4Y-O4Y-C1Z
8	A	1106	PCW	O2-C2-C3-O3
8	A	1108	PCW	O2-C2-C3-O3
8	A	1109	PCW	O2-C2-C3-O3
8	C	1106	PCW	O2-C2-C3-O3
7	A	1104	CLR	C13-C17-C20-C22
7	C	1104	CLR	C13-C17-C20-C22
8	C	1107	PCW	O3P-C1-C2-O2
8	A	1106	PCW	C1-O3P-P-O4P
8	A	1106	PCW	C4-O4P-P-O3P
8	A	1107	PCW	C4-O4P-P-O3P
8	A	1108	PCW	C1-O3P-P-O4P
8	B	403	PCW	C1-O3P-P-O4P
8	B	403	PCW	C4-O4P-P-O3P
8	C	1108	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
8	C	1106	PCW	C1-O3P-P-O4P
8	C	1106	PCW	C4-O4P-P-O3P
7	C	1104	CLR	C22-C23-C24-C25
7	A	1104	CLR	C16-C17-C20-C21
7	D	402	CLR	C23-C24-C25-C26
8	A	1106	PCW	C1-C2-C3-O3
8	A	1108	PCW	C12-C11-O3-C3
8	A	1106	PCW	C4-O4P-P-O2P
8	A	1107	PCW	C4-O4P-P-O2P
8	B	403	PCW	C1-O3P-P-O2P
8	B	403	PCW	C4-O4P-P-O2P

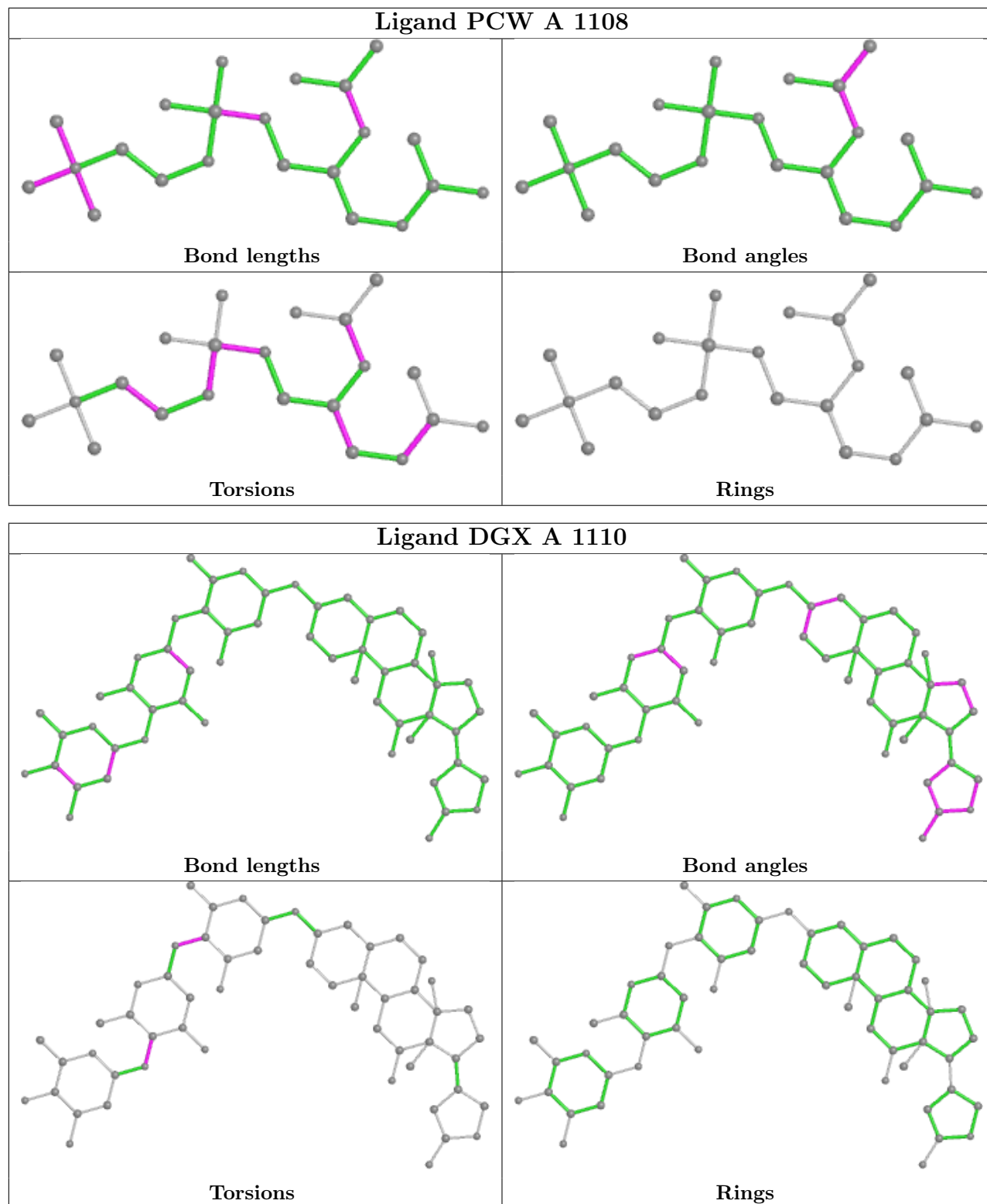
There are no ring outliers.

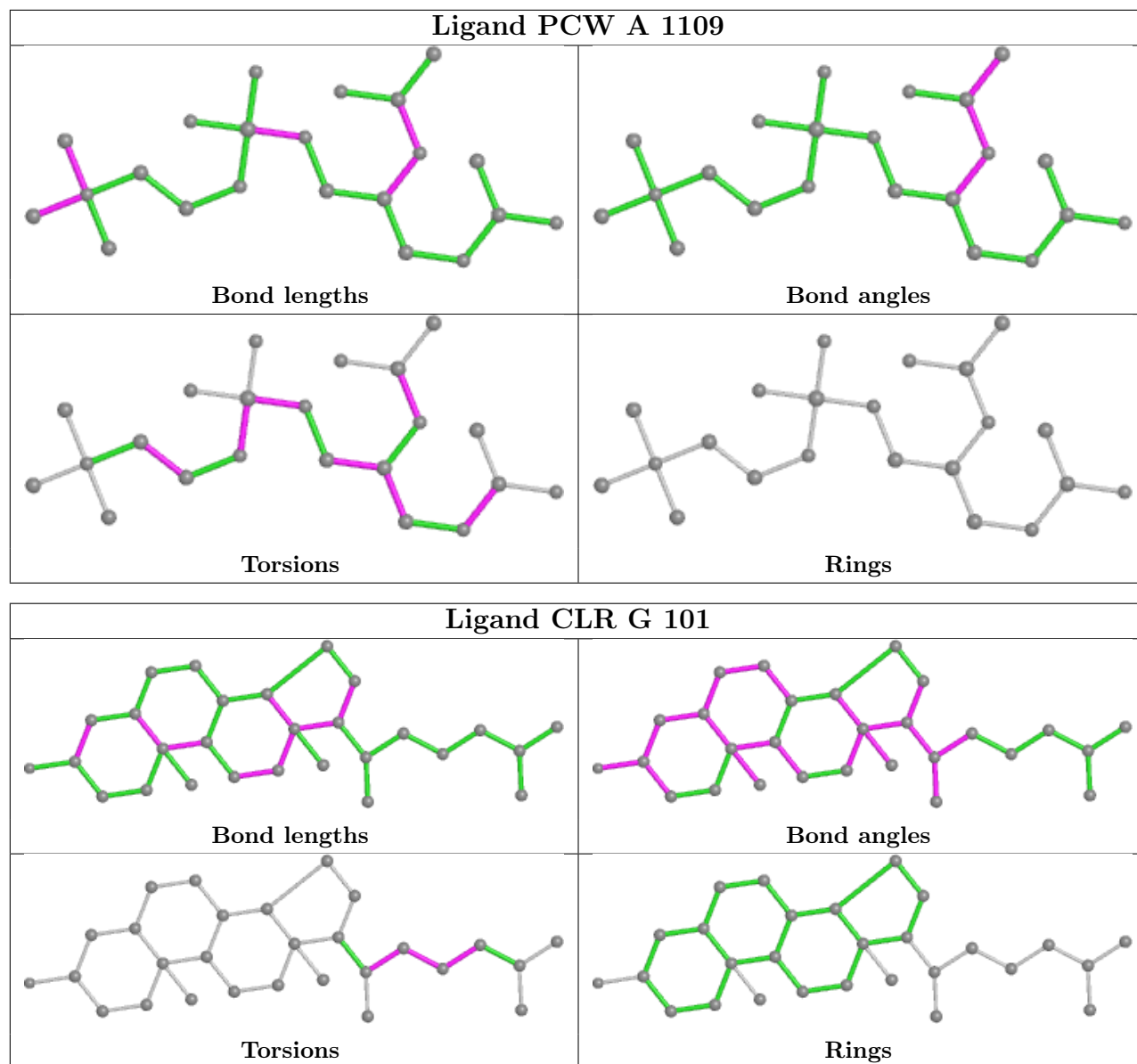
14 monomers are involved in 31 short contacts:

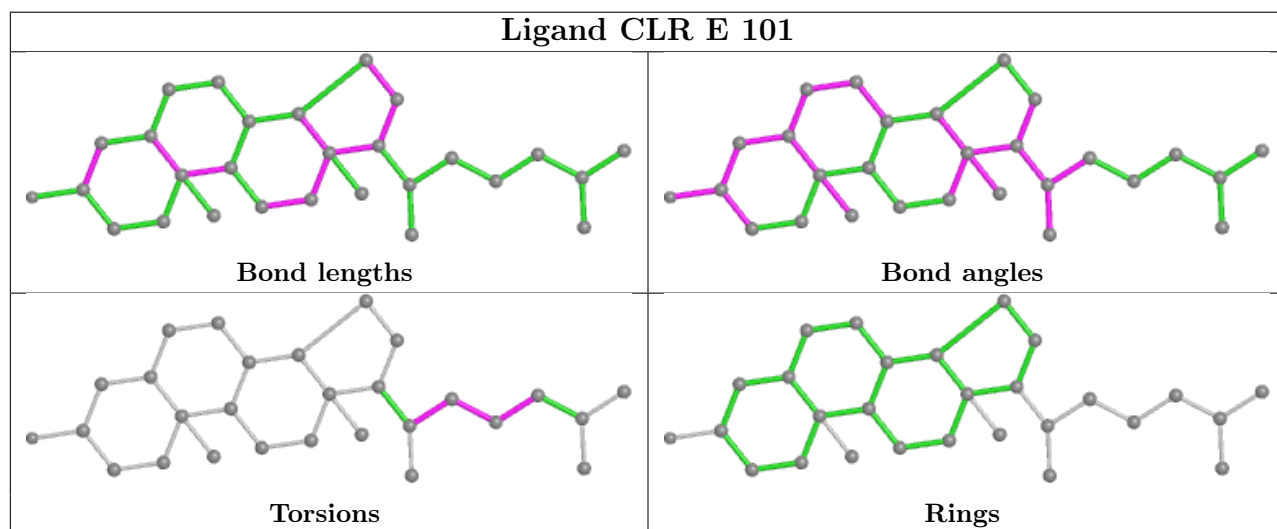
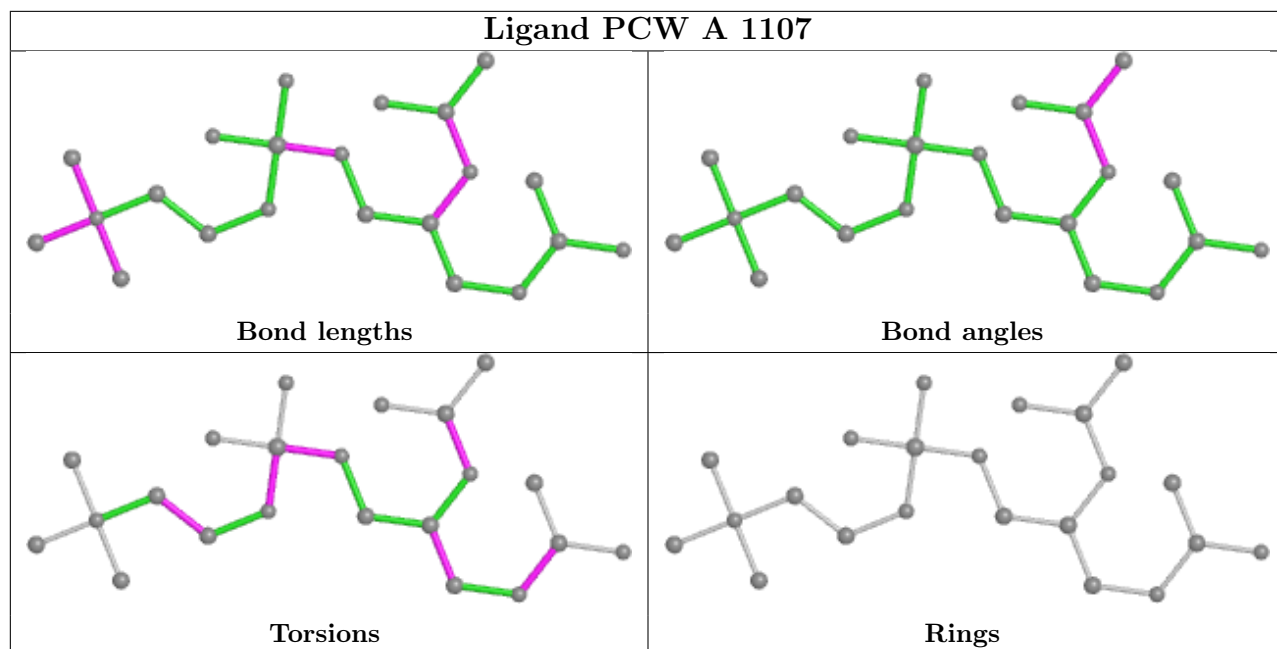
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1108	PCW	2	0
9	A	1110	DGX	1	0
8	A	1109	PCW	1	0
7	G	101	CLR	1	0
7	E	101	CLR	6	0
8	C	1107	PCW	2	0
7	C	1104	CLR	3	0
9	C	1121	DGX	2	0
8	A	1106	PCW	4	0
8	A	1105	PCW	2	0
8	C	1105	PCW	2	0
8	B	403	PCW	2	0
7	A	1104	CLR	2	0
7	D	402	CLR	1	0

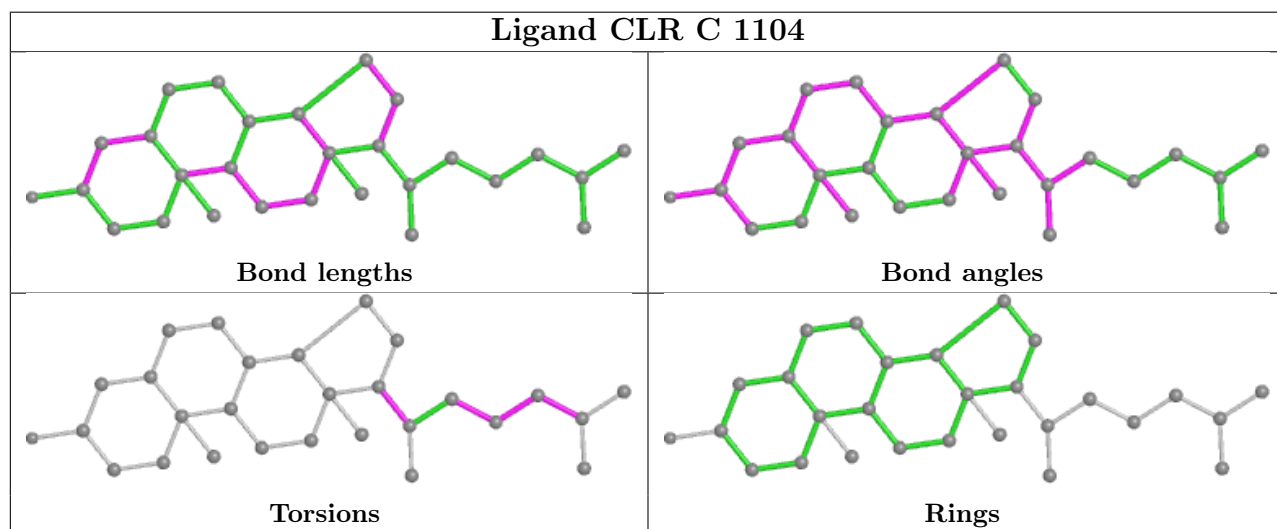
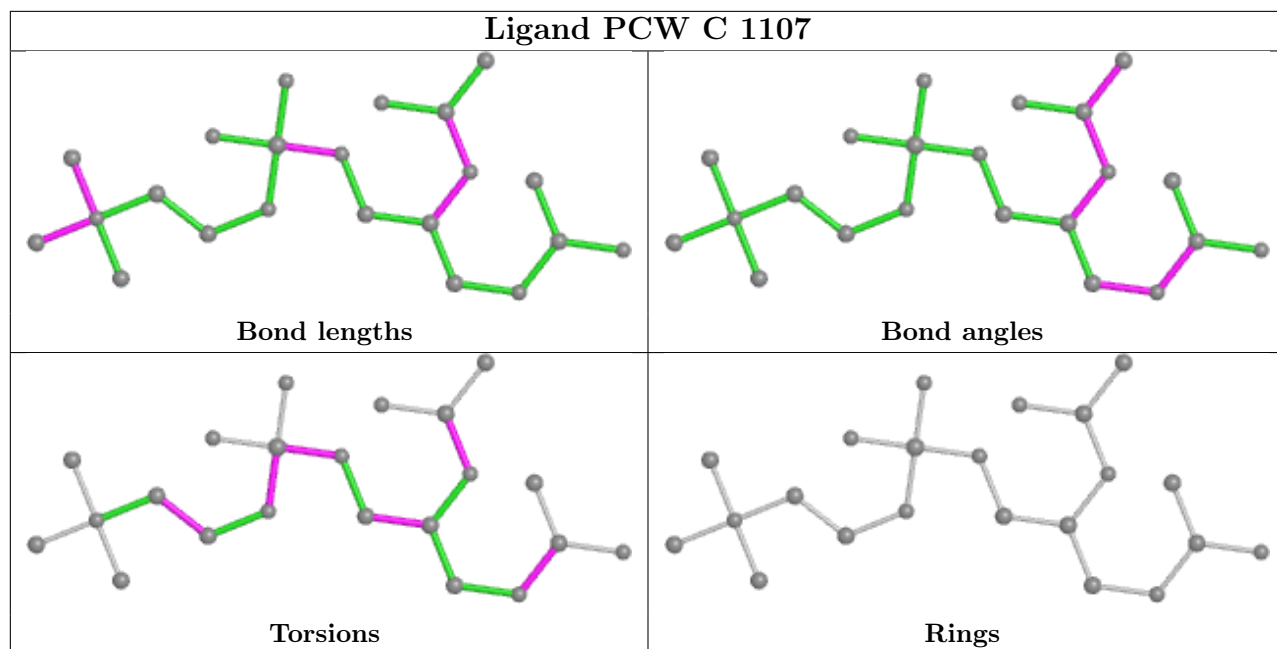
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

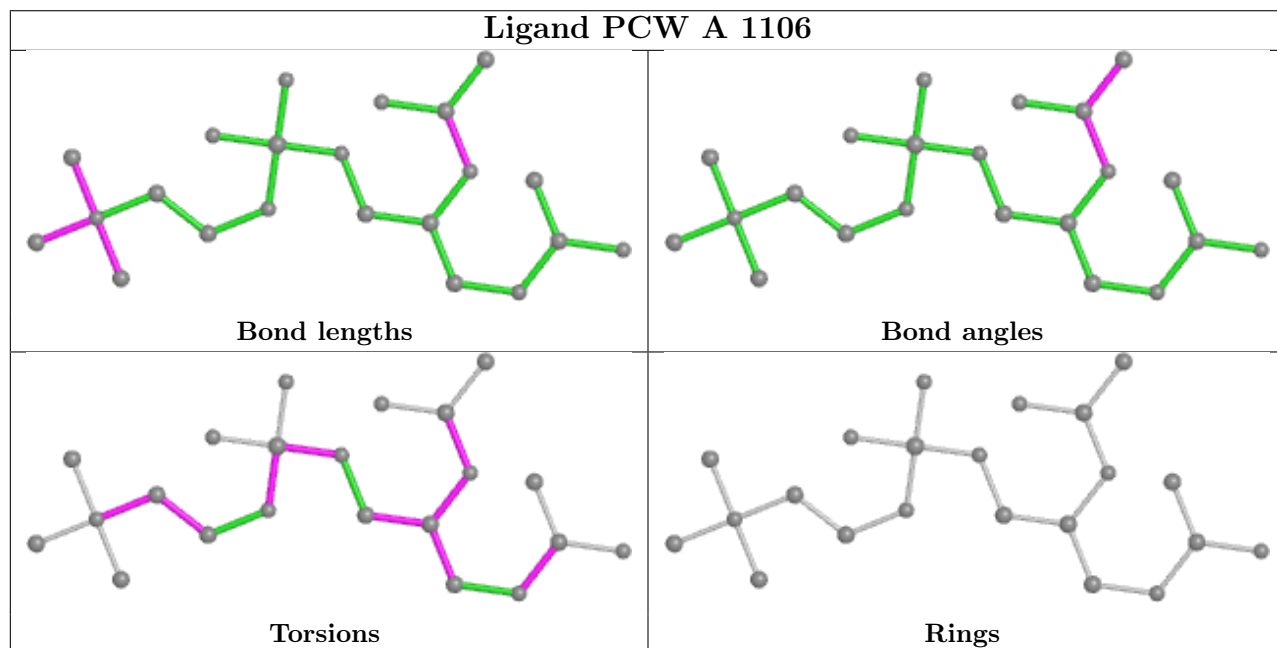
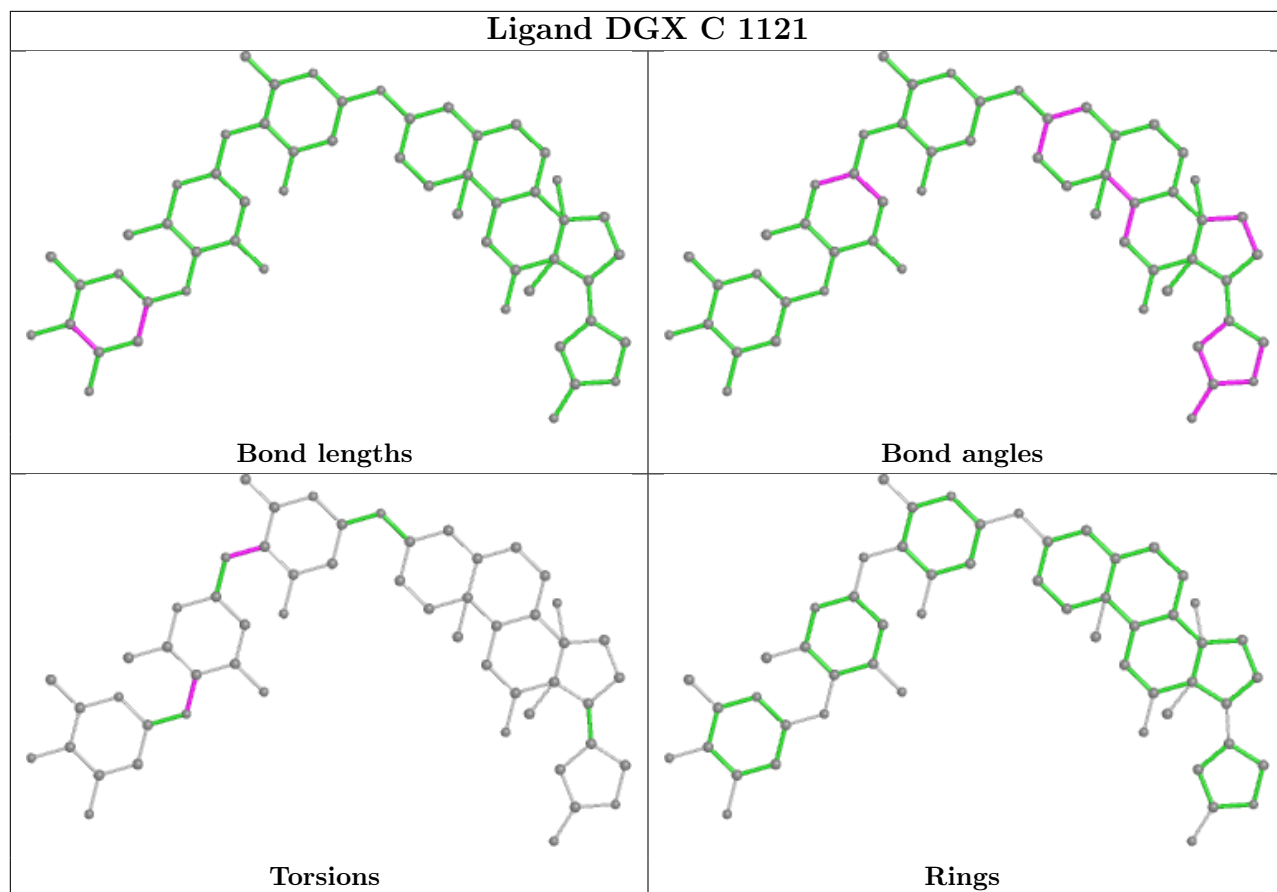
equivalents in the CSD to analyse the geometry.

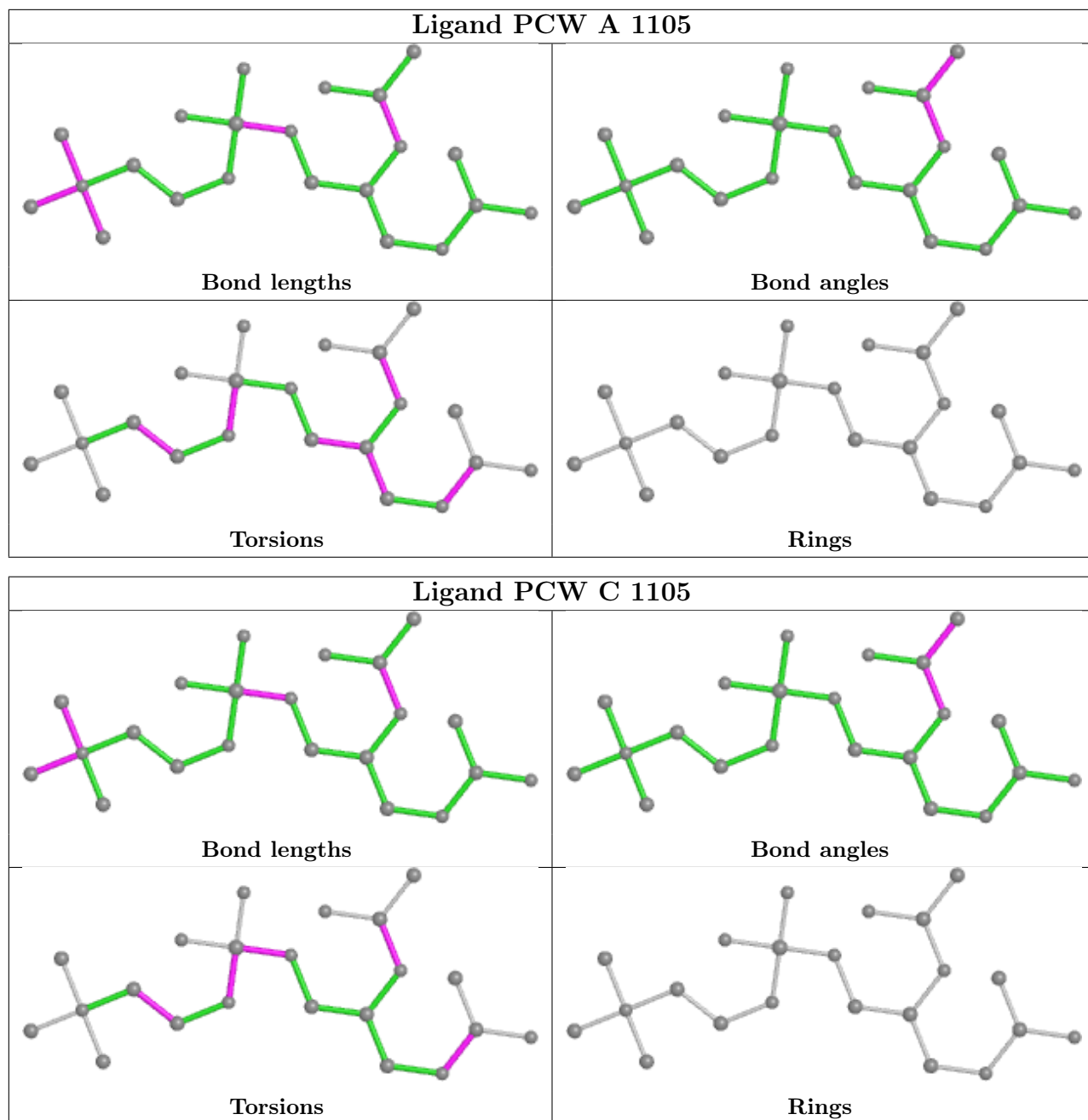


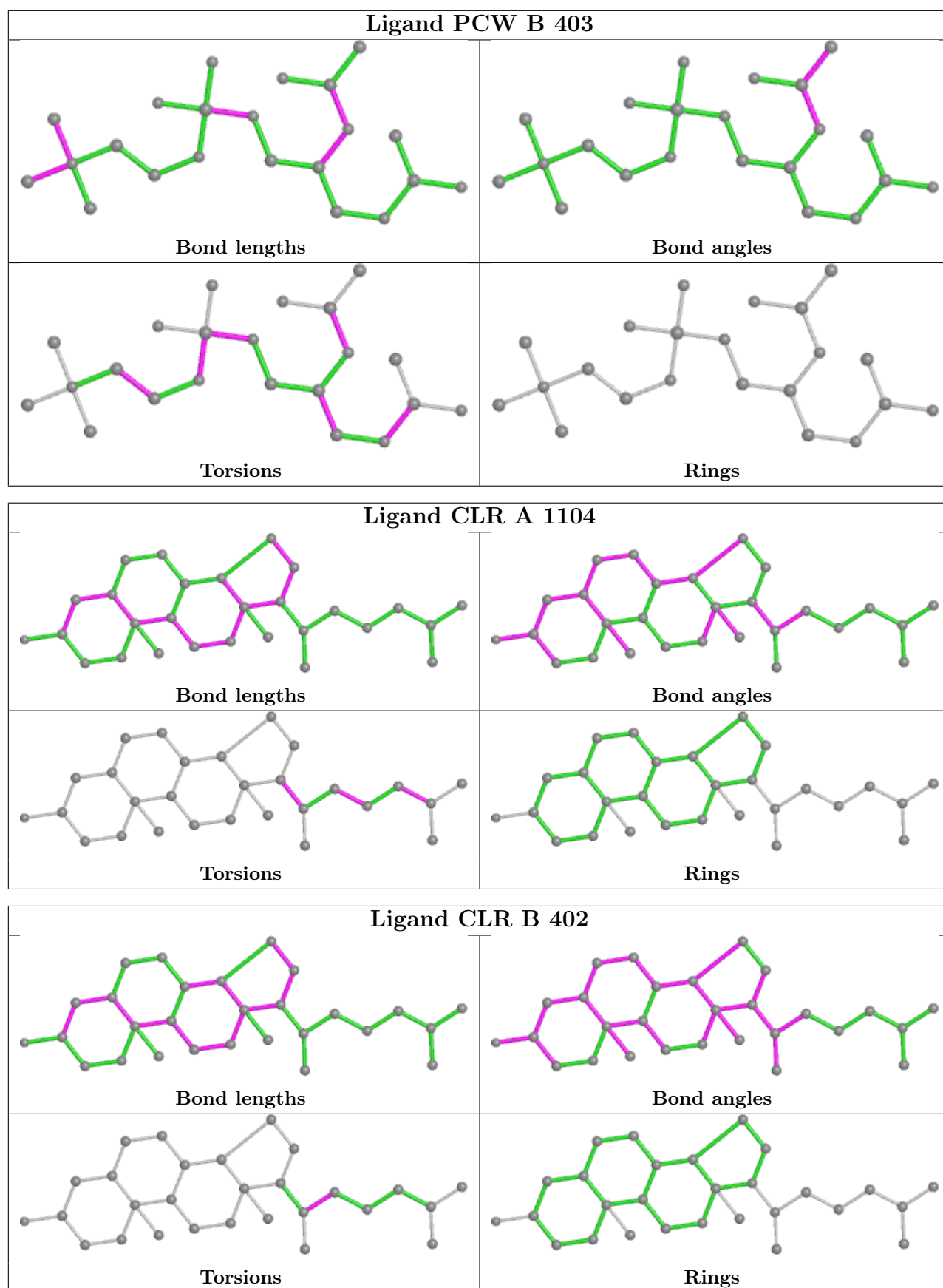


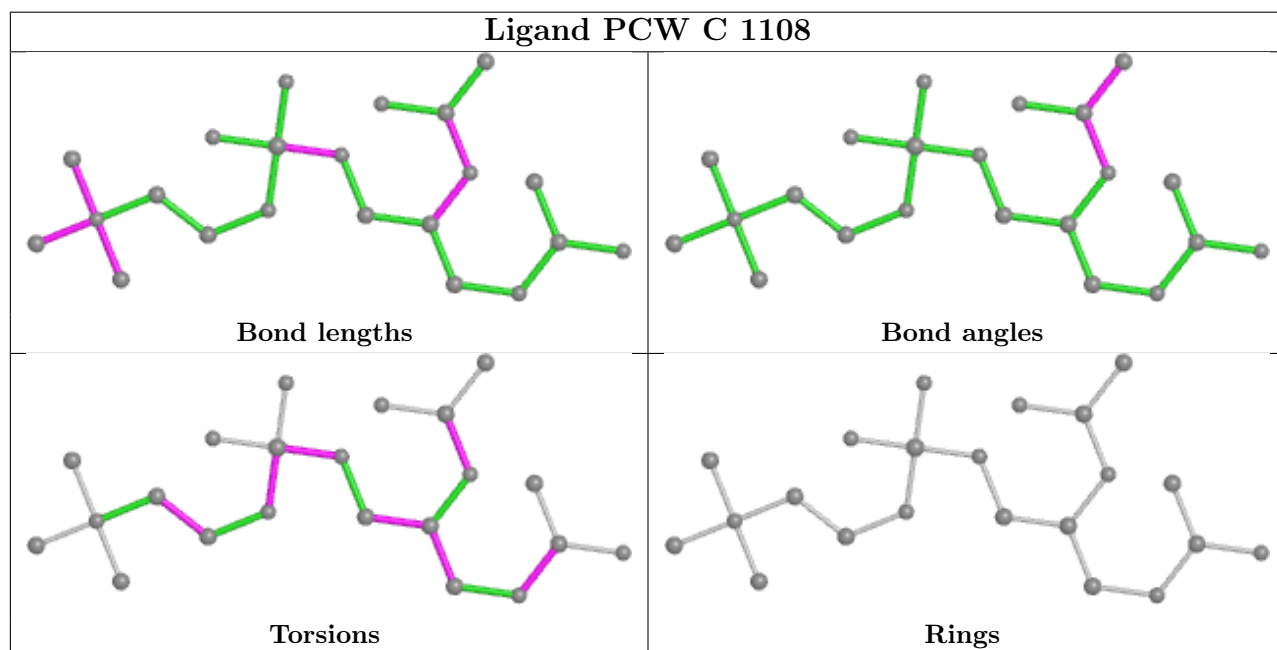
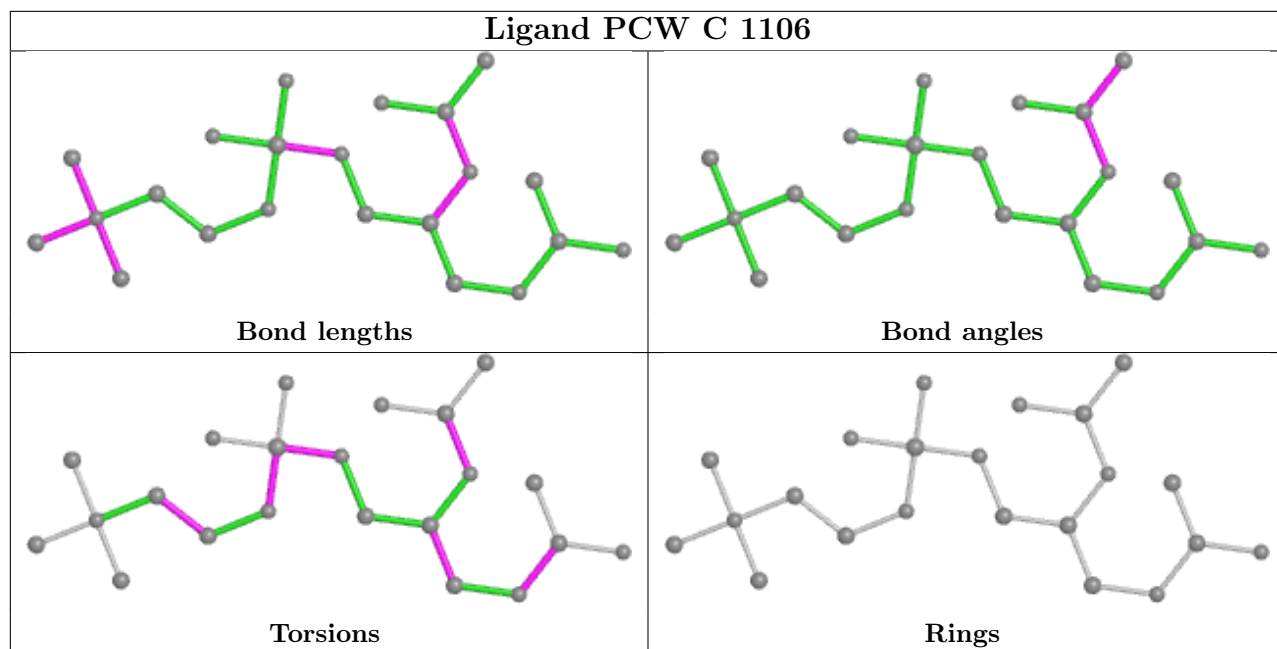


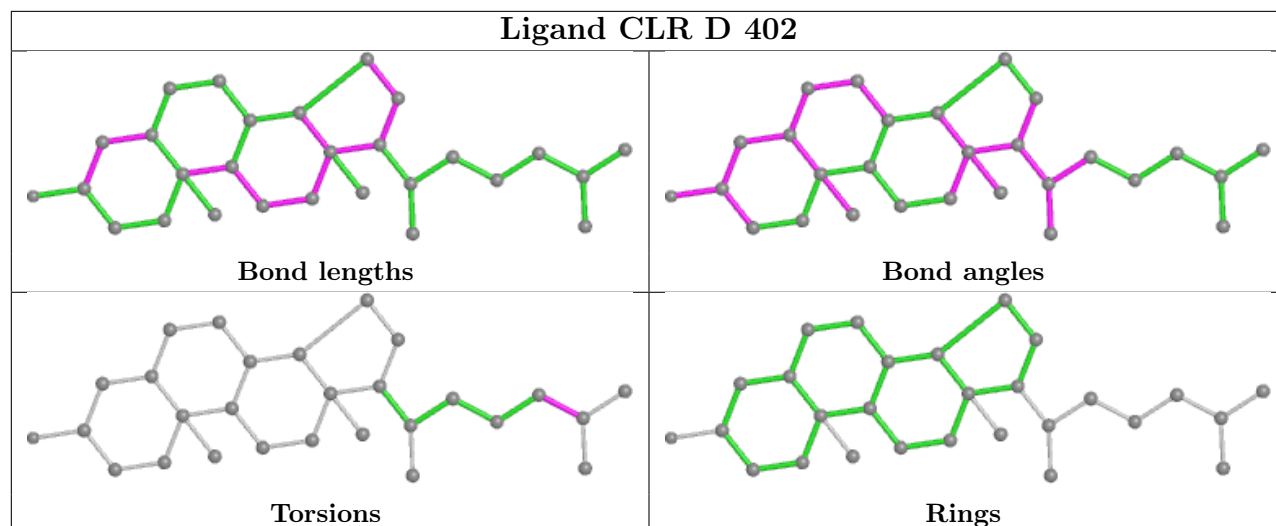












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	995/1016 (97%)	0.16	43 (4%) 35 34	50, 103, 209, 236	0
1	C	995/1016 (97%)	0.14	32 (3%) 47 46	51, 107, 185, 211	0
2	B	291/303 (96%)	0.10	21 (7%) 15 17	66, 134, 178, 209	0
2	D	285/303 (94%)	0.00	11 (3%) 39 38	58, 124, 176, 202	0
3	E	32/65 (49%)	-0.01	0 100 100	60, 84, 119, 143	0
3	G	32/65 (49%)	0.08	0 100 100	57, 85, 120, 130	0
All	All	2630/2768 (95%)	0.12	107 (4%) 37 36	50, 110, 196, 236	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	571	PHE	8.7
2	B	165	GLU	8.0
1	C	579	VAL	6.1
1	A	550	HIS	6.1
1	A	489	PRO	6.0
1	A	552	PHE	5.6
1	C	548	PHE	5.5
1	A	553	LEU	5.4
1	C	582	ILE	5.3
1	A	491	THR	5.1
1	A	578	PHE	5.1
2	B	166	THR	4.8
1	A	748	PHE	4.7
1	A	490	ASN	4.7
1	A	498	LEU	4.7
2	D	184	LEU	4.7
1	C	33	SER	4.6
1	A	514	ILE	4.5
1	A	522	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	203	LYS	4.5
2	B	211	VAL	4.4
2	B	198	THR	4.2
1	A	497	LEU	4.2
2	B	64	PHE	4.2
1	A	526	GLU	4.1
1	C	501	LYS	3.9
2	B	176	VAL	3.8
1	A	515	LEU	3.8
1	A	527	LEU	3.8
1	A	545	VAL	3.7
1	C	545	VAL	3.7
1	C	578	PHE	3.6
1	C	497	LEU	3.6
2	B	199	TYR	3.5
1	A	486	HIS	3.5
1	A	581	LEU	3.4
1	C	571	PHE	3.4
1	C	546	LEU	3.3
1	C	480	LYS	3.3
2	D	64	PHE	3.2
1	A	466	ARG	3.2
2	B	216	LYS	3.2
1	A	467	TYR	3.2
1	C	93	PHE	3.1
1	C	748	PHE	3.1
1	A	504	PRO	3.1
1	C	449	LEU	3.1
1	A	582	ILE	3.1
2	D	199	TYR	3.1
2	B	263	PHE	3.1
1	A	551	LEU	3.1
2	D	151	PHE	3.0
2	B	178	ILE	2.9
1	A	492	ALA	2.9
1	C	581	LEU	2.9
1	A	524	ASP	2.9
1	C	440	VAL	2.8
1	C	96	LEU	2.8
1	A	418	ALA	2.7
1	C	402	VAL	2.7
2	D	20	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	69	GLN	2.7
1	C	504	PRO	2.7
1	A	519	LYS	2.7
1	A	420	LEU	2.6
1	A	354	LEU	2.6
1	C	73	LEU	2.6
1	C	196	LEU	2.5
2	D	197	GLU	2.5
1	C	34	MET	2.5
2	D	198	THR	2.5
2	B	164	ASP	2.5
2	B	258	LEU	2.5
1	C	708	THR	2.4
2	D	156	LEU	2.4
1	A	488	ASN	2.4
2	B	167	TYR	2.4
2	B	224	VAL	2.4
1	A	419	GLY	2.3
1	C	390	ILE	2.3
1	A	542	GLY	2.3
2	D	260	ALA	2.3
1	A	607	ILE	2.3
1	A	606	VAL	2.2
1	C	580	GLY	2.2
2	D	258	LEU	2.2
1	C	236	ALA	2.2
2	B	299	ILE	2.2
1	A	546	LEU	2.1
2	B	77	LEU	2.1
1	A	366	ILE	2.1
1	A	496	HIS	2.1
1	A	449	LEU	2.1
1	A	460	VAL	2.1
2	B	177	ILE	2.1
1	A	73	LEU	2.1
1	A	179	VAL	2.1
1	C	694	ILE	2.0
1	C	259	VAL	2.0
2	B	196	LEU	2.0
1	C	260	MET	2.0
1	C	883	TRP	2.0
1	C	72	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	773	LEU	2.0
2	B	184	LEU	2.0
2	B	25	LEU	2.0
1	A	548	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PHD	A	369	12/13	0.98	0.22	73,73,97,101	0
1	PHD	C	369	12/13	0.99	0.21	86,86,118,125	0

6.3 Carbohydrates [i](#)

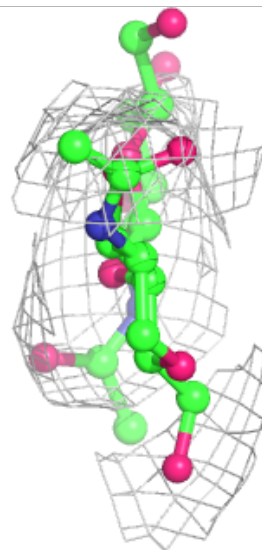
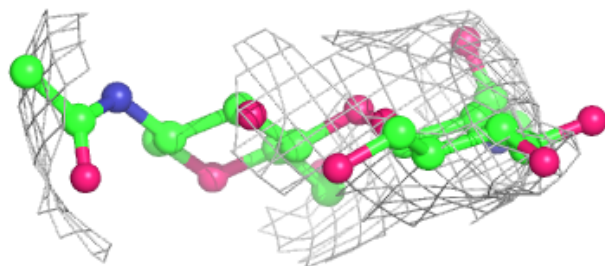
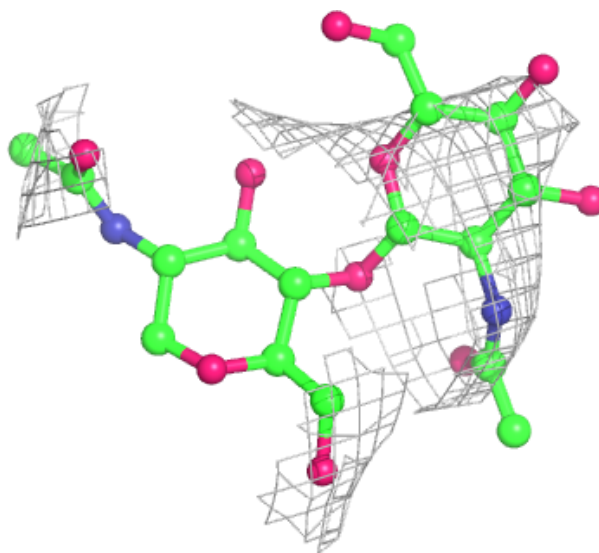
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	2	14/15	0.53	0.69	193,205,230,231	0
4	NAG	H	1	14/15	0.74	0.20	179,187,213,237	0
4	NAG	F	1	14/15	0.80	0.13	155,159,180,196	0
4	NAG	J	2	14/15	0.80	0.57	184,196,213,213	0
4	NAG	J	1	14/15	0.84	0.29	176,187,213,219	0
4	NAG	F	2	14/15	0.87	0.38	168,187,196,201	0
4	NAG	I	1	14/15	0.88	0.14	143,151,166,188	0
4	NAG	I	2	14/15	0.93	0.11	150,162,174,178	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.

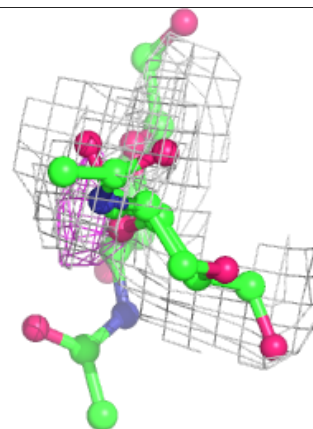
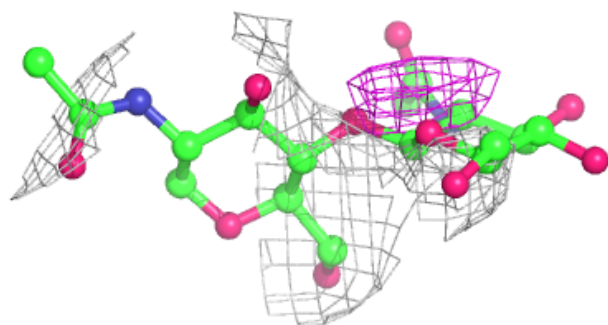
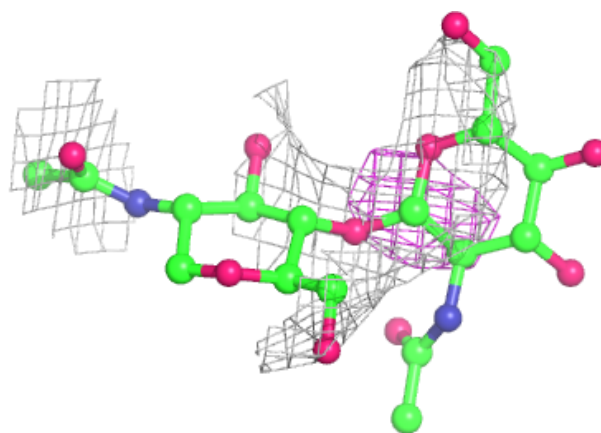
Electron density around Chain F:

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



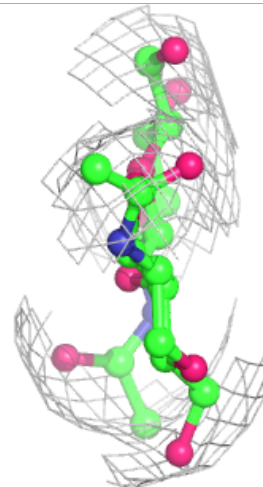
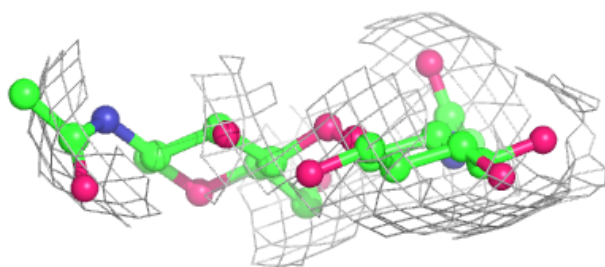
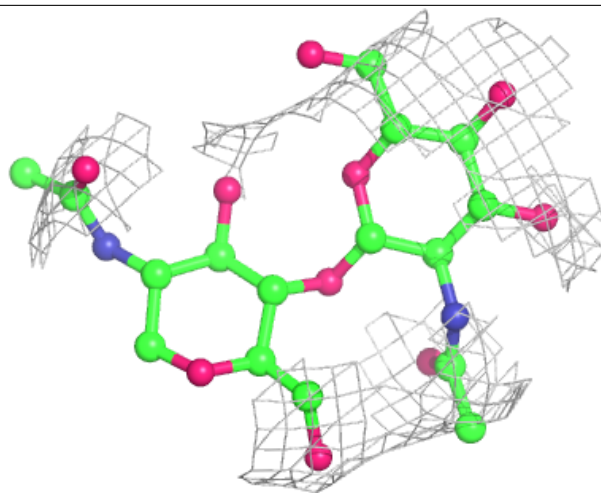
Electron density around Chain H:

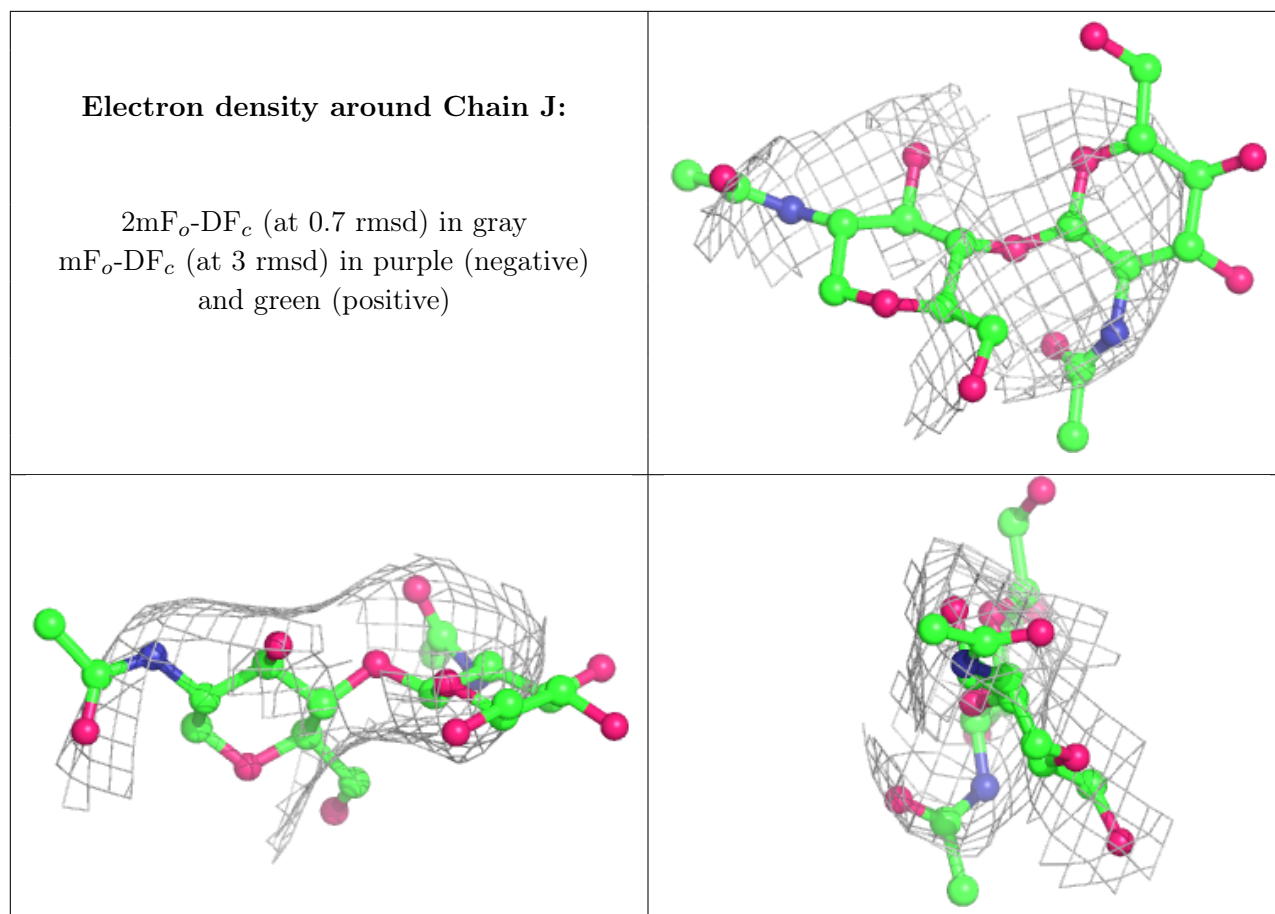
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

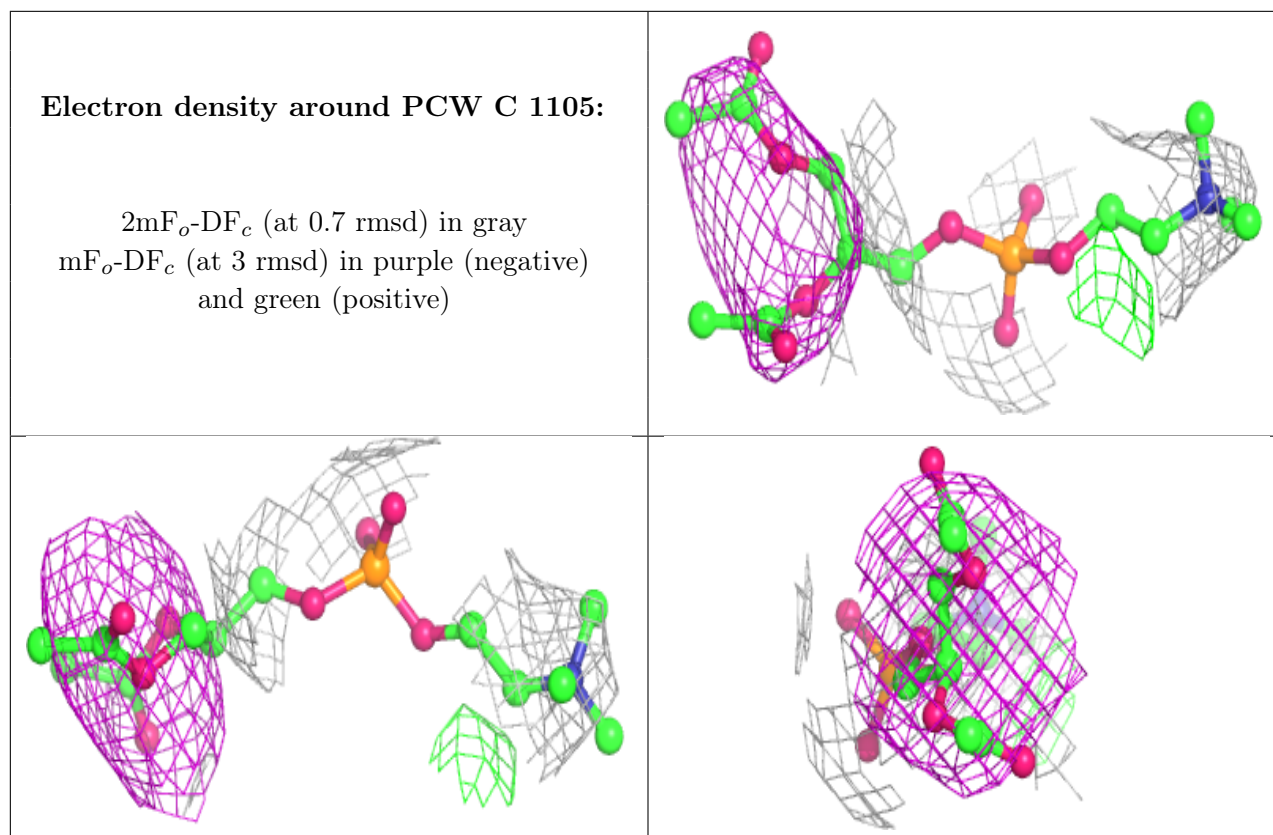
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PCW	C	1105	22/54	0.55	0.65	119,157,191,204	0
8	PCW	A	1107	22/54	0.67	0.42	154,180,205,211	0
10	NAG	B	401	14/15	0.74	0.20	161,177,190,195	0
8	PCW	A	1106	22/54	0.75	0.42	118,158,195,209	0
8	PCW	A	1108	22/54	0.75	0.69	130,163,204,216	0
10	NAG	D	401	14/15	0.77	0.18	164,178,198,201	0
8	PCW	C	1106	22/54	0.78	0.36	122,158,180,196	0
7	CLR	D	402	28/28	0.85	0.71	97,120,149,166	0
8	PCW	A	1105	22/54	0.86	0.22	93,140,181,190	0
7	CLR	A	1104	28/28	0.86	0.91	83,111,135,145	0
7	CLR	C	1104	28/28	0.88	0.70	67,104,133,144	0
9	DGX	A	1110	55/55	0.88	0.26	102,119,149,165	0

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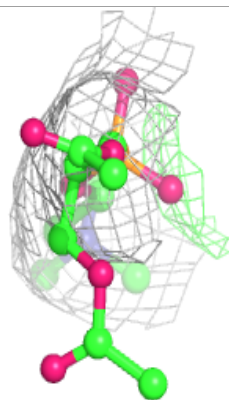
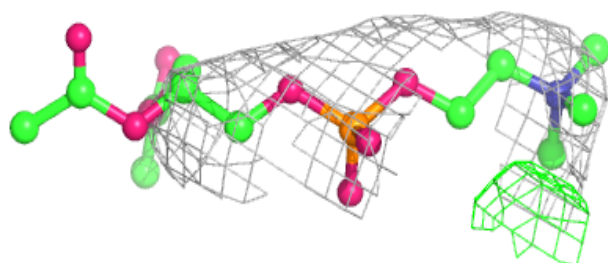
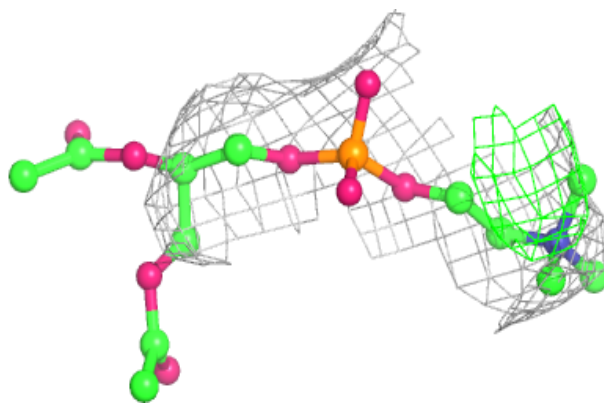
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PCW	C	1108	22/54	0.90	0.21	106,125,142,161	0
8	PCW	A	1109	22/54	0.90	0.39	83,118,149,157	0
8	PCW	B	403	22/54	0.90	0.45	118,165,189,206	0
7	CLR	B	402	28/28	0.92	0.83	107,128,142,152	0
9	DGX	C	1121	55/55	0.92	0.30	80,90,126,132	0
7	CLR	E	101	28/28	0.93	0.46	54,55,75,88	0
8	PCW	C	1107	22/54	0.93	0.32	82,112,165,171	0
7	CLR	G	101	28/28	0.95	0.47	61,63,95,121	0
6	NA	C	1102	1/1	0.97	0.38	41,41,41,41	0
5	MG	C	1103	1/1	0.97	0.20	55,55,55,55	0
6	NA	A	1102	1/1	0.97	0.29	50,50,50,50	0
5	MG	A	1103	1/1	0.98	0.28	67,67,67,67	0
5	MG	A	1101	1/1	0.98	0.20	87,87,87,87	0
5	MG	C	1101	1/1	0.99	0.22	87,87,87,87	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.

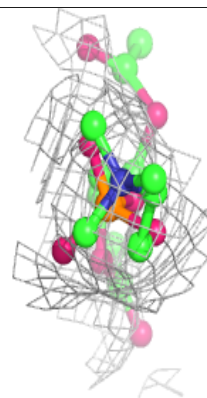
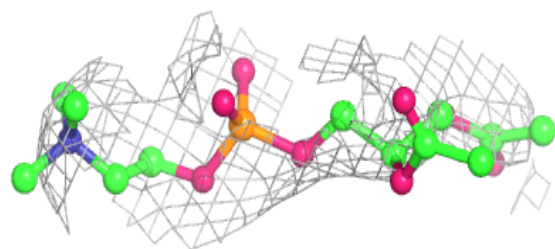
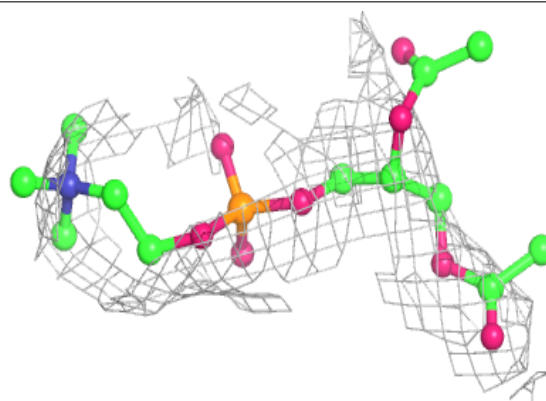


Electron density around PCW A 1107:

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

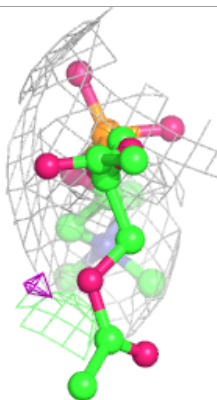
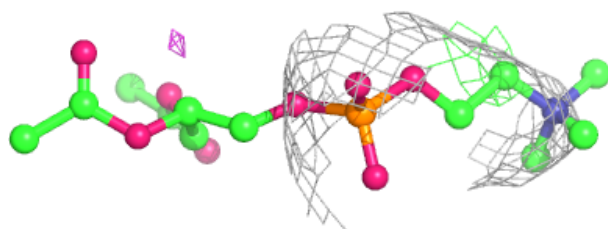
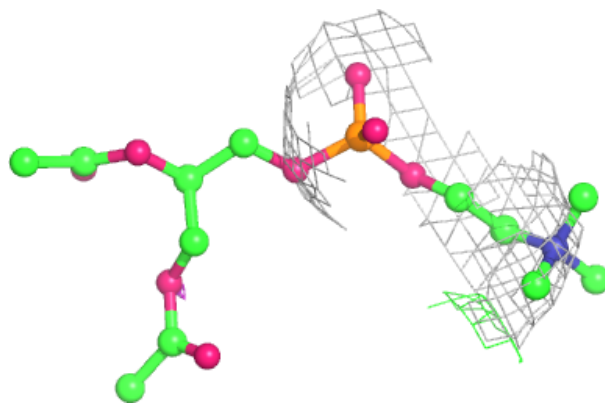
**Electron density around PCW A 1106:**

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

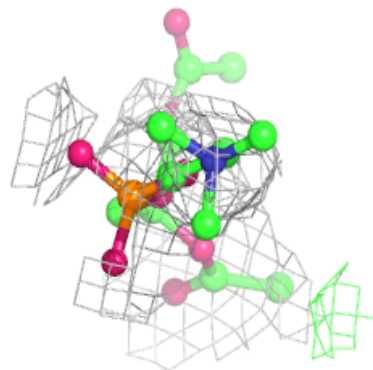
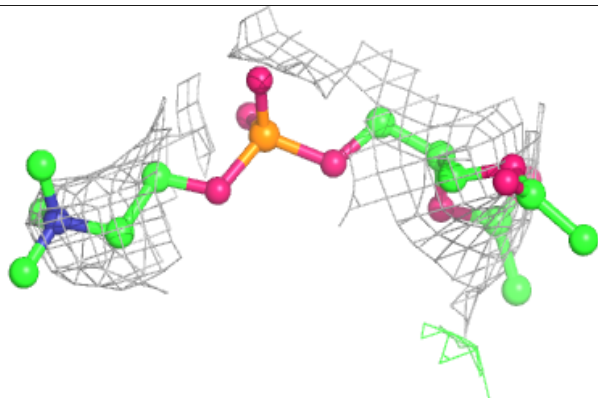
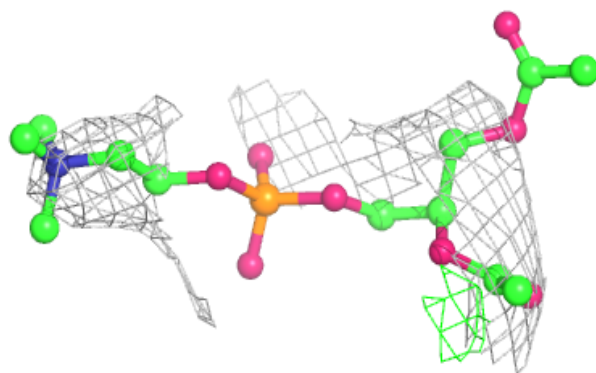


Electron density around PCW A 1108:

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

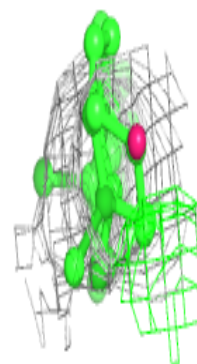
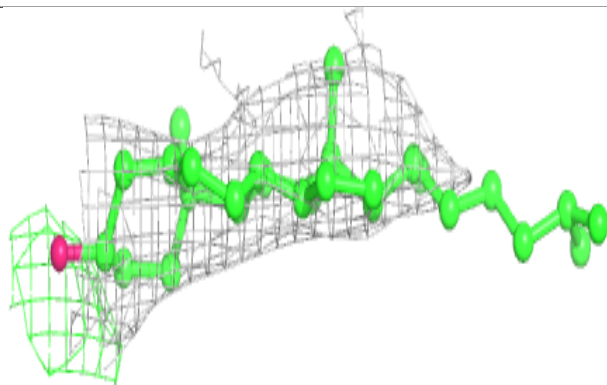
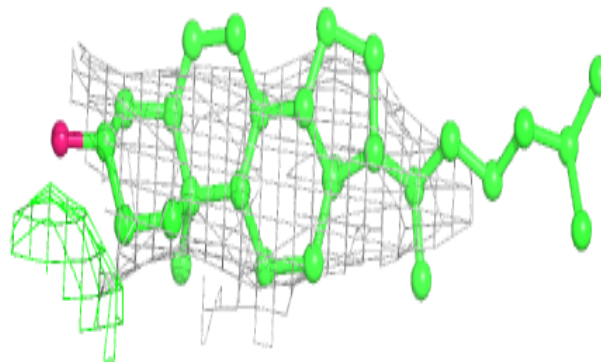
**Electron density around PCW C 1106:**

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

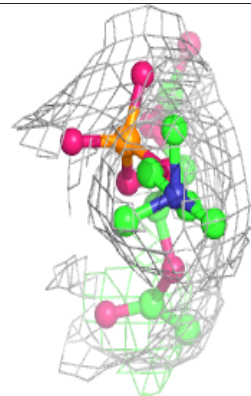
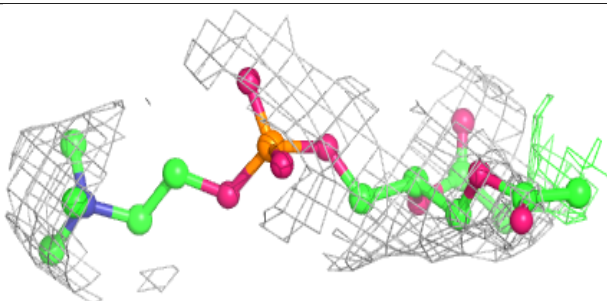
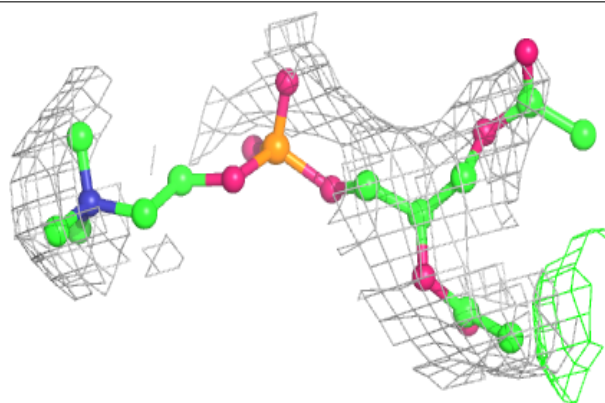


Electron density around CLR D 402:

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

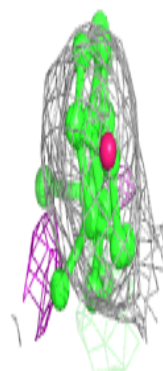
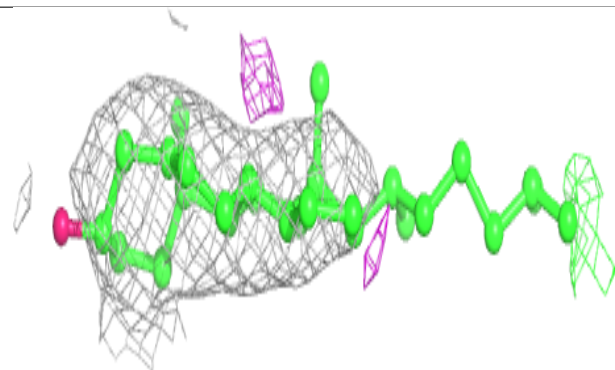
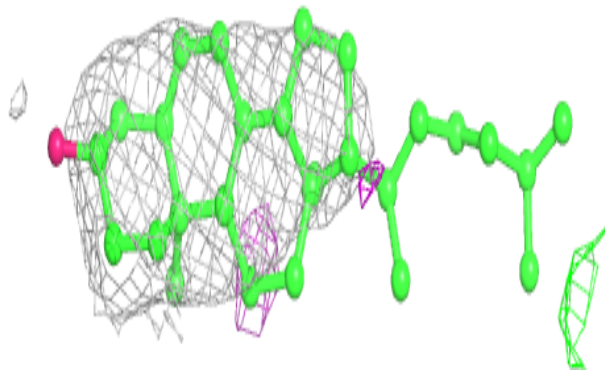
**Electron density around PCW A 1105:**

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

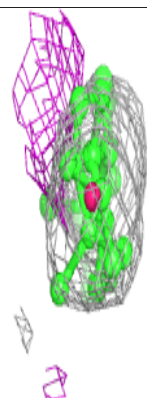
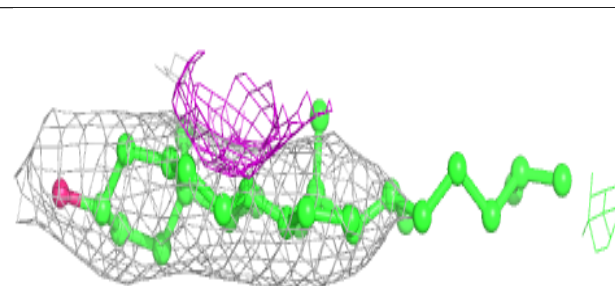
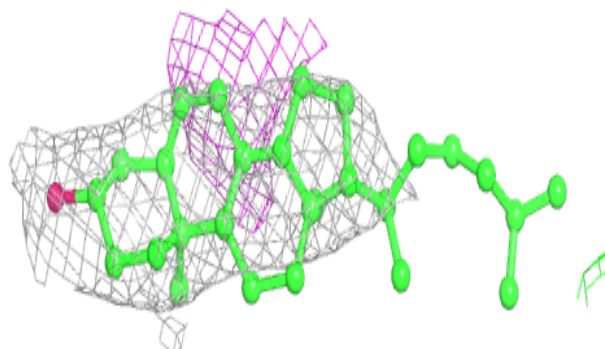


Electron density around CLR A 1104:

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

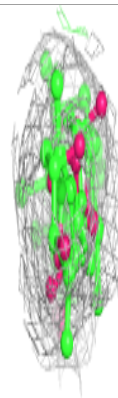
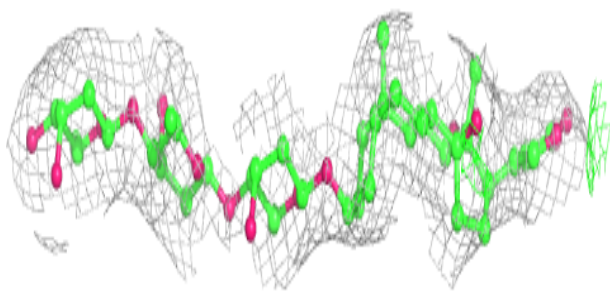
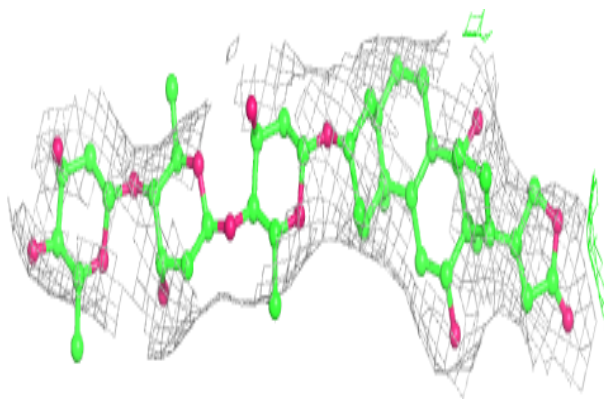
**Electron density around CLR C 1104:**

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

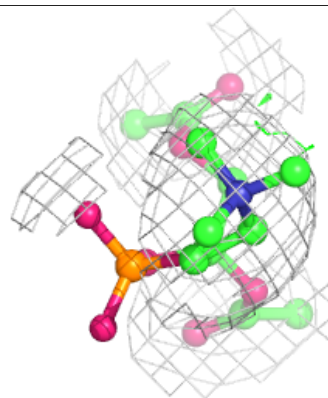
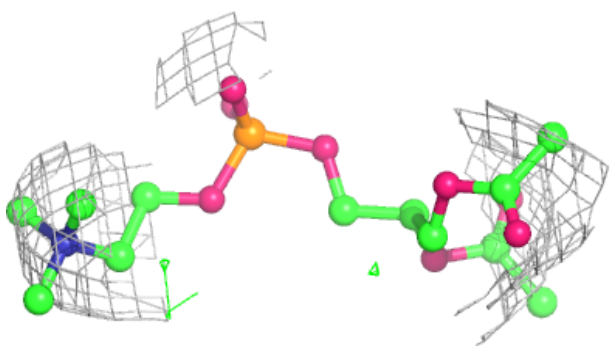
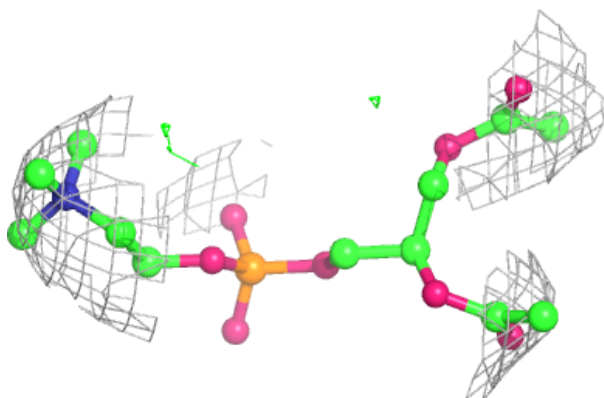


Electron density around DGX A 1110:

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

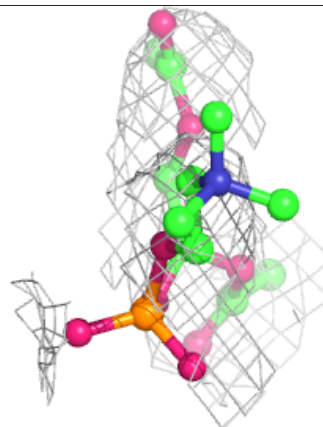
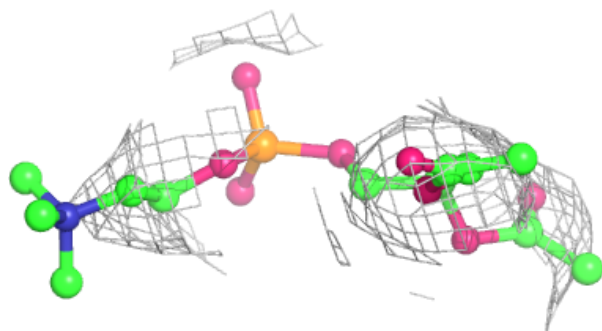
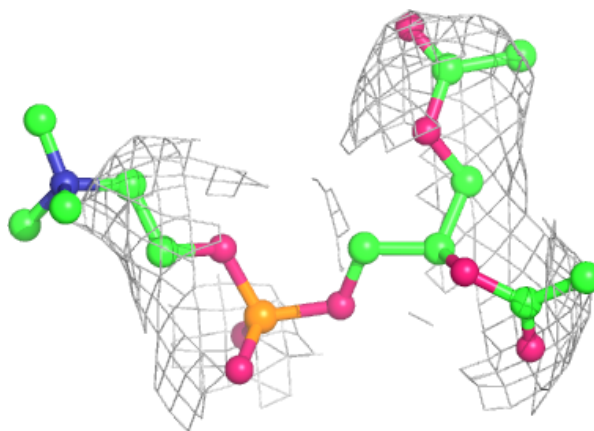
**Electron density around PCW C 1108:**

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

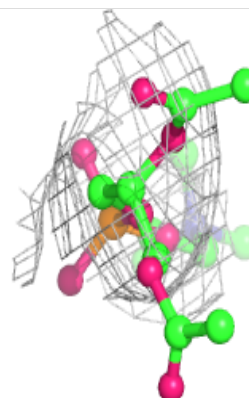
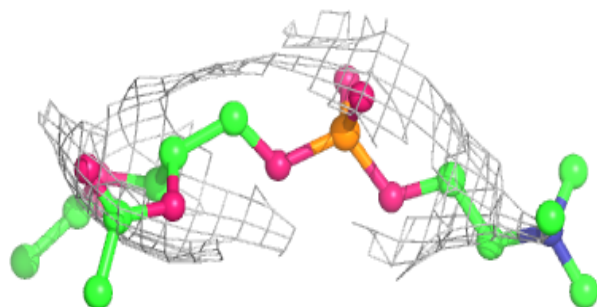
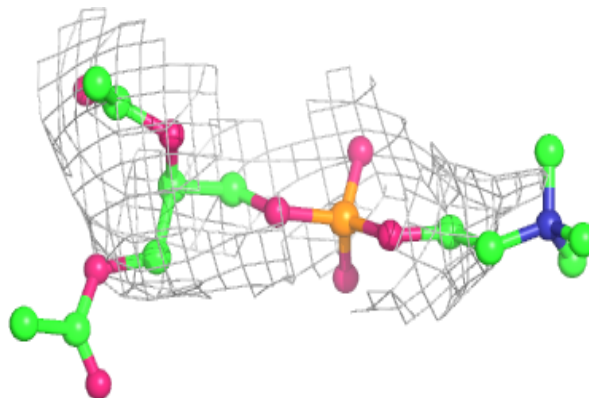


Electron density around PCW A 1109:

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

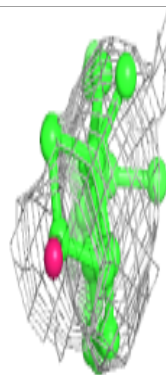
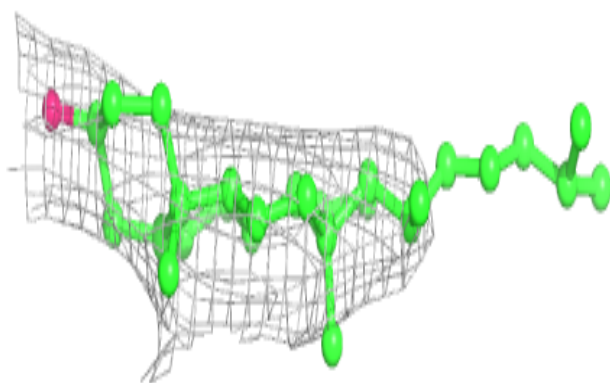
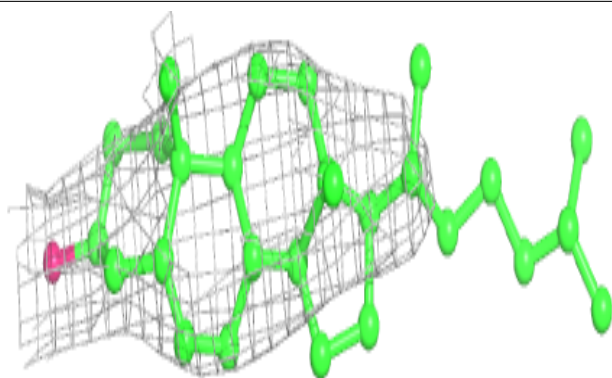
**Electron density around PCW B 403:**

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

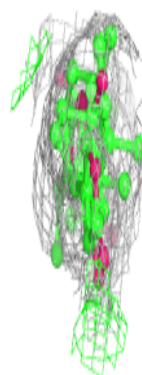
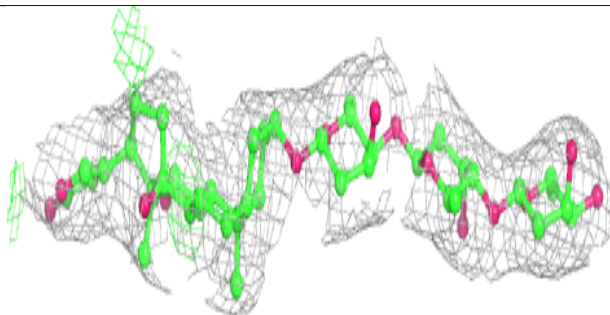
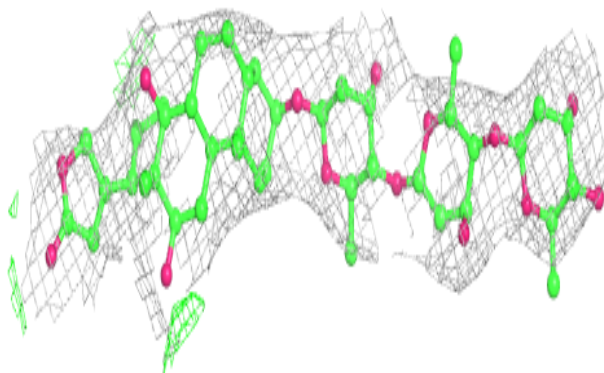


Electron density around CLR B 402:

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

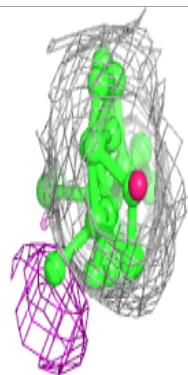
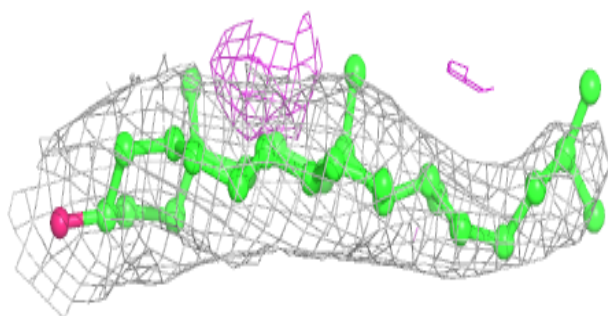
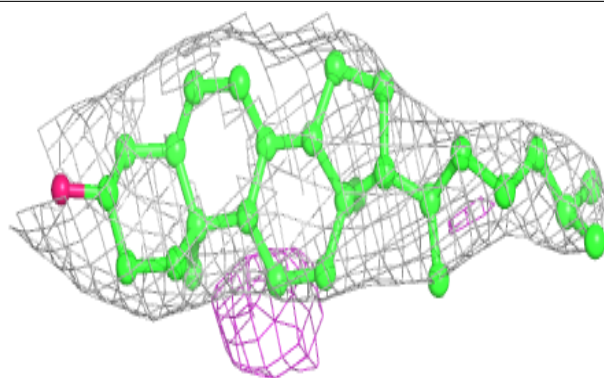
**Electron density around DGX C 1121:**

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

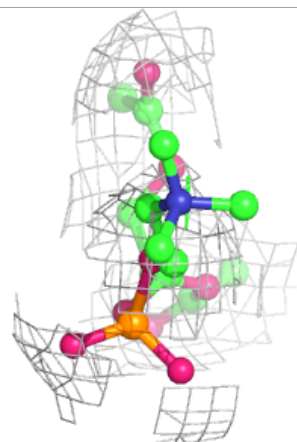
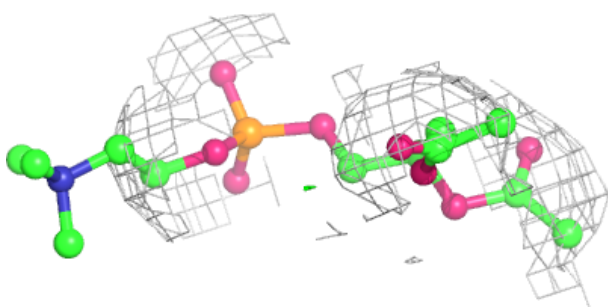
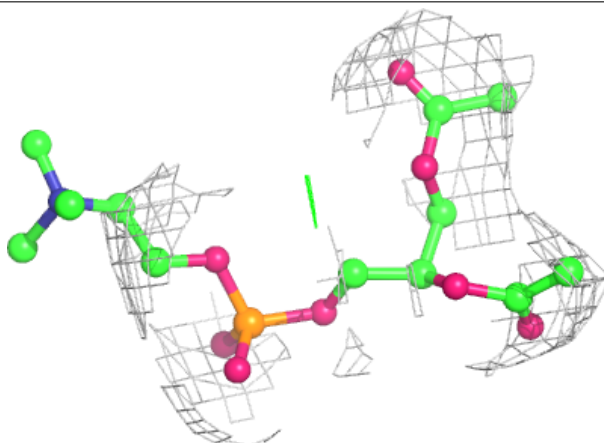


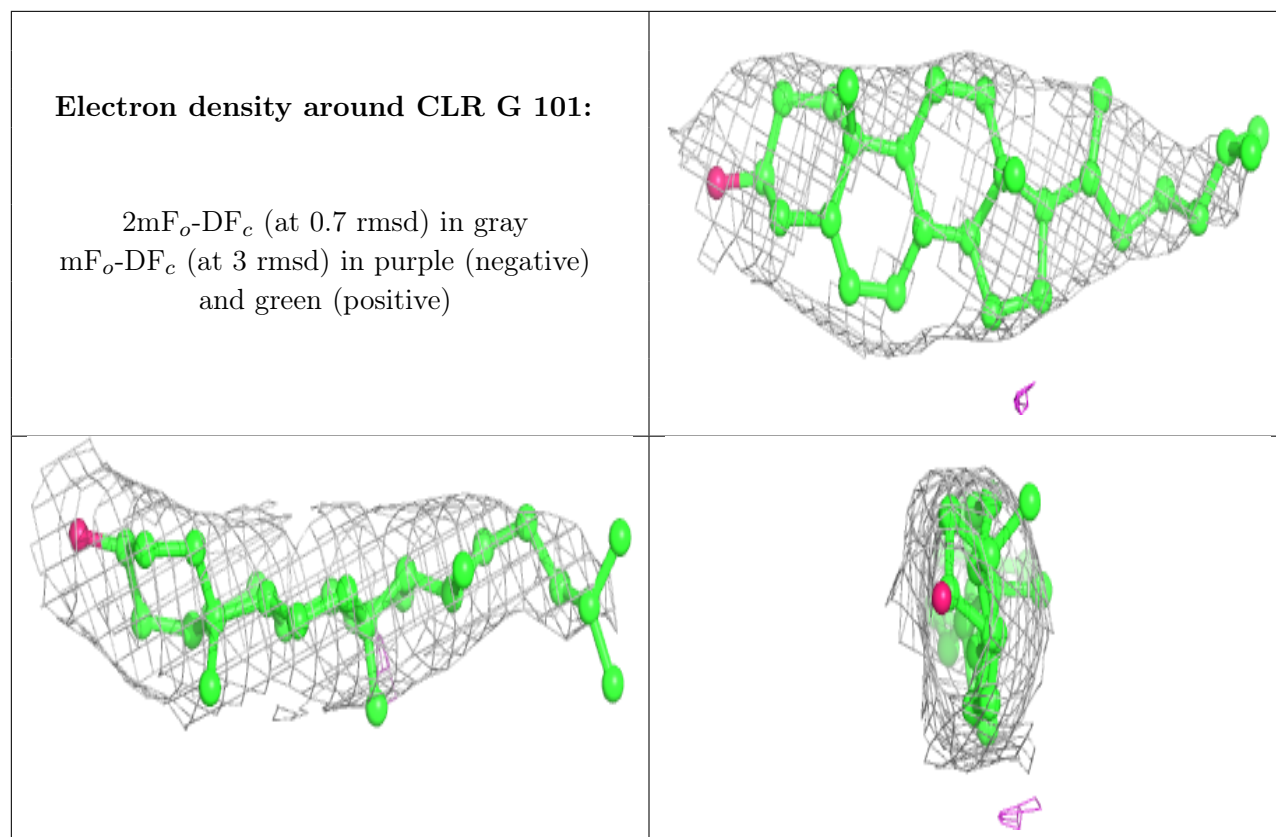
Electron density around CLR E 101:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.