



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:43 AM UTC

PDB ID : 9VJ2 / pdb_00009vj2
Title : Crystal structure of palytoxin-bound Na⁺,K⁺-ATPase in the E2P state
Authors : Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2025-06-19
Resolution : 3.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

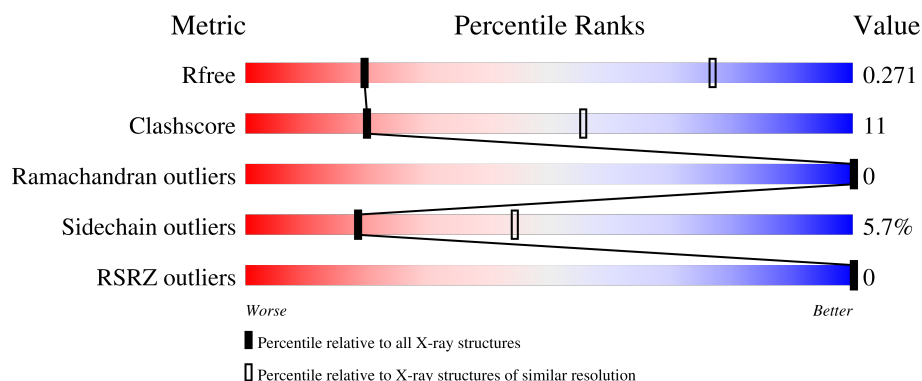
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

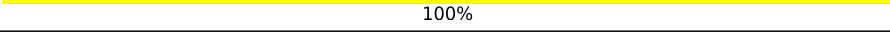
The reported resolution of this entry is 3.79 Å.

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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	1021	
2	B	303	
3	G	65	
4	C	2	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10796 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	996	Total	Be	C	F	N	O	S	0	0	0
			7736	1	4929	3	1303	1453	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			

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

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

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

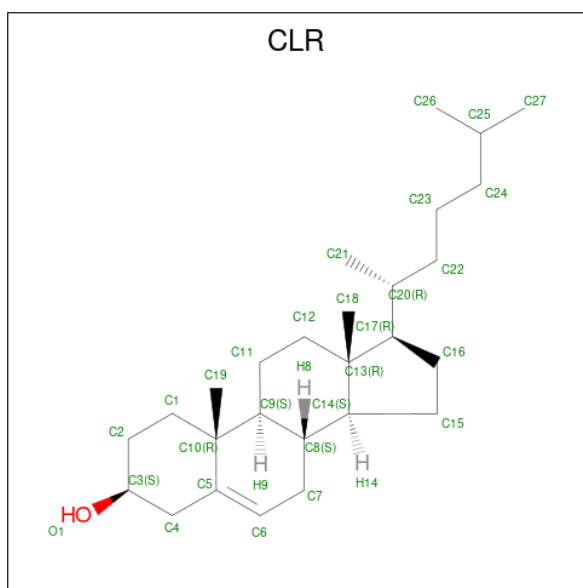


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

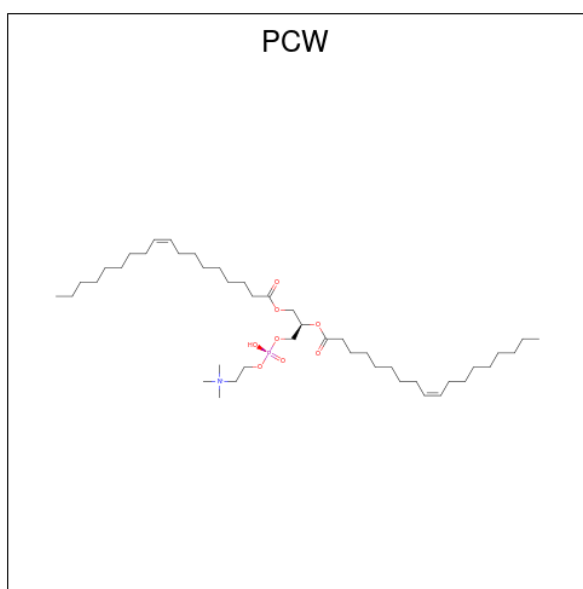
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



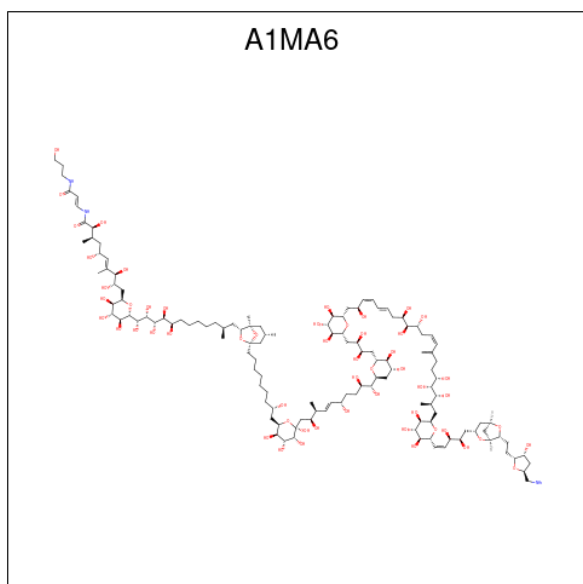
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			28	27	1		
6	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



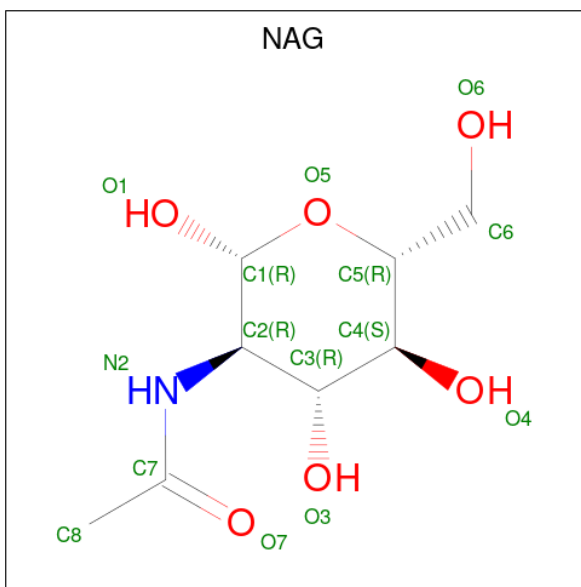
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 8 is palytoxin (CCD ID: A1MA6) (formula: $C_{129}H_{223}N_3O_{54}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			184	129	3	52		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

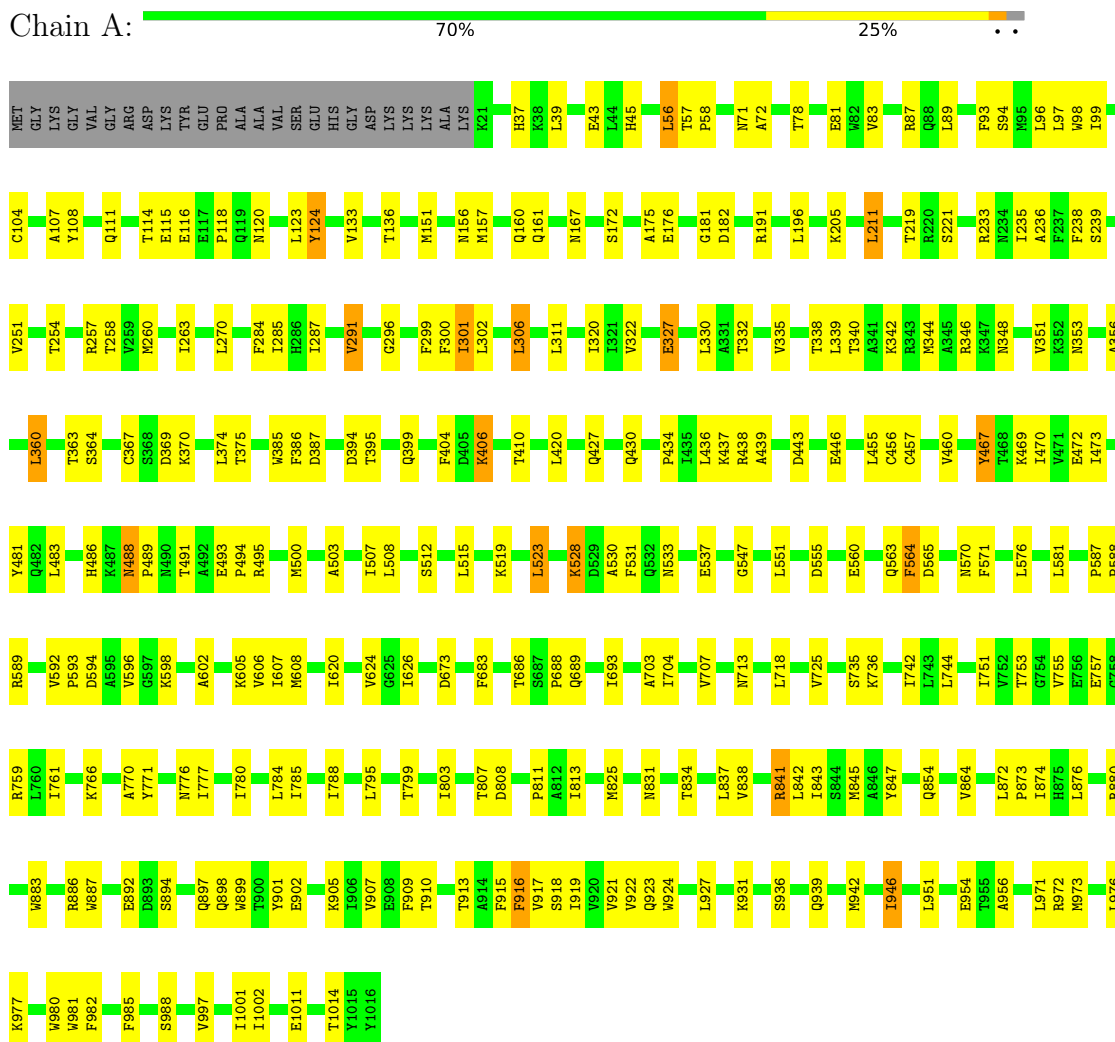
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	O	0	0
			3	3		

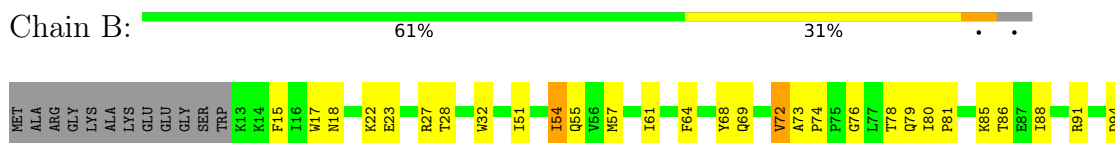
3 Residue-property plots

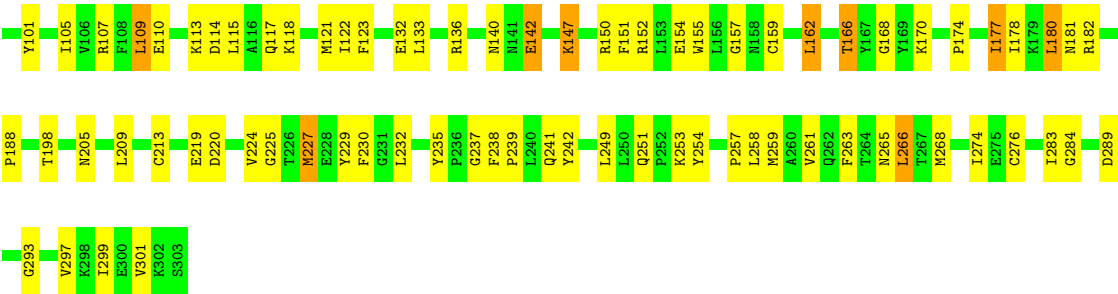
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

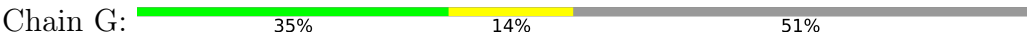


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1





● Molecule 3: FXYP domain-containing ion transport regulator



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.02Å 85.02Å 646.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.79 10.00 – 3.79	Depositor EDS
% Data completeness (in resolution range)	44.1 (10.00-3.79) 41.4 (10.00-3.79)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.227 , 0.276 0.253 , 0.271	Depositor DCC
R_{free} test set	519 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	123.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10796	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, A1MA6, PCW, BFD, MG, NAG

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	0.18	0/7873	0.49	0/10680
2	B	0.16	0/2449	0.47	0/3301
3	G	0.14	0/261	0.39	0/354
All	All	0.18	0/10583	0.49	0/14335

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	7736	0	7788	178	0
2	B	2386	0	2362	68	0
3	G	255	0	259	7	0
4	C	28	0	25	0	0
5	A	2	0	0	0	0
6	A	56	0	92	7	0
7	A	132	0	108	1	0
8	A	184	0	0	3	0
9	B	14	0	13	0	0
10	A	3	0	0	0	0
All	All	10796	0	10647	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (244) 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)
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.55	0.89
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.54	0.87
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.40	0.84
2:B:266:LEU:HD13	2:B:301:VAL:HG21	1.62	0.80
2:B:157:GLY:H	2:B:230:PHE:HB3	1.48	0.79
1:A:807:THR:HB	1:A:954:GLU:HG3	1.66	0.77
1:A:375:THR:HA	1:A:588:PRO:HA	1.66	0.75
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.75	0.69
1:A:898:GLN:HE21	2:B:181:ASN:HD22	1.42	0.67
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.31	0.66
1:A:238:PHE:HD2	1:A:258:THR:HG21	1.62	0.65
1:A:985:PHE:HZ	6:A:1103:CLR:H20	1.62	0.64
1:A:469:LYS:HD3	1:A:472:GLU:HB3	1.80	0.64
2:B:177:ILE:HD11	2:B:258:LEU:HD22	1.79	0.64
1:A:348:ASN:HB3	1:A:744:LEU:HB2	1.81	0.63
1:A:254:THR:HG23	1:A:257:ARG:HH21	1.62	0.63
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.80	0.63
1:A:104:CYS:SG	1:A:322:VAL:HG11	2.39	0.63
1:A:931:LYS:HE3	1:A:942:MET:HA	1.81	0.62
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.65	0.61
2:B:166:THR:HG22	2:B:168:GLY:H	1.65	0.61
1:A:370:LYS:HZ3	1:A:620:ILE:HG13	1.66	0.60
1:A:443:ASP:HB3	1:A:446:GLU:OE1	2.01	0.60
2:B:122:ILE:HG21	2:B:253:LYS:HE2	1.82	0.59
1:A:564:PHE:HB3	1:A:571:PHE:HZ	1.67	0.59
2:B:166:THR:HG21	2:B:170:LYS:H	1.67	0.59
1:A:72:ALA:HB2	1:A:176:GLU:HG2	1.84	0.59
1:A:946:ILE:HD13	3:G:45:ILE:HD11	1.85	0.58
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	1.86	0.58
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.86	0.58
1:A:114:THR:HG21	8:A:1111:A1MA6:C95	2.34	0.57
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.87	0.57
2:B:110:GLU:HG2	2:B:113:LYS:HE3	1.86	0.57
1:A:93:PHE:HD1	1:A:285:ILE:HD11	1.70	0.57
2:B:91:ARG:HE	2:B:94:ASP:HB2	1.70	0.56
1:A:263:ILE:HD13	1:A:688:PRO:HG2	1.86	0.56
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:NE1	1:A:133:VAL:HG11	2.20	0.56
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.87	0.56
1:A:564:PHE:HB3	1:A:571:PHE:CZ	2.40	0.55
1:A:924:TRP:HD1	1:A:951:LEU:HD22	1.72	0.55
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.88	0.55
1:A:924:TRP:CD1	1:A:951:LEU:HD22	2.42	0.54
1:A:874:ILE:H	1:A:874:ILE:HD12	1.73	0.54
2:B:18:ASN:HA	2:B:23:GLU:O	2.07	0.54
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.73	0.54
1:A:470:ILE:HG21	1:A:564:PHE:CZ	2.42	0.54
1:A:98:TRP:HE1	1:A:133:VAL:HG11	1.73	0.54
1:A:108:TYR:CG	1:A:123:LEU:HB2	2.43	0.54
1:A:531:PHE:HE2	1:A:581:LEU:HD21	1.73	0.54
1:A:360:LEU:HD12	1:A:755:VAL:HB	1.90	0.53
1:A:488:ASN:ND2	1:A:494:PRO:HD2	2.22	0.53
1:A:404:PHE:CZ	1:A:456:CYS:HB3	2.43	0.53
1:A:500:MET:HE3	1:A:507:ILE:HD12	1.89	0.53
1:A:161:GLN:NE2	1:A:172:SER:HB3	2.24	0.53
1:A:831:ASN:HB3	1:A:834:THR:HB	1.90	0.53
2:B:220:ASP:O	2:B:224:VAL:HG23	2.09	0.53
1:A:238:PHE:HD1	1:A:239:SER:N	2.07	0.53
1:A:843:ILE:HG23	1:A:847:TYR:HD2	1.74	0.52
1:A:977:LYS:HD2	1:A:980:TRP:CZ2	2.44	0.52
2:B:81:PRO:HD3	2:B:105:ILE:HD11	1.90	0.52
1:A:530:ALA:HA	1:A:533:ASN:OD1	2.10	0.52
1:A:902:GLU:HB2	2:B:289:ASP:OD2	2.10	0.52
1:A:917:VAL:O	1:A:921:VAL:HG23	2.09	0.52
1:A:924:TRP:CZ3	6:A:1103:CLR:H231	2.45	0.52
1:A:332:THR:HA	1:A:813:ILE:HD11	1.92	0.52
1:A:565:ASP:HB2	1:A:570:ASN:CB	2.39	0.52
1:A:547:GLY:HA2	1:A:581:LEU:HD23	1.92	0.51
1:A:825:MET:HA	1:A:825:MET:HE2	1.92	0.51
2:B:136:ARG:HD2	2:B:147:LYS:HG2	1.92	0.51
7:A:1105:PCW:H11	7:A:1105:PCW:O31	2.09	0.51
2:B:166:THR:HG21	2:B:170:LYS:HB2	1.91	0.51
2:B:239:PRO:HD2	2:B:257:PRO:HB3	1.91	0.50
1:A:196:LEU:HB2	1:A:236:ALA:HB3	1.93	0.50
1:A:191:ARG:HE	1:A:239:SER:HA	1.77	0.50
1:A:58:PRO:HD3	1:A:167:ASN:HB2	1.94	0.50
1:A:488:ASN:OD1	1:A:494:PRO:HG2	2.11	0.50
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:HA	1:A:704:ILE:HB	1.93	0.49
1:A:887:TRP:CE3	2:B:86:THR:HG23	2.47	0.49
1:A:335:VAL:O	1:A:339:LEU:HG	2.12	0.49
1:A:977:LYS:HD3	2:B:68:TYR:CZ	2.47	0.49
1:A:96:LEU:HD22	1:A:285:ILE:HG23	1.93	0.49
1:A:96:LEU:HD12	1:A:99:ILE:HD11	1.94	0.49
1:A:395:THR:HB	1:A:587:PRO:CB	2.43	0.49
1:A:913:THR:HB	1:A:976:LEU:HD21	1.95	0.48
1:A:299:PHE:HB3	1:A:320:ILE:HD13	1.95	0.48
3:G:21:TYR:HD1	3:G:22:ASP:N	2.11	0.48
1:A:915:PHE:O	1:A:919:ILE:HG12	2.13	0.48
1:A:491:THR:HA	1:A:493:GLU:OE2	2.13	0.48
1:A:602:ALA:HB1	1:A:759:ARG:HH12	1.76	0.48
6:A:1103:CLR:H162	6:A:1103:CLR:H222	1.53	0.48
1:A:181:GLY:H	1:A:251:VAL:HB	1.79	0.48
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.96	0.48
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.95	0.48
1:A:766:LYS:HG2	1:A:837:LEU:O	2.14	0.48
2:B:136:ARG:HB3	2:B:147:LYS:HE2	1.95	0.48
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.95	0.48
1:A:898:GLN:HE21	2:B:181:ASN:ND2	2.10	0.48
1:A:404:PHE:CE2	1:A:406:LYS:HB3	2.48	0.48
1:A:467:TYR:CZ	1:A:489:PRO:HB3	2.49	0.48
1:A:854:GLN:HG2	1:A:922:VAL:HB	1.96	0.48
2:B:178:ILE:HB	2:B:259:MET:HE2	1.96	0.48
1:A:93:PHE:HD2	1:A:330:LEU:HD13	1.79	0.47
1:A:892:GLU:HA	1:A:897:GLN:O	2.15	0.47
1:A:898:GLN:HG3	2:B:182:ARG:HB2	1.97	0.47
1:A:108:TYR:CE2	1:A:123:LEU:HD22	2.50	0.47
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.95	0.47
1:A:410:THR:HG23	1:A:515:LEU:HD23	1.97	0.47
1:A:495:ARG:HB3	1:A:555:ASP:HB3	1.96	0.47
2:B:81:PRO:HG3	2:B:101:TYR:HB3	1.97	0.47
2:B:115:LEU:O	2:B:118:LYS:HG3	2.14	0.47
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.96	0.47
1:A:924:TRP:CH2	6:A:1103:CLR:H162	2.49	0.47
1:A:94:SER:O	1:A:98:TRP:HD1	1.97	0.47
1:A:898:GLN:NE2	2:B:181:ASN:HD22	2.09	0.47
2:B:268:MET:HA	2:B:301:VAL:HG23	1.97	0.47
1:A:71:ASN:HB3	1:A:175:ALA:O	2.15	0.46
2:B:51:ILE:O	2:B:54:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:SER:HB3	1:A:939:GLN:HG3	1.97	0.46
1:A:300:PHE:HD1	1:A:301:ILE:HD12	1.80	0.46
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.85	0.46
1:A:771:TYR:CE2	1:A:811:PRO:HB2	2.51	0.46
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.51	0.46
2:B:232:LEU:HD13	2:B:239:PRO:HG3	1.98	0.46
1:A:594:ASP:O	1:A:598:LYS:HG2	2.16	0.46
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.51	0.46
1:A:803:ILE:HG12	1:A:916:PHE:HD2	1.81	0.46
2:B:15:PHE:C	2:B:17:TRP:H	2.23	0.46
1:A:688:PRO:HG3	1:A:713:ASN:CB	2.46	0.46
1:A:97:LEU:HD21	1:A:327:GLU:HA	1.98	0.45
1:A:776:ASN:HB2	1:A:847:TYR:HE1	1.79	0.45
2:B:229:TYR:CD1	2:B:261:VAL:HG12	2.51	0.45
1:A:296:GLY:HA2	1:A:320:ILE:HD13	1.98	0.45
1:A:364:SER:OG	1:A:703:ALA:HB1	2.16	0.45
2:B:51:ILE:O	2:B:55:GLN:HG2	2.17	0.45
1:A:605:LYS:HE2	1:A:607:ILE:HD11	1.98	0.45
6:A:1103:CLR:H71	3:G:33:PHE:CE2	2.51	0.45
2:B:154:GLU:HG3	2:B:162:LEU:HD13	1.99	0.45
2:B:263:PHE:O	2:B:266:LEU:HG	2.16	0.45
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.99	0.45
1:A:841:ARG:HE	1:A:841:ARG:HB2	1.55	0.45
2:B:157:GLY:HA3	2:B:230:PHE:CD1	2.52	0.45
2:B:209:LEU:O	2:B:237:GLY:HA3	2.16	0.45
1:A:302:LEU:HD23	1:A:306:LEU:HD23	1.98	0.45
1:A:353:ASN:HB3	1:A:356:ALA:HB2	1.99	0.45
1:A:360:LEU:HB3	1:A:755:VAL:HA	1.97	0.45
1:A:872:LEU:HD23	1:A:894:SER:HB2	1.99	0.45
8:A:1111:A1MA6:CBE	8:A:1111:A1MA6:CA1	2.92	0.45
1:A:107:ALA:HB1	8:A:1111:A1MA6:CA5	2.47	0.45
2:B:225:GLY:HA3	2:B:265:ASN:O	2.16	0.45
1:A:83:VAL:O	1:A:87:ARG:HG2	2.17	0.44
1:A:467:TYR:CE1	1:A:489:PRO:HB3	2.53	0.44
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.99	0.44
1:A:515:LEU:HD12	1:A:519:LYS:O	2.17	0.44
1:A:565:ASP:HB2	1:A:570:ASN:HB2	1.98	0.44
1:A:785:ILE:HA	1:A:788:ILE:HB	1.99	0.44
2:B:174:PRO:HD2	2:B:266:LEU:HD21	2.00	0.44
2:B:213:CYS:HA	2:B:276:CYS:HA	2.00	0.44
1:A:221:SER:H	1:A:233:ARG:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD21	1:A:182:ASP:HB3	1.99	0.44
1:A:306:LEU:HD13	1:A:306:LEU:HA	1.72	0.44
1:A:956:ALA:HB2	3:G:37:ALA:HB3	1.98	0.44
1:A:385:TRP:CH2	1:A:531:PHE:HB2	2.52	0.44
2:B:205:ASN:HB2	2:B:235:TYR:CE1	2.53	0.44
1:A:596:VAL:HG13	1:A:606:VAL:HG21	2.00	0.44
1:A:608:MET:HE3	1:A:626:ILE:HD12	2.00	0.44
2:B:123:PHE:HB3	2:B:150:ARG:HG3	1.99	0.44
2:B:140:ASN:HB2	2:B:142:GLU:HG2	2.00	0.44
1:A:287:ILE:O	1:A:291:VAL:HG22	2.18	0.43
1:A:887:TRP:CZ2	2:B:85:LYS:HA	2.53	0.43
1:A:918:SER:O	1:A:922:VAL:HG22	2.18	0.43
2:B:76:GLY:HA2	2:B:293:GLY:H	1.83	0.43
1:A:551:LEU:HD22	1:A:576:LEU:HD23	1.99	0.43
1:A:982:PHE:HA	1:A:985:PHE:CD1	2.53	0.43
1:A:427:GLN:HB2	1:A:430:GLN:OE1	2.19	0.43
1:A:115:GLU:HG3	1:A:118:PRO:HG3	2.01	0.43
1:A:777:ILE:HG12	1:A:847:TYR:HD1	1.83	0.43
2:B:117:GLN:HB3	2:B:150:ARG:HG2	1.99	0.43
3:G:42:LEU:HA	3:G:45:ILE:HG22	2.01	0.43
1:A:689:GLN:O	1:A:693:ILE:HG12	2.19	0.43
1:A:766:LYS:HG3	1:A:837:LEU:HD12	2.00	0.43
1:A:770:ALA:HA	1:A:842:LEU:HD21	2.01	0.43
2:B:109:LEU:HD13	2:B:109:LEU:HA	1.84	0.42
6:A:1104:CLR:H162	6:A:1104:CLR:H222	1.64	0.42
2:B:151:PHE:CE2	2:B:258:LEU:HB2	2.54	0.42
1:A:565:ASP:HB2	1:A:570:ASN:HB3	2.01	0.42
1:A:799:THR:HG22	1:A:973:MET:HE3	2.01	0.42
1:A:899:TRP:CD2	2:B:72:VAL:HG13	2.54	0.42
2:B:69:GLN:O	2:B:72:VAL:HG23	2.18	0.42
1:A:211:LEU:O	1:A:713:ASN:HB3	2.20	0.42
1:A:367:CYS:HB2	1:A:707:VAL:HG22	2.02	0.42
1:A:386:PHE:HD1	1:A:387:ASP:OD2	2.03	0.42
1:A:736:LYS:HG3	1:A:742:ILE:HD12	2.01	0.42
2:B:22:LYS:O	2:B:28:THR:HA	2.19	0.42
2:B:152:ARG:HG3	2:B:155:TRP:CZ3	2.54	0.42
1:A:205:LYS:HA	1:A:219:THR:HA	2.00	0.42
1:A:340:THR:O	1:A:344:MET:HG2	2.18	0.42
1:A:913:THR:HG23	1:A:973:MET:HE2	2.01	0.42
1:A:508:LEU:HD11	1:A:528:LYS:HE2	2.01	0.42
1:A:593:PRO:HA	1:A:624:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:THR:O	1:A:757:GLU:HG2	2.19	0.42
2:B:91:ARG:NE	2:B:94:ASP:HB2	2.33	0.42
1:A:136:THR:HG21	1:A:330:LEU:HG	2.01	0.41
1:A:430:GLN:HG2	1:A:439:ALA:O	2.19	0.41
1:A:997:VAL:O	1:A:1001:ILE:HG12	2.20	0.41
2:B:297:VAL:HG12	2:B:299:ILE:HG23	2.01	0.41
1:A:374:LEU:O	1:A:592:VAL:HG21	2.19	0.41
1:A:880:ARG:HA	1:A:883:TRP:HB3	2.02	0.41
1:A:981:TRP:CG	6:A:1103:CLR:H191	2.55	0.41
1:A:108:TYR:CD1	1:A:123:LEU:HB2	2.55	0.41
1:A:473:ILE:HD12	1:A:483:LEU:HD11	2.02	0.41
1:A:512:SER:HA	1:A:523:LEU:HD23	2.02	0.41
1:A:845:MET:SD	1:A:1014:THR:HB	2.60	0.41
2:B:73:ALA:HB2	3:G:19:PHE:HB3	2.02	0.41
1:A:907:VAL:HA	1:A:910:THR:HG22	2.02	0.41
1:A:982:PHE:HA	1:A:985:PHE:HD1	1.86	0.41
2:B:180:LEU:HD22	2:B:180:LEU:HA	1.87	0.41
1:A:151:MET:HE2	1:A:151:MET:HA	2.02	0.41
1:A:287:ILE:HD13	1:A:287:ILE:HA	1.82	0.41
2:B:54:ILE:HD12	2:B:54:ILE:HA	1.90	0.41
1:A:342:LYS:O	1:A:346:ARG:HG3	2.21	0.41
1:A:780:ILE:O	1:A:784:LEU:HG	2.20	0.41
1:A:808:ASP:CG	1:A:923:GLN:HE21	2.29	0.41
2:B:229:TYR:HD1	2:B:261:VAL:HG12	1.86	0.41
2:B:241:GLN:HG3	2:B:242:TYR:CD1	2.56	0.41
1:A:905:LYS:HD3	1:A:905:LYS:HA	1.91	0.41
1:A:338:THR:O	1:A:342:LYS:HG2	2.20	0.40
1:A:374:LEU:HD22	1:A:592:VAL:HG13	2.02	0.40
1:A:488:ASN:ND2	1:A:489:PRO:HD2	2.36	0.40
1:A:503:ALA:O	1:A:507:ILE:HG12	2.21	0.40
1:A:909:PHE:CE2	1:A:972:ARG:HD2	2.56	0.40
2:B:227:MET:HE2	2:B:227:MET:HB2	2.01	0.40
1:A:977:LYS:H	1:A:980:TRP:CD1	2.39	0.40
1:A:260:MET:HE2	1:A:260:MET:HB2	1.94	0.40
1:A:921:VAL:HG12	1:A:988:SER:OG	2.21	0.40
1:A:120:ASN:O	1:A:124:TYR:HB2	2.21	0.40
1:A:160:GLN:HE22	1:A:191:ARG:HD3	1.87	0.40
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.90	0.40
1:A:784:LEU:O	1:A:788:ILE:HG12	2.20	0.40
2:B:74:PRO:HG2	2:B:284:GLY:HA3	2.03	0.40
2:B:132:GLU:OE2	2:B:133:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LEU:HD12	1:A:735:SER:HB2	2.03	0.40
3:G:38:PHE:CE2	3:G:42:LEU:HD11	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	993/1021 (97%)	932 (94%)	61 (6%)	0	100	100
2	B	289/303 (95%)	273 (94%)	16 (6%)	0	100	100
3	G	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
All	All	1312/1389 (94%)	1233 (94%)	79 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	845/863 (98%)	806 (95%)	39 (5%)	24	48
2	B	261/269 (97%)	236 (90%)	25 (10%)	8	29
3	G	26/52 (50%)	25 (96%)	1 (4%)	29	53
All	All	1132/1184 (96%)	1067 (94%)	65 (6%)	18	44

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	56	LEU
1	A	57	THR
1	A	78	THR
1	A	81	GLU
1	A	89	LEU
1	A	111	GLN
1	A	116	GLU
1	A	124	TYR
1	A	156	ASN
1	A	157	MET
1	A	211	LEU
1	A	291	VAL
1	A	301	ILE
1	A	306	LEU
1	A	311	LEU
1	A	327	GLU
1	A	351	VAL
1	A	360	LEU
1	A	394	ASP
1	A	406	LYS
1	A	455	LEU
1	A	457	CYS
1	A	460	VAL
1	A	467	TYR
1	A	481	TYR
1	A	488	ASN
1	A	523	LEU
1	A	528	LYS
1	A	537	GLU
1	A	560	GLU
1	A	563	GLN
1	A	564	PHE
1	A	673	ASP
1	A	761	ILE
1	A	841	ARG
1	A	916	PHE
1	A	946	ILE
1	A	971	LEU
2	B	27	ARG
2	B	32	TRP
2	B	54	ILE

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Mol	Chain	Res	Type
2	B	61	ILE
2	B	64	PHE
2	B	72	VAL
2	B	78	THR
2	B	79	GLN
2	B	107	ARG
2	B	109	LEU
2	B	114	ASP
2	B	121	MET
2	B	142	GLU
2	B	147	LYS
2	B	159	CYS
2	B	162	LEU
2	B	166	THR
2	B	177	ILE
2	B	180	LEU
2	B	198	THR
2	B	219	GLU
2	B	227	MET
2	B	249	LEU
2	B	266	LEU
2	B	274	ILE
3	G	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	GLN
1	A	122	ASN
1	A	160	GLN
1	A	161	GLN
1	A	324	ASN
1	A	399	GLN
1	A	427	GLN
1	A	521	GLN
1	A	563	GLN
1	A	570	ASN
1	A	747	ASN
1	A	849	GLN
2	B	69	GLN
2	B	79	GLN

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Mol	Chain	Res	Type
2	B	82	GLN
2	B	140	ASN
2	B	181	ASN
2	B	212	HIS
2	B	256	GLN
2	B	262	GLN
2	B	292	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	BFD	A	369	1,5	8,11,12	1.17	0	2,15,17	2.29	1 (50%)

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	BFD	A	369	1,5	-	0/5/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	BFD	OD2-CG-CB	-2.79	118.16	124.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 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	C	1	4,2	14,14,15	0.71	0	17,19,21	2.01	4 (23%)
4	NAG	C	2	4	14,14,15	0.77	0	17,19,21	1.25	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C2-N2-C7	4.05	128.33	122.90
4	C	1	NAG	C1-O5-C5	3.94	117.47	112.19
4	C	1	NAG	O3-C3-C2	-3.15	102.87	109.40
4	C	1	NAG	O3-C3-C4	3.10	117.69	110.38
4	C	2	NAG	C2-N2-C7	3.04	126.97	122.90
4	C	2	NAG	O5-C1-C2	-2.37	107.62	111.29

There are no chirality outliers.

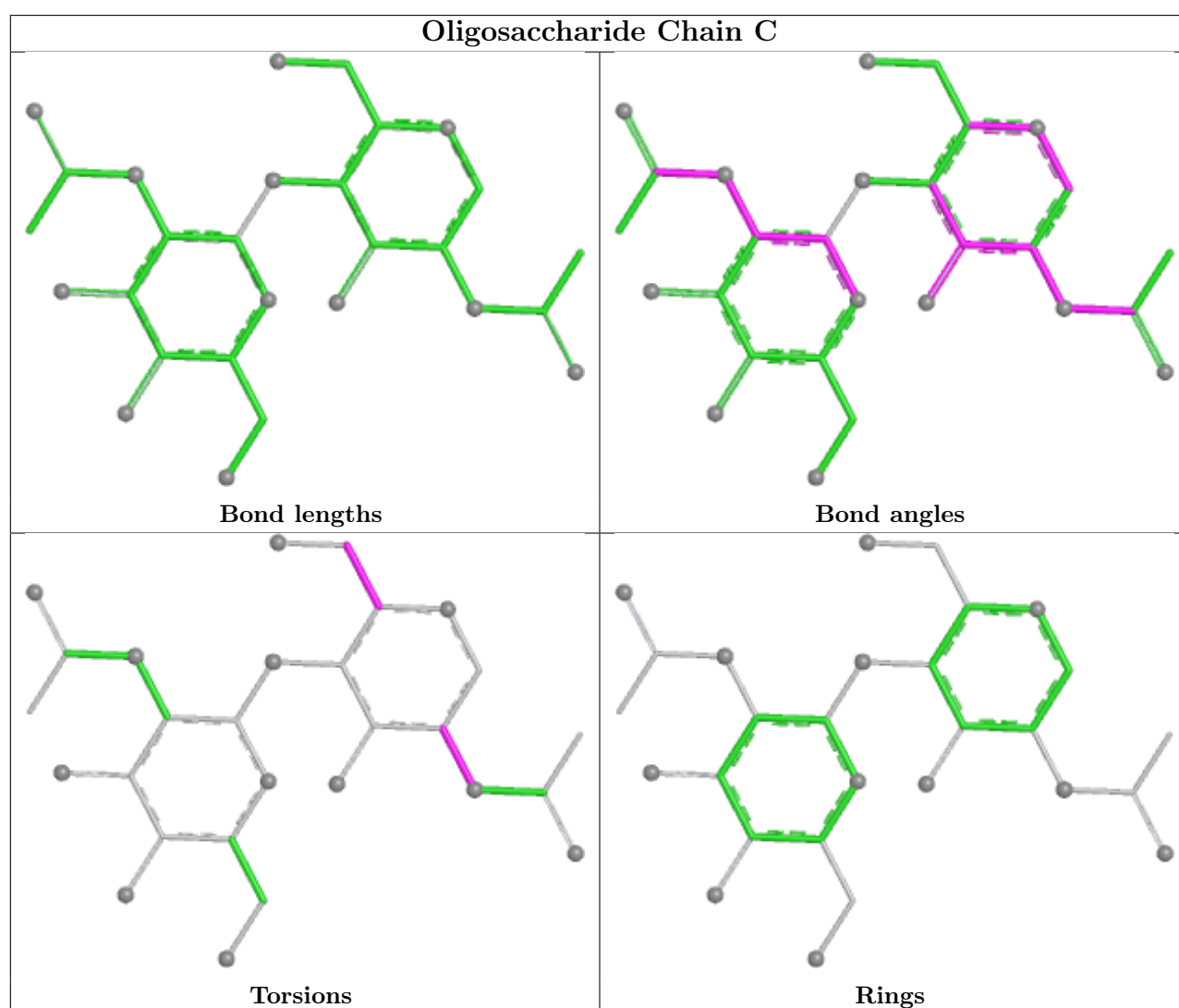
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	C4-C5-C6-O6
4	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
7	PCW	A	1107	-	21,21,53	0.86	0	27,29,61	1.26	3 (11%)
8	A1MA6	A	1111	-	190,193,195	1.32	19 (10%)	225,274,278	1.67	44 (19%)
9	NAG	B	401	2	14,14,15	0.85	1 (7%)	17,19,21	1.56	2 (11%)
6	CLR	A	1103	-	31,31,31	1.33	2 (6%)	48,48,48	1.36	5 (10%)
7	PCW	A	1110	-	21,21,53	0.86	0	27,29,61	0.94	1 (3%)
7	PCW	A	1105	-	21,21,53	0.85	0	27,29,61	0.97	1 (3%)
7	PCW	A	1108	-	21,21,53	0.86	0	27,29,61	1.08	2 (7%)
6	CLR	A	1104	-	31,31,31	1.35	5 (16%)	48,48,48	1.53	9 (18%)
7	PCW	A	1106	-	21,21,53	0.87	0	27,29,61	1.25	3 (11%)
7	PCW	A	1109	-	21,21,53	0.85	0	27,29,61	1.22	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	A	1107	-	-	5/23/23/57	-
8	A1MA6	A	1111	-	-	100/189/343/350	1/12/10/10
9	NAG	B	401	2	-	1/6/23/26	0/1/1/1
6	CLR	A	1103	-	-	4/10/68/68	0/4/4/4
7	PCW	A	1110	-	-	9/23/23/57	-
7	PCW	A	1105	-	-	9/23/23/57	-
7	PCW	A	1108	-	-	5/23/23/57	-
6	CLR	A	1104	-	-	4/10/68/68	0/4/4/4
7	PCW	A	1106	-	-	7/23/23/57	-
7	PCW	A	1109	-	-	7/23/23/57	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1111	A1MA6	OC2-C43	5.76	1.54	1.43
8	A	1111	A1MA6	OA0-CAP	5.47	1.57	1.45
8	A	1111	A1MA6	OC2-C47	5.05	1.51	1.43
8	A	1111	A1MA6	CBL-CBM	-4.78	1.43	1.52
8	A	1111	A1MA6	CA3-CA4	4.17	1.54	1.45
6	A	1104	CLR	C16-C17	3.72	1.62	1.54
8	A	1111	A1MA6	CAN-CAM	-3.62	1.45	1.52
8	A	1111	A1MA6	C48-C49	-3.54	1.46	1.53
6	A	1103	CLR	C16-C17	3.41	1.61	1.54
8	A	1111	A1MA6	C51-C49	-3.41	1.46	1.53
8	A	1111	A1MA6	CAV-CAW	-3.39	1.45	1.52
8	A	1111	A1MA6	C95-C94	3.00	1.53	1.44
6	A	1103	CLR	C13-C17	2.92	1.60	1.55
8	A	1111	A1MA6	C07-C06	2.63	1.53	1.48
8	A	1111	A1MA6	O46-C44	-2.59	1.41	1.45
8	A	1111	A1MA6	CAN-CB0	-2.54	1.47	1.52
8	A	1111	A1MA6	CAL-CAK	-2.52	1.46	1.52
6	A	1104	CLR	C12-C13	2.47	1.58	1.54
8	A	1111	A1MA6	C15-C17	2.42	1.53	1.50
6	A	1104	CLR	C2-C3	2.38	1.57	1.51
8	A	1111	A1MA6	CAH-CAG	2.34	1.53	1.50
8	A	1111	A1MA6	O76-C75	2.29	1.50	1.44
9	B	401	NAG	C1-C2	2.29	1.55	1.52
8	A	1111	A1MA6	O76-C77	-2.24	1.38	1.44
6	A	1104	CLR	C13-C17	2.18	1.59	1.55
6	A	1104	CLR	C8-C14	-2.17	1.49	1.53
8	A	1111	A1MA6	CAT-CAS	2.12	1.58	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1111	A1MA6	C97-C96-C95	-8.15	115.06	125.44
8	A	1111	A1MA6	CAH-CAG-CAF	-6.41	115.19	124.94
9	B	401	NAG	C1-O5-C5	5.03	118.92	112.19
8	A	1111	A1MA6	CA1-CA2-CA3	-4.95	115.23	125.93
7	A	1109	PCW	C2-O2-C31	-4.60	109.73	117.85
8	A	1111	A1MA6	C44-O46-C47	-4.57	101.65	110.68
8	A	1111	A1MA6	CAE-CAF-CAG	-4.53	115.18	125.02
8	A	1111	A1MA6	C92-C93-C94	-4.41	115.11	124.78
7	A	1107	PCW	C2-O2-C31	-4.35	110.17	117.85
8	A	1111	A1MA6	C70-C69-C68	-4.11	115.03	124.74
8	A	1111	A1MA6	CAR-CAS-CAT	-3.99	107.83	116.24
7	A	1106	PCW	C2-O2-C31	-3.94	110.88	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1111	A1MA6	C63-O62-C61	-3.71	109.88	114.61
7	A	1106	PCW	C3-O3-C11	-3.65	108.09	117.08
8	A	1111	A1MA6	C67-C68-C69	-3.60	114.93	125.81
8	A	1111	A1MA6	CAQ-CAP-CB0	-3.45	108.60	116.18
8	A	1111	A1MA6	OAZ-CAW-CAV	-3.37	100.81	105.07
8	A	1111	A1MA6	C53-C52-C47	-3.35	109.68	114.64
6	A	1104	CLR	C22-C20-C17	-3.31	103.47	110.33
8	A	1111	A1MA6	C08-N09-C10	-3.30	117.01	123.65
7	A	1108	PCW	C2-O2-C31	-3.25	112.11	117.85
6	A	1103	CLR	C7-C8-C14	-3.10	106.54	110.93
8	A	1111	A1MA6	C13-C14-C15	-3.03	109.40	115.08
8	A	1111	A1MA6	C21-C19-C18	-2.98	109.56	113.66
8	A	1111	A1MA6	CAS-OAZ-CAW	-2.92	102.15	108.95
8	A	1111	A1MA6	C37-C36-C34	-2.92	109.33	114.11
8	A	1111	A1MA6	CAA-CAB-CAC	-2.91	109.60	115.35
7	A	1108	PCW	C3-O3-C11	-2.90	109.93	117.08
8	A	1111	A1MA6	C72-C73-C74	-2.83	109.48	113.97
8	A	1111	A1MA6	O62-C61-C60	2.78	109.44	105.95
8	A	1111	A1MA6	CA6-CA7-CA8	-2.78	109.57	113.97
8	A	1111	A1MA6	C36-C34-C32	-2.78	109.57	113.97
8	A	1111	A1MA6	C32-C30-C28	-2.75	109.45	113.24
7	A	1110	PCW	C3-O3-C11	-2.73	110.34	117.08
8	A	1111	A1MA6	C22-C23-CC7	-2.70	109.58	114.10
8	A	1111	A1MA6	C30-C28-C26	-2.69	109.54	113.24
6	A	1104	CLR	C10-C5-C6	2.68	126.85	122.93
7	A	1105	PCW	C3-O3-C11	-2.66	110.53	117.08
8	A	1111	A1MA6	C78-C77-CB0	-2.63	109.21	113.47
8	A	1111	A1MA6	CAA-CA9-CA8	-2.61	109.58	114.69
8	A	1111	A1MA6	CA5-CA6-CA7	-2.60	109.49	114.81
6	A	1104	CLR	C18-C13-C12	2.59	114.43	110.61
8	A	1111	A1MA6	C60-C61-CBV	-2.56	109.32	113.47
8	A	1111	A1MA6	C71-C72-C73	-2.55	109.45	113.43
8	A	1111	A1MA6	CCB-C18-C19	2.55	120.07	115.33
6	A	1104	CLR	C1-C2-C3	2.54	113.85	110.48
6	A	1104	CLR	C7-C8-C9	2.54	112.66	109.72
8	A	1111	A1MA6	C91-C90-C85	-2.53	109.36	113.47
8	A	1111	A1MA6	C81-C82-C83	-2.52	109.38	113.47
8	A	1111	A1MA6	CA0-C99-C98	-2.45	109.49	113.57
7	A	1107	PCW	C3-O3-C11	-2.39	111.18	117.08
8	A	1111	A1MA6	CAB-CAC-CB8	-2.38	109.61	113.47
6	A	1103	CLR	C18-C13-C12	2.38	114.11	110.61
6	A	1103	CLR	C10-C5-C6	2.34	126.34	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1104	CLR	C16-C17-C20	-2.28	108.73	112.18
8	A	1111	A1MA6	C77-O76-C75	-2.25	109.25	113.19
6	A	1104	CLR	C24-C23-C22	-2.22	103.31	113.28
8	A	1111	A1MA6	C61-C60-C59	-2.22	109.54	114.49
7	A	1109	PCW	O2-C31-C32	2.21	115.02	111.09
8	A	1111	A1MA6	OC2-C43-C44	-2.20	101.58	104.68
7	A	1107	PCW	O2-C31-C32	2.20	115.01	111.09
9	B	401	NAG	C2-N2-C7	2.20	125.84	122.90
8	A	1111	A1MA6	CAP-OAO-CAM	-2.18	103.88	108.95
8	A	1111	A1MA6	C04-C03-C02	-2.18	109.64	112.95
8	A	1111	A1MA6	CA0-CA1-CA2	-2.17	109.48	112.88
8	A	1111	A1MA6	C98-C97-C96	-2.16	109.49	112.88
6	A	1103	CLR	C22-C20-C17	-2.13	105.91	110.33
8	A	1111	A1MA6	CAC-OAD-CAE	-2.11	109.84	112.65
6	A	1104	CLR	C4-C5-C10	-2.08	113.76	116.42
6	A	1103	CLR	C2-C3-C4	-2.06	107.39	110.29
7	A	1109	PCW	C3-O3-C11	-2.04	112.05	117.08
6	A	1104	CLR	C21-C20-C17	2.04	115.94	112.88
7	A	1106	PCW	O2-C31-C32	2.03	114.70	111.09

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1105	PCW	C1-O3P-P-O1P
7	A	1105	PCW	C1-O3P-P-O2P
7	A	1105	PCW	C1-O3P-P-O4P
7	A	1105	PCW	C4-O4P-P-O1P
7	A	1105	PCW	C4-O4P-P-O2P
7	A	1105	PCW	C4-O4P-P-O3P
7	A	1106	PCW	C1-O3P-P-O1P
7	A	1106	PCW	C1-O3P-P-O2P
7	A	1106	PCW	C1-O3P-P-O4P
7	A	1106	PCW	C4-O4P-P-O3P
7	A	1107	PCW	C1-O3P-P-O1P
7	A	1107	PCW	C1-O3P-P-O2P
7	A	1107	PCW	C1-O3P-P-O4P
7	A	1108	PCW	C1-O3P-P-O2P
7	A	1108	PCW	C4-O4P-P-O1P
7	A	1108	PCW	C4-O4P-P-O2P
7	A	1108	PCW	C4-O4P-P-O3P
7	A	1109	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
7	A	1109	PCW	C1-O3P-P-O2P
7	A	1109	PCW	C1-O3P-P-O4P
7	A	1109	PCW	C4-O4P-P-O1P
7	A	1109	PCW	C4-O4P-P-O2P
7	A	1109	PCW	C4-O4P-P-O3P
7	A	1110	PCW	C1-O3P-P-O1P
7	A	1110	PCW	C1-O3P-P-O2P
7	A	1110	PCW	C1-O3P-P-O4P
7	A	1110	PCW	C4-O4P-P-O1P
7	A	1110	PCW	C4-O4P-P-O2P
7	A	1110	PCW	C4-O4P-P-O3P
8	A	1111	A1MA6	C02-C03-C04-N05
8	A	1111	A1MA6	N09-C10-C11-O12
8	A	1111	A1MA6	C10-C11-C13-C14
8	A	1111	A1MA6	C10-C11-C13-CCC
8	A	1111	A1MA6	O12-C11-C13-C14
8	A	1111	A1MA6	O12-C11-C13-CCC
8	A	1111	A1MA6	C18-C19-C21-C22
8	A	1111	A1MA6	O24-C25-C26-O27
8	A	1111	A1MA6	O24-C25-C26-C28
8	A	1111	A1MA6	CC4-C25-C26-O27
8	A	1111	A1MA6	CC4-C25-C26-C28
8	A	1111	A1MA6	C26-C28-C30-O31
8	A	1111	A1MA6	C26-C28-C30-C32
8	A	1111	A1MA6	O29-C28-C30-C32
8	A	1111	A1MA6	C30-C32-C34-O35
8	A	1111	A1MA6	O33-C32-C34-O35
8	A	1111	A1MA6	O33-C32-C34-C36
8	A	1111	A1MA6	C40-C41-C42-C43
8	A	1111	A1MA6	CC3-C41-C42-C43
8	A	1111	A1MA6	C41-C42-C43-OC2
8	A	1111	A1MA6	C58-C59-C60-C61
8	A	1111	A1MA6	OC1-C59-C60-C61
8	A	1111	A1MA6	C59-C60-C61-O62
8	A	1111	A1MA6	C59-C60-C61-CBV
8	A	1111	A1MA6	C65-C66-C67-C68
8	A	1111	A1MA6	C65-C66-C67-CBT
8	A	1111	A1MA6	OBU-C66-C67-C68
8	A	1111	A1MA6	OBU-C66-C67-CBT
8	A	1111	A1MA6	C69-C70-C71-C72
8	A	1111	A1MA6	OBS-C70-C71-C72
8	A	1111	A1MA6	C71-C72-C73-OB

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Mol	Chain	Res	Type	Atoms
8	A	1111	A1MA6	C72-C73-C74-C75
8	A	1111	A1MA6	C72-C73-C74-OBQ
8	A	1111	A1MA6	OBR-C73-C74-C75
8	A	1111	A1MA6	OBR-C73-C74-OBQ
8	A	1111	A1MA6	O76-C77-C78-C79
8	A	1111	A1MA6	CBO-C77-C78-C79
8	A	1111	A1MA6	C78-C79-C80-C81
8	A	1111	A1MA6	C78-C79-C80-OBJ
8	A	1111	A1MA6	OBK-C79-C80-C81
8	A	1111	A1MA6	OBK-C79-C80-OBJ
8	A	1111	A1MA6	C90-C91-C92-C93
8	A	1111	A1MA6	C90-C91-C92-OB1
8	A	1111	A1MA6	C96-C97-C98-C99
8	A	1111	A1MA6	C96-C97-C98-OBH
8	A	1111	A1MA6	C98-C99-CA0-CA1
8	A	1111	A1MA6	C98-C99-CA0-OBF
8	A	1111	A1MA6	OBG-C99-CA0-CA1
8	A	1111	A1MA6	OBG-C99-CA0-OBF
8	A	1111	A1MA6	C99-CA0-CA1-CA2
8	A	1111	A1MA6	OBF-CA0-CA1-CA2
8	A	1111	A1MA6	CA5-CA6-CA7-OBD
8	A	1111	A1MA6	CA7-CA8-CA9-OB8
8	A	1111	A1MA6	OBC-CA8-CA9-CAA
8	A	1111	A1MA6	CBA-CAA-CAB-CAC
8	A	1111	A1MA6	CAA-CAB-CAC-OAD
8	A	1111	A1MA6	CAA-CAB-CAC-CB8
8	A	1111	A1MA6	OAO-CAP-CAQ-CAR
8	A	1111	A1MA6	CB0-CAP-CAQ-CAR
8	A	1111	A1MA6	CAV-CAW-CAX-NAY
8	A	1111	A1MA6	OAZ-CAW-CAX-NAY
8	A	1111	A1MA6	O29-C28-C30-O31
8	A	1111	A1MA6	OBC-CA8-CA9-OB8
8	A	1111	A1MA6	O35-C34-C36-C37
8	A	1111	A1MA6	CA7-CA8-CA9-CAA
8	A	1111	A1MA6	CA5-CA6-CA7-CA8
8	A	1111	A1MA6	CAF-CAG-CAH-OB3
8	A	1111	A1MA6	CAI-CAJ-CAK-OB1
8	A	1111	A1MA6	CAI-CAJ-CAK-CAL
8	A	1111	A1MA6	O20-C19-C21-C22
8	A	1111	A1MA6	CBT-C67-C68-C69
6	A	1104	CLR	C20-C22-C23-C24
8	A	1111	A1MA6	C68-C69-C70-C71

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Mol	Chain	Res	Type	Atoms
8	A	1111	A1MA6	C91-C92-C93-C94
8	A	1111	A1MA6	C52-C53-C54-C55
8	A	1111	A1MA6	C11-C13-C14-C15
6	A	1103	CLR	C13-C17-C20-C21
9	B	401	NAG	O5-C5-C6-O6
8	A	1111	A1MA6	C55-C56-C57-C58
8	A	1111	A1MA6	CCC-C13-C14-C15
8	A	1111	A1MA6	C66-C67-C68-C69
8	A	1111	A1MA6	CA0-CA1-CA2-CA3
6	A	1103	CLR	C16-C17-C20-C21
6	A	1104	CLR	C23-C24-C25-C26
8	A	1111	A1MA6	C68-C69-C70-OBS
8	A	1111	A1MA6	OBI-C92-C93-C94
6	A	1103	CLR	C13-C17-C20-C22
8	A	1111	A1MA6	C77-C78-C79-OBK
8	A	1111	A1MA6	CA9-CAA-CAB-CAC
8	A	1111	A1MA6	CA4-CA5-CA6-CA7
8	A	1111	A1MA6	C54-C55-C56-C57
8	A	1111	A1MA6	OAD-CAE-CAF-CAG
7	A	1106	PCW	C5-C4-O4P-P
8	A	1111	A1MA6	OCD-C10-C11-O12
7	A	1105	PCW	O4P-C4-C5-N
7	A	1106	PCW	O4P-C4-C5-N
7	A	1107	PCW	O4P-C4-C5-N
7	A	1108	PCW	O4P-C4-C5-N
7	A	1109	PCW	O4P-C4-C5-N
7	A	1110	PCW	O4P-C4-C5-N
8	A	1111	A1MA6	C30-C32-C34-C36
8	A	1111	A1MA6	CAF-CAG-CAH-CAI
8	A	1111	A1MA6	C56-C57-C58-C59
6	A	1103	CLR	C16-C17-C20-C22
8	A	1111	A1MA6	C80-C81-C82-C83
7	A	1106	PCW	C4-O4P-P-O2P
7	A	1107	PCW	C4-O4P-P-O1P
8	A	1111	A1MA6	C37-C38-C39-C40
6	A	1104	CLR	C23-C24-C25-C27
8	A	1111	A1MA6	C80-C81-C82-O89
8	A	1111	A1MA6	CA2-CA3-CA4-CA5
8	A	1111	A1MA6	CAP-CAQ-CAR-CAS
8	A	1111	A1MA6	O31-C30-C32-O33
6	A	1104	CLR	C13-C17-C20-C21
7	A	1105	PCW	C1-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
7	A	1105	PCW	C3-C2-O2-C31
7	A	1110	PCW	C3-C2-O2-C31
8	A	1111	A1MA6	CA2-CA3-CA4-CBE
8	A	1111	A1MA6	CCB-C18-C19-C21
8	A	1111	A1MA6	C15-C17-C18-C19
8	A	1111	A1MA6	OB3-CAH-CAI-CAJ
7	A	1110	PCW	C1-C2-O2-C31

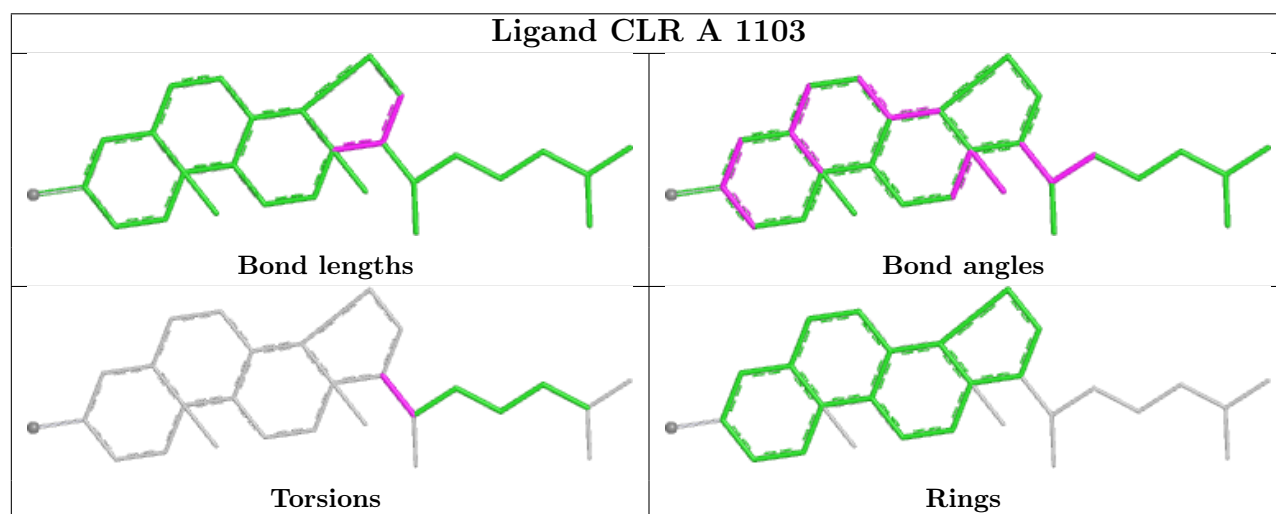
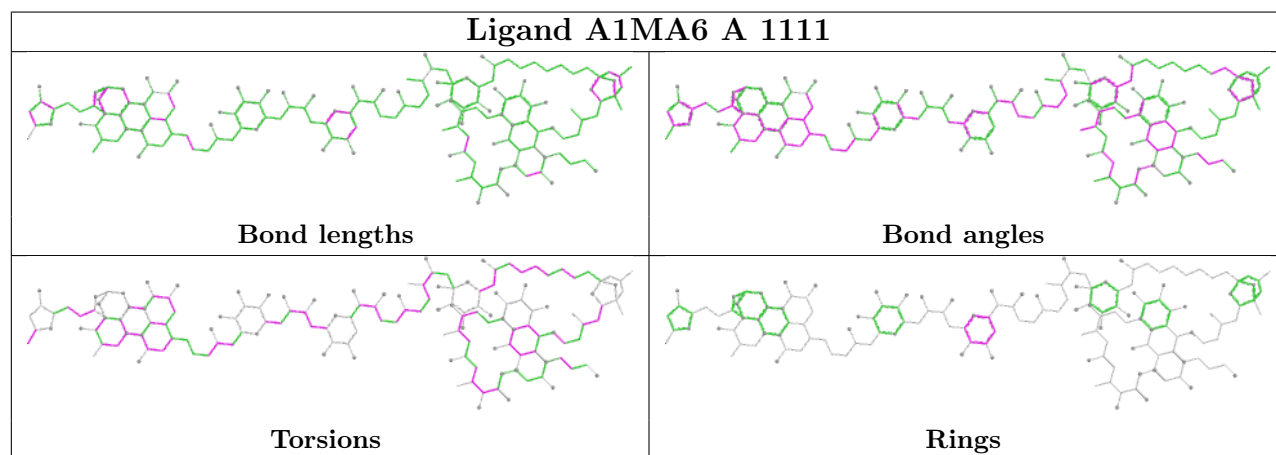
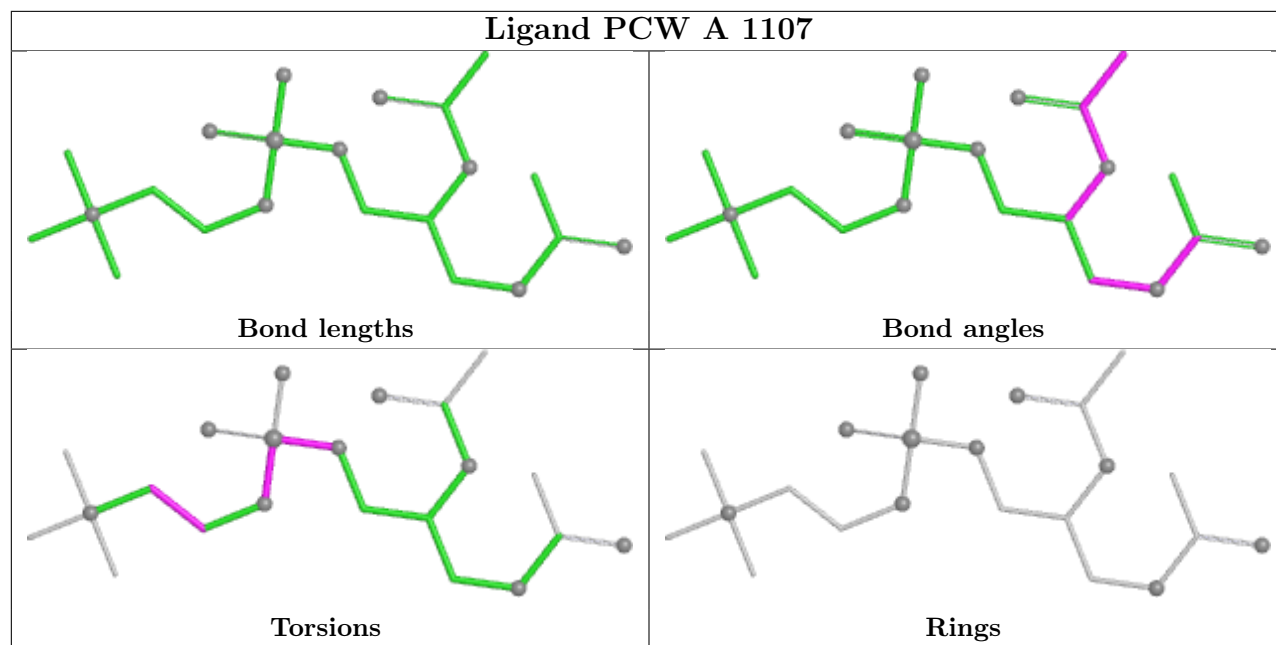
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1111	A1MA6	C75-C77-CBL-CBM-CBO-O76

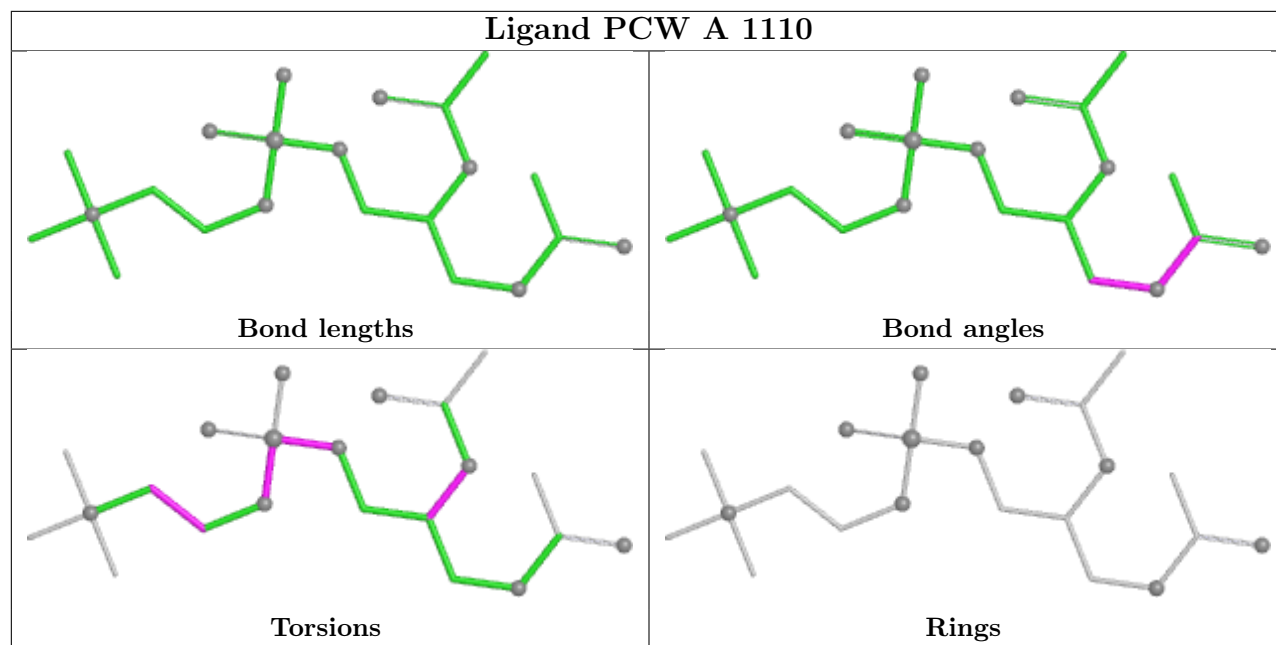
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1111	A1MA6	3	0
6	A	1103	CLR	6	0
7	A	1105	PCW	1	0
6	A	1104	CLR	1	0

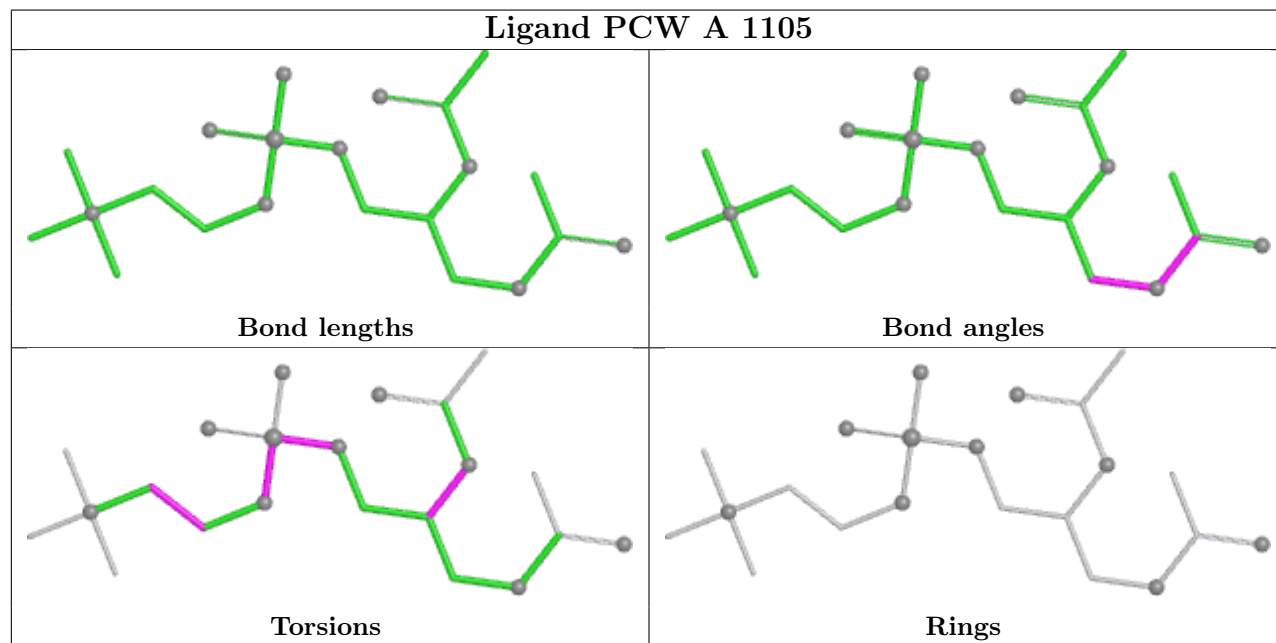
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



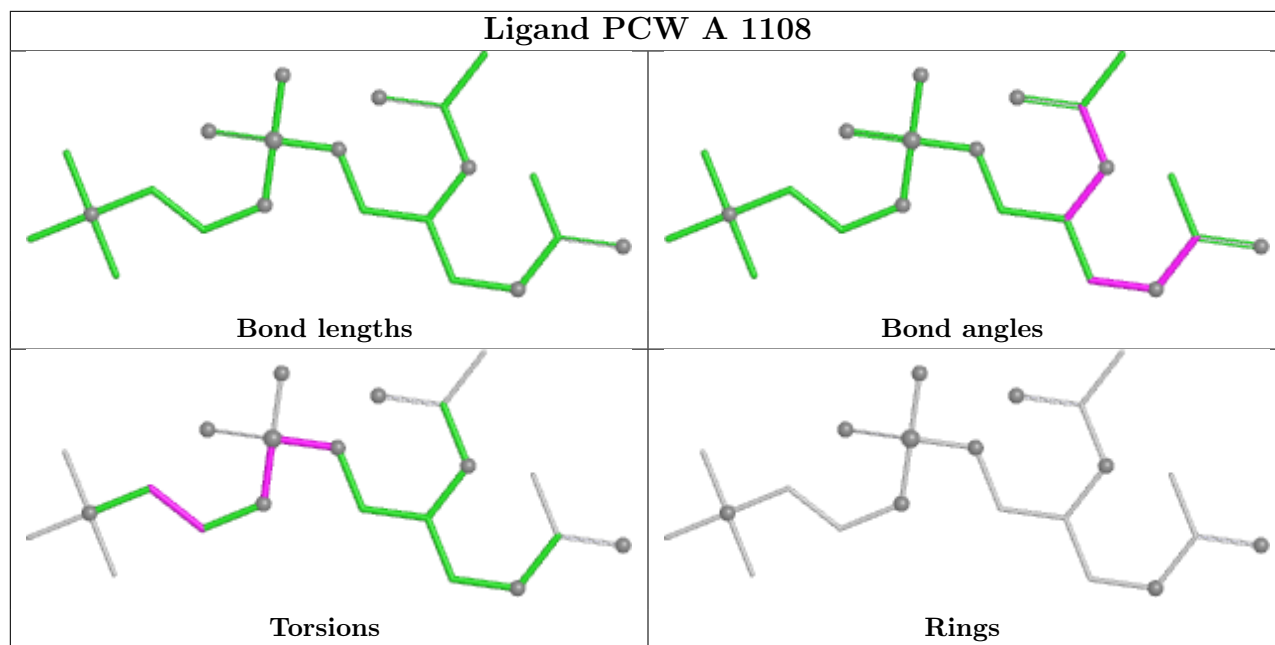
Ligand PCW A 1110



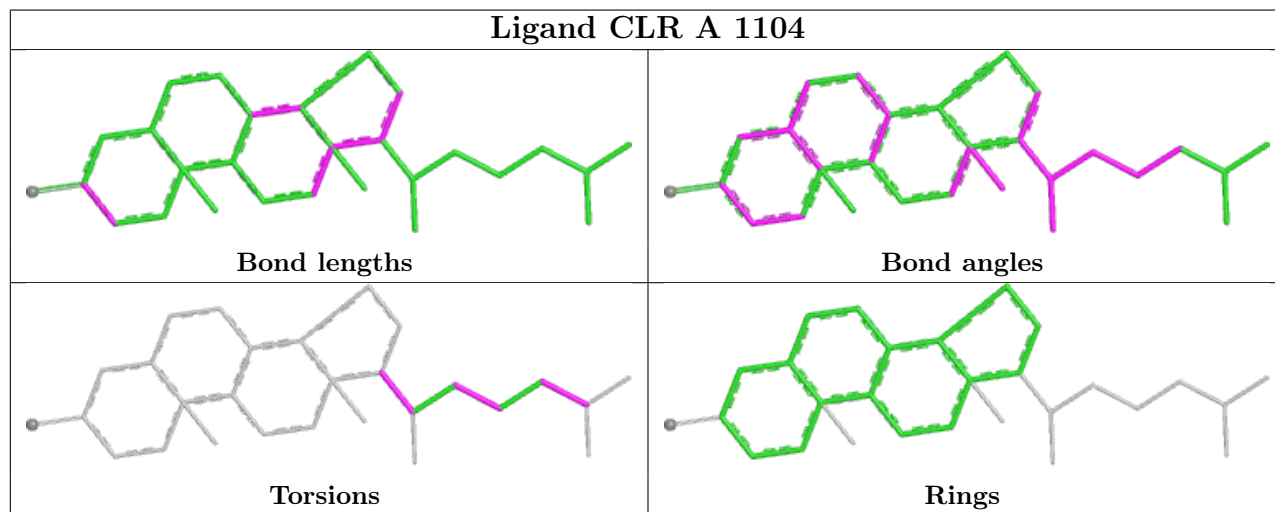
Ligand PCW A 1105

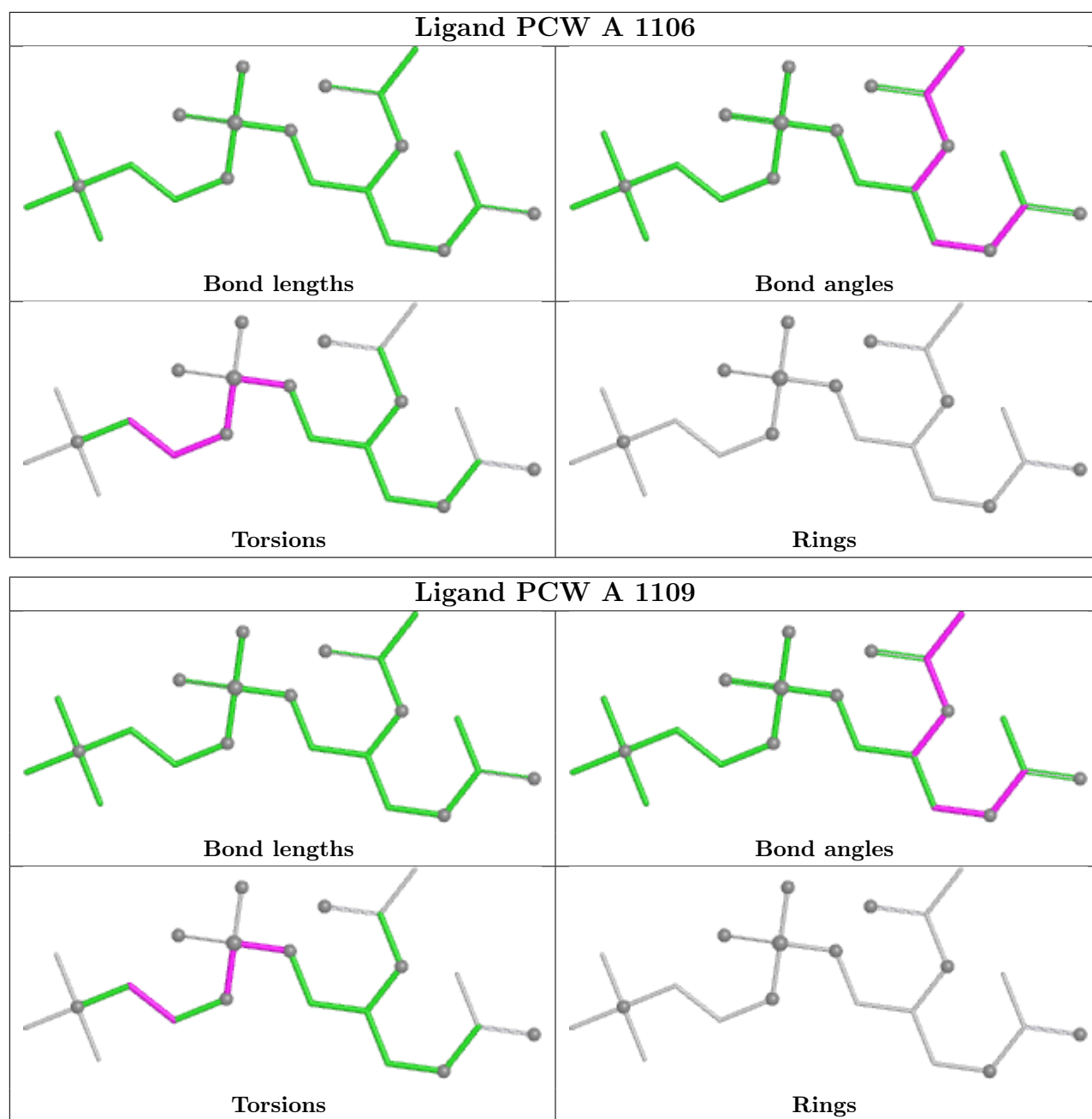


Ligand PCW A 1108



Ligand CLR A 1104





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	995/1021 (97%)	-0.93	0 100 100	74, 126, 179, 226	0
2	B	291/303 (96%)	-0.88	0 100 100	98, 142, 184, 210	0
3	G	32/65 (49%)	-0.98	0 100 100	79, 109, 140, 167	0
All	All	1318/1389 (94%)	-0.92	0 100 100	74, 130, 180, 226	0

There are no RSRZ outliers to report.

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.

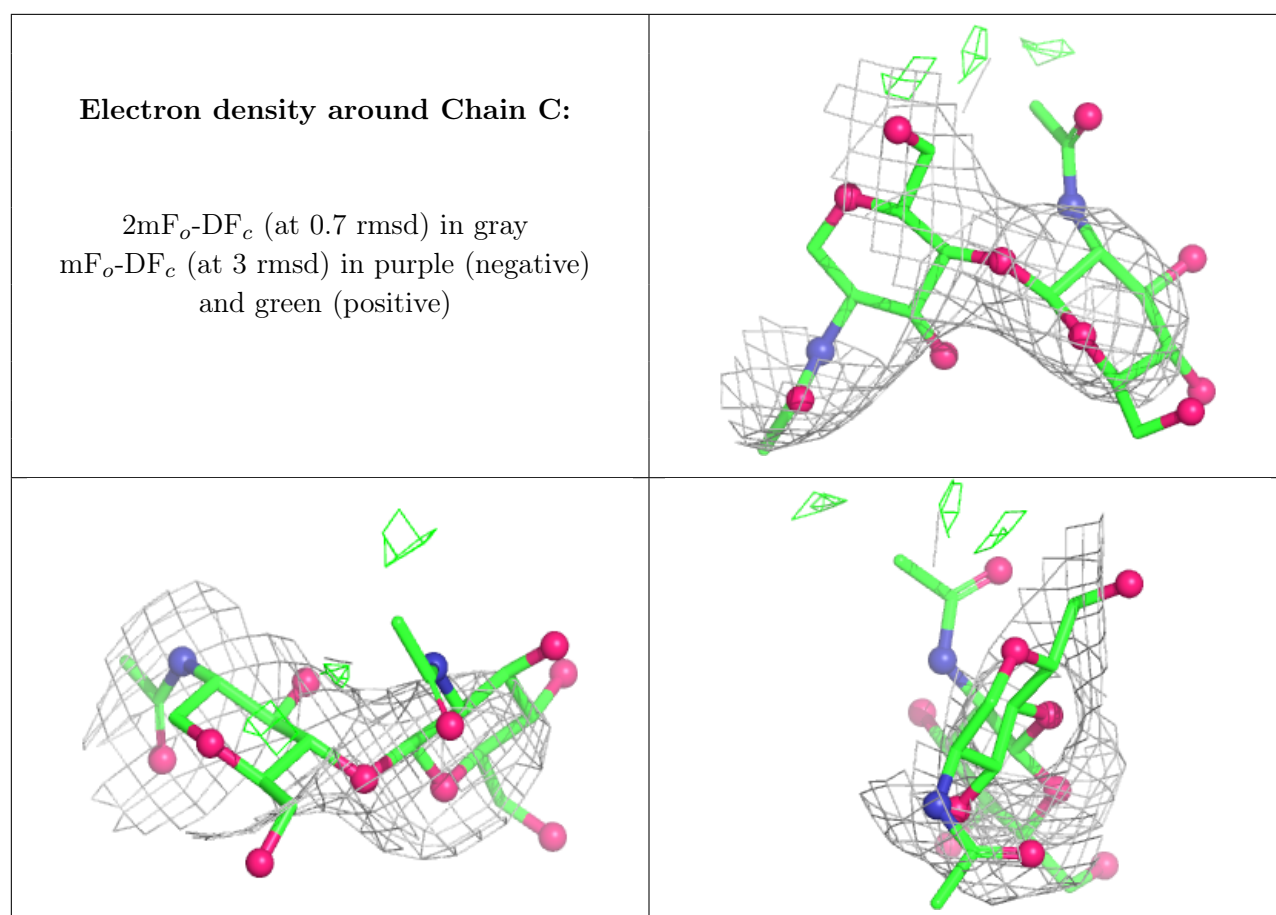
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	BFD	A	369	12/13	0.95	0.06	91,102,121,129	0

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	C	1	14/15	-	-	136,180,203,203	0
4	NAG	C	2	14/15	-	-	149,194,205,209	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.



6.4 Ligands [i](#)

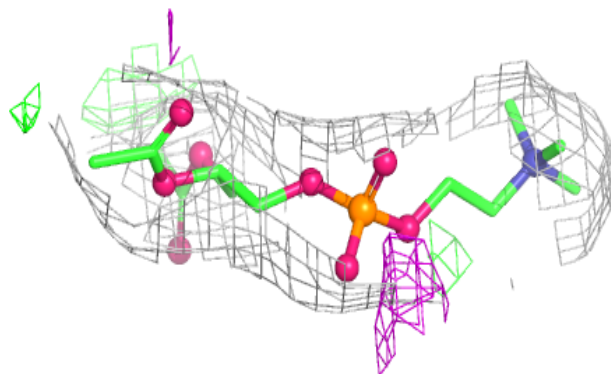
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PCW	A	1107	22/54	0.73	0.08	128,165,205,234	0
7	PCW	A	1108	22/54	0.81	0.07	117,154,172,175	0
8	A1MA6	A	1111	184/186	0.82	0.08	130,171,213,230	0
7	PCW	A	1110	22/54	0.83	0.09	108,158,183,197	0
7	PCW	A	1109	22/54	0.83	0.07	128,161,183,193	0
7	PCW	A	1105	22/54	0.86	0.07	134,187,207,245	0
9	NAG	B	401	14/15	0.88	0.08	183,197,206,212	0
7	PCW	A	1106	22/54	0.89	0.07	127,174,202,214	0
6	CLR	A	1104	28/28	0.90	0.07	112,128,134,150	0
6	CLR	A	1103	28/28	0.91	0.08	105,121,138,161	0
5	MG	A	1102	1/1	0.98	0.10	100,100,100,100	0
5	MG	A	1101	1/1	0.99	0.03	116,116,116,116	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.

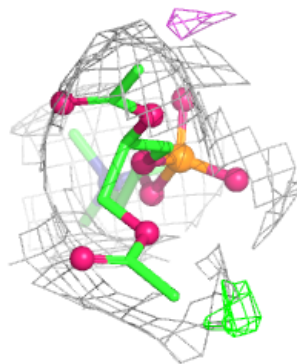
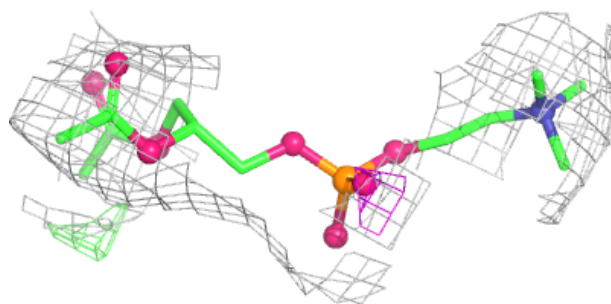
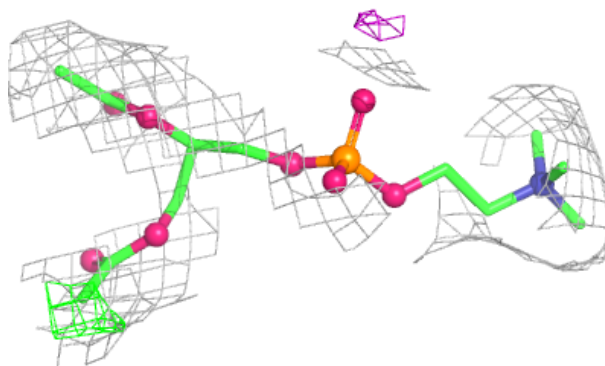
Electron density around PCW A 1107:

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



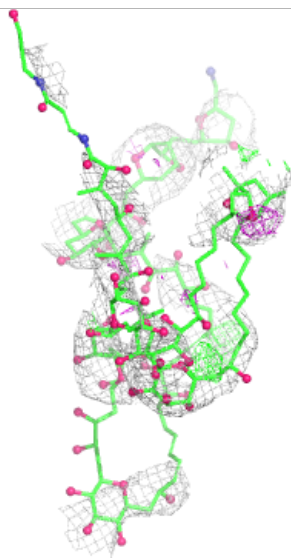
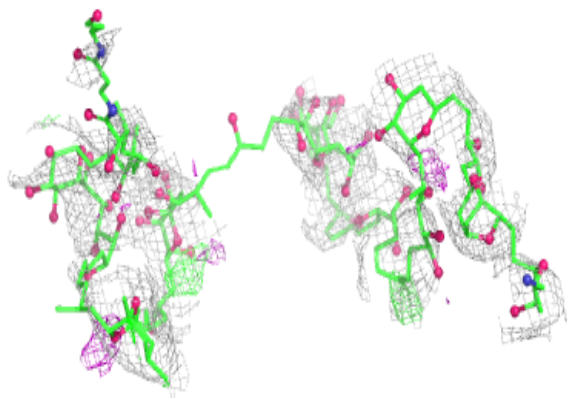
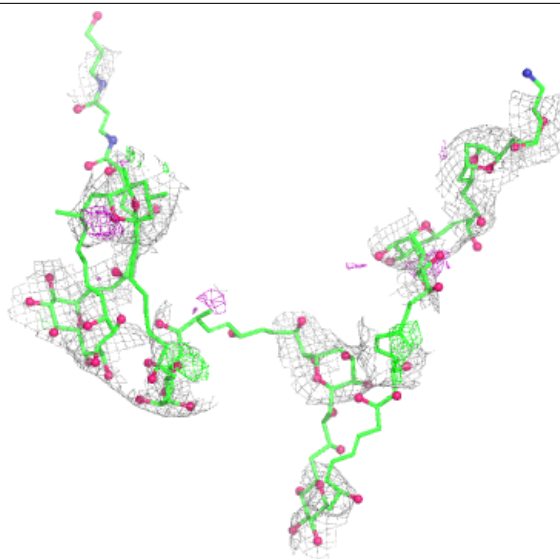
Electron density around PCW A 1108:

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



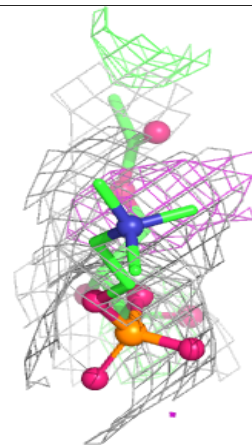
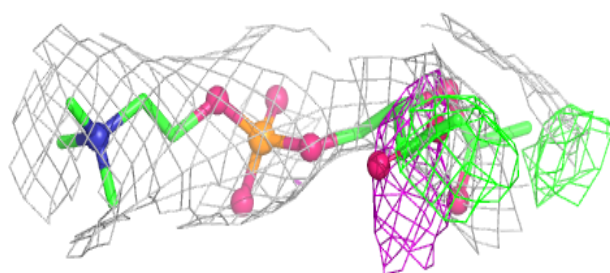
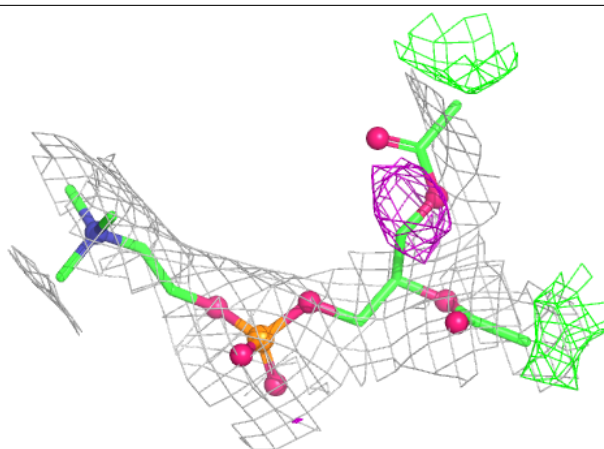
Electron density around A1MA6 A 1111:

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and green (positive)

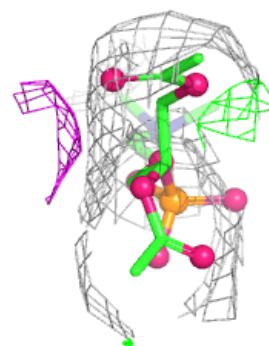
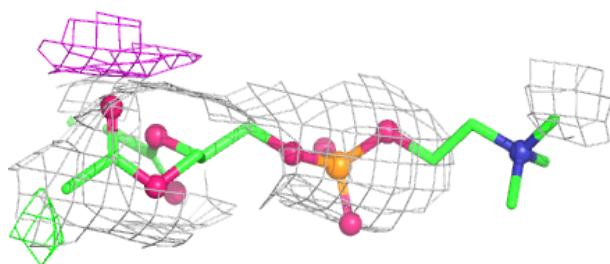
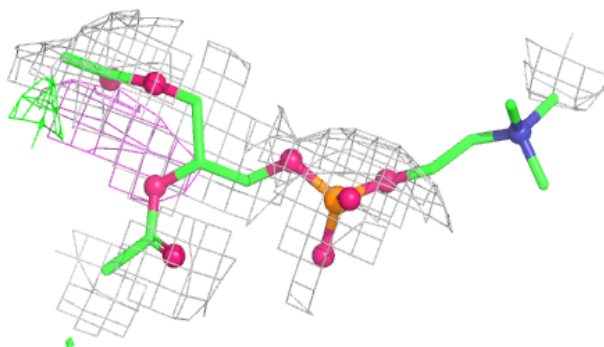


Electron density around PCW A 1110:

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and green (positive)

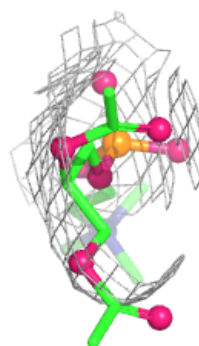
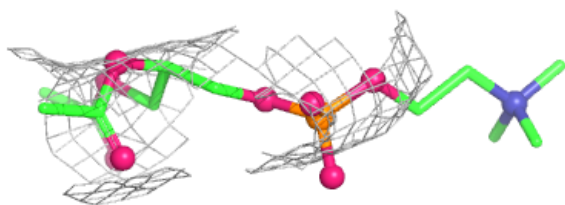
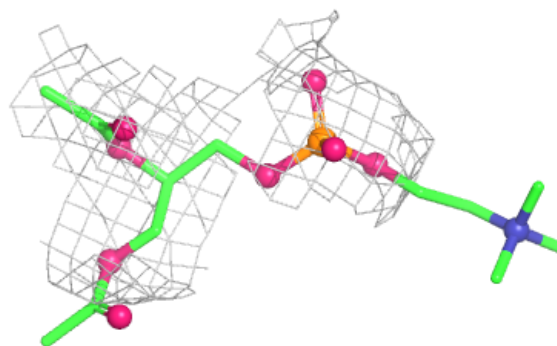
**Electron density around PCW A 1109:**

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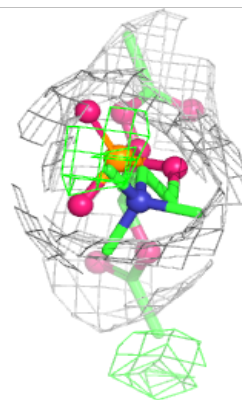
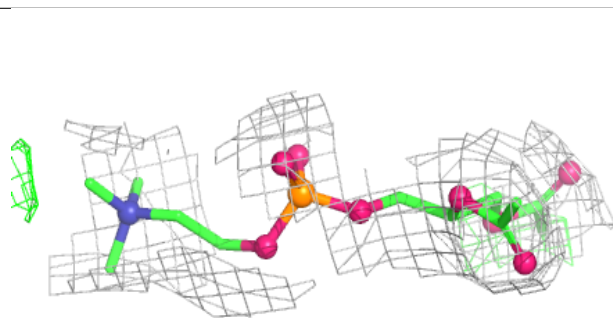
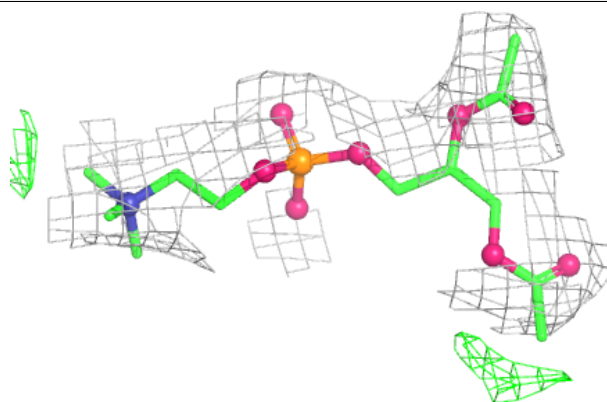


Electron density around PCW A 1105:

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

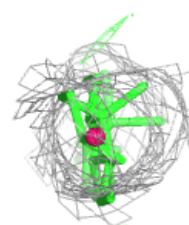
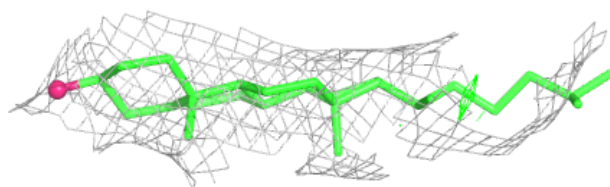
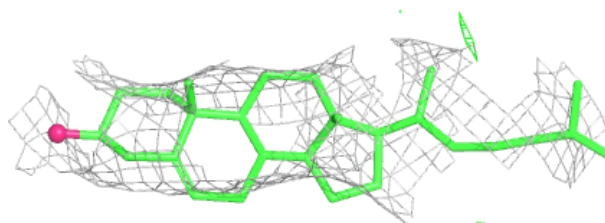
**Electron density around PCW A 1106:**

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and green (positive)

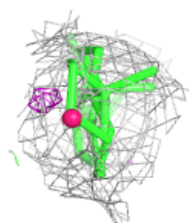
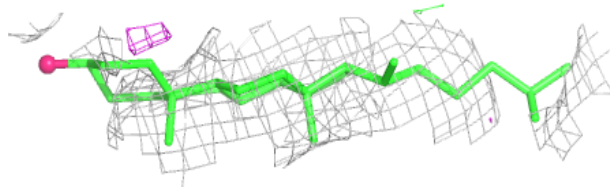
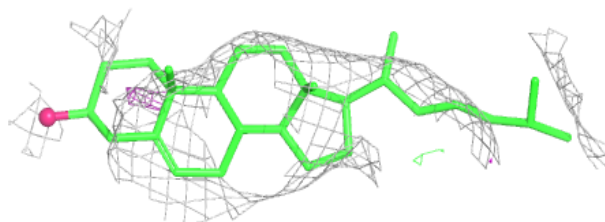


Electron density around CLR A 1104:

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

**Electron density around CLR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.