



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 06:06 PM EST

PDB ID : 6MGK
Title : Crystal structure of the catalytic domain from GH74 enzyme PoGH74 from *Paenibacillus odorifer*, in complex with XLX xyloglucan
Authors : Stogios, P.J.; Skarina, T.; Nocek, B.; Arnal, G.; Brumer, H.; Savchenko, A.
Deposited on : 2018-09-14
Resolution : 2.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

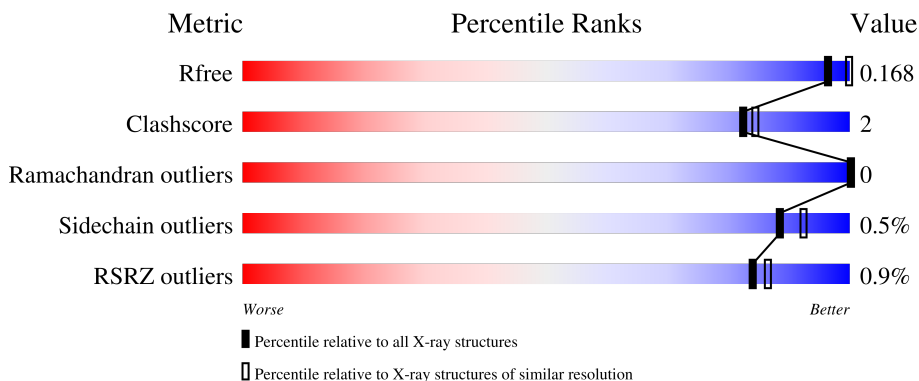
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

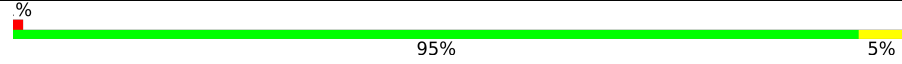
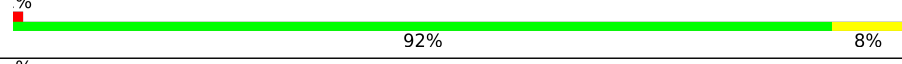
The reported resolution of this entry is 2.10 Å.

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.



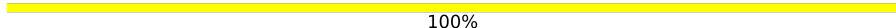
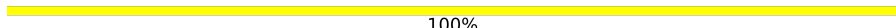

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	747	
1	B	747	
1	C	747	
1	D	747	
2	E	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	5	 100%
2	H	5	 100%
3	F	7	 86% 14%

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	GOL	B	817	-	-	-	X
4	GOL	D	817	-	-	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 26723 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.

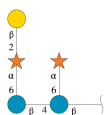
- Molecule 1 is a protein called Xyloglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	747	5668	3576	953	1121	18	0	2	0
1	B	747	5677	3581	953	1124	19	0	4	0
1	C	747	5663	3571	953	1121	18	0	1	0
1	D	747	5663	3571	953	1121	18	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

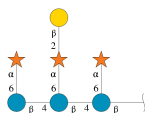
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A1R0YRH0
A	0	MSE	-	expression tag	UNP A0A1R0YRH0
A	600	GLY	ALA	variant	UNP A0A1R0YRH0
A	680	SER	ALA	variant	UNP A0A1R0YRH0
B	-1	GLY	-	expression tag	UNP A0A1R0YRH0
B	0	MSE	-	expression tag	UNP A0A1R0YRH0
B	600	GLY	ALA	variant	UNP A0A1R0YRH0
B	680	SER	ALA	variant	UNP A0A1R0YRH0
C	-1	GLY	-	expression tag	UNP A0A1R0YRH0
C	0	MSE	-	expression tag	UNP A0A1R0YRH0
C	600	GLY	ALA	variant	UNP A0A1R0YRH0
C	680	SER	ALA	variant	UNP A0A1R0YRH0
D	-1	GLY	-	expression tag	UNP A0A1R0YRH0
D	0	MSE	-	expression tag	UNP A0A1R0YRH0
D	600	GLY	ALA	variant	UNP A0A1R0YRH0
D	680	SER	ALA	variant	UNP A0A1R0YRH0

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose.



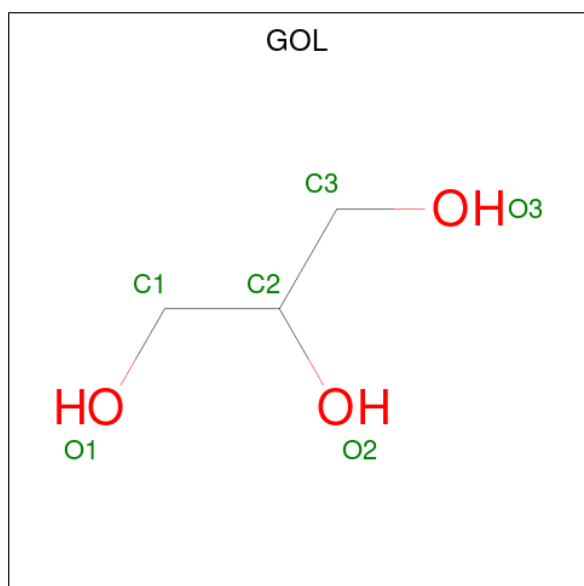
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	5	Total	C	O	0	0	0
			52	28	24			
2	G	5	Total	C	O	0	0	0
			52	28	24			
2	H	5	Total	C	O	0	0	0
			52	28	24			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	7	Total	C	O	0	0	0
			72	39	33			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

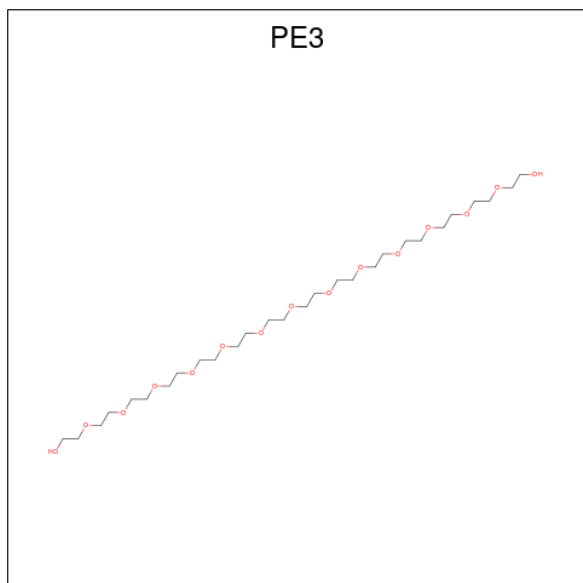
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			12	8	4		
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			12	8	4		
5	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0

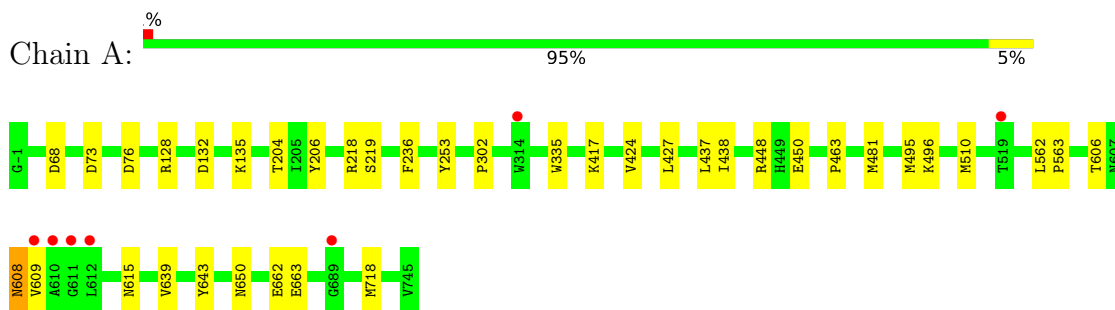
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	857	Total O 886 886	0	29
7	B	777	Total O 800 800	0	23
7	C	876	Total O 898 898	0	22
7	D	867	Total O 886 886	0	21

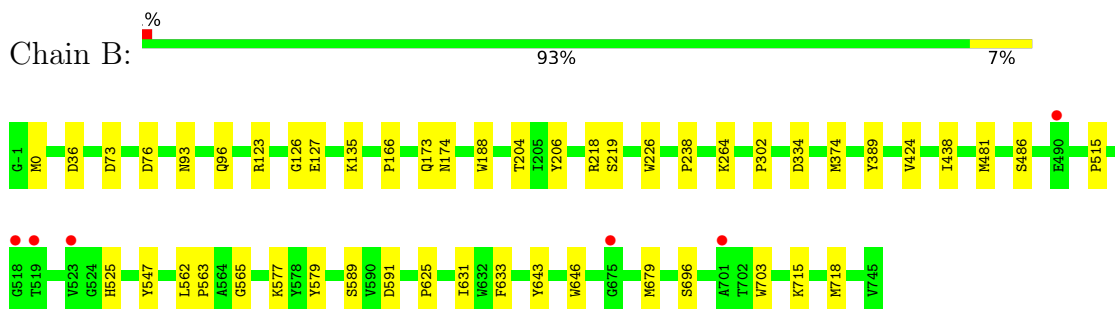
3 Residue-property plots [i](#)

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.

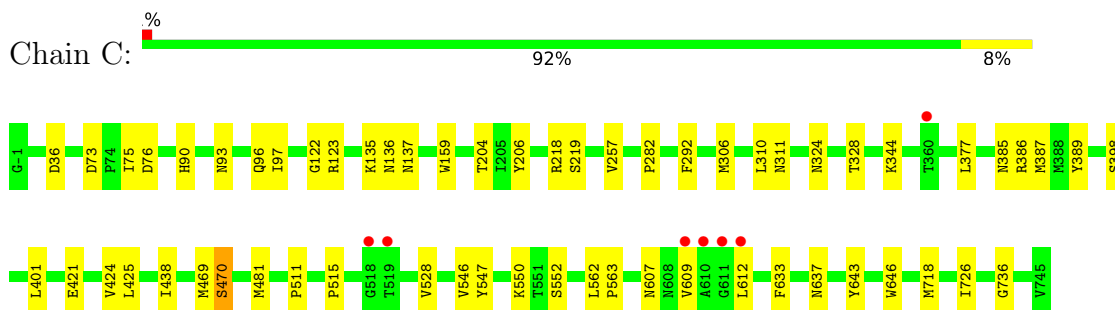
- Molecule 1: Xyloglucanase



- Molecule 1: Xyloglucanase

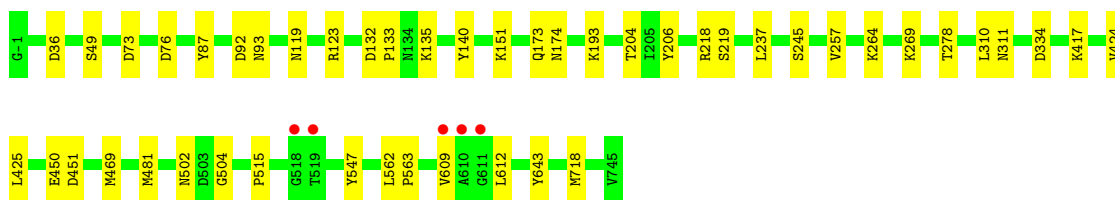


- Molecule 1: Xyloglucanase



- Molecule 1: Xyloglucanase





- Molecule 2: beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose

Chain E: 100%

BGC1
BGC2
XYS3
GAL4
XYS5

- Molecule 2: beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose

Chain G: 100%

BGC1
BGC2
XYS3
GAL4
XYS5

- Molecule 2: beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose

Chain H: 100%

BGC1
BGC2
XYS3
GAL4
XYS5

- Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose

Chain F: 86% 14%

BGC1
BGC2
BGC3
XYS4
XYS5
GAL6
XYS7

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	239.26Å 212.47Å 91.65Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	39.29 – 2.10 39.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.7 (39.29-2.10) 89.6 (39.29-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (DEV_3092: ???)	Depositor
R, R_{free}	0.158 , 0.181 0.159 , 0.168	Depositor DCC
R_{free} test set	2000 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26723	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: CL, PE3, XYS, BGC, GOL, GAL

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	0.26	0/5817	0.51	0/7921
1	B	0.26	0/5832	0.49	0/7940
1	C	0.28	0/5809	0.49	0/7910
1	D	0.27	0/5809	0.50	0/7910
All	All	0.27	0/23267	0.50	0/31681

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	5668	0	5372	24	0
1	B	5677	0	5381	30	0
1	C	5663	0	5361	34	0
1	D	5663	0	5361	24	0
2	E	52	0	43	0	0
2	G	52	0	43	0	0
2	H	52	0	43	0	0
3	F	72	0	59	1	0
4	A	66	0	88	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	78	0	104	5	0
4	C	54	0	72	0	0
4	D	72	0	96	3	0
5	A	23	0	30	0	0
5	B	25	0	31	0	0
5	C	19	0	23	3	0
5	D	13	0	17	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	886	0	0	1	0
7	B	800	0	0	4	0
7	C	898	0	0	3	0
7	D	886	0	0	0	0
All	All	26723	0	22124	112	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 2.

All (112) 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:609:VAL:HG11	1:A:639:VAL:HG11	1.57	0.84
1:B:0[A]:MSE:CE	7:B:1669:HOH:O	2.26	0.82
1:D:451:ASP:H	4:D:812:GOL:H11	1.52	0.73
1:A:302:PRO:HG2	1:B:302:PRO:HG2	1.75	0.69
1:B:0[A]:MSE:HE1	7:B:1669:HOH:O	1.92	0.68
1:D:49:SER:HB3	1:D:417:LYS:HE3	1.77	0.65
1:A:417:LYS:HE2	4:A:806:GOL:H31	1.80	0.64
1:D:450:GLU:HB2	4:D:812:GOL:H11	1.80	0.62
1:C:562:LEU:HD12	1:C:563:PRO:HD2	1.83	0.61
1:A:495:MSE:SE	1:A:510:MSE:SE	3.20	0.60
1:B:577:LYS:HE2	7:B:1412:HOH:O	2.01	0.59
1:B:135:LYS:HG2	4:B:813:GOL:H32	1.86	0.57
1:B:218:ARG:HH22	4:B:814:GOL:H31	1.71	0.55
1:A:606:THR:O	1:A:608:ASN:N	2.38	0.55
1:A:335:TRP:CD1	4:A:809:GOL:H12	2.43	0.53
1:A:335:TRP:HD1	4:A:809:GOL:H12	1.72	0.53
1:C:387:MSE:HB2	1:C:401:LEU:HD22	1.92	0.52
1:D:133:PRO:HB2	1:D:193:LYS:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:LEU:HD12	1:B:563:PRO:HD2	1.92	0.52
1:B:486:SER:HB2	1:B:525:HIS:CE1	2.46	0.51
1:D:245:SER:HA	4:D:810:GOL:H32	1.92	0.50
1:A:615:ASN:ND2	7:A:908:HOH:O	2.44	0.50
1:C:324:ASN:ND2	1:C:328:THR:OG1	2.41	0.50
1:C:515:PRO:HB3	1:C:547:TYR:CG	2.46	0.50
1:C:609:VAL:HB	1:C:612:LEU:HD12	1.92	0.50
1:A:662:GLU:HG2	1:A:663:GLU:HG3	1.92	0.49
1:C:607:ASN:OD1	1:C:637:ASN:ND2	2.45	0.49
1:A:606:THR:O	1:A:606:THR:OG1	2.30	0.49
1:B:204:THR:HA	1:B:219:SER:O	2.13	0.49
1:A:650:ASN:HA	4:A:814:GOL:H32	1.95	0.49
1:B:438:ILE:HD12	1:B:481:MSE:SE	2.62	0.49
1:B:577:LYS:HA	1:B:589:SER:O	2.13	0.49
1:A:463:PRO:HB3	1:A:510:MSE:SE	2.63	0.48
1:B:625:PRO:HD2	1:B:679:MSE:HE1	1.94	0.48
1:A:438:ILE:HD12	1:A:481:MSE:SE	2.64	0.47
1:C:306:MSE:HE1	1:C:387:MSE:SE	2.63	0.47
1:D:73:ASP:HB3	1:D:76:ASP:O	2.15	0.47
4:B:810:GOL:H2	1:C:385:ASN:ND2	2.29	0.47
1:C:424:VAL:O	1:C:718:MSE:HB3	2.13	0.47
1:B:36:ASP:HB3	1:B:123:ARG:HD2	1.95	0.47
1:A:73:ASP:HB3	1:A:76:ASP:O	2.15	0.47
1:C:36:ASP:HB3	1:C:123:ARG:HD2	1.95	0.47
5:C:816:PE3:H411	5:C:816:PE3:H381	1.65	0.47
1:D:481:MSE:HE3	1:D:504:GLY:HA2	1.97	0.46
1:D:269:LYS:HG2	1:D:278:THR:HB	1.96	0.46
1:A:496:LYS:H	1:A:510:MSE:SE	2.48	0.46
1:D:515:PRO:HB3	1:D:547:TYR:CG	2.51	0.46
1:A:424:VAL:O	1:A:718:MSE:HB3	2.16	0.46
1:C:73:ASP:HB3	1:C:76:ASP:O	2.16	0.46
1:C:633:PHE:HB3	1:C:646:TRP:HB2	1.97	0.46
1:B:424:VAL:O	1:B:718:MSE:HB3	2.16	0.45
1:B:515:PRO:HB3	1:B:547:TYR:CG	2.51	0.45
1:C:90:HIS:HB3	5:C:816:PE3:C42	2.45	0.45
1:A:562:LEU:HD12	1:A:563:PRO:HD2	1.98	0.45
1:B:565:GLY:HA2	4:B:819:GOL:H31	1.97	0.45
1:B:633:PHE:HB3	1:B:646:TRP:HB2	1.97	0.45
1:D:264:LYS:HD2	1:D:264:LYS:HA	1.79	0.45
1:B:579:TYR:CZ	1:B:631:ILE:HD11	2.52	0.44
1:A:427:LEU:HD22	1:A:437:LEU:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:HB3	5:C:816:PE3:H321	1.98	0.44
1:D:425:LEU:HD22	1:D:469:MSE:SE	2.68	0.44
1:D:424:VAL:O	1:D:718:MSE:HB3	2.18	0.44
1:B:73:ASP:HB3	1:B:76:ASP:O	2.18	0.44
1:A:204:THR:HA	1:A:219:SER:O	2.18	0.43
1:D:173:GLN:HG2	1:D:174:ASN:ND2	2.33	0.43
1:C:386:ARG:HA	1:C:398:SER:O	2.19	0.43
1:A:68:ASP:CG	1:A:128:ARG:HH12	2.22	0.43
1:D:36:ASP:HB3	1:D:123:ARG:HD2	2.01	0.43
1:C:122:GLY:HA2	1:C:257:VAL:O	2.18	0.43
1:C:511:PRO:HB3	1:C:552:SER:O	2.18	0.43
1:D:92:ASP:OD1	1:D:93:ASN:N	2.52	0.43
1:A:236:PHE:HB3	1:A:253:TYR:HB3	2.00	0.43
1:C:206:TYR:CE2	1:C:218:ARG:HD3	2.54	0.43
1:A:206:TYR:CE2	1:A:218:ARG:HD3	2.54	0.42
1:C:470:SER:OG	1:C:528:VAL:HG12	2.18	0.42
1:A:132:ASP:HB3	1:A:135:LYS:O	2.19	0.42
1:C:204:THR:HA	1:C:219:SER:O	2.20	0.42
1:C:470:SER:HB2	7:C:1287:HOH:O	2.18	0.42
1:C:425:LEU:HD22	1:C:469:MSE:SE	2.70	0.42
4:B:811:GOL:H11	1:C:726:ILE:HG23	2.00	0.42
1:C:97:ILE:HG21	1:C:159:TRP:CZ2	2.55	0.42
1:D:310:LEU:HA	1:D:311:ASN:HA	1.87	0.42
1:D:562:LEU:HD12	1:D:563:PRO:HD2	2.01	0.42
1:A:448:ARG:NH1	1:A:450:GLU:OE2	2.44	0.42
1:C:344:LYS:NZ	7:C:906:HOH:O	2.36	0.42
1:D:204:THR:HA	1:D:219:SER:O	2.20	0.42
1:D:609:VAL:HB	1:D:612:LEU:HD22	2.02	0.41
1:B:206:TYR:CE2	1:B:218:ARG:HD3	2.55	0.41
1:C:421:GLU:HA	1:C:736:GLY:O	2.20	0.41
1:D:132:ASP:HB3	1:D:135:LYS:O	2.18	0.41
1:B:591:ASP:OD1	1:B:591:ASP:N	2.51	0.41
1:B:715:LYS:HG2	3:F:4:XYS:H4	2.02	0.41
1:D:140:TYR:OH	1:D:151:LYS:HE3	2.20	0.41
1:D:237:LEU:HD13	1:D:257:VAL:HG13	2.03	0.41
1:C:377:LEU:HD12	1:C:389:TYR:HB3	2.03	0.41
1:C:546:VAL:HG21	1:C:562:LEU:HD23	2.03	0.41
1:B:126:GLY:HA3	1:B:127:GLU:HA	1.83	0.41
1:B:696:SER:HB2	1:B:703:TRP:CE3	2.56	0.41
1:C:75:ILE:HD12	1:C:136:ASN:HB3	2.03	0.41
1:D:206:TYR:CE2	1:D:218:ARG:HD3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HD3	1:B:226:TRP:HB2	2.02	0.41
1:B:188:TRP:HE1	1:B:238:PRO:HB2	1.86	0.41
1:B:374:MSE:HE3	1:B:389:TYR:CD2	2.56	0.41
1:C:282:PRO:HD2	1:C:292:PHE:CZ	2.56	0.41
1:C:310:LEU:HA	1:C:311:ASN:HA	1.86	0.41
1:D:87:TYR:CE1	1:D:119:ASN:HB3	2.55	0.41
1:C:438:ILE:HD12	1:C:481:MSE:SE	2.71	0.41
1:B:173:GLN:HG2	1:B:174:ASN:ND2	2.35	0.40
1:B:0[A]:MSE:HE2	7:B:1669:HOH:O	2.06	0.40
1:B:264:LYS:HD2	1:B:264:LYS:HA	1.95	0.40
1:C:550:LYS:HG2	7:C:954:HOH:O	2.21	0.40
1:C:135:LYS:HD2	1:C:137:ASN:OD1	2.22	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	747/747 (100%)	717 (96%)	30 (4%)	0	100	100
1	B	749/747 (100%)	722 (96%)	27 (4%)	0	100	100
1	C	746/747 (100%)	717 (96%)	29 (4%)	0	100	100
1	D	746/747 (100%)	717 (96%)	29 (4%)	0	100	100
All	All	2988/2988 (100%)	2873 (96%)	115 (4%)	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	601/581 (103%)	599 (100%)	2 (0%)	92	95
1	B	603/581 (104%)	599 (99%)	4 (1%)	84	88
1	C	600/581 (103%)	597 (100%)	3 (0%)	88	92
1	D	600/581 (103%)	597 (100%)	3 (0%)	88	92
All	All	2404/2324 (103%)	2392 (100%)	12 (0%)	88	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	608	ASN
1	A	643	TYR
1	B	93	ASN
1	B	96	GLN
1	B	334	ASP
1	B	643	TYR
1	C	96	GLN
1	C	470	SER
1	C	643	TYR
1	D	334	ASP
1	D	502	ASN
1	D	643	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

22 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
2	BGC	E	1	2	12,12,12	1.13	1 (8%)	17,17,17	0.75	0
2	BGC	E	2	2	11,11,12	1.78	3 (27%)	15,15,17	1.09	1 (6%)
2	XYS	E	3	2	9,9,10	1.91	3 (33%)	10,12,14	0.91	0
2	GAL	E	4	2	11,11,12	1.78	2 (18%)	15,15,17	1.09	1 (6%)
2	XYS	E	5	2	9,9,10	2.01	3 (33%)	10,12,14	0.85	1 (10%)
3	BGC	F	1	3	12,12,12	1.13	1 (8%)	17,17,17	0.72	0
3	BGC	F	2	3	11,11,12	1.65	2 (18%)	15,15,17	1.13	2 (13%)
3	BGC	F	3	3	11,11,12	1.72	3 (27%)	15,15,17	0.64	0
3	XYS	F	4	3	9,9,10	1.94	3 (33%)	10,12,14	1.01	1 (10%)
3	XYS	F	5	3	9,9,10	1.88	3 (33%)	10,12,14	1.22	1 (10%)
3	GAL	F	6	3	11,11,12	1.77	2 (18%)	15,15,17	0.99	1 (6%)
3	XYS	F	7	3	9,9,10	1.95	3 (33%)	10,12,14	0.82	1 (10%)
2	BGC	G	1	2	12,12,12	1.15	1 (8%)	17,17,17	0.72	0
2	BGC	G	2	2	11,11,12	1.75	3 (27%)	15,15,17	0.88	1 (6%)
2	XYS	G	3	2	9,9,10	1.94	3 (33%)	10,12,14	1.11	1 (10%)
2	GAL	G	4	2	11,11,12	1.77	2 (18%)	15,15,17	1.59	2 (13%)
2	XYS	G	5	2	9,9,10	1.99	3 (33%)	10,12,14	0.87	0
2	BGC	H	1	2	12,12,12	1.16	1 (8%)	17,17,17	0.76	0
2	BGC	H	2	2	11,11,12	1.72	3 (27%)	15,15,17	0.97	1 (6%)
2	XYS	H	3	2	9,9,10	1.90	3 (33%)	10,12,14	1.12	1 (10%)
2	GAL	H	4	2	11,11,12	1.78	3 (27%)	15,15,17	1.18	1 (6%)
2	XYS	H	5	2	9,9,10	2.00	3 (33%)	10,12,14	0.98	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
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	XYS	E	3	2	-	-	0/1/1/1
2	GAL	E	4	2	-	2/2/19/22	0/1/1/1
2	XYS	E	5	2	-	-	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	F	3	3	-	0/2/19/22	0/1/1/1
3	XYS	F	4	3	-	-	0/1/1/1
3	XYS	F	5	3	-	-	0/1/1/1
3	GAL	F	6	3	-	2/2/19/22	0/1/1/1
3	XYS	F	7	3	-	-	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	XYS	G	3	2	-	-	0/1/1/1
2	GAL	G	4	2	-	2/2/19/22	0/1/1/1
2	XYS	G	5	2	-	-	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
2	XYS	H	3	2	-	-	0/1/1/1
2	GAL	H	4	2	-	2/2/19/22	0/1/1/1
2	XYS	H	5	2	-	-	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	GAL	O5-C1	4.69	1.51	1.43
2	E	4	GAL	O5-C1	4.65	1.51	1.43
2	H	4	GAL	O5-C1	4.62	1.51	1.43
2	E	2	BGC	O5-C1	4.62	1.51	1.43
3	F	6	GAL	O5-C1	4.59	1.51	1.43
2	G	2	BGC	O5-C1	4.56	1.51	1.43
2	H	2	BGC	O5-C1	4.39	1.50	1.43
3	F	3	BGC	O5-C1	4.34	1.50	1.43
3	F	2	BGC	O5-C1	4.13	1.50	1.43
2	H	5	XYS	O5-C1	4.11	1.50	1.42
2	G	5	XYS	O5-C1	4.02	1.50	1.42
2	E	5	XYS	O5-C1	4.01	1.50	1.42
3	F	7	XYS	O5-C1	3.94	1.50	1.42
3	F	4	XYS	O5-C1	3.91	1.50	1.42
2	G	3	XYS	O5-C1	3.88	1.50	1.42
2	H	3	XYS	O5-C1	3.86	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	XYS	O5-C1	3.86	1.50	1.42
3	F	5	XYS	O5-C1	3.84	1.50	1.42
2	E	5	XYS	O5-C5	3.02	1.48	1.42
2	G	1	BGC	O5-C1	3.02	1.50	1.42
2	H	1	BGC	O5-C1	3.00	1.50	1.42
2	G	5	XYS	O5-C5	2.97	1.48	1.42
2	E	1	BGC	O5-C1	2.96	1.50	1.42
2	H	5	XYS	O5-C5	2.95	1.48	1.42
3	F	7	XYS	O5-C5	2.92	1.48	1.42
3	F	1	BGC	O5-C1	2.90	1.50	1.42
2	G	3	XYS	O5-C5	2.88	1.48	1.42
3	F	4	XYS	O5-C5	2.88	1.48	1.42
2	E	3	XYS	O5-C5	2.82	1.48	1.42
3	F	5	XYS	O5-C5	2.81	1.48	1.42
2	H	3	XYS	O5-C5	2.76	1.48	1.42
2	H	4	GAL	C2-C3	-2.54	1.48	1.52
3	F	3	BGC	C2-C3	-2.51	1.48	1.52
2	E	4	GAL	C2-C3	-2.49	1.48	1.52
3	F	6	GAL	C2-C3	-2.48	1.48	1.52
3	F	2	BGC	C2-C3	-2.36	1.49	1.52
2	E	5	XYS	C2-C3	-2.36	1.49	1.52
2	G	2	BGC	C2-C3	-2.35	1.49	1.52
2	G	4	GAL	C2-C3	-2.33	1.49	1.52
2	H	2	BGC	C2-C3	-2.32	1.49	1.52
3	F	4	XYS	C2-C3	-2.29	1.49	1.52
2	E	3	XYS	C2-C3	-2.26	1.49	1.52
2	E	2	BGC	C2-C3	-2.25	1.49	1.52
3	F	7	XYS	C2-C3	-2.24	1.49	1.52
2	G	3	XYS	C2-C3	-2.20	1.49	1.52
2	G	5	XYS	C2-C3	-2.18	1.49	1.52
3	F	5	XYS	C2-C3	-2.17	1.49	1.52
2	H	5	XYS	C2-C3	-2.11	1.49	1.52
2	H	2	BGC	O5-C5	2.11	1.47	1.43
2	H	3	XYS	C2-C3	-2.10	1.49	1.52
3	F	3	BGC	O5-C5	2.09	1.47	1.43
2	E	2	BGC	O5-C5	2.08	1.47	1.43
2	H	4	GAL	O5-C5	2.07	1.47	1.43
2	G	2	BGC	O5-C5	2.05	1.47	1.43

All (16) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	GAL	C1-C2-C3	4.55	115.26	109.67
2	E	4	GAL	C1-C2-C3	2.96	113.31	109.67
3	F	5	XYS	C5-C4-C3	2.53	112.78	109.67
3	F	4	XYS	C5-C4-C3	2.53	112.78	109.67
3	F	2	BGC	C1-C2-C3	2.50	112.74	109.67
2	H	4	GAL	C1-C2-C3	2.43	112.65	109.67
2	H	2	BGC	C1-C2-C3	2.41	112.62	109.67
2	E	2	BGC	C1-C2-C3	2.40	112.61	109.67
2	G	2	BGC	C1-C2-C3	2.39	112.61	109.67
3	F	6	GAL	C1-C2-C3	2.32	112.51	109.67
2	G	4	GAL	O5-C1-C2	2.29	114.30	110.77
3	F	7	XYS	C5-C4-C3	2.19	112.36	109.67
2	E	5	XYS	C5-C4-C3	2.16	112.32	109.67
2	H	3	XYS	C5-C4-C3	2.15	112.31	109.67
2	G	3	XYS	C1-C2-C3	2.06	112.20	109.67
3	F	2	BGC	C2-C3-C4	2.04	114.43	110.89

There are no chirality outliers.

All (8) torsion outliers are listed below:

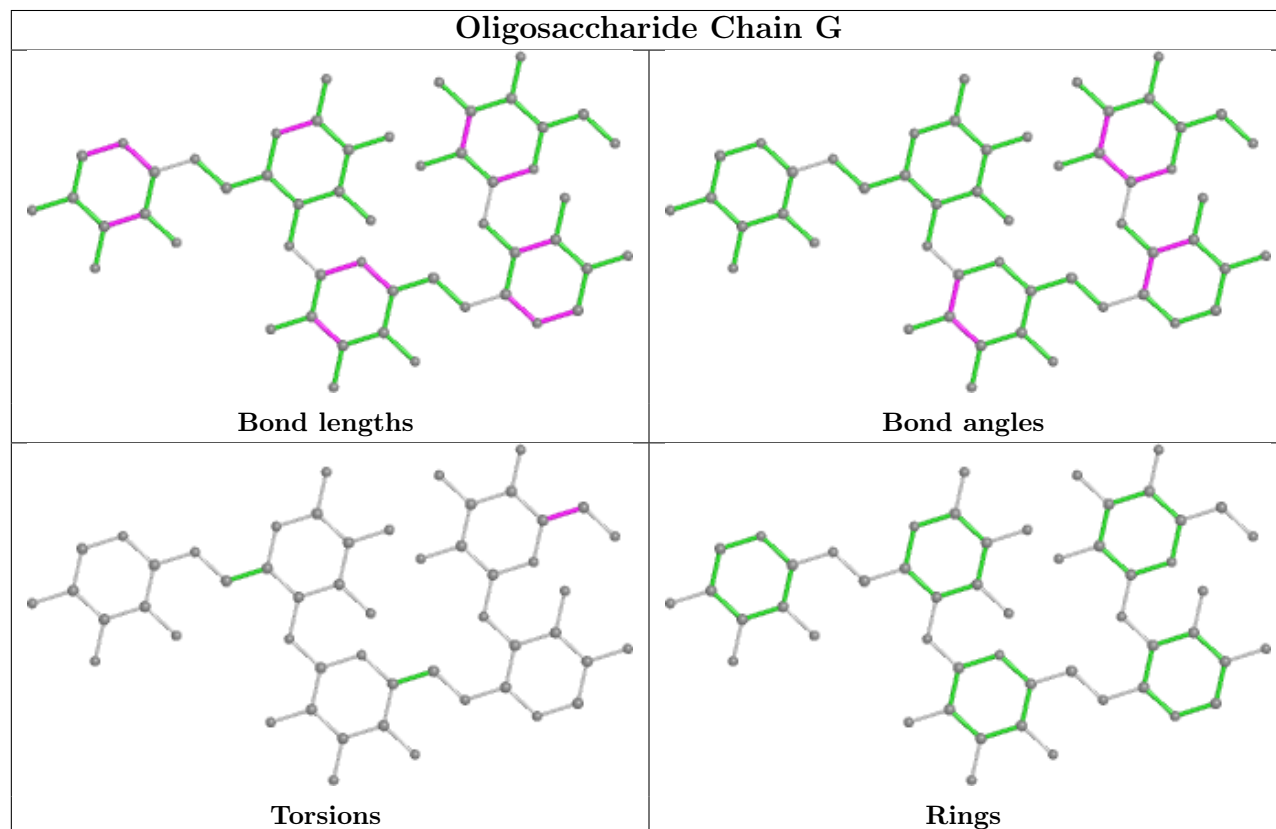
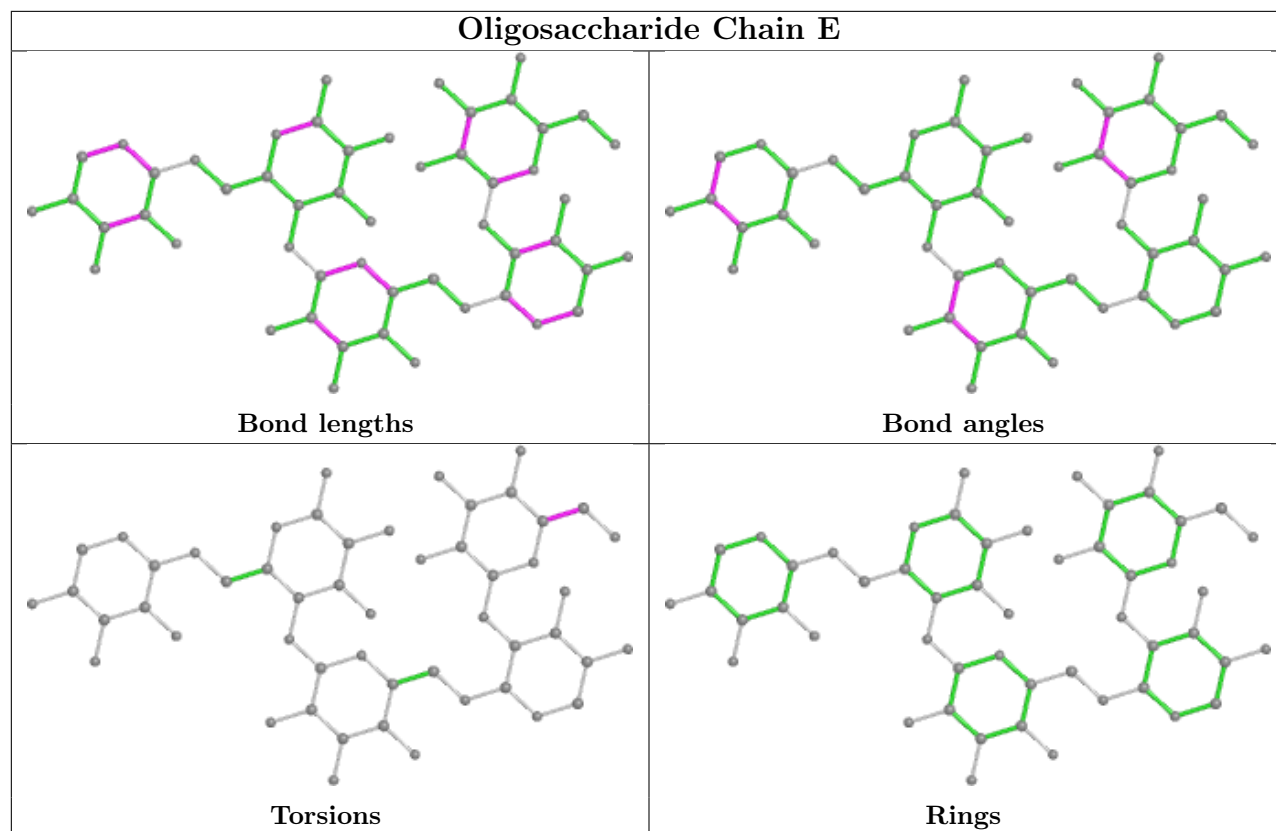
Mol	Chain	Res	Type	Atoms
3	F	6	GAL	O5-C5-C6-O6
2	H	4	GAL	O5-C5-C6-O6
2	E	4	GAL	O5-C5-C6-O6
2	G	4	GAL	O5-C5-C6-O6
2	E	4	GAL	C4-C5-C6-O6
2	G	4	GAL	C4-C5-C6-O6
2	H	4	GAL	C4-C5-C6-O6
3	F	6	GAL	C4-C5-C6-O6

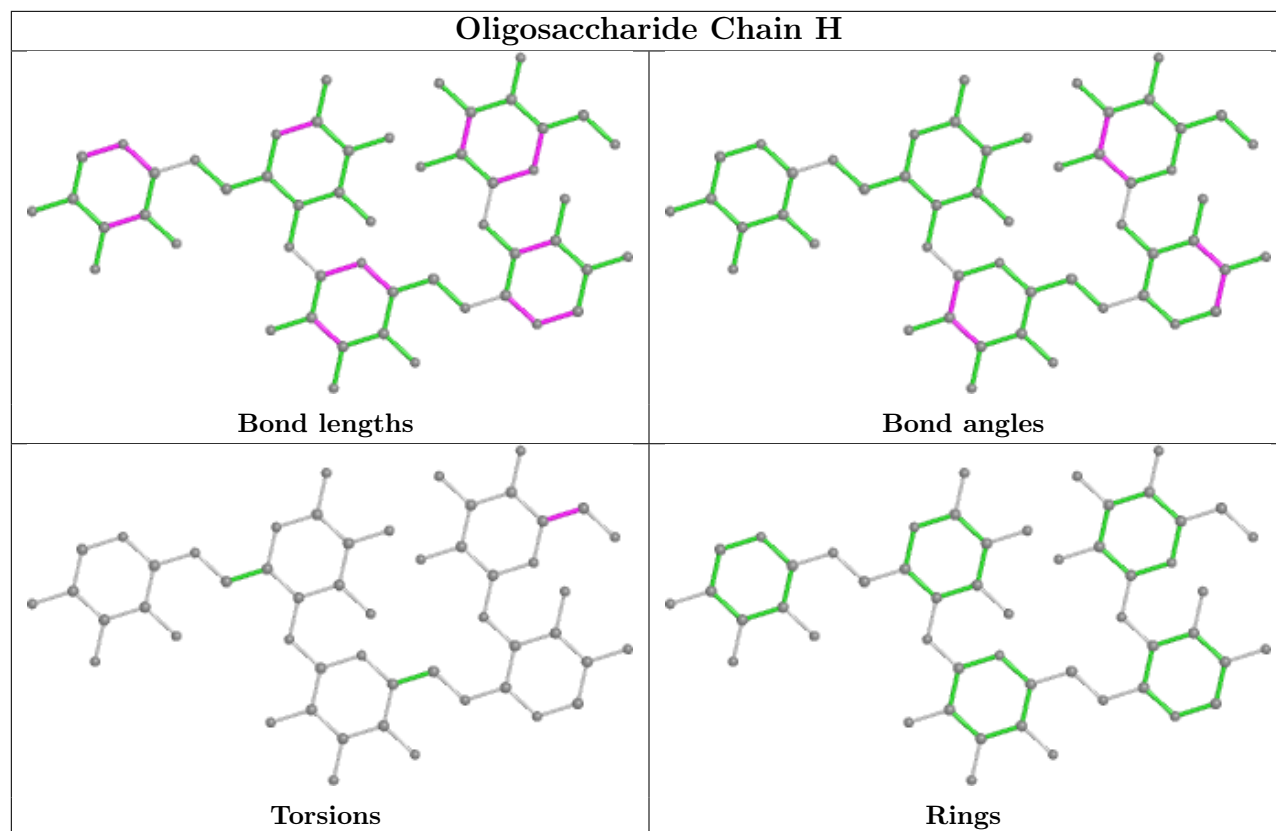
There are no ring outliers.

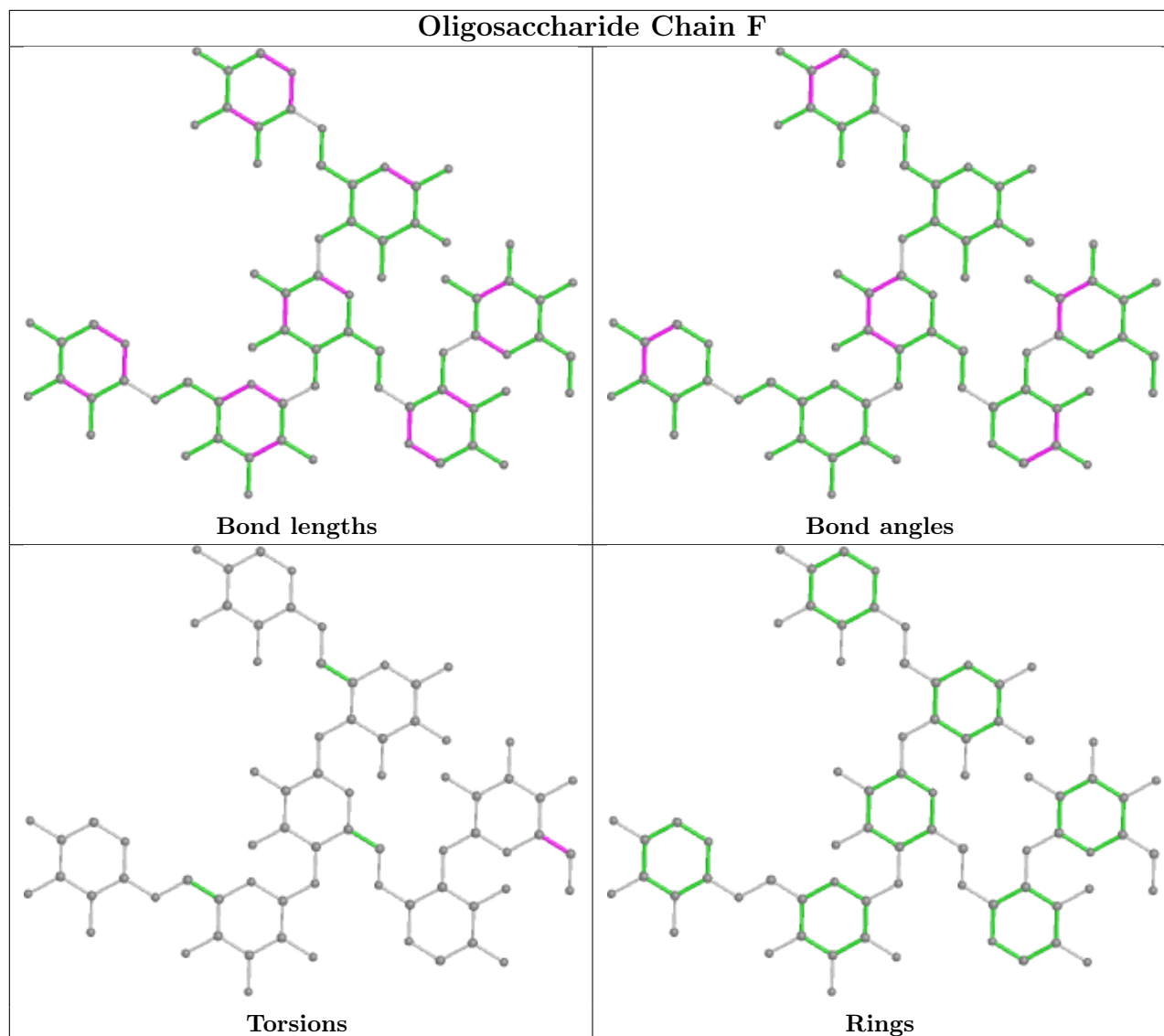
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	XYS	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 56 ligands modelled in this entry, 4 are monoatomic - leaving 52 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
4	GOL	A	806	-	5,5,5	0.89	0	5,5,5	0.99	0
4	GOL	D	810	-	5,5,5	0.91	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	816	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	B	820	-	5,5,5	0.25	0	5,5,5	0.58	0
4	GOL	C	808	-	5,5,5	0.88	0	5,5,5	1.02	0
4	GOL	B	809	-	5,5,5	0.90	0	5,5,5	1.02	0
4	GOL	A	808	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	D	816	-	5,5,5	0.88	0	5,5,5	1.04	0
4	GOL	A	807	-	5,5,5	0.89	0	5,5,5	1.00	0
4	GOL	D	809	-	5,5,5	0.90	0	5,5,5	0.98	0
5	PE3	C	815	-	6,6,42	0.59	0	5,5,41	0.66	0
5	PE3	D	818	-	12,12,42	0.58	0	11,11,41	0.64	0
4	GOL	A	815	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	A	819	-	5,5,5	0.90	0	5,5,5	1.02	0
4	GOL	B	818	-	5,5,5	0.88	0	5,5,5	1.01	0
4	GOL	C	813	-	5,5,5	0.87	0	5,5,5	0.99	0
4	GOL	C	814	-	5,5,5	0.88	0	5,5,5	1.03	0
4	GOL	B	808	-	5,5,5	0.91	0	5,5,5	1.01	0
4	GOL	D	814	-	5,5,5	0.90	0	5,5,5	0.99	0
4	GOL	A	810	-	5,5,5	0.89	0	5,5,5	1.02	0
4	GOL	A	813	-	5,5,5	0.89	0	5,5,5	1.00	0
4	GOL	B	814	-	5,5,5	0.88	0	5,5,5	1.01	0
4	GOL	C	810	-	5,5,5	0.90	0	5,5,5	0.99	0
4	GOL	D	813	-	5,5,5	0.93	0	5,5,5	1.01	0
4	GOL	B	815	-	5,5,5	0.91	0	5,5,5	0.99	0
4	GOL	D	806	-	5,5,5	0.90	0	5,5,5	1.01	0
4	GOL	D	808	-	5,5,5	0.92	0	5,5,5	0.99	0
4	GOL	B	813	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	C	807	-	5,5,5	0.91	0	5,5,5	1.00	0
4	GOL	B	819	-	5,5,5	0.88	0	5,5,5	1.01	0
4	GOL	D	807	-	5,5,5	0.92	0	5,5,5	0.96	0
4	GOL	D	811	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	A	809	-	5,5,5	0.89	0	5,5,5	1.05	0
4	GOL	A	811	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	C	811	-	5,5,5	0.87	0	5,5,5	1.03	0
4	GOL	C	809	-	5,5,5	0.91	0	5,5,5	0.99	0
5	PE3	A	817	-	9,9,42	0.70	0	8,8,41	1.45	2 (25%)
5	PE3	A	816	-	12,12,42	0.57	0	11,11,41	0.58	0
5	PE3	C	816	-	11,11,42	0.73	0	10,10,41	1.88	2 (20%)
4	GOL	B	811	-	5,5,5	0.92	0	5,5,5	1.01	0
4	GOL	C	812	-	5,5,5	0.90	0	5,5,5	0.99	0
4	GOL	A	812	-	5,5,5	0.89	0	5,5,5	0.98	0
4	GOL	D	815	-	5,5,5	0.91	0	5,5,5	1.02	0
4	GOL	A	814	-	5,5,5	0.89	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PE3	B	821	-	11,11,42	0.59	0	10,10,41	2.05	3 (30%)
4	GOL	B	817	-	5,5,5	0.90	0	5,5,5	1.01	0
4	GOL	D	817	-	5,5,5	0.88	0	5,5,5	1.03	0
5	PE3	B	822	-	12,12,42	0.62	0	11,11,41	0.71	0
4	GOL	D	812	-	5,5,5	0.86	0	5,5,5	0.94	0
4	GOL	C	806	-	5,5,5	0.86	0	5,5,5	1.07	0
4	GOL	B	812	-	5,5,5	0.89	0	5,5,5	1.04	0
4	GOL	B	810	-	5,5,5	0.93	0	5,5,5	0.98	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	GOL	A	806	-	-	2/4/4/4	-
4	GOL	D	810	-	-	4/4/4/4	-
4	GOL	B	816	-	-	0/4/4/4	-
4	GOL	B	820	-	-	4/4/4/4	-
4	GOL	C	808	-	-	0/4/4/4	-
4	GOL	B	809	-	-	2/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	D	816	-	-	0/4/4/4	-
4	GOL	A	807	-	-	2/4/4/4	-
4	GOL	D	809	-	-	1/4/4/4	-
5	PE3	C	815	-	-	1/4/4/40	-
5	PE3	D	818	-	-	3/10/10/40	-
4	GOL	A	815	-	-	2/4/4/4	-
4	GOL	A	819	-	-	0/4/4/4	-
4	GOL	B	818	-	-	1/4/4/4	-
4	GOL	C	813	-	-	0/4/4/4	-
4	GOL	C	814	-	-	2/4/4/4	-
4	GOL	B	808	-	-	3/4/4/4	-
4	GOL	D	814	-	-	0/4/4/4	-
4	GOL	A	810	-	-	2/4/4/4	-
4	GOL	A	813	-	-	2/4/4/4	-
4	GOL	B	814	-	-	2/4/4/4	-
4	GOL	C	810	-	-	0/4/4/4	-
4	GOL	D	813	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	815	-	-	2/4/4/4	-
4	GOL	D	806	-	-	1/4/4/4	-
4	GOL	D	808	-	-	2/4/4/4	-
4	GOL	B	813	-	-	2/4/4/4	-
4	GOL	C	807	-	-	1/4/4/4	-
4	GOL	B	819	-	-	2/4/4/4	-
4	GOL	D	807	-	-	0/4/4/4	-
4	GOL	D	811	-	-	1/4/4/4	-
4	GOL	A	809	-	-	0/4/4/4	-
4	GOL	A	811	-	-	1/4/4/4	-
4	GOL	C	811	-	-	1/4/4/4	-
4	GOL	C	809	-	-	4/4/4/4	-
5	PE3	A	817	-	-	3/7/7/40	-
5	PE3	A	816	-	-	3/10/10/40	-
5	PE3	C	816	-	-	3/9/9/40	-
4	GOL	B	811	-	-	0/4/4/4	-
4	GOL	C	812	-	-	2/4/4/4	-
4	GOL	A	812	-	-	2/4/4/4	-
4	GOL	D	815	-	-	2/4/4/4	-
4	GOL	A	814	-	-	1/4/4/4	-
5	PE3	B	821	-	-	1/9/9/40	-
4	GOL	B	817	-	-	0/4/4/4	-
4	GOL	D	817	-	-	2/4/4/4	-
5	PE3	B	822	-	-	1/10/10/40	-
4	GOL	D	812	-	-	2/4/4/4	-
4	GOL	C	806	-	-	0/4/4/4	-
4	GOL	B	812	-	-	1/4/4/4	-
4	GOL	B	810	-	-	2/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	821	PE3	O37-C38-C39	4.60	131.12	110.39
5	C	816	PE3	O37-C36-C35	4.40	130.21	110.39
5	A	817	PE3	O37-C38-C39	2.89	123.41	110.39
5	B	821	PE3	O40-C39-C38	2.71	122.61	110.39
5	C	816	PE3	C41-O40-C39	-2.69	103.26	112.90
5	B	821	PE3	C41-O40-C39	-2.65	103.41	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	817	PE3	C36-O37-C38	2.04	122.14	113.29

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	O1-C1-C2-O2
4	A	806	GOL	O1-C1-C2-C3
4	A	813	GOL	O1-C1-C2-C3
4	A	815	GOL	O1-C1-C2-C3
4	B	808	GOL	O2-C2-C3-O3
4	B	810	GOL	O1-C1-C2-C3
4	B	813	GOL	C1-C2-C3-O3
4	B	813	GOL	O2-C2-C3-O3
4	B	814	GOL	O1-C1-C2-C3
4	B	819	GOL	C1-C2-C3-O3
4	C	809	GOL	O1-C1-C2-C3
4	C	812	GOL	O1-C1-C2-C3
4	C	814	GOL	C1-C2-C3-O3
4	D	815	GOL	C1-C2-C3-O3
4	D	817	GOL	O1-C1-C2-C3
4	C	812	GOL	O1-C1-C2-O2
4	D	810	GOL	O2-C2-C3-O3
4	D	815	GOL	O2-C2-C3-O3
4	A	807	GOL	C1-C2-C3-O3
4	A	812	GOL	C1-C2-C3-O3
4	B	808	GOL	C1-C2-C3-O3
4	B	815	GOL	O1-C1-C2-C3
4	B	820	GOL	O1-C1-C2-C3
4	C	809	GOL	C1-C2-C3-O3
4	D	809	GOL	O1-C1-C2-C3
4	D	810	GOL	O1-C1-C2-C3
4	D	810	GOL	C1-C2-C3-O3
4	D	812	GOL	C1-C2-C3-O3
4	A	807	GOL	O2-C2-C3-O3
4	A	812	GOL	O2-C2-C3-O3
4	A	813	GOL	O1-C1-C2-O2
4	B	814	GOL	O1-C1-C2-O2
4	B	819	GOL	O2-C2-C3-O3
4	C	809	GOL	O1-C1-C2-O2
4	C	814	GOL	O2-C2-C3-O3
4	D	810	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

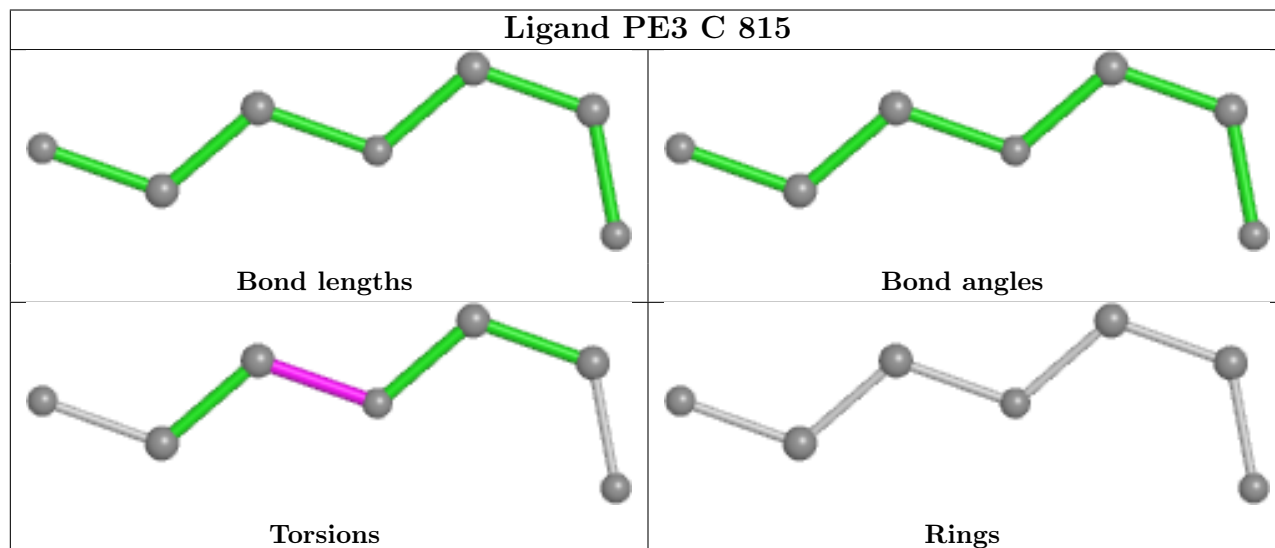
Mol	Chain	Res	Type	Atoms
4	D	812	GOL	O2-C2-C3-O3
4	B	815	GOL	O1-C1-C2-O2
4	A	810	GOL	O2-C2-C3-O3
4	A	815	GOL	O1-C1-C2-O2
4	D	817	GOL	O1-C1-C2-O2
5	B	821	PE3	C39-C38-O37-C36
5	C	816	PE3	C35-C36-O37-C38
5	A	816	PE3	C36-C35-O34-C33
4	B	809	GOL	O2-C2-C3-O3
4	B	812	GOL	O2-C2-C3-O3
5	A	817	PE3	C39-C38-O37-C36
4	D	808	GOL	C1-C2-C3-O3
5	D	818	PE3	C42-C41-O40-C39
4	C	809	GOL	O2-C2-C3-O3
5	C	815	PE3	C38-C39-O40-C41
5	A	816	PE3	C42-C41-O40-C39
4	B	820	GOL	C1-C2-C3-O3
4	B	820	GOL	O1-C1-C2-O2
5	C	816	PE3	C38-C39-O40-C41
5	D	818	PE3	C35-C36-O37-C38
4	A	814	GOL	O1-C1-C2-O2
4	A	811	GOL	C1-C2-C3-O3
4	B	809	GOL	C1-C2-C3-O3
4	C	807	GOL	O1-C1-C2-C3
4	D	806	GOL	O1-C1-C2-C3
5	A	817	PE3	C35-C36-O37-C38
4	B	810	GOL	O1-C1-C2-O2
4	D	808	GOL	O2-C2-C3-O3
5	C	816	PE3	O34-C35-C36-O37
5	D	818	PE3	O34-C35-C36-O37
4	B	820	GOL	O2-C2-C3-O3
5	A	816	PE3	O34-C35-C36-O37
5	A	817	PE3	O37-C38-C39-O40
5	B	822	PE3	O34-C35-C36-O37
4	A	810	GOL	C1-C2-C3-O3
4	B	808	GOL	O1-C1-C2-C3
4	B	818	GOL	C1-C2-C3-O3
4	D	811	GOL	O1-C1-C2-C3
4	C	811	GOL	O1-C1-C2-O2

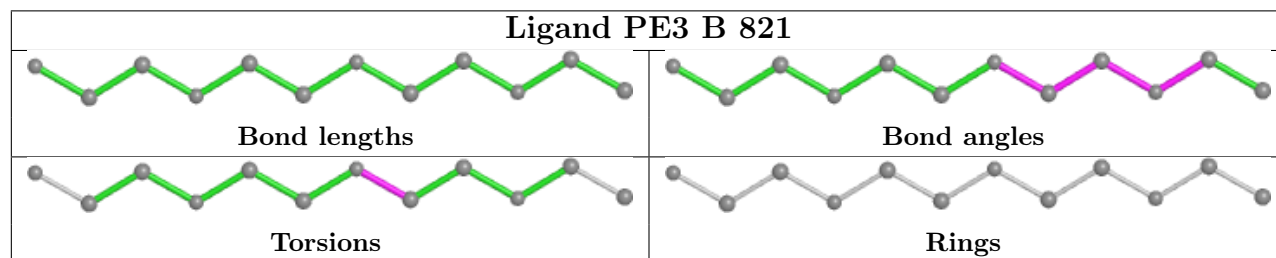
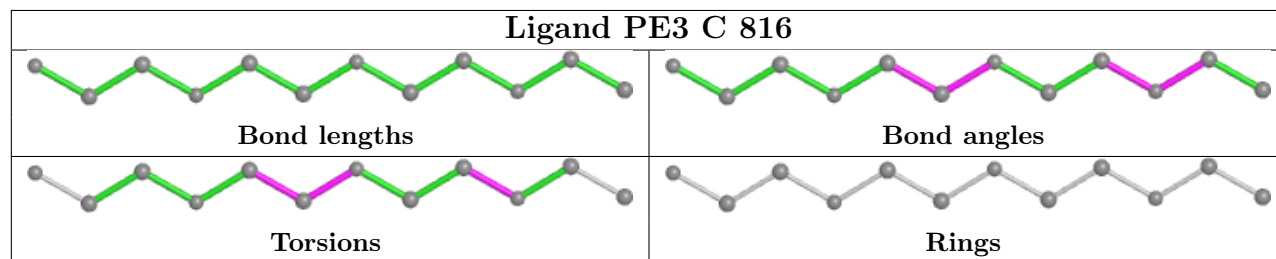
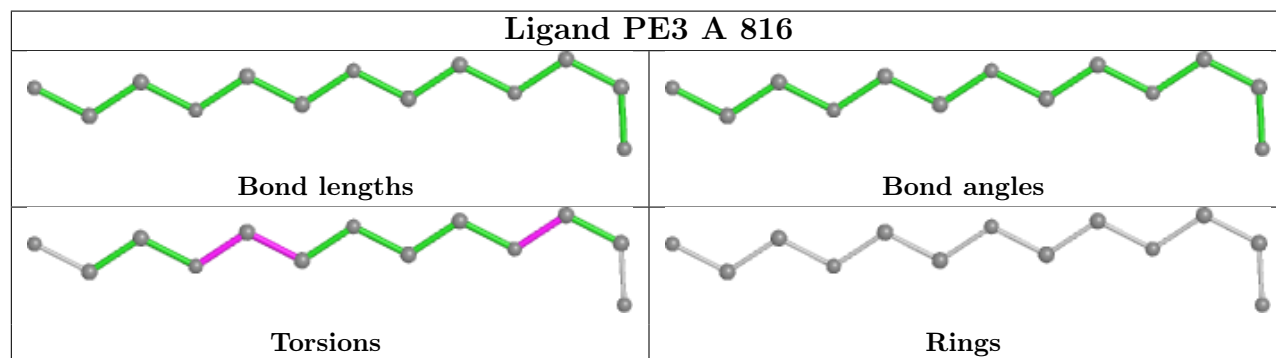
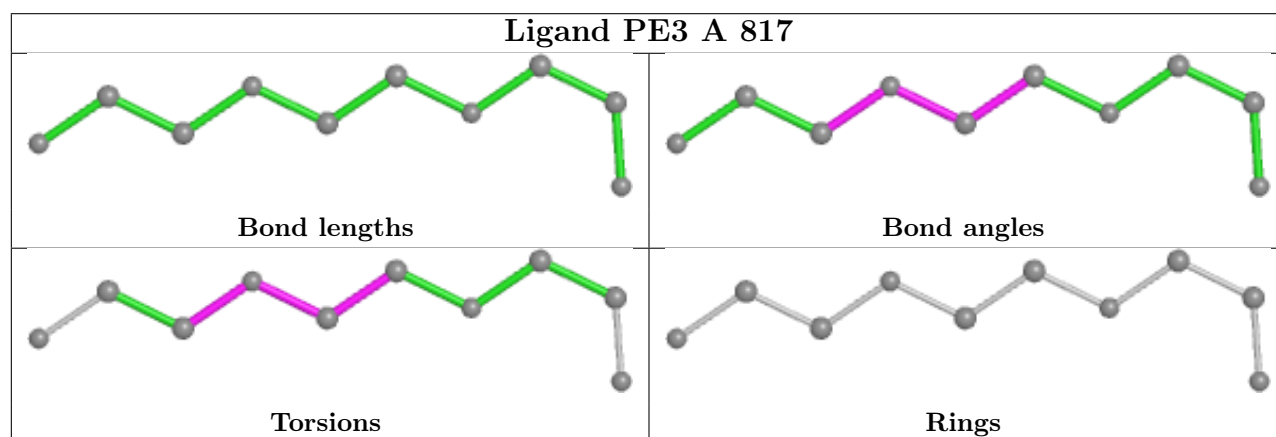
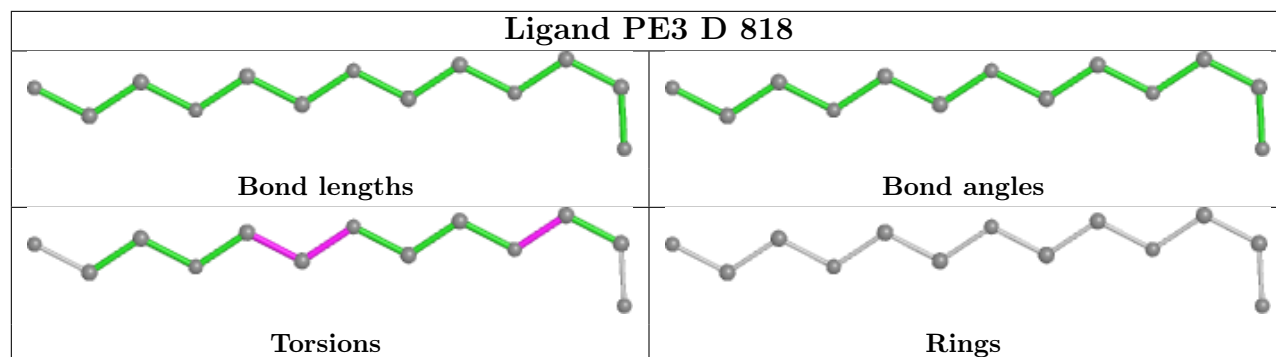
There are no ring outliers.

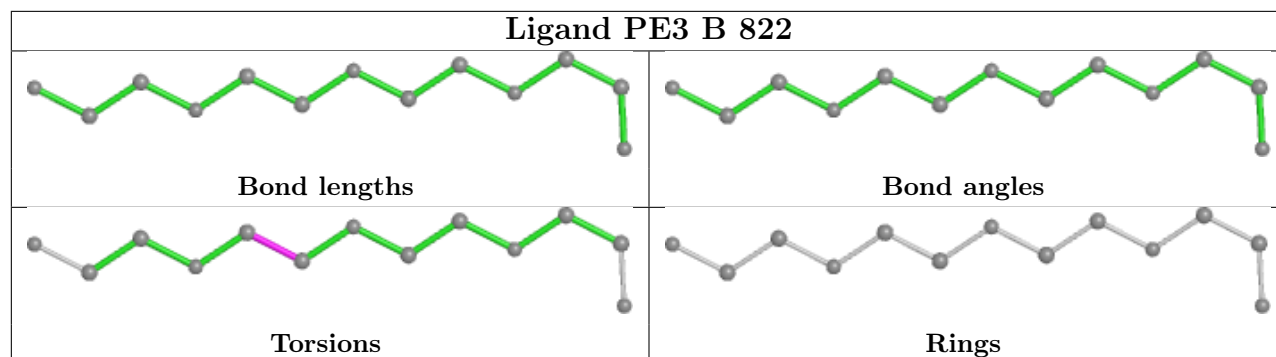
11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	GOL	1	0
4	D	810	GOL	1	0
4	B	814	GOL	1	0
4	B	813	GOL	1	0
4	B	819	GOL	1	0
4	A	809	GOL	2	0
5	C	816	PE3	3	0
4	B	811	GOL	1	0
4	A	814	GOL	1	0
4	D	812	GOL	2	0
4	B	810	GOL	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	729/747 (97%)	-0.45	7 (0%) 82 85	14, 24, 44, 102	0
1	B	729/747 (97%)	-0.42	6 (0%) 86 88	14, 26, 56, 93	0
1	C	729/747 (97%)	-0.38	7 (0%) 82 85	15, 27, 50, 109	0
1	D	729/747 (97%)	-0.48	5 (0%) 87 89	15, 26, 43, 74	0
All	All	2916/2988 (97%)	-0.43	25 (0%) 84 86	14, 26, 51, 109	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	611	GLY	5.9
1	C	610	ALA	5.6
1	A	610	ALA	4.6
1	D	519	THR	4.0
1	C	609	VAL	4.0
1	A	609	VAL	3.9
1	C	612	LEU	3.8
1	C	518	GLY	3.7
1	C	519	THR	3.4
1	C	611	GLY	3.2
1	A	612	LEU	3.1
1	A	519	THR	2.9
1	B	675	GLY	2.8
1	D	518	GLY	2.5
1	B	518	GLY	2.5
1	D	611	GLY	2.5
1	B	519	THR	2.4
1	D	610	ALA	2.3
1	C	360	THR	2.3
1	B	701	ALA	2.2
1	A	689	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	314	TRP	2.2
1	B	490	GLU	2.2
1	B	523	VAL	2.1
1	D	609	VAL	2.1

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

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

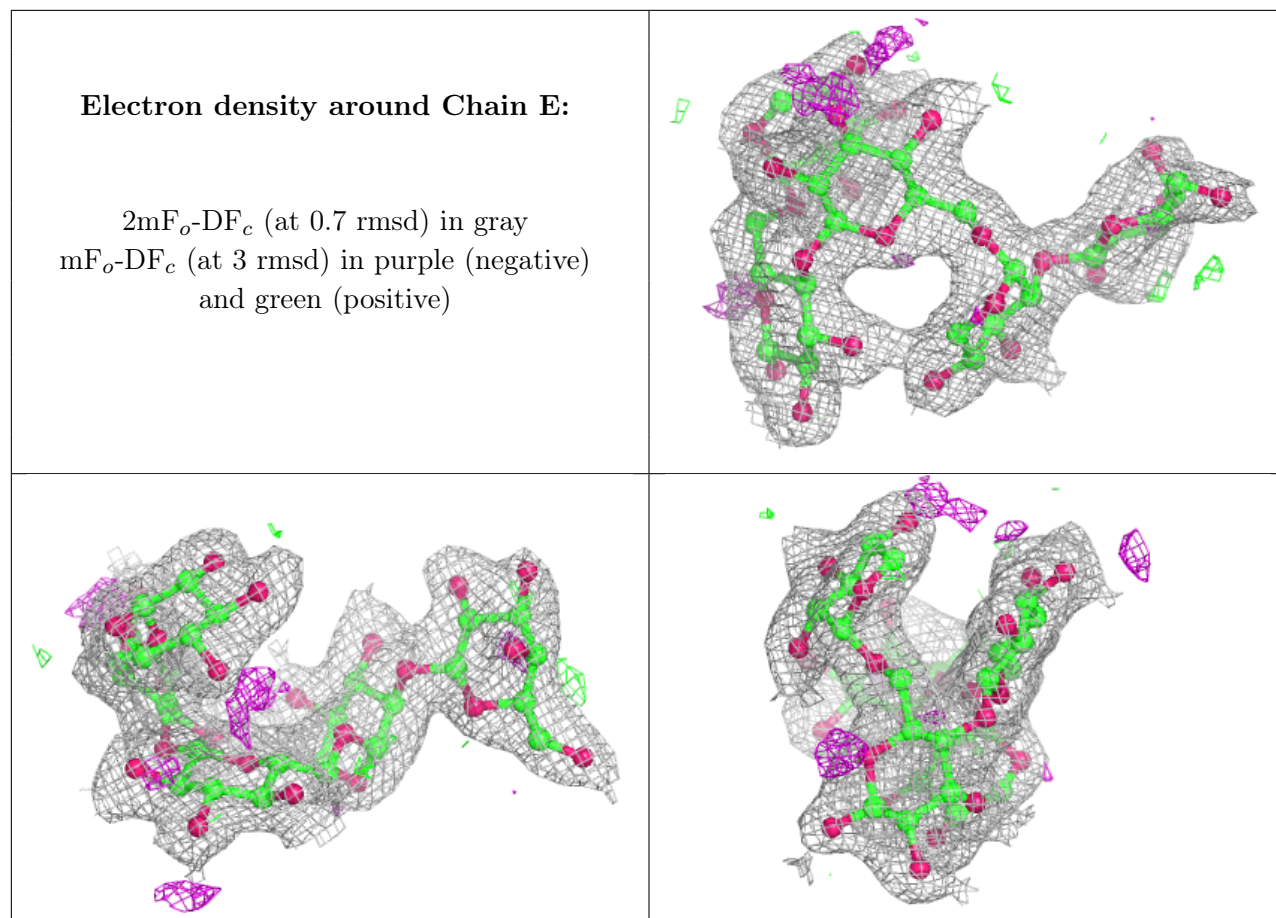
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	GAL	G	4	11/12	0.77	0.27	53,62,65,65	0
2	GAL	H	4	11/12	0.81	0.28	67,79,82,83	0
2	GAL	E	4	11/12	0.85	0.23	54,61,66,67	0
3	GAL	F	6	11/12	0.88	0.14	42,48,52,54	0
3	BGC	F	3	11/12	0.94	0.09	29,33,35,36	0
2	BGC	G	2	11/12	0.95	0.10	25,27,30,31	0
2	XYS	G	5	9/10	0.96	0.13	31,35,39,43	0
2	BGC	H	1	12/12	0.96	0.12	22,26,30,33	0
2	XYS	E	3	9/10	0.96	0.10	26,29,31,41	0
2	XYS	H	5	9/10	0.96	0.15	31,34,41,43	0
3	BGC	F	1	12/12	0.96	0.11	17,23,28,30	0
2	XYS	G	3	9/10	0.96	0.09	24,31,36,41	0
3	XYS	F	4	9/10	0.96	0.12	32,34,38,43	0
2	BGC	G	1	12/12	0.96	0.12	25,28,33,33	0
3	XYS	F	7	9/10	0.96	0.15	31,35,39,44	0
2	BGC	E	2	11/12	0.97	0.11	21,23,25,28	0
2	XYS	E	5	9/10	0.97	0.10	27,30,35,37	0
2	BGC	E	1	12/12	0.97	0.10	21,22,27,34	0
2	BGC	H	2	11/12	0.98	0.09	23,24,26,28	0
3	XYS	F	5	9/10	0.98	0.08	21,23,28,35	0
3	BGC	F	2	11/12	0.98	0.09	19,22,25,27	0
2	XYS	H	3	9/10	0.98	0.08	29,34,39,52	0

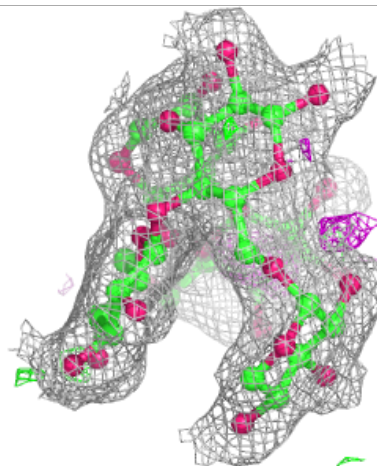
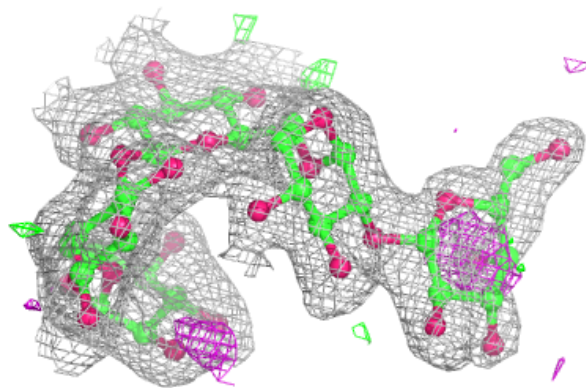
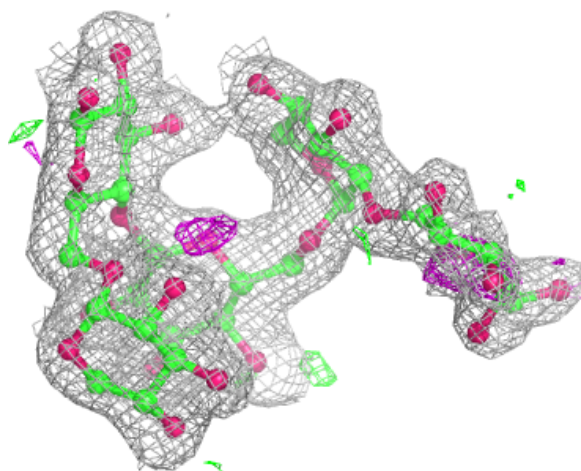
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

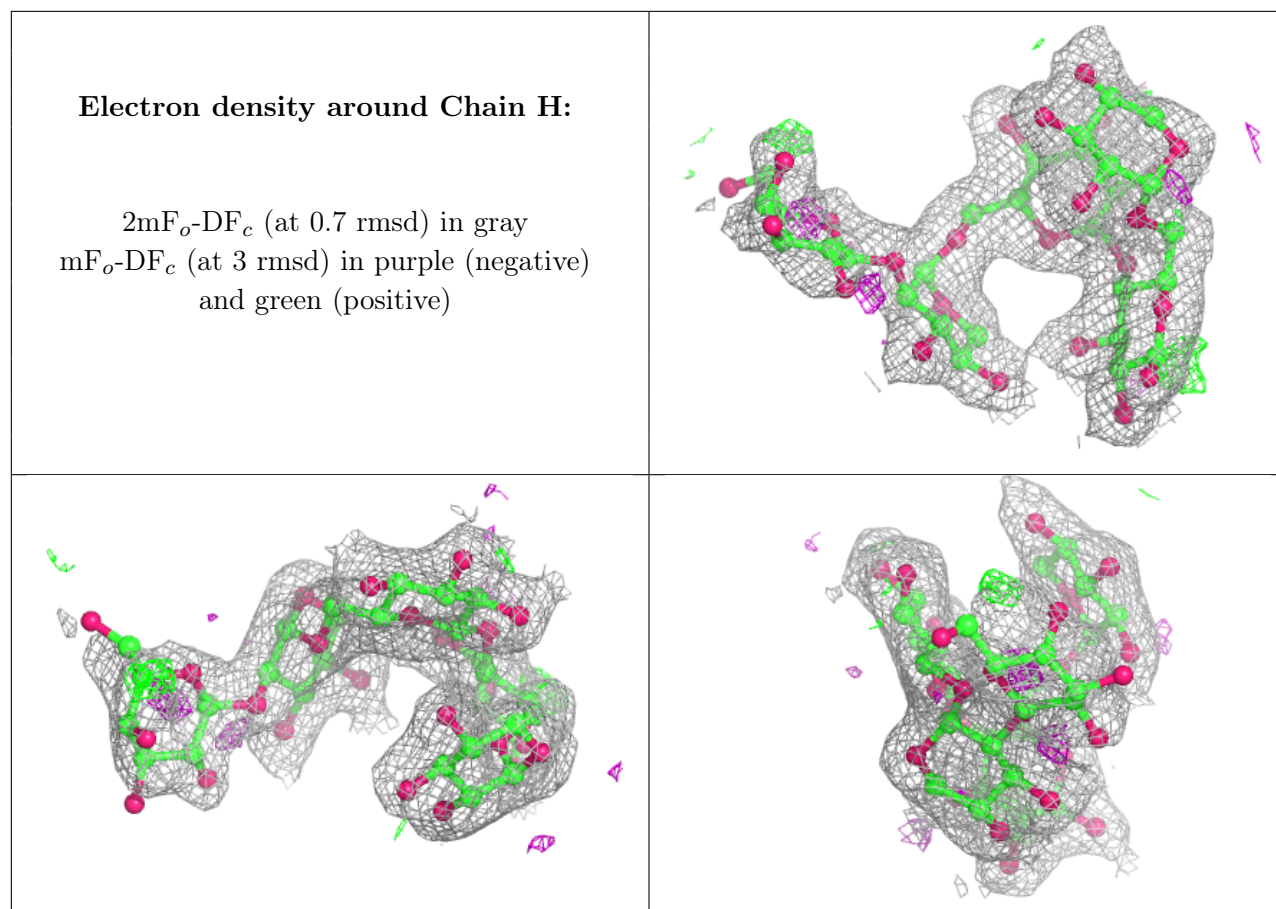
charide. Each fit is shown from different orientation to approximate a three-dimensional view.

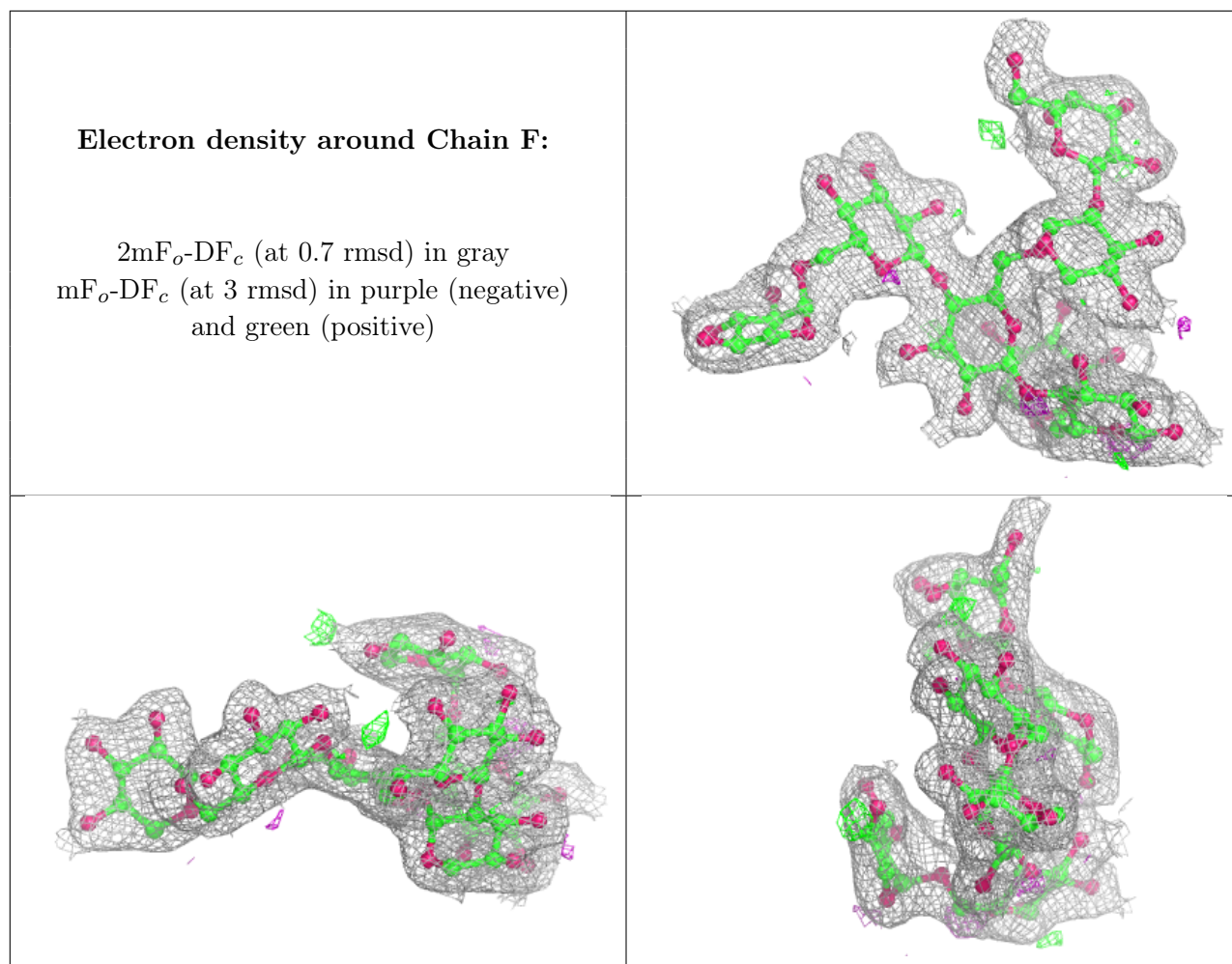


Electron density around Chain G:

$2mF_o-DF_c$ (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
4	GOL	B	820	6/6	0.37	0.37	91,94,96,96	0
4	GOL	B	808	6/6	0.54	0.29	77,82,83,83	0
5	PE3	A	816	13/43	0.60	0.23	78,86,89,90	0
5	PE3	C	816	12/43	0.60	0.28	66,74,83,85	0
5	PE3	B	822	13/43	0.63	0.25	80,82,84,84	0
4	GOL	C	808	6/6	0.63	0.31	74,76,77,77	0
5	PE3	C	815	7/43	0.64	0.29	76,78,82,83	0
4	GOL	D	813	6/6	0.65	0.25	65,66,68,69	0
5	PE3	A	817	10/43	0.66	0.30	78,86,92,94	0
4	GOL	D	817	6/6	0.66	0.58	103,106,106,107	0

Continued on next page...

Continued from previous page...

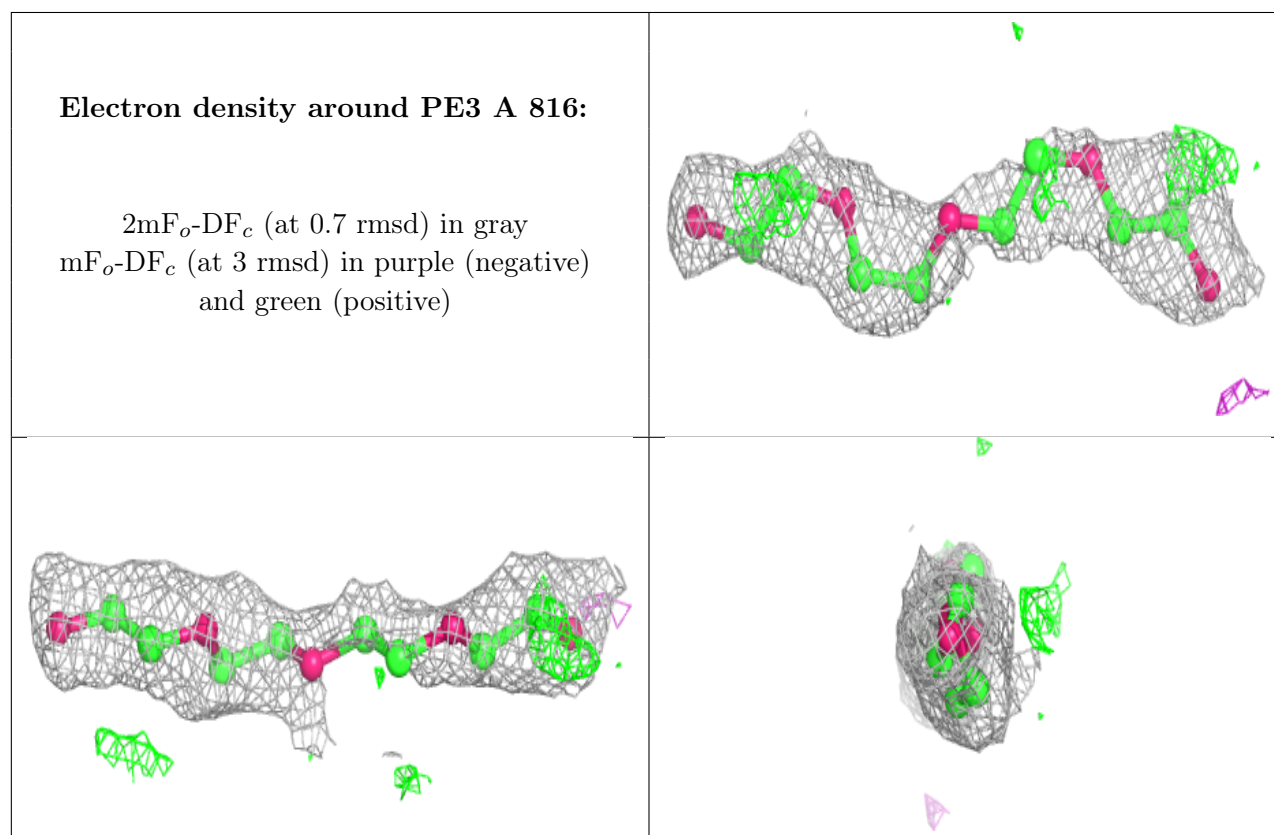
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	818	6/6	0.67	0.36	71,75,77,79	0
4	GOL	A	810	6/6	0.67	0.33	64,72,73,74	0
4	GOL	B	817	6/6	0.68	0.41	85,90,92,93	0
4	GOL	C	814	6/6	0.69	0.24	80,83,84,84	0
5	PE3	D	818	13/43	0.70	0.30	73,77,83,83	0
4	GOL	B	809	6/6	0.71	0.24	63,70,70,73	0
4	GOL	B	813	6/6	0.72	0.20	60,65,66,67	0
4	GOL	A	806	6/6	0.72	0.21	61,65,68,70	0
4	GOL	B	811	6/6	0.72	0.27	76,80,81,81	0
4	GOL	D	811	6/6	0.72	0.22	76,78,78,79	0
4	GOL	C	810	6/6	0.76	0.23	54,58,67,70	0
4	GOL	D	808	6/6	0.77	0.18	68,74,74,75	0
4	GOL	A	813	6/6	0.78	0.23	55,57,58,58	0
5	PE3	B	821	12/43	0.78	0.21	51,55,60,62	0
4	GOL	D	810	6/6	0.78	0.22	52,56,59,61	0
4	GOL	A	815	6/6	0.79	0.32	75,75,76,78	0
4	GOL	D	816	6/6	0.80	0.30	83,84,84,84	0
4	GOL	B	812	6/6	0.80	0.19	71,74,74,75	0
4	GOL	A	809	6/6	0.80	0.26	63,64,68,70	0
4	GOL	C	811	6/6	0.82	0.17	61,67,69,70	0
4	GOL	D	812	6/6	0.82	0.20	30,43,48,51	0
4	GOL	B	819	6/6	0.82	0.29	83,84,85,87	0
4	GOL	A	814	6/6	0.83	0.23	81,84,86,86	0
4	GOL	B	814	6/6	0.83	0.22	62,62,63,63	0
6	CL	B	823	1/1	0.83	0.11	80,80,80,80	0
4	GOL	D	814	6/6	0.84	0.44	71,73,78,80	0
4	GOL	D	807	6/6	0.86	0.17	34,55,60,65	0
4	GOL	A	807	6/6	0.86	0.20	60,62,63,64	0
4	GOL	D	809	6/6	0.86	0.15	51,53,59,62	0
4	GOL	A	812	6/6	0.87	0.17	56,58,59,60	0
4	GOL	A	811	6/6	0.87	0.19	46,55,59,60	0
4	GOL	C	806	6/6	0.88	0.22	47,50,54,56	0
4	GOL	D	815	6/6	0.88	0.21	70,72,72,74	0
4	GOL	C	809	6/6	0.88	0.17	59,64,65,66	0
6	CL	D	819	1/1	0.88	0.15	77,77,77,77	0
4	GOL	A	808	6/6	0.89	0.34	81,83,84,84	0
4	GOL	C	807	6/6	0.89	0.16	37,53,57,59	0
4	GOL	C	812	6/6	0.89	0.30	57,64,66,67	0
6	CL	C	817	1/1	0.90	0.09	70,70,70,70	0
4	GOL	B	816	6/6	0.90	0.18	86,86,86,87	0
4	GOL	C	813	6/6	0.91	0.18	30,50,57,60	0
6	CL	A	818	1/1	0.92	0.11	70,70,70,70	0

Continued on next page...

Continued from previous page...

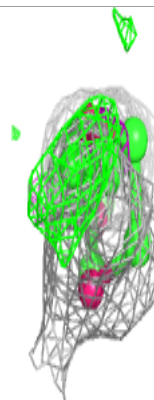
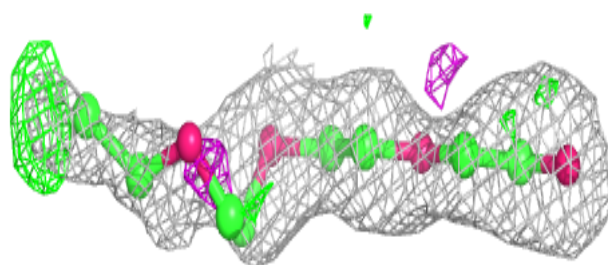
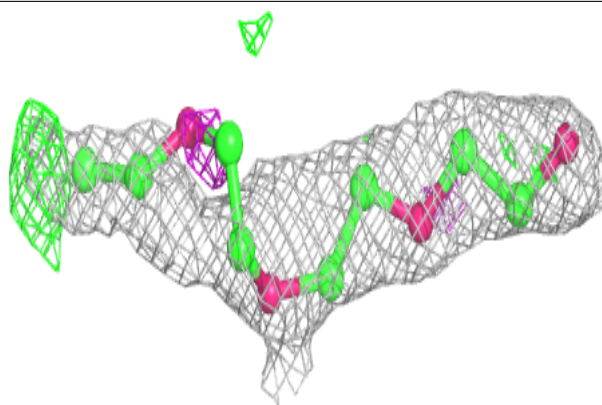
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	806	6/6	0.92	0.14	47,48,51,53	0
4	GOL	B	815	6/6	0.93	0.27	83,84,86,88	0
4	GOL	B	810	6/6	0.94	0.20	51,56,58,61	0
4	GOL	A	819	6/6	0.95	0.18	52,57,59,61	0

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.

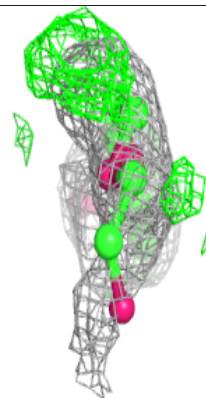
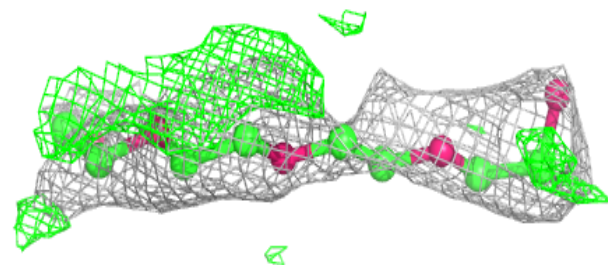
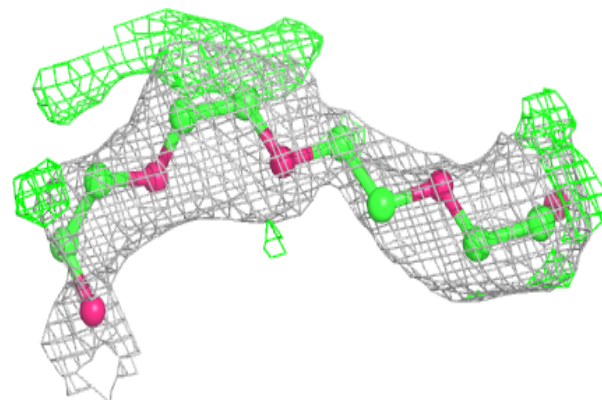


Electron density around PE3 C 816:

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

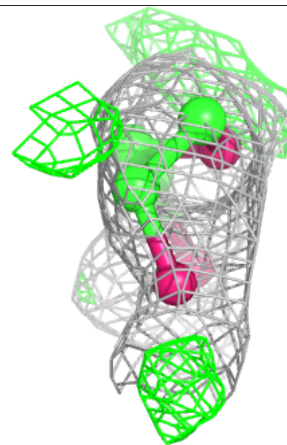
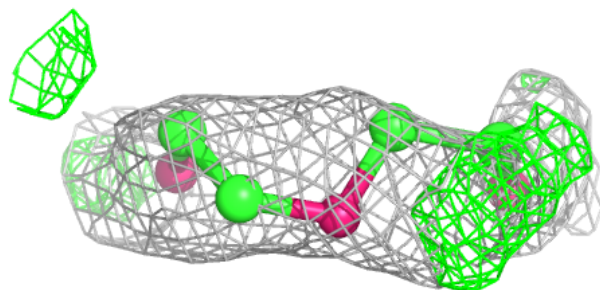
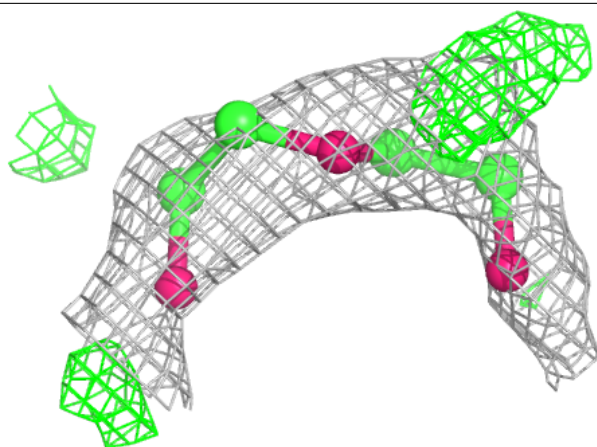
**Electron density around PE3 B 822:**

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

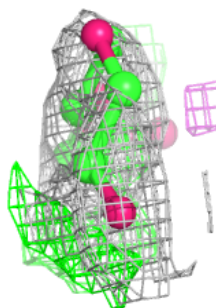
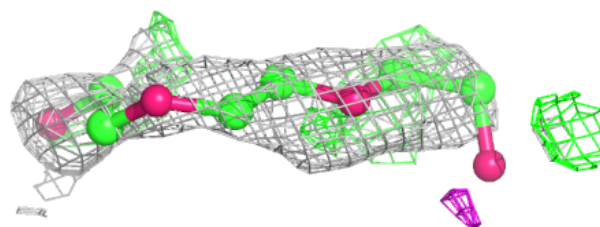
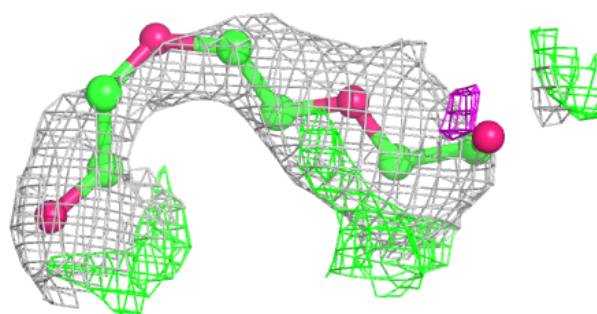


Electron density around PE3 C 815:

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

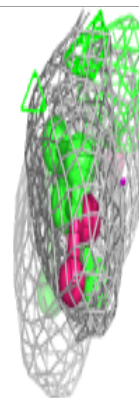
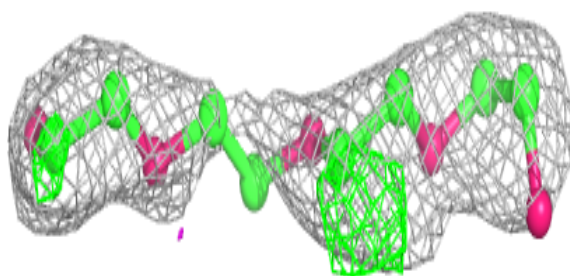
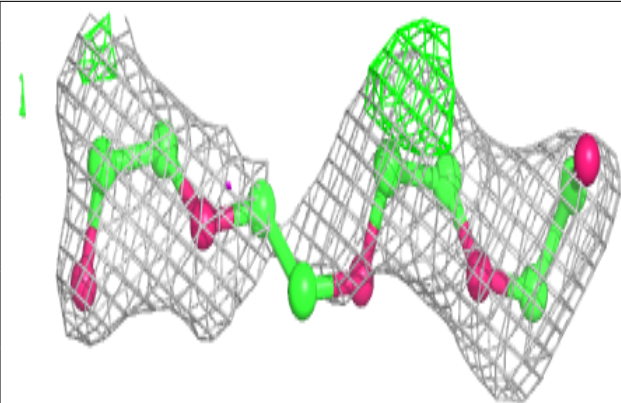
**Electron density around PE3 A 817:**

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

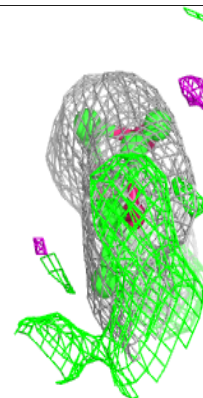
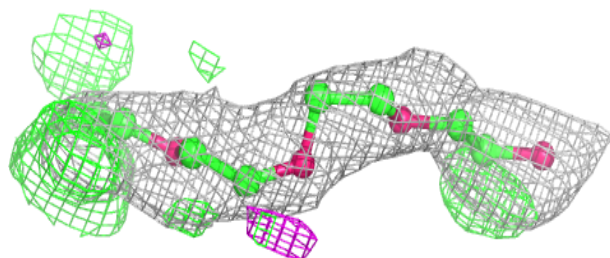
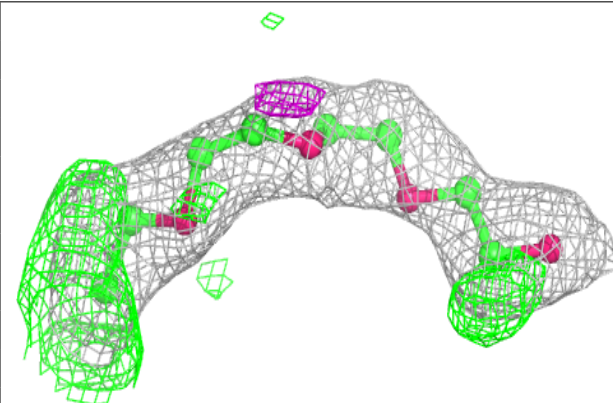


Electron density around PE3 D 818:

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

**Electron density around PE3 B 821:**

$2mF_o-DF_c$ (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.