Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2022 – 01:20 am BST

PDB ID	:	7OV2
Title	:	Crystal structure of pig purple acid phosphatase in complex with L-glutamine, (poly)ethylene glycol fragments and glycerol
Authors	:	Feder, D.; McGeary, R.P.; Guddat, L.W.; Schenk, G.
Deposited on	:	2021-06-14
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 following versions of software and data (see references ⓘ) were used in the production of this report:

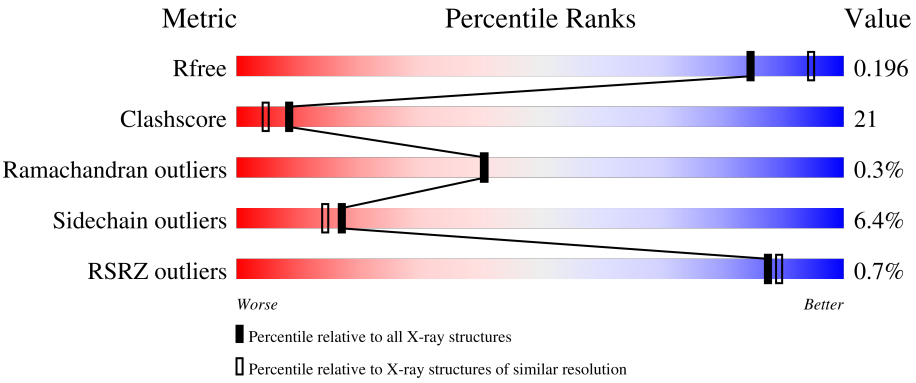
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

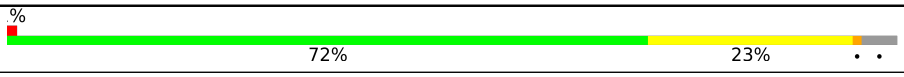
The reported resolution of this entry is 2.10 Å.

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 <=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	313	
2	B	4	

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
3	1PE	A	604	-	-	X	-
6	GLN	A	618	-	-	-	X
7	PO4	A	619[A]	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 3423 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.

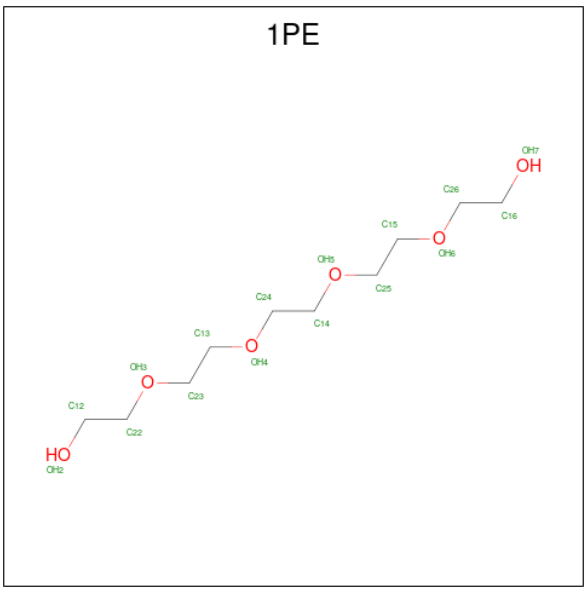
- Molecule 1 is a protein called Tartrate-resistant acid phosphatase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	302	2457	1581	436	433	7	3	12	0

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

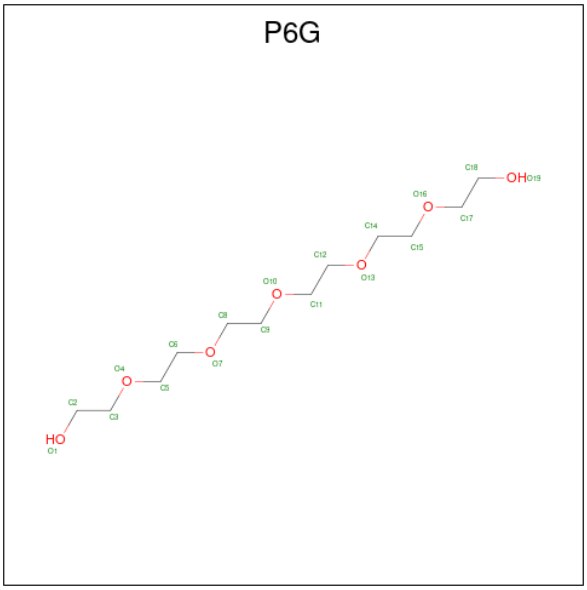
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



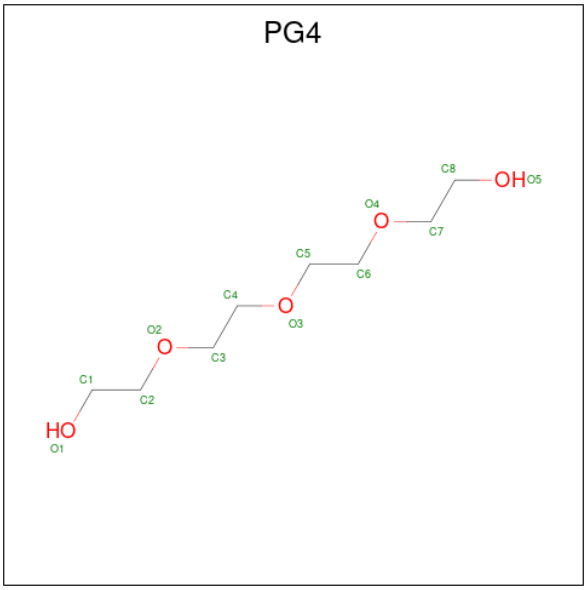
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 16 10 6	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



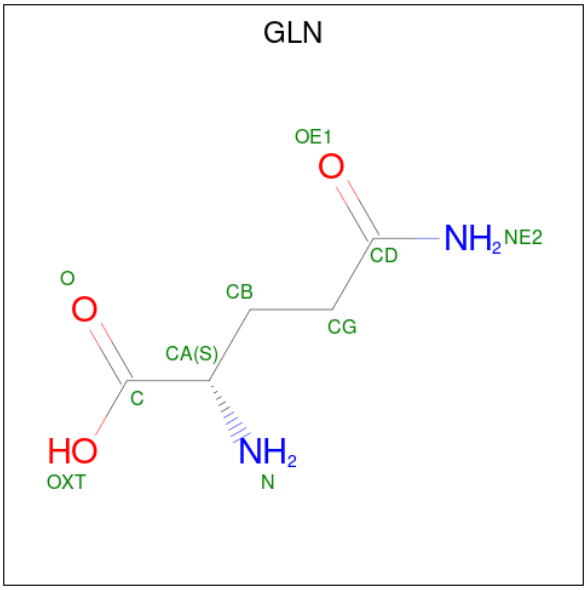
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 19 12 7	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 26 16 10	0	1

- Molecule 6 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 10 5 2 3	0	0

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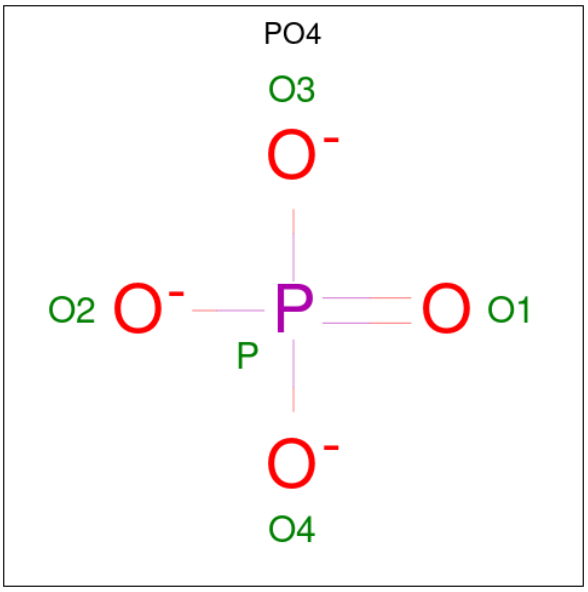
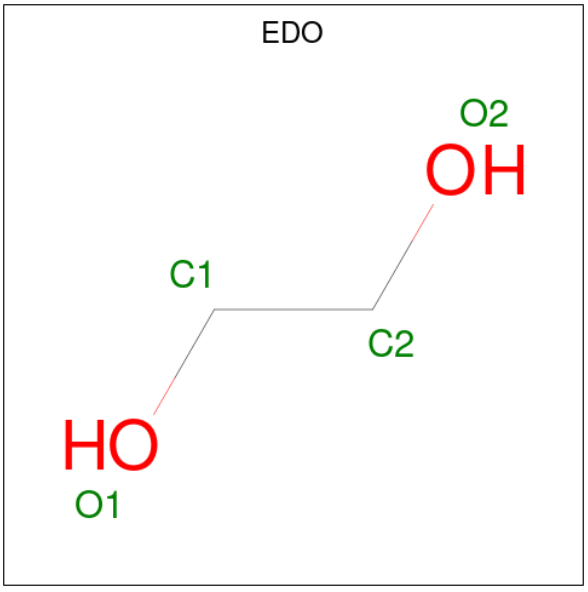
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 20 10 4 6	0	1
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0
6	A	1	Total C N O 10 5 2 3	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 10 8 2	0	1

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

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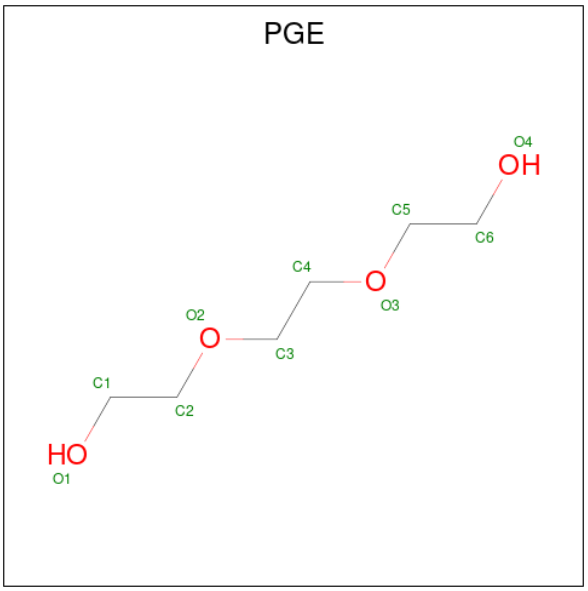
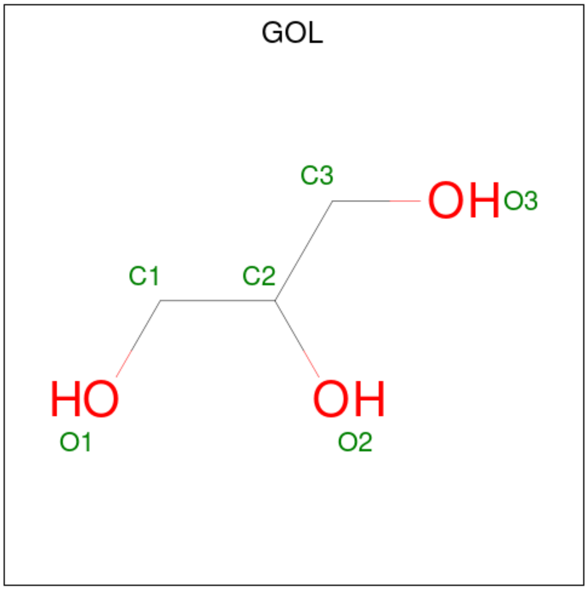
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



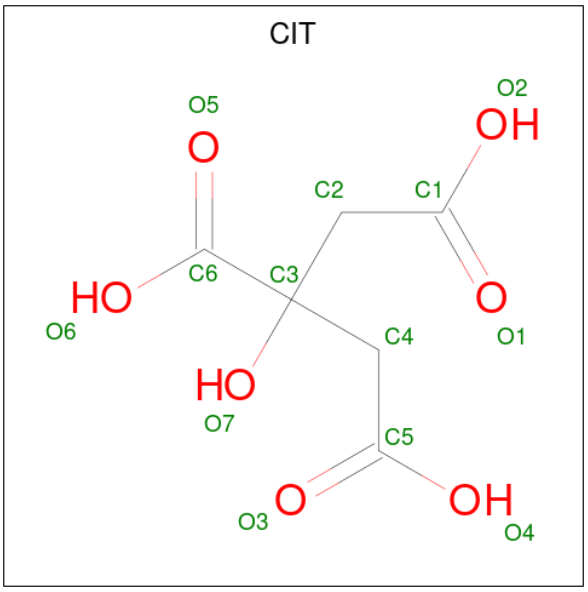
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 10 6 4	0	0
9	A	1	Total C O 10 6 4	0	0
9	A	1	Total C O 10 6 4	0	0
9	A	1	Total C O 20 12 8	0	1
9	A	1	Total C O 20 12 8	0	1
9	A	1	Total C O 10 6 4	0	0
9	A	1	Total C O 10 6 4	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 11 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 13 6 7	0	0

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Na 1 1	0	0

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	2	Total Fe 2 2	0	0

- Molecule 14 is water.

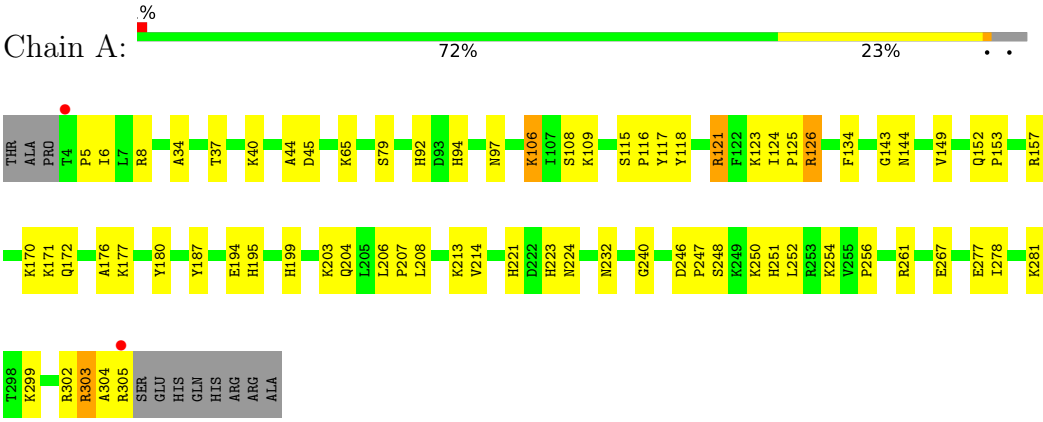
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	200	Total O 203 203	0	3

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: Tartrate-resistant acid phosphatase type 5

Chain A:



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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.45Å 68.67Å 77.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.25 – 2.10 51.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.25-2.10) 99.8 (51.25-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.142 , 0.196 0.142 , 0.196	Depositor DCC
R_{free} test set	1050 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3423	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 1PE, FE, BMA, PG4, CIT, PGE, EDO, GOL, P6G, NA, PO4

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	0.40	0/2559	0.54	0/3475

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2457	0	2452	85	3
2	B	50	0	43	5	1
3	A	26	0	34	8	0
4	A	19	0	26	2	0
5	A	39	0	54	8	0
6	A	360	0	252	62	3
7	A	10	0	0	2	0
8	A	68	0	102	13	0
9	A	97	0	135	13	1
10	A	78	0	104	14	0
11	A	13	0	5	2	0
12	A	1	0	0	0	0
13	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	203	0	0	25	0
All	All	3423	0	3207	132	4

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 21.

All (132) 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)
8:A:635:EDO:H11	2:B:4:BMA:H62	1.36	1.07
1:A:109:LYS:H	3:A:604:1PE:H261	1.39	0.85
1:A:195:HIS:HE1	8:A:628:EDO:H12	1.42	0.83
6:A:665:GLN:N	14:A:705:HOH:O	2.16	0.78
1:A:109:LYS:HA	3:A:604:1PE:H131	1.66	0.78
6:A:613:GLN:O	14:A:701:HOH:O	2.02	0.77
1:A:302:ARG:HH22	6:A:616[A]:GLN:HG3	1.49	0.76
6:A:673:GLN:NE2	14:A:705:HOH:O	2.19	0.74
3:A:604:1PE:H262	10:A:655:GOL:H31	1.71	0.73
1:A:250:LYS:HZ2	6:A:612[B]:GLN:HG3	1.52	0.72
1:A:126:ARG:HH11	6:A:606:GLN:HB3	1.53	0.72
1:A:163[A]:ARG:HH21	9:A:637:PGE:H4	1.55	0.71
1:A:109:LYS:HB2	3:A:604:1PE:H252	1.72	0.71
6:A:618:GLN:OXT	14:A:702:HOH:O	2.08	0.71
1:A:5:PRO:HB3	1:A:125:PRO:O	1.88	0.71
1:A:109:LYS:HD3	10:A:656:GOL:H12	1.75	0.69
1:A:248:SER:HB2	9:A:641[B]:PGE:H2	1.73	0.69
6:A:605:GLN:N	8:A:634:EDO:HO1	1.91	0.68
1:A:195:HIS:CE1	8:A:628:EDO:H12	2.25	0.68
6:A:666:GLN:N	14:A:713:HOH:O	2.27	0.67
1:A:295:LEU:O	6:A:674:GLN:N	2.28	0.66
1:A:34:ALA:HA	9:A:640:PGE:H32	1.77	0.66
8:A:632:EDO:H21	2:B:2:NAG:H3	1.76	0.66
1:A:161:LEU:HD23	6:A:611[A]:GLN:NE2	2.10	0.66
1:A:126:ARG:NH1	6:A:606:GLN:HB3	2.12	0.65
1:A:163[A]:ARG:HD3	9:A:637:PGE:H4	1.77	0.65
1:A:121:ARG:H	6:A:666:GLN:HG3	1.62	0.65
1:A:157:ARG:NH1	9:A:644:PGE:O1	2.31	0.63
1:A:297:LYS:HZ2	6:A:607:GLN:N	1.97	0.63
8:A:635:EDO:H11	2:B:4:BMA:C6	2.23	0.63
1:A:144:ASN:HD22	6:A:611[B]:GLN:HG3	1.64	0.62
1:A:267[A]:GLU:OE2	14:A:704:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:N	3:A:604:1PE:H261	2.12	0.61
1:A:170:LYS:HZ2	4:A:602:P6G:H121	1.67	0.60
1:A:149:VAL:H	10:A:657:GOL:H31	1.66	0.59
1:A:176:ALA:O	1:A:303:ARG:NH2	2.34	0.59
6:A:613:GLN:N	6:A:617[A]:GLN:OE1	2.37	0.58
5:A:660[B]:PG4:H42	6:A:661:GLN:HB3	1.86	0.57
10:A:654:GOL:O2	14:A:706:HOH:O	2.17	0.56
6:A:611[B]:GLN:OXT	6:A:611[B]:GLN:HG2	2.06	0.56
1:A:214:VAL:O	6:A:610:GLN:N	2.39	0.55
1:A:152:GLN:HE22	1:A:199:HIS:H	1.54	0.54
6:A:612[A]:GLN:N	14:A:727:HOH:O	2.41	0.54
1:A:144:ASN:ND2	6:A:611[B]:GLN:HG3	2.23	0.53
1:A:252:LEU:HD11	10:A:654:GOL:H31	1.90	0.53
1:A:118:TYR:HA	6:A:671[B]:GLN:HG3	1.91	0.53
1:A:256:PRO:HG3	10:A:645:GOL:H32	1.89	0.53
6:A:611[A]:GLN:NE2	14:A:716:HOH:O	2.29	0.52
3:A:604:1PE:H262	10:A:655:GOL:C3	2.40	0.52
1:A:106:LYS:NZ	8:A:636:EDO:H22	2.25	0.52
1:A:144:ASN:HB2	6:A:611[B]:GLN:OXT	2.09	0.51
6:A:612[A]:GLN:NE2	9:A:641[A]:PGE:O1	2.43	0.51
1:A:247:PRO:HD3	1:A:267[B]:GLU:HG3	1.92	0.51
11:A:659:CIT:H22	5:A:660[B]:PG4:H11	1.93	0.51
5:A:660[B]:PG4:H62	6:A:661:GLN:HE21	1.76	0.51
6:A:608[B]:GLN:NE2	14:A:707:HOH:O	2.20	0.50
1:A:121:ARG:HB3	6:A:666:GLN:N	2.26	0.50
1:A:213:LYS:HA	6:A:610:GLN:HA	1.93	0.50
1:A:116:PRO:HG2	6:A:661:GLN:HB2	1.92	0.50
1:A:199:HIS:ND1	10:A:648:GOL:O2	2.37	0.50
8:A:632:EDO:H21	2:B:2:NAG:HN2	1.77	0.50
1:A:177:LYS:NZ	14:A:733:HOH:O	2.45	0.50
1:A:251:HIS:CE1	6:A:608[A]:GLN:HG3	2.47	0.50
6:A:611[A]:GLN:HG2	11:A:659:CIT:O2	2.12	0.49
1:A:246:ASP:OD1	9:A:641[B]:PGE:H12	2.13	0.49
1:A:92:HIS:NE2	7:A:619[A]:PO4:O2	2.24	0.49
6:A:675:GLN:OXT	6:A:675:GLN:HG2	2.13	0.49
5:A:603:PG4:H42	6:A:667:GLN:N	2.27	0.49
6:A:607:GLN:NE2	8:A:623:EDO:O2	2.46	0.48
1:A:302:ARG:NH2	6:A:616[A]:GLN:HG3	2.25	0.48
1:A:206:LEU:HD21	10:A:653:GOL:H32	1.96	0.47
1:A:207:PRO:HA	5:A:603:PG4:H62	1.95	0.47
1:A:221:HIS:HA	14:A:718[B]:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:642[A]:PGE:H4	2:B:1:NAG:H82	1.96	0.47
10:A:645:GOL:O3	6:A:667:GLN:O	2.27	0.47
10:A:653:GOL:O1	6:A:667:GLN:NE2	2.41	0.47
1:A:6:ILE:HD11	1:A:277:GLU:HB3	1.96	0.47
6:A:605:GLN:O	6:A:606:GLN:NE2	2.48	0.47
1:A:124:ILE:HD11	1:A:278:ILE:HG22	1.96	0.47
1:A:204:GLN:NE2	14:A:722:HOH:O	2.34	0.46
6:A:669[A]:GLN:N	14:A:737:HOH:O	2.48	0.46
1:A:153:PRO:HG3	1:A:187:TYR:CE2	2.51	0.46
1:A:299:LYS:HD3	14:A:702:HOH:O	2.16	0.46
1:A:152:GLN:NE2	1:A:199:HIS:H	2.14	0.46
1:A:232:ASN:ND2	10:A:650:GOL:H2	2.31	0.46
1:A:134:PHE:CE1	1:A:172:GLN:HB3	2.51	0.46
9:A:638:PGE:O4	14:A:703:HOH:O	2.15	0.46
3:A:601:1PE:H232	9:A:639:PGE:H62	1.99	0.45
6:A:605:GLN:NE2	8:A:634:EDO:O1	2.49	0.45
5:A:660[A]:PG4:H32	5:A:660[A]:PG4:H52	1.63	0.45
1:A:94:HIS:HB3	6:A:611[B]:GLN:HB2	1.99	0.45
1:A:254:LYS:NZ	6:A:609:GLN:HE21	2.13	0.45
1:A:254:LYS:NZ	8:A:629:EDO:O1	2.48	0.45
6:A:607:GLN:OE1	6:A:675:GLN:N	2.50	0.45
1:A:126:ARG:N	1:A:126:ARG:HD3	2.32	0.44
1:A:163[A]:ARG:HB3	9:A:637:PGE:H42	1.99	0.44
1:A:8[A]:ARG:NH1	6:A:605:GLN:OXT	2.49	0.43
1:A:115[A]:SER:OG	1:A:117:TYR:O	2.34	0.43
1:A:250:LYS:NZ	6:A:608[B]:GLN:OXT	2.34	0.43
10:A:653:GOL:H31	6:A:667:GLN:HG2	2.01	0.43
1:A:208:LEU:HD23	8:A:620:EDO:H11	2.01	0.43
1:A:8[A]:ARG:NH1	14:A:741:HOH:O	2.51	0.43
1:A:92:HIS:HE2	7:A:619[A]:PO4:P	2.39	0.43
1:A:251:HIS:NE2	6:A:608[B]:GLN:HG2	2.34	0.43
1:A:44:ALA:O	6:A:605:GLN:N	2.52	0.42
6:A:671[B]:GLN:HG2	14:A:814:HOH:O	2.20	0.42
1:A:203:LYS:HE2	6:A:672:GLN:O	2.19	0.42
1:A:299:LYS:NZ	14:A:744:HOH:O	2.52	0.42
1:A:180:TYR:CE1	1:A:302:ARG:HA	2.55	0.42
6:A:610:GLN:NE2	14:A:725:HOH:O	2.39	0.42
6:A:613:GLN:N	14:A:747:HOH:O	2.53	0.42
1:A:223:HIS:HA	1:A:240:GLY:O	2.20	0.41
1:A:207:PRO:HG3	5:A:603:PG4:H32	2.02	0.41
1:A:8[A]:ARG:HD3	14:A:715:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HE2	1:A:79:SER:HB3	2.02	0.41
1:A:143:GLY:HA2	6:A:611[A]:GLN:OXT	2.21	0.41
1:A:170:LYS:NZ	4:A:602:P6G:H152	2.36	0.41
1:A:194:GLU:HB2	14:A:727:HOH:O	2.19	0.41
1:A:45:ASP:HA	8:A:634:EDO:H21	2.03	0.41
6:A:674:GLN:O	6:A:674:GLN:HG2	2.21	0.41
6:A:672:GLN:O	6:A:672:GLN:HG2	2.21	0.41
1:A:125:PRO:O	1:A:126:ARG:HB2	2.20	0.41
1:A:108:SER:HA	3:A:604:1PE:H261	2.02	0.41
1:A:97:ASN:HB2	9:A:642[A]:PGE:H12	2.02	0.40
6:A:618:GLN:HB3	14:A:702:HOH:O	2.20	0.40
6:A:666:GLN:NE2	14:A:750:HOH:O	2.54	0.40
1:A:37:THR:HG22	9:A:640:PGE:H6	2.03	0.40
5:A:660[A]:PG4:H22	6:A:661:GLN:OXT	2.21	0.40
1:A:149:VAL:HB	10:A:657:GOL:H31	2.02	0.40
1:A:254:LYS:HD2	6:A:668:GLN:HB3	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:O	9:A:643:PGE:C4[3_655]	1.38	0.82
2:B:4:BMA:O2	6:A:606:GLN:NE2[3_645]	2.09	0.11
1:A:261:ARG:NH1	6:A:617[B]:GLN:OE1[3_555]	2.15	0.05
1:A:281:LYS:O	6:A:612[B]:GLN:NE2[3_555]	2.18	0.02

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	312/313 (100%)	300 (96%)	11 (4%)	1 (0%)	41 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	ALA

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	265/263 (101%)	256 (97%)	9 (3%)	37 39

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	106	LYS
1	A	121	ARG
1	A	126	ARG
1	A	171	LYS
1	A	224[A]	ASN
1	A	224[B]	ASN
1	A	303	ARG
1	A	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	232	ASN

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)

4 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	NAG	B	1	2,1	14,14,15	0.51	0	17,19,21	0.44	0
2	NAG	B	2	2	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
2	BMA	B	3	2	11,11,12	1.02	0	15,15,17	1.87	5 (33%)
2	BMA	B	4	2	11,11,12	2.04	3 (27%)	15,15,17	2.38	7 (46%)

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	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	BMA	O5-C1	4.55	1.51	1.43
2	B	4	BMA	C2-C3	-3.05	1.48	1.52
2	B	4	BMA	C1-C2	2.49	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	BMA	C1-O5-C5	4.77	118.65	112.19
2	B	4	BMA	C3-C4-C5	-4.02	103.07	110.24
2	B	3	BMA	C3-C4-C5	-3.79	103.48	110.24
2	B	4	BMA	O2-C2-C3	-3.78	102.56	110.14
2	B	3	BMA	O5-C5-C6	2.95	111.83	107.20
2	B	3	BMA	C1-C2-C3	-2.75	106.29	109.67
2	B	4	BMA	C2-C3-C4	-2.49	106.58	110.89
2	B	4	BMA	C1-C2-C3	2.44	112.67	109.67
2	B	4	BMA	O5-C1-C2	2.43	114.53	110.77
2	B	4	BMA	O2-C2-C1	-2.43	104.18	109.15
2	B	2	NAG	O4-C4-C3	-2.24	105.16	110.35
2	B	3	BMA	C1-O5-C5	-2.21	109.19	112.19
2	B	3	BMA	O3-C3-C2	2.15	114.11	109.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6

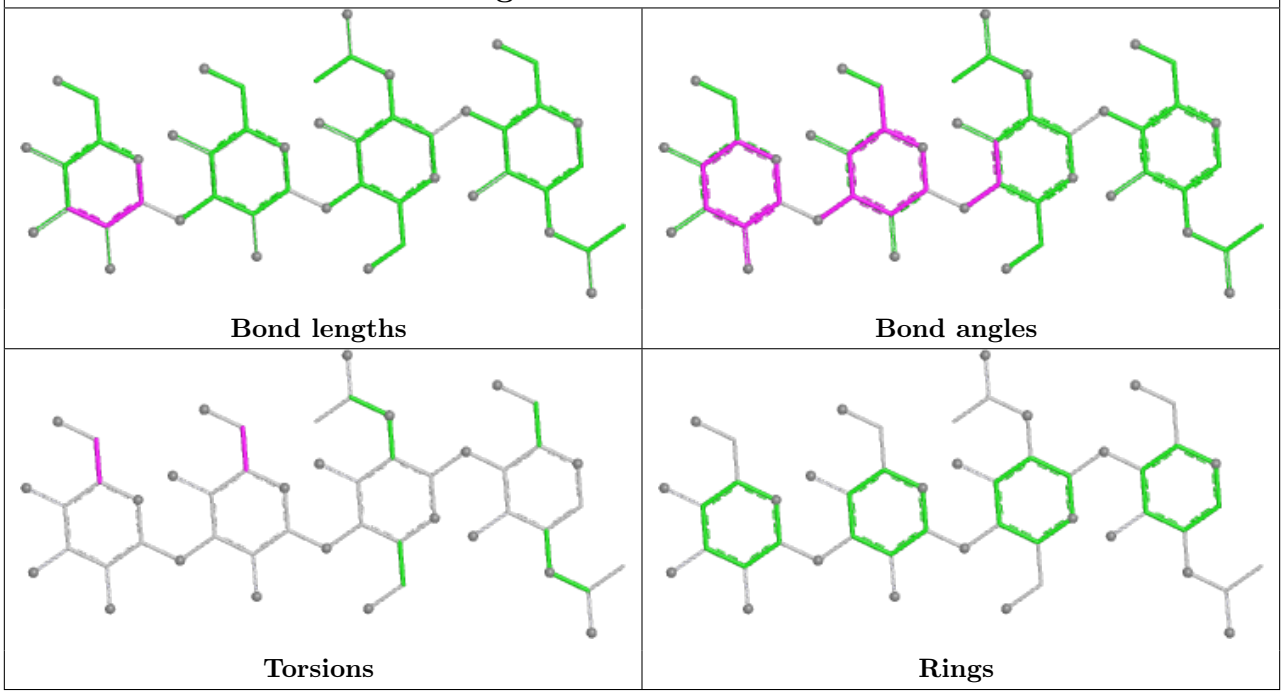
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0
2	B	1	NAG	1	0
2	B	4	BMA	2	1

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 88 ligands modelled in this entry, 3 are monoatomic - leaving 85 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CIT	A	659	-	3,12,12	1.36	0	3,17,17	1.35	1 (33%)
6	GLN	A	614	-	5,9,9	0.22	0	5,11,11	0.06	0
6	GLN	A	667	-	5,9,9	0.29	0	5,11,11	0.08	0
10	GOL	A	649	-	5,5,5	0.95	0	5,5,5	1.05	0
10	GOL	A	656	-	5,5,5	0.98	0	5,5,5	0.93	0
6	GLN	A	610	-	5,9,9	0.35	0	5,11,11	0.19	0
6	GLN	A	612[B]	-	5,9,9	0.22	0	5,11,11	0.31	0
6	GLN	A	611[B]	-	5,9,9	0.25	0	5,11,11	0.90	1 (20%)
9	PGE	A	643	-	9,9,9	0.71	0	8,8,8	0.69	0
9	PGE	A	640	-	9,9,9	0.29	0	8,8,8	0.45	0
10	GOL	A	645	-	5,5,5	0.99	0	5,5,5	0.89	0
8	EDO	A	624	-	3,3,3	0.44	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PGE	A	642[B]	-	9,9,9	0.30	0	8,8,8	0.26	0
8	EDO	A	631	-	3,3,3	0.48	0	2,2,2	0.37	0
10	GOL	A	653	-	5,5,5	1.01	1 (20%)	5,5,5	1.00	0
8	EDO	A	625	-	3,3,3	0.46	0	2,2,2	0.33	0
6	GLN	A	608[A]	-	5,9,9	0.31	0	5,11,11	0.11	0
8	EDO	A	629	-	3,3,3	0.45	0	2,2,2	0.37	0
5	PG4	A	660[A]	-	12,12,12	0.52	0	11,11,11	0.79	0
8	EDO	A	620	-	3,3,3	0.48	0	2,2,2	0.26	0
9	PGE	A	638	-	9,9,9	0.29	0	8,8,8	0.24	0
9	PGE	A	639	-	9,9,9	0.31	0	8,8,8	0.36	0
6	GLN	A	673	-	5,9,9	0.37	0	5,11,11	0.32	0
8	EDO	A	621	-	3,3,3	0.48	0	2,2,2	0.26	0
10	GOL	A	648	-	5,5,5	0.96	0	5,5,5	0.95	0
10	GOL	A	650	-	5,5,5	0.79	0	5,5,5	1.04	0
8	EDO	A	635	-	3,3,3	0.45	0	2,2,2	0.25	0
10	GOL	A	652	-	5,5,5	0.81	0	5,5,5	1.20	0
6	GLN	A	618	-	5,9,9	0.36	0	5,11,11	0.14	0
6	GLN	A	606	-	5,9,9	0.92	0	5,11,11	0.42	0
6	GLN	A	616[A]	-	5,9,9	0.19	0	5,11,11	0.10	0
8	EDO	A	633	-	3,3,3	0.49	0	2,2,2	0.37	0
5	PG4	A	603	-	12,12,12	0.52	0	11,11,11	0.79	0
10	GOL	A	646	-	5,5,5	1.00	0	5,5,5	1.19	1 (20%)
6	GLN	A	666	-	5,9,9	0.49	0	5,11,11	0.27	0
6	GLN	A	675	-	5,9,9	0.39	0	5,11,11	0.11	0
10	GOL	A	647	-	5,5,5	0.95	0	5,5,5	1.02	0
6	GLN	A	661	-	5,9,9	0.32	0	5,11,11	0.33	0
8	EDO	A	627	-	3,3,3	0.47	0	2,2,2	0.24	0
9	PGE	A	641[A]	-	9,9,9	0.31	0	8,8,8	0.34	0
6	GLN	A	608[B]	-	5,9,9	0.21	0	5,11,11	0.07	0
10	GOL	A	655	-	5,5,5	0.93	0	5,5,5	0.96	0
10	GOL	A	651	-	5,5,5	0.78	0	5,5,5	0.98	0
5	PG4	A	660[B]	-	12,12,12	0.49	0	11,11,11	0.92	0
10	GOL	A	657	-	5,5,5	0.84	0	5,5,5	1.04	0
6	GLN	A	670	-	5,9,9	0.27	0	5,11,11	0.10	0
6	GLN	A	672	-	5,9,9	0.35	0	5,11,11	0.70	0
8	EDO	A	628	-	3,3,3	0.40	0	2,2,2	0.55	0
6	GLN	A	609	-	5,9,9	0.27	0	5,11,11	0.06	0
6	GLN	A	671[A]	-	5,9,9	0.23	0	5,11,11	0.11	0
9	PGE	A	644	-	9,9,9	0.29	0	8,8,8	0.34	0
6	GLN	A	669[A]	-	5,9,9	0.30	0	5,11,11	0.21	0
8	EDO	A	636	-	3,3,3	0.46	0	2,2,2	0.29	0
6	GLN	A	658	-	5,9,9	0.61	0	5,11,11	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	EDO	A	626	-	3,3,3	0.48	0	2,2,2	0.30	0
6	GLN	A	615[A]	-	5,9,9	0.25	0	5,11,11	0.21	0
6	GLN	A	616[B]	-	5,9,9	0.27	0	5,11,11	0.20	0
6	GLN	A	613	-	5,9,9	0.25	0	5,11,11	0.12	0
4	P6G	A	602	-	18,18,18	0.54	0	17,17,17	0.26	0
6	GLN	A	605	-	5,9,9	0.28	0	5,11,11	0.17	0
6	GLN	A	617[A]	-	5,9,9	0.31	0	5,11,11	0.12	0
9	PGE	A	641[B]	-	9,9,9	0.32	0	8,8,8	0.28	0
6	GLN	A	607	-	5,9,9	0.20	0	5,11,11	0.04	0
3	1PE	A	601	-	9,9,15	0.51	0	8,8,14	0.76	0
7	PO4	A	619[B]	13	4,4,4	1.10	0	6,6,6	0.64	0
6	GLN	A	674	-	5,9,9	0.42	0	5,11,11	0.77	0
6	GLN	A	671[B]	-	5,9,9	0.29	0	5,11,11	0.42	0
7	PO4	A	619[A]	13	4,4,4	0.95	0	6,6,6	0.57	0
6	GLN	A	669[B]	-	5,9,9	0.24	0	5,11,11	0.16	0
10	GOL	A	654	-	5,5,5	0.98	0	5,5,5	0.94	0
6	GLN	A	615[B]	-	5,9,9	0.26	0	5,11,11	0.14	0
6	GLN	A	668	-	5,9,9	0.25	0	5,11,11	0.21	0
8	EDO	A	622	-	3,3,3	0.47	0	2,2,2	0.30	0
3	1PE	A	604	12	15,15,15	0.47	0	14,14,14	0.95	0
6	GLN	A	612[A]	-	5,9,9	0.21	0	5,11,11	0.17	0
6	GLN	A	611[A]	-	5,9,9	0.25	0	5,11,11	0.13	0
9	PGE	A	637	-	6,6,9	0.30	0	5,5,8	0.66	0
8	EDO	A	630	-	3,3,3	0.47	0	2,2,2	0.24	0
8	EDO	A	634	-	3,3,3	0.47	0	2,2,2	0.29	0
9	PGE	A	642[A]	-	9,9,9	0.30	0	8,8,8	0.24	0
8	EDO	A	623	-	3,3,3	0.49	0	2,2,2	0.26	0
6	GLN	A	617[B]	-	5,9,9	0.27	0	5,11,11	0.17	0
6	GLN	A	665	-	5,9,9	0.30	0	5,11,11	0.29	0
6	GLN	A	676	-	5,9,9	0.48	0	5,11,11	0.72	0
8	EDO	A	632	-	3,3,3	0.43	0	2,2,2	0.53	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
11	CIT	A	659	-	-	0/6/16/16	-
6	GLN	A	614	-	-	1/5/9/9	-
6	GLN	A	667	-	-	1/5/9/9	-
10	GOL	A	649	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	A	656	-	-	4/4/4/4	-
6	GLN	A	610	-	-	2/5/9/9	-
6	GLN	A	612[B]	-	-	2/5/9/9	-
6	GLN	A	611[B]	-	-	5/5/9/9	-
9	PGE	A	643	-	-	3/7/7/7	-
9	PGE	A	640	-	-	5/7/7/7	-
10	GOL	A	645	-	-	2/4/4/4	-
8	EDO	A	624	-	-	0/1/1/1	-
9	PGE	A	642[B]	-	-	4/7/7/7	-
8	EDO	A	631	-	-	0/1/1/1	-
10	GOL	A	653	-	-	0/4/4/4	-
8	EDO	A	625	-	-	0/1/1/1	-
6	GLN	A	608[A]	-	-	2/5/9/9	-
8	EDO	A	629	-	-	0/1/1/1	-
5	PG4	A	660[A]	-	-	6/10/10/10	-
8	EDO	A	620	-	-	0/1/1/1	-
9	PGE	A	638	-	-	2/7/7/7	-
9	PGE	A	639	-	-	3/7/7/7	-
6	GLN	A	673	-	-	1/5/9/9	-
8	EDO	A	621	-	-	0/1/1/1	-
10	GOL	A	648	-	-	2/4/4/4	-
10	GOL	A	650	-	-	4/4/4/4	-
8	EDO	A	635	-	-	1/1/1/1	-
10	GOL	A	652	-	-	2/4/4/4	-
6	GLN	A	618	-	-	2/5/9/9	-
6	GLN	A	606	-	-	3/5/9/9	-
6	GLN	A	616[A]	-	-	3/5/9/9	-
8	EDO	A	633	-	-	1/1/1/1	-
5	PG4	A	603	-	-	4/10/10/10	-
10	GOL	A	646	-	-	2/4/4/4	-
6	GLN	A	666	-	-	1/5/9/9	-
6	GLN	A	675	-	-	3/5/9/9	-
10	GOL	A	647	-	-	4/4/4/4	-
6	GLN	A	661	-	-	1/5/9/9	-
8	EDO	A	627	-	-	0/1/1/1	-
9	PGE	A	641[A]	-	-	4/7/7/7	-
6	GLN	A	608[B]	-	-	1/5/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	A	655	-	-	0/4/4/4	-
10	GOL	A	651	-	-	0/4/4/4	-
5	PG4	A	660[B]	-	-	1/10/10/10	-
10	GOL	A	657	-	-	4/4/4/4	-
6	GLN	A	670	-	-	2/5/9/9	-
6	GLN	A	672	-	-	0/5/9/9	-
8	EDO	A	628	-	-	1/1/1/1	-
6	GLN	A	609	-	-	3/5/9/9	-
6	GLN	A	671[A]	-	-	2/5/9/9	-
9	PGE	A	644	-	-	4/7/7/7	-
6	GLN	A	669[A]	-	-	3/5/9/9	-
8	EDO	A	636	-	-	1/1/1/1	-
6	GLN	A	658	-	-	2/5/9/9	-
8	EDO	A	626	-	-	1/1/1/1	-
6	GLN	A	615[A]	-	-	1/5/9/9	-
6	GLN	A	616[B]	-	-	5/5/9/9	-
6	GLN	A	613	-	-	2/5/9/9	-
4	P6G	A	602	-	-	10/16/16/16	-
6	GLN	A	605	-	-	1/5/9/9	-
6	GLN	A	617[A]	-	-	4/5/9/9	-
9	PGE	A	641[B]	-	-	5/7/7/7	-
6	GLN	A	607	-	-	1/5/9/9	-
3	1PE	A	601	-	-	4/7/7/13	-
6	GLN	A	674	-	-	5/5/9/9	-
6	GLN	A	671[B]	-	-	3/5/9/9	-
6	GLN	A	669[B]	-	-	2/5/9/9	-
10	GOL	A	654	-	-	4/4/4/4	-
6	GLN	A	615[B]	-	-	3/5/9/9	-
6	GLN	A	668	-	-	0/5/9/9	-
8	EDO	A	622	-	-	0/1/1/1	-
3	1PE	A	604	12	-	7/13/13/13	-
6	GLN	A	612[A]	-	-	5/5/9/9	-
6	GLN	A	611[A]	-	-	2/5/9/9	-
9	PGE	A	637	-	-	1/4/4/7	-
8	EDO	A	630	-	-	0/1/1/1	-
8	EDO	A	634	-	-	1/1/1/1	-
9	PGE	A	642[A]	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	623	-	-	0/1/1/1	-
6	GLN	A	617[B]	-	-	1/5/9/9	-
6	GLN	A	665	-	-	2/5/9/9	-
6	GLN	A	676	-	-	3/5/9/9	-
8	EDO	A	632	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	653	GOL	O2-C2	-2.04	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	646	GOL	C3-C2-C1	-2.24	102.99	111.70
11	A	659	CIT	C3-C2-C1	-2.22	111.43	114.98
6	A	611[B]	GLN	CG-CB-CA	2.01	118.54	113.84

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	605	GLN	N-CA-CB-CG
6	A	606	GLN	N-CA-CB-CG
6	A	606	GLN	C-CA-CB-CG
6	A	608[A]	GLN	C-CA-CB-CG
6	A	611[A]	GLN	C-CA-CB-CG
6	A	611[B]	GLN	N-CA-CB-CG
6	A	611[B]	GLN	C-CA-CB-CG
6	A	612[A]	GLN	N-CA-CB-CG
6	A	612[A]	GLN	C-CA-CB-CG
6	A	612[B]	GLN	N-CA-CB-CG
6	A	612[B]	GLN	C-CA-CB-CG
6	A	616[B]	GLN	N-CA-CB-CG
6	A	616[B]	GLN	C-CA-CB-CG
6	A	617[A]	GLN	N-CA-CB-CG
6	A	617[A]	GLN	C-CA-CB-CG
6	A	618	GLN	C-CA-CB-CG
6	A	669[A]	GLN	N-CA-CB-CG
6	A	669[A]	GLN	C-CA-CB-CG
6	A	670	GLN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
6	A	670	GLN	C-CA-CB-CG
6	A	671[A]	GLN	N-CA-CB-CG
6	A	671[A]	GLN	C-CA-CB-CG
6	A	671[B]	GLN	C-CA-CB-CG
6	A	674	GLN	N-CA-CB-CG
6	A	674	GLN	C-CA-CB-CG
6	A	675	GLN	C-CA-CB-CG
10	A	645	GOL	O1-C1-C2-C3
10	A	648	GOL	O1-C1-C2-C3
10	A	649	GOL	C1-C2-C3-O3
10	A	654	GOL	O1-C1-C2-C3
10	A	654	GOL	C1-C2-C3-O3
10	A	656	GOL	O1-C1-C2-C3
10	A	657	GOL	O1-C1-C2-C3
10	A	657	GOL	C1-C2-C3-O3
9	A	639	PGE	C3-C4-O3-C5
4	A	602	P6G	C15-C14-O13-C12
6	A	667	GLN	CA-CB-CG-CD
6	A	675	GLN	CA-CB-CG-CD
6	A	676	GLN	CA-CB-CG-CD
4	A	602	P6G	O13-C14-C15-O16
5	A	603	PG4	O1-C1-C2-O2
9	A	644	PGE	O1-C1-C2-O2
9	A	641[A]	PGE	C4-C3-O2-C2
9	A	641[B]	PGE	O2-C3-C4-O3
4	A	602	P6G	C18-C17-O16-C15
9	A	642[B]	PGE	O3-C5-C6-O4
9	A	642[B]	PGE	O2-C3-C4-O3
6	A	606	GLN	CA-CB-CG-CD
6	A	612[A]	GLN	CA-CB-CG-CD
6	A	615[A]	GLN	CA-CB-CG-CD
6	A	616[A]	GLN	CA-CB-CG-CD
6	A	616[B]	GLN	CA-CB-CG-CD
6	A	666	GLN	CA-CB-CG-CD
6	A	669[A]	GLN	CA-CB-CG-CD
6	A	671[B]	GLN	CA-CB-CG-CD
6	A	673	GLN	CA-CB-CG-CD
6	A	674	GLN	CA-CB-CG-CD
4	A	602	P6G	O16-C17-C18-O19
9	A	641[B]	PGE	O3-C5-C6-O4
9	A	643	PGE	O3-C5-C6-O4
5	A	603	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
10	A	646	GOL	C1-C2-C3-O3
10	A	647	GOL	O1-C1-C2-C3
10	A	647	GOL	C1-C2-C3-O3
10	A	650	GOL	O1-C1-C2-C3
10	A	652	GOL	C1-C2-C3-O3
10	A	656	GOL	C1-C2-C3-O3
9	A	642[A]	PGE	O3-C5-C6-O4
6	A	665	GLN	OE1-CD-CG-CB
6	A	669[B]	GLN	OE1-CD-CG-CB
6	A	669[B]	GLN	NE2-CD-CG-CB
6	A	674	GLN	OE1-CD-CG-CB
6	A	674	GLN	NE2-CD-CG-CB
6	A	614	GLN	CA-CB-CG-CD
4	A	602	P6G	O4-C5-C6-O7
9	A	643	PGE	C1-C2-O2-C3
10	A	645	GOL	O1-C1-C2-O2
10	A	646	GOL	O2-C2-C3-O3
10	A	648	GOL	O1-C1-C2-O2
10	A	650	GOL	O1-C1-C2-O2
10	A	654	GOL	O1-C1-C2-O2
10	A	654	GOL	O2-C2-C3-O3
10	A	656	GOL	O2-C2-C3-O3
10	A	657	GOL	O1-C1-C2-O2
10	A	657	GOL	O2-C2-C3-O3
8	A	634	EDO	O1-C1-C2-O2
8	A	635	EDO	O1-C1-C2-O2
6	A	665	GLN	NE2-CD-CG-CB
9	A	641[A]	PGE	O1-C1-C2-O2
3	A	604	1PE	OH7-C16-C26-OH6
9	A	639	PGE	O3-C5-C6-O4
9	A	640	PGE	O1-C1-C2-O2
9	A	640	PGE	O3-C5-C6-O4
10	A	650	GOL	O2-C2-C3-O3
10	A	652	GOL	O2-C2-C3-O3
10	A	656	GOL	O1-C1-C2-O2
4	A	602	P6G	O10-C11-C12-O13
6	A	615[B]	GLN	OE1-CD-CG-CB
3	A	604	1PE	OH6-C15-C25-OH5
8	A	628	EDO	O1-C1-C2-O2
8	A	632	EDO	O1-C1-C2-O2
6	A	609	GLN	OE1-CD-CG-CB
6	A	609	GLN	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
6	A	611[B]	GLN	OE1-CD-CG-CB
6	A	617[A]	GLN	OE1-CD-CG-CB
6	A	617[A]	GLN	NE2-CD-CG-CB
6	A	658	GLN	OE1-CD-CG-CB
6	A	658	GLN	NE2-CD-CG-CB
6	A	610	GLN	CA-CB-CG-CD
6	A	611[B]	GLN	CA-CB-CG-CD
6	A	676	GLN	OE1-CD-CG-CB
8	A	633	EDO	O1-C1-C2-O2
6	A	612[A]	GLN	NE2-CD-CG-CB
6	A	615[B]	GLN	NE2-CD-CG-CB
6	A	616[A]	GLN	OE1-CD-CG-CB
6	A	616[B]	GLN	OE1-CD-CG-CB
6	A	611[B]	GLN	NE2-CD-CG-CB
6	A	612[A]	GLN	OE1-CD-CG-CB
9	A	641[A]	PGE	C3-C4-O3-C5
9	A	641[A]	PGE	C1-C2-O2-C3
9	A	644	PGE	C4-C3-O2-C2
4	A	602	P6G	C12-C11-O10-C9
9	A	639	PGE	C1-C2-O2-C3
9	A	640	PGE	C6-C5-O3-C4
9	A	642[A]	PGE	C4-C3-O2-C2
3	A	604	1PE	C15-C25-OH5-C14
9	A	642[B]	PGE	C4-C3-O2-C2
5	A	660[A]	PG4	C4-C3-O2-C2
3	A	604	1PE	C25-C15-OH6-C26
5	A	603	PG4	C8-C7-O4-C6
9	A	640	PGE	C1-C2-O2-C3
9	A	641[B]	PGE	C6-C5-O3-C4
9	A	642[B]	PGE	C1-C2-O2-C3
6	A	616[A]	GLN	NE2-CD-CG-CB
8	A	626	EDO	O1-C1-C2-O2
9	A	644	PGE	C1-C2-O2-C3
6	A	607	GLN	N-CA-CB-CG
6	A	608[B]	GLN	N-CA-CB-CG
6	A	610	GLN	N-CA-CB-CG
6	A	611[A]	GLN	N-CA-CB-CG
6	A	618	GLN	N-CA-CB-CG
6	A	661	GLN	N-CA-CB-CG
6	A	675	GLN	N-CA-CB-CG
6	A	616[B]	GLN	NE2-CD-CG-CB
9	A	638	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	A	604	1PE	OH4-C13-C23-OH3
10	A	649	GOL	O2-C2-C3-O3
9	A	638	PGE	O3-C5-C6-O4
9	A	644	PGE	C6-C5-O3-C4
8	A	636	EDO	O1-C1-C2-O2
9	A	642[A]	PGE	C1-C2-O2-C3
3	A	601	1PE	C14-C24-OH4-C13
9	A	637	PGE	C6-C5-O3-C4
9	A	641[B]	PGE	C1-C2-O2-C3
4	A	602	P6G	O1-C2-C3-O4
5	A	660[A]	PG4	O1-C1-C2-O2
6	A	609	GLN	CA-CB-CG-CD
10	A	647	GOL	O1-C1-C2-O2
10	A	647	GOL	O2-C2-C3-O3
6	A	676	GLN	NE2-CD-CG-CB
6	A	617[B]	GLN	CA-CB-CG-CD
5	A	660[A]	PG4	C3-C4-O3-C5
4	A	602	P6G	C9-C8-O7-C6
9	A	641[B]	PGE	C4-C3-O2-C2
5	A	603	PG4	C4-C3-O2-C2
10	A	650	GOL	C1-C2-C3-O3
6	A	613	GLN	NE2-CD-CG-CB
5	A	660[A]	PG4	C5-C6-O4-C7
5	A	660[A]	PG4	O3-C5-C6-O4
4	A	602	P6G	C8-C9-O10-C11
3	A	604	1PE	C14-C24-OH4-C13
6	A	615[B]	GLN	CA-CB-CG-CD
5	A	660[B]	PG4	O2-C3-C4-O3
3	A	601	1PE	C23-C13-OH4-C24
3	A	601	1PE	OH2-C12-C22-OH3
9	A	642[A]	PGE	O1-C1-C2-O2
6	A	613	GLN	OE1-CD-CG-CB
9	A	643	PGE	C4-C3-O2-C2
3	A	601	1PE	C13-C23-OH3-C22
6	A	608[A]	GLN	N-CA-CB-CG
6	A	671[B]	GLN	N-CA-CB-CG
3	A	604	1PE	OH5-C14-C24-OH4
9	A	640	PGE	O2-C3-C4-O3
5	A	660[A]	PG4	O2-C3-C4-O3

There are no ring outliers.

62 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	659	CIT	2	0
6	A	614	GLN	1	0
6	A	667	GLN	4	0
10	A	656	GOL	1	0
6	A	610	GLN	3	0
6	A	612[B]	GLN	1	1
6	A	611[B]	GLN	5	0
9	A	643	PGE	0	1
9	A	640	PGE	2	0
10	A	645	GOL	2	0
10	A	653	GOL	3	0
6	A	608[A]	GLN	1	0
8	A	629	EDO	1	0
5	A	660[A]	PG4	2	0
8	A	620	EDO	1	0
9	A	638	PGE	1	0
9	A	639	PGE	1	0
6	A	673	GLN	1	0
10	A	648	GOL	1	0
10	A	650	GOL	1	0
8	A	635	EDO	2	0
6	A	618	GLN	2	0
6	A	606	GLN	3	1
6	A	616[A]	GLN	2	0
5	A	603	PG4	3	0
6	A	666	GLN	4	0
6	A	675	GLN	2	0
6	A	661	GLN	4	0
9	A	641[A]	PGE	1	0
6	A	608[B]	GLN	3	0
10	A	655	GOL	2	0
5	A	660[B]	PG4	3	0
10	A	657	GOL	2	0
6	A	672	GLN	2	0
8	A	628	EDO	2	0
6	A	609	GLN	1	0
9	A	644	PGE	1	0
6	A	669[A]	GLN	1	0
8	A	636	EDO	1	0
6	A	616[B]	GLN	1	0
6	A	613	GLN	3	0
4	A	602	P6G	2	0
6	A	605	GLN	5	0

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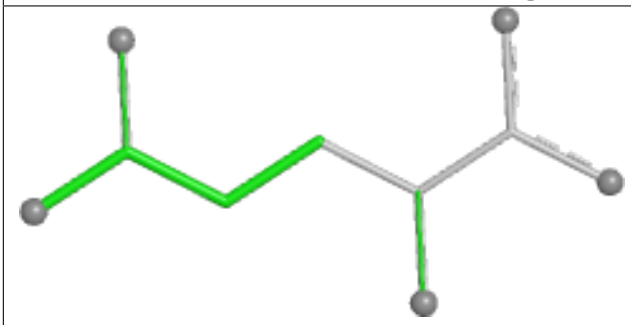
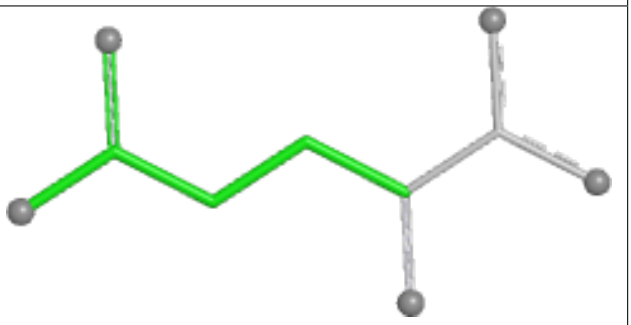
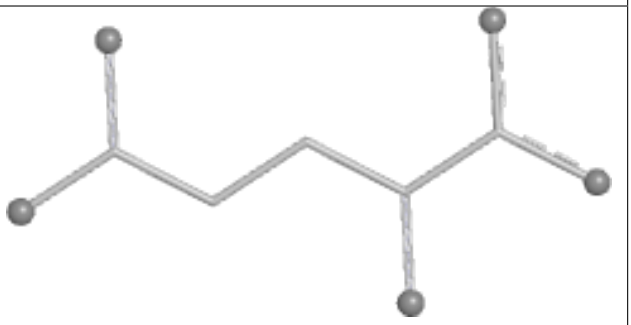
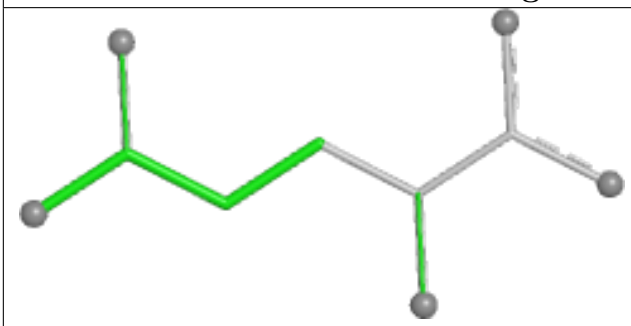
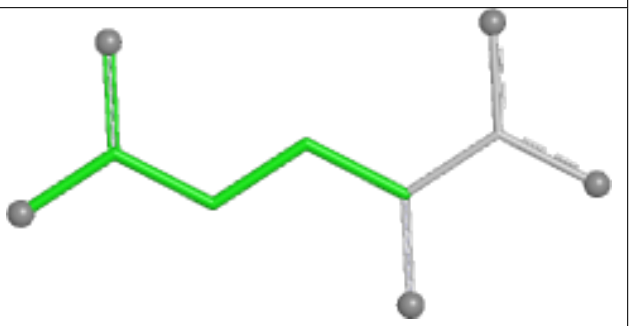
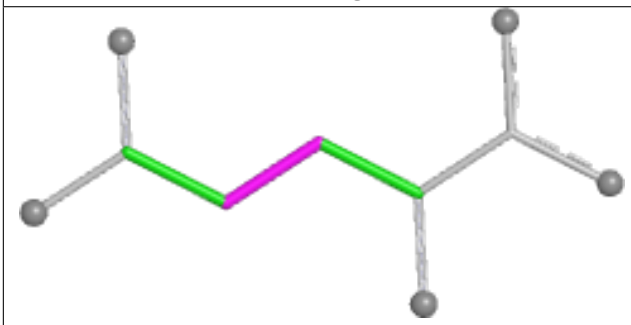
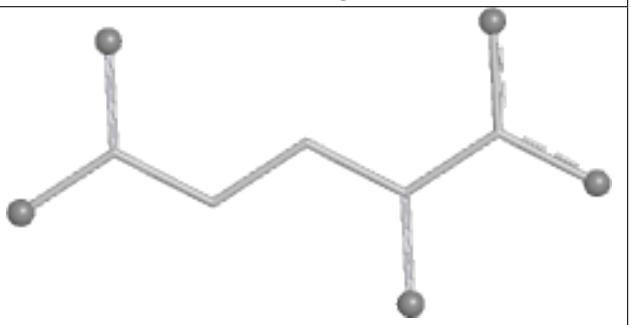
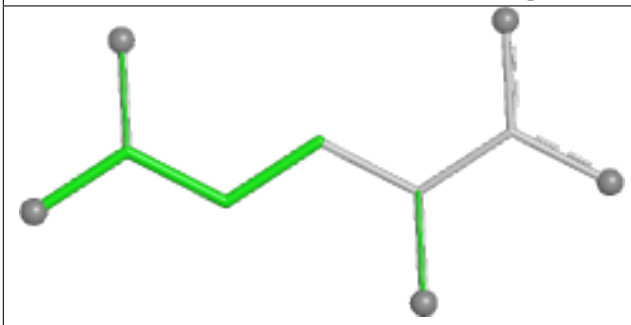
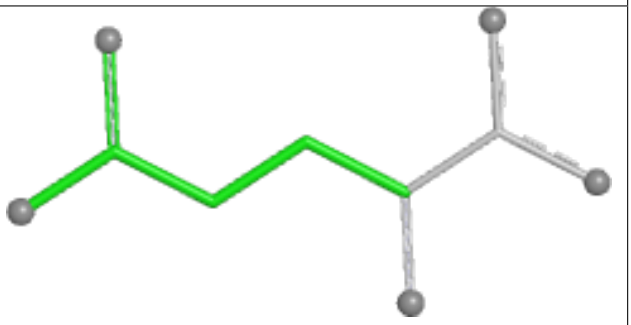
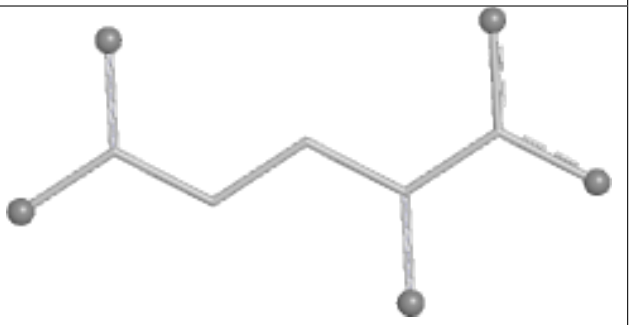
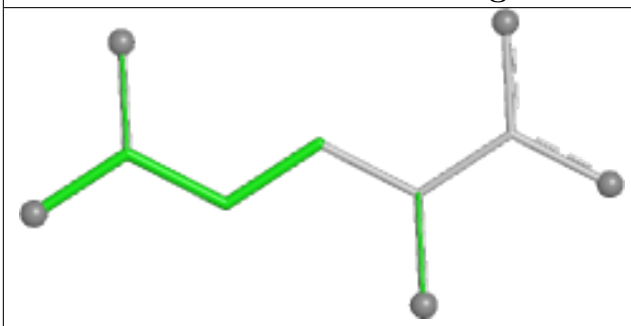
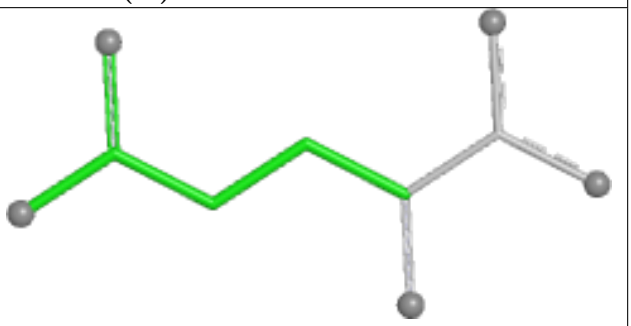
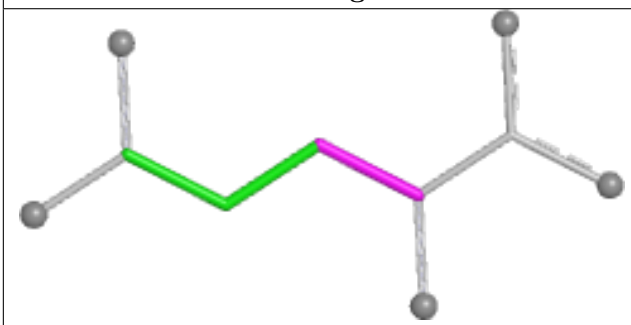
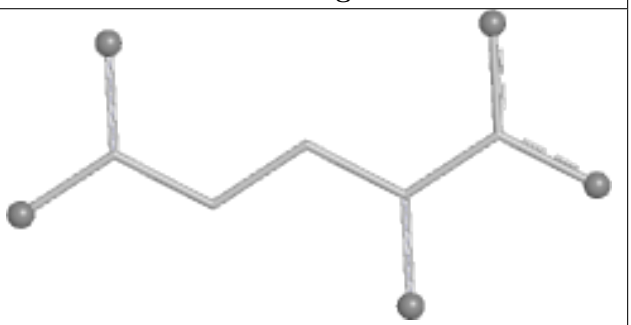
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	617[A]	GLN	1	0
9	A	641[B]	PGE	2	0
6	A	607	GLN	3	0
3	A	601	1PE	1	0
6	A	674	GLN	2	0
6	A	671[B]	GLN	2	0
7	A	619[A]	PO4	2	0
10	A	654	GOL	2	0
6	A	668	GLN	1	0
3	A	604	1PE	7	0
6	A	612[A]	GLN	2	0
6	A	611[A]	GLN	4	0
9	A	637	PGE	3	0
8	A	634	EDO	3	0
9	A	642[A]	PGE	2	0
8	A	623	EDO	1	0
6	A	617[B]	GLN	0	1
6	A	665	GLN	1	0
8	A	632	EDO	2	0

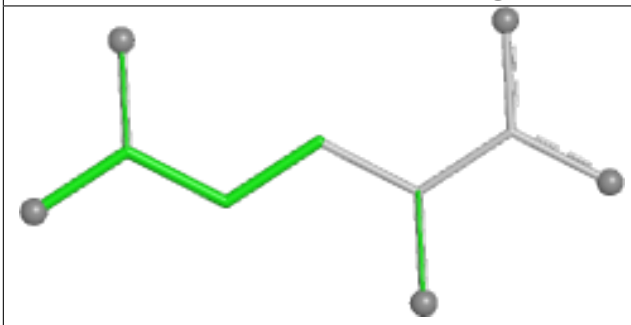
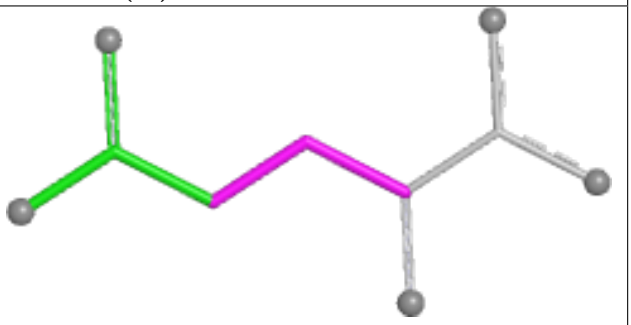
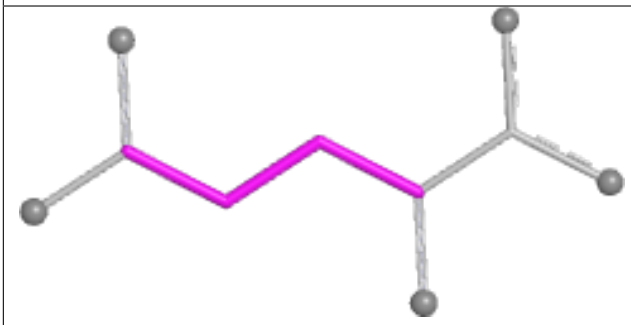
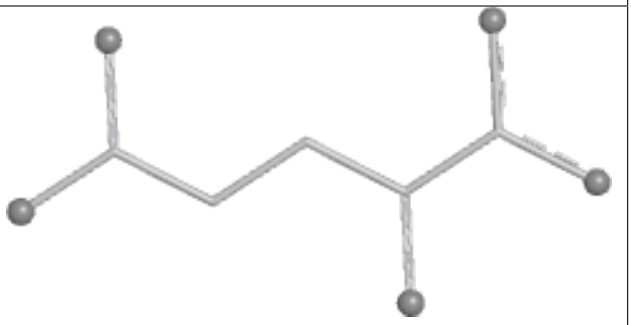
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

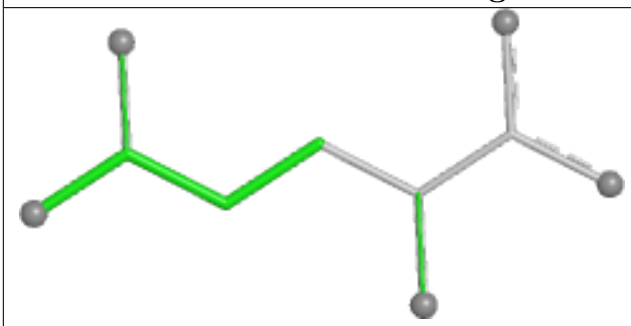
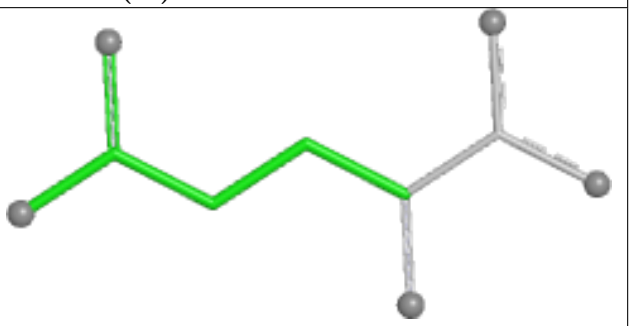
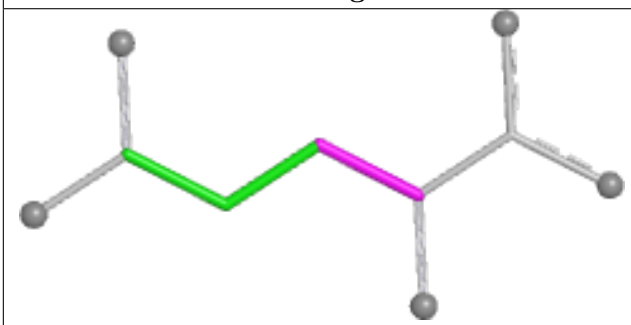
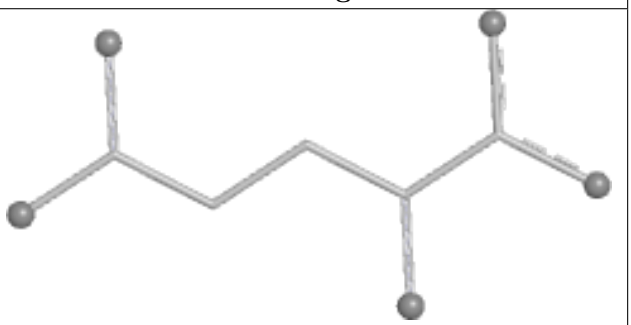
Ligand GLN A 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

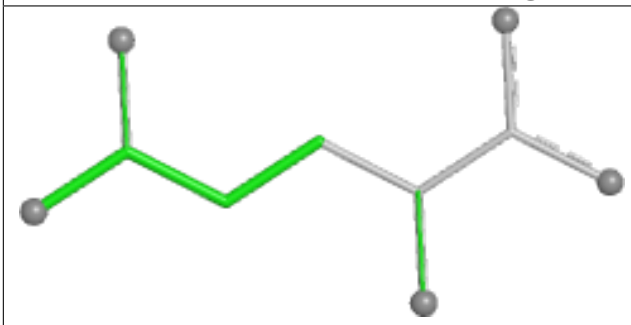
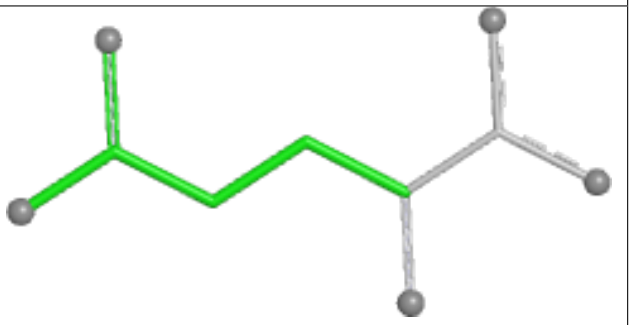
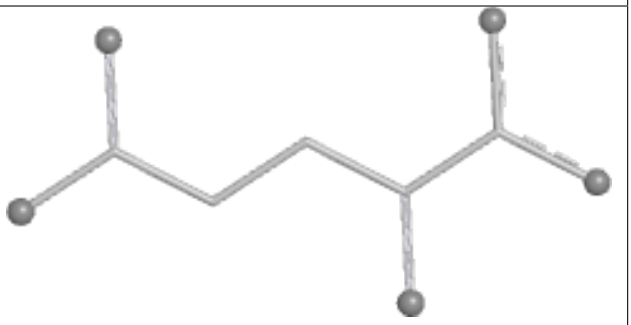
Ligand GLN A 667	
 Bond lengths	 Bond angles
 Torsions	 Rings

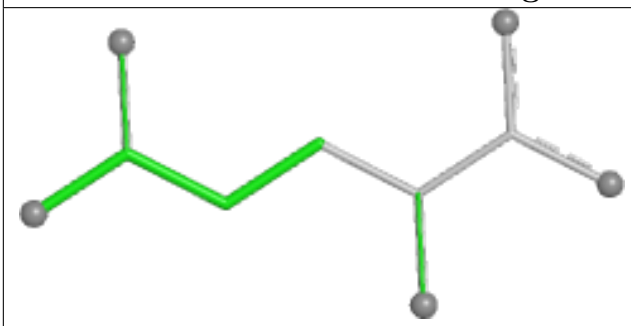
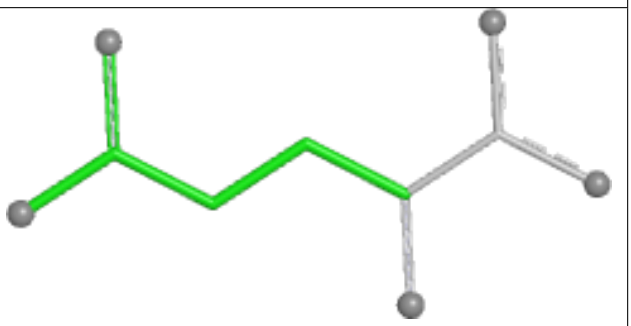
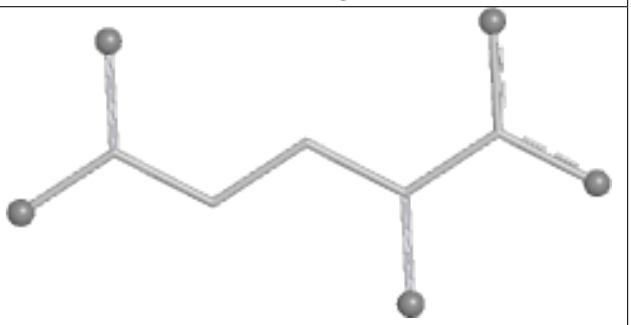
Ligand GLN A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

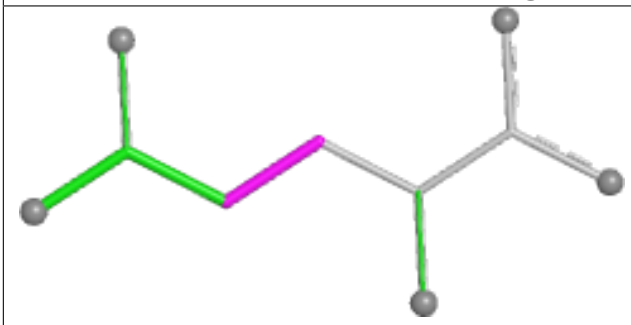
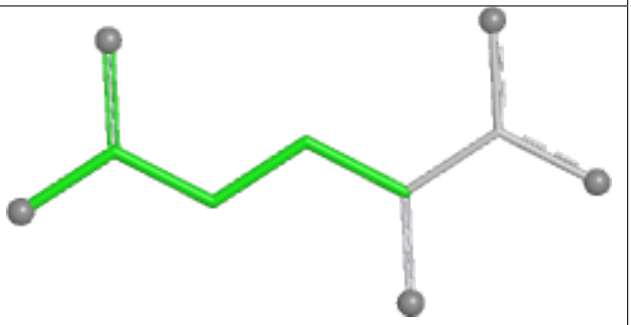
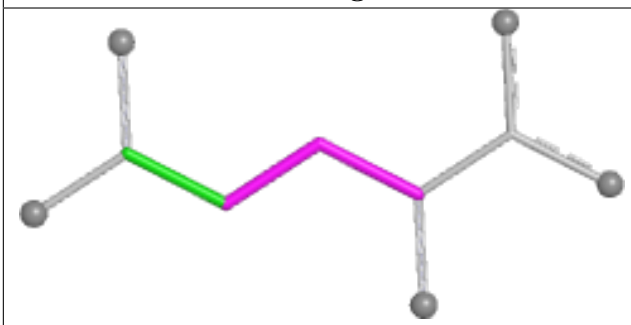
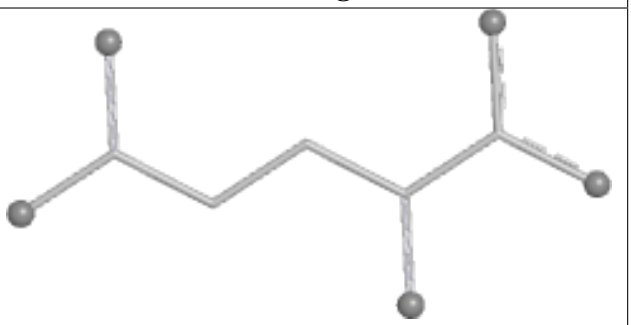
Ligand GLN A 612 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

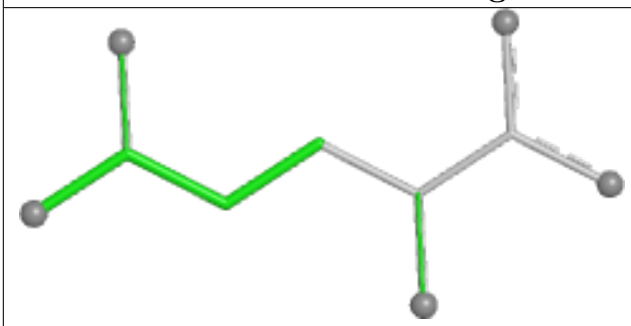
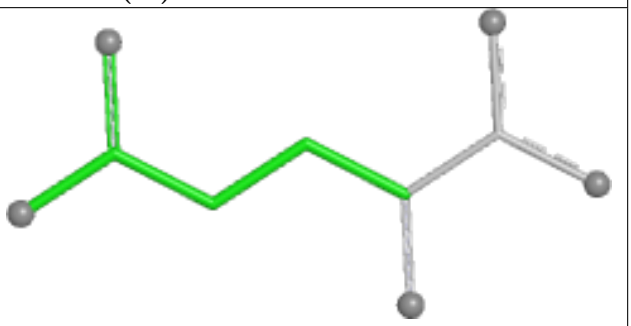
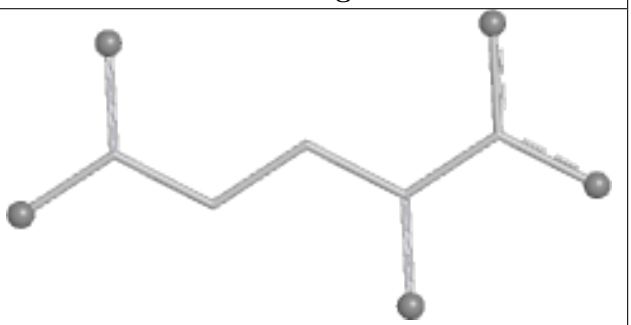
Ligand GLN A 611 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

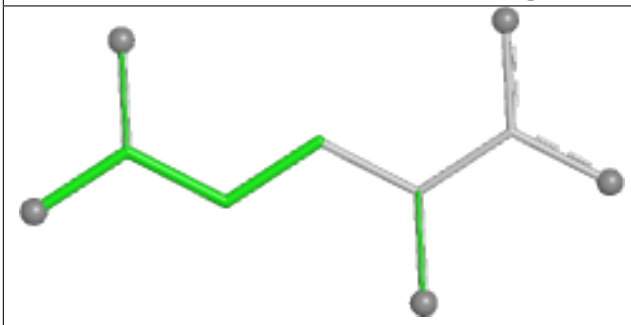
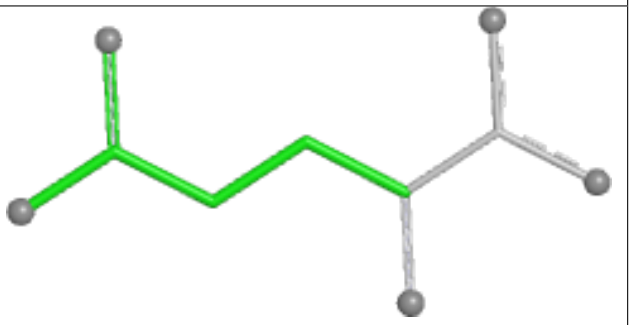
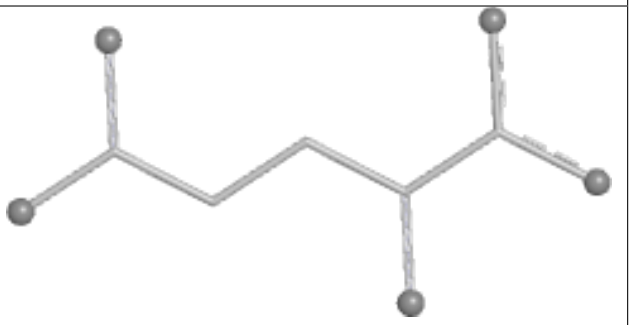
Ligand GLN A 608 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

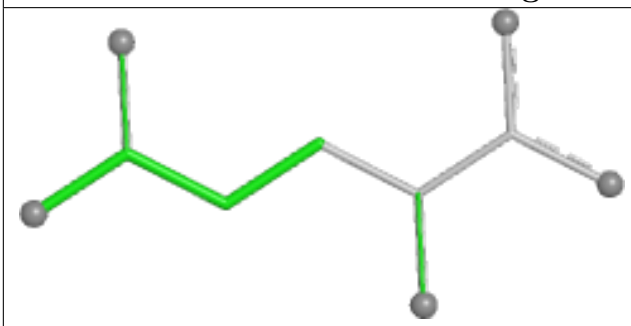
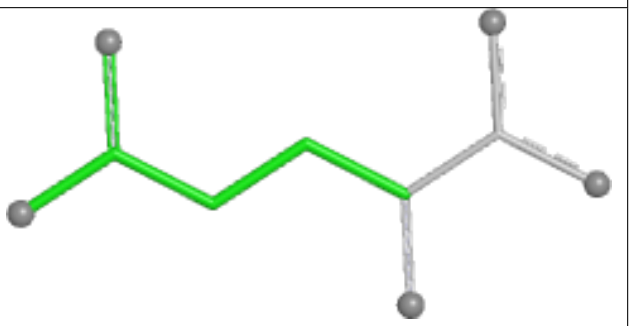
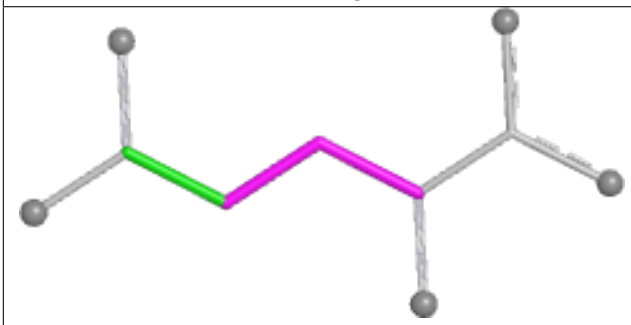
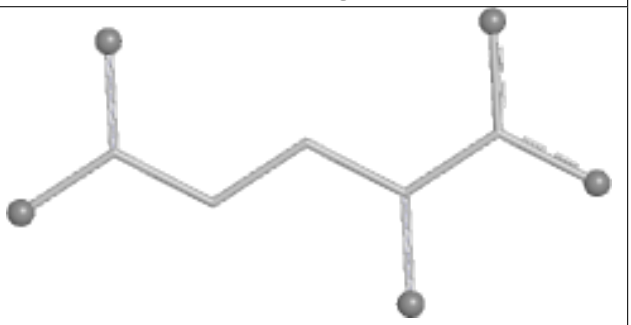
Ligand GLN A 673	
 Bond lengths	 Bond angles
 Torsions	 Rings

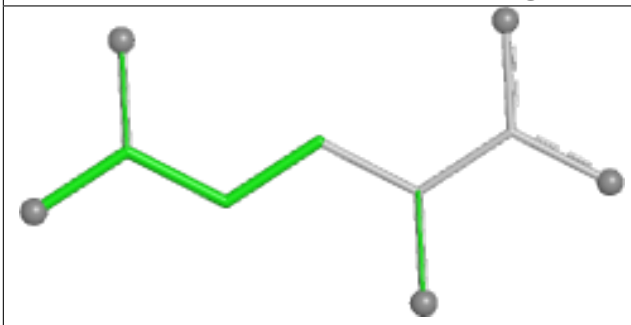
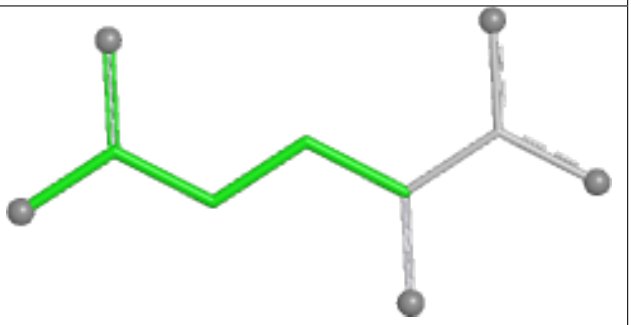
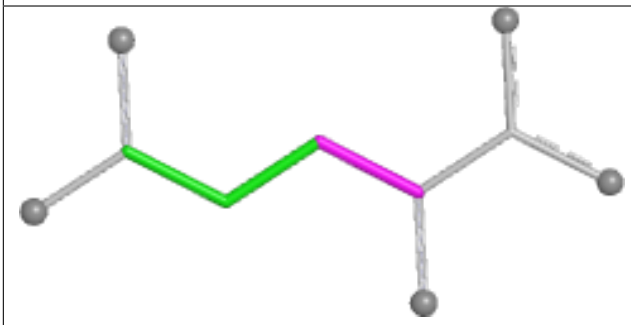
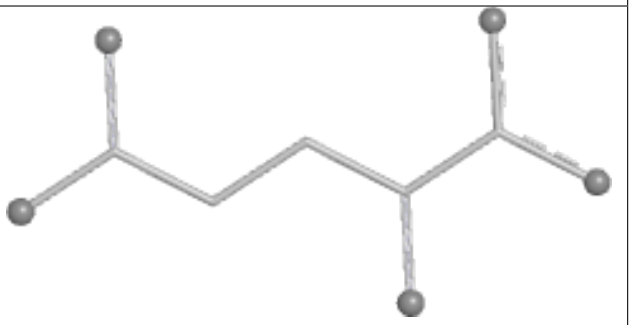
Ligand GLN A 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

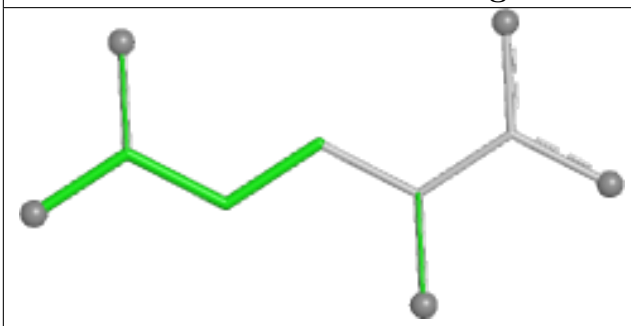
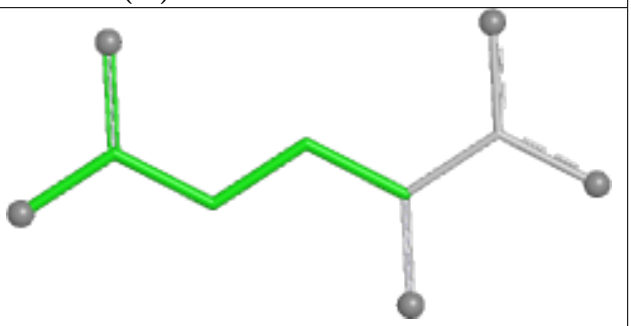
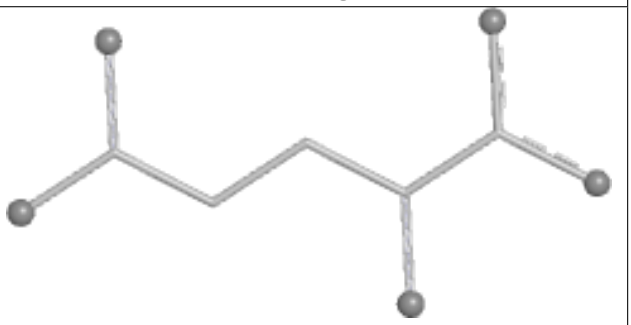
Ligand GLN A 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

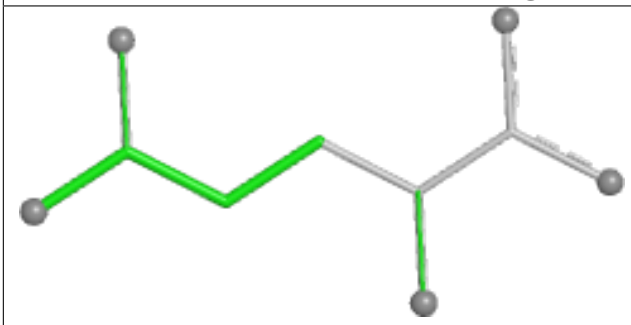
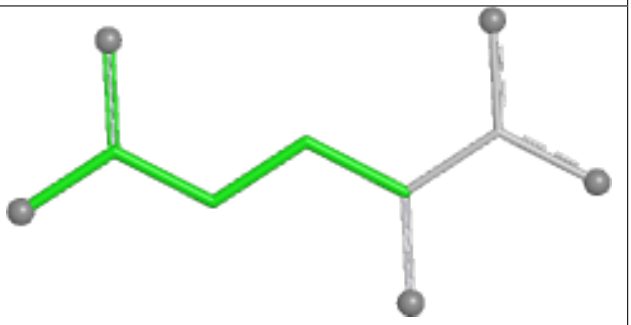
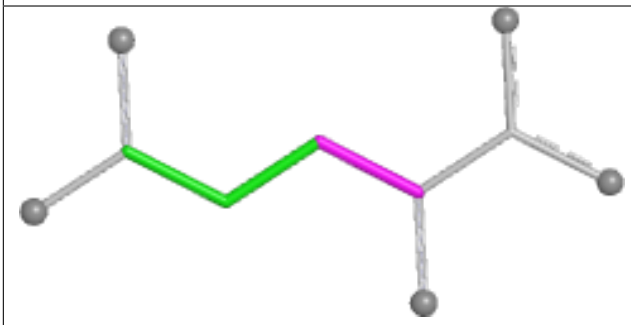
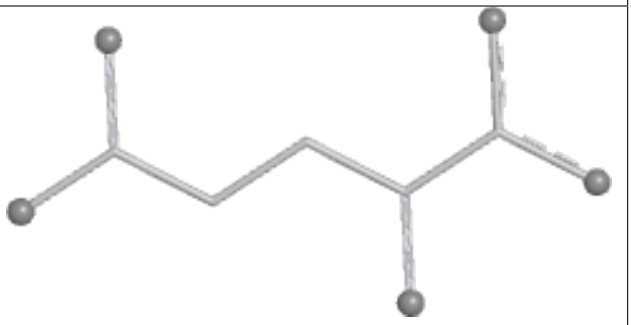
Ligand GLN A 616 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

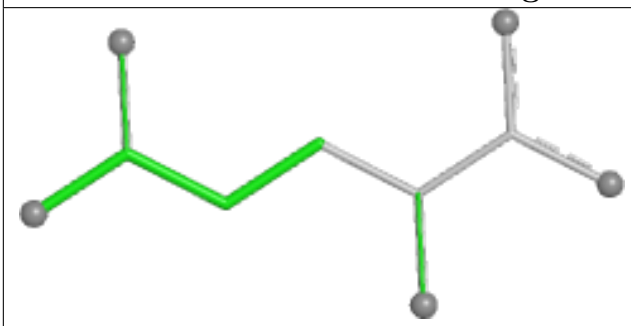
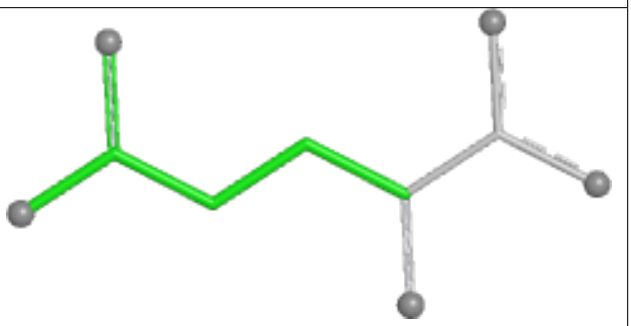
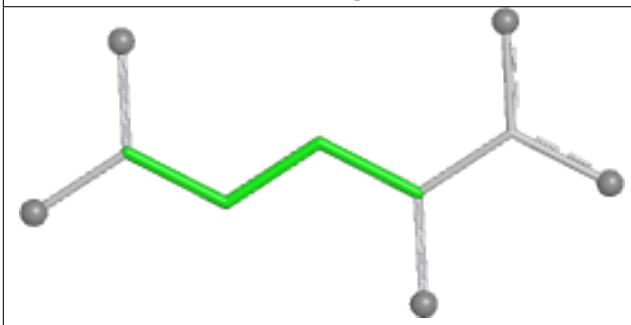
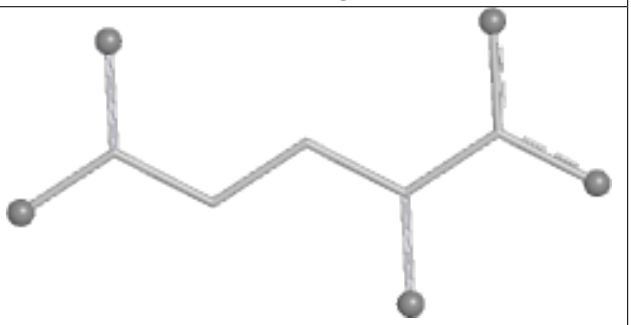
Ligand GLN A 666	
 Bond lengths	 Bond angles
 Torsions	 Rings

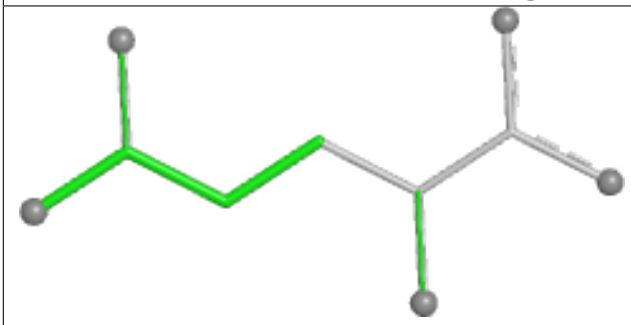
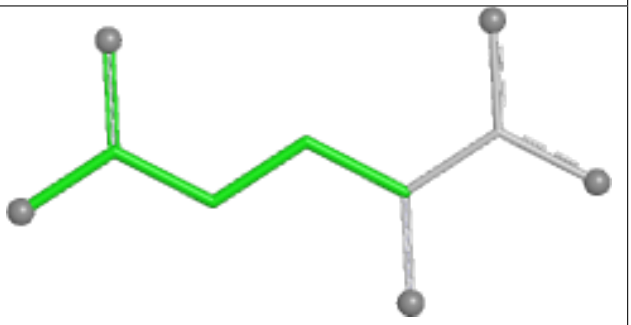
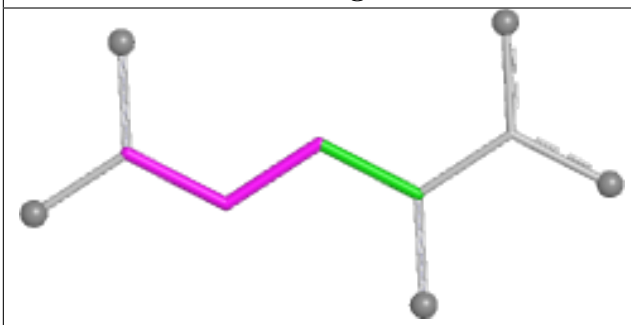
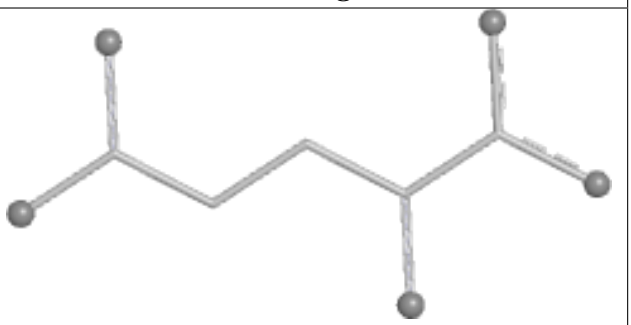
Ligand GLN A 675	
 Bond lengths	 Bond angles
 Torsions	 Rings

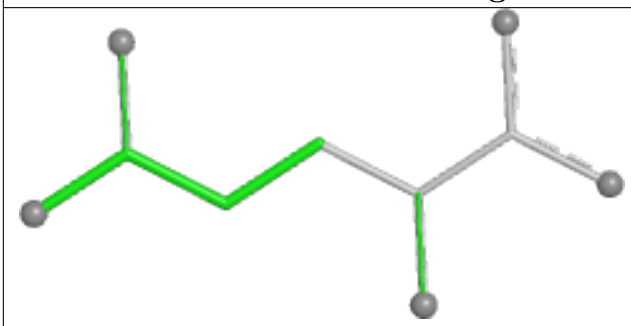
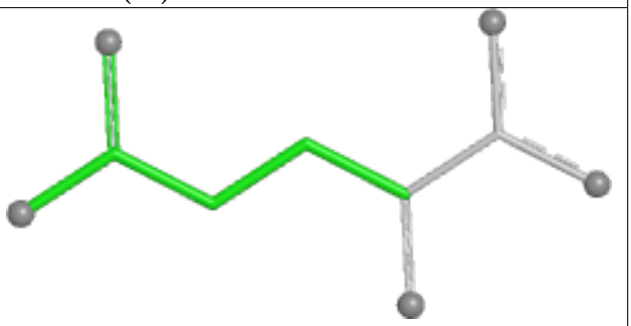
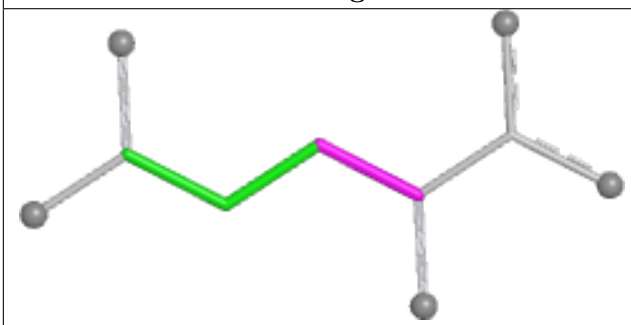
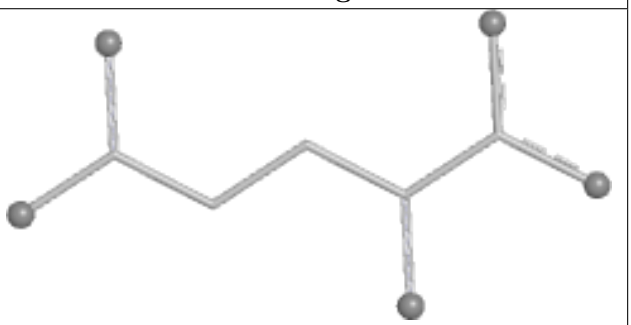
Ligand GLN A 661	
 Bond lengths	 Bond angles
 Torsions	 Rings

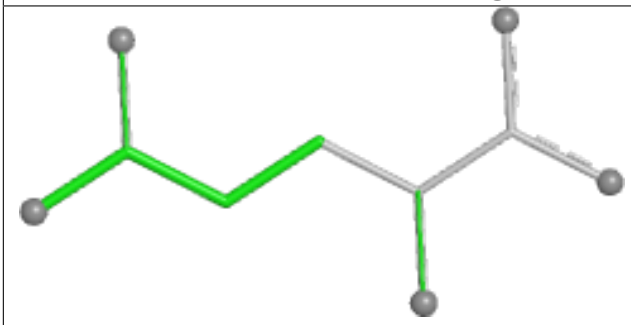
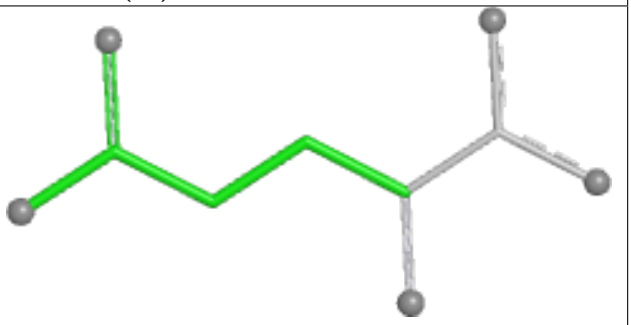
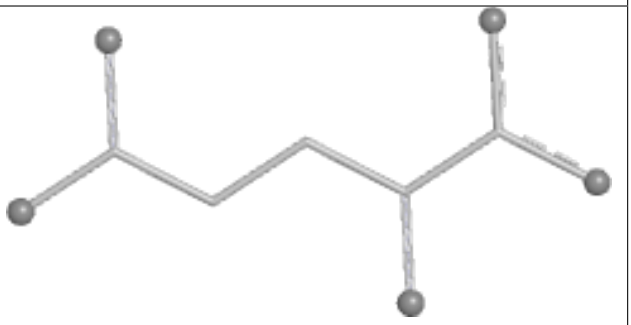
Ligand GLN A 608 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 670	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 672	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 671 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 669 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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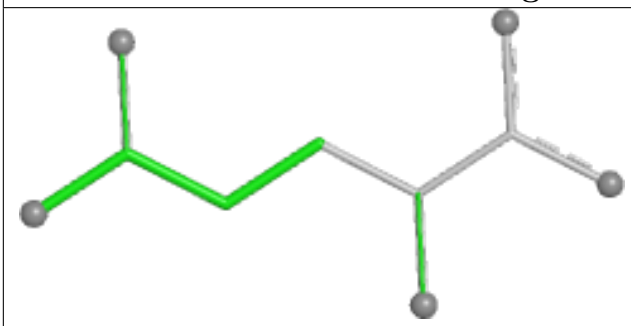
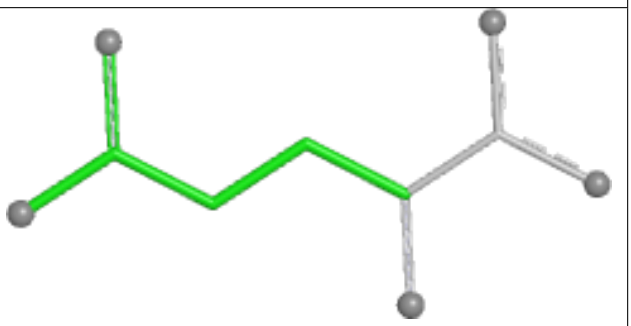
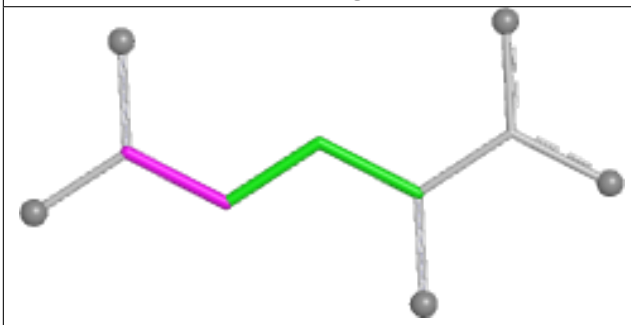
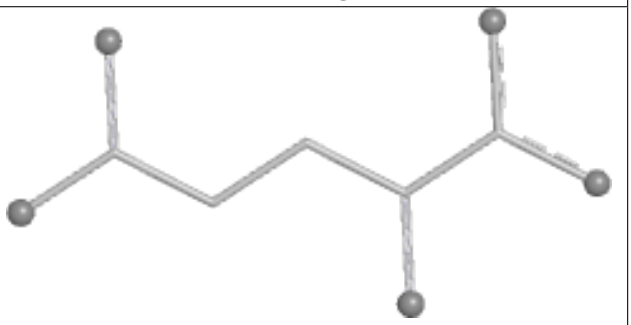
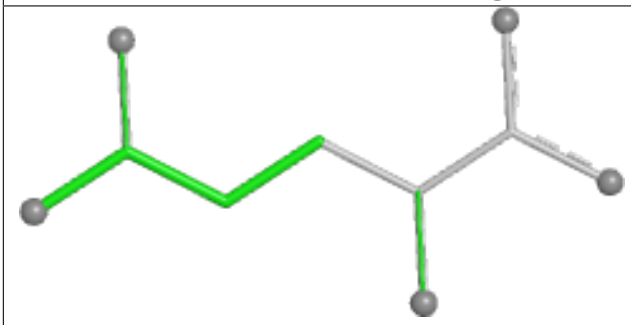
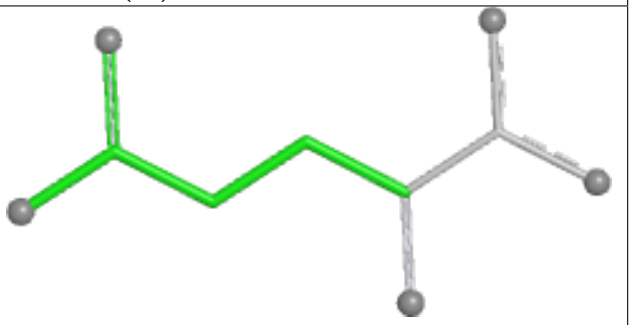
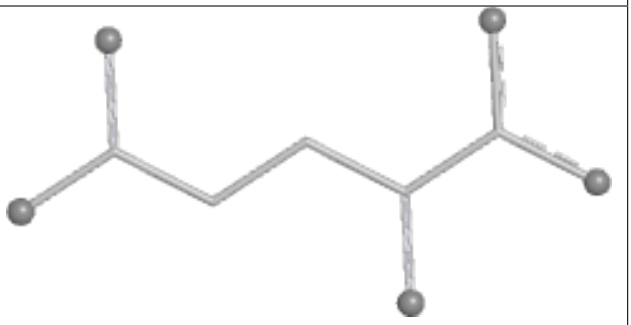
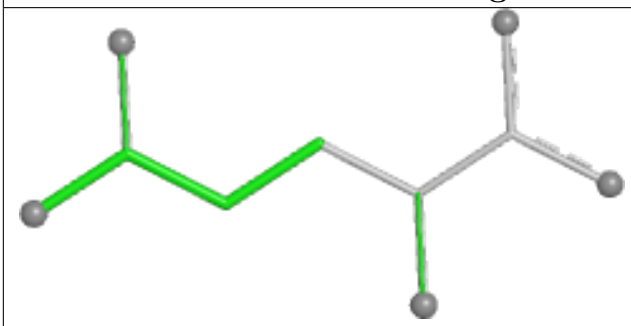
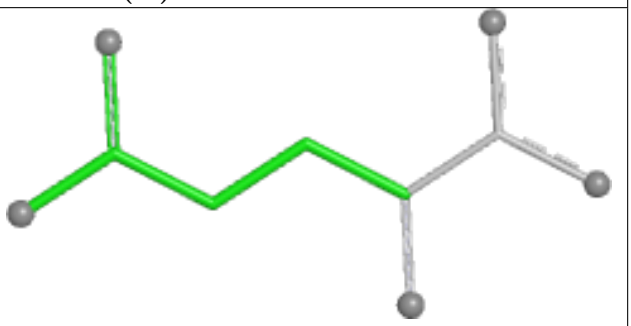
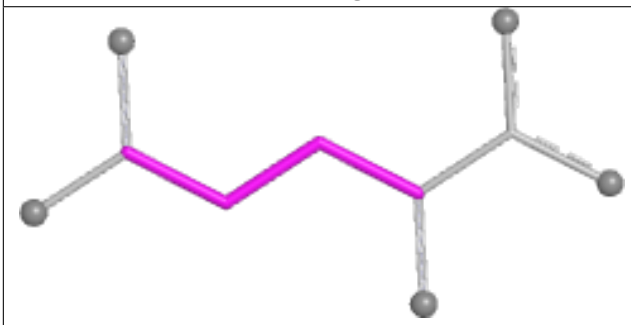
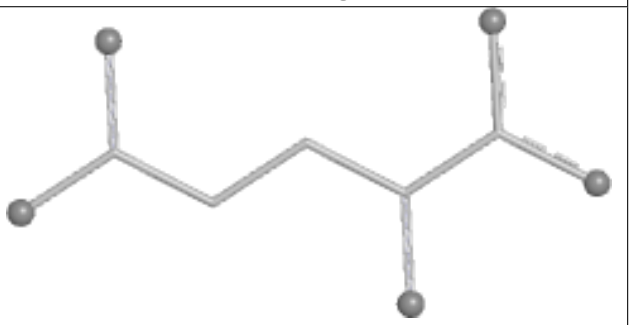
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 615 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 616 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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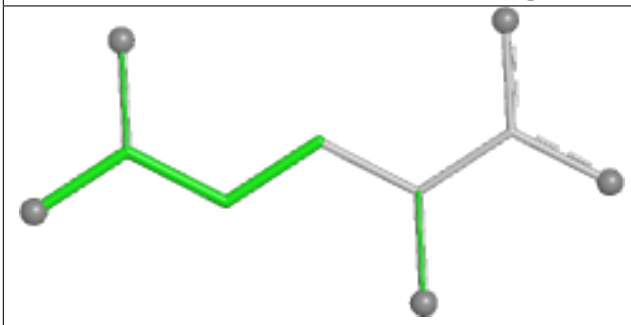
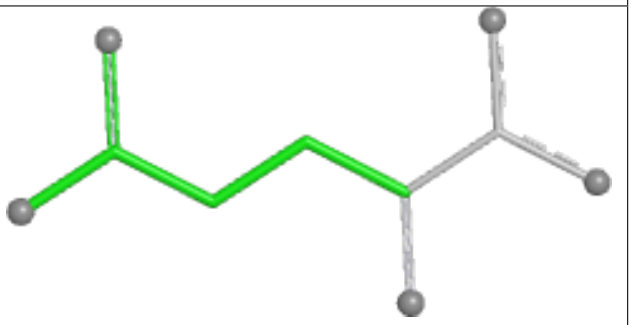
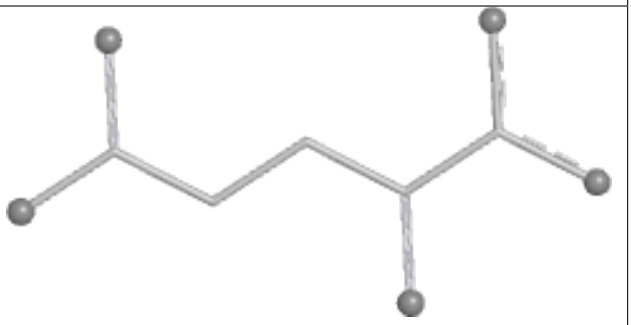
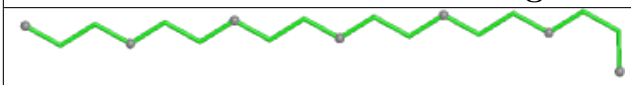
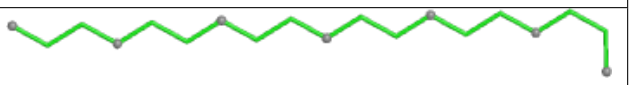
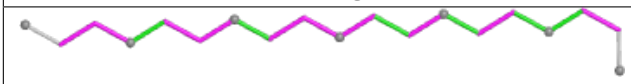
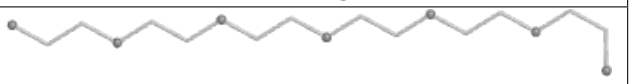
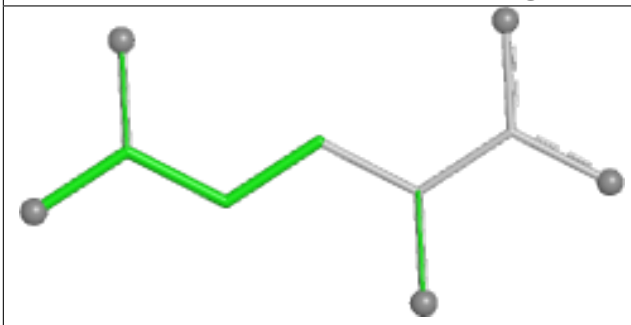
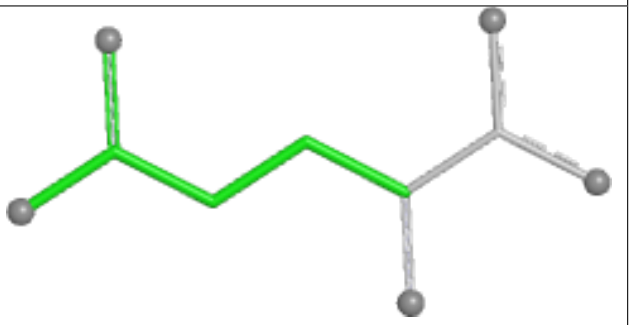
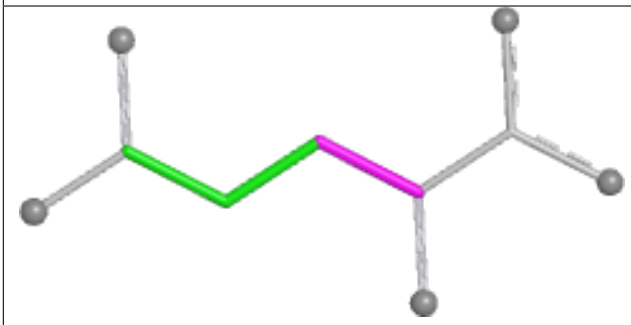
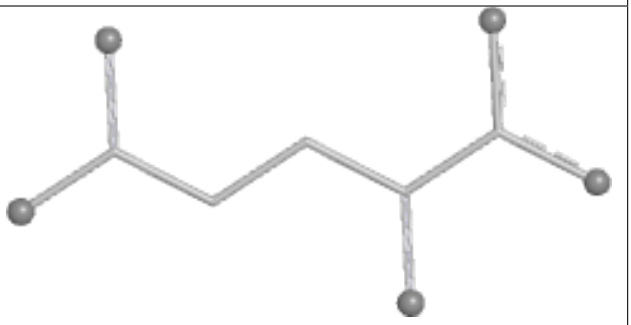
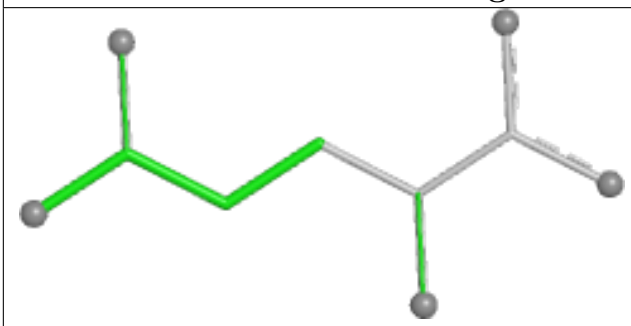
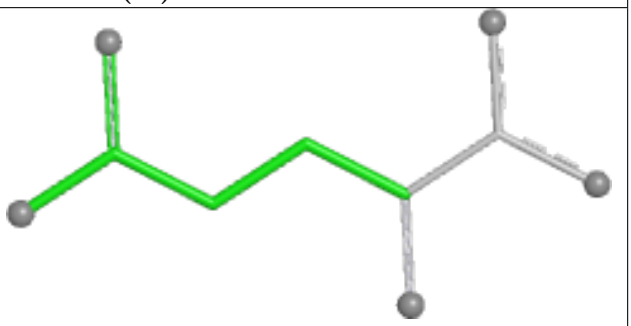
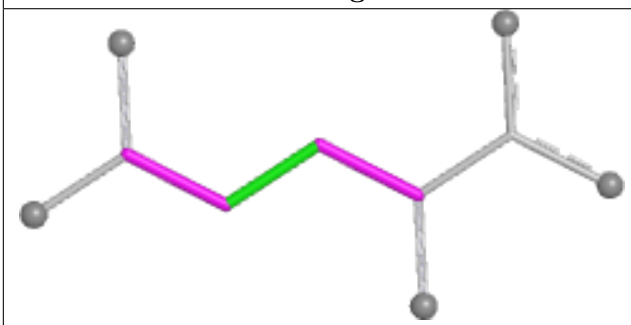
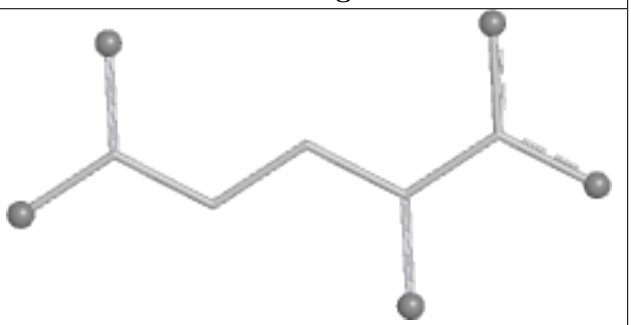
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand P6G A 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 617 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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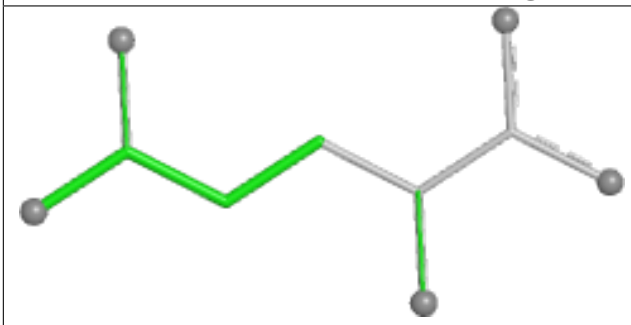
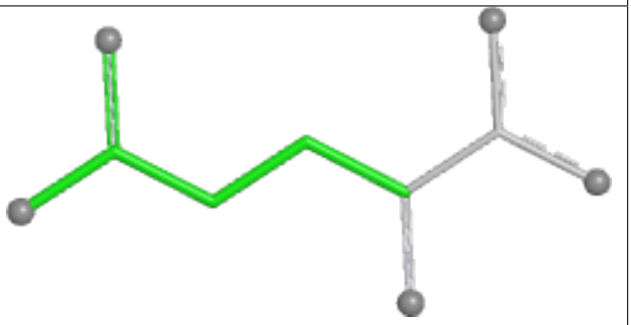
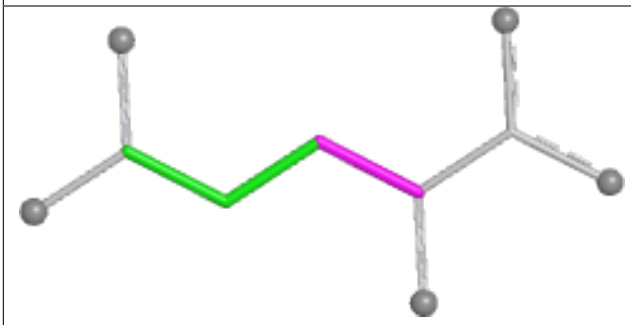
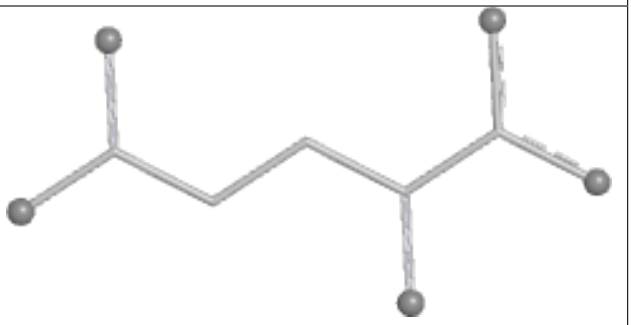
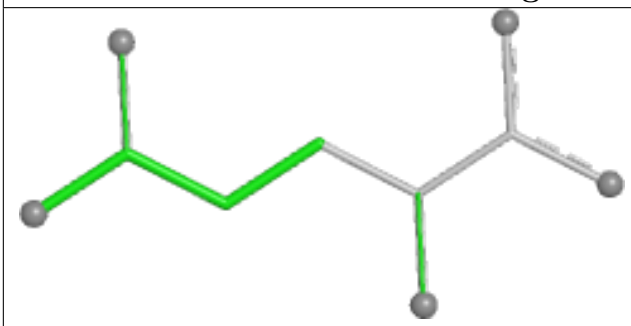
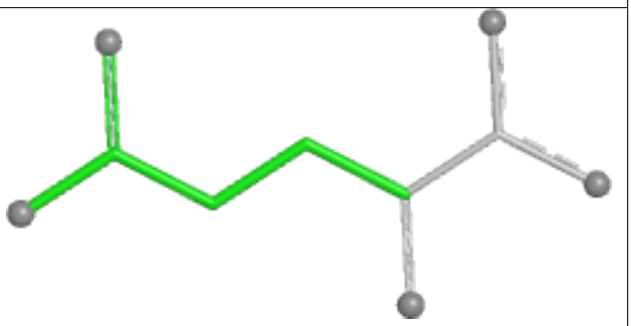
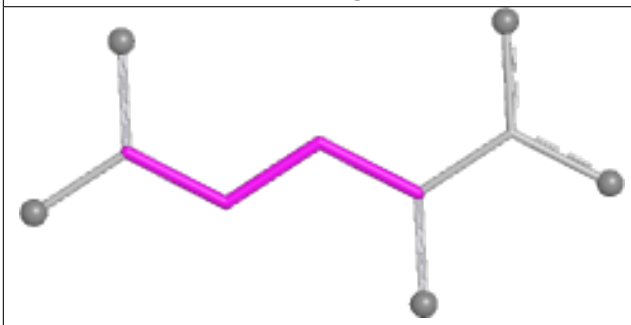
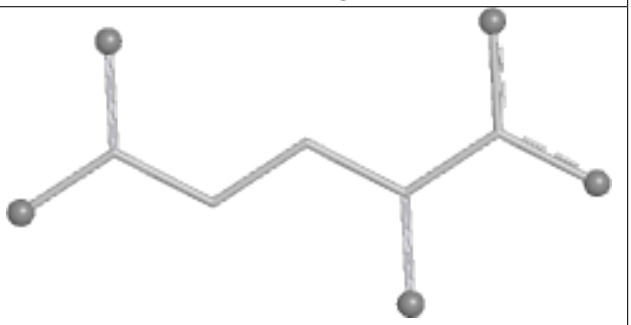
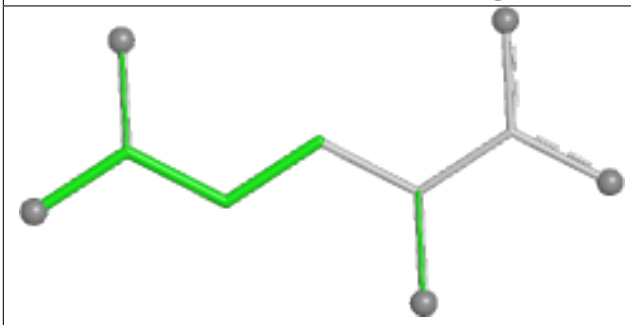
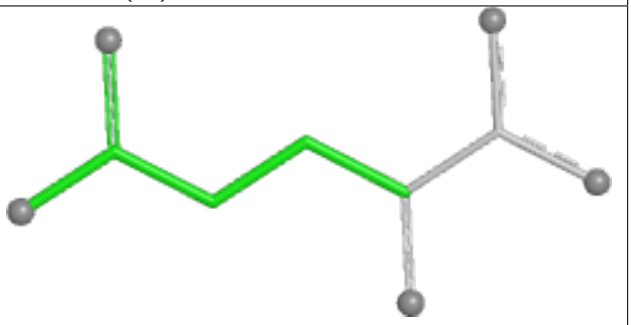
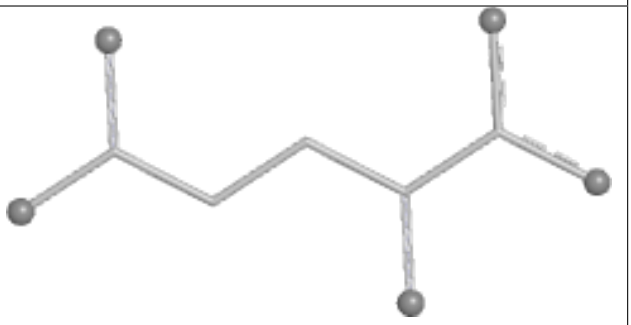
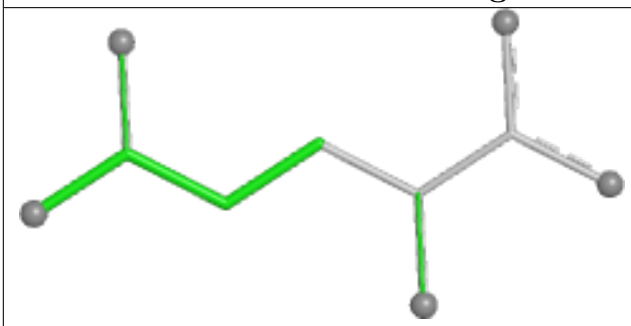
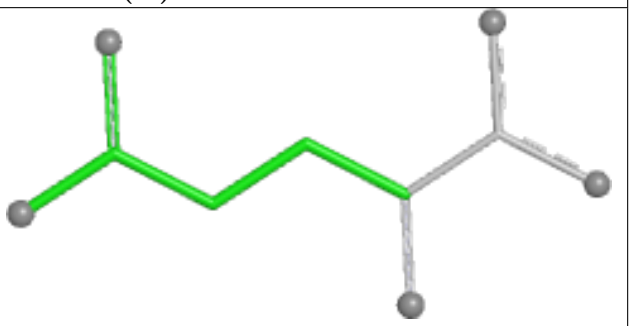
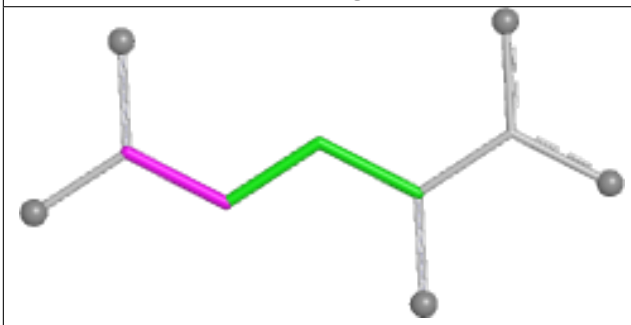
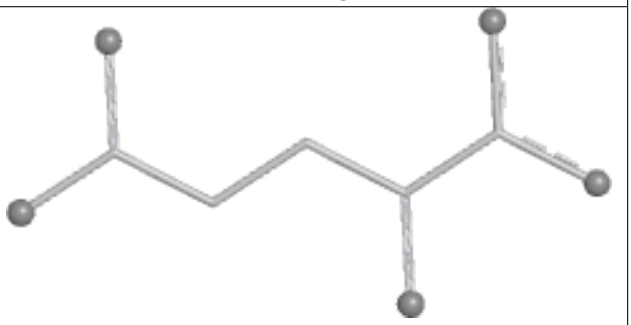
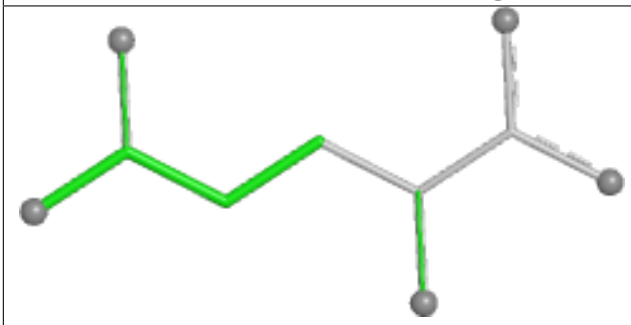
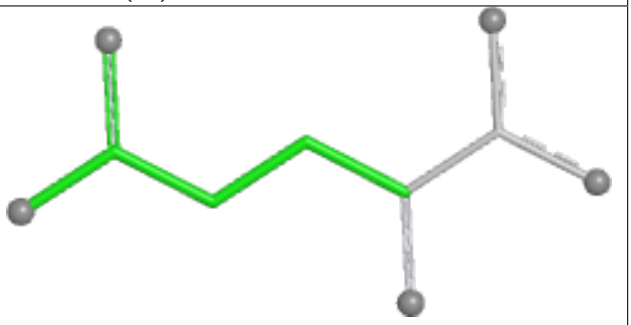
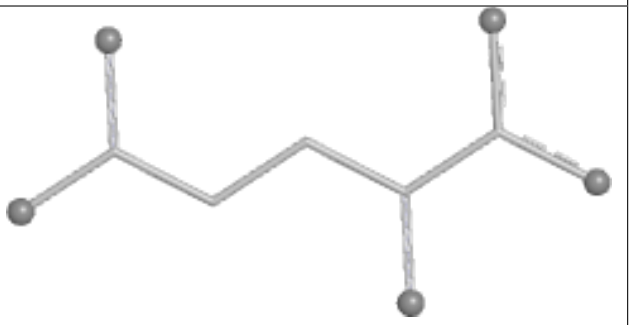
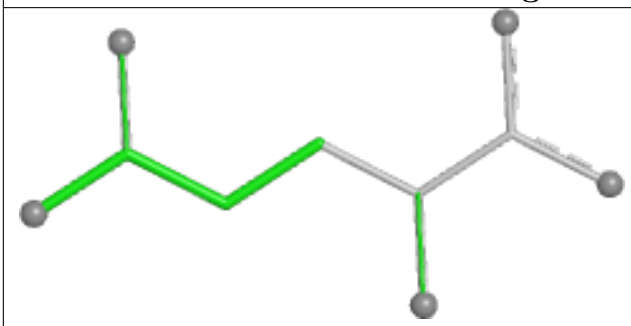
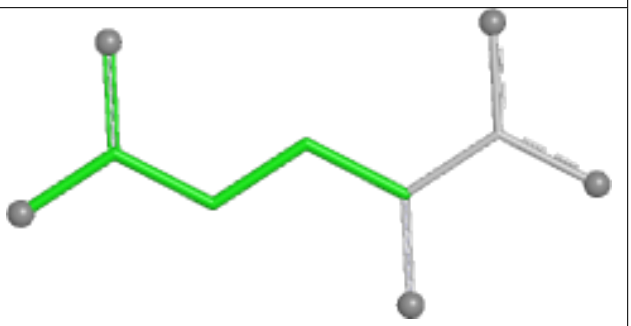
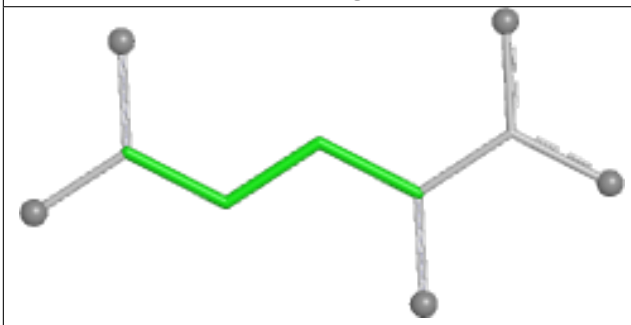
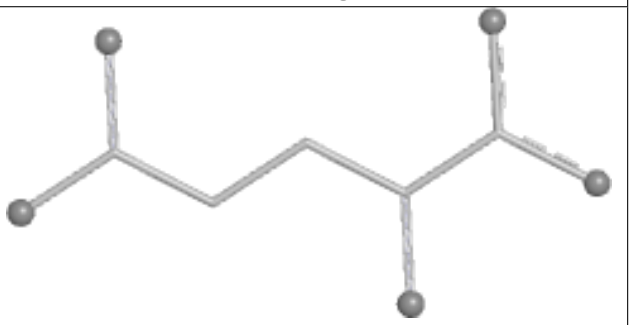
 Bond lengths	 Bond angles
 Torsions	 Rings

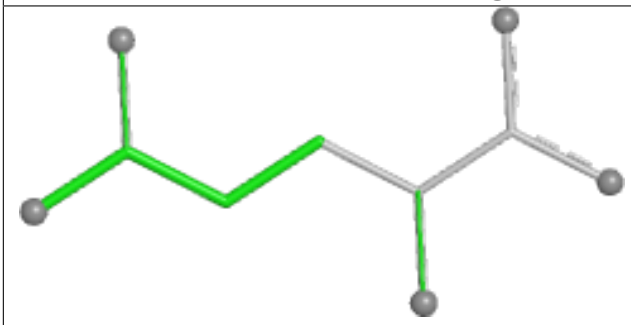
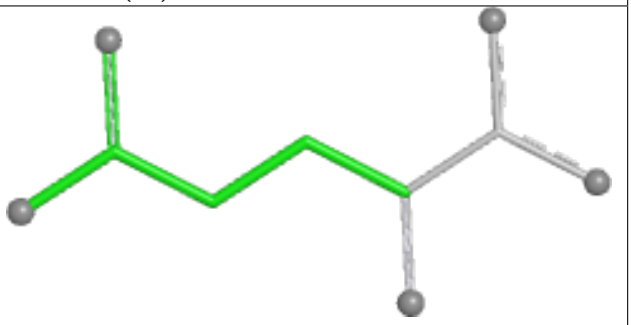
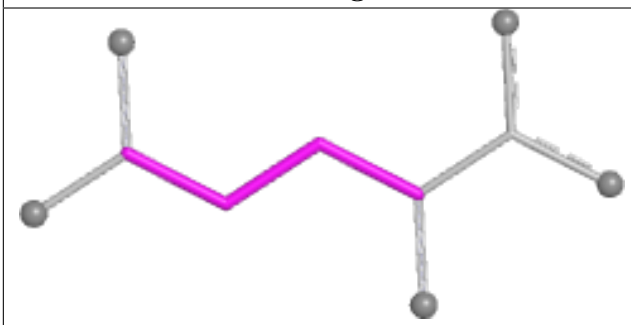
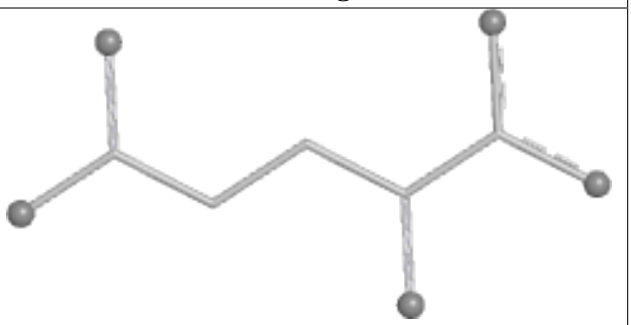
Ligand GLN A 674	
 Bond lengths	 Bond angles
 Torsions	 Rings

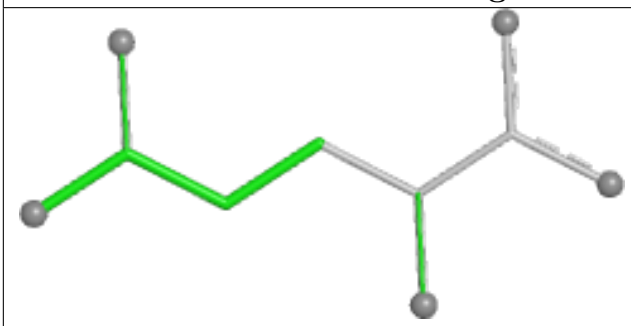
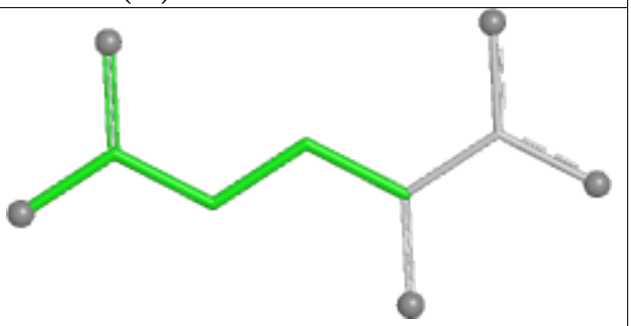
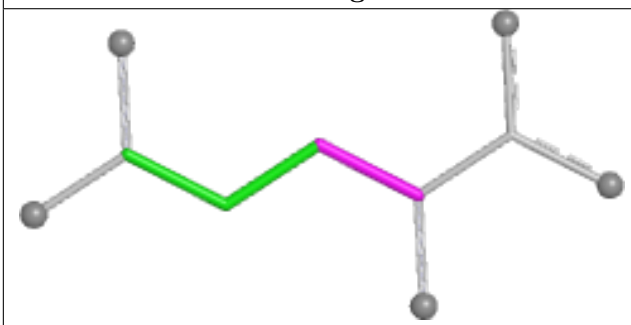
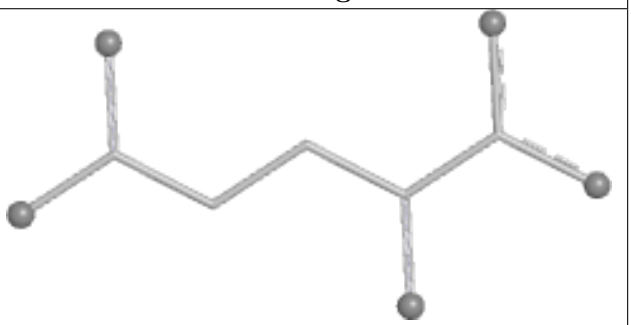
Ligand GLN A 671 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

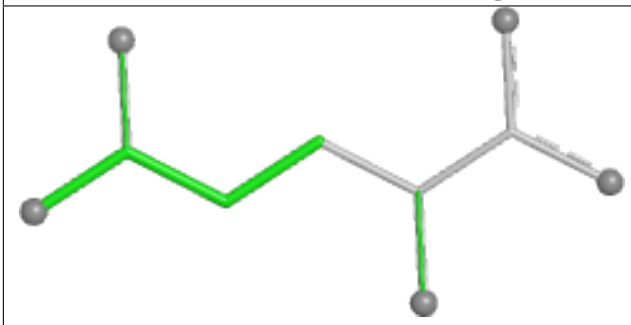
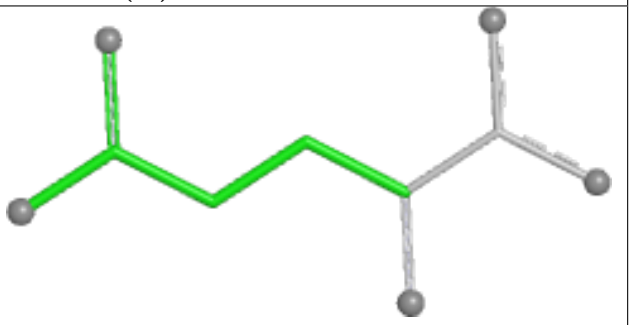
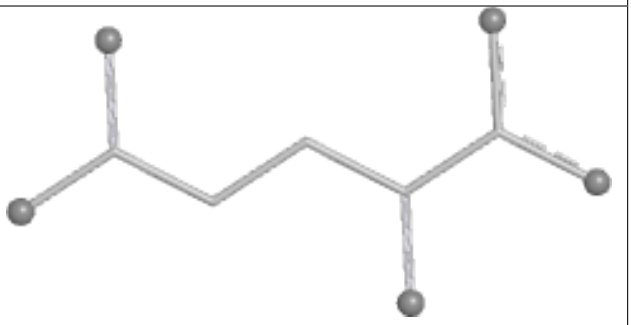
Ligand GLN A 669 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

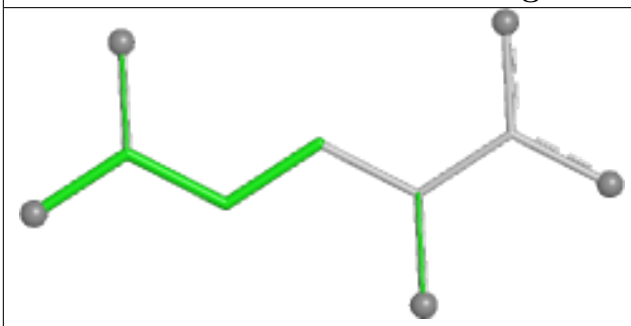
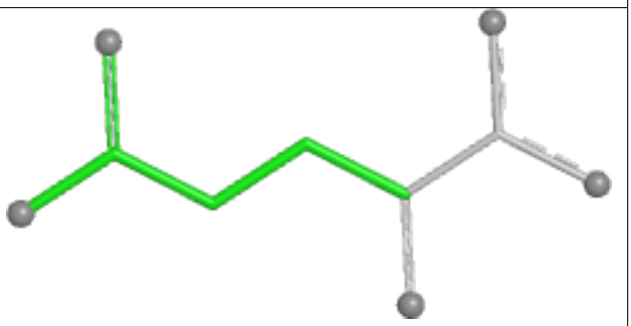
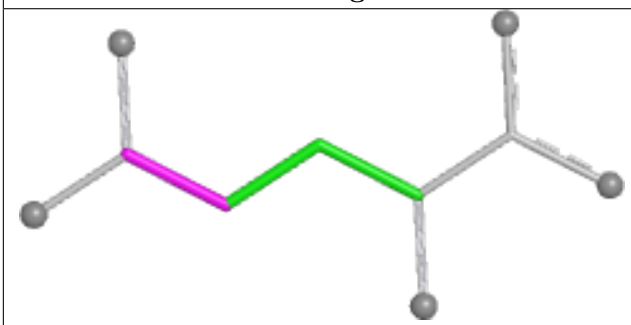
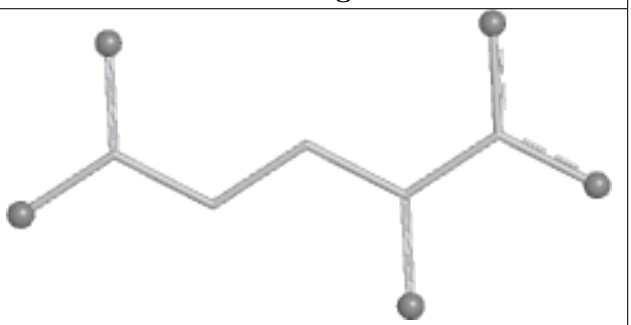
Ligand GLN A 615 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

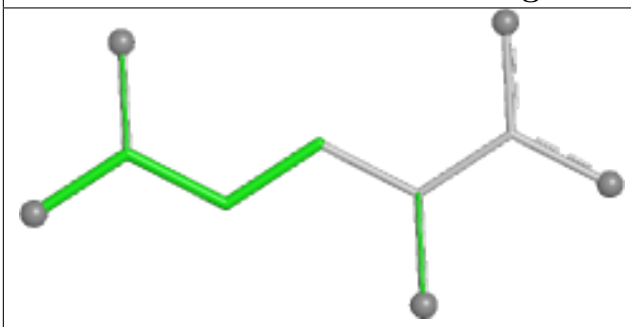
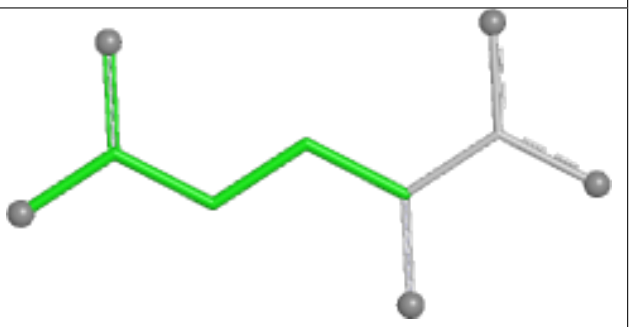
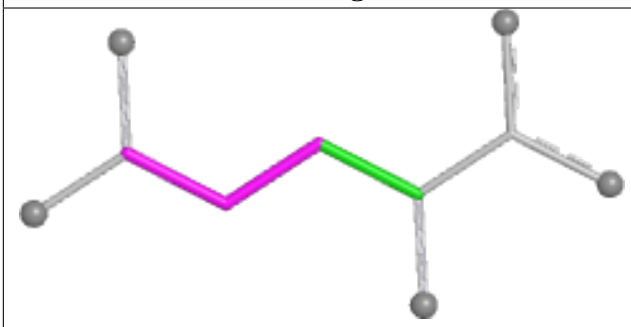
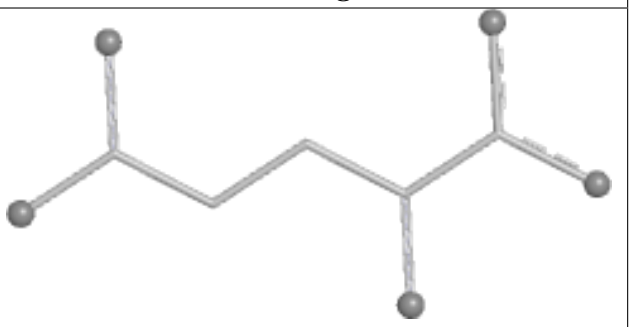
Ligand GLN A 668	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 612 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 611 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 617 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 665	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 676	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	302/313 (96%)	-0.63	2 (0%)	87	89	11, 18, 40, 74	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	THR	3.4
1	A	305	ARG	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

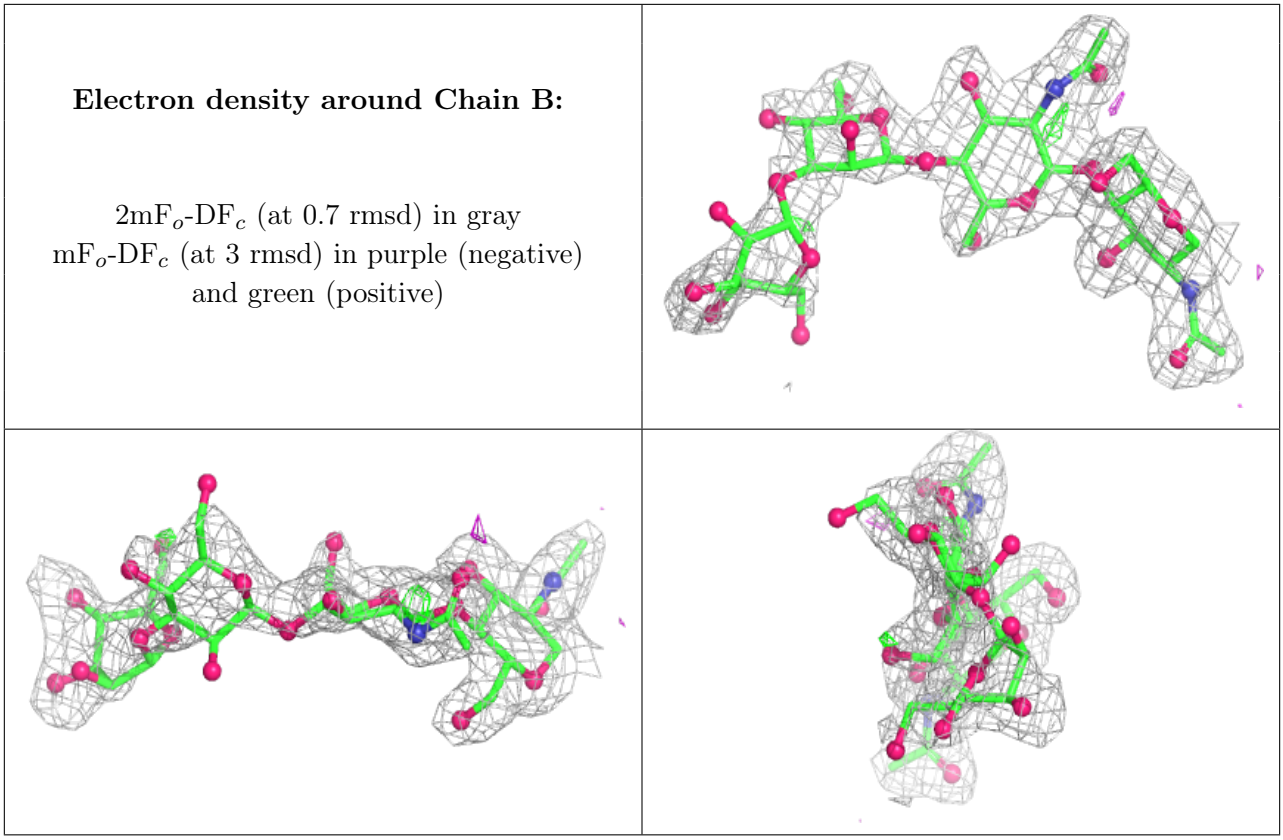
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	B	4	11/12	0.52	0.26	70,93,98,99	0
2	BMA	B	3	11/12	0.77	0.22	68,79,91,91	0
2	NAG	B	2	14/15	0.92	0.17	29,36,57,67	14
2	NAG	B	1	14/15	0.97	0.10	17,26,29,31	0

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

Electron density around Chain B:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GLN	A	606	10/10	0.59	0.26	61,64,71,87	10
6	GLN	A	618	10/10	0.59	0.44	28,40,44,48	10
9	PGE	A	643	10/10	0.60	0.34	53,60,64,70	10
6	GLN	A	668	10/10	0.67	0.25	50,61,70,79	10
6	GLN	A	612[B]	10/10	0.68	0.39	30,43,46,51	10
6	GLN	A	612[A]	10/10	0.68	0.39	32,42,46,52	10
6	GLN	A	676	10/10	0.72	0.32	41,63,74,78	10
6	GLN	A	672	10/10	0.72	0.20	63,74,78,81	0
10	GOL	A	650	6/6	0.74	0.25	33,37,44,46	6
6	GLN	A	671[A]	10/10	0.76	0.27	20,36,40,42	10
6	GLN	A	671[B]	10/10	0.76	0.27	25,34,39,39	10
6	GLN	A	669[A]	10/10	0.77	0.24	27,42,53,54	10
6	GLN	A	669[B]	10/10	0.77	0.24	33,43,51,53	10
6	GLN	A	611[A]	10/10	0.77	0.34	20,24,34,36	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GLN	A	611[B]	10/10	0.77	0.34	24,32,35,36	10
8	EDO	A	634	4/4	0.78	0.20	38,47,50,54	4
8	EDO	A	635	4/4	0.78	0.23	73,76,77,80	0
9	PGE	A	641[A]	10/10	0.79	0.28	36,39,44,45	10
9	PGE	A	641[B]	10/10	0.79	0.28	31,37,42,44	10
6	GLN	A	615[A]	10/10	0.79	0.28	38,48,59,62	10
6	GLN	A	615[B]	10/10	0.79	0.28	39,49,59,63	10
6	GLN	A	616[B]	10/10	0.80	0.28	50,59,66,70	10
6	GLN	A	605	10/10	0.80	0.24	37,44,55,72	10
6	GLN	A	616[A]	10/10	0.80	0.28	54,58,67,70	10
8	EDO	A	633	4/4	0.81	0.19	30,39,46,56	4
6	GLN	A	608[B]	10/10	0.82	0.22	36,46,50,51	10
6	GLN	A	610	10/10	0.82	0.24	23,31,36,40	10
8	EDO	A	621	4/4	0.82	0.16	43,49,56,66	4
5	PG4	A	603	13/13	0.82	0.21	32,42,61,73	13
6	GLN	A	608[A]	10/10	0.82	0.22	15,45,51,53	10
6	GLN	A	665	10/10	0.83	0.28	18,32,45,48	10
8	EDO	A	625	4/4	0.83	0.17	49,50,51,55	0
3	1PE	A	601	10/16	0.83	0.20	32,46,54,54	10
9	PGE	A	639	10/10	0.84	0.22	19,32,41,46	10
6	GLN	A	658	10/10	0.84	0.25	22,34,41,48	10
6	GLN	A	666	10/10	0.84	0.20	27,44,53,61	10
6	GLN	A	675	10/10	0.84	0.32	45,59,72,74	10
8	EDO	A	636	4/4	0.84	0.18	45,49,54,63	0
10	GOL	A	652	6/6	0.84	0.23	20,29,38,40	6
9	PGE	A	640	10/10	0.85	0.18	32,39,44,47	10
10	GOL	A	649	6/6	0.85	0.20	46,46,48,58	6
6	GLN	A	613	10/10	0.85	0.23	25,36,41,42	10
6	GLN	A	607	10/10	0.85	0.25	24,34,42,56	10
10	GOL	A	656	6/6	0.85	0.23	36,42,57,59	6
6	GLN	A	667	10/10	0.86	0.21	28,39,45,47	10
6	GLN	A	673	10/10	0.86	0.24	36,54,59,69	10
6	GLN	A	674	10/10	0.86	0.28	41,58,67,84	10
6	GLN	A	661	10/10	0.86	0.23	30,38,44,45	10
6	GLN	A	609	10/10	0.88	0.17	40,53,58,63	10
9	PGE	A	644	10/10	0.88	0.17	48,57,70,73	10
10	GOL	A	645	6/6	0.88	0.21	24,30,42,51	6
8	EDO	A	626	4/4	0.88	0.14	50,53,58,64	0
5	PG4	A	660[B]	13/13	0.88	0.27	28,36,46,48	13
10	GOL	A	651	6/6	0.88	0.28	15,28,33,40	6
4	P6G	A	602	19/19	0.88	0.14	33,54,72,77	19
5	PG4	A	660[A]	13/13	0.88	0.27	31,37,47,48	13

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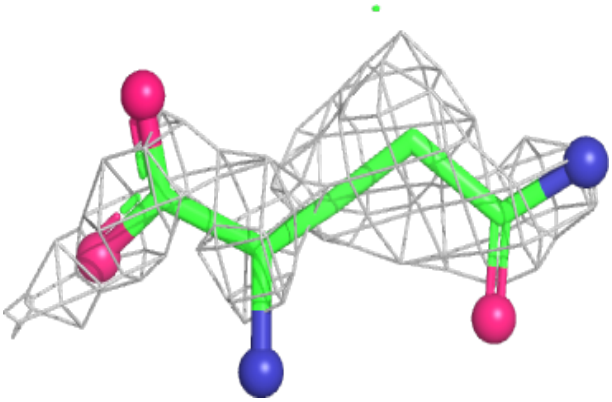
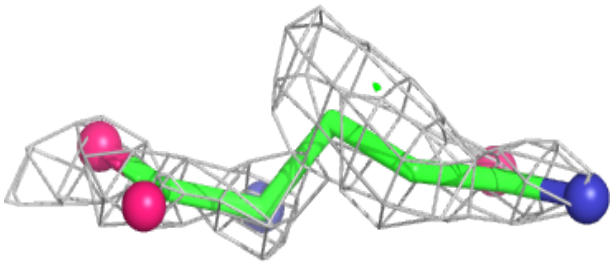
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PGE	A	642[B]	10/10	0.89	0.21	32,33,38,38	10
6	GLN	A	617[A]	10/10	0.89	0.30	28,35,37,39	10
6	GLN	A	617[B]	10/10	0.89	0.30	28,35,43,43	10
3	1PE	A	604	16/16	0.89	0.24	21,32,44,45	16
6	GLN	A	670	10/10	0.89	0.19	32,49,61,62	10
8	EDO	A	629	4/4	0.89	0.21	63,65,67,84	4
8	EDO	A	630	4/4	0.89	0.16	43,52,53,54	0
6	GLN	A	614	10/10	0.89	0.21	32,43,59,60	10
9	PGE	A	642[A]	10/10	0.89	0.21	29,35,37,38	10
10	GOL	A	657	6/6	0.89	0.17	26,29,55,60	6
8	EDO	A	620	4/4	0.90	0.19	43,44,51,59	4
10	GOL	A	648	6/6	0.90	0.14	43,47,52,61	6
8	EDO	A	631	4/4	0.91	0.16	29,37,49,51	0
8	EDO	A	632	4/4	0.91	0.14	37,39,44,56	0
10	GOL	A	655	6/6	0.92	0.14	30,47,58,61	6
8	EDO	A	622	4/4	0.92	0.12	51,54,59,59	0
8	EDO	A	628	4/4	0.92	0.31	18,20,32,32	4
9	PGE	A	638	10/10	0.93	0.12	23,39,51,55	10
11	CIT	A	659	13/13	0.93	0.12	18,27,36,38	13
8	EDO	A	624	4/4	0.94	0.12	25,26,38,40	4
10	GOL	A	653	6/6	0.94	0.19	26,30,36,41	6
8	EDO	A	623	4/4	0.94	0.12	29,30,38,48	4
8	EDO	A	627	4/4	0.95	0.12	23,27,34,41	4
10	GOL	A	646	6/6	0.95	0.19	13,21,26,42	6
10	GOL	A	647	6/6	0.95	0.12	26,36,44,48	6
10	GOL	A	654	6/6	0.95	0.17	15,38,41,50	6
9	PGE	A	637	7/10	0.97	0.08	20,20,25,39	0
12	NA	A	662	1/1	0.97	0.07	19,19,19,19	0
7	PO4	A	619[A]	5/5	0.99	0.09	14,15,17,20	5
7	PO4	A	619[B]	5/5	0.99	0.09	12,13,17,20	5
13	FE	A	663	1/1	1.00	0.03	13,13,13,13	0
13	FE	A	664	1/1	1.00	0.06	10,10,10,10	1

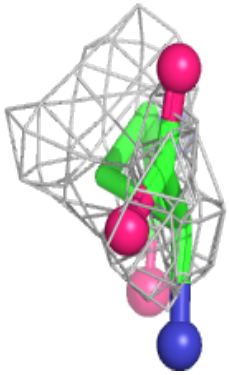
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GLN A 606:

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

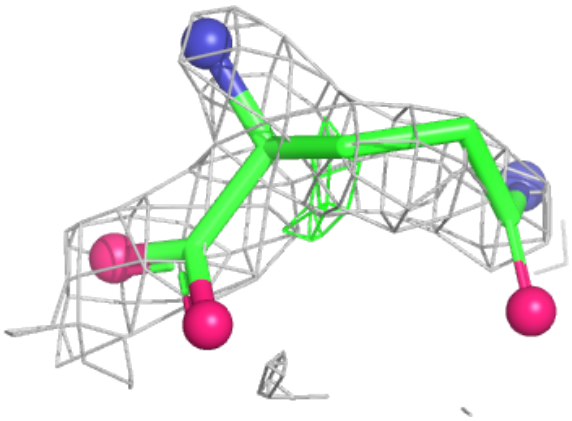


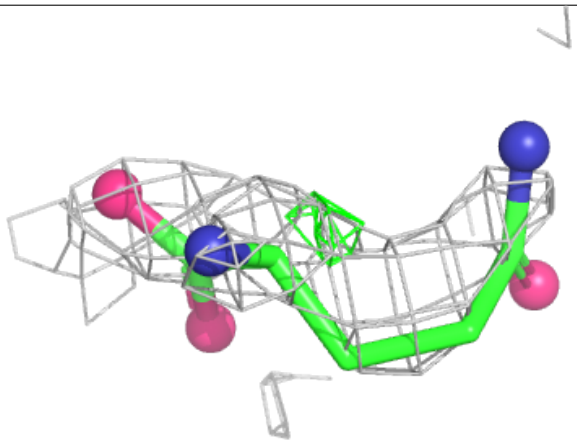


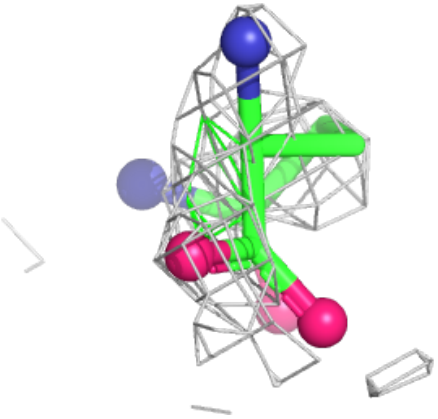


Electron density around GLN A 618:

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

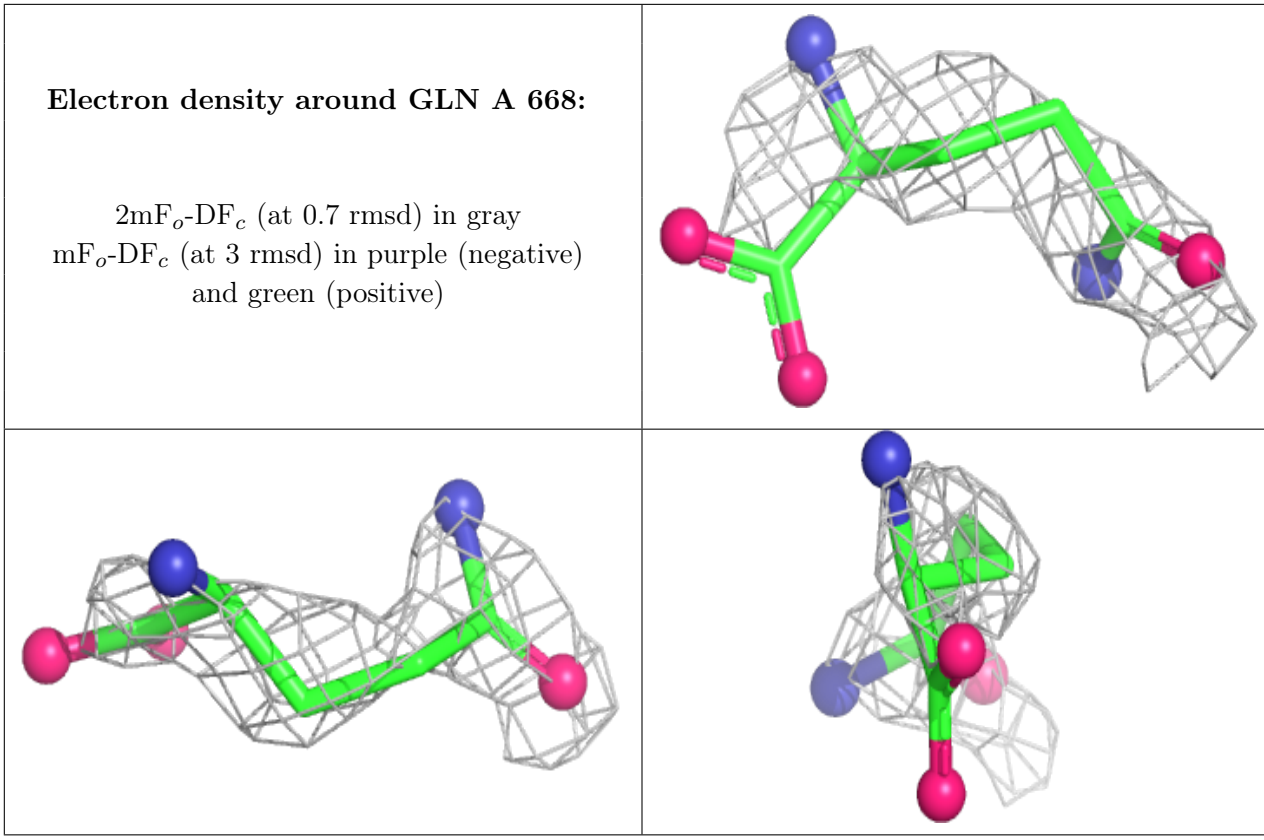






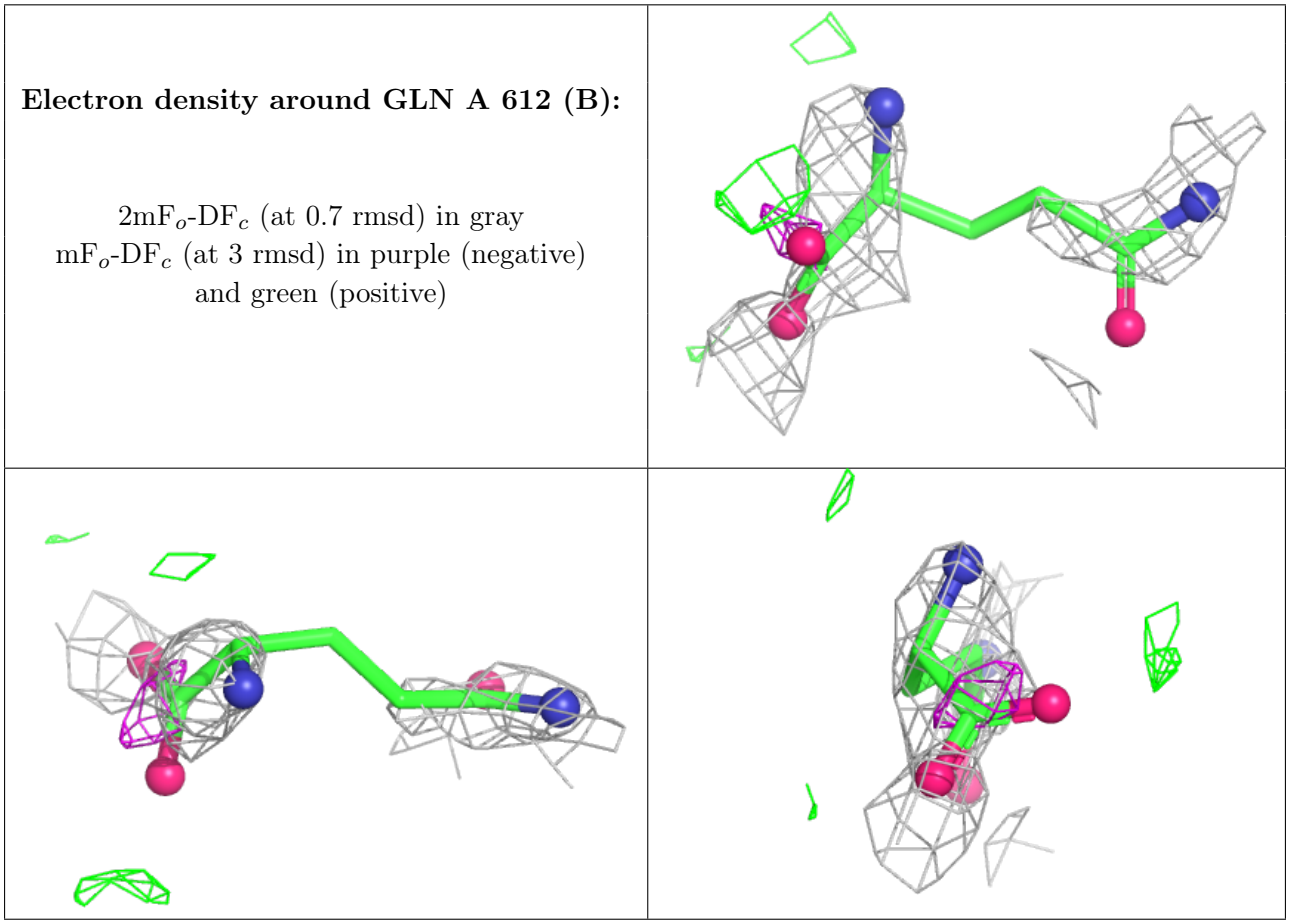
Electron density around GLN A 668:

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



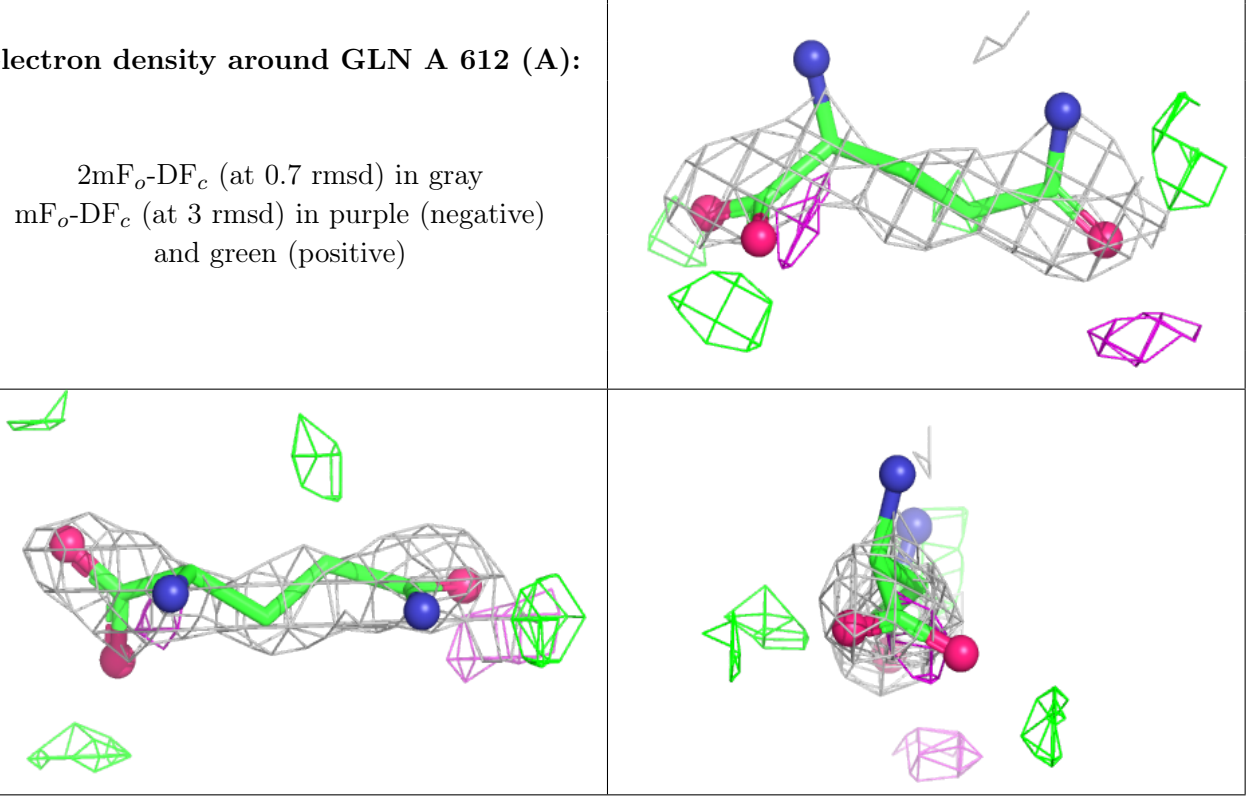
Electron density around GLN A 612 (B):

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



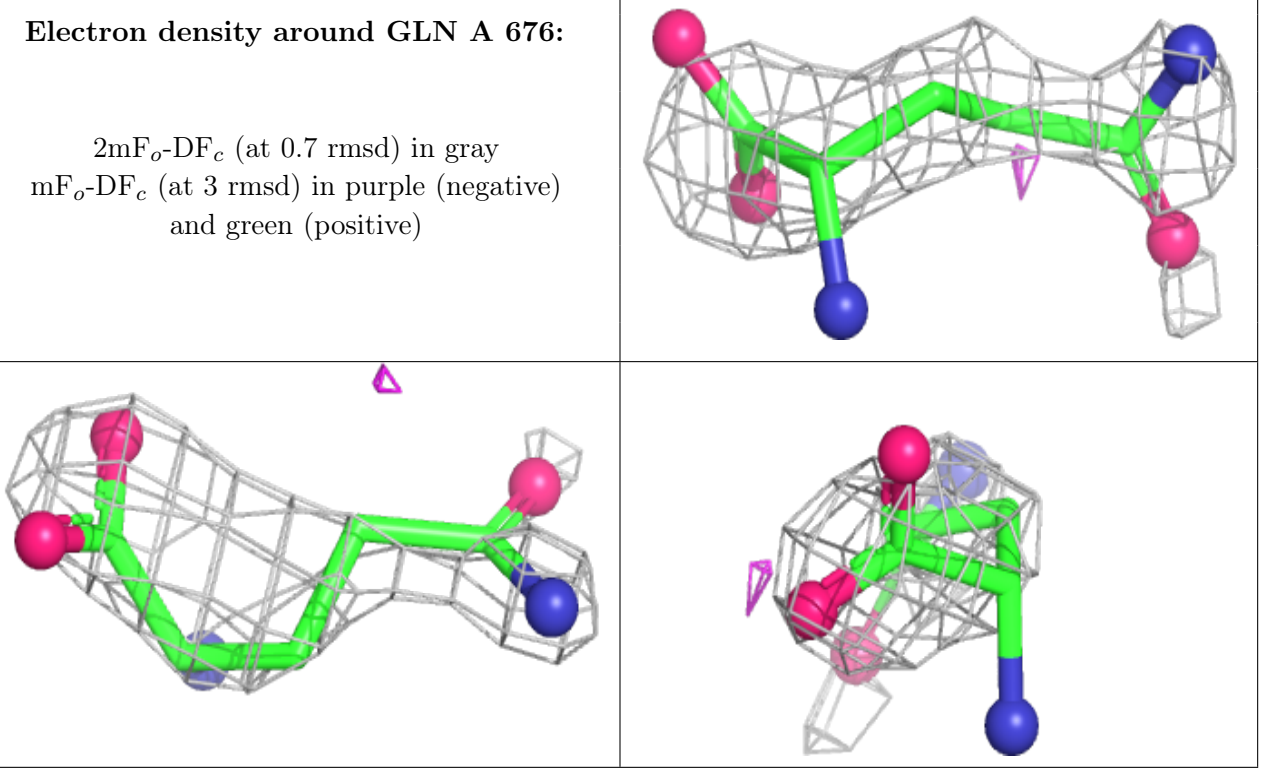
Electron density around GLN A 612 (A):

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



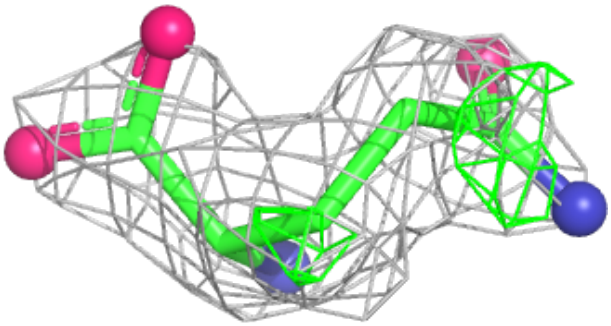
Electron density around GLN A 676:

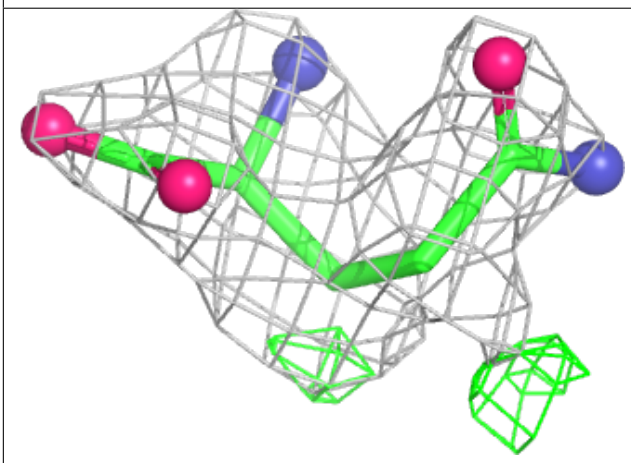
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

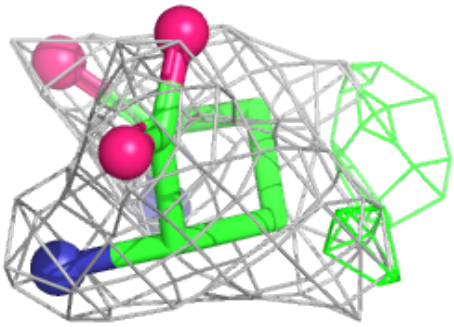


Electron density around GLN A 672:

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

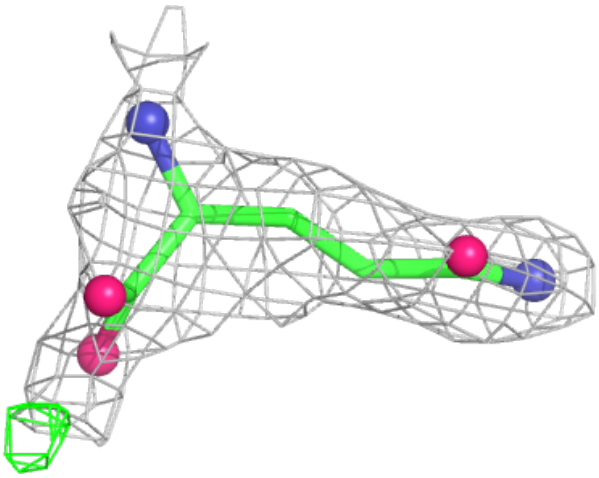


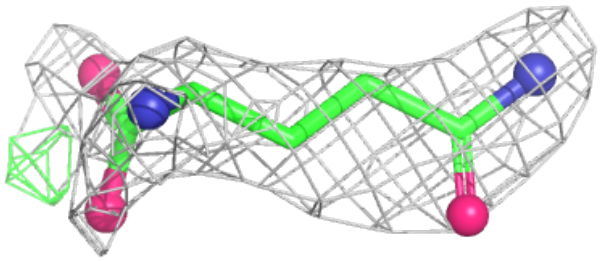


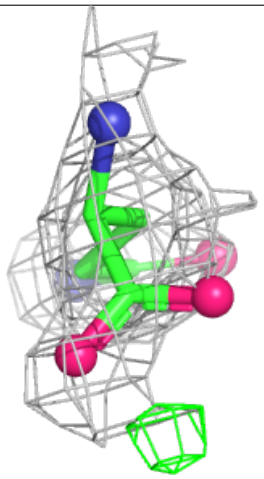


Electron density around GLN A 671 (A):

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

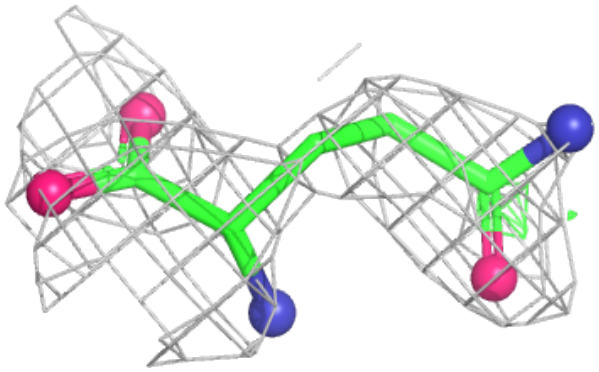


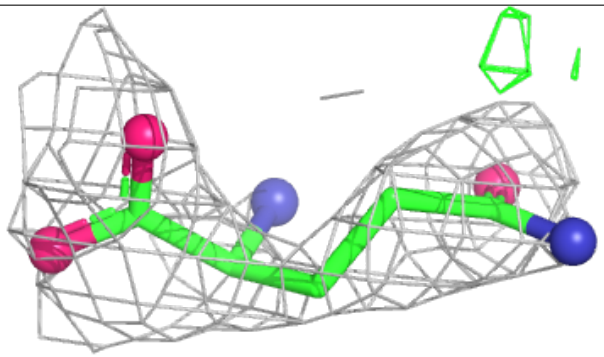


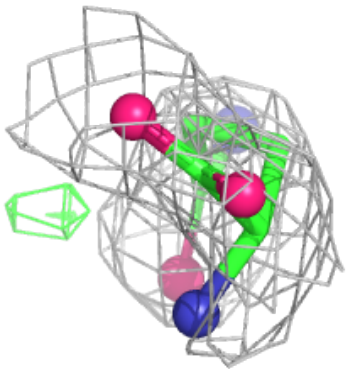


Electron density around GLN A 671 (B):

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

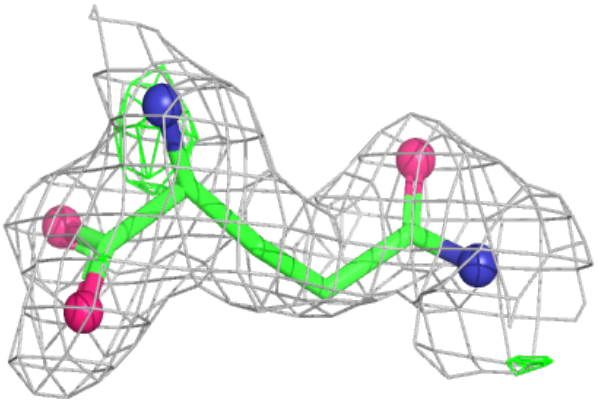


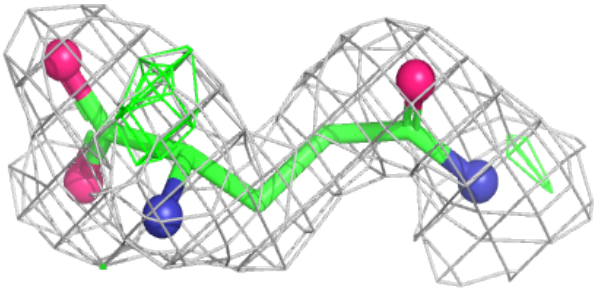


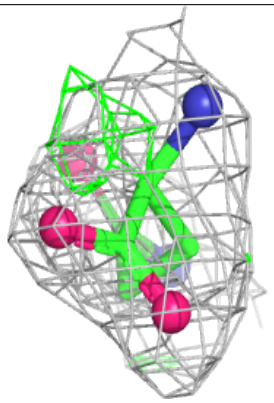


Electron density around GLN A 669 (A):

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

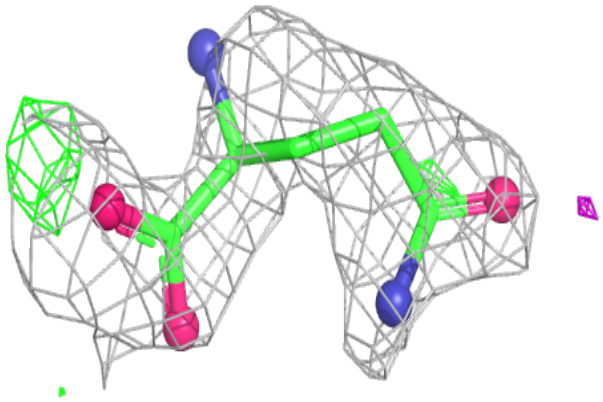


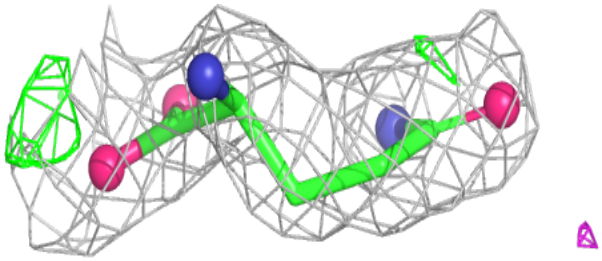


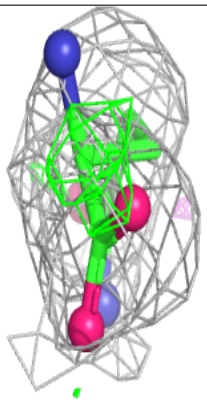


Electron density around GLN A 669 (B):

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

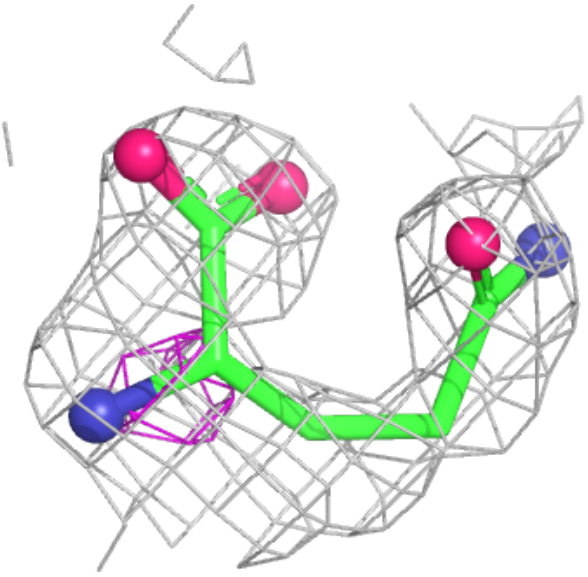


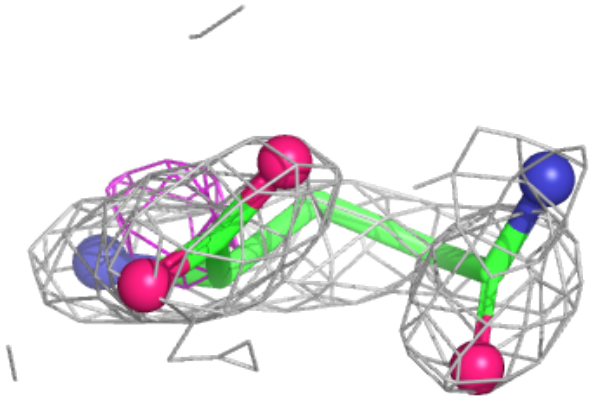


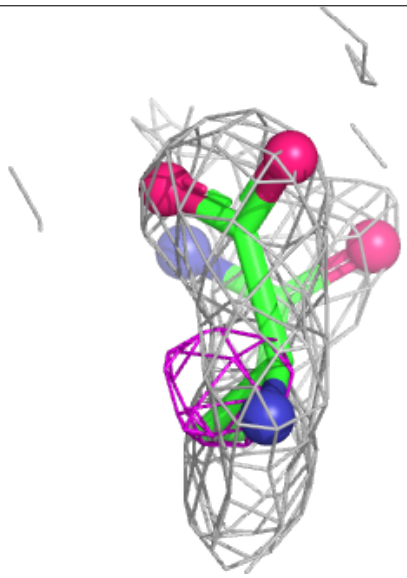


Electron density around GLN A 611 (A):

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

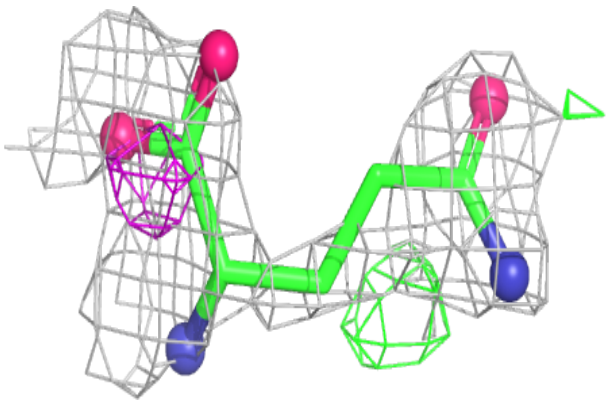


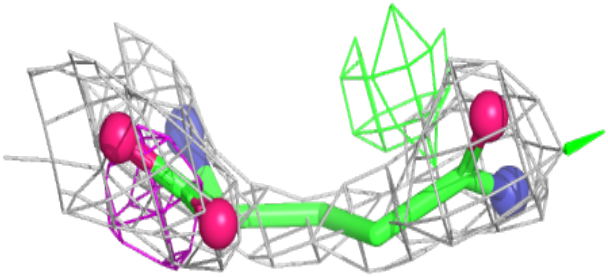


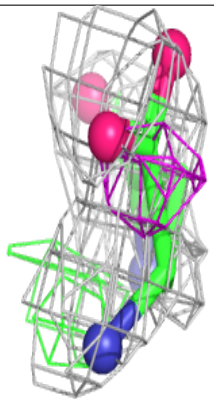


Electron density around GLN A 611 (B):

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

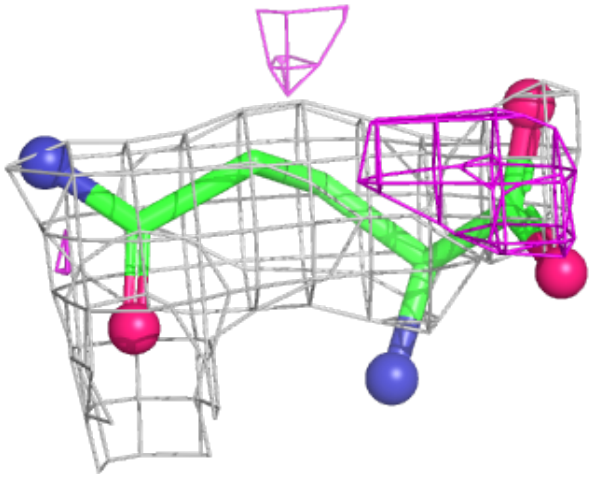


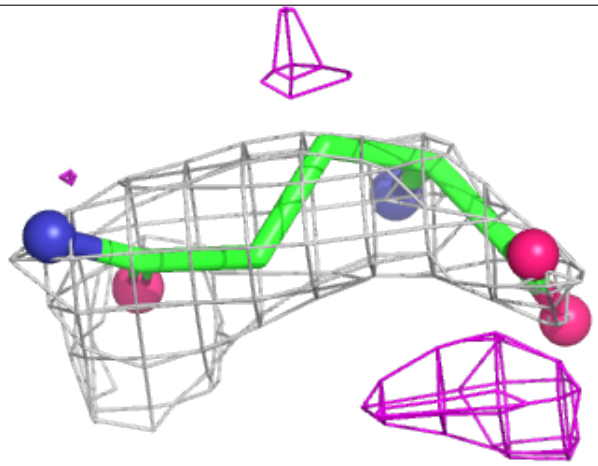


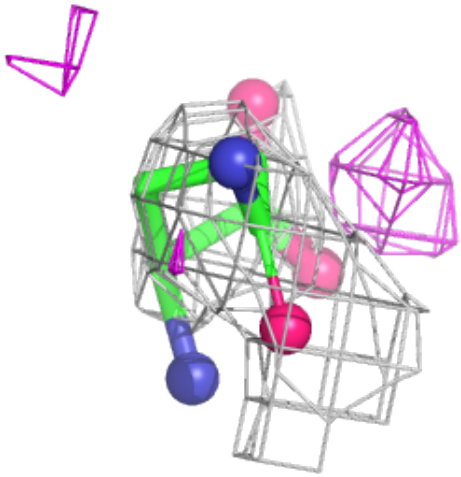


Electron density around GLN A 615 (A):

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

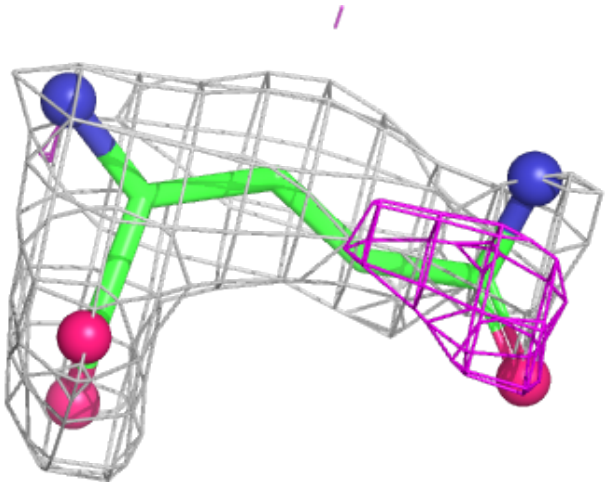


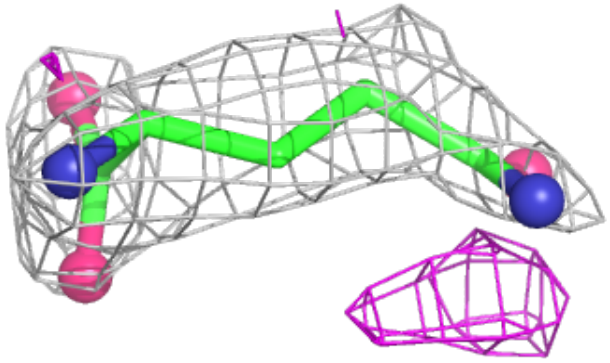


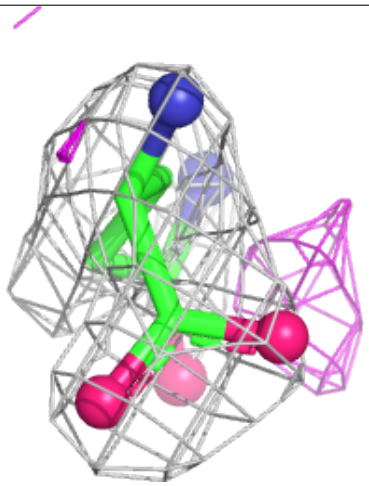


Electron density around GLN A 615 (B):

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

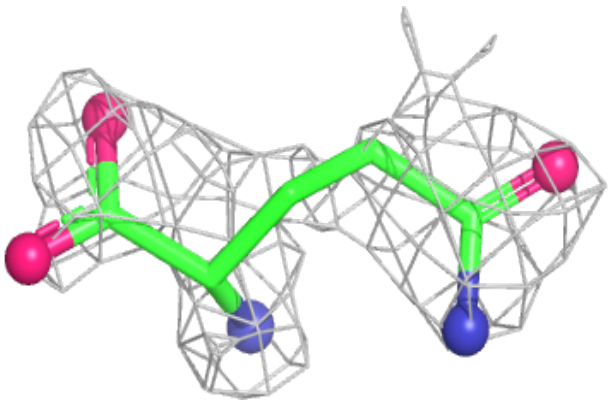


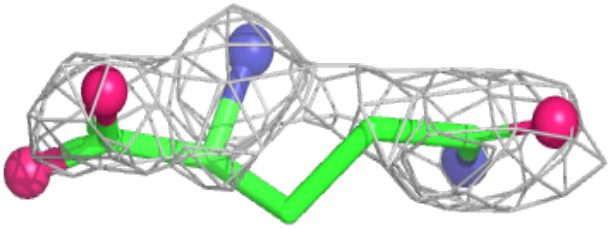


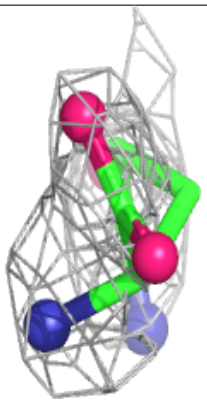


Electron density around GLN A 616 (B):

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

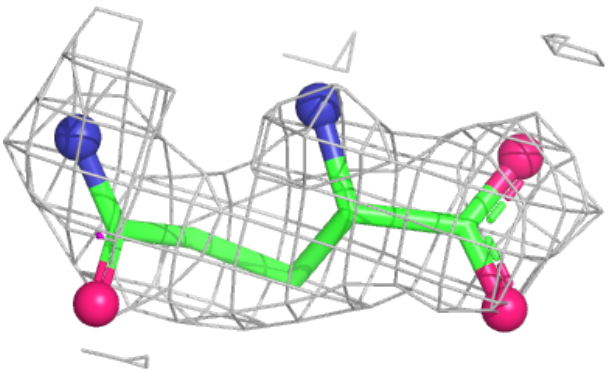


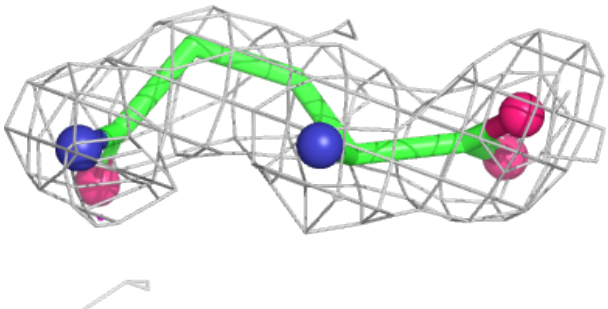


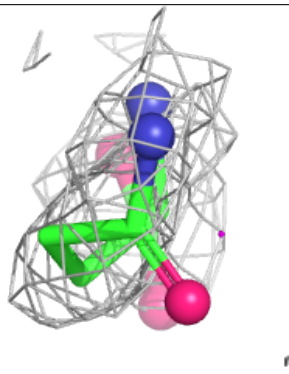


Electron density around GLN A 605:

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

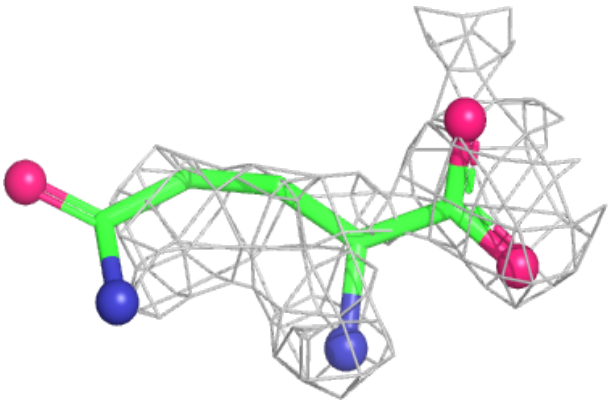


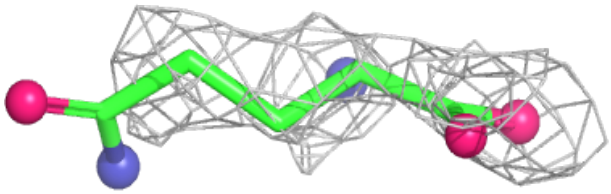


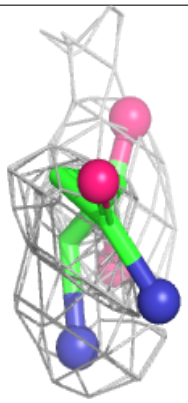


Electron density around GLN A 616 (A):

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

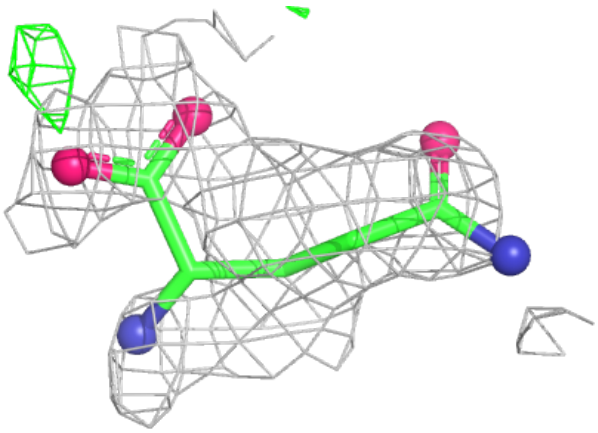


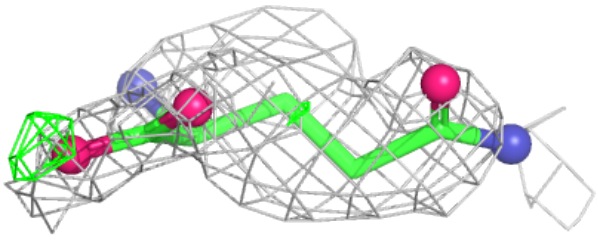


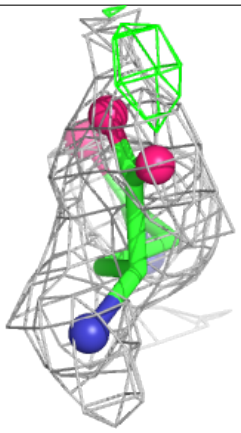


Electron density around GLN A 608 (B):

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

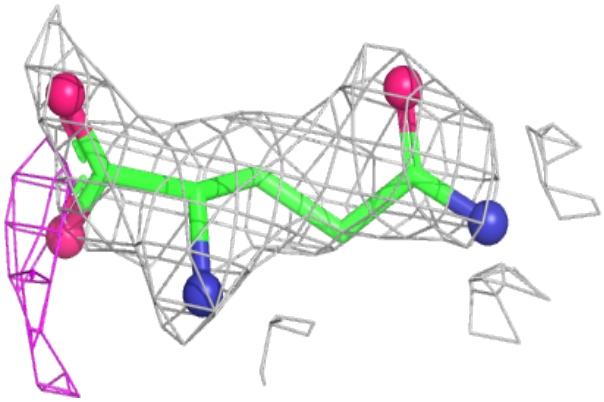


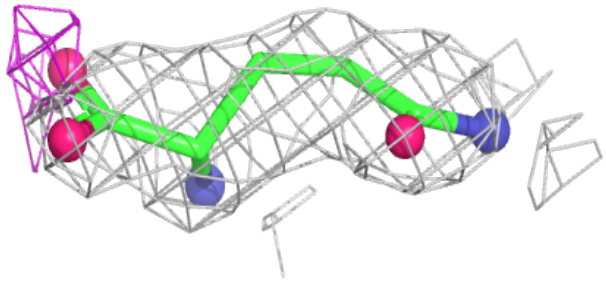


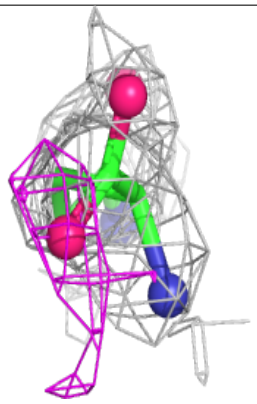


Electron density around GLN A 610:

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

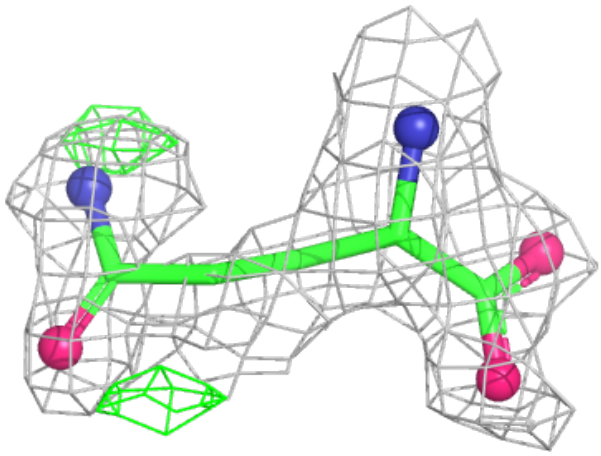


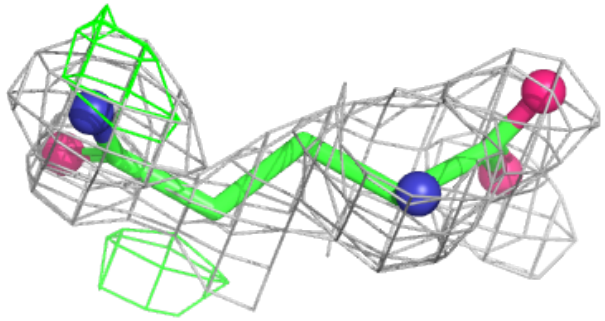


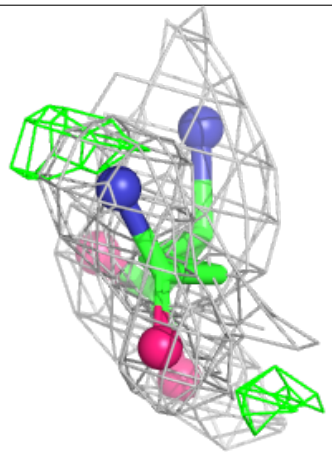


Electron density around GLN A 608 (A):

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

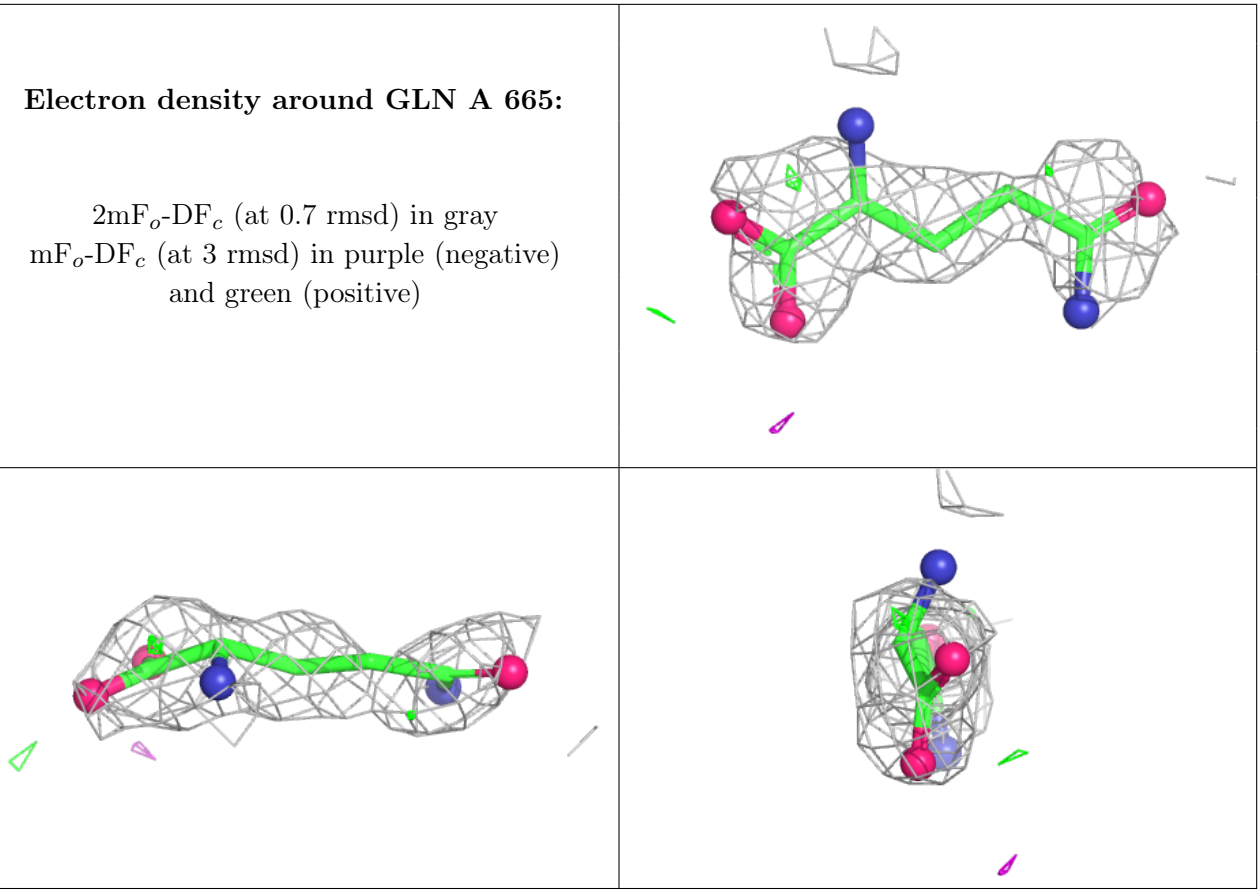






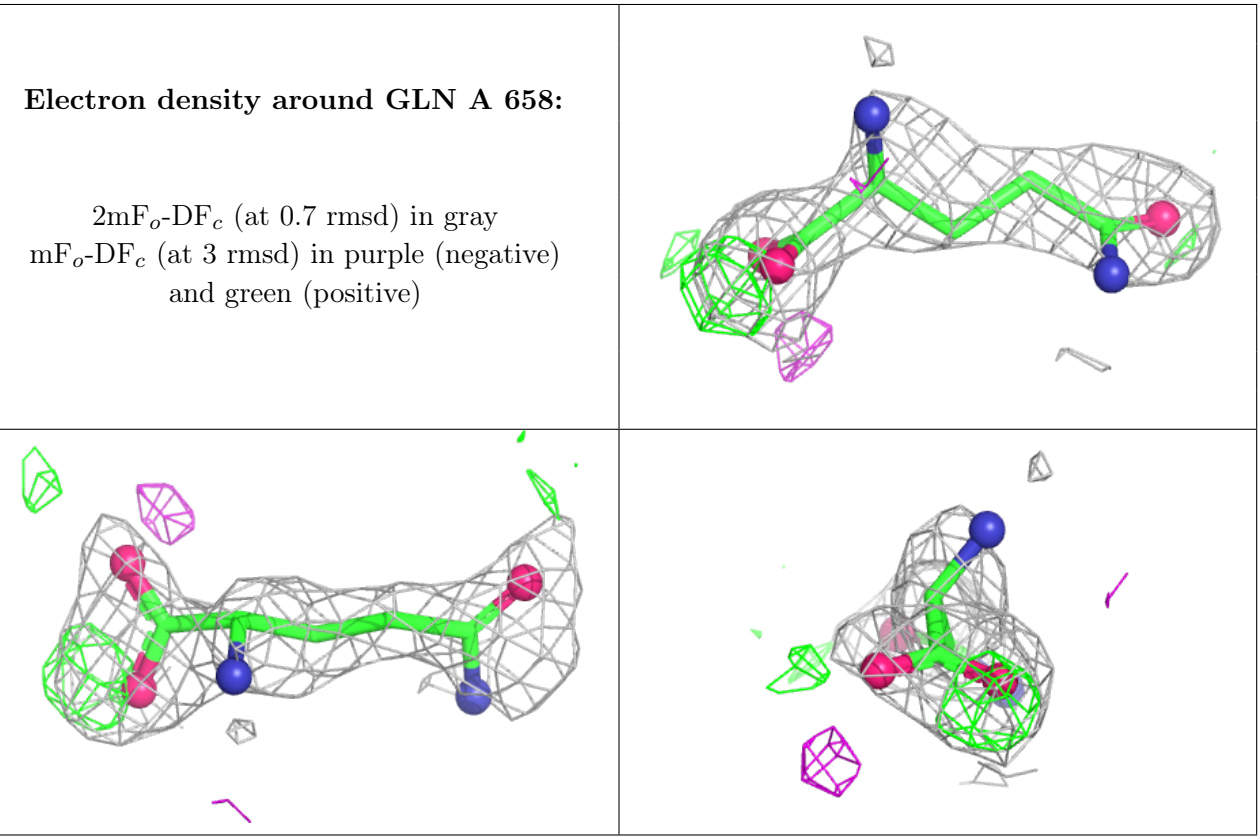
Electron density around GLN A 665:

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



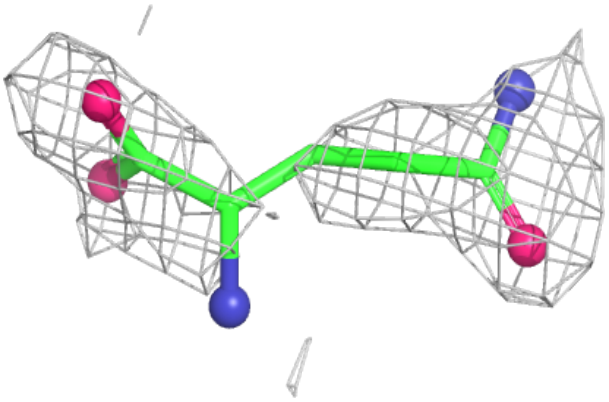
Electron density around GLN A 658:

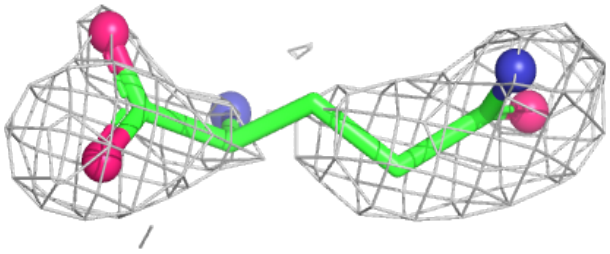
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

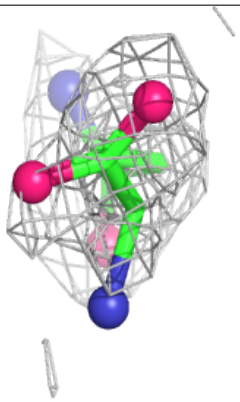


Electron density around GLN A 666:

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

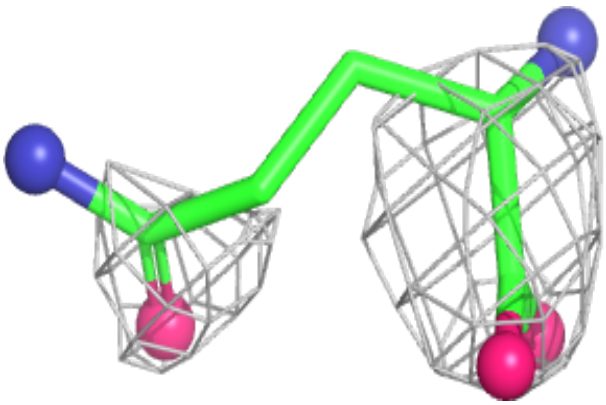


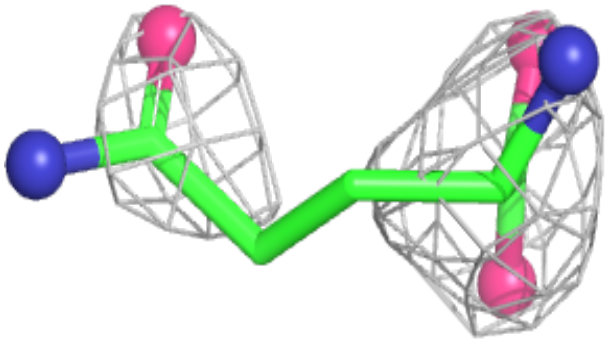


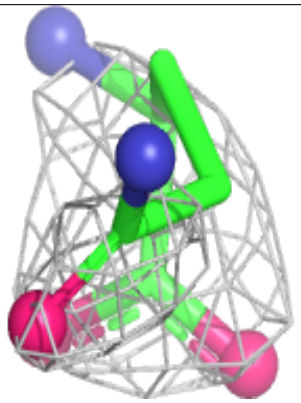


Electron density around GLN A 675:

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

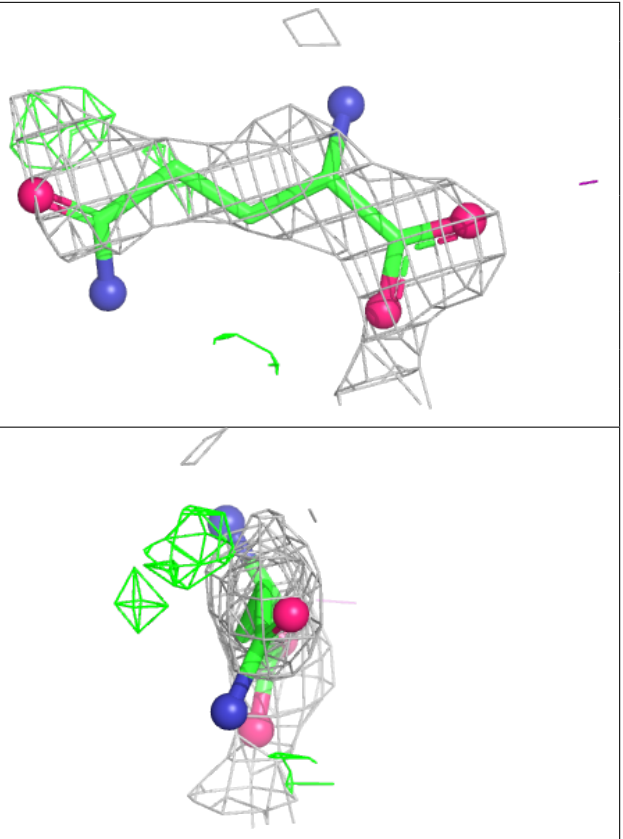


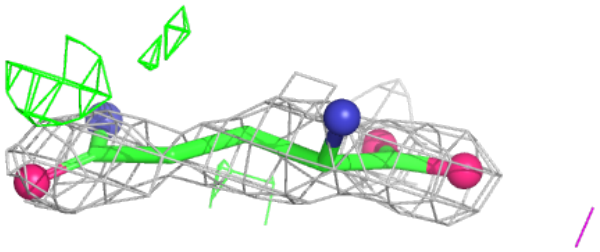




Electron density around GLN A 613:

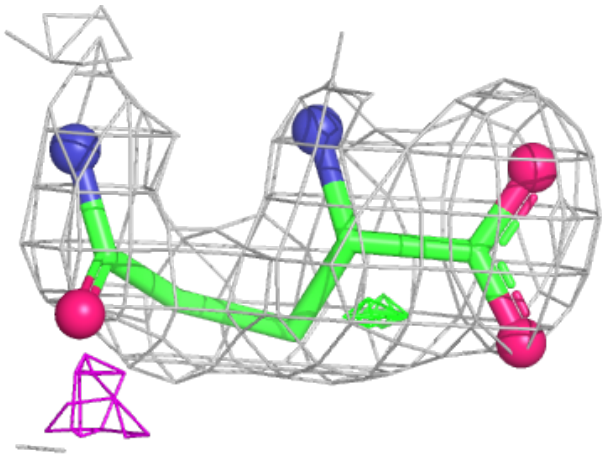
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

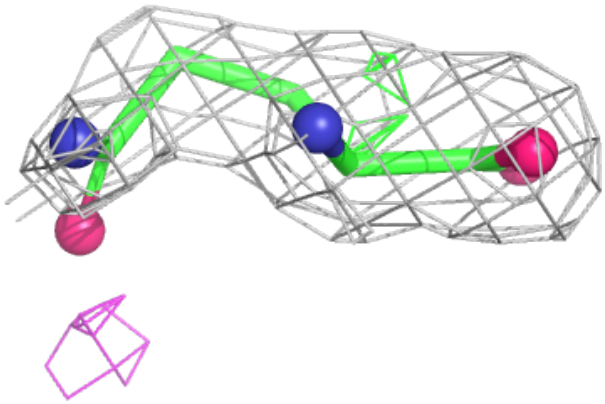


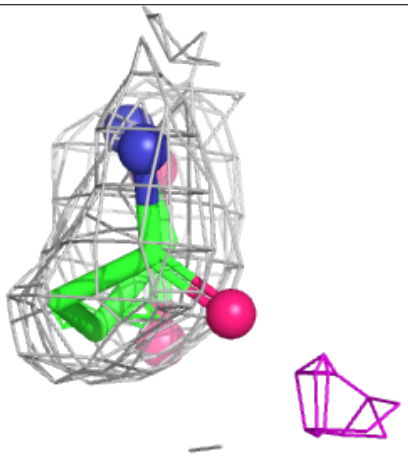


Electron density around GLN A 607:

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

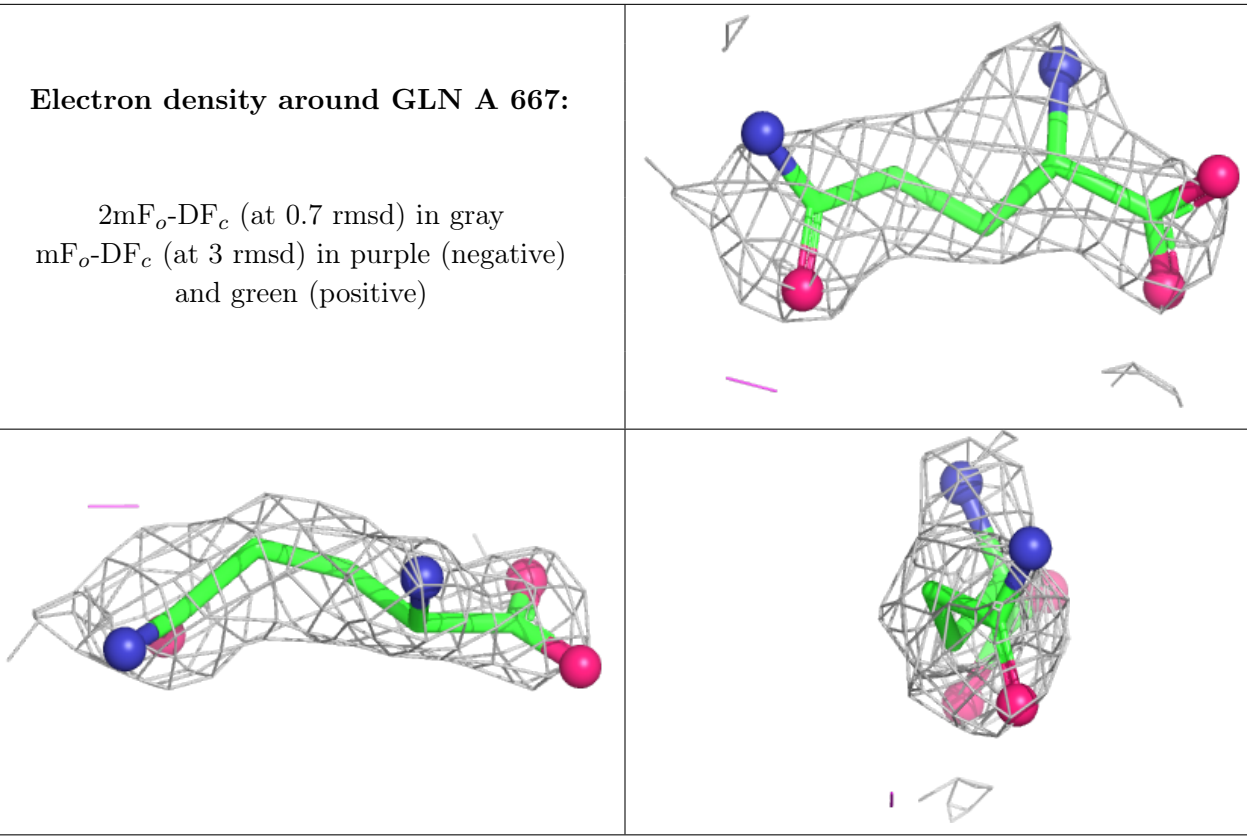






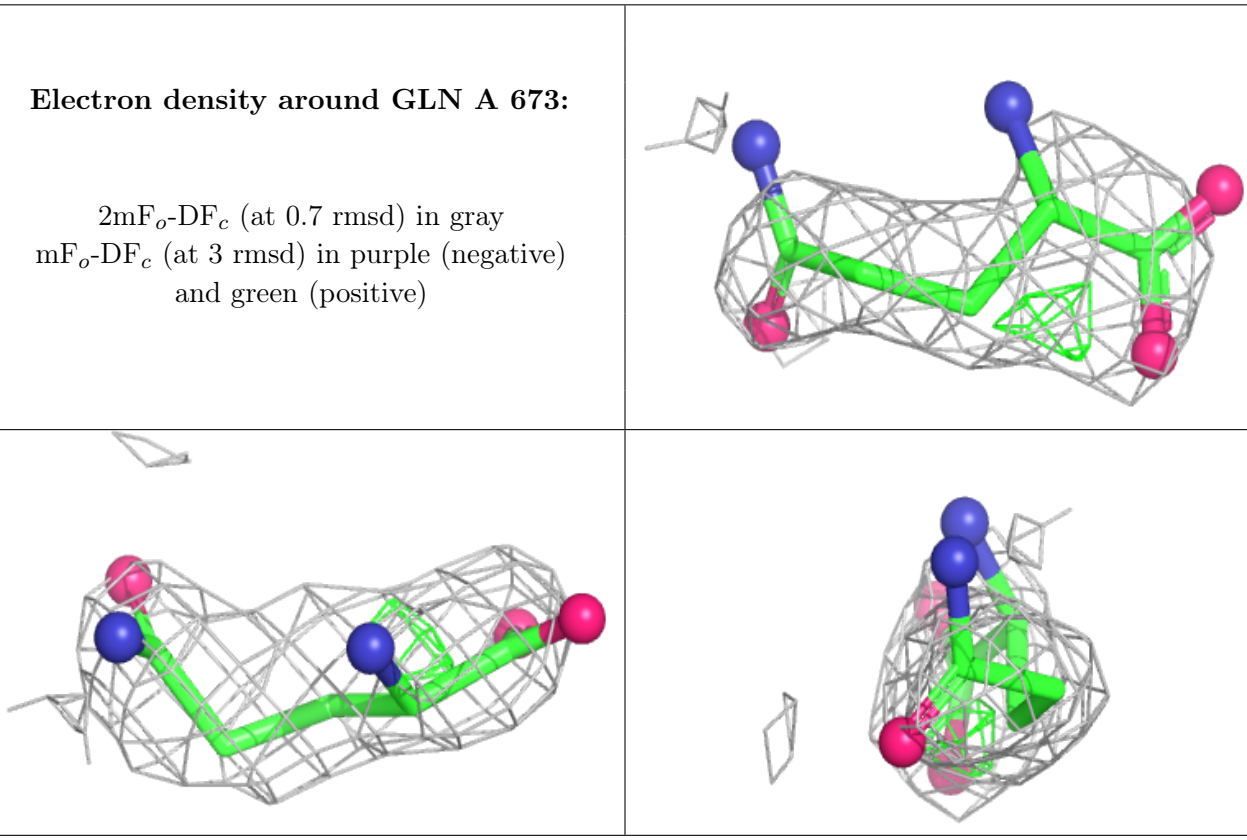
Electron density around GLN A 667:

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



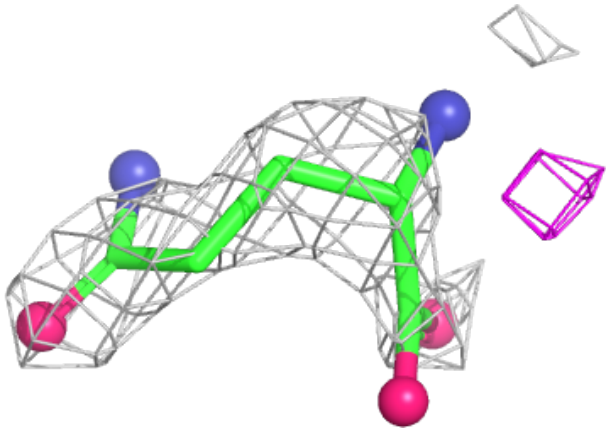
Electron density around GLN A 673:

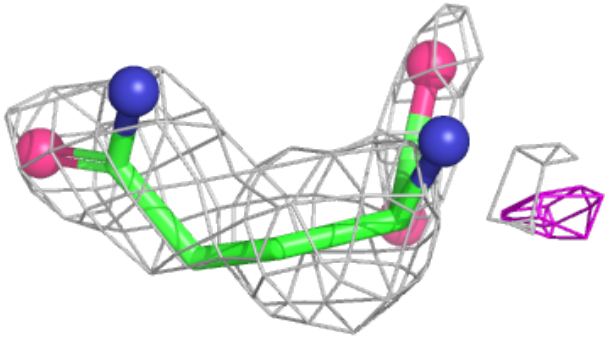
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

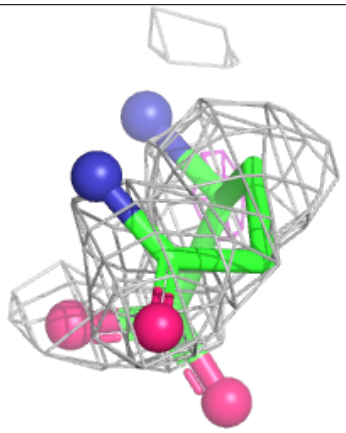


Electron density around GLN A 674:

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

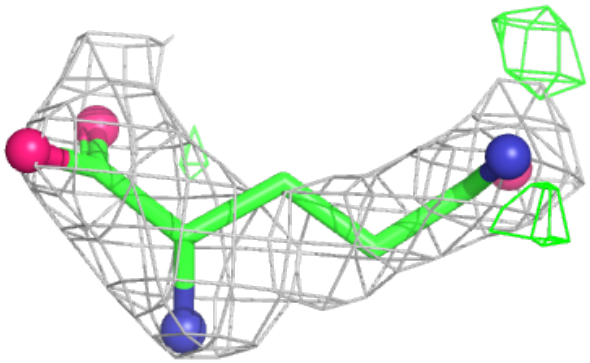


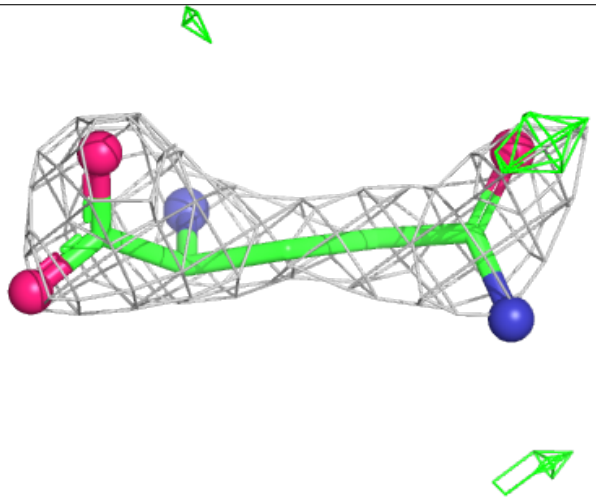


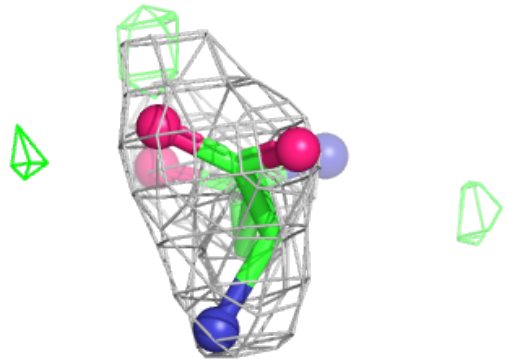


Electron density around GLN A 661:

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

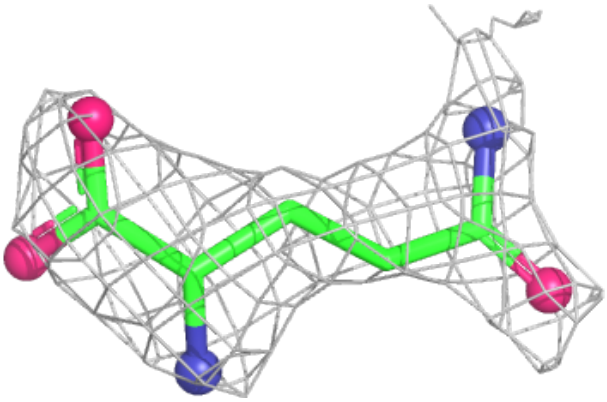


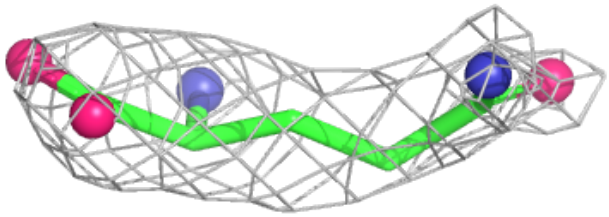


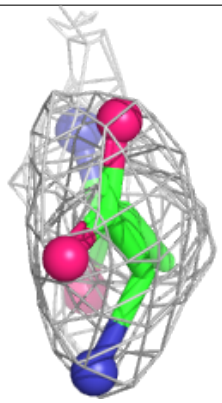


Electron density around GLN A 609:

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

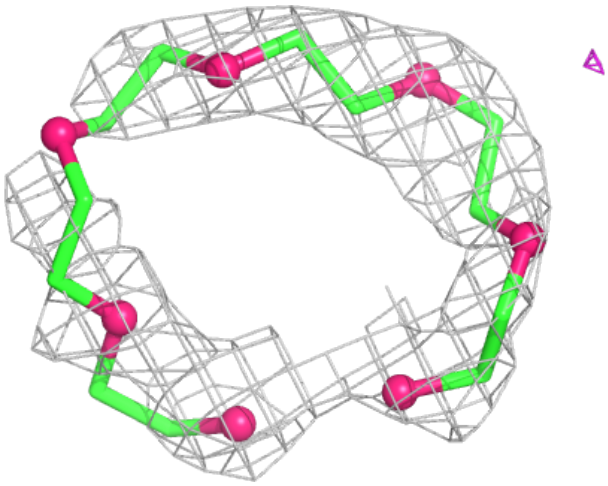


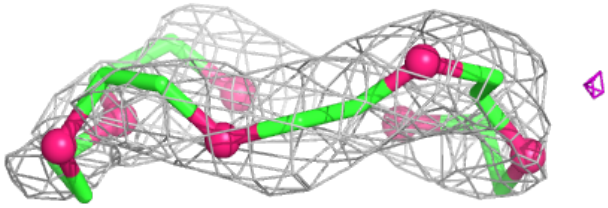


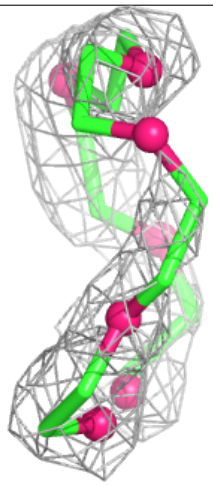


Electron density around P6G A 602:

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

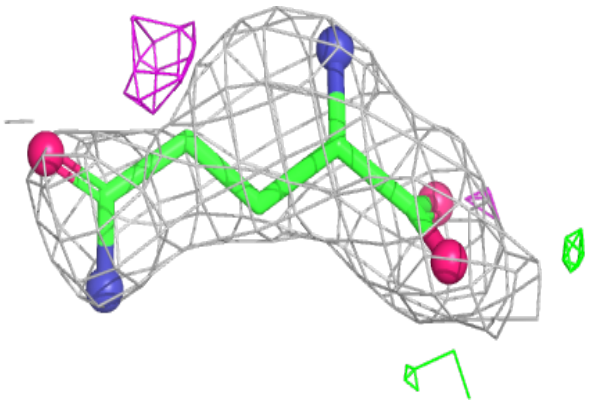


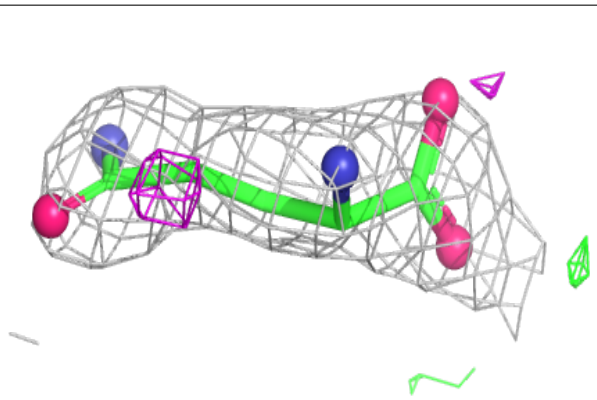


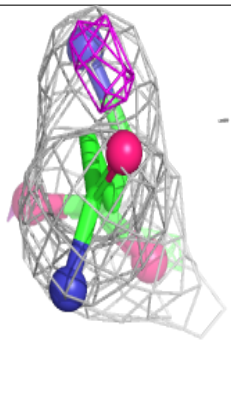


Electron density around GLN A 617 (A):

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

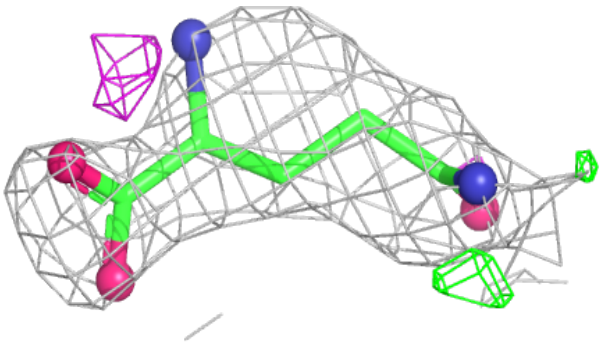


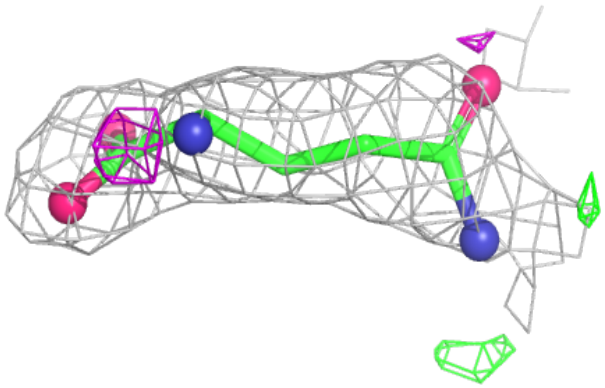


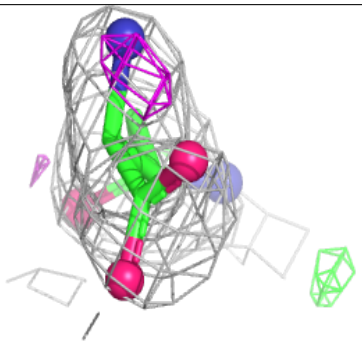


Electron density around GLN A 617 (B):

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

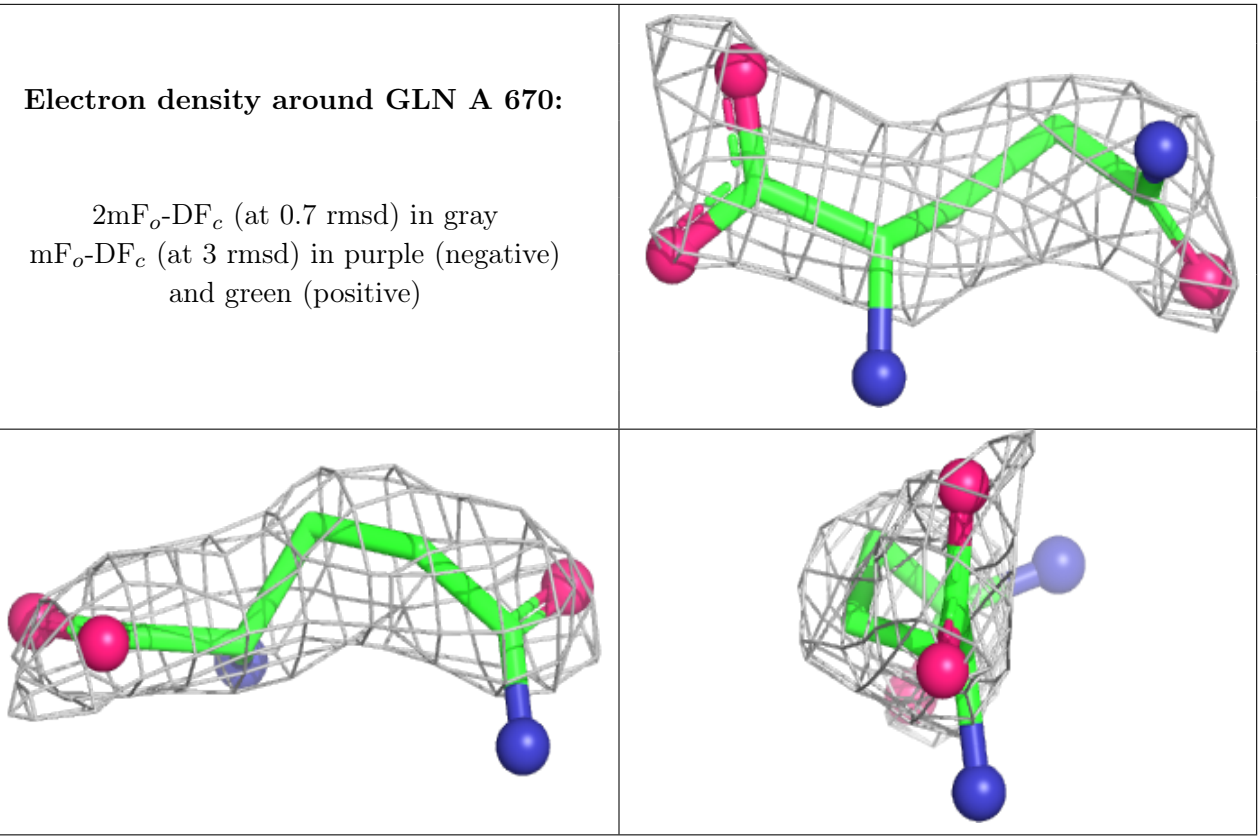






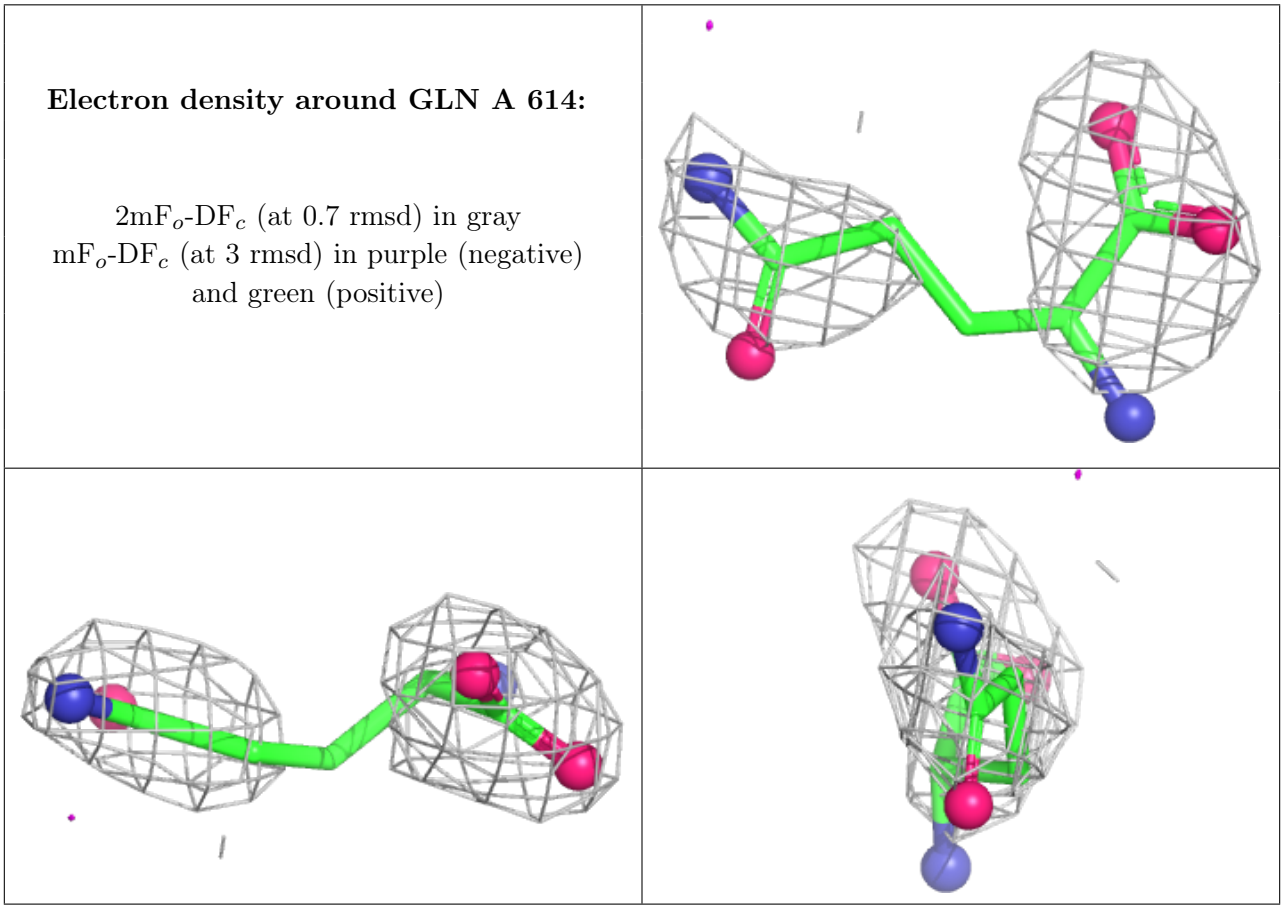
Electron density around GLN A 670:

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



Electron density around GLN A 614:

$2mF_o$-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.