



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 12:09 PM UTC

PDB ID : 2ABM / pdb_00002abm
Title : Crystal Structure of Aquaporin Z Tetramer Reveals both Open and Closed Water-conducting Channels
Authors : Jiang, J.; Daniels, B.V.; Fu, D.
Deposited on : 2005-07-15
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

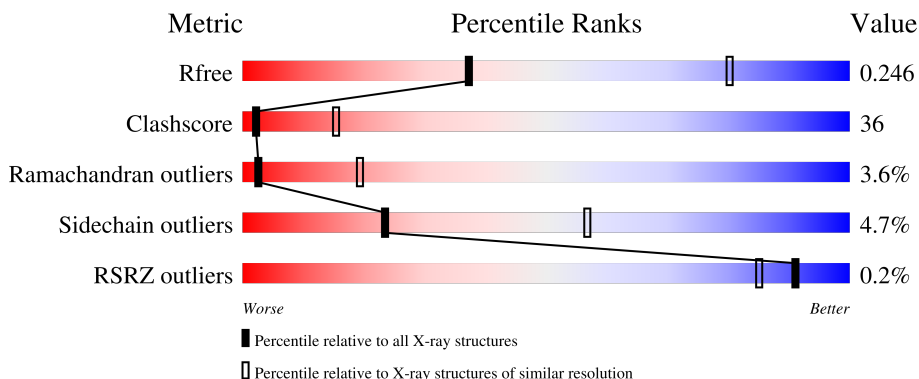
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	
1	E	231	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	

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
2	BGL	A	609	X	-	-	-
2	BGL	E	608	X	-	-	-
3	POQ	A	600	X	-	-	-
5	PO4	B	626	-	-	X	-
5	PO4	F	636	-	-	X	-
6	3PG	C	627	X	X	-	-
6	3PG	G	637	X	X	-	-
7	AGA	C	629	-	X	-	-
7	AGA	G	639	-	X	-	-

2 Entry composition

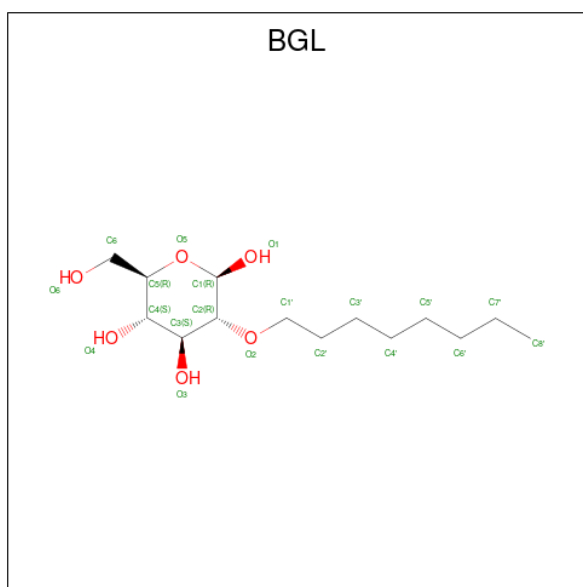
There are 8 unique types of molecules in this entry. The entry contains 13946 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aquaporin Z.

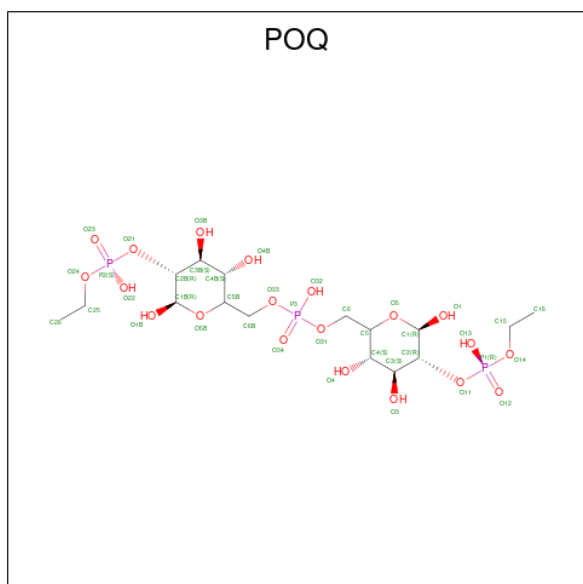
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1643	1095	265	278	5	0	0	0
1	B	227	1643	1095	265	278	5	0	0	0
1	C	227	1643	1095	265	278	5	0	0	0
1	D	227	1643	1095	265	278	5	0	0	0
1	E	227	1643	1095	265	278	5	0	0	0
1	F	227	1643	1095	265	278	5	0	0	0
1	G	227	1643	1095	265	278	5	0	0	0
1	H	227	1643	1095	265	278	5	0	0	0

- Molecule 2 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



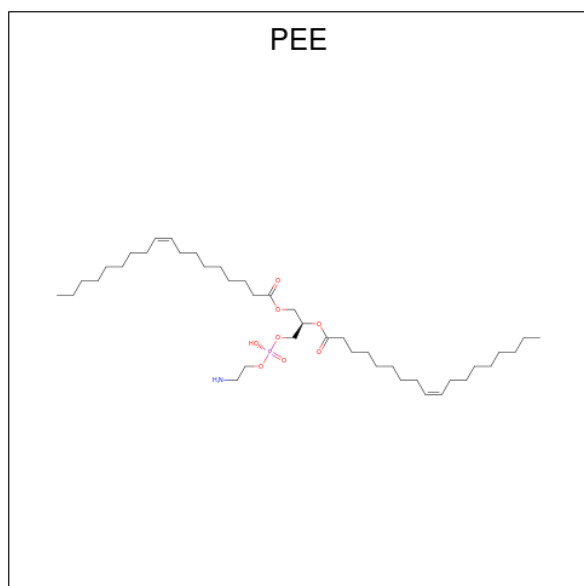
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			16	11 5		
2	B	1	Total	C O	0	0
			18	12 6		
2	B	1	Total	C O	0	0
			18	12 6		
2	E	1	Total	C O	0	0
			16	11 5		

- Molecule 3 is BIS(((3S,4S,5R,6R)-5-(ETHYL(PHOSPHORYLOXY))-3,4,6-TRIHYDROXY-TETRAHYDRO-2H-PYRAN-2-YL)METHYL) HYDROGEN PHOSPHATE (CCD ID: POQ) (formula: C₁₆H₃₃O₂₀P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	39	16	20	3	0	0

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



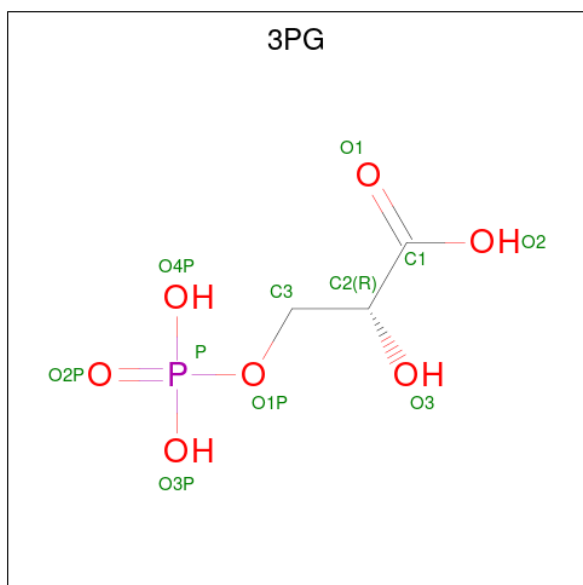
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			9	9		
4	B	1	Total	C	0	0
			14	14		
4	B	1	Total	C	0	0
			10	10		
4	E	1	Total	C	0	0
			16	16		
4	F	1	Total	C	0	0
			14	14		
4	F	1	Total	C	0	0
			10	10		
4	G	1	Total	C	0	0
			9	9		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



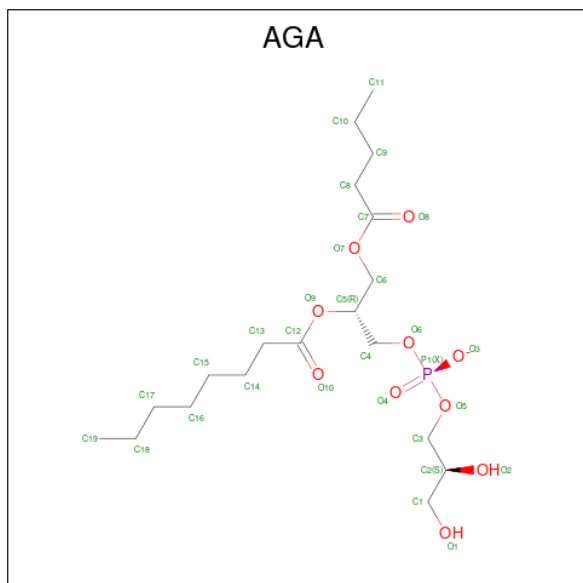
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	G	1	Total O P 5 4 1	0	0

- Molecule 6 is 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: C₃H₇O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	P	0	0
			11	3	7	1		
6	G	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 7 is (1S)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYL)OXY]METHYL]ETHYL OCTANOATE (CCD ID: AGA) (formula: C₁₉H₃₆O₁₀P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			16	11	5		
7	G	1	Total	C	O	0	0
			16	11	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	78	Total	O	0	0
			78	78		
8	C	69	Total	O	0	0
			69	69		
8	D	60	Total	O	0	0
			60	60		
8	E	65	Total	O	0	0
			65	65		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	68	Total 68	O 68	0	0
8	G	69	Total 69	O 69	0	0
8	H	61	Total 61	O 61	0	0

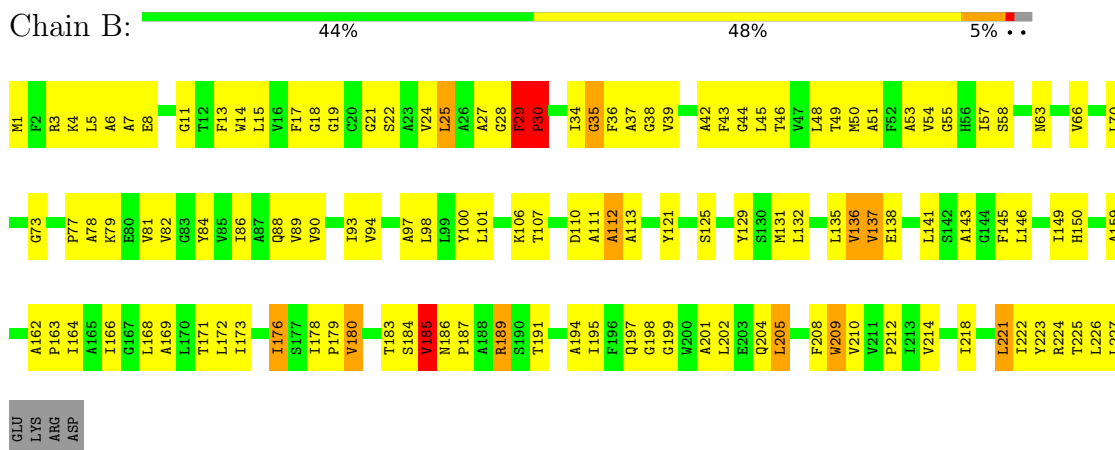
3 Residue-property plots [i](#)

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

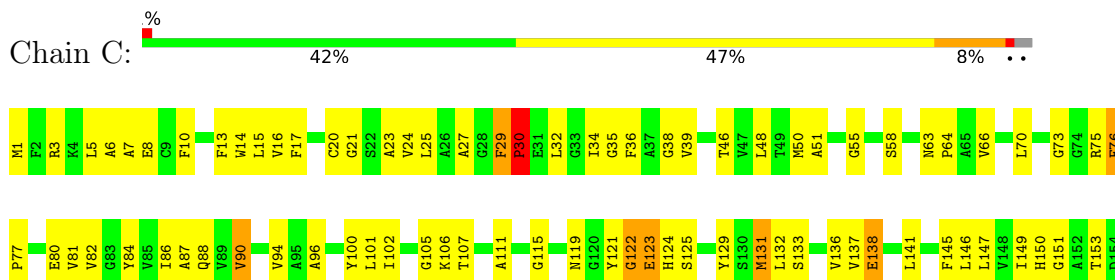
• Molecule 1: Aquaporin Z

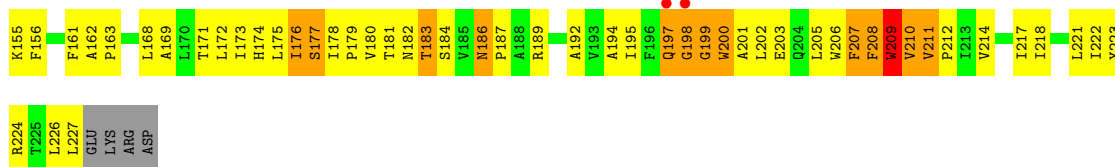


• Molecule 1: Aquaporin Z



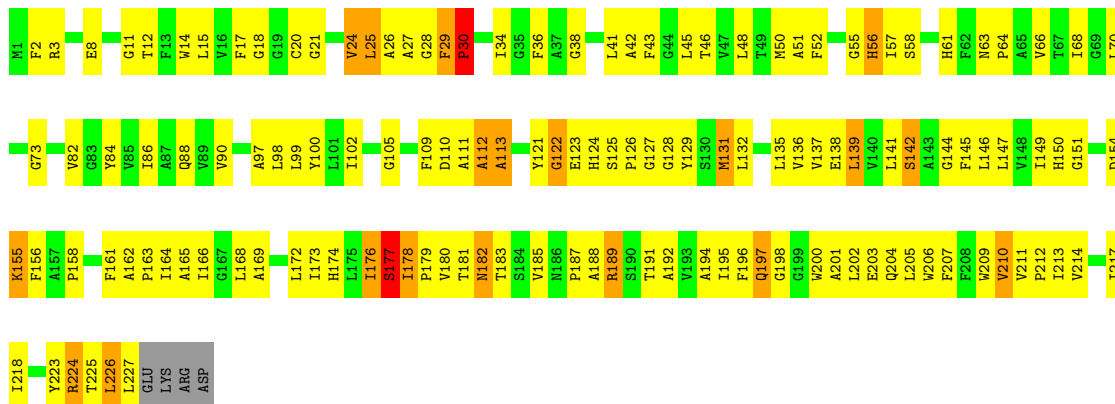
• Molecule 1: Aquaporin Z





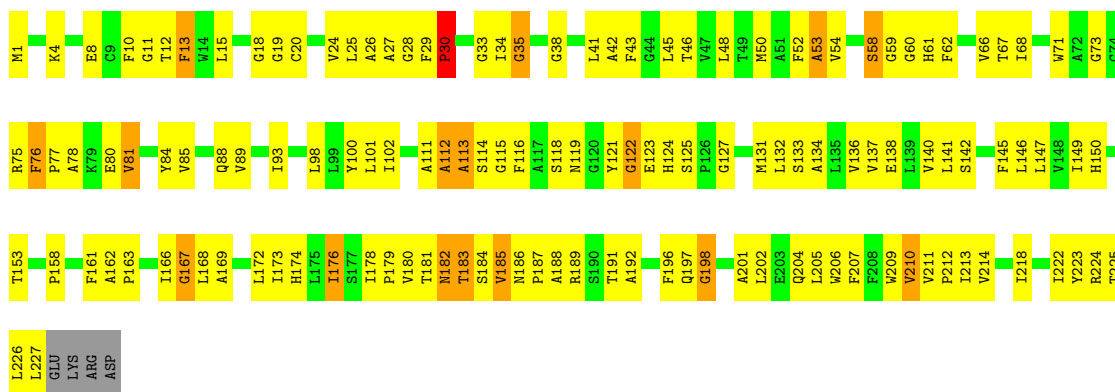
- Molecule 1: Aquaporin Z

Chain D: ..



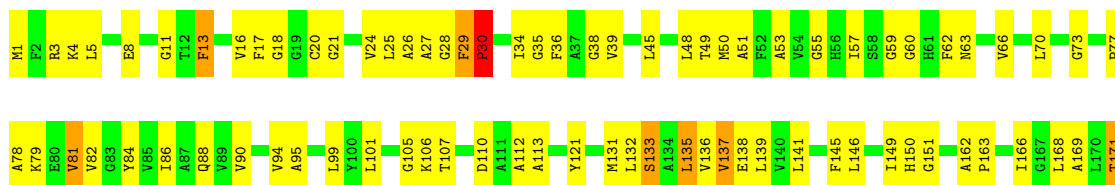
- Molecule 1: Aquaporin Z

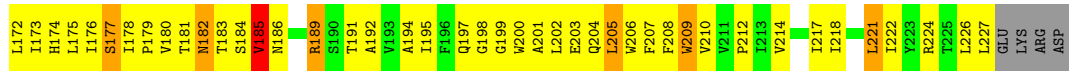
Chain E: .



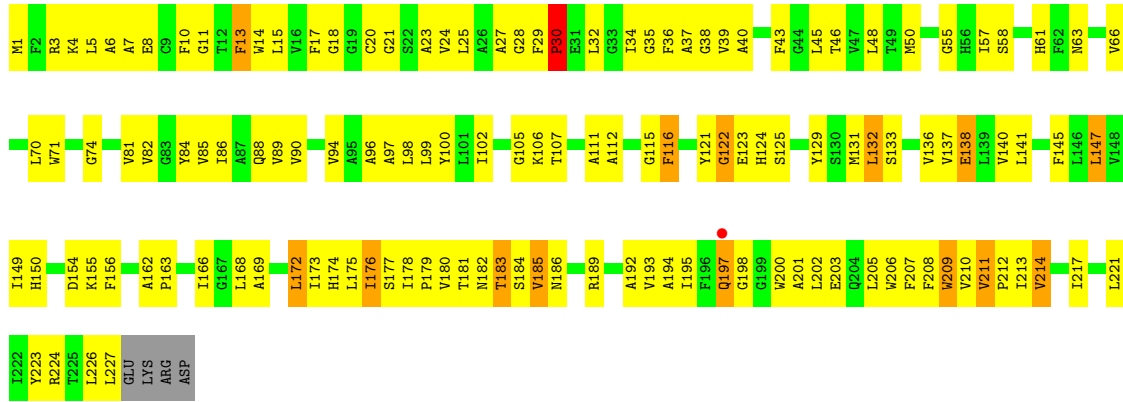
- Molecule 1: Aquaporin Z

Chain F: ..

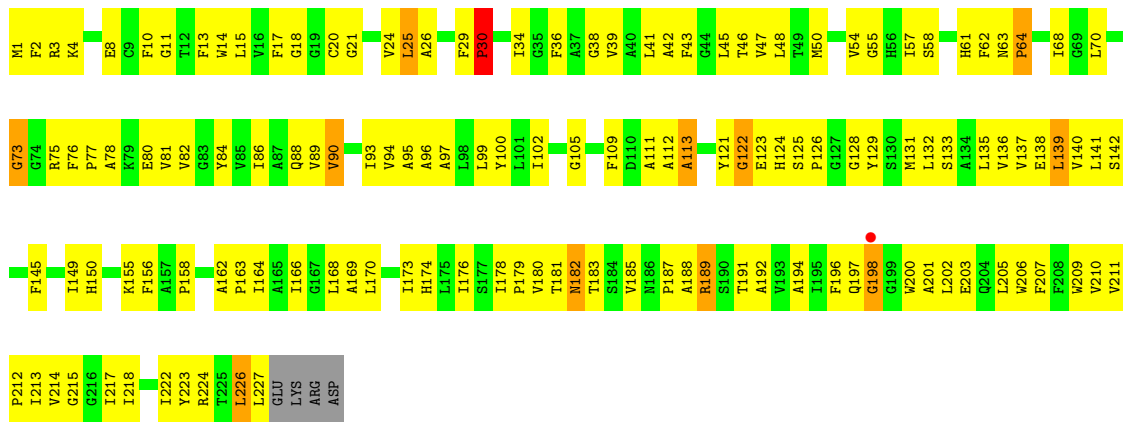




• Molecule 1: Aquaporin Z



• Molecule 1: Aquaporin Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.15Å 119.15Å 380.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 10.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-3.20) 96.2 (10.00-3.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.19Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.242 0.197 , 0.246	Depositor DCC
R_{free} test set	2306 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 100.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13946	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POQ, PEE, PO4, BGL, AGA, 3PG

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	0.56	0/1689	1.10	12/2305 (0.5%)
1	B	0.57	0/1689	1.11	12/2305 (0.5%)
1	C	0.55	0/1689	1.11	15/2305 (0.7%)
1	D	0.57	0/1689	1.08	10/2305 (0.4%)
1	E	0.54	0/1689	1.06	7/2305 (0.3%)
1	F	0.58	0/1689	1.09	10/2305 (0.4%)
1	G	0.51	0/1689	1.07	8/2305 (0.3%)
1	H	0.55	0/1689	1.02	4/2305 (0.2%)
All	All	0.55	0/13512	1.08	78/18440 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ILE	CB-CA-C	-9.51	104.67	113.70
1	A	178	ILE	N-CA-CB	9.03	116.57	110.52
1	A	176	ILE	N-CA-C	7.95	118.53	110.82
1	D	24	VAL	N-CA-C	7.32	117.45	110.42
1	D	177	SER	CA-C-O	-7.17	112.82	120.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	196	PHE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1643	0	1673	127	0
1	B	1643	0	1673	121	0
1	C	1643	0	1673	127	0
1	D	1643	0	1673	146	0
1	E	1643	0	1673	137	0
1	F	1643	0	1673	127	0
1	G	1643	0	1673	135	0
1	H	1643	0	1673	142	0
2	A	16	0	15	1	0
2	B	36	0	42	9	0
2	E	16	0	15	1	0
3	A	39	0	26	8	0
4	A	9	0	17	0	0
4	B	24	0	46	0	0
4	E	16	0	31	0	0
4	F	24	0	46	0	0
4	G	9	0	17	0	0
5	B	5	0	0	2	0
5	C	5	0	0	0	0
5	F	5	0	0	3	0
5	G	5	0	0	0	0
6	C	11	0	5	0	0
6	G	11	0	5	0	0
7	C	16	0	11	0	0
7	G	16	0	9	2	0
8	A	69	0	0	4	0
8	B	78	0	0	3	0
8	C	69	0	0	2	0
8	D	60	0	0	5	0
8	E	65	0	0	2	0
8	F	68	0	0	5	0
8	G	69	0	0	3	0
8	H	61	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13946	0	13669	987	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

The worst 5 of 987 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)
7:G:639:AGA:C10	7:G:639:AGA:C9	1.76	1.64
2:B:605:BGL:C4'	2:B:605:BGL:C3'	1.74	1.57
2:B:605:BGL:C5'	2:B:605:BGL:C6'	1.80	1.56
2:B:604:BGL:C6'	2:B:604:BGL:C5'	1.79	1.54
3:A:600:POQ:C1	3:A:600:POQ:O5	1.69	1.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/231 (97%)	191 (85%)	26 (12%)	8 (4%)	2	19
1	B	225/231 (97%)	204 (91%)	13 (6%)	8 (4%)	2	19
1	C	225/231 (97%)	194 (86%)	22 (10%)	9 (4%)	2	17
1	D	225/231 (97%)	181 (80%)	35 (16%)	9 (4%)	2	17
1	E	225/231 (97%)	196 (87%)	19 (8%)	10 (4%)	2	15
1	F	225/231 (97%)	205 (91%)	14 (6%)	6 (3%)	4	25
1	G	225/231 (97%)	196 (87%)	22 (10%)	7 (3%)	3	22
1	H	225/231 (97%)	190 (84%)	28 (12%)	7 (3%)	3	22
All	All	1800/1848 (97%)	1557 (86%)	179 (10%)	64 (4%)	2	19

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	183	THR
1	B	29	PHE
1	B	30	PRO
1	C	30	PRO

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	158/162 (98%)	154 (98%)	4 (2%)	42 69
1	B	158/162 (98%)	148 (94%)	10 (6%)	16 48
1	C	158/162 (98%)	150 (95%)	8 (5%)	21 54
1	D	158/162 (98%)	149 (94%)	9 (6%)	18 51
1	E	158/162 (98%)	155 (98%)	3 (2%)	50 73
1	F	158/162 (98%)	148 (94%)	10 (6%)	16 48
1	G	158/162 (98%)	151 (96%)	7 (4%)	25 59
1	H	158/162 (98%)	150 (95%)	8 (5%)	21 54
All	All	1264/1296 (98%)	1205 (95%)	59 (5%)	23 57

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	210	VAL
1	H	182	ASN
1	F	107	THR
1	H	139	LEU
1	G	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	150	HIS
1	H	124	HIS
1	E	124	HIS
1	G	197	GLN
1	E	119	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands 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
5	PO4	F	636	-	4,4,4	1.58	0	6,6,6	0.47	0
6	3PG	G	637	-	9,10,10	3.42	5 (55%)	11,14,14	3.15	5 (45%)
5	PO4	G	635	-	4,4,4	1.48	0	6,6,6	0.47	0
4	PEE	E	613	-	15,15,50	1.92	3 (20%)	14,14,55	1.75	4 (28%)
5	PO4	C	625	-	4,4,4	1.88	3 (75%)	6,6,6	0.48	0
7	AGA	C	629	-	15,15,29	5.84	9 (60%)	17,17,35	6.42	14 (82%)
3	POQ	A	600	-	40,40,40	5.39	29 (72%)	53,60,60	2.79	16 (30%)
4	PEE	B	602	-	13,13,50	1.02	1 (7%)	12,12,55	1.12	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	3PG	C	627	-	9,10,10	2.90	4 (44%)	11,14,14	3.45	5 (45%)
4	PEE	F	607	-	9,9,50	1.59	2 (22%)	8,8,55	1.33	1 (12%)
4	PEE	G	611	-	8,8,50	0.90	0	7,7,55	1.03	1 (14%)
2	BGL	B	604	-	18,18,20	2.84	7 (38%)	22,23,25	2.32	9 (40%)
2	BGL	E	608	-	16,16,20	4.13	9 (56%)	20,21,25	3.52	11 (55%)
4	PEE	B	606	-	9,9,50	1.68	2 (22%)	8,8,55	1.35	1 (12%)
4	PEE	A	612	-	8,8,50	0.99	0	7,7,55	1.06	1 (14%)
2	BGL	A	609	-	16,16,20	4.10	10 (62%)	20,21,25	3.47	11 (55%)
7	AGA	G	639	-	14,14,29	6.40	8 (57%)	16,16,35	8.22	13 (81%)
4	PEE	F	603	-	13,13,50	1.04	1 (7%)	12,12,55	1.10	1 (8%)
5	PO4	B	626	-	4,4,4	1.92	3 (75%)	6,6,6	0.44	0
2	BGL	B	605	-	18,18,20	3.21	8 (44%)	22,23,25	2.40	10 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AGA	G	639	-	-	10/15/15/34	-
4	PEE	F	607	-	-	2/7/7/54	-
4	PEE	B	606	-	-	2/7/7/54	-
4	PEE	G	611	-	-	0/6/6/54	-
6	3PG	G	637	-	1/1/3/3	10/10/10/10	-
2	BGL	B	604	-	-	2/9/29/31	0/1/1/1
7	AGA	C	629	-	-	9/17/17/34	-
2	BGL	E	608	-	1/1/5/5	2/6/26/31	0/1/1/1
4	PEE	F	603	-	-	3/11/11/54	-
3	POQ	A	600	-	2/2/13/13	11/30/70/70	0/2/2/2
4	PEE	A	612	-	-	0/6/6/54	-
2	BGL	A	609	-	1/1/5/5	2/6/26/31	0/1/1/1
4	PEE	B	602	-	-	3/11/11/54	-
6	3PG	C	627	-	1/1/3/3	10/10/10/10	-
4	PEE	E	613	-	-	4/13/13/54	-
2	BGL	B	605	-	-	2/9/29/31	0/1/1/1

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	639	AGA	O8-C7	12.18	1.58	1.22
7	G	639	AGA	O9-C12	11.91	1.67	1.34
7	C	629	AGA	O8-C7	11.59	1.57	1.22
7	C	629	AGA	O9-C12	11.54	1.66	1.34
3	A	600	POQ	O5B-C1B	10.92	1.69	1.42

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	639	AGA	C5-O9-C12	25.18	154.11	117.78
7	C	629	AGA	C5-O9-C12	14.33	152.08	117.80
7	G	639	AGA	O9-C12-O10	-9.64	101.17	123.70
7	C	629	AGA	O9-C12-O10	-9.57	101.32	123.70
7	C	629	AGA	C9-C8-C7	9.27	151.78	114.36

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	609	BGL	C5
2	E	608	BGL	C5
3	A	600	POQ	C5
3	A	600	POQ	C5B
6	C	627	3PG	C2

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	POQ	C3-C2-O11-P1
3	A	600	POQ	C4-C5-C6-O31
3	A	600	POQ	O5-C5-C6-O31
3	A	600	POQ	C6B-O33-P3-O32
3	A	600	POQ	C3B-C2B-O21-P2

There are no ring outliers.

8 monomers are involved in 26 short contacts:

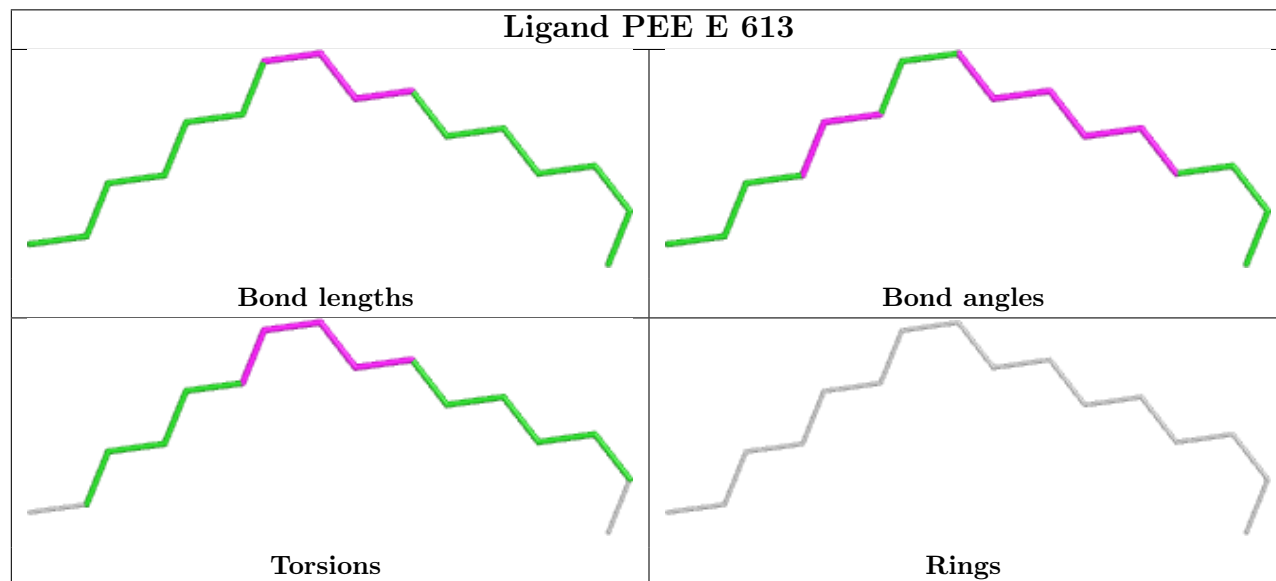
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	636	PO4	3	0
3	A	600	POQ	8	0
2	B	604	BGL	3	0
2	E	608	BGL	1	0
2	A	609	BGL	1	0

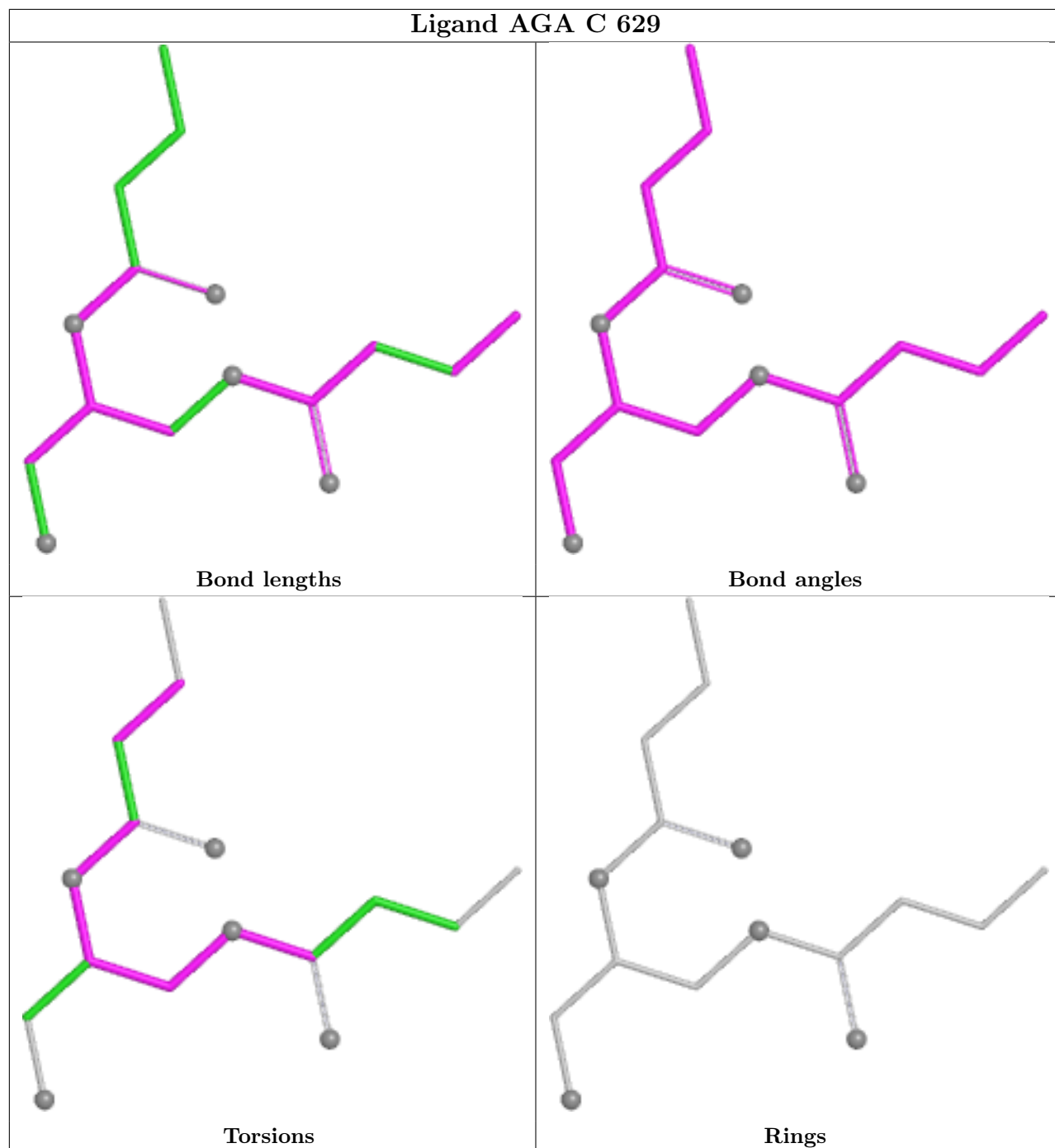
Continued on next page...

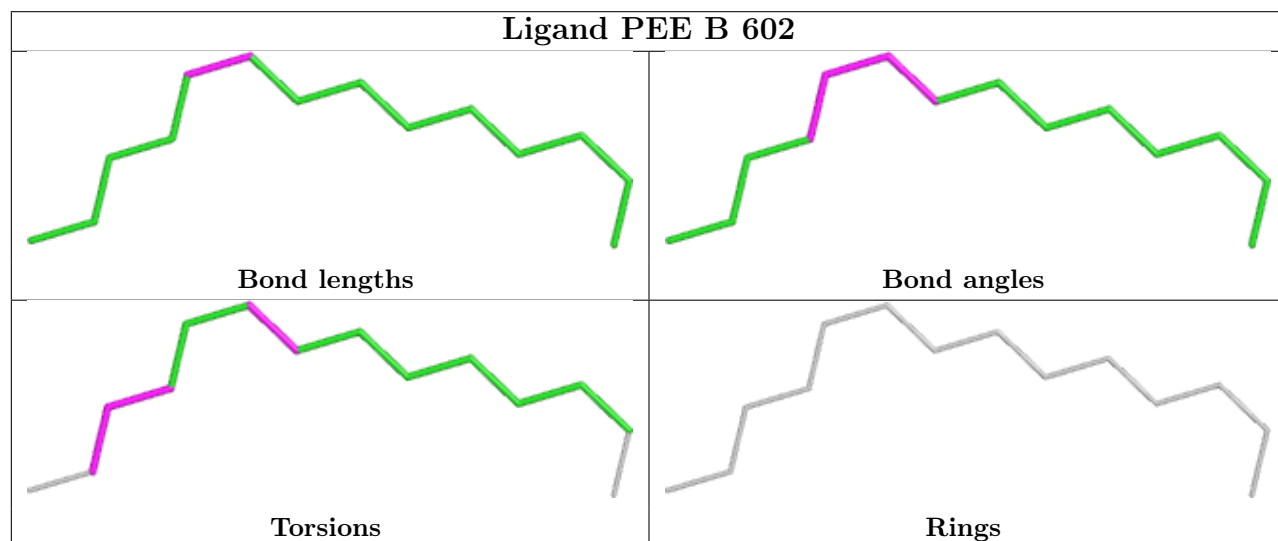
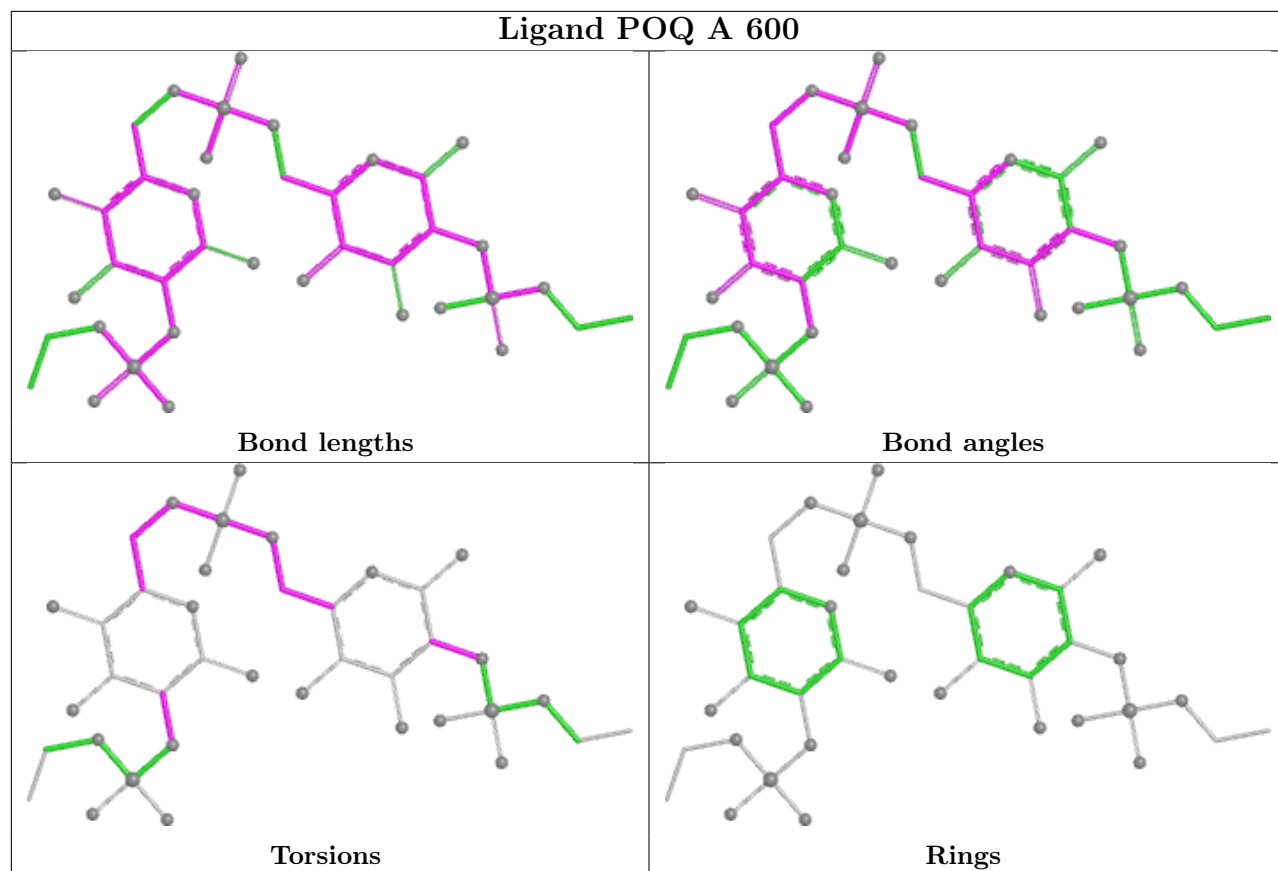
Continued from previous page...

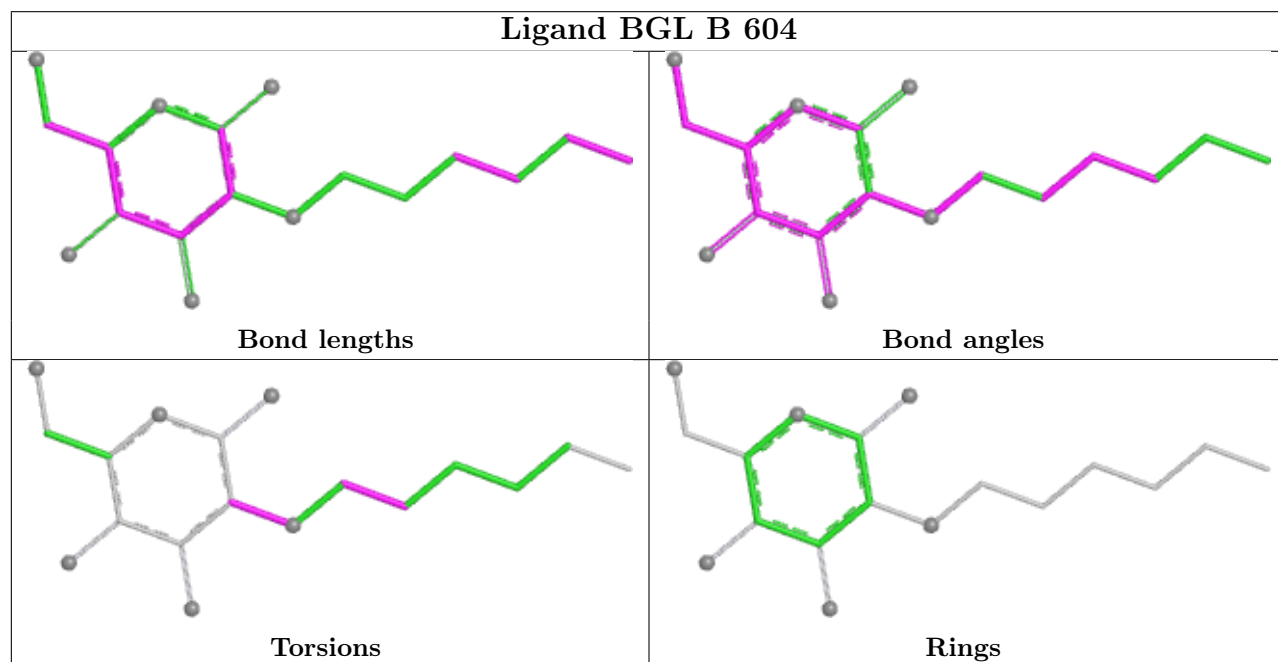
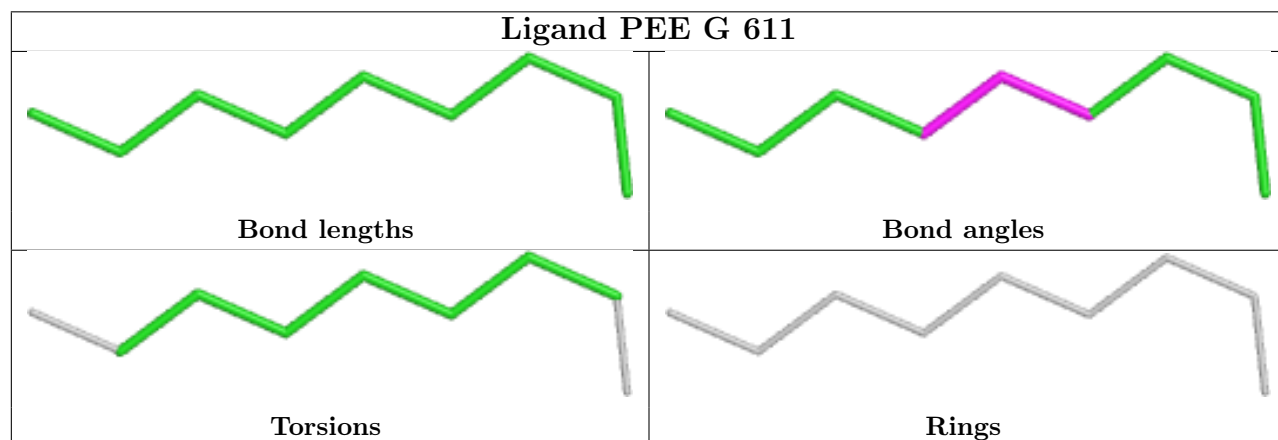
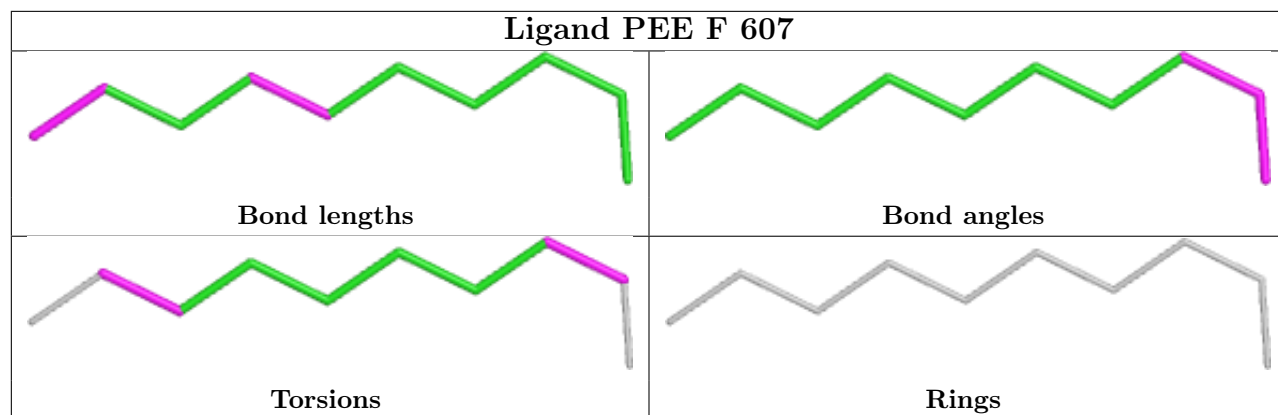
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	639	AGA	2	0
5	B	626	PO4	2	0
2	B	605	BGL	6	0

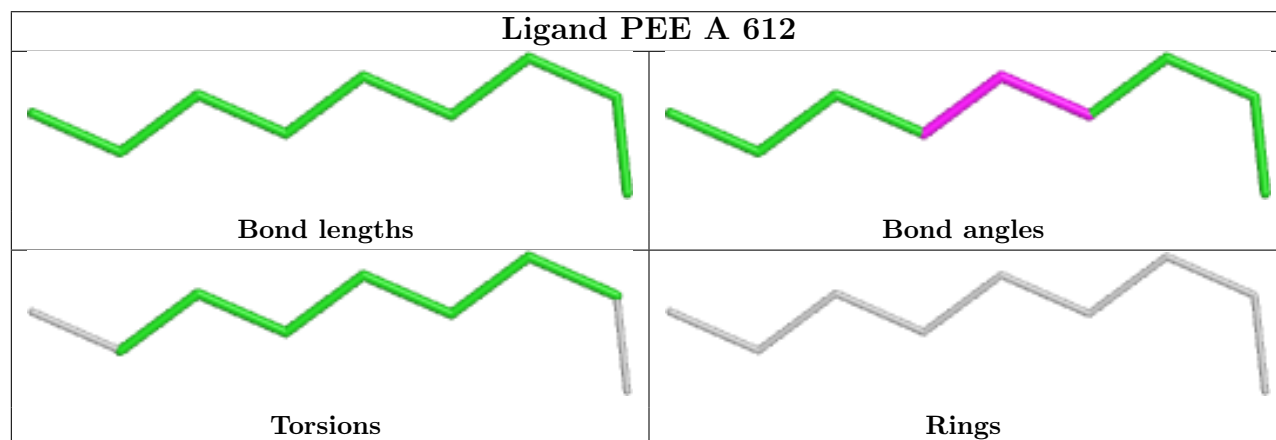
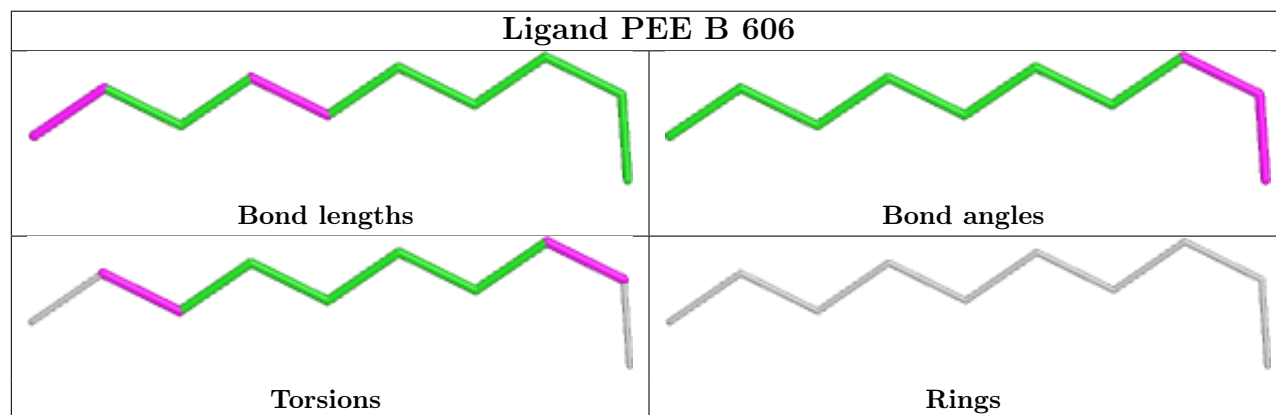
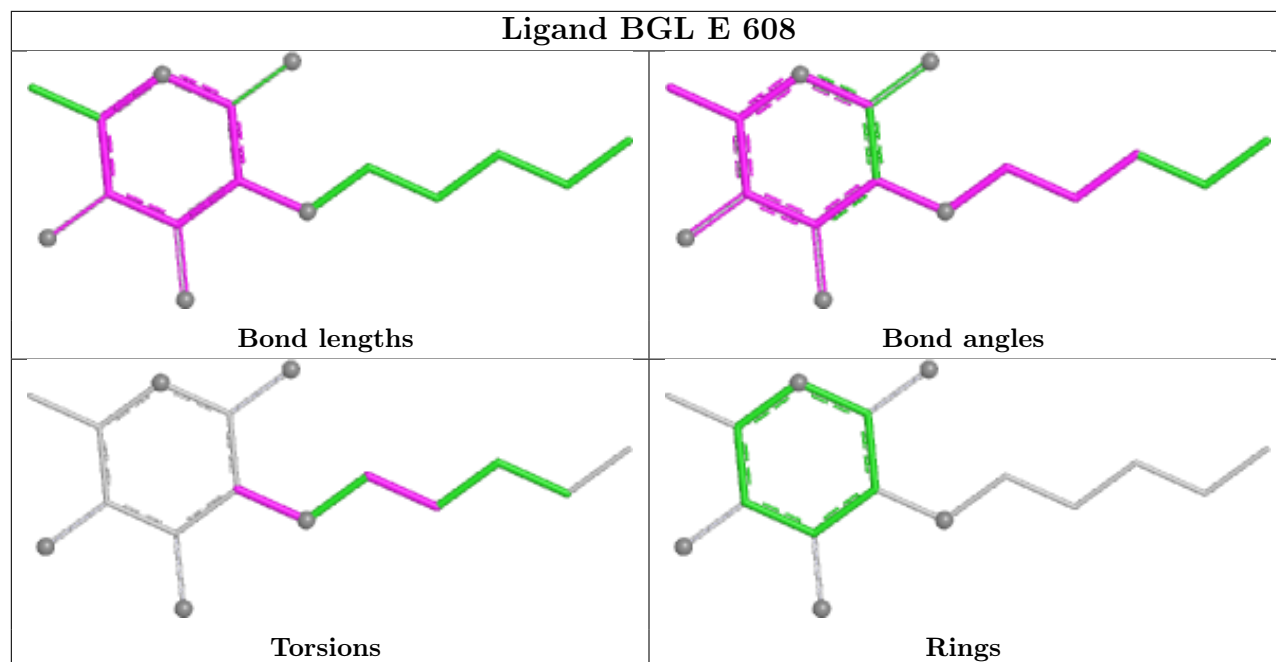
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

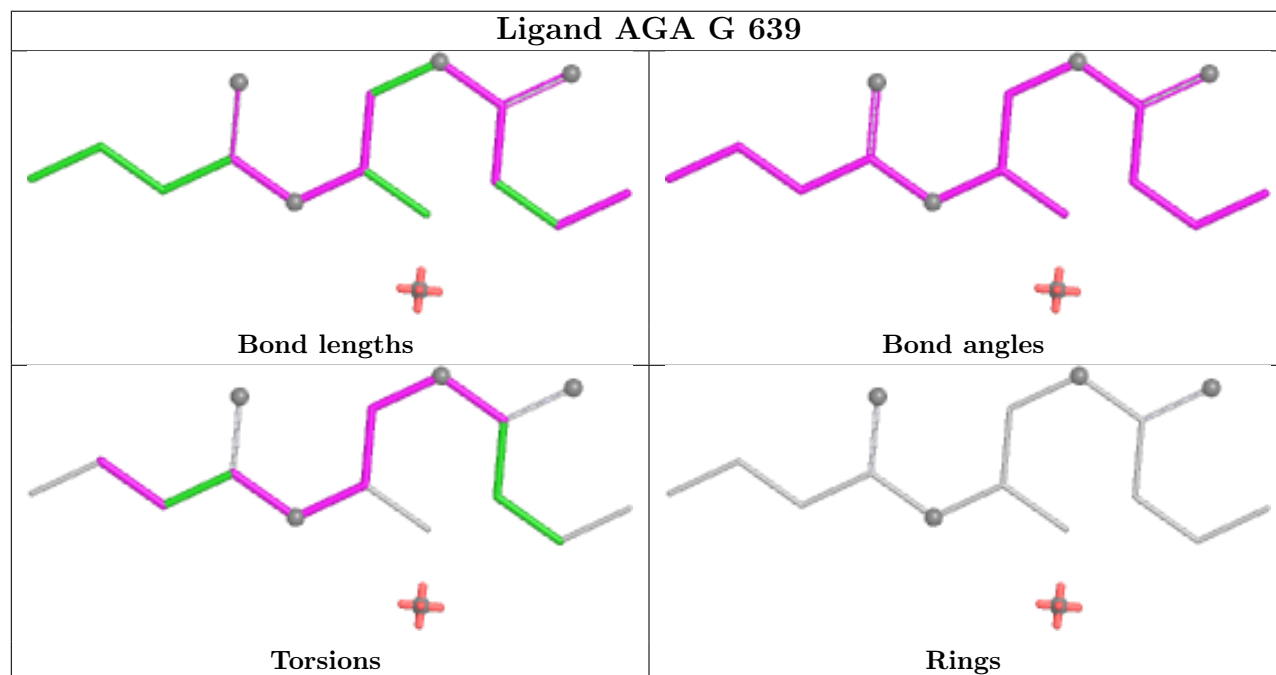
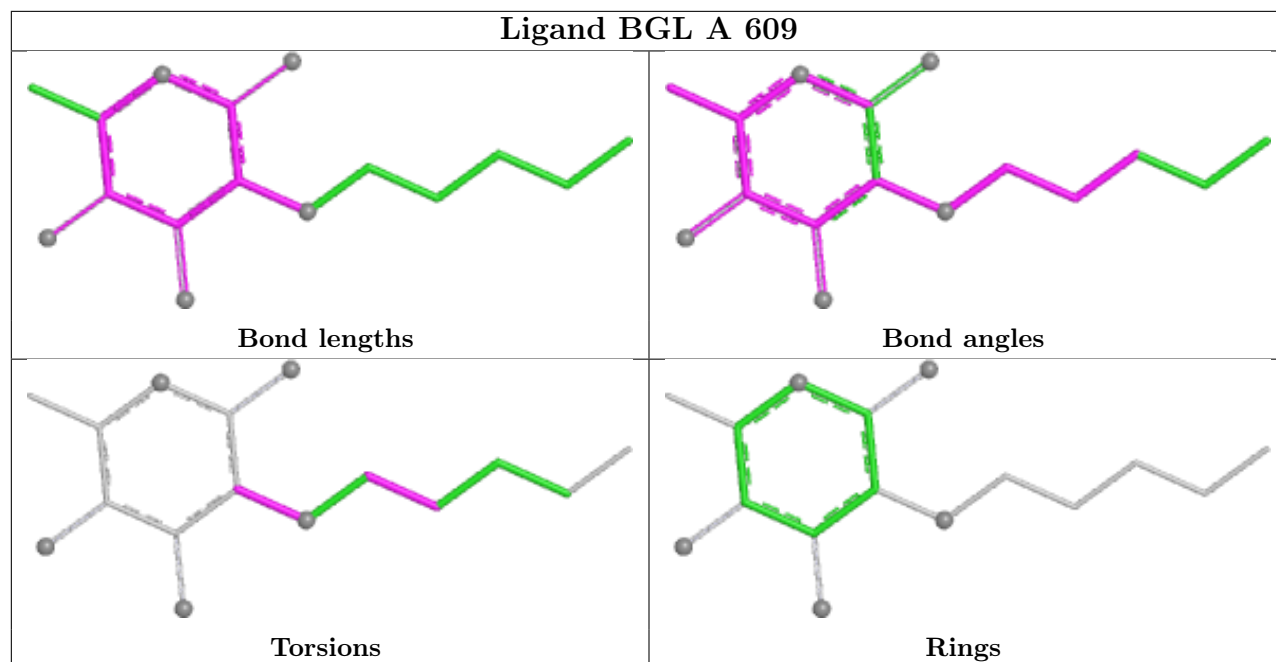


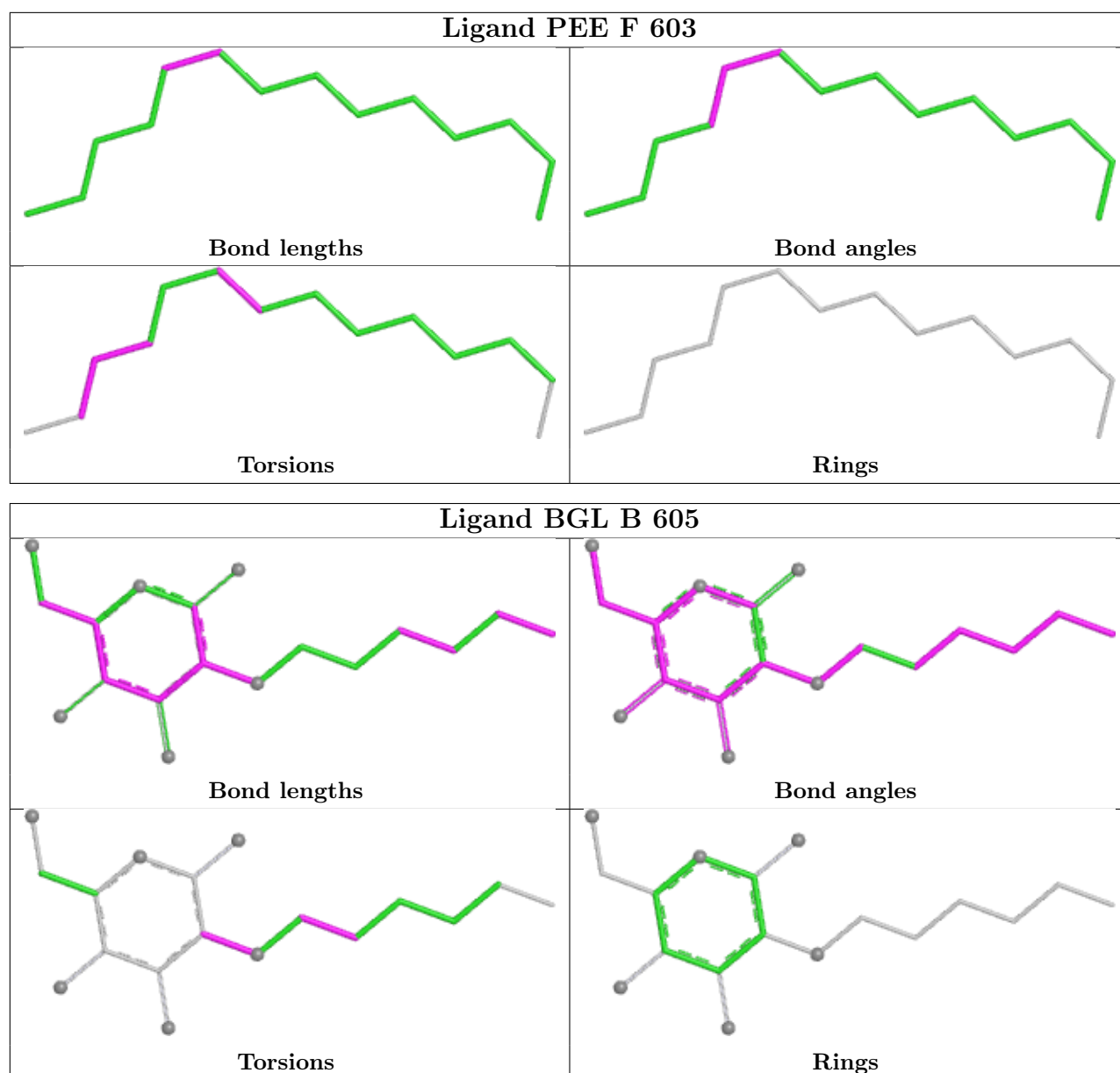












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/231 (98%)	-0.92	0 100 100	15, 32, 51, 66	0
1	B	227/231 (98%)	-0.93	0 100 100	14, 28, 48, 74	0
1	C	227/231 (98%)	-0.77	2 (0%) 81 64	18, 38, 57, 77	0
1	D	227/231 (98%)	-0.83	0 100 100	17, 37, 52, 78	0
1	E	227/231 (98%)	-0.89	0 100 100	16, 34, 53, 67	0
1	F	227/231 (98%)	-0.99	0 100 100	15, 29, 50, 75	0
1	G	227/231 (98%)	-0.76	1 (0%) 88 79	21, 42, 59, 80	0
1	H	227/231 (98%)	-0.86	1 (0%) 88 79	20, 38, 52, 77	0
All	All	1816/1848 (98%)	-0.87	4 (0%) 91 85	14, 35, 54, 80	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	GLY	5.1
1	G	197	GLN	2.9
1	C	197	GLN	2.1
1	H	198	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

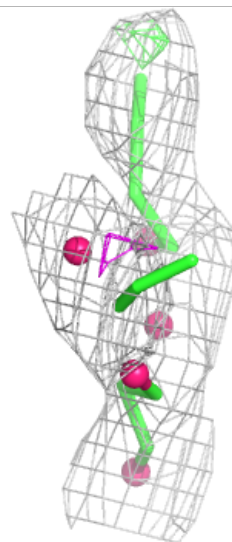
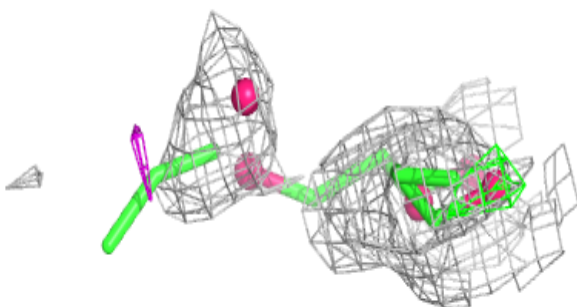
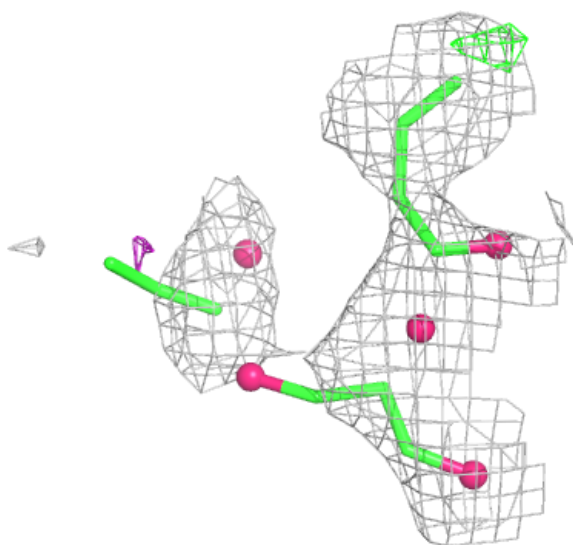
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	G	635	5/5	0.52	0.22	68,68,69,70	5
7	AGA	G	639	16/30	0.65	0.12	40,48,61,61	9
6	3PG	G	637	11/11	0.68	0.14	54,57,60,60	5
4	PEE	E	613	16/51	0.78	0.10	35,41,45,46	0
5	PO4	C	625	5/5	0.79	0.22	54,54,55,56	5
6	3PG	C	627	11/11	0.80	0.11	42,49,51,52	5
7	AGA	C	629	16/30	0.83	0.14	38,44,52,52	9
4	PEE	F	607	10/51	0.87	0.09	35,40,42,42	0
2	BGL	B	605	18/20	0.89	0.11	40,78,81,82	0
2	BGL	E	608	16/20	0.90	0.08	33,40,42,45	0
3	POQ	A	600	39/39	0.90	0.08	34,64,67,70	1
4	PEE	A	612	9/51	0.91	0.06	40,42,44,44	0
4	PEE	B	606	10/51	0.92	0.07	35,37,40,40	0
2	BGL	B	604	18/20	0.93	0.08	46,74,79,79	0
4	PEE	G	611	9/51	0.93	0.06	45,46,50,50	0
5	PO4	F	636	5/5	0.94	0.10	38,39,40,40	5
5	PO4	B	626	5/5	0.94	0.14	29,29,30,31	5
4	PEE	B	602	14/51	0.95	0.05	36,39,48,49	0
4	PEE	F	603	14/51	0.95	0.06	37,41,47,48	0
2	BGL	A	609	16/20	0.95	0.06	38,42,45,46	0

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

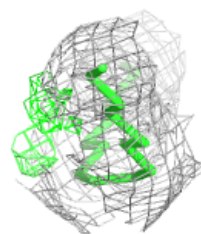
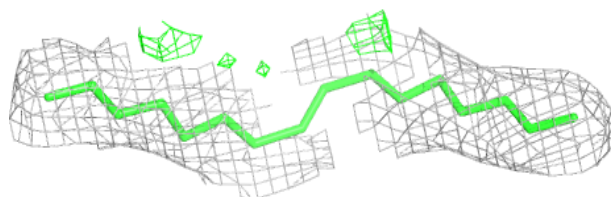
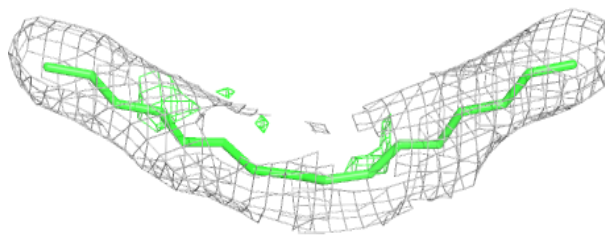
Electron density around AGA G 639:

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



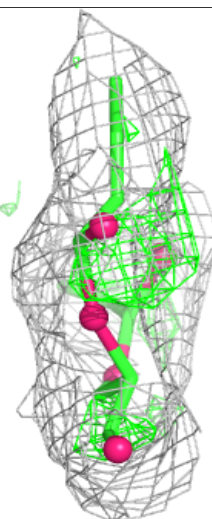
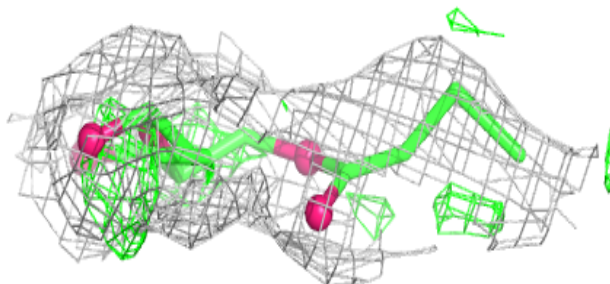
Electron density around PEE E 613:

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



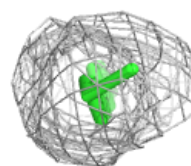
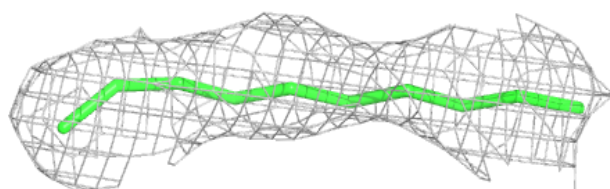
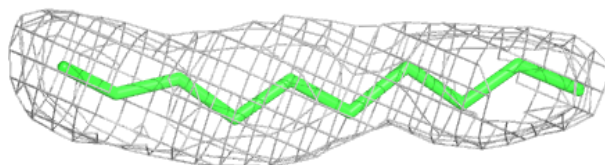
Electron density around AGA C 629:

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

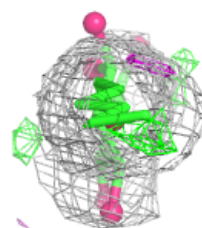
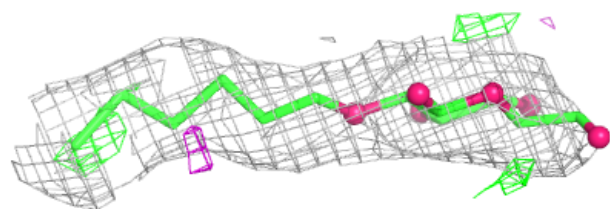
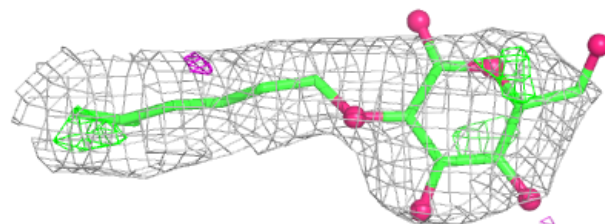


Electron density around PEE F 607:

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

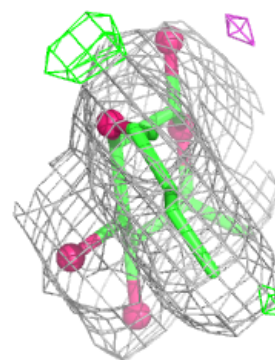
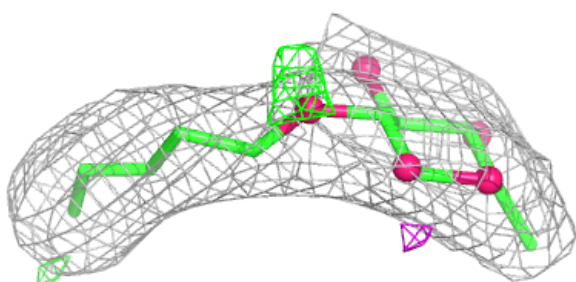
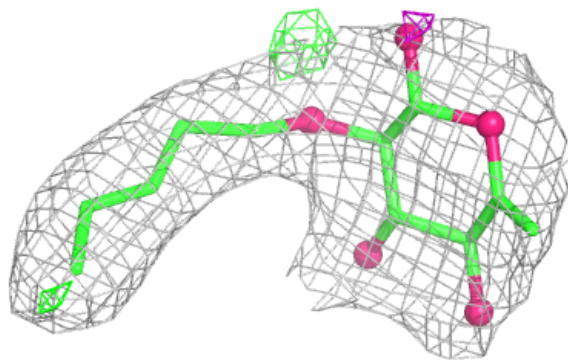
**Electron density around BGL B 605:**

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

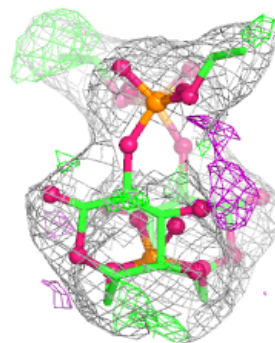
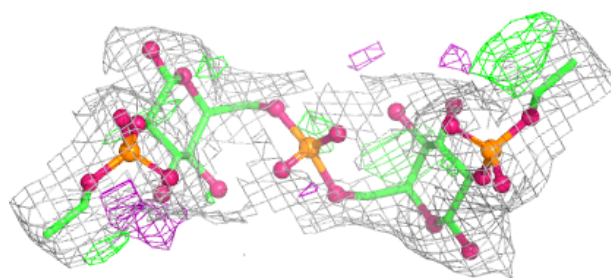
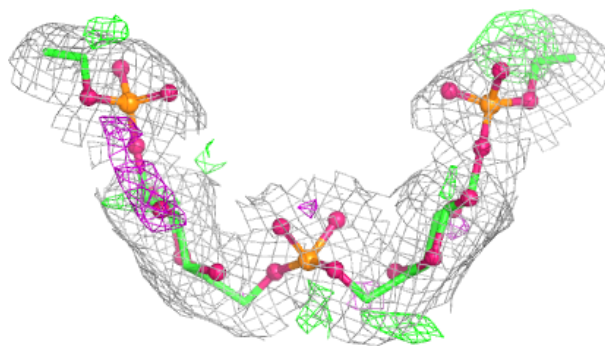


Electron density around BGL E 608:

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

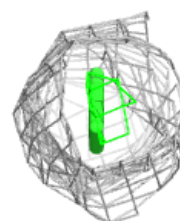
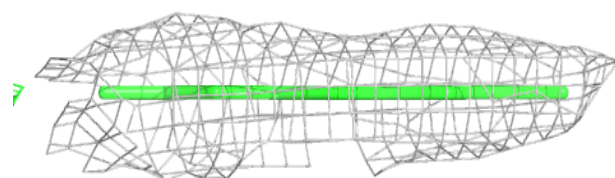
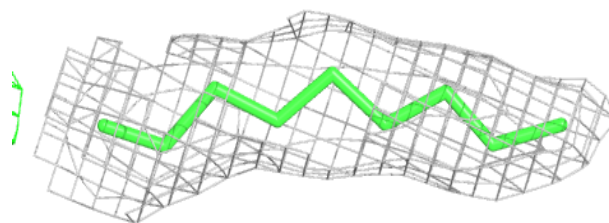
**Electron density around POQ A 600:**

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

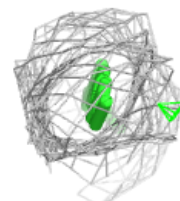
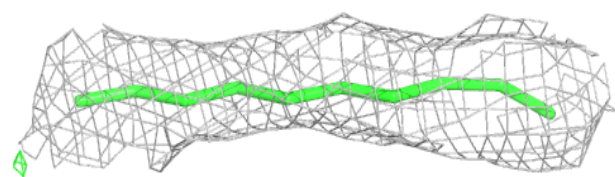
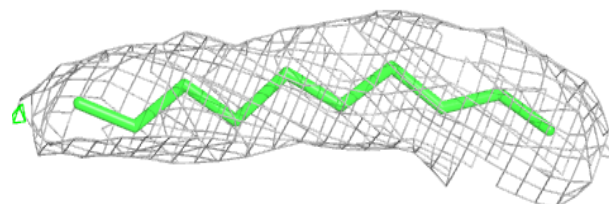


Electron density around PEE A 612:

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

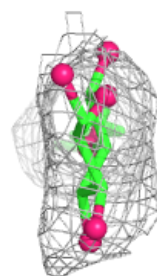
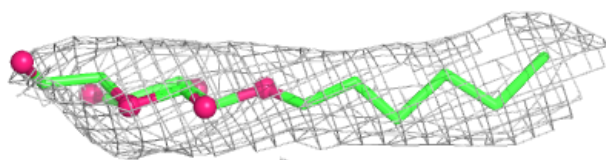
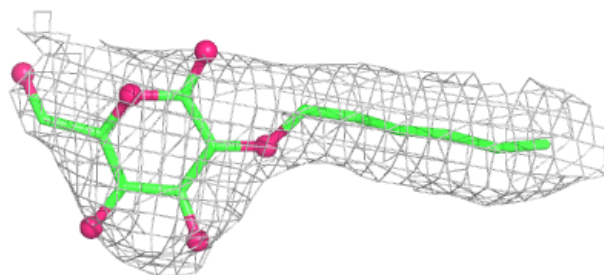
**Electron density around PEE B 606:**

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

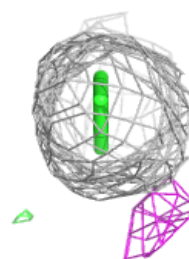
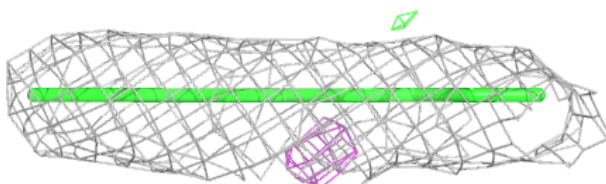
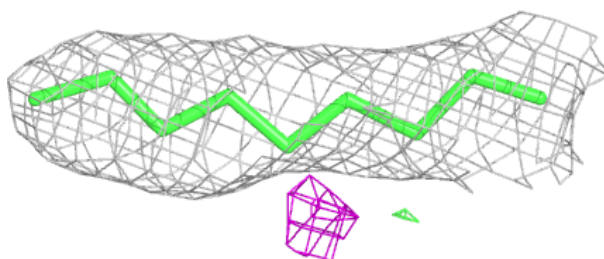


Electron density around BGL B 604:

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

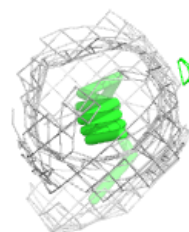
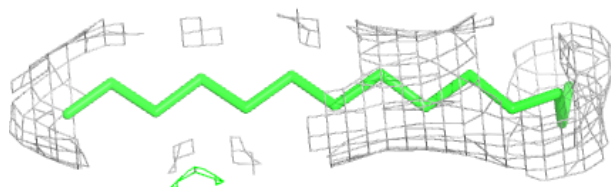
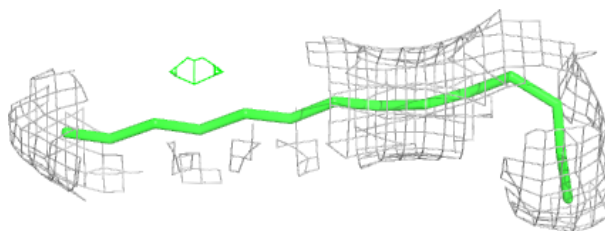
**Electron density around PEE G 611:**

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

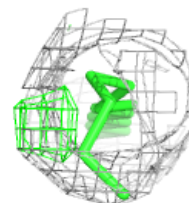
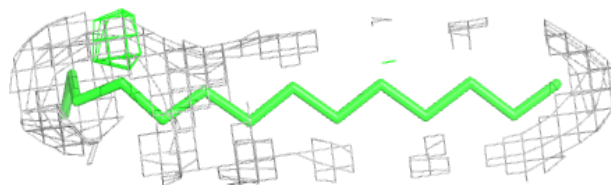
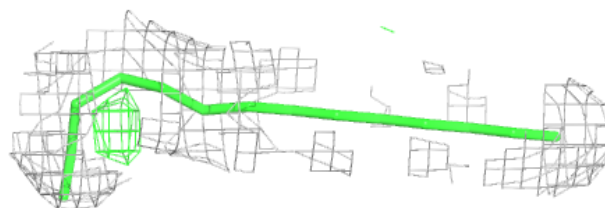


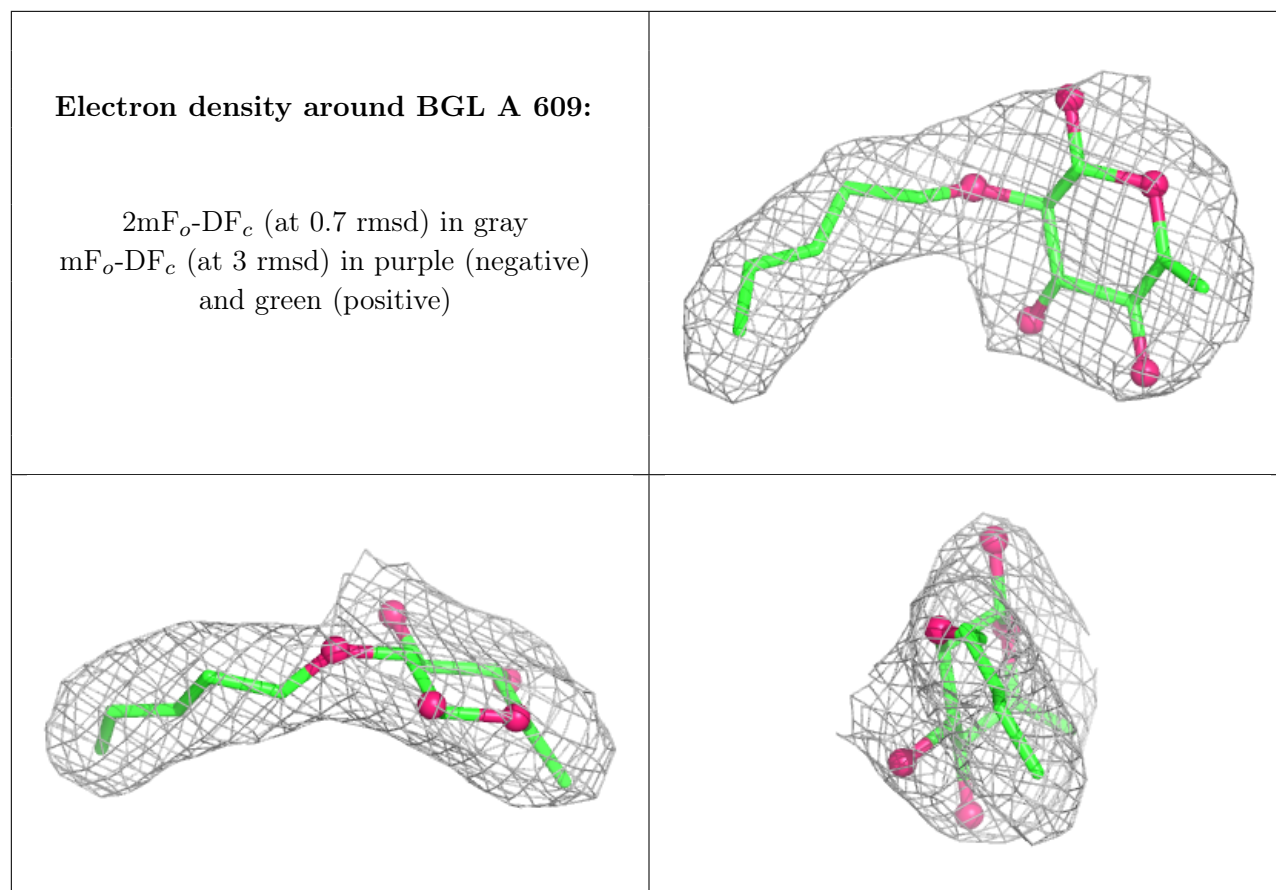
Electron density around PEE B 602:

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

**Electron density around PEE F 603:**

$2mF_o-DF_c$ (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.