wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 11:24 PM EDT

PDB ID	:	4KI0
Title	:	Crystal structure of the maltose-binding protein/maltose transporter complex in an outward-facing conformation bound to maltohexaose
Authors	:	Oldham, M.L.; Chen, S.; Chen, J.
Deposited on	:	2013-05-01
Resolution	:	2.38 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 (i) 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 (i)) were used in the production of this report:

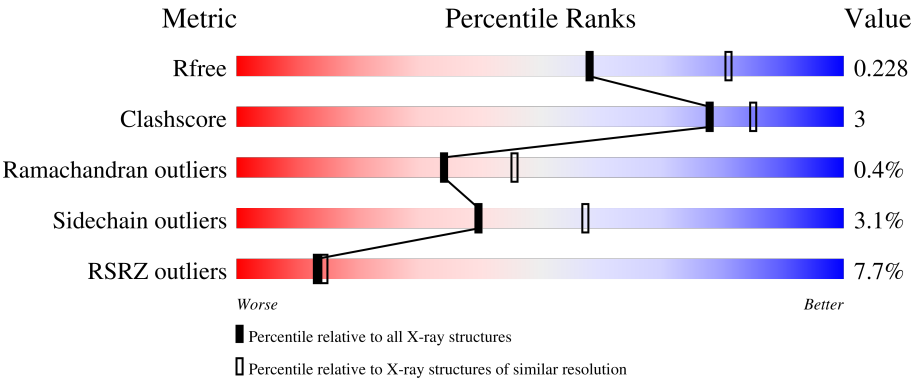
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	381	5% 87% 10% ·
1	B	381	11% 86% 11% ·
2	E	380	7% 94% · ·
3	F	514	8% 85% 9% · 5%
4	G	296	5% 88% 9% ··

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Mol	Chain	Length	Quality of chain
5	C	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
5	GLC	C	2	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15618 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 ABC transporter related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	1	0
			2884	1824	518	529	13			
1	B	371	Total	C	N	O	S	0	0	0
			2876	1819	515	529	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP C9QV42
A	373	SER	-	expression tag	UNP C9QV42
A	374	ALA	-	expression tag	UNP C9QV42
A	375	SER	-	expression tag	UNP C9QV42
A	376	HIS	-	expression tag	UNP C9QV42
A	377	HIS	-	expression tag	UNP C9QV42
A	378	HIS	-	expression tag	UNP C9QV42
A	379	HIS	-	expression tag	UNP C9QV42
A	380	HIS	-	expression tag	UNP C9QV42
A	381	HIS	-	expression tag	UNP C9QV42
B	372	ALA	-	expression tag	UNP C9QV42
B	373	SER	-	expression tag	UNP C9QV42
B	374	ALA	-	expression tag	UNP C9QV42
B	375	SER	-	expression tag	UNP C9QV42
B	376	HIS	-	expression tag	UNP C9QV42
B	377	HIS	-	expression tag	UNP C9QV42
B	378	HIS	-	expression tag	UNP C9QV42
B	379	HIS	-	expression tag	UNP C9QV42
B	380	HIS	-	expression tag	UNP C9QV42
B	381	HIS	-	expression tag	UNP C9QV42

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	370	2877	1853	469	549	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	371	ALA	-	expression tag	UNP P0AEX9
E	372	SER	-	expression tag	UNP P0AEX9
E	373	ALA	-	expression tag	UNP P0AEX9
E	374	SER	-	expression tag	UNP P0AEX9
E	375	HIS	-	expression tag	UNP P0AEX9
E	376	HIS	-	expression tag	UNP P0AEX9
E	377	HIS	-	expression tag	UNP P0AEX9
E	378	HIS	-	expression tag	UNP P0AEX9
E	379	HIS	-	expression tag	UNP P0AEX9
E	380	HIS	-	expression tag	UNP P0AEX9

- Molecule 3 is a protein called Maltose transport system permease protein MalF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	490	3819	2512	607	683	17	0	1	0

- Molecule 4 is a protein called Binding-protein-dependent transport systems inner membrane component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	289	2238	1500	357	373	8	0	1	0

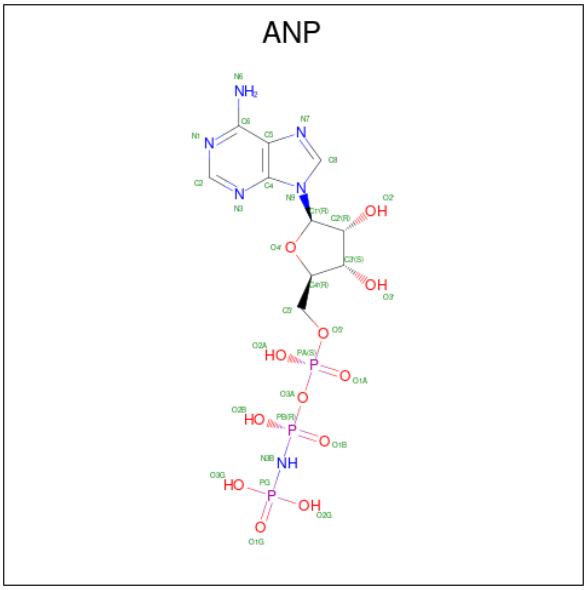
- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
5	C	4	34	18	16	0	0	1

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

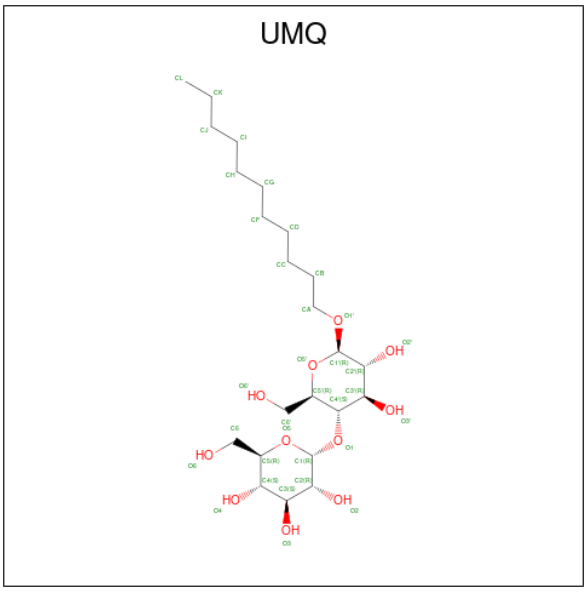
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



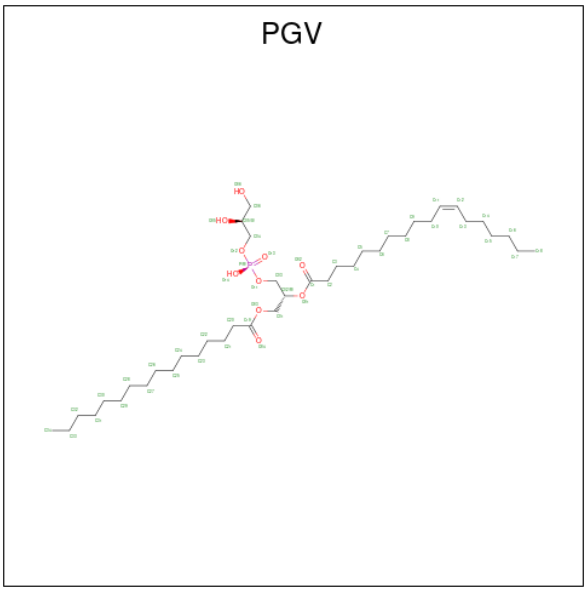
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 31 10 6 12 3	0	0
7	B	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 8 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 34 23 11	0	0
8	F	1	Total C O 13 12 1	0	0
8	F	1	Total C O 13 12 1	0	0
8	F	1	Total C O 13 12 1	0	0
8	G	1	Total C O 34 23 11	0	0
8	G	1	Total C O 13 12 1	0	0
8	G	1	Total C O 13 12 1	0	0
8	G	1	Total C O 13 12 1	0	0
8	G	1	Total C O 23 17 6	0	0
8	G	1	Total C O 13 12 1	0	0
8	G	1	Total C O 34 23 11	0	0

- Molecule 9 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	F	1	Total 51	C 40	O 10	P 1	0	0
9	F	1	Total 51	C 40	O 10	P 1	0	0

- Molecule 10 is water.

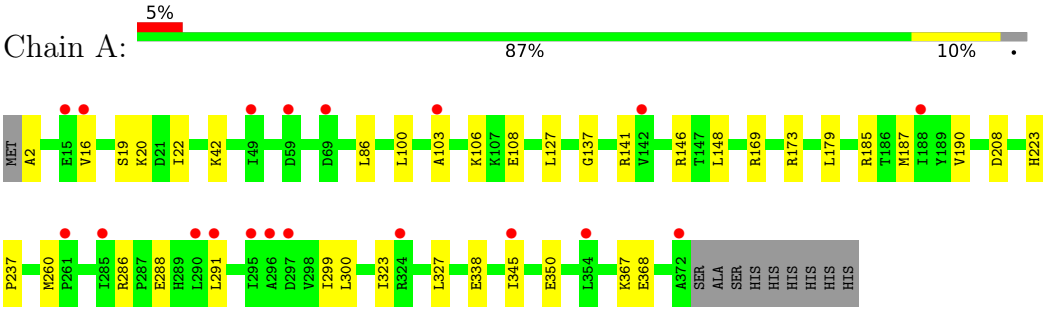
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	112	Total 112	O 112	0	0
10	B	123	Total 123	O 123	0	0
10	E	105	Total 105	O 105	0	0
10	F	87	Total 87	O 87	0	0
10	G	81	Total 81	O 81	0	0

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.

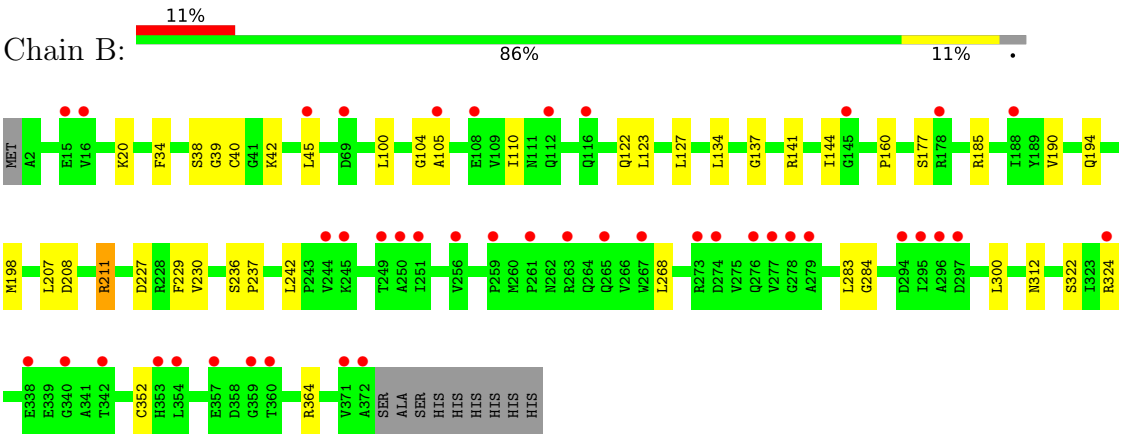
• Molecule 1: ABC transporter related protein

Chain A:



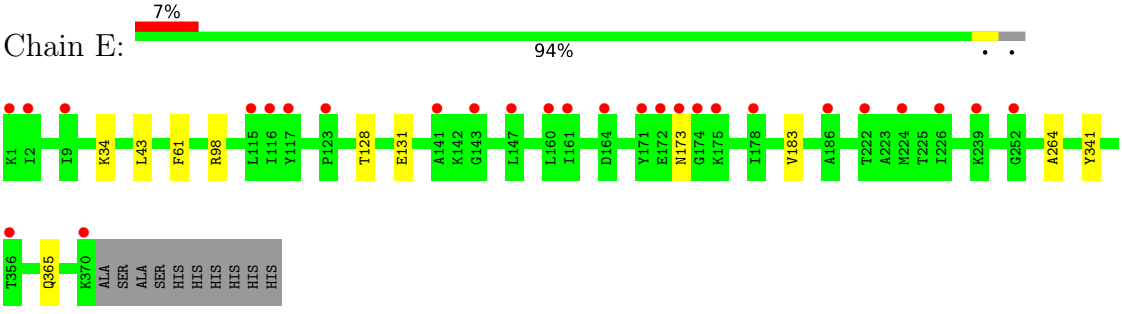
• Molecule 1: ABC transporter related protein

Chain B:



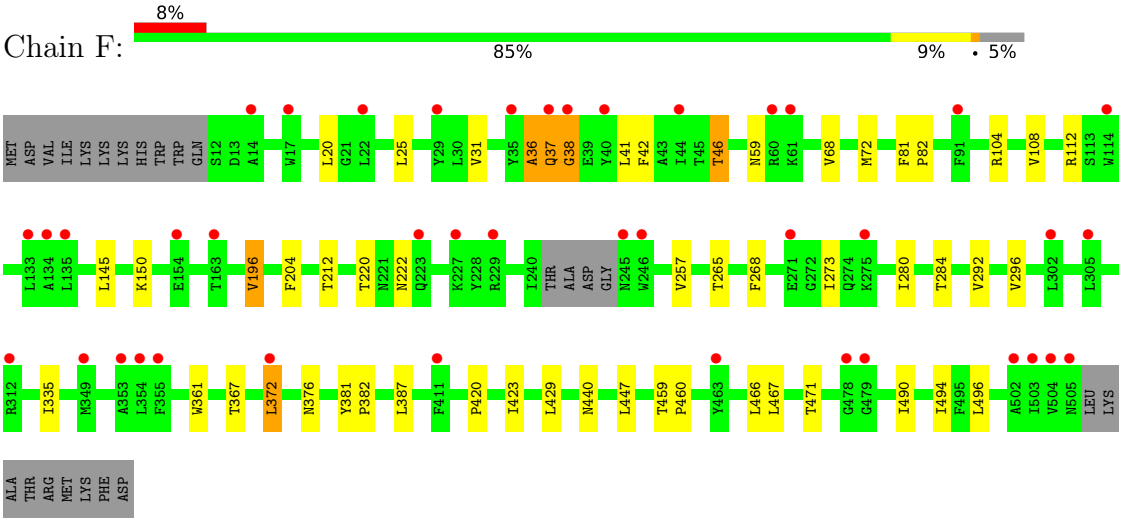
• Molecule 2: Maltose-binding periplasmic protein

Chain E:



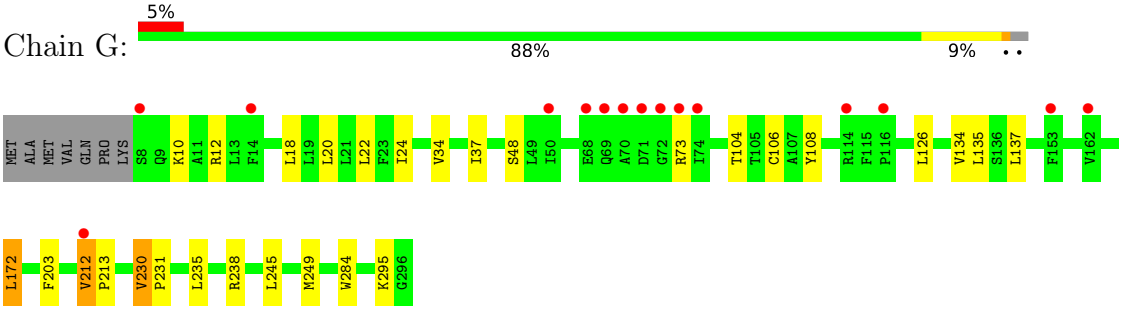
• Molecule 3: Maltose transport system permease protein MalF

Chain F:



• Molecule 4: Binding-protein-dependent transport systems inner membrane component

Chain G:



• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.59Å 96.63Å 112.32Å 85.30° 79.11° 73.00°	Depositor
Resolution (Å)	19.82 – 2.38 19.81 – 2.38	Depositor EDS
% Data completeness (in resolution range)	87.9 (19.82-2.38) 88.1 (19.81-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.228 0.196 , 0.228	Depositor DCC
R_{free} test set	5670 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15618	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: ANP, MG, UMQ, GLC, PGV

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	0.31	0/2937	0.55	0/3982
1	B	0.31	0/2926	0.54	0/3968
2	E	0.32	0/2946	0.48	0/3998
3	F	0.32	0/3917	0.51	0/5333
4	G	0.33	0/2304	0.52	0/3150
All	All	0.32	0/15030	0.52	0/20431

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	2884	0	2954	22	0
1	B	2876	0	2942	19	0
2	E	2877	0	2859	6	0
3	F	3819	0	3853	29	0
4	G	2238	0	2323	20	0
5	C	34	0	28	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	31	0	13	0	0
7	B	31	0	13	1	0
8	E	34	0	44	0	0
8	F	39	0	69	0	0
8	G	143	0	213	1	0
9	F	102	0	152	0	0
10	A	112	0	0	6	0
10	B	123	0	0	3	0
10	E	105	0	0	1	0
10	F	87	0	0	1	0
10	G	81	0	0	2	0
All	All	15618	0	15463	90	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 3.

The worst 5 of 90 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)
3:F:429:LEU:HD23	4:G:172:LEU:HD12	1.53	0.88
1:A:173:ARG:CZ	10:A:1690:HOH:O	2.36	0.73
4:G:295:LYS:NZ	10:G:410:HOH:O	2.21	0.73
1:A:223:HIS:CE1	1:A:368:GLU:HG2	2.27	0.68
4:G:212:VAL:HG22	4:G:284[A]:TRP:CD2	2.30	0.67

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	370/381 (97%)	363 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/381 (97%)	349 (95%)	18 (5%)	2 (0%)	29	39
2	E	368/380 (97%)	360 (98%)	7 (2%)	1 (0%)	41	53
3	F	487/514 (95%)	469 (96%)	15 (3%)	3 (1%)	25	34
4	G	288/296 (97%)	283 (98%)	4 (1%)	1 (0%)	41	53
All	All	1882/1952 (96%)	1824 (97%)	51 (3%)	7 (0%)	34	46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	37	GLN
2	E	173	ASN
3	F	38	GLY
1	B	38	SER
3	F	36	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	315/323 (98%)	305 (97%)	10 (3%)	39	56
1	B	314/323 (97%)	303 (96%)	11 (4%)	36	52
2	E	297/305 (97%)	296 (100%)	1 (0%)	92	97
3	F	402/424 (95%)	385 (96%)	17 (4%)	30	44
4	G	232/237 (98%)	222 (96%)	10 (4%)	29	43
All	All	1560/1612 (97%)	1511 (97%)	49 (3%)	40	57

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	112	ARG
3	F	376	ASN
3	F	145	LEU
3	F	220	THR

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Mol	Chain	Res	Type
3	F	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	376	ASN
3	F	437	ASN
4	G	241	ASN
3	F	440	ASN
3	F	37	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

Of 4 monosaccharides modelled in this entry, 3 were used 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	$\#\|Z\| > 2$
5	GLC	C	2	5	11,11,12	0.66	0	15,15,17	1.63	5 (33%)
5	GLC	C	3	5	11,11,12	0.67	0	15,15,17	1.03	1 (6%)
5	GLC	C	4	5	11,11,12	0.63	0	15,15,17	0.66	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
5	GLC	C	2	5	1/1/4/5	0/2/19/22	0/1/1/1
5	GLC	C	3	5	-	0/2/19/22	0/1/1/1
5	GLC	C	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	GLC	O5-C1-C2	3.62	116.36	110.77
5	C	3	GLC	C1-O5-C5	2.83	116.03	112.19
5	C	2	GLC	O4-C4-C3	-2.70	104.11	110.35
5	C	2	GLC	C3-C4-C5	2.41	114.54	110.24
5	C	2	GLC	C2-C3-C4	2.10	114.54	110.89

All (1) chirality outliers are listed below:

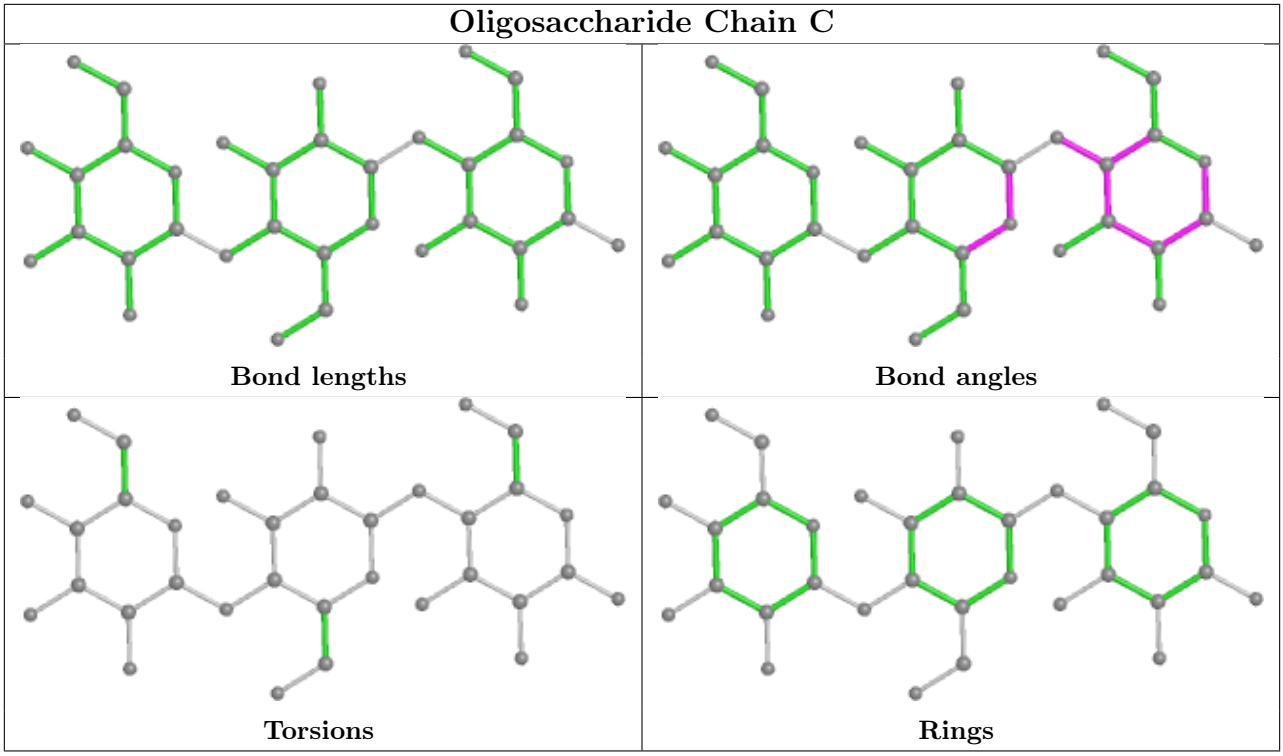
Mol	Chain	Res	Type	Atom
5	C	2	GLC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	UMQ	G	301	-	35,35,35	0.53	1 (2%)	46,46,46	0.97	2 (4%)
7	ANP	A	1502	6	29,33,33	1.73	8 (27%)	31,52,52	1.73	6 (19%)
8	UMQ	G	305	-	23,23,35	0.50	0	28,28,46	0.67	0
7	ANP	B	402	6	29,33,33	1.74	8 (27%)	31,52,52	1.88	6 (19%)
8	UMQ	E	401	-	35,35,35	0.42	0	46,46,46	0.68	0
8	UMQ	F	609	-	12,12,35	0.36	0	11,11,46	0.41	0
9	PGV	F	606	-	50,50,50	1.10	3 (6%)	53,56,56	0.92	2 (3%)
8	UMQ	G	307	-	35,35,35	0.54	1 (2%)	46,46,46	1.01	3 (6%)
9	PGV	F	605	-	50,50,50	1.10	3 (6%)	53,56,56	1.03	3 (5%)
8	UMQ	F	607	-	12,12,35	0.36	0	11,11,46	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	UMQ	G	303	-	12,12,35	0.35	0	11,11,46	0.41	0
8	UMQ	G	302	-	12,12,35	0.38	0	11,11,46	0.43	0
8	UMQ	G	304	-	12,12,35	0.38	0	11,11,46	0.37	0
8	UMQ	G	306	-	12,12,35	0.37	0	11,11,46	0.41	0
8	UMQ	F	608	-	12,12,35	0.38	0	11,11,46	0.37	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
8	UMQ	G	301	-	-	9/20/60/60	0/2/2/2
7	ANP	A	1502	6	-	4/14/38/38	0/3/3/3
8	UMQ	G	305	-	-	8/14/34/60	0/1/1/2
7	ANP	B	402	6	-	4/14/38/38	0/3/3/3
8	UMQ	E	401	-	-	9/20/60/60	0/2/2/2
8	UMQ	F	609	-	-	6/10/10/60	-
9	PGV	F	606	-	-	19/55/55/55	-
8	UMQ	G	307	-	-	14/20/60/60	0/2/2/2
9	PGV	F	605	-	-	23/55/55/55	-
8	UMQ	F	607	-	-	3/10/10/60	-
8	UMQ	G	303	-	-	3/10/10/60	-
8	UMQ	G	302	-	-	4/10/10/60	-
8	UMQ	G	304	-	-	5/10/10/60	-
8	UMQ	G	306	-	-	3/10/10/60	-
8	UMQ	F	608	-	-	2/10/10/60	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	606	PGV	O01-C1	4.46	1.46	1.34
9	F	605	PGV	O01-C1	4.44	1.46	1.34
9	F	606	PGV	O03-C19	4.38	1.46	1.33
9	F	605	PGV	O03-C19	4.11	1.45	1.33
7	B	402	ANP	PB-N3B	3.88	1.73	1.63

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	402	ANP	O1G-PG-N3B	-5.31	103.95	111.77
7	A	1502	ANP	O2B-PB-O1B	4.86	120.11	109.92
7	B	402	ANP	O2B-PB-O1B	4.27	118.88	109.92
7	A	1502	ANP	O1G-PG-N3B	-4.05	105.81	111.77
7	B	402	ANP	N3-C2-N1	-3.90	122.58	128.68

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1502	ANP	PB-N3B-PG-O1G
7	A	1502	ANP	PG-N3B-PB-O1B
7	A	1502	ANP	PA-O3A-PB-O1B
7	A	1502	ANP	PA-O3A-PB-O2B
7	B	402	ANP	PB-N3B-PG-O1G

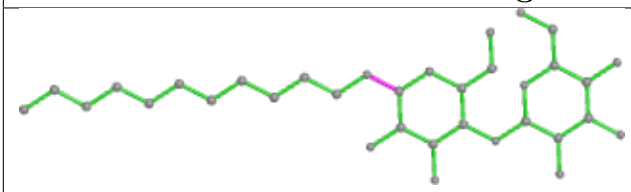
There are no ring outliers.

2 monomers are involved in 2 short contacts:

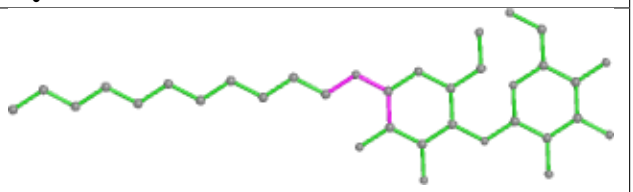
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	402	ANP	1	0
8	G	307	UMQ	1	0

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

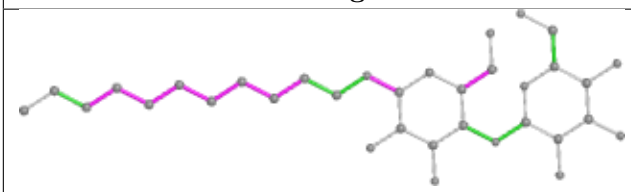
Ligand UMQ G 301



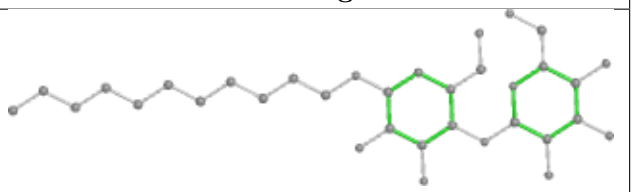
Bond lengths



Bond angles

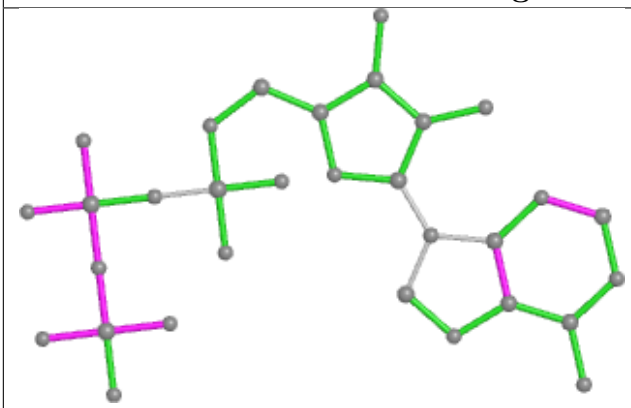


Torsions

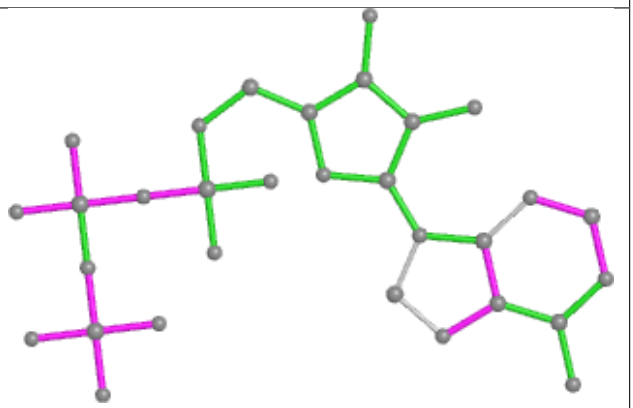


Rings

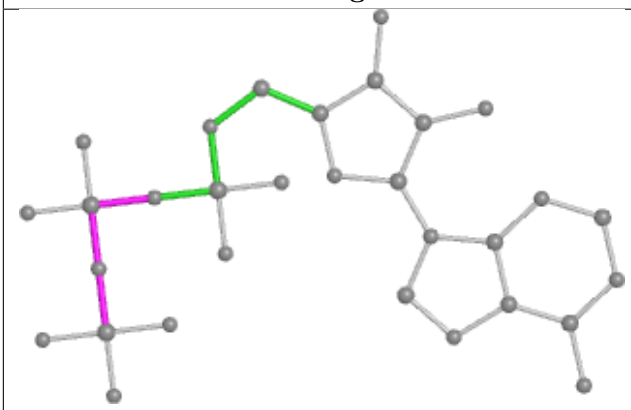
Ligand ANP A 1502



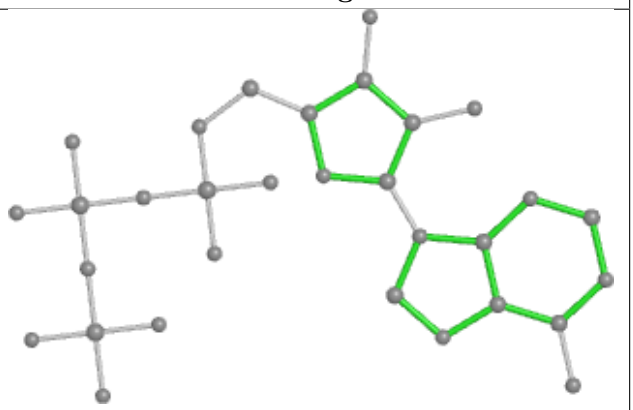
Bond lengths



Bond angles

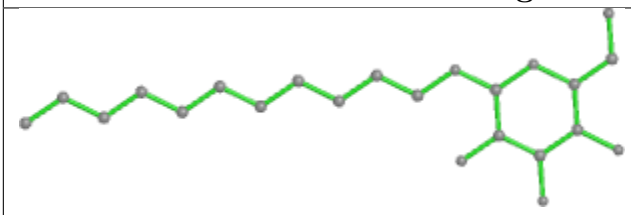


Torsions

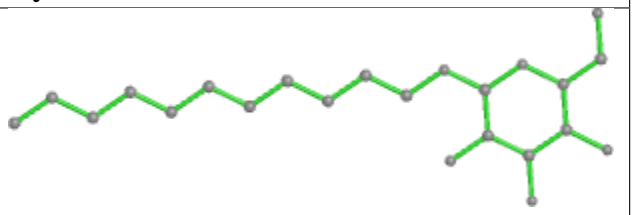


Rings

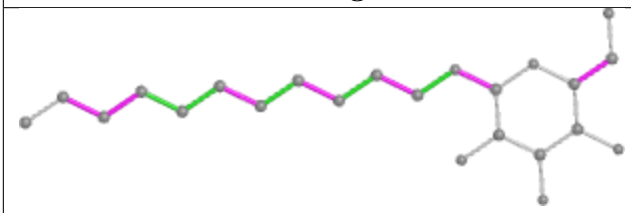
Ligand UMQ G 305



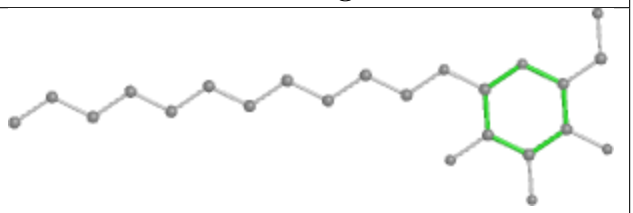
Bond lengths



Bond angles

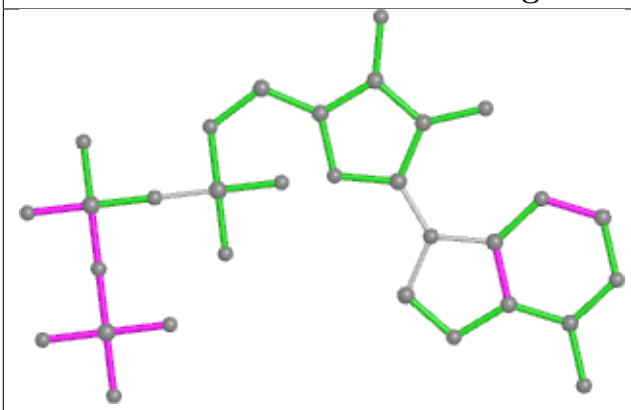


Torsions

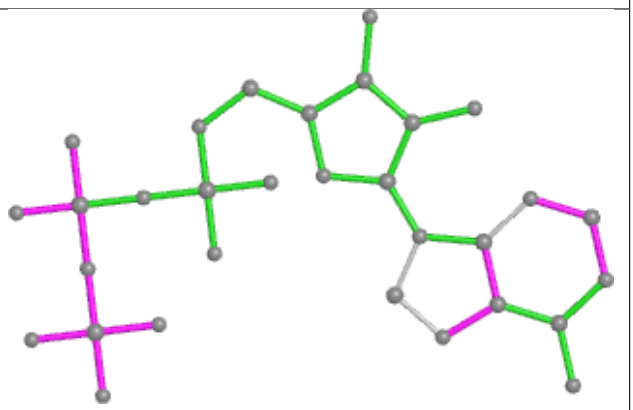


Rings

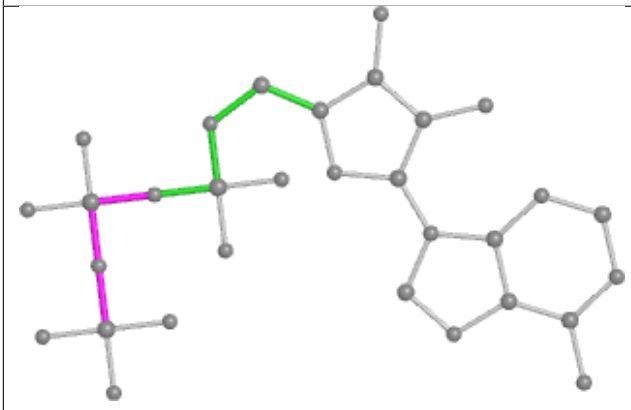
Ligand ANP B 402



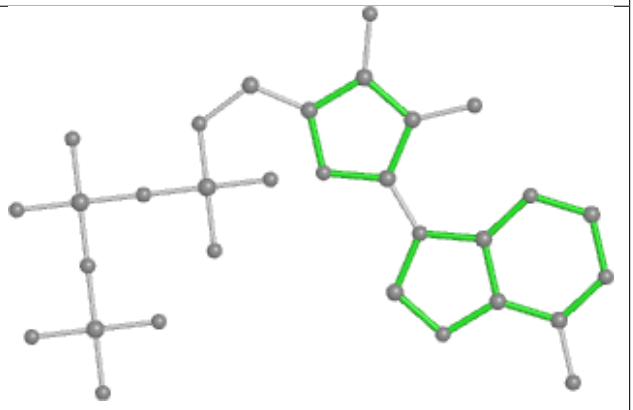
Bond lengths



Bond angles

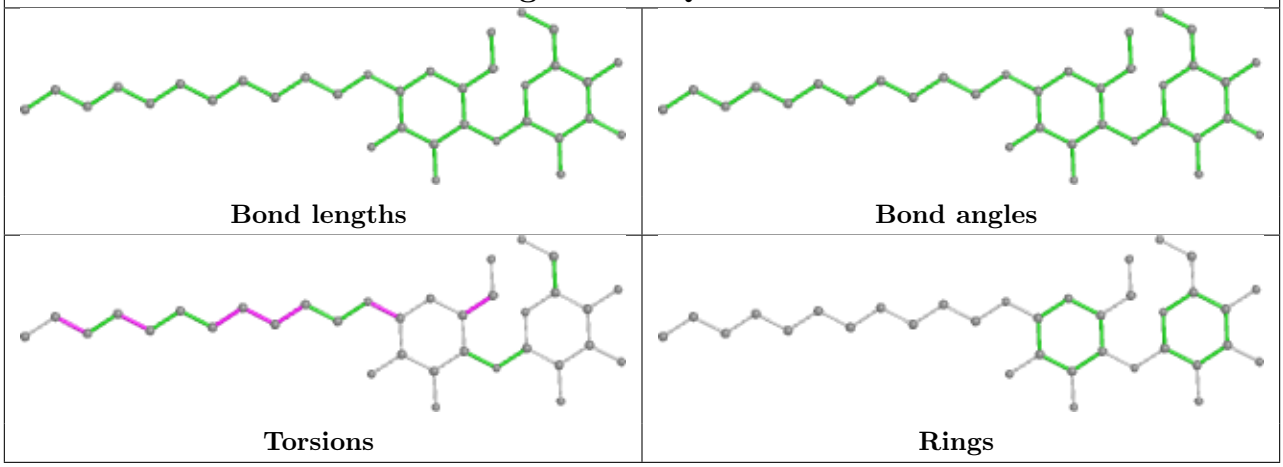


Torsions

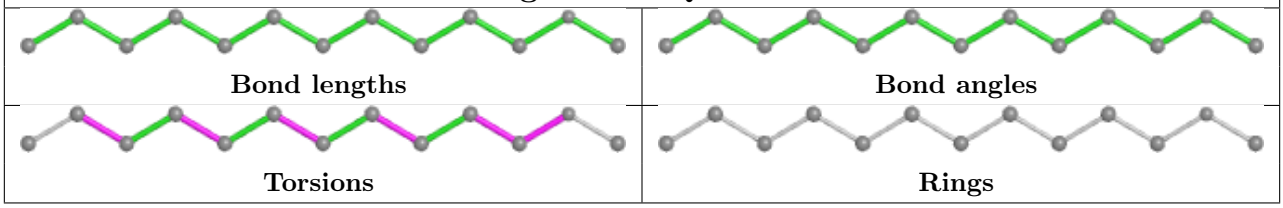


Rings

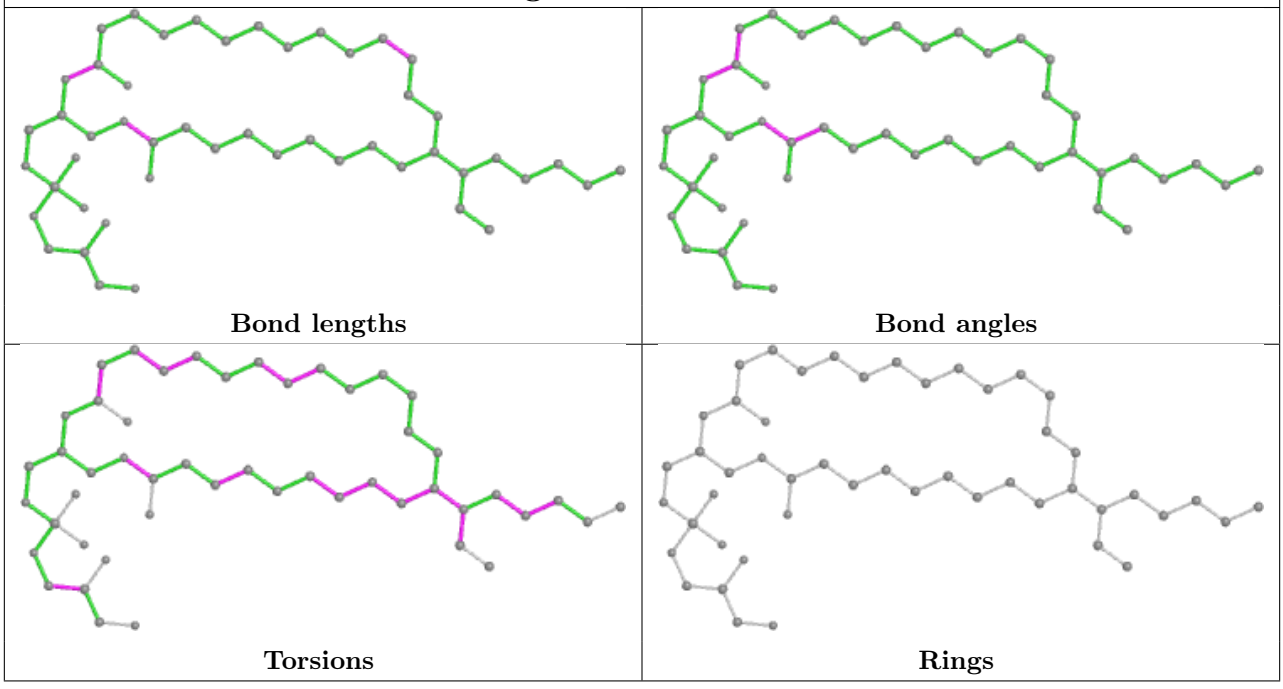
Ligand UMQ E 401



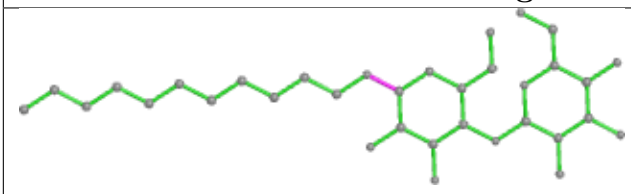
Ligand UMQ F 609

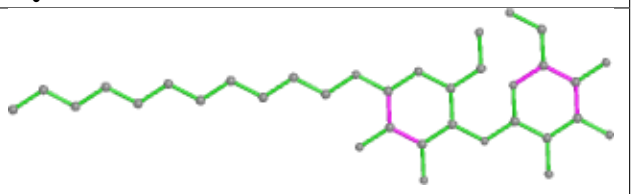


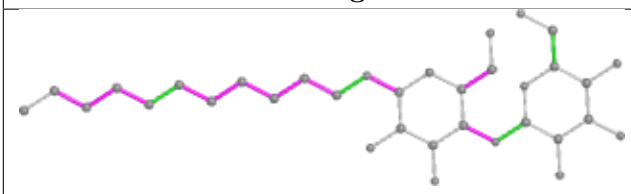
Ligand PGV F 606

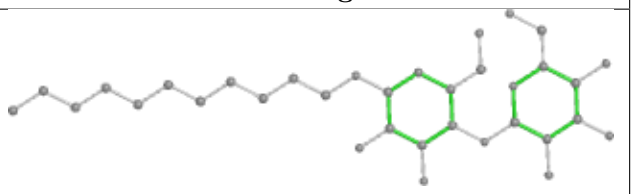


Ligand UMQ G 307

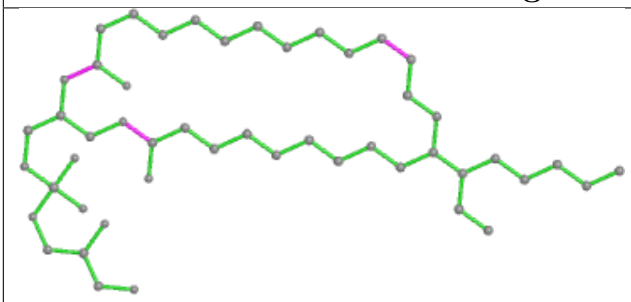

Bond lengths

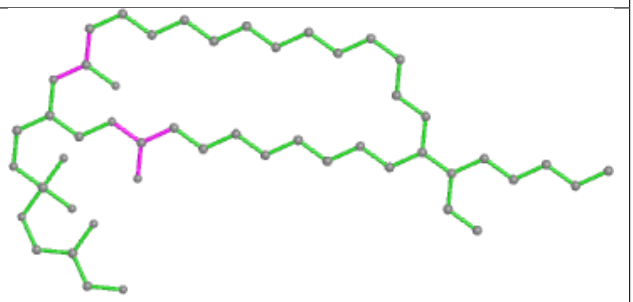

Bond angles

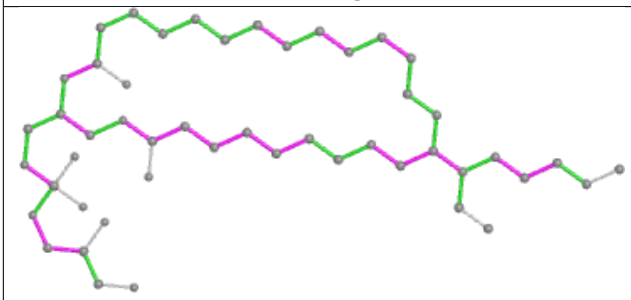

Torsions

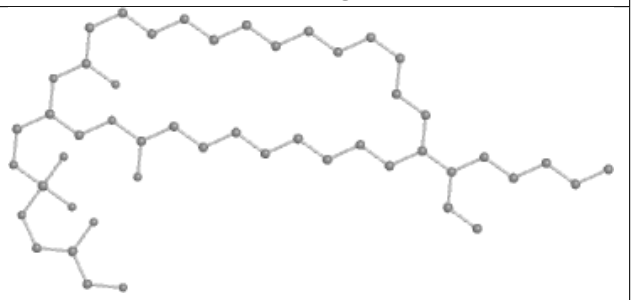

Rings

Ligand PGV F 605


Bond lengths

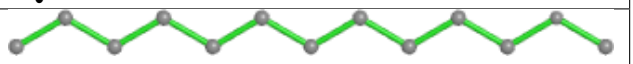

Bond angles


Torsions


Rings

Ligand UMQ F 607

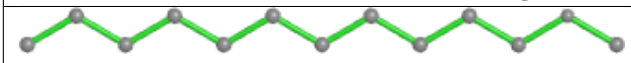

Bond lengths

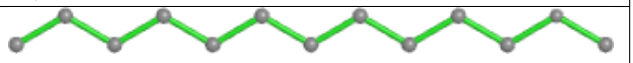

Bond angles


Torsions


Rings

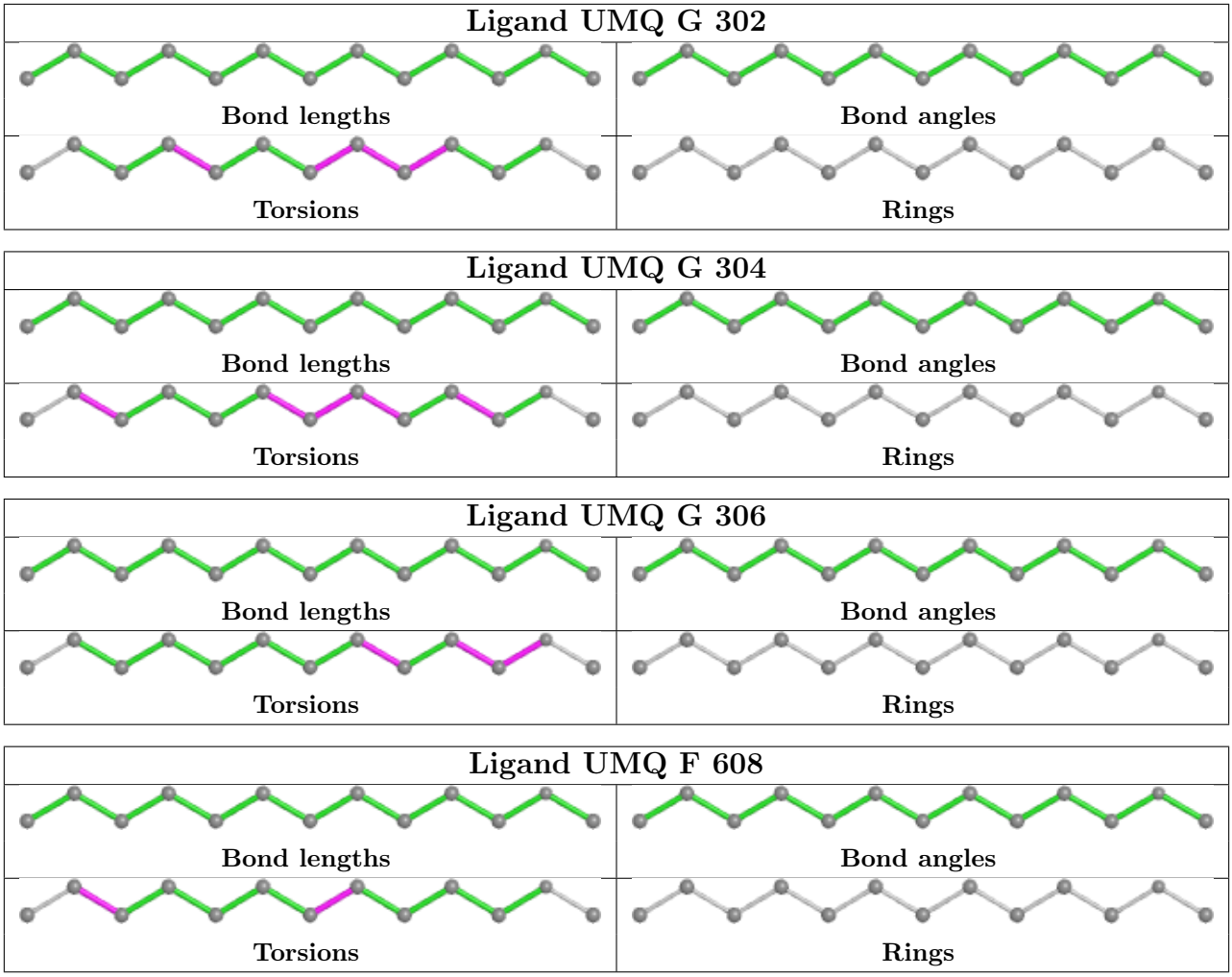
Ligand UMQ G 303


Bond lengths


Bond angles


Torsions


Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	371/381 (97%)	0.24	19 (5%) 28 30	54, 79, 108, 126	0
1	B	371/381 (97%)	0.52	43 (11%) 4 5	54, 92, 147, 170	0
2	E	370/380 (97%)	0.21	27 (7%) 15 16	59, 83, 111, 132	0
3	F	490/514 (95%)	0.43	41 (8%) 11 12	53, 85, 134, 153	0
4	G	289/296 (97%)	0.24	15 (5%) 27 30	51, 71, 115, 148	0
All	All	1891/1952 (96%)	0.34	145 (7%) 13 14	51, 82, 130, 170	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	ALA	9.2
1	B	251	ILE	8.5
1	B	295	ILE	6.8
4	G	70	ALA	6.8
4	G	71	ASP	6.3

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.

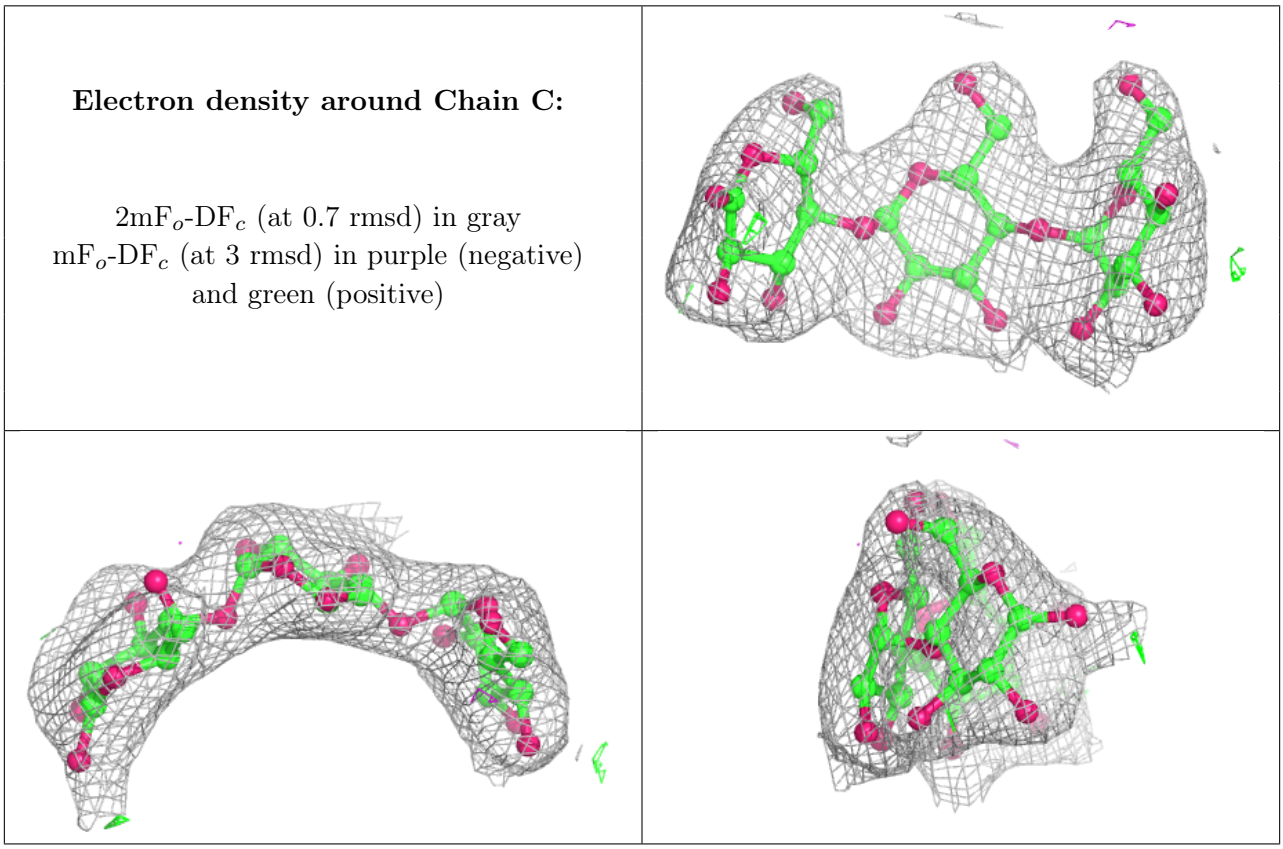
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLC	C	1	1/12	0.82	0.27	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLC	C	2	11/12	0.94	0.12	73,80,87,95	0
5	GLC	C	3	11/12	0.98	0.08	61,64,68,68	0
5	GLC	C	4	11/12	0.99	0.08	61,62,66,67	0

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UMQ	G	306	13/34	0.67	0.29	90,99,118,119	0
8	UMQ	G	301	34/34	0.68	0.33	91,132,157,158	0
8	UMQ	F	608	13/34	0.71	0.28	97,100,115,115	0
8	UMQ	G	307	34/34	0.75	0.34	99,135,156,157	0
8	UMQ	G	305	23/34	0.79	0.22	94,106,127,136	0

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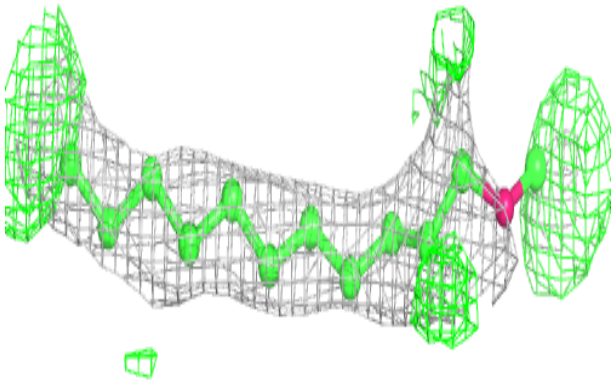
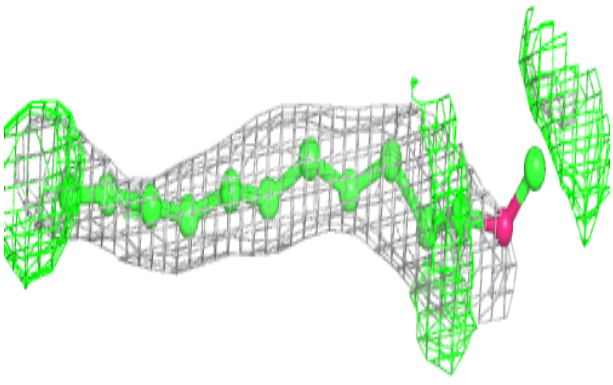
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PGV	F	606	51/51	0.79	0.24	86,106,129,134	0
8	UMQ	F	607	13/34	0.81	0.26	87,90,92,94	0
8	UMQ	G	302	13/34	0.81	0.21	86,93,96,99	0
8	UMQ	F	609	13/34	0.81	0.36	95,101,111,111	0
8	UMQ	G	304	13/34	0.82	0.28	88,100,110,111	0
8	UMQ	G	303	13/34	0.87	0.19	78,86,99,101	0
9	PGV	F	605	51/51	0.88	0.23	89,98,109,111	0
8	UMQ	E	401	34/34	0.94	0.20	80,87,96,97	0
7	ANP	B	402	31/31	0.96	0.11	58,70,84,89	0
6	MG	B	401	1/1	0.96	0.10	59,59,59,59	0
7	ANP	A	1502	31/31	0.98	0.11	55,62,75,81	0
6	MG	A	1501	1/1	0.99	0.04	57,57,57,57	0

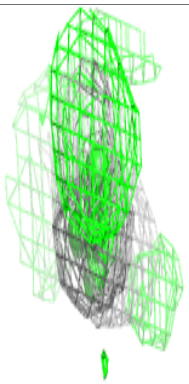
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMQ G 306:

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

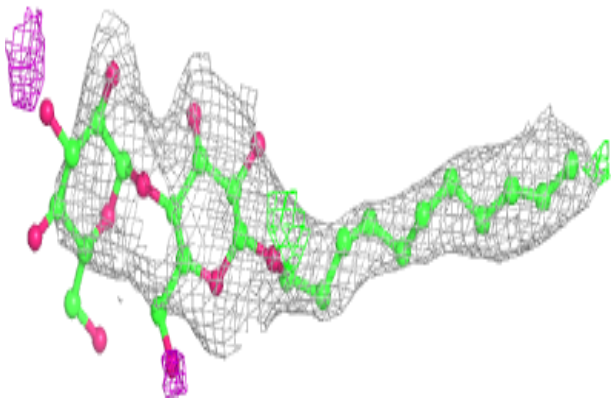


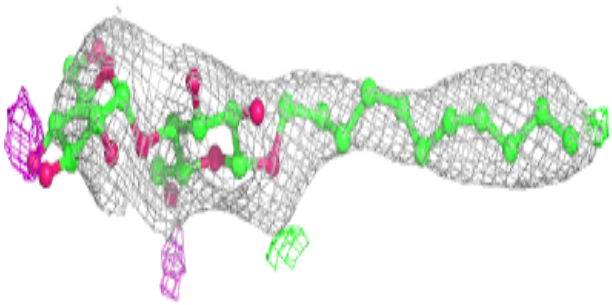


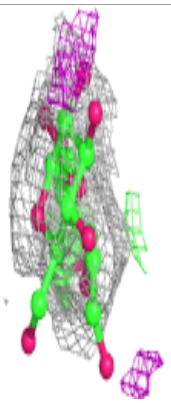


Electron density around UMQ G 301:

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

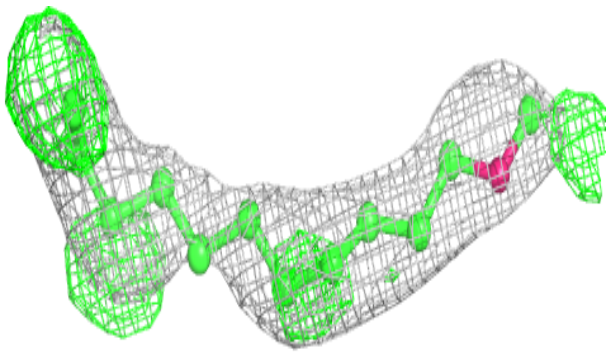


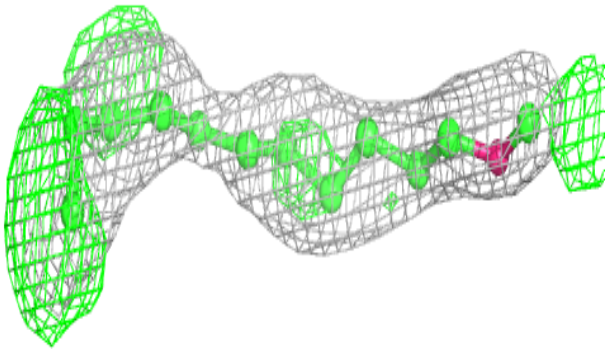


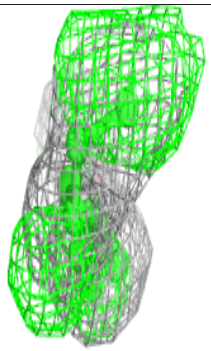


Electron density around UMQ F 608:

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

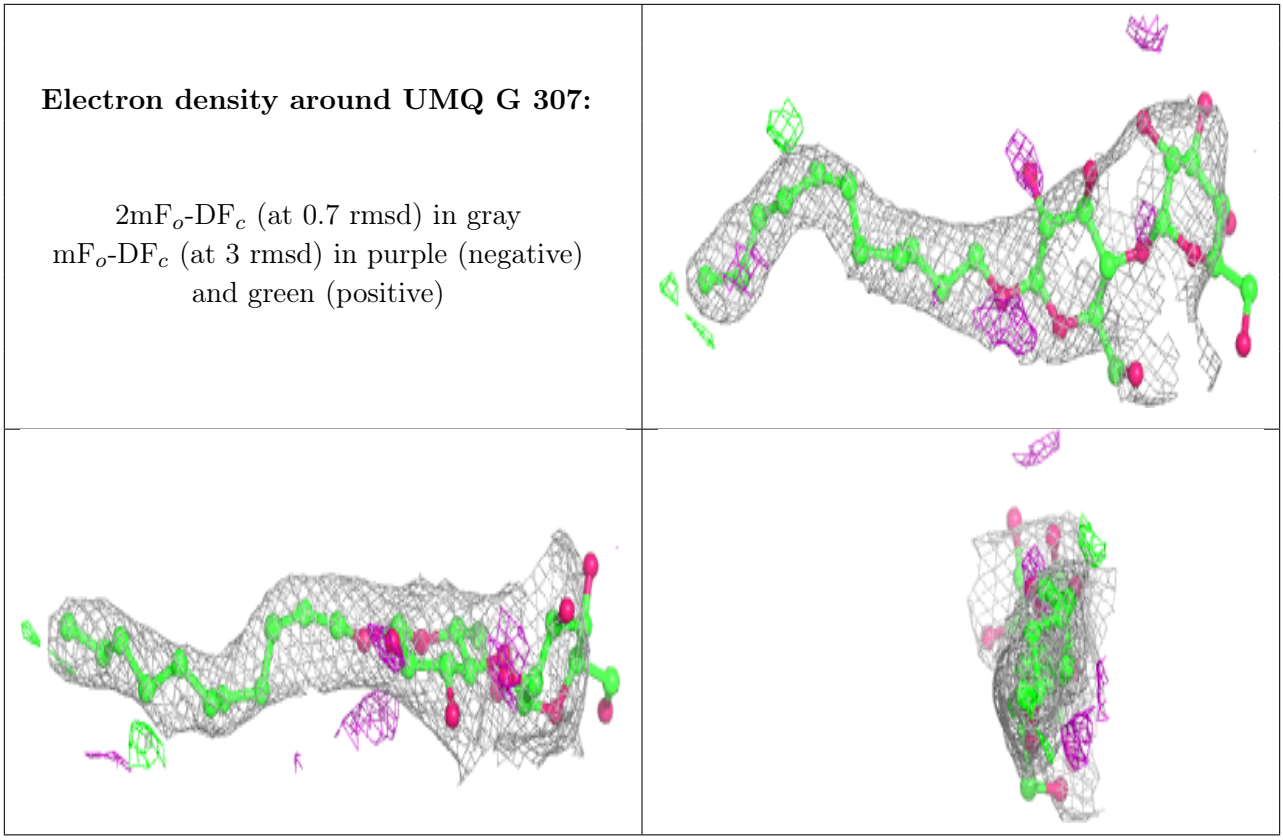






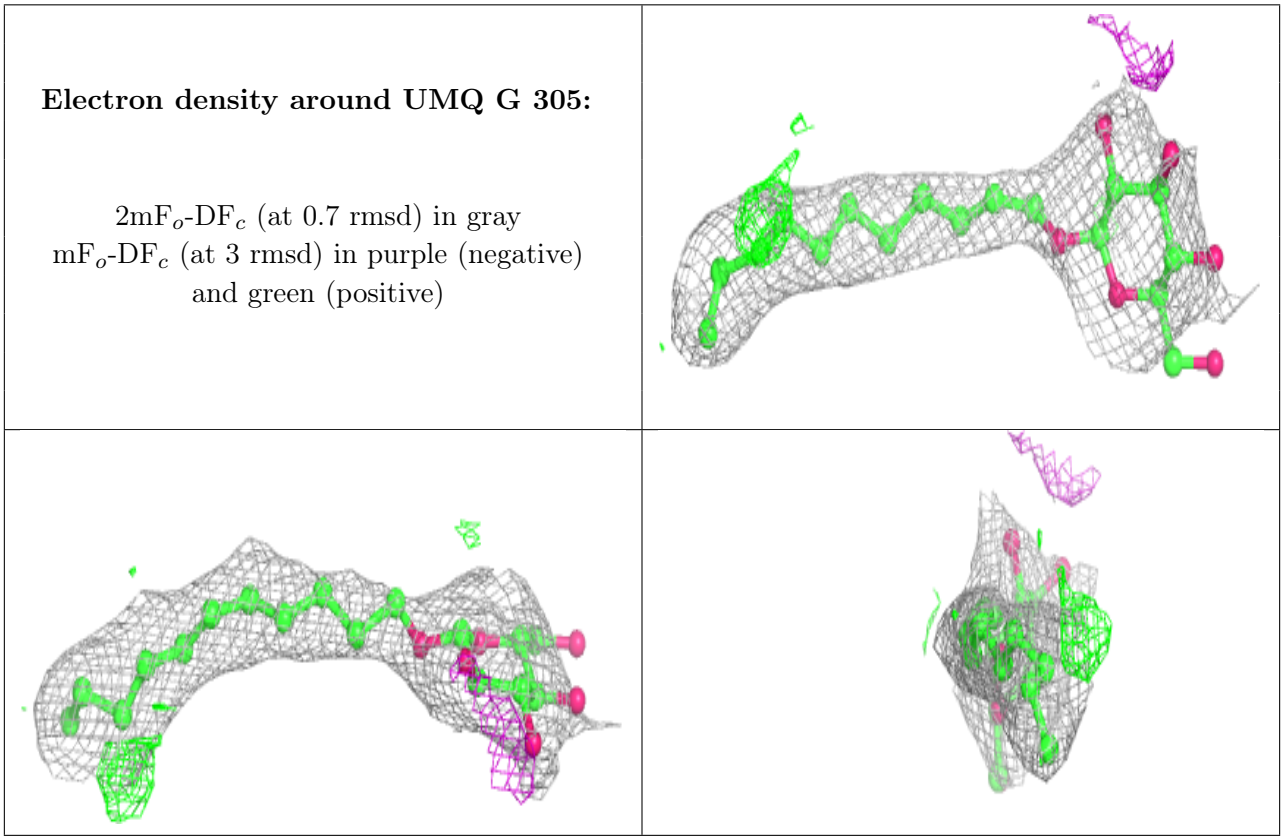
Electron density around UMQ G 307:

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



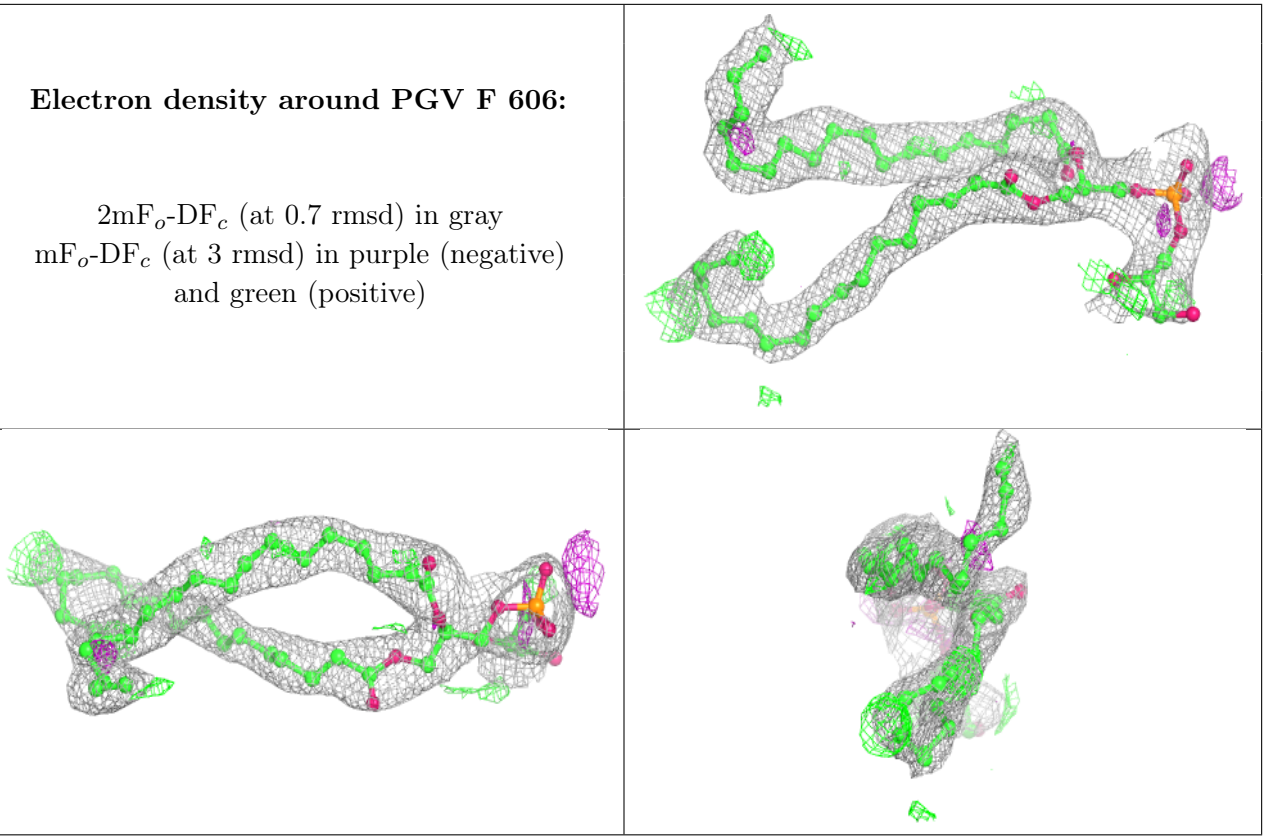
Electron density around UMQ G 305:

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



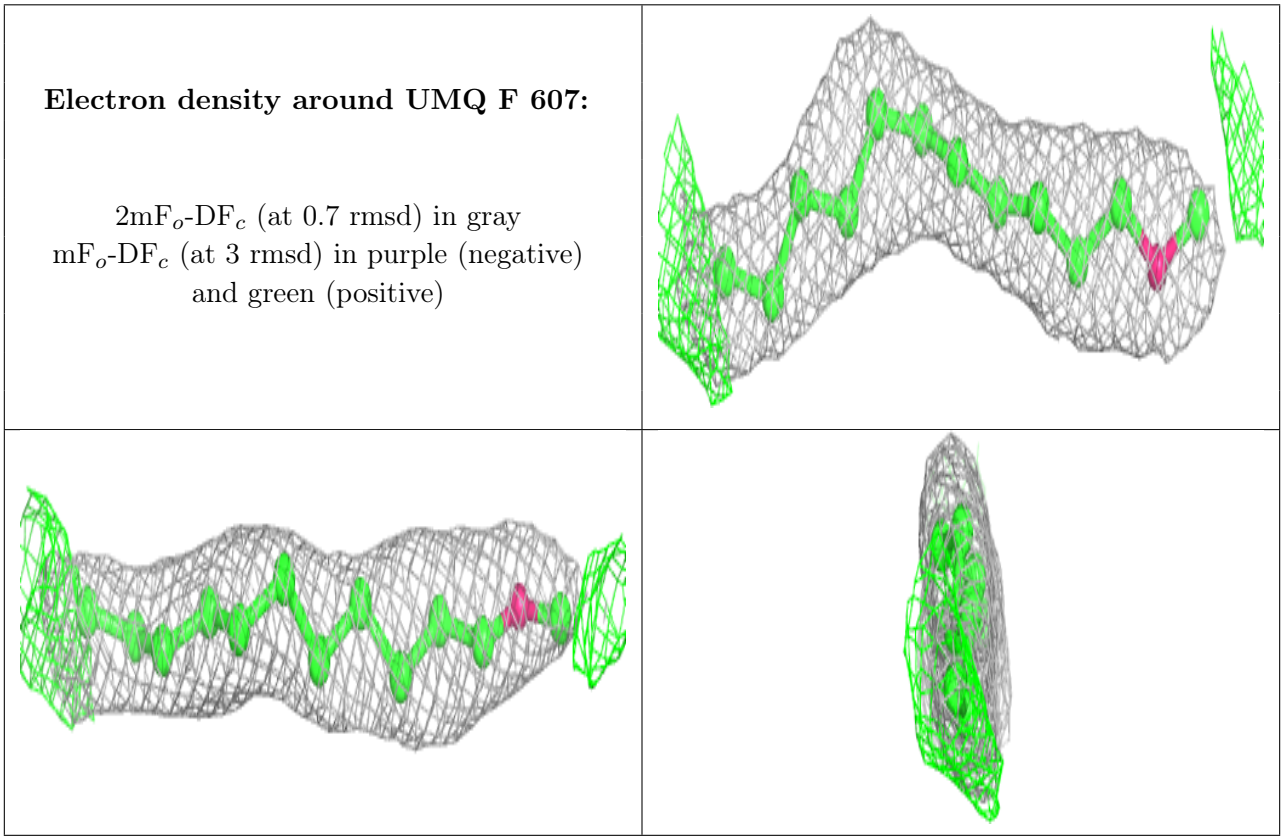
Electron density around PGV F 606:

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



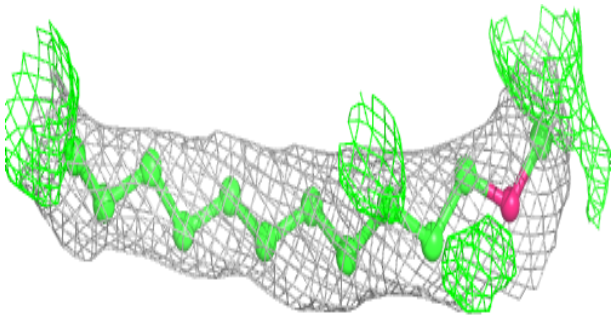
Electron density around UMQ F 607:

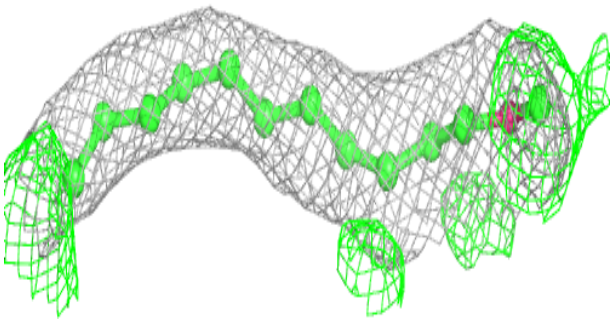
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

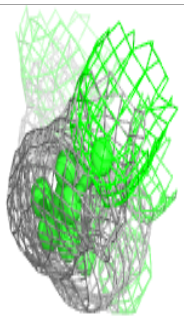


Electron density around UMQ G 302:

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

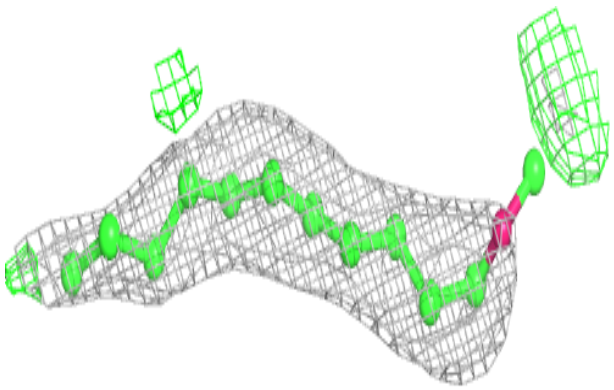


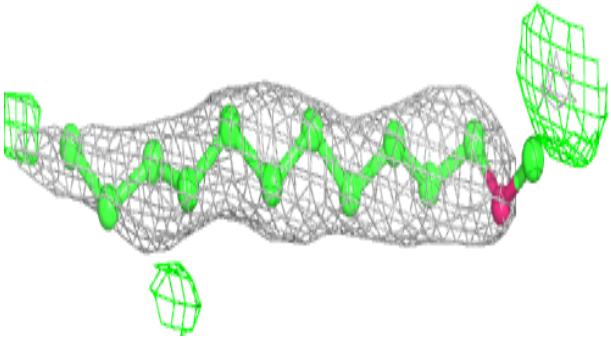


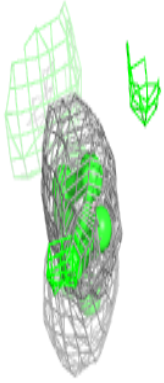


Electron density around UMQ F 609:

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

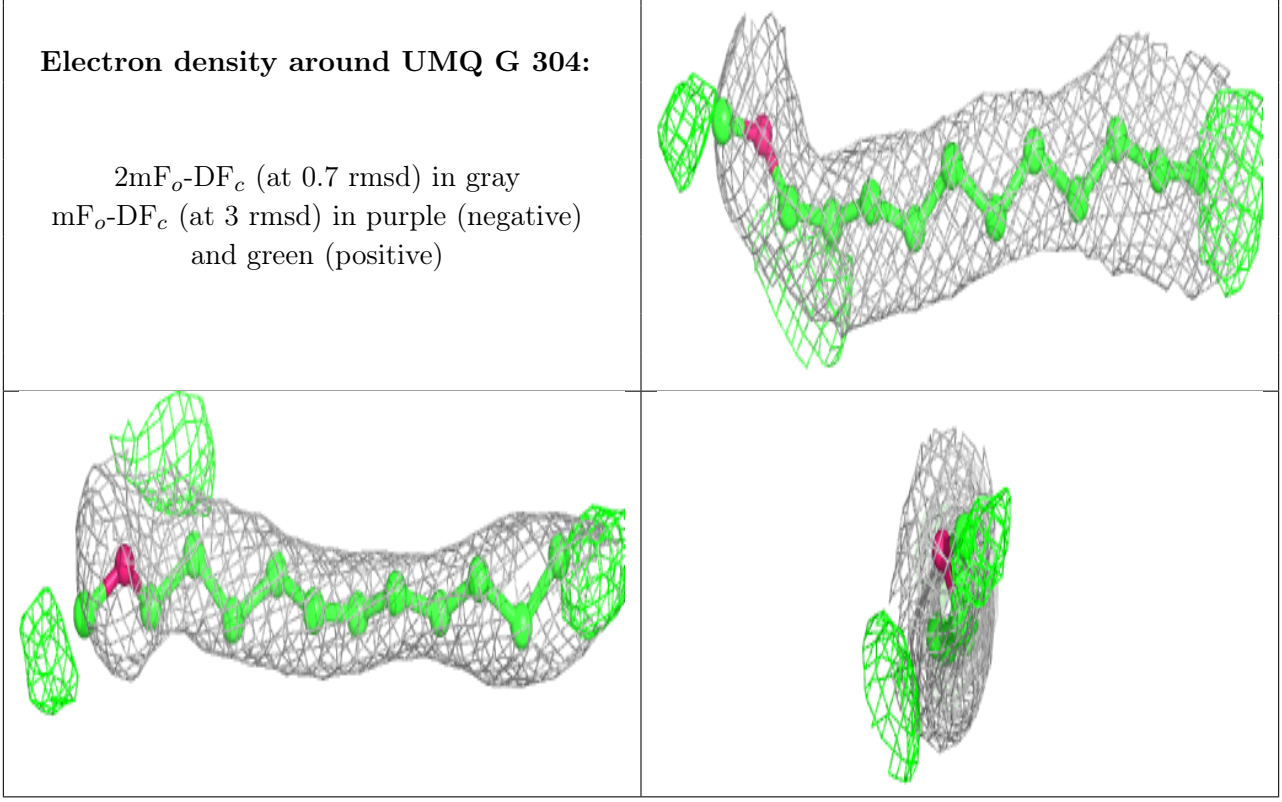






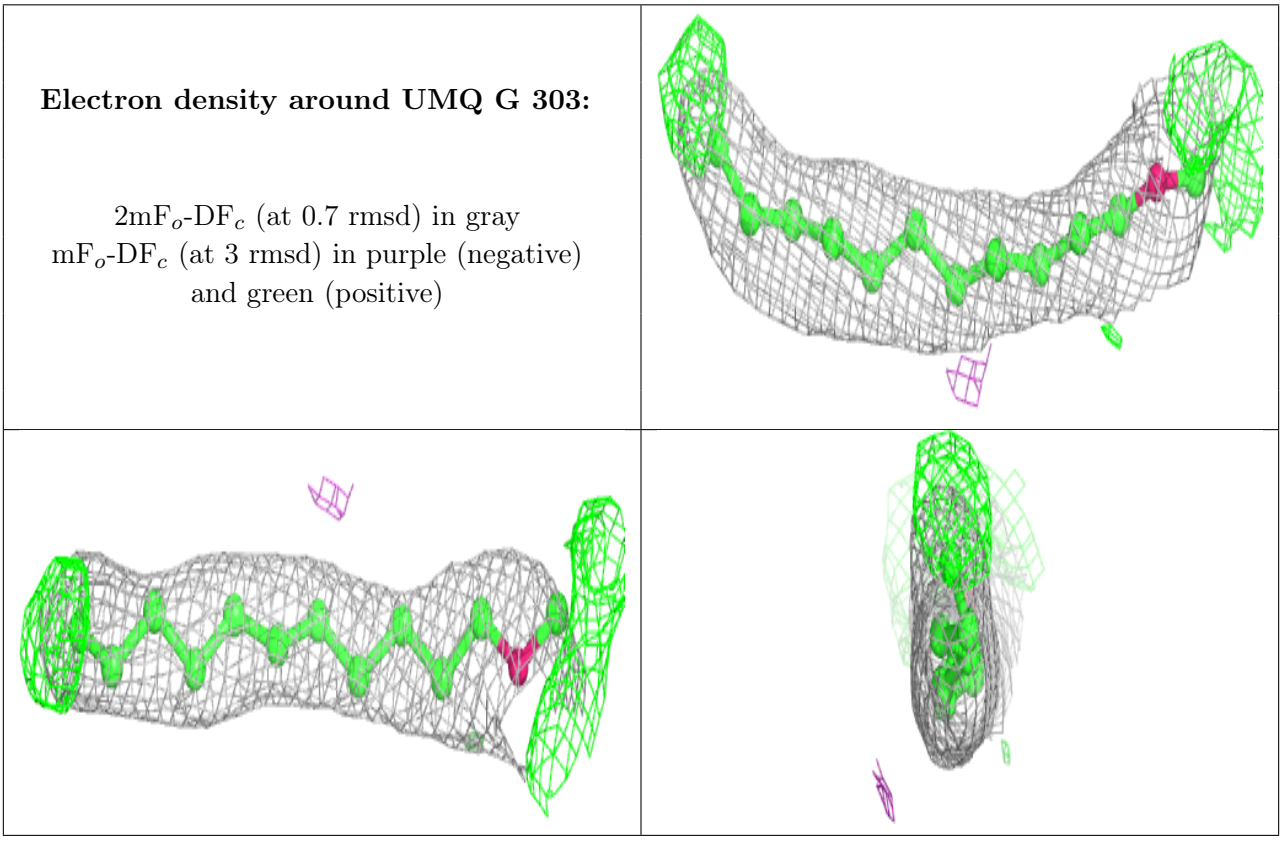
Electron density around UMQ G 304:

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



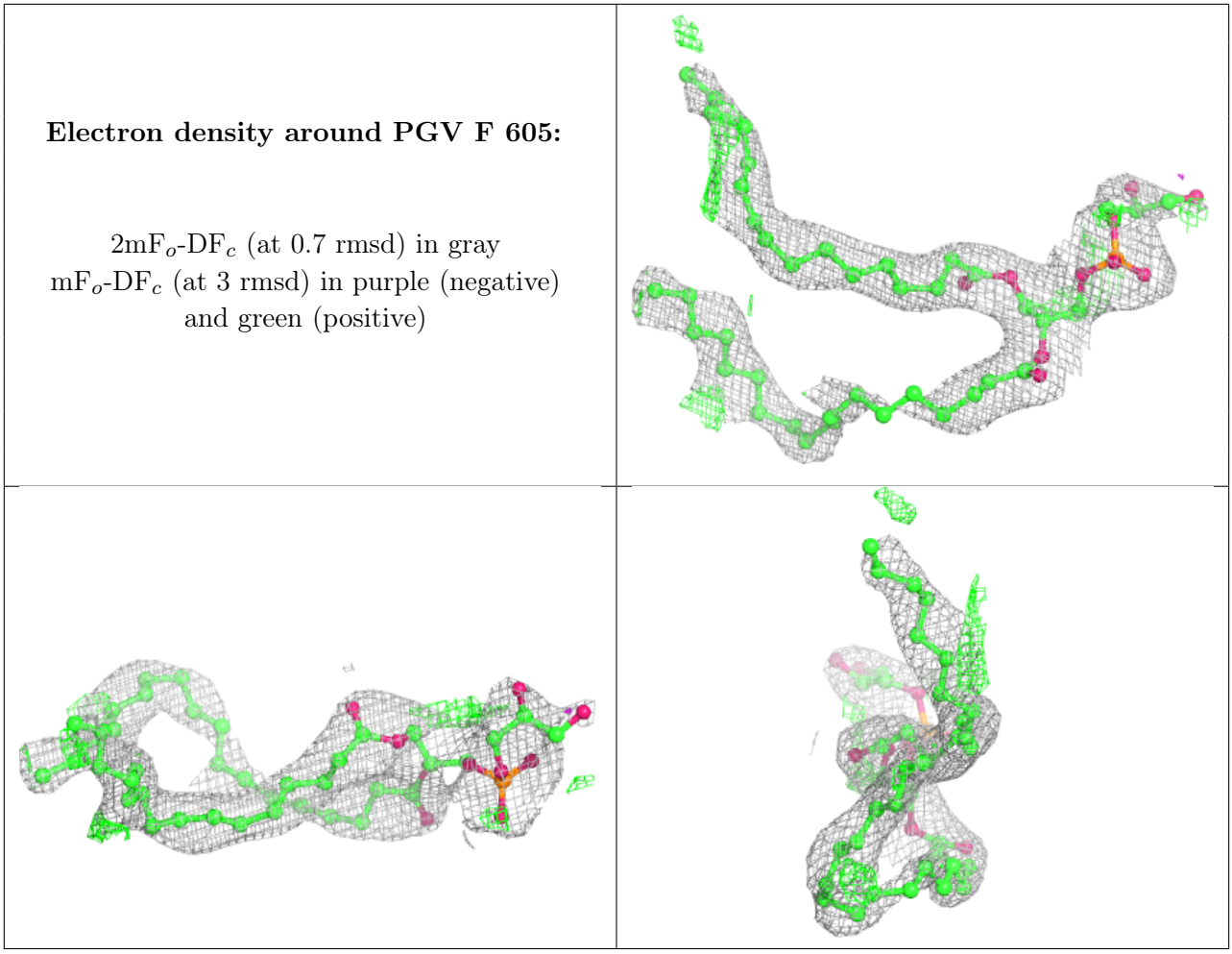
Electron density around UMQ G 303:

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



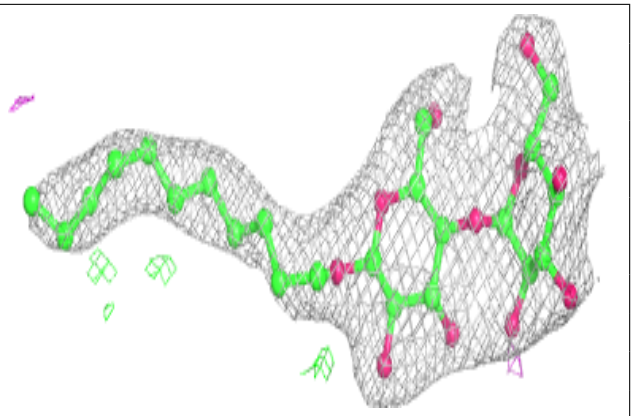
Electron density around PGV F 605:

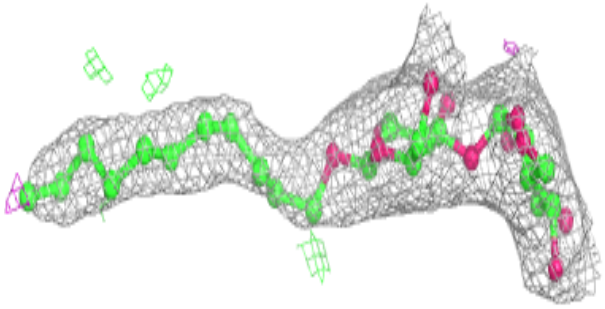
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

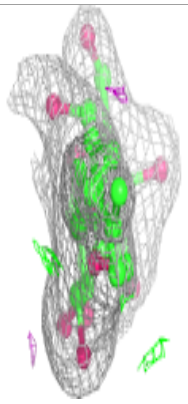


Electron density around UMQ E 401:

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

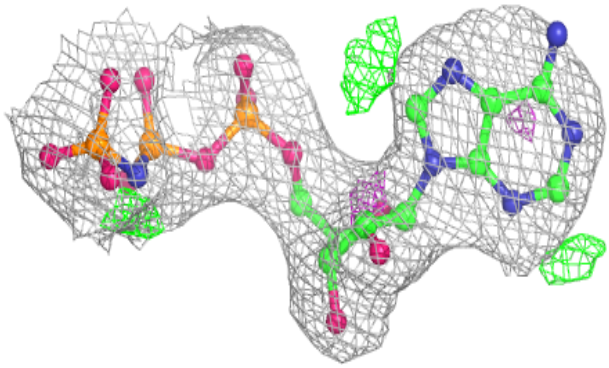


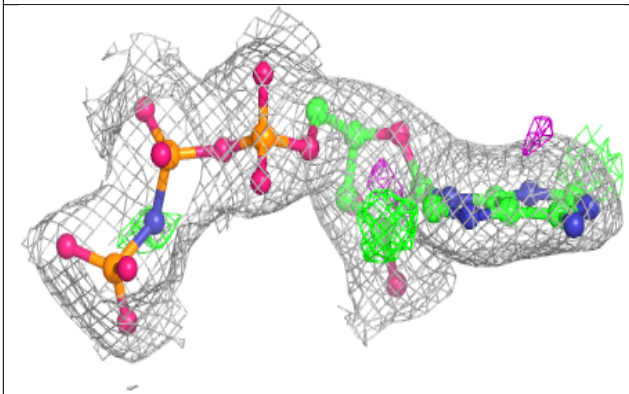


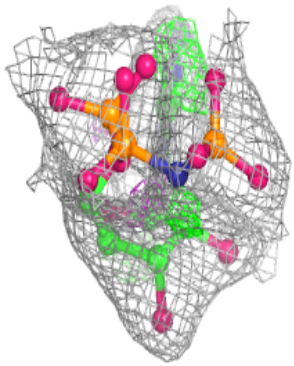


Electron density around ANP B 402:

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

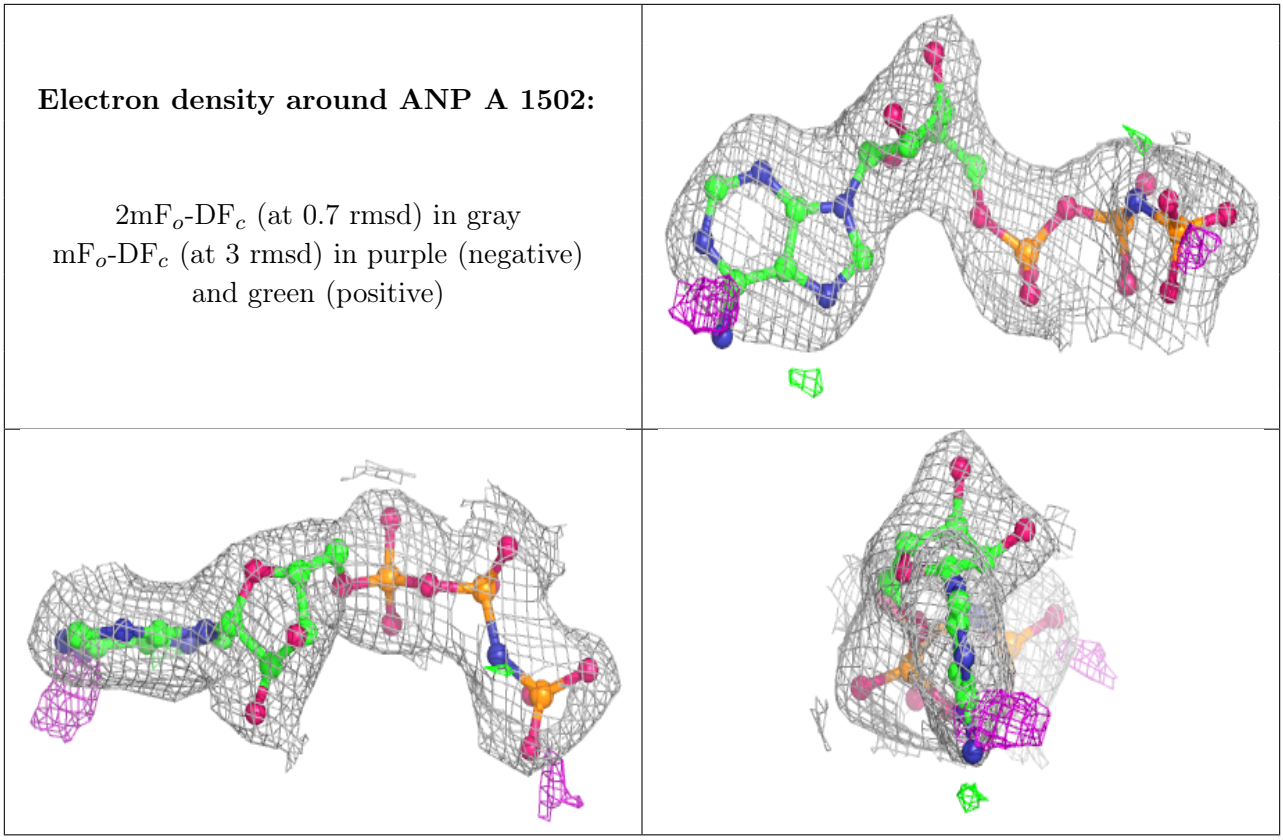






Electron density around ANP A 1502:

$2mF_o$-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.