



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:52 PM BST

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 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

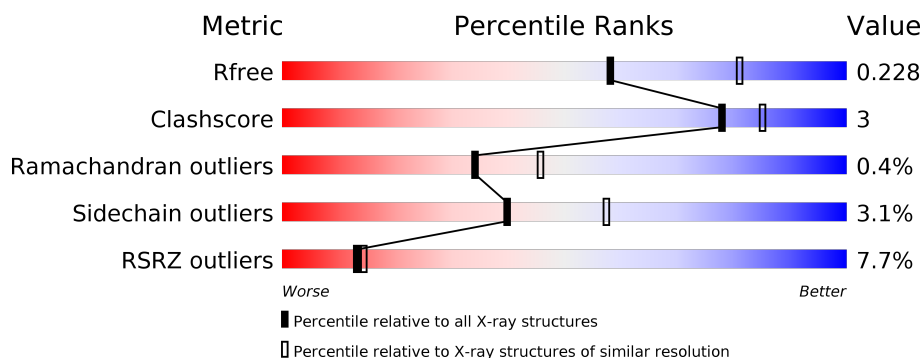
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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 on 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	381	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
1	B	381	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>
2	E	380	<div> <div>7%</div> <div> <div></div> <div>94%</div> <div>•</div> <div>•</div> </div> </div>
3	F	514	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>•</div> <div>5%</div> </div> </div>
4	G	296	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> <div>•</div> </div> </div>
5	C	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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
2	E	370	Total	C	N	O	S	0	0	0
			2877	1853	469	549	6			

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
3	F	490	Total	C	N	O	S	0	1	0
			3819	2512	607	683	17			

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

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

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

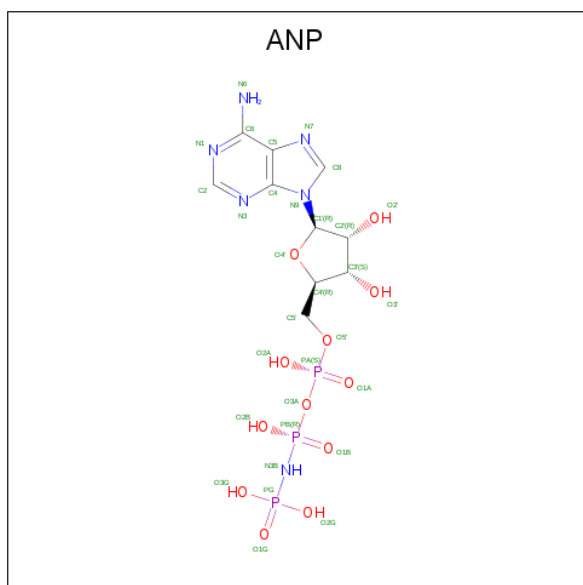


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	4	Total	C	O	0	0	1
			34	18	16			

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

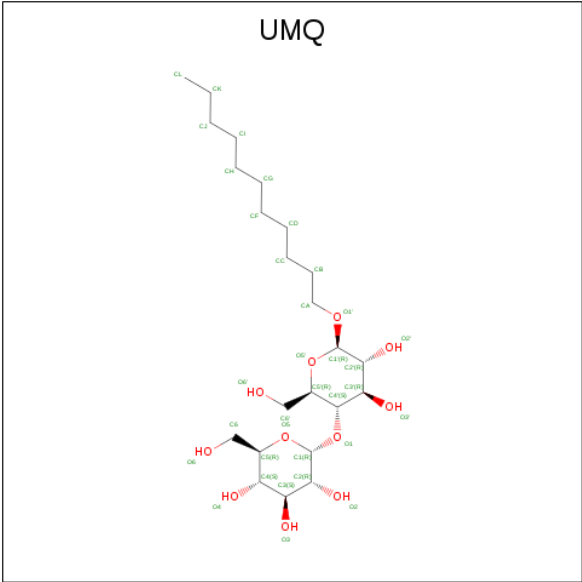
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

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



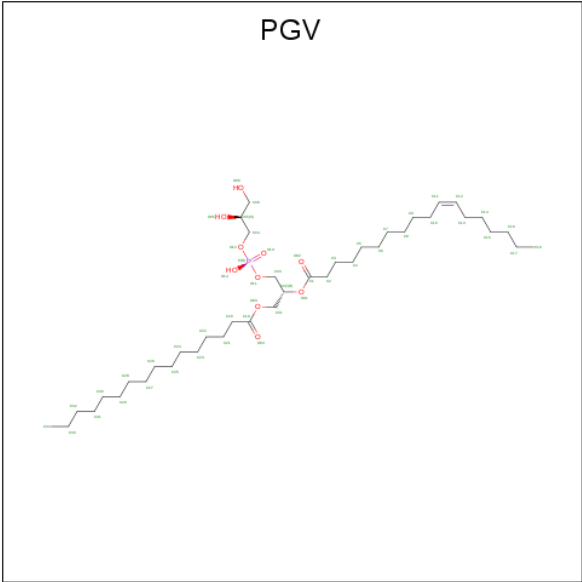
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- 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	0	0
			34	23	11		
8	F	1	Total	C	O	0	0
			13	12	1		
8	F	1	Total	C	O	0	0
			13	12	1		
8	F	1	Total	C	O	0	0
			13	12	1		
8	G	1	Total	C	O	0	0
			34	23	11		
8	G	1	Total	C	O	0	0
			13	12	1		
8	G	1	Total	C	O	0	0
			13	12	1		
8	G	1	Total	C	O	0	0
			13	12	1		
8	G	1	Total	C	O	0	0
			23	17	6		
8	G	1	Total	C	O	0	0
			13	12	1		
8	G	1	Total	C	O	0	0
			34	23	11		

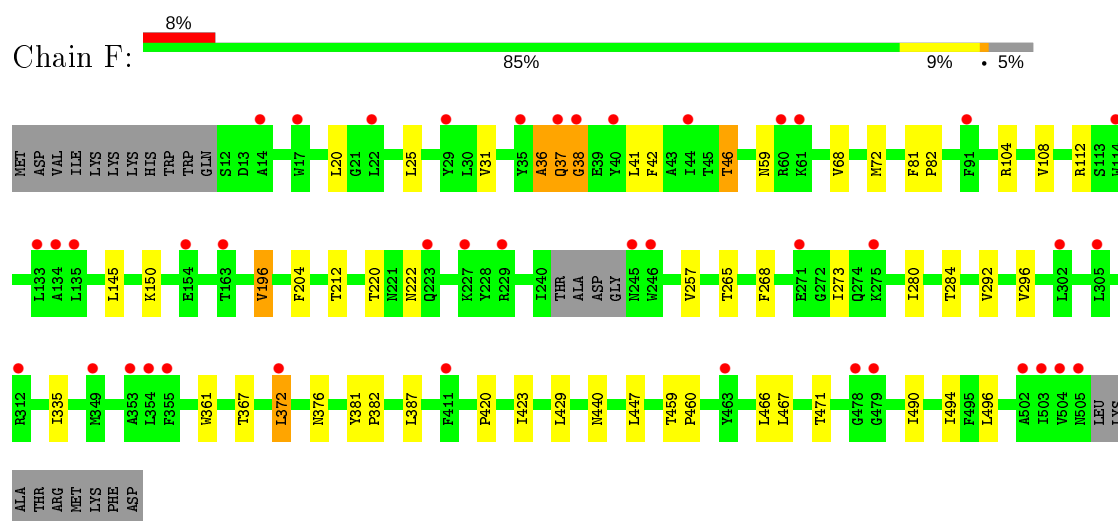
- Molecule 9 is (1R)-2-[[[(2S)-2,3-dihydroxypropyl]oxy](hydroxy)phosphoryl]oxy-1-[(palmitoyloxy)methyl]ethyl (11E)-octadec-11-enoate (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



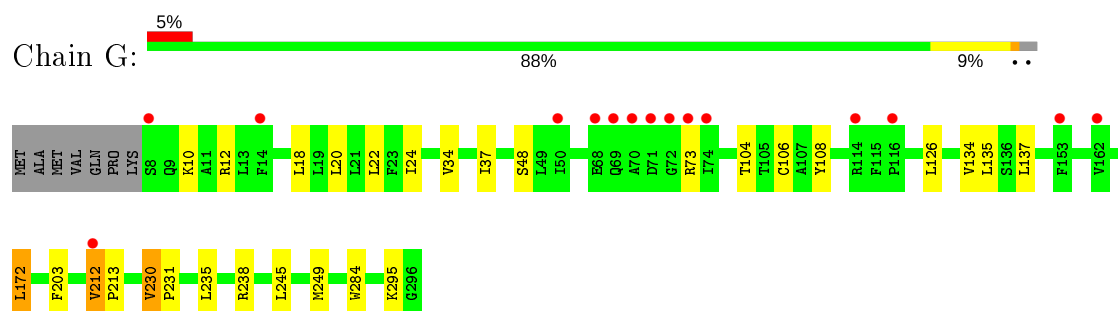
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	F	1	Total	C	O	P	0	0
			51	40	10	1		
9	F	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 10 is water.

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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.59 Å 96.63 Å 112.32 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.38 Å)	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	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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.*

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: PGV, ANP, MG, GLC, UMQ

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 [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	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.

All (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
3:F:284:THR:HG22	3:F:466:LEU:HA	1.77	0.66
3:F:280:ILE:O	3:F:284:THR:HG23	1.97	0.64
1:A:100:LEU:O	1:A:103:ALA:O	2.14	0.63
1:B:45:LEU:HD12	1:B:207:LEU:HD11	1.82	0.62
4:G:238:ARG:NH1	10:G:474:HOH:O	2.34	0.60
3:F:212:THR:HG23	3:F:222:ASN:HD21	1.68	0.58
1:B:364:ARG:NH1	10:B:563:HOH:O	2.35	0.57
3:F:387:LEU:HD13	3:F:429:LEU:HD13	1.85	0.57
1:A:260:MET:HE2	1:A:300:LEU:HD22	1.87	0.57
3:F:372:LEU:HD13	3:F:447:LEU:HD23	1.86	0.57
3:F:36:ALA:O	3:F:38:GLY:N	2.38	0.56
1:A:260:MET:CE	1:A:300:LEU:HD22	2.36	0.55
3:F:196:VAL:CG1	3:F:204:PHE:HB3	2.37	0.55
1:B:122:GLN:NE2	10:B:576:HOH:O	2.39	0.55
1:B:194:GLN:NE2	10:B:598:HOH:O	2.40	0.54
4:G:20:LEU:O	4:G:24:ILE:HG12	2.07	0.54
3:F:335:ILE:CD1	4:G:34:VAL:HG22	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:284:THR:HG21	3:F:467:LEU:H	1.73	0.53
2:E:43:LEU:HD12	2:E:43:LEU:C	2.30	0.52
1:B:236:SER:HA	1:B:237:PRO:C	2.30	0.52
1:A:288:GLU:HG2	1:B:312:ASN:HB2	1.93	0.51
1:A:16:VAL:HG11	10:A:1702:HOH:O	2.09	0.51
3:F:273:ILE:HG22	3:F:459:THR:HG21	1.93	0.51
4:G:212:VAL:HG22	4:G:284[A]:TRP:CE3	2.45	0.51
3:F:335:ILE:HD12	4:G:34:VAL:HG22	1.92	0.51
3:F:265:THR:O	3:F:268:PHE:N	2.44	0.50
1:A:42:LYS:HD2	1:A:190:VAL:HG13	1.93	0.50
1:A:327:LEU:CD2	1:A:345:ILE:HD11	2.41	0.50
4:G:134:VAL:HG23	4:G:135:LEU:CD1	2.42	0.50
3:F:196:VAL:HG13	3:F:204:PHE:HB3	1.93	0.50
2:E:341:TYR:CE2	3:F:460:PRO:HB2	2.47	0.50
3:F:471:THR:CG2	3:F:490:ILE:HG21	2.42	0.50
1:A:19:SER:HB3	1:A:22:ILE:HD12	1.94	0.49
1:A:291:LEU:HD12	10:A:1679:HOH:O	2.12	0.49
1:A:148:LEU:CD2	1:A:179:LEU:HD22	2.42	0.49
2:E:61:PHE:CE2	2:E:264:ALA:HB2	2.49	0.48
4:G:134:VAL:HG23	4:G:135:LEU:HD13	1.95	0.47
1:A:187:MET:HB3	10:A:1678:HOH:O	2.13	0.47
1:A:286:ARG:HB3	1:A:288:GLU:OE1	2.14	0.47
1:A:2:ALA:N	10:A:1672:HOH:O	2.48	0.47
3:F:471:THR:HG21	3:F:490:ILE:HG21	1.97	0.47
1:A:208:ASP:HB2	1:A:229:PHE:CE2	2.49	0.47
1:B:268:LEU:HD22	1:B:352:CYS:HB2	1.96	0.47
4:G:104:THR:HG22	4:G:203:PHE:HZ	1.80	0.47
3:F:68:VAL:HG12	3:F:72:MET:HG2	1.97	0.47
1:B:194:GLN:O	1:B:198:MET:HG2	2.16	0.46
4:G:212:VAL:HG12	4:G:213:PRO:HD3	1.97	0.46
3:F:361:TRP:NE1	10:F:758:HOH:O	2.36	0.46
3:F:372:LEU:CD1	3:F:447:LEU:HD23	2.45	0.46
4:G:230:VAL:HB	4:G:231:PRO:HD3	1.97	0.46
1:A:146:ARG:HD2	10:A:1610:HOH:O	2.14	0.46
1:A:260:MET:HE3	1:A:323:ILE:HD11	1.98	0.46
1:A:137:GLY:O	1:A:141:ARG:HD3	2.17	0.45
4:G:245:LEU:HG	4:G:249:MET:CE	2.46	0.45
3:F:81:PHE:HB3	3:F:82:PRO:HD3	1.98	0.45
3:F:31:VAL:HG22	3:F:46:THR:CG2	2.46	0.45
1:B:208:ASP:HB2	1:B:229:PHE:CE2	2.52	0.45
1:B:34:PHE:HB2	1:B:190:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:ARG:NH2	10:E:597:HOH:O	2.51	0.44
2:E:183:VAL:HG22	2:E:365:GLN:OE1	2.18	0.44
1:B:283:LEU:HD23	1:B:284:GLY:N	2.33	0.44
3:F:361:TRP:CE3	3:F:367:THR:HG22	2.53	0.44
3:F:335:ILE:HD11	4:G:37:ILE:HD12	2.00	0.43
1:B:137:GLY:O	1:B:141:ARG:HD3	2.19	0.43
3:F:381:TYR:N	3:F:382:PRO:CD	2.82	0.43
4:G:18:LEU:HD23	4:G:22:LEU:HD23	2.01	0.42
3:F:42:PHE:O	3:F:46:THR:HB	2.19	0.42
3:F:104:ARG:O	3:F:108:VAL:HG23	2.20	0.42
1:A:86:LEU:HA	1:A:146:ARG:NH2	2.35	0.42
1:A:236:SER:HA	1:A:237:PRO:C	2.40	0.42
1:B:40:CYS:SG	1:B:42:LYS:HG3	2.60	0.41
2:E:128:THR:OG1	2:E:131:GLU:HB2	2.19	0.41
4:G:108:TYR:CZ	4:G:203:PHE:HB2	2.55	0.41
1:B:144:ILE:HD11	1:B:160:PRO:O	2.21	0.41
3:F:420:PRO:HA	3:F:423:ILE:HG12	2.02	0.41
4:G:212:VAL:HG13	4:G:284[B]:TRP:HB3	2.02	0.41
1:B:105:ALA:HA	1:B:110:ILE:HD11	2.01	0.41
1:B:208:ASP:OD2	1:B:211:ARG:NH1	2.52	0.41
4:G:104:THR:HG22	4:G:203:PHE:CZ	2.56	0.41
3:F:292:VAL:O	3:F:296:VAL:HG23	2.21	0.40
1:B:227:ASP:OD1	1:B:230:VAL:HG23	2.20	0.40
4:G:212:VAL:HG21	8:G:307:UMQ:O2'	2.21	0.40
1:B:300:LEU:N	1:B:300:LEU:HD12	2.37	0.40
1:A:299:ILE:O	1:A:300:LEU:HD23	2.21	0.40
1:B:39:GLY:N	7:B:402:ANP:HNB1	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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

All (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
4	G	230	VAL
1	B	104	GLY

5.3.2 Protein sidechains ⓘ

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

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS

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Mol	Chain	Res	Type
1	A	106	LYS
1	A	108	GLU
1	A	127	LEU
1	A	169[A]	ARG
1	A	169[B]	ARG
1	A	185	ARG
1	A	338	GLU
1	A	350	GLU
1	A	367	LYS
1	B	20	LYS
1	B	100	LEU
1	B	123	LEU
1	B	127	LEU
1	B	134	LEU
1	B	177	SER
1	B	185	ARG
1	B	211	ARG
1	B	242	LEU
1	B	322	SER
1	B	324	ARG
2	E	34	LYS
3	F	20	LEU
3	F	25	LEU
3	F	37	GLN
3	F	41	LEU
3	F	46	THR
3	F	59	ASN
3	F	112	ARG
3	F	145	LEU
3	F	150	LYS
3	F	196	VAL
3	F	220	THR
3	F	257	VAL
3	F	372	LEU
3	F	376	ASN
3	F	440	ASN
3	F	494	ILE
3	F	496	LEU
4	G	10	LYS
4	G	12	ARG
4	G	48	SER
4	G	73	ARG

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Mol	Chain	Res	Type
4	G	106	CYS
4	G	126	LEU
4	G	137	LEU
4	G	172	LEU
4	G	212	VAL
4	G	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	GLN
1	B	8	ASN
1	B	125	HIS
2	E	218	ASN
3	F	37	GLN
3	F	106	GLN
3	F	232	ASN
3	F	376	ASN
3	F	437	ASN
3	F	440	ASN
4	G	241	ASN

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.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	C	2	GLC	C1-C2-C3	2.07	112.21	109.67

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.

5.6 Ligand geometry

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	F	609	-	12,12,35	0.36	0	11,11,46	0.41	0
8	UMQ	E	401	-	35,35,35	0.42	0	46,46,46	0.68	0
8	UMQ	F	607	-	12,12,35	0.36	0	11,11,46	0.40	0
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%)
9	PGV	F	605	-	50,50,50	1.10	3 (6%)	53,56,56	1.03	3 (5%)
8	UMQ	G	305	-	23,23,35	0.50	0	28,28,46	0.67	0
8	UMQ	G	302	-	12,12,35	0.38	0	11,11,46	0.43	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
8	UMQ	G	303	-	12,12,35	0.35	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%)
7	ANP	B	402	6	29,33,33	1.74	8 (27%)	31,52,52	1.88	6 (19%)
8	UMQ	G	307	-	35,35,35	0.54	1 (2%)	46,46,46	1.01	3 (6%)
8	UMQ	G	304	-	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	F	609	-	-	6/10/10/60	-
8	UMQ	E	401	-	-	9/20/60/60	0/2/2/2
8	UMQ	F	607	-	-	3/10/10/60	-
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
9	PGV	F	605	-	-	23/55/55/55	-
8	UMQ	G	305	-	-	8/14/34/60	0/1/1/2
8	UMQ	G	302	-	-	4/10/10/60	-
8	UMQ	G	306	-	-	3/10/10/60	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	UMQ	F	608	-	-	2/10/10/60	-
8	UMQ	G	303	-	-	3/10/10/60	-
9	PGV	F	606	-	-	19/55/55/55	-
7	ANP	B	402	6	-	4/14/38/38	0/3/3/3
8	UMQ	G	307	-	-	14/20/60/60	0/2/2/2
8	UMQ	G	304	-	-	5/10/10/60	-

All (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
7	A	1502	ANP	PB-O1B	3.82	1.52	1.46
9	F	605	PGV	C12-C11	3.77	1.53	1.31
7	A	1502	ANP	PG-N3B	3.69	1.73	1.63
7	B	402	ANP	PG-N3B	3.61	1.72	1.63
9	F	606	PGV	C12-C11	3.61	1.52	1.31
7	A	1502	ANP	PB-N3B	3.57	1.72	1.63
7	B	402	ANP	PG-O1G	3.50	1.51	1.46
7	B	402	ANP	PB-O1B	3.08	1.51	1.46
7	A	1502	ANP	PG-O1G	2.95	1.50	1.46
7	B	402	ANP	C5-C4	2.56	1.47	1.40
7	A	1502	ANP	C5-C4	2.47	1.47	1.40
8	G	301	UMQ	O1'-C1'	2.46	1.44	1.40
8	G	307	UMQ	O1'-C1'	2.34	1.44	1.40
7	A	1502	ANP	C2-N3	2.25	1.35	1.32
7	B	402	ANP	PG-O3G	-2.18	1.50	1.56
7	B	402	ANP	PG-O2G	-2.16	1.50	1.56
7	A	1502	ANP	PG-O3G	-2.11	1.51	1.56
7	A	1502	ANP	PB-O2B	-2.07	1.51	1.56
7	B	402	ANP	C2-N3	2.02	1.35	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
9	F	605	PGV	O01-C1-C2	3.85	119.80	111.50
7	A	1502	ANP	N3-C2-N1	-3.71	122.88	128.68
8	G	301	UMQ	O1'-C1'-C2'	3.61	113.93	108.30
9	F	606	PGV	O01-C1-C2	3.50	119.05	111.50
9	F	605	PGV	O03-C19-C20	3.27	122.16	111.91
8	G	307	UMQ	C3-C4-C5	2.93	115.46	110.24
7	B	402	ANP	O1B-PB-N3B	-2.81	107.64	111.77
9	F	606	PGV	O03-C19-C20	2.80	120.68	111.91
8	G	301	UMQ	CA-O1'-C1'	2.65	118.24	113.84
9	F	605	PGV	O03-C19-O04	-2.51	117.25	123.59
7	A	1502	ANP	PA-O3A-PB	-2.40	124.17	132.62
7	B	402	ANP	O3G-PG-O2G	2.37	113.96	107.64
8	G	307	UMQ	O5-C5-C4	2.30	113.88	109.69
7	A	1502	ANP	O3G-PG-O2G	2.27	113.68	107.64
8	G	307	UMQ	C1'-C2'-C3'	2.19	114.56	110.00
7	A	1502	ANP	C4-C5-N7	-2.19	107.12	109.40
7	B	402	ANP	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	605	PGV	C2-C1-O01-C02
9	F	605	PGV	C10-C11-C12-C13
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
8	G	305	UMQ	C2'-C1'-O1'-CA
8	G	305	UMQ	O5'-C1'-O1'-CA
7	B	402	ANP	PB-N3B-PG-O1G
7	B	402	ANP	PG-N3B-PB-O1B
7	B	402	ANP	PA-O3A-PB-O1B
7	B	402	ANP	PA-O3A-PB-O2B
8	G	307	UMQ	O5'-C1'-O1'-CA
9	F	605	PGV	O02-C1-O01-C02
8	G	307	UMQ	C4'-C5'-C6'-O6'
9	F	606	PGV	O12-C04-C05-C06
8	G	301	UMQ	C2'-C1'-O1'-CA
8	G	307	UMQ	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
9	F	605	PGV	C19-C20-C21-C22
8	G	304	UMQ	O1'-CA-CB-CC
8	G	305	UMQ	O1'-CA-CB-CC
9	F	606	PGV	O12-C04-C05-O05
9	F	605	PGV	C20-C19-O03-C01
9	F	605	PGV	C22-C23-C24-C25
9	F	605	PGV	C05-C04-O12-P
8	E	401	UMQ	C2'-C1'-O1'-CA
8	E	401	UMQ	CC-CD-CF-CG
8	G	305	UMQ	CH-CI-CJ-CK
9	F	606	PGV	C20-C21-C22-C23
9	F	606	PGV	C7-C8-C9-C10
8	G	301	UMQ	CD-CF-CG-CH
8	G	302	UMQ	CG-CH-CI-CJ
8	G	301	UMQ	CG-CH-CI-CJ
9	F	605	PGV	C6-C7-C8-C9
8	G	306	UMQ	O1'-CA-CB-CC
8	E	401	UMQ	O5'-C1'-O1'-CA
9	F	605	PGV	C29-C30-C31-C32
8	G	301	UMQ	CA-CB-CC-CD
8	G	302	UMQ	CB-CC-CD-CF
8	F	609	UMQ	O1'-CA-CB-CC
9	F	605	PGV	O04-C19-O03-C01
9	F	606	PGV	C29-C30-C31-C32
8	G	305	UMQ	CD-CF-CG-CH
8	F	607	UMQ	CF-CG-CH-CI
8	G	307	UMQ	CD-CF-CG-CH
8	G	301	UMQ	CB-CC-CD-CF
9	F	606	PGV	C27-C28-C29-C30
8	G	307	UMQ	C2'-C1'-O1'-CA
8	F	607	UMQ	CA-CB-CC-CD
8	G	301	UMQ	O5'-C5'-C6'-O6'
9	F	605	PGV	C11-C10-C9-C8
8	G	307	UMQ	CH-CI-CJ-CK
8	G	306	UMQ	CB-CA-O1'-C1'
8	G	303	UMQ	CG-CH-CI-CJ
8	G	301	UMQ	CH-CI-CJ-CK
8	G	305	UMQ	O5'-C5'-C6'-O6'
9	F	606	PGV	C15-C16-C17-C18
8	F	609	UMQ	CG-CH-CI-CJ
9	F	606	PGV	C6-C7-C8-C9
8	E	401	UMQ	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
9	F	605	PGV	O03-C01-C02-O01
8	F	608	UMQ	CC-CD-CF-CG
9	F	606	PGV	C26-C27-C28-C29
8	E	401	UMQ	C4'-C5'-C6'-O6'
8	E	401	UMQ	CI-CJ-CK-CL
8	G	303	UMQ	CC-CD-CF-CG
9	F	606	PGV	C30-C31-C32-C33
8	G	301	UMQ	CF-CG-CH-CI
9	F	605	PGV	C30-C31-C32-C33
8	G	307	UMQ	O1'-CA-CB-CC
8	G	306	UMQ	CB-CC-CD-CF
8	G	307	UMQ	CB-CC-CD-CF
8	E	401	UMQ	CG-CH-CI-CJ
8	G	301	UMQ	CC-CD-CF-CG
8	G	304	UMQ	CD-CF-CG-CH
8	G	304	UMQ	CI-CJ-CK-CL
9	F	605	PGV	C03-O11-P-O12
8	G	304	UMQ	CC-CD-CF-CG
8	G	307	UMQ	CA-CB-CC-CD
9	F	606	PGV	C20-C19-O03-C01
9	F	605	PGV	O03-C01-C02-C03
9	F	606	PGV	C24-C25-C26-C27
8	F	609	UMQ	CB-CA-O1'-C1'
9	F	606	PGV	C23-C24-C25-C26
9	F	606	PGV	O04-C19-O03-C01
8	G	304	UMQ	CB-CC-CD-CF
9	F	605	PGV	C27-C28-C29-C30
8	G	303	UMQ	CI-CJ-CK-CL
8	G	307	UMQ	CG-CH-CI-CJ
8	G	307	UMQ	C3'-C4'-O1-C1
9	F	605	PGV	C20-C21-C22-C23
9	F	606	PGV	C2-C3-C4-C5
8	G	307	UMQ	C5'-C4'-O1-C1
9	F	606	PGV	C3-C4-C5-C6
8	G	302	UMQ	CA-CB-CC-CD
8	G	307	UMQ	CC-CD-CF-CG
8	E	401	UMQ	CA-CB-CC-CD
9	F	605	PGV	C26-C27-C28-C29
8	G	305	UMQ	CI-CJ-CK-CL
8	F	607	UMQ	CI-CJ-CK-CL
8	G	305	UMQ	CB-CC-CD-CF
8	E	401	UMQ	CB-CC-CD-CF

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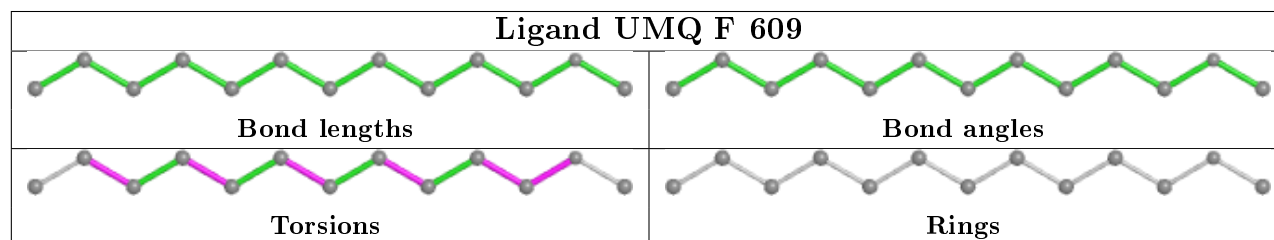
Mol	Chain	Res	Type	Atoms
9	F	606	PGV	C25-C26-C27-C28
9	F	605	PGV	C25-C26-C27-C28
8	G	302	UMQ	CC-CD-CF-CG
9	F	605	PGV	O03-C19-C20-C21
8	F	608	UMQ	CI-CJ-CK-CL
9	F	606	PGV	O01-C1-C2-C3
8	F	609	UMQ	CD-CF-CG-CH
8	F	609	UMQ	CB-CC-CD-CF
8	F	609	UMQ	CI-CJ-CK-CL
9	F	605	PGV	O04-C19-C20-C21
9	F	605	PGV	O12-C04-C05-C06
9	F	606	PGV	O02-C1-C2-C3
9	F	605	PGV	C21-C22-C23-C24
8	G	307	UMQ	CI-CJ-CK-CL

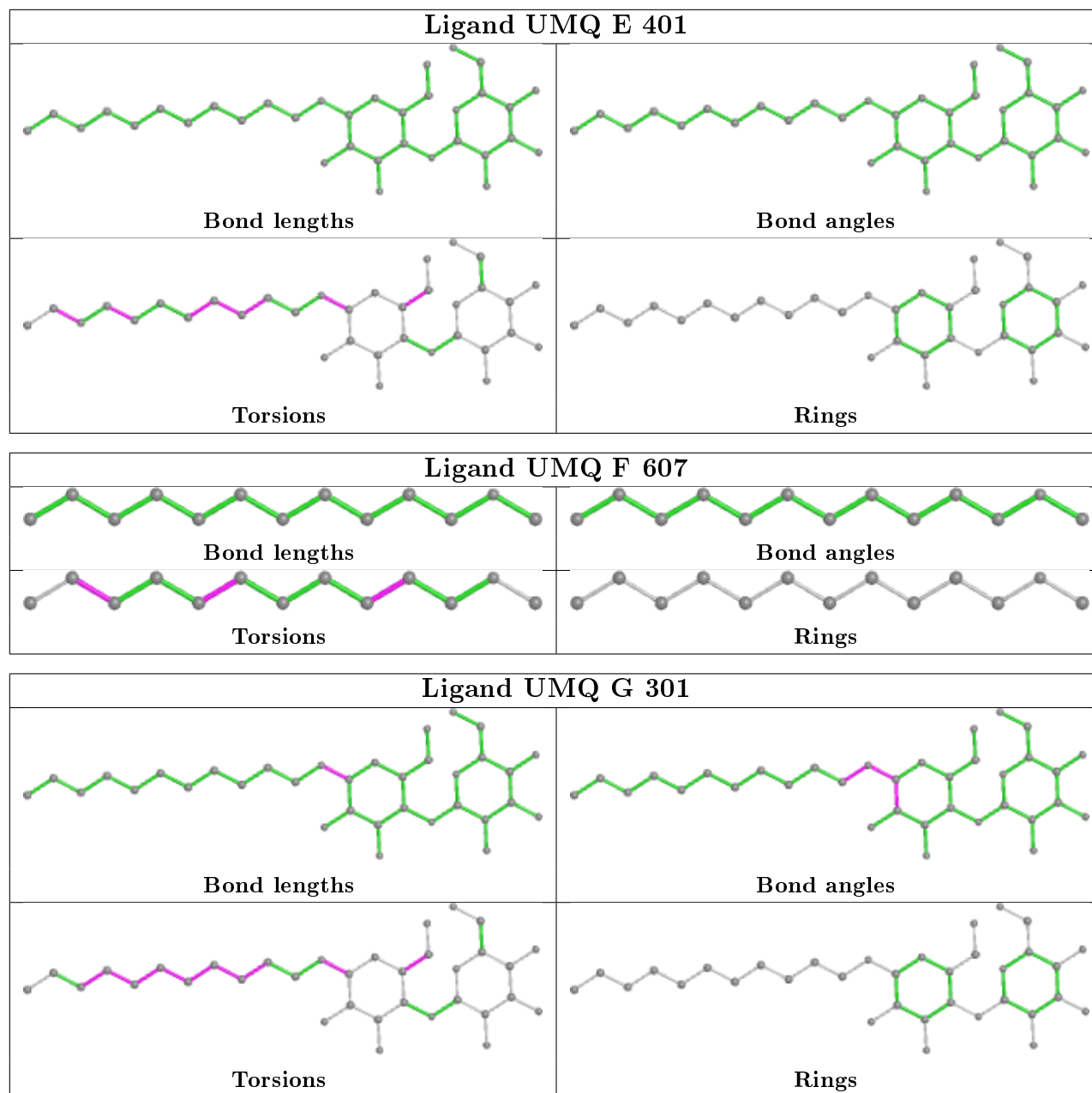
There are no ring outliers.

2 monomers are involved in 2 short contacts:

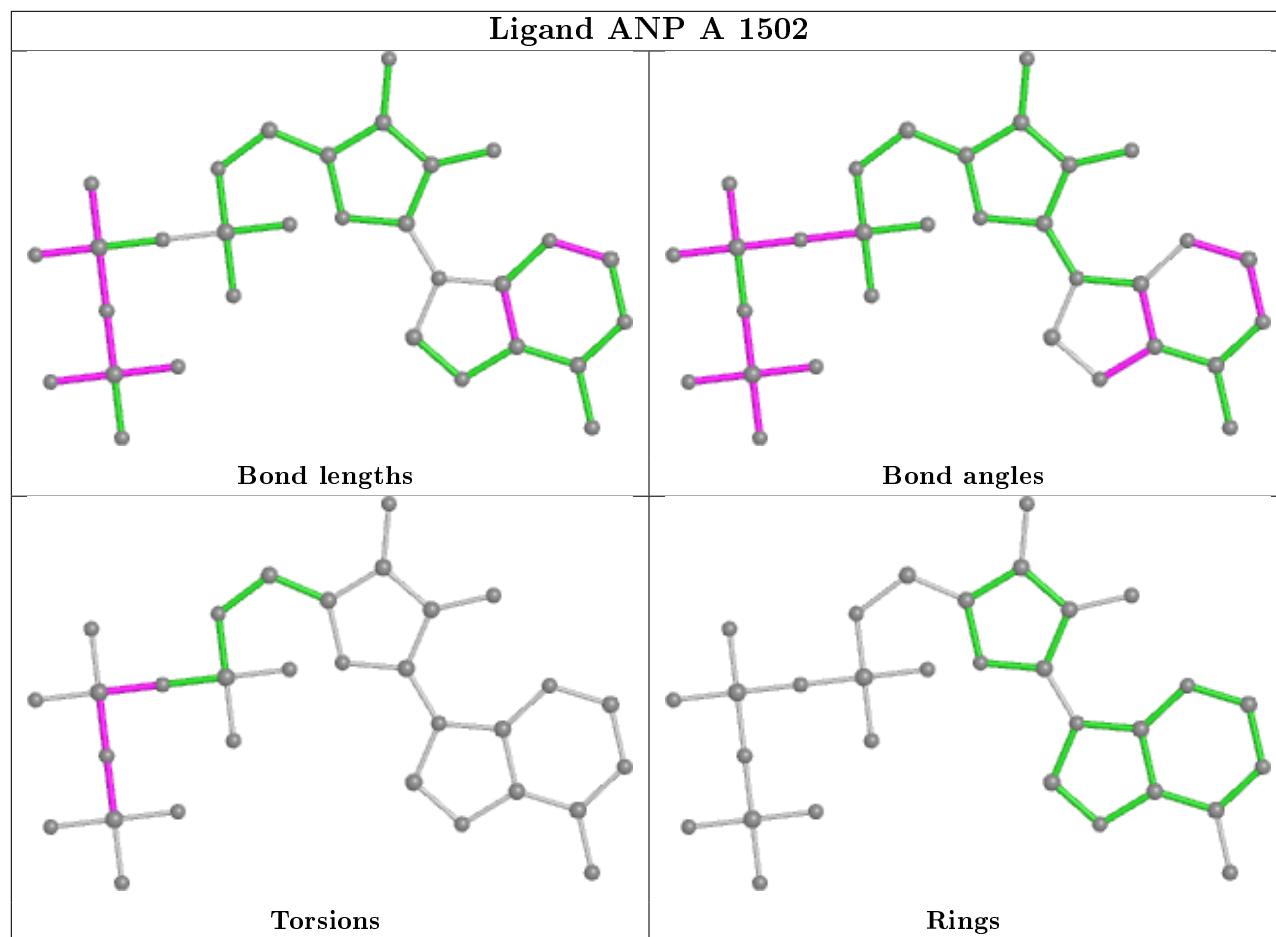
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	402	ANP	1	0
8	G	307	UMQ	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

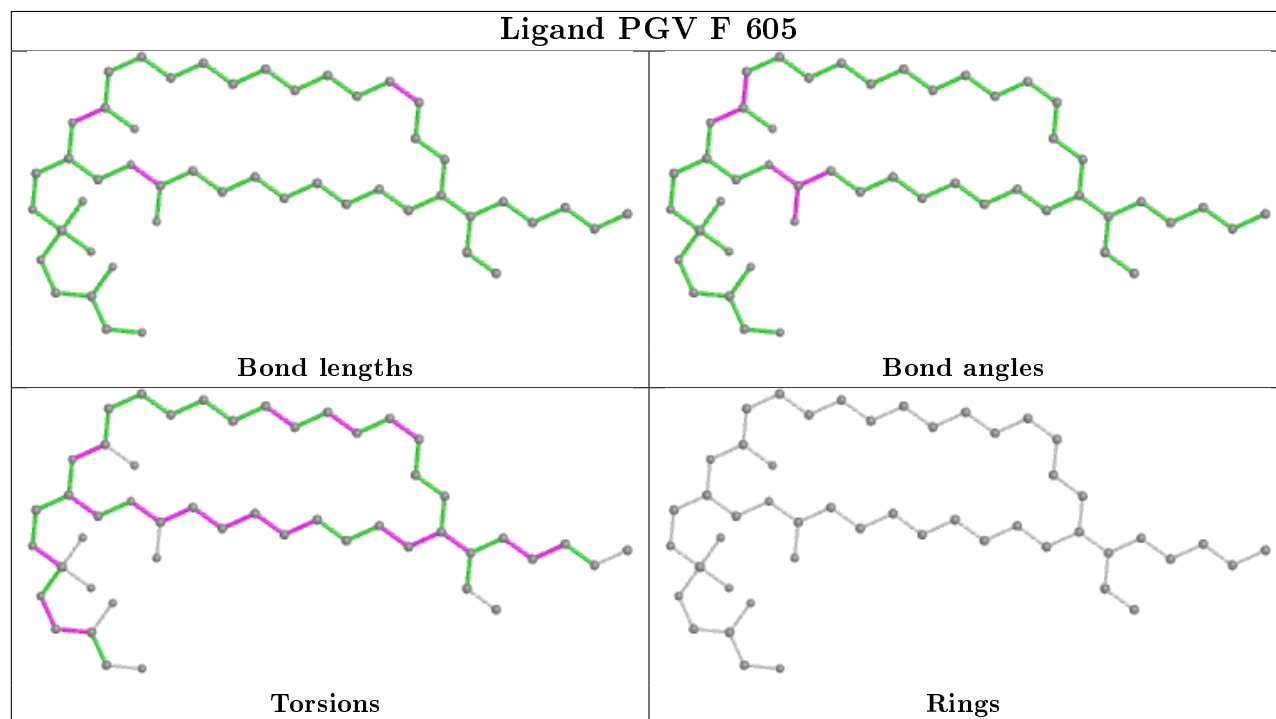


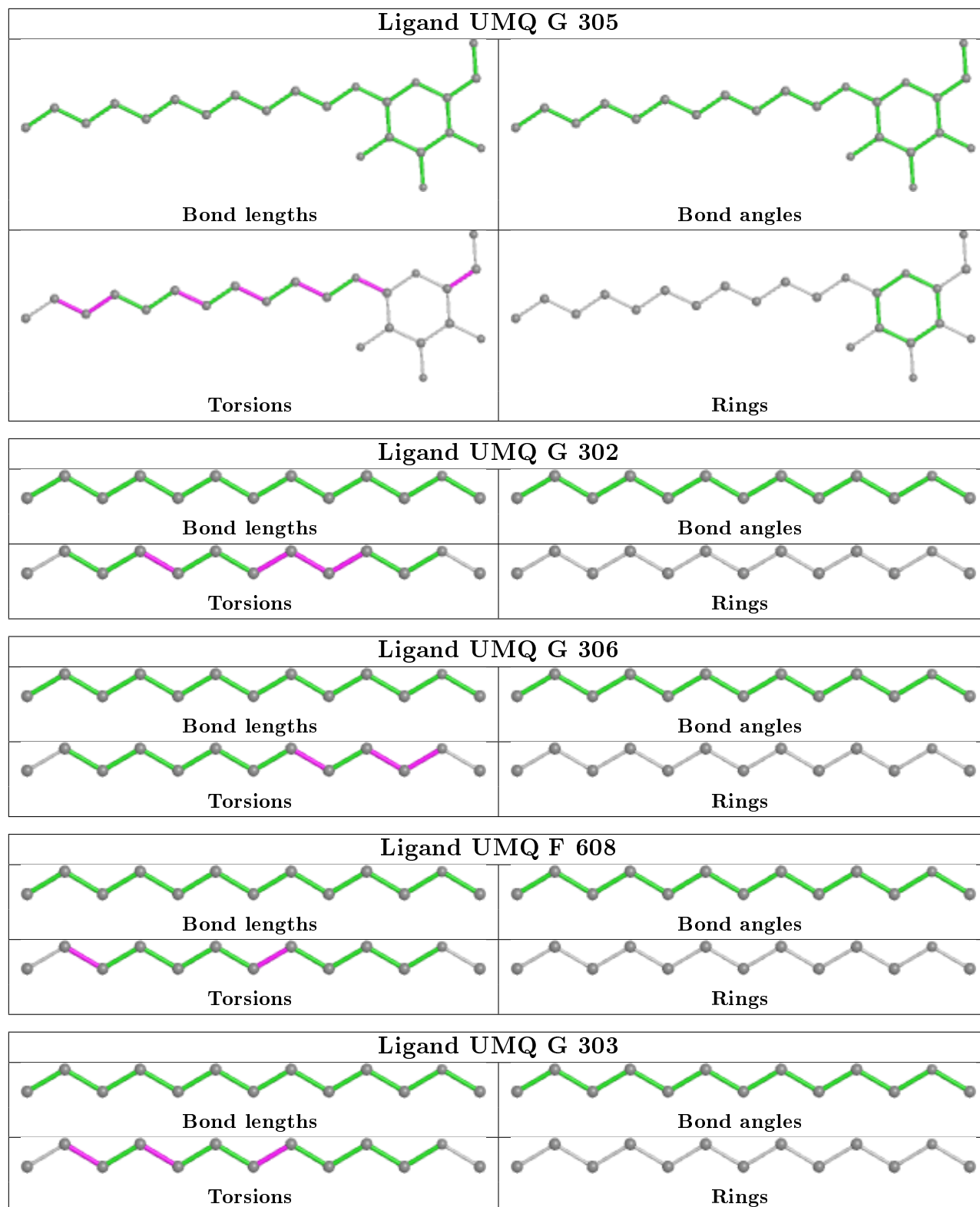


Ligand ANP A 1502

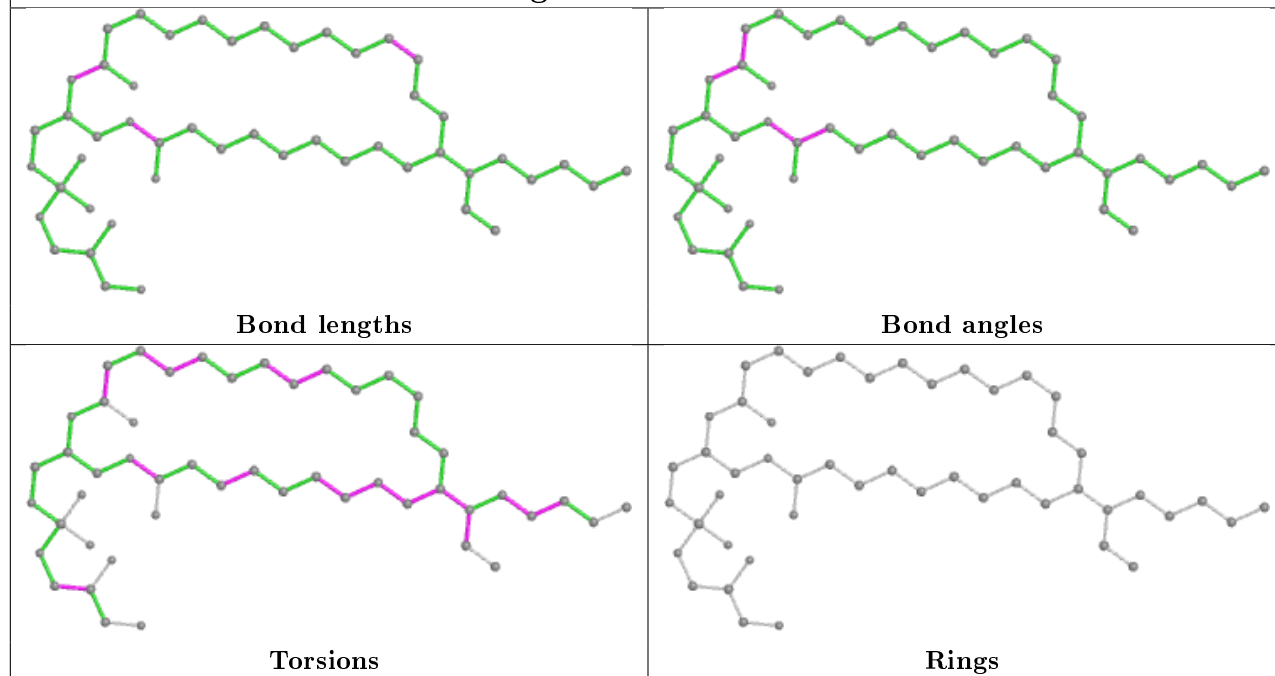


Ligand PGV F 605

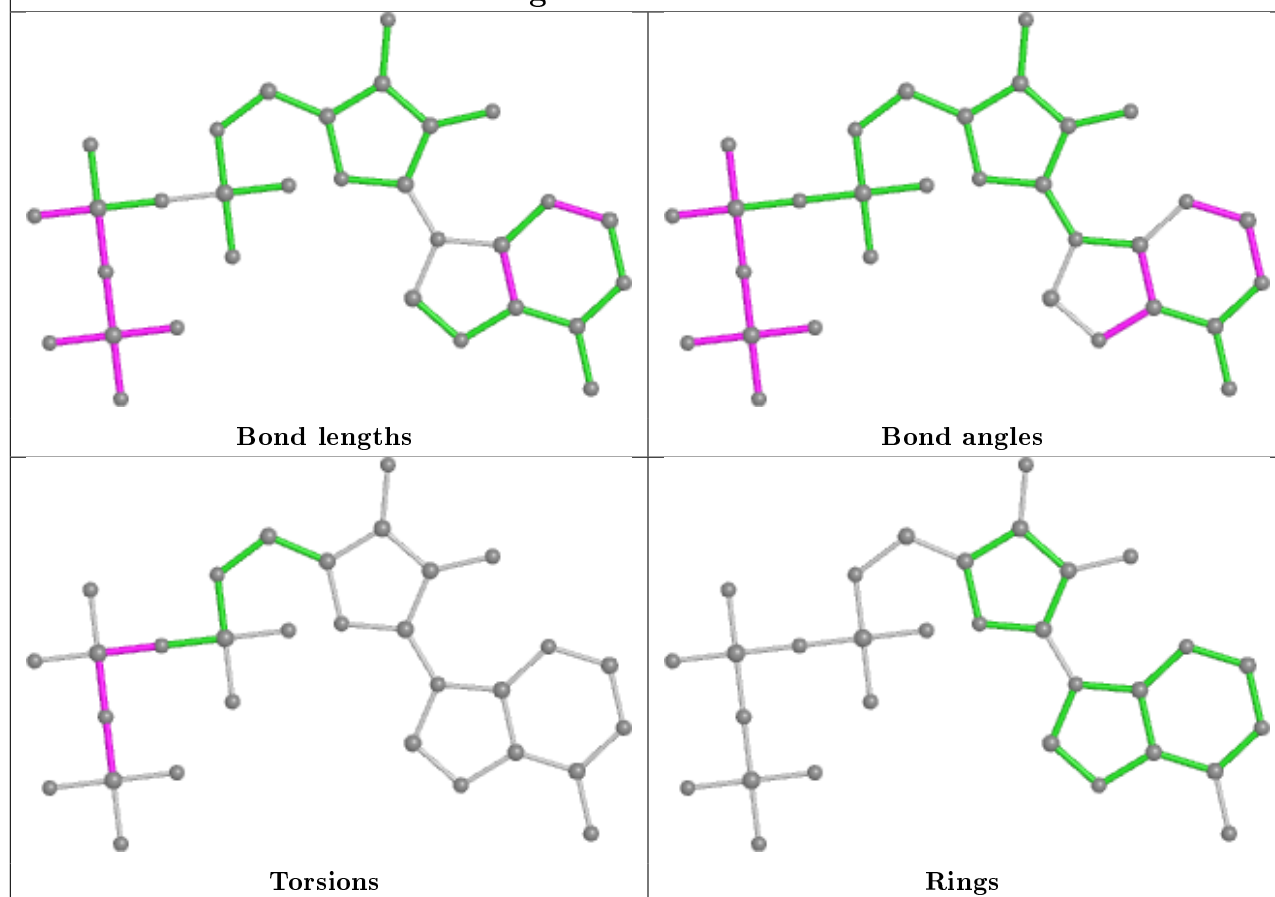


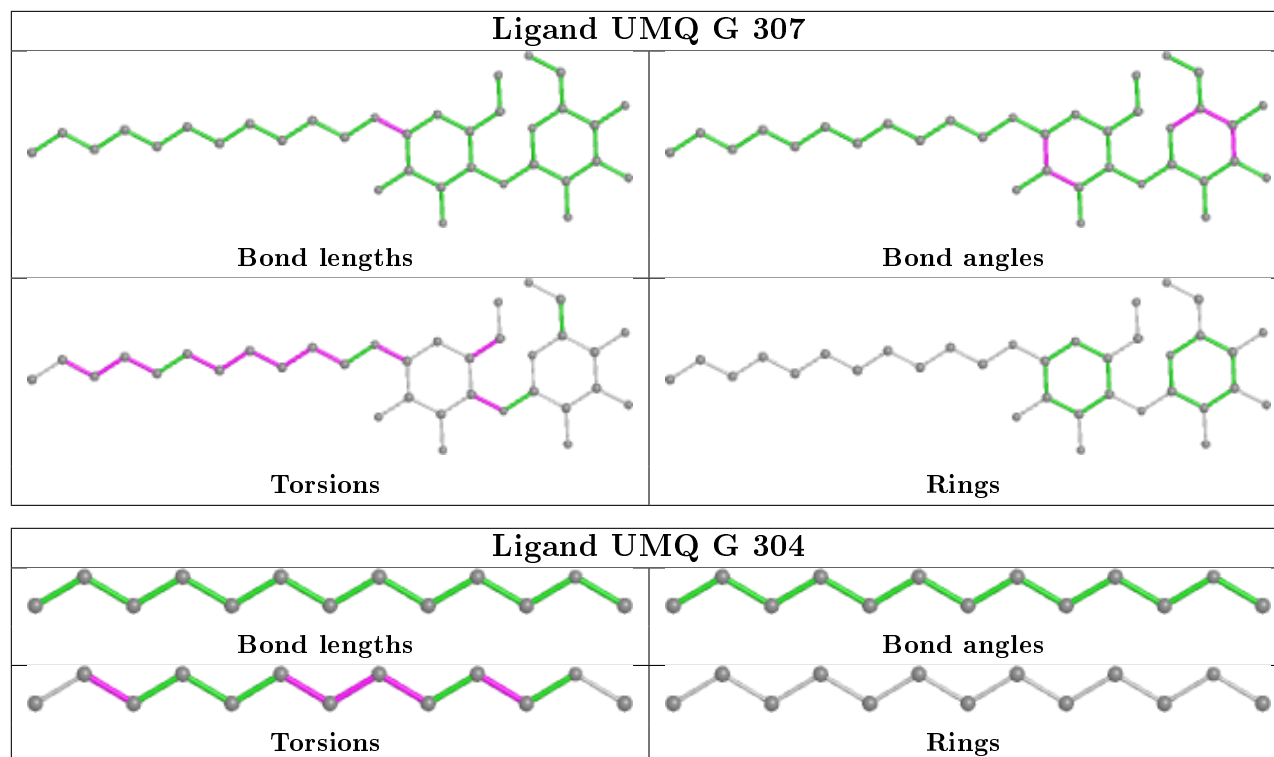


Ligand PGV F 606



Ligand ANP B 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

All (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
3	F	37	GLN	6.2
2	E	1	LYS	5.0
1	B	276	GLN	5.0
3	F	40	TYR	4.9
1	B	261	PRO	4.6
3	F	503	ILE	4.5
3	F	354	LEU	4.5
4	G	69	GLN	4.4
1	B	105	ALA	4.4
3	F	312	ARG	4.4
1	A	324	ARG	4.2
1	B	16	VAL	4.2
1	B	277	VAL	4.1
3	F	245	ASN	4.1
2	E	174	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	4.1
1	A	372	ALA	4.0
1	B	45	LEU	4.0
3	F	353	ALA	4.0
2	E	173	ASN	3.8
1	B	263	ARG	3.8
2	E	115	LEU	3.8
3	F	134	ALA	3.8
3	F	355	PHE	3.7
3	F	246	TRP	3.7
4	G	73	ARG	3.6
3	F	349	MET	3.6
1	B	359	GLY	3.5
4	G	114	ARG	3.5
3	F	29	TYR	3.4
2	E	224	MET	3.4
3	F	133	LEU	3.4
1	A	188	ILE	3.4
1	B	357	GLU	3.4
2	E	172	GLU	3.4
3	F	504	VAL	3.3
2	E	370	LYS	3.3
1	A	69	ASP	3.3
1	B	353	HIS	3.3
3	F	505	ASN	3.2
1	B	274	ASP	3.2
1	A	297	ASP	3.2
1	B	265	GLN	3.2
1	B	340	GLY	3.2
1	B	267	TRP	3.2
1	B	278	GLY	3.1
1	B	245	LYS	3.0
3	F	61	LYS	3.0
4	G	74	ILE	3.0
4	G	68	GLU	3.0
1	A	285	ILE	3.0
2	E	226	ILE	3.0
3	F	478	GLY	3.0
1	A	16	VAL	3.0
1	B	279	ALA	2.9
1	B	354	LEU	2.9
2	E	161	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	249	THR	2.9
3	F	271	GLU	2.8
1	B	294	ASP	2.8
1	B	273	ARG	2.8
3	F	154	GLU	2.8
2	E	147	LEU	2.8
4	G	116	PRO	2.8
1	B	324	ARG	2.8
1	A	49	ILE	2.8
1	B	296	ALA	2.7
2	E	252	GLY	2.7
3	F	114	TRP	2.7
1	B	15	GLU	2.7
1	B	244	VAL	2.7
1	B	116	GLN	2.7
2	E	239	LYS	2.6
3	F	479	GLY	2.6
2	E	186	ALA	2.6
2	E	2	ILE	2.6
4	G	162	VAL	2.5
1	A	345	ILE	2.5
1	A	261	PRO	2.5
3	F	463	TYR	2.5
4	G	72	GLY	2.5
1	A	15	GLU	2.5
3	F	227	LYS	2.5
3	F	22	LEU	2.5
1	B	112	GLN	2.5
3	F	305	LEU	2.4
3	F	372	LEU	2.4
3	F	502	ALA	2.4
4	G	14	PHE	2.4
3	F	38	GLY	2.4
1	B	69	ASP	2.4
1	B	108	GLU	2.4
3	F	17	TRP	2.4
1	B	342	THR	2.4
4	G	153	PHE	2.4
2	E	178	ILE	2.4
2	E	160	LEU	2.4
2	E	356	THR	2.4
3	F	275	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	35	TYR	2.3
1	B	360	THR	2.3
1	A	142	VAL	2.3
3	F	163	THR	2.3
3	F	302	LEU	2.3
3	F	135	LEU	2.2
1	B	338	GLU	2.2
1	B	297	ASP	2.2
1	B	259	PRO	2.2
1	A	103	ALA	2.2
2	E	141	ALA	2.2
3	F	44	ILE	2.2
4	G	8	SER	2.2
3	F	91	PHE	2.2
2	E	9	ILE	2.1
2	E	164	ASP	2.1
3	F	223	GLN	2.1
2	E	123	PRO	2.1
2	E	143	GLY	2.1
1	A	296	ALA	2.1
2	E	117	TYR	2.1
1	A	59	ASP	2.1
4	G	212	VAL	2.1
3	F	60	ARG	2.1
1	B	371	VAL	2.1
3	F	411	PHE	2.1
1	A	290	LEU	2.0
2	E	222	THR	2.0
1	B	256	VAL	2.0
1	A	291	LEU	2.0
1	B	145	GLY	2.0
1	B	250	ALA	2.0
3	F	229	ARG	2.0
2	E	175	LYS	2.0
2	E	171	TYR	2.0
1	A	354	LEU	2.0
1	B	188	ILE	2.0
2	E	116	ILE	2.0
4	G	50	ILE	2.0
1	B	178	ARG	2.0
3	F	14	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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

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

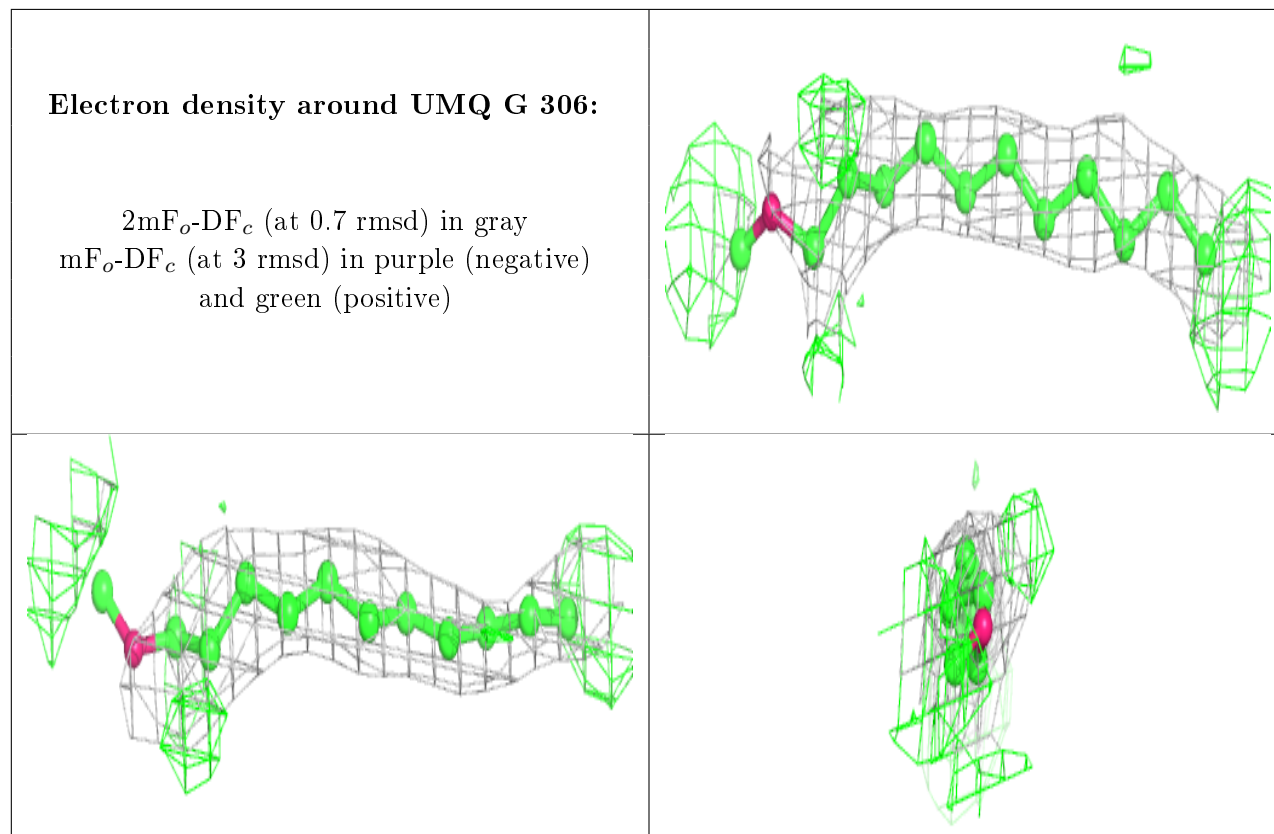
6.4 Ligands [i](#)

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
9	PGV	F	606	51/51	0.79	0.24	86,106,129,134	0
8	UMQ	G	305	23/34	0.79	0.22	94,106,127,136	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
6	MG	B	401	1/1	0.96	0.10	59,59,59,59	0
7	ANP	B	402	31/31	0.96	0.11	58,70,84,89	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

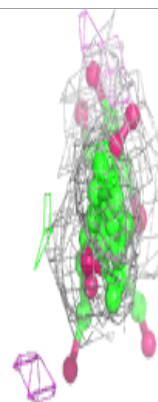
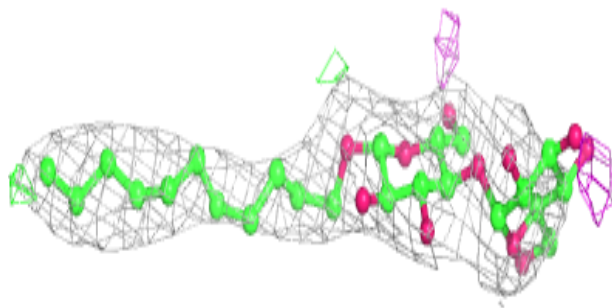
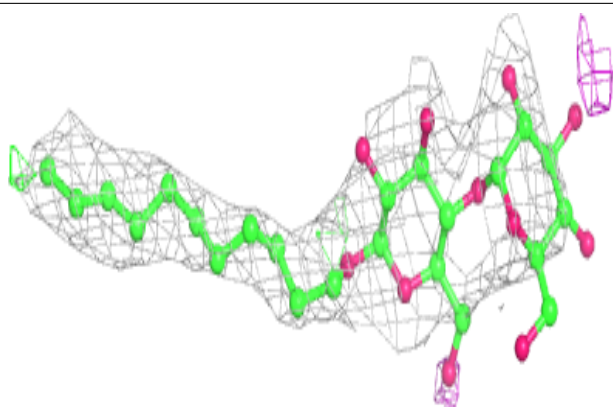
The following is a graphical depiction of the model fit to experimental electron density of all

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.

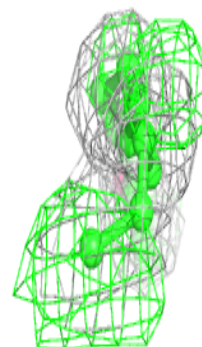
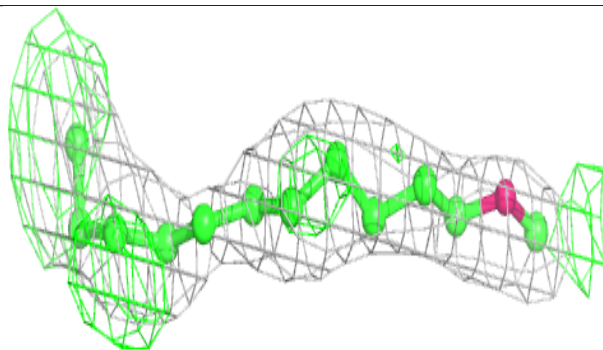
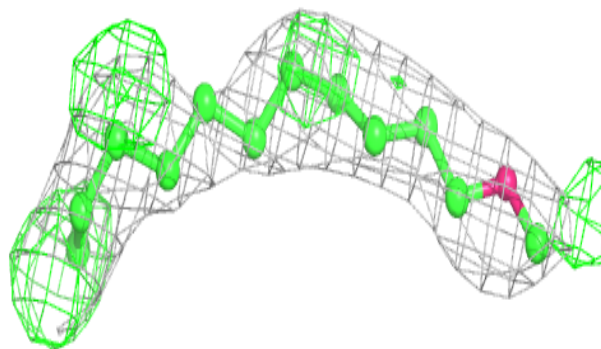


Electron density around UMQ G 301:

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

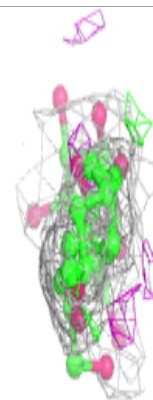
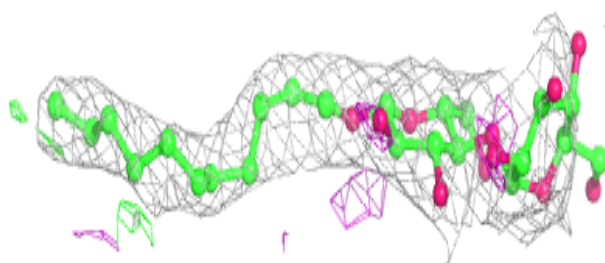
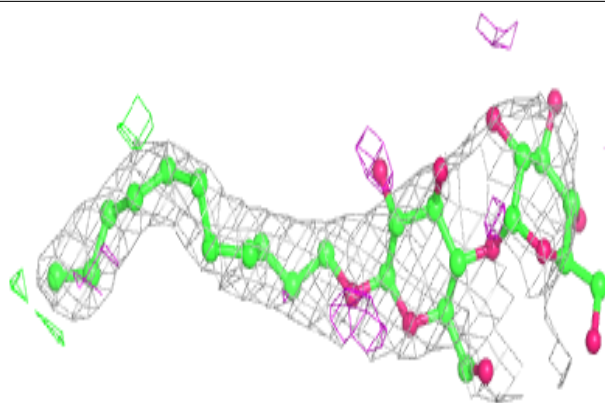
**Electron density around UMQ F 608:**

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

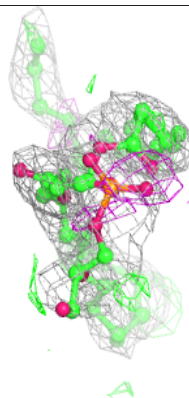
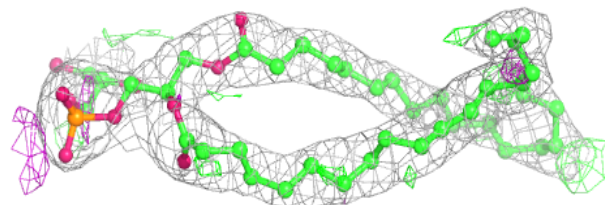
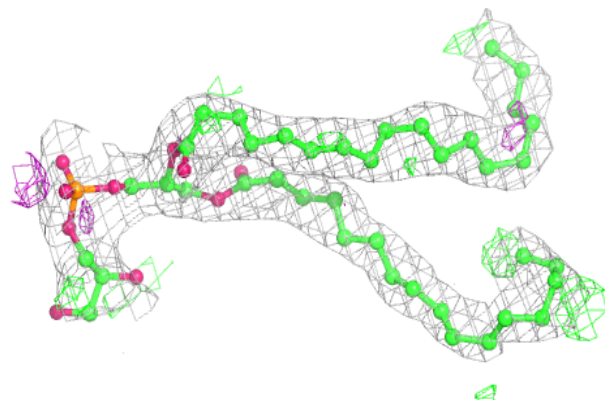


Electron density around UMQ G 307:

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

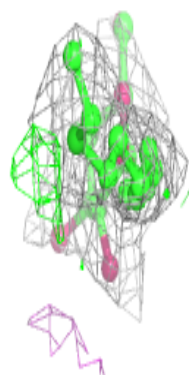
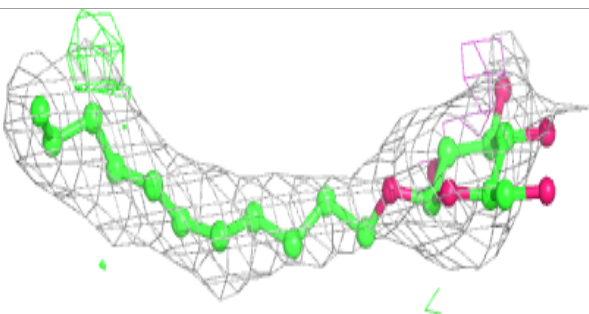
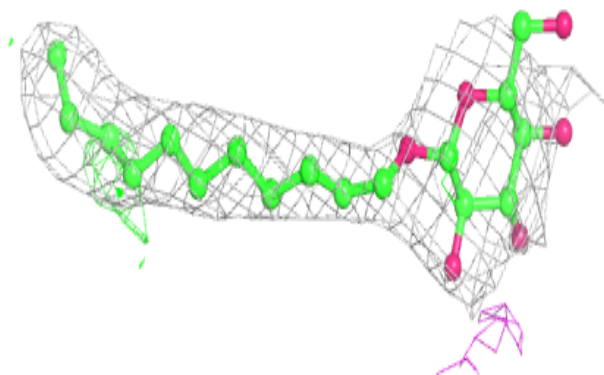
**Electron density around PGV F 606:**

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

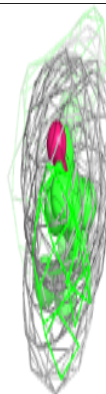
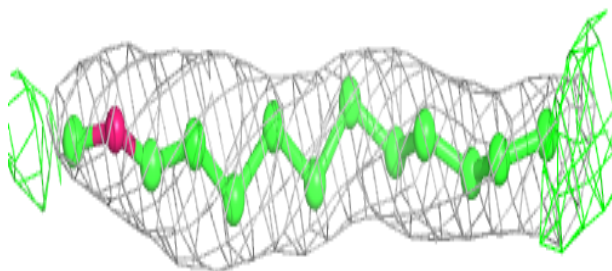
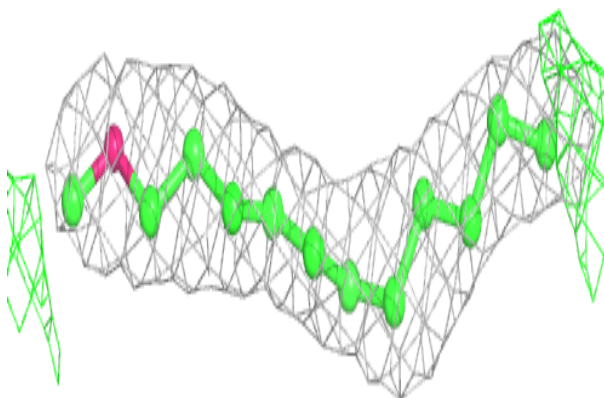


Electron density around UMQ G 305:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

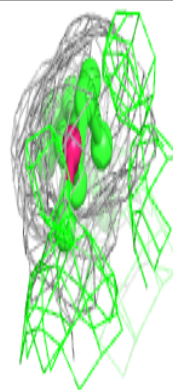
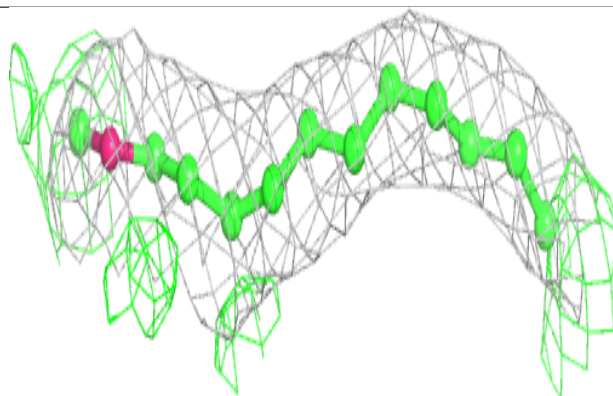
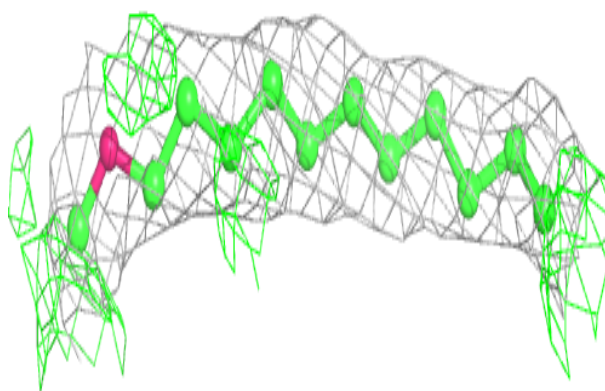
**Electron density around UMQ F 607:**

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

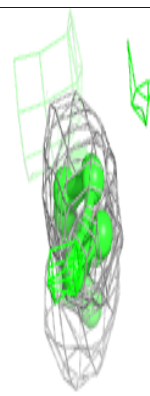
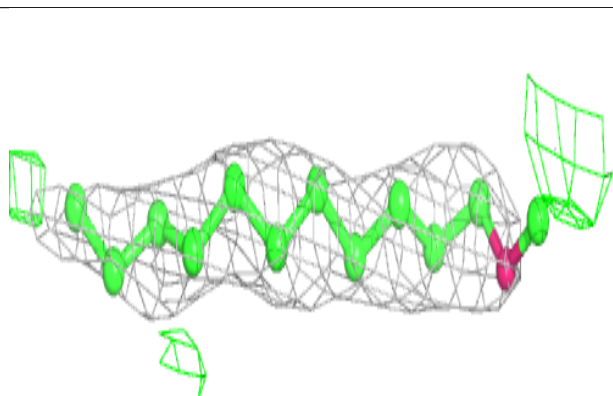
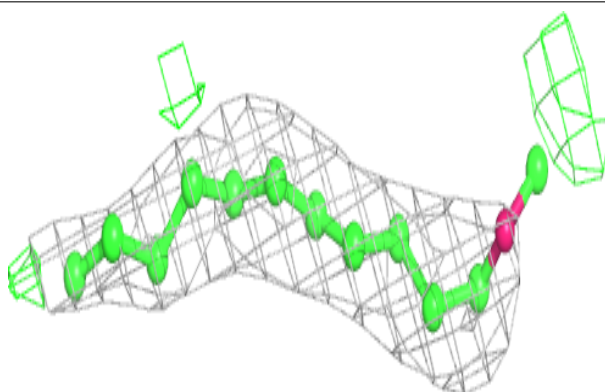


Electron density around UMQ G 302:

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

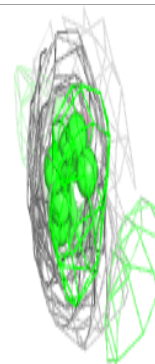
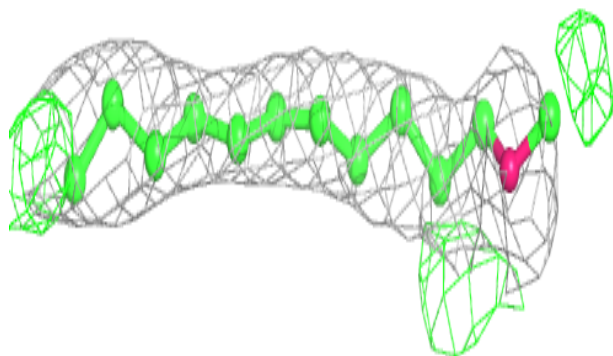
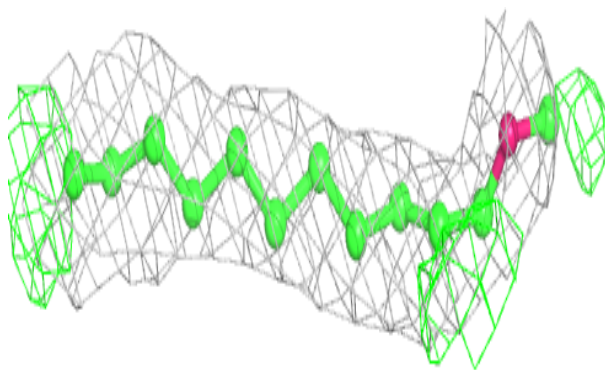
**Electron density around UMQ F 609:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

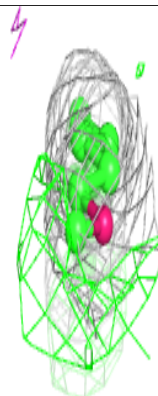
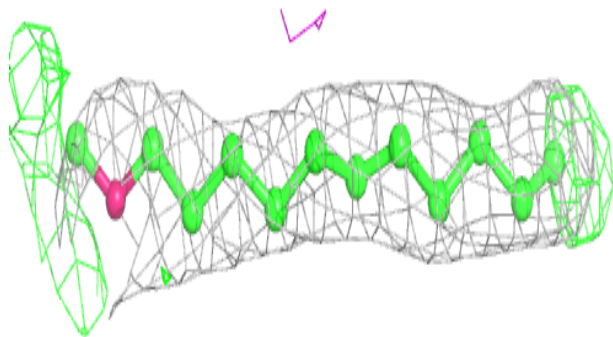
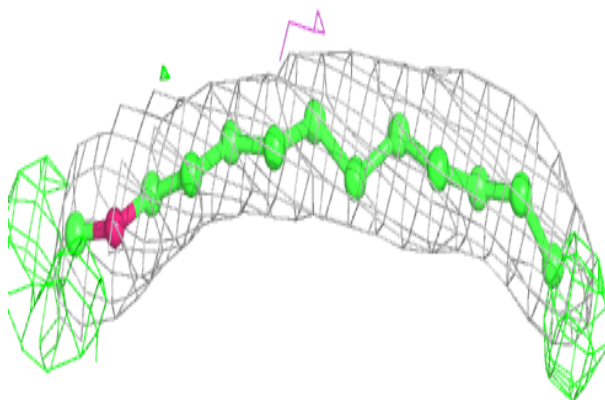


Electron density around UMQ G 304:

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and green (positive)

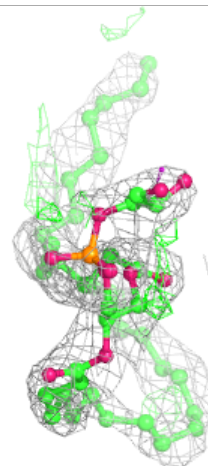
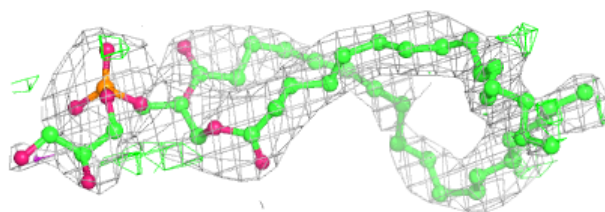
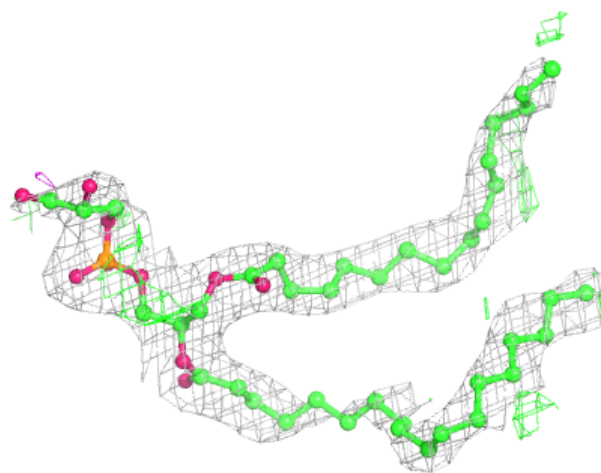
**Electron density around UMQ G 303:**

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



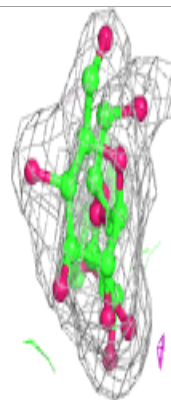
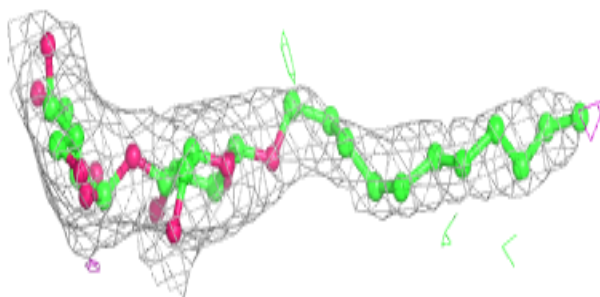
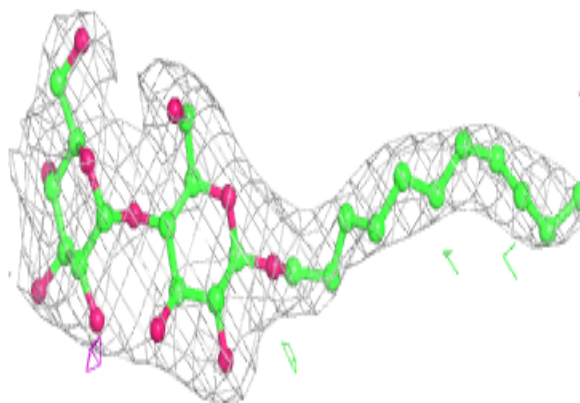
Electron density around PGV F 605:

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

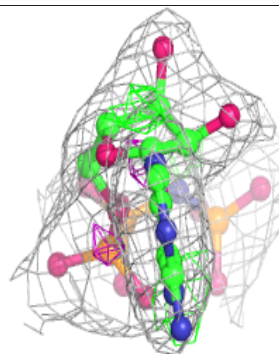
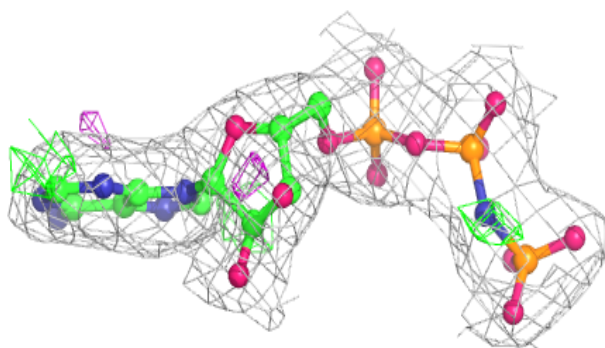
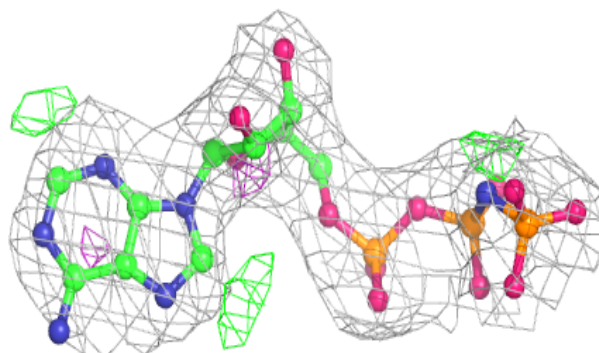


Electron density around UMQ E 401:

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

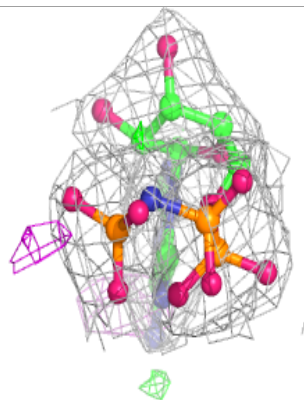
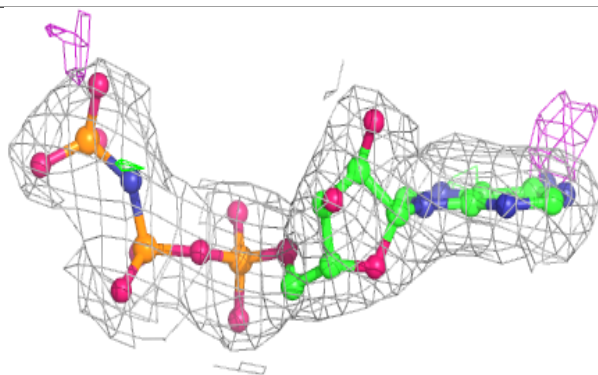
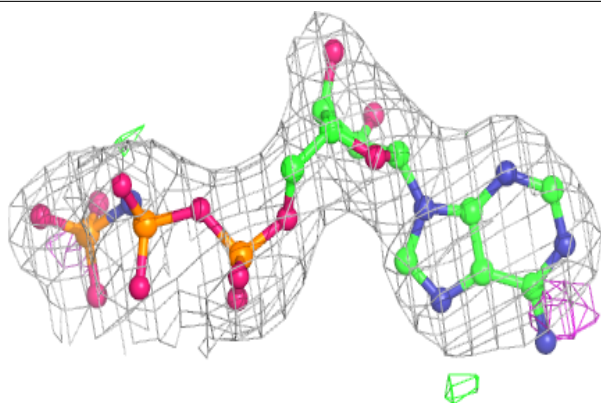
**Electron density around ANP B 402:**

$2mF_o-DF_c$ (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.