



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:41 PM UTC

PDB ID : 5V7P / pdb_00005v7p
Title : Atomic structure of the eukaryotic intramembrane Ras methyltransferase ICMT (isoprenylcysteine carboxyl methyltransferase), in complex with a monobody
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Deposited on : 2017-03-20
Resolution : 2.30 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

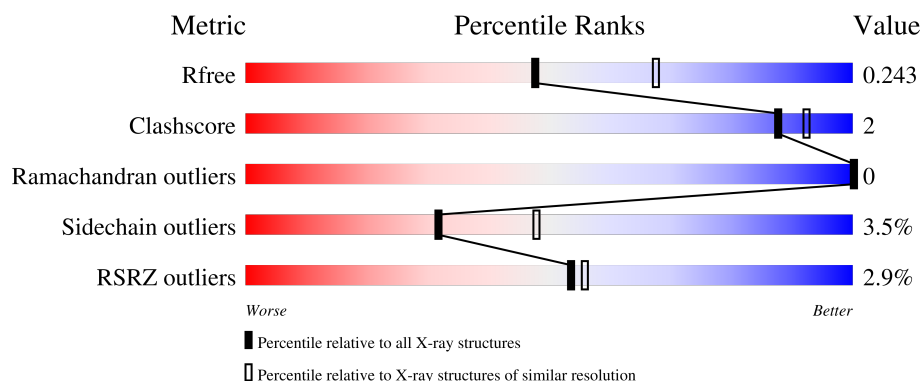
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

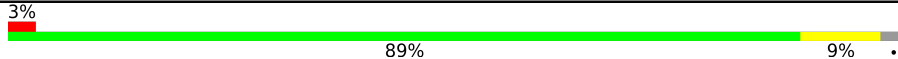
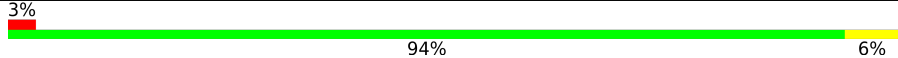
The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	288	
2	D	95	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3450 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 Protein-S-isoprenylcysteine O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	4	0
			2292	1550	347	383	12			

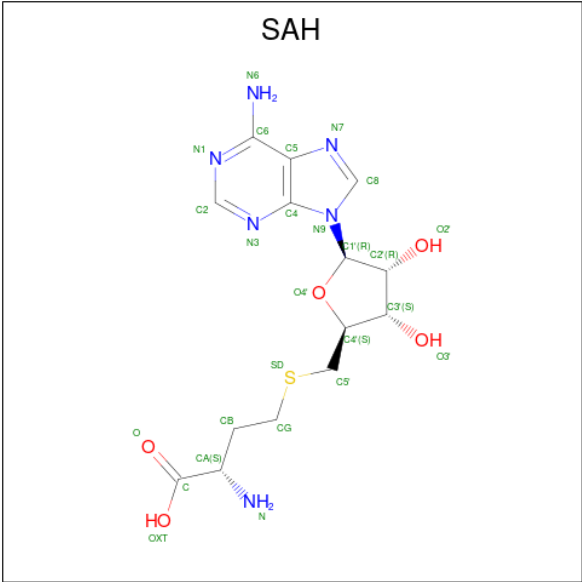
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	ALA	-	expression tag	UNP D6WJ77
A	283	ALA	-	expression tag	UNP D6WJ77
A	284	GLU	-	expression tag	UNP D6WJ77
A	285	GLY	-	expression tag	UNP D6WJ77
A	286	GLU	-	expression tag	UNP D6WJ77
A	287	GLU	-	expression tag	UNP D6WJ77
A	288	PHE	-	expression tag	UNP D6WJ77

- Molecule 2 is a protein called monobody.

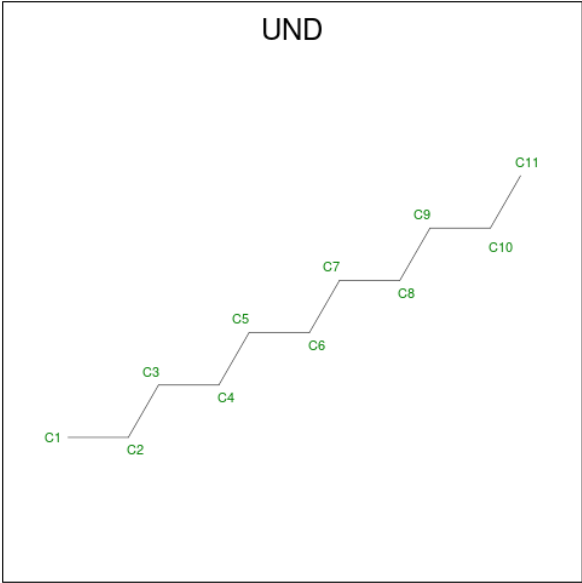
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	95	Total	C	N	O	0	1	0
			721	470	108	143			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



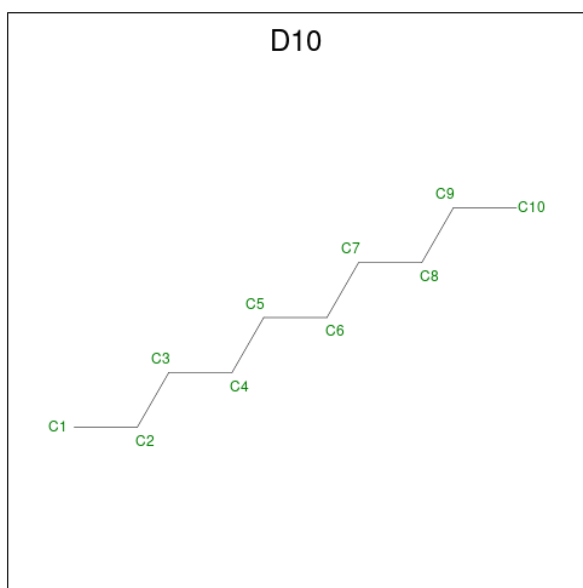
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄).



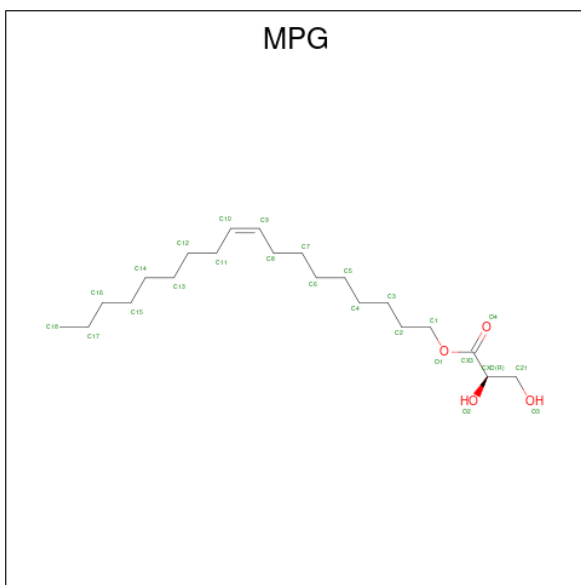
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			11	11		
4	A	1	Total	C	0	0
			11	11		
4	A	1	Total	C	0	0
			11	11		

- Molecule 5 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 9 9	0	0
5	A	1	Total C 10 10	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 5 5	0	0
5	A	1	Total C 10 10	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0

- Molecule 6 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 20 16 4	0	0
6	A	1	Total C O 21 17 4	0	0
6	A	1	Total C O 20 16 4	0	0
6	A	1	Total C O 11 7 4	0	0
6	A	1	Total C O 19 15 4	0	0
6	A	1	Total C O 21 17 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 20 16 4	0	0
6	A	1	Total C O 18 14 4	0	0
6	A	1	Total C O 23 19 4	0	0

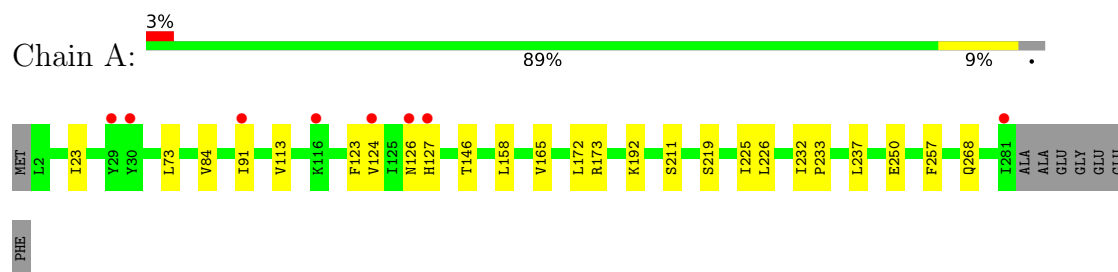
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	51	Total O 51 51	0	0
7	D	41	Total O 41 41	0	0

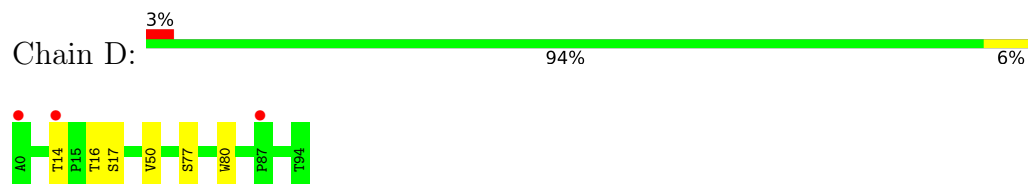
3 Residue-property plots

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: Protein-S-isoprenylcysteine O-methyltransferase



- Molecule 2: monobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.55Å 87.69Å 147.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.30 29.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.77-2.30) 95.7 (29.77-2.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.214 , 0.247 (Not available) , 0.243	Depositor DCC
R_{free} test set	1132 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3450	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, MPG, UND, D10

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	0.11	0/2381	0.29	0/3243
2	D	0.13	0/745	0.28	0/1026
All	All	0.12	0/3126	0.29	0/4269

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	2292	0	2281	10	0
2	D	721	0	721	4	0
3	A	26	0	19	1	0
4	A	33	0	72	0	0
5	A	88	0	159	0	0
6	A	198	0	271	4	0
7	A	51	0	0	1	0
7	D	41	0	0	0	0
All	All	3450	0	3523	14	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:HA	1:A:127:HIS:HB2	1.78	0.66
1:A:268:GLN:NE2	7:A:403:HOH:O	2.43	0.51
6:A:325:MPG:H42C	2:D:80:TRP:CZ2	2.46	0.50
1:A:219:SER:HB2	6:A:325:MPG:H52C	1.94	0.49
1:A:232:ILE:HB	1:A:233:PRO:HD3	1.97	0.47
2:D:14:THR:HG23	2:D:16:THR:H	1.80	0.45
1:A:192:LYS:NZ	1:A:257:PHE:O	2.51	0.44
2:D:14:THR:HG22	2:D:17:SER:OG	2.19	0.43
6:A:325:MPG:H131	2:D:77:SER:HB3	2.02	0.41
1:A:123:PHE:O	1:A:124:VAL:HG12	2.21	0.41
1:A:173:ARG:HD2	1:A:211:SER:O	2.20	0.41
1:A:250:GLU:OE2	3:A:301:SAH:H8	2.21	0.41
1:A:91:ILE:CG2	1:A:225:ILE:O	2.68	0.40
1:A:23:ILE:HG12	6:A:324:MPG:H31C	2.03	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	282/288 (98%)	277 (98%)	5 (2%)	0	100	100
2	D	94/95 (99%)	92 (98%)	2 (2%)	0	100	100
All	All	376/383 (98%)	369 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	210/249 (84%)	200 (95%)	10 (5%)	23	35
2	D	82/81 (101%)	81 (99%)	1 (1%)	63	79
All	All	292/330 (88%)	281 (96%)	11 (4%)	32	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	84	VAL
1	A	113	VAL
1	A	146	THR
1	A	158	LEU
1	A	165	VAL
1	A	172	LEU
1	A	226	LEU
1	A	237[A]	LEU
1	A	237[B]	LEU
2	D	50	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	268	GLN
2	D	91	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MPG	A	322	-	24,24,24	0.91	1 (4%)	24,25,25	1.16	2 (8%)
6	MPG	A	321	-	20,20,24	0.99	1 (5%)	20,21,25	1.16	2 (10%)
5	D10	A	305	-	9,9,9	0.29	0	8,8,8	0.83	0
4	UND	A	302	-	10,10,10	0.31	0	9,9,9	0.81	0
6	MPG	A	319	-	10,10,24	1.35	1 (10%)	10,11,25	1.60	2 (20%)
5	D10	A	315	-	7,7,9	0.31	0	6,6,8	0.74	0
4	UND	A	309	-	10,10,10	0.32	0	9,9,9	0.77	0
3	SAH	A	301	-	27,28,28	1.07	5 (18%)	36,40,40	1.93	9 (25%)
5	D10	A	312	-	4,4,9	0.34	0	3,3,8	0.57	0
6	MPG	A	323	-	19,19,24	1.02	1 (5%)	19,20,25	1.26	2 (10%)
5	D10	A	307	-	5,5,9	0.32	0	4,4,8	0.60	0
5	D10	A	310	-	8,8,9	0.31	0	7,7,8	0.79	0
5	D10	A	306	-	5,5,9	0.31	0	4,4,8	0.63	0
5	D10	A	311	-	7,7,9	0.31	0	6,6,8	0.75	0
5	D10	A	304	-	8,8,9	0.32	0	7,7,8	0.75	0
5	D10	A	308	-	8,8,9	0.31	0	7,7,8	0.77	0
6	MPG	A	316	-	19,19,24	1.00	1 (5%)	19,20,25	1.13	1 (5%)
5	D10	A	314	-	7,7,9	0.31	0	6,6,8	0.71	0
4	UND	A	303	-	10,10,10	0.30	0	9,9,9	0.81	0
6	MPG	A	320	-	18,18,24	1.04	1 (5%)	18,19,25	1.23	2 (11%)
6	MPG	A	317	-	20,20,24	0.98	1 (5%)	20,21,25	1.17	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	D10	A	313	-	9,9,9	0.32	0	8,8,8	0.77	0
6	MPG	A	318	-	19,19,24	1.00	1 (5%)	19,20,25	1.17	2 (10%)
6	MPG	A	324	-	17,17,24	1.06	1 (5%)	17,18,25	1.34	2 (11%)
6	MPG	A	325	-	22,22,24	0.97	2 (9%)	22,23,25	0.99	1 (4%)

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
6	MPG	A	322	-	-	10/25/25/25	-
6	MPG	A	321	-	-	11/21/21/25	-
5	D10	A	305	-	-	5/7/7/7	-
4	UND	A	302	-	-	0/8/8/8	-
6	MPG	A	319	-	-	6/11/11/25	-
5	D10	A	315	-	-	0/5/5/7	-
4	UND	A	309	-	-	5/8/8/8	-
3	SAH	A	301	-	-	0/15/31/31	0/3/3/3
5	D10	A	312	-	-	0/2/2/7	-
6	MPG	A	323	-	-	9/20/20/25	-
5	D10	A	307	-	-	0/3/3/7	-
5	D10	A	310	-	-	0/6/6/7	-
5	D10	A	306	-	-	1/3/3/7	-
5	D10	A	311	-	-	0/5/5/7	-
5	D10	A	304	-	-	3/6/6/7	-
5	D10	A	308	-	-	0/6/6/7	-
6	MPG	A	316	-	-	4/20/20/25	-
5	D10	A	314	-	-	0/5/5/7	-
4	UND	A	303	-	-	2/8/8/8	-
6	MPG	A	320	-	-	3/19/19/25	-
6	MPG	A	317	-	-	5/21/21/25	-
5	D10	A	313	-	-	1/7/7/7	-
6	MPG	A	318	-	-	11/20/20/25	-
6	MPG	A	324	-	-	9/18/18/25	-
6	MPG	A	325	-	-	9/23/23/25	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	323	MPG	O1-CX3	3.50	1.40	1.33
6	A	319	MPG	O1-CX3	3.43	1.40	1.33
6	A	321	MPG	O1-CX3	3.43	1.40	1.33
6	A	320	MPG	O1-CX3	3.39	1.40	1.33
6	A	322	MPG	O1-CX3	3.37	1.40	1.33
6	A	316	MPG	O1-CX3	3.37	1.40	1.33
6	A	317	MPG	O1-CX3	3.35	1.40	1.33
6	A	318	MPG	O1-CX3	3.31	1.40	1.33
6	A	324	MPG	O1-CX3	3.31	1.40	1.33
6	A	325	MPG	O1-CX3	3.21	1.40	1.33
3	A	301	SAH	C2-N1	2.43	1.38	1.33
3	A	301	SAH	C2-N3	2.37	1.38	1.33
3	A	301	SAH	OXT-C	-2.21	1.23	1.30
6	A	325	MPG	O1-C1	-2.08	1.39	1.45
3	A	301	SAH	C8-N7	2.04	1.35	1.31
3	A	301	SAH	C5-N7	-2.04	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	SAH	N3-C2-N1	-5.60	120.10	128.58
3	A	301	SAH	C5-C4-N3	-4.25	120.86	126.72
6	A	319	MPG	O1-CX3-CXD	3.88	120.76	111.78
6	A	323	MPG	O1-CX3-CXD	3.84	120.67	111.78
6	A	322	MPG	O1-CX3-CXD	3.60	120.11	111.78
3	A	301	SAH	N9-C8-N7	-3.56	108.88	113.94
6	A	324	MPG	O1-CX3-CXD	3.54	119.97	111.78
6	A	317	MPG	O1-CX3-CXD	3.54	119.96	111.78
6	A	320	MPG	O1-CX3-CXD	3.50	119.87	111.78
6	A	321	MPG	O1-CX3-CXD	3.49	119.86	111.78
6	A	318	MPG	O1-CX3-CXD	3.40	119.63	111.78
6	A	316	MPG	O1-CX3-CXD	3.29	119.38	111.78
3	A	301	SAH	C2-N3-C4	3.28	119.85	111.83
3	A	301	SAH	C5-N7-C8	3.17	108.42	103.45
6	A	325	MPG	O1-CX3-CXD	2.86	118.39	111.78
3	A	301	SAH	OXT-C-O	-2.82	117.68	124.08
3	A	301	SAH	N3-C4-N9	2.66	131.70	127.17
6	A	319	MPG	O1-CX3-O4	-2.53	119.52	124.14
3	A	301	SAH	C5'-SD-CG	-2.49	94.87	102.26
6	A	322	MPG	O1-CX3-O4	-2.39	119.78	124.14
6	A	324	MPG	O1-CX3-O4	-2.26	120.00	124.14
3	A	301	SAH	C4-C5-N7	-2.24	108.02	110.58
6	A	317	MPG	O1-CX3-O4	-2.24	120.04	124.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	320	MPG	O1-CX3-O4	-2.21	120.10	124.14
6	A	318	MPG	O1-CX3-O4	-2.19	120.14	124.14
6	A	323	MPG	O1-CX3-O4	-2.16	120.18	124.14
6	A	321	MPG	O1-CX3-O4	-2.06	120.38	124.14

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	316	MPG	O3-C21-CXD-O2
6	A	317	MPG	O3-C21-CXD-O2
6	A	318	MPG	C10-C11-C12-C13
6	A	319	MPG	CXD-CX3-O1-C1
6	A	319	MPG	O4-CX3-O1-C1
6	A	319	MPG	O3-C21-CXD-O2
6	A	320	MPG	O3-C21-CXD-O2
6	A	321	MPG	O3-C21-CXD-O2
6	A	321	MPG	O1-CX3-CXD-C21
6	A	324	MPG	CXD-CX3-O1-C1
6	A	324	MPG	O4-CX3-O1-C1
6	A	324	MPG	O3-C21-CXD-O2
6	A	325	MPG	O3-C21-CXD-O2
6	A	325	MPG	O1-CX3-CXD-C21
6	A	318	MPG	O4-CX3-O1-C1
6	A	321	MPG	O4-CX3-O1-C1
6	A	318	MPG	CXD-CX3-O1-C1
6	A	323	MPG	O4-CX3-O1-C1
6	A	322	MPG	O4-CX3-O1-C1
6	A	321	MPG	CXD-CX3-O1-C1
6	A	322	MPG	CXD-CX3-O1-C1
6	A	323	MPG	CXD-CX3-O1-C1
6	A	324	MPG	O1-C1-C2-C3
6	A	318	MPG	O1-C1-C2-C3
4	A	309	UND	C7-C8-C9-C10
6	A	324	MPG	C1-C2-C3-C4
6	A	321	MPG	O1-C1-C2-C3
6	A	321	MPG	C1-C2-C3-C4
6	A	323	MPG	C4-C5-C6-C7
6	A	322	MPG	C11-C12-C13-C14
4	A	303	UND	C6-C7-C8-C9
4	A	309	UND	C2-C3-C4-C5
6	A	323	MPG	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	A	322	MPG	C5-C6-C7-C8
6	A	324	MPG	C4-C5-C6-C7
6	A	318	MPG	C3-C4-C5-C6
6	A	320	MPG	O1-C1-C2-C3
6	A	318	MPG	C6-C7-C8-C9
6	A	317	MPG	O3-C21-CXD-CX3
6	A	319	MPG	O3-C21-CXD-CX3
6	A	324	MPG	O3-C21-CXD-CX3
6	A	325	MPG	O3-C21-CXD-CX3
5	A	305	D10	C6-C7-C8-C9
6	A	321	MPG	C10-C11-C12-C13
6	A	325	MPG	C13-C14-C15-C16
6	A	323	MPG	C2-C3-C4-C5
6	A	318	MPG	C5-C6-C7-C8
6	A	325	MPG	C5-C6-C7-C8
6	A	318	MPG	C7-C8-C9-C10
6	A	321	MPG	C6-C7-C8-C9
5	A	306	D10	C3-C4-C5-C6
6	A	322	MPG	O1-C1-C2-C3
5	A	304	D10	C3-C4-C5-C6
6	A	318	MPG	C4-C5-C6-C7
6	A	316	MPG	O1-C1-C2-C3
6	A	318	MPG	C9-C10-C11-C12
6	A	318	MPG	O3-C21-CXD-O2
5	A	305	D10	C5-C6-C7-C8
6	A	323	MPG	C5-C6-C7-C8
6	A	316	MPG	C3-C4-C5-C6
6	A	321	MPG	O4-CX3-CXD-C21
6	A	325	MPG	O4-CX3-CXD-C21
6	A	316	MPG	O4-CX3-CXD-O2
6	A	320	MPG	C9-C10-C11-C12
6	A	317	MPG	C2-C3-C4-C5
4	A	303	UND	C3-C4-C5-C6
6	A	322	MPG	C6-C7-C8-C9
5	A	305	D10	C2-C3-C4-C5
6	A	323	MPG	C10-C11-C12-C13
5	A	304	D10	C5-C6-C7-C8
6	A	322	MPG	C13-C14-C15-C16
6	A	325	MPG	O1-C1-C2-C3
6	A	322	MPG	C7-C8-C9-C10
6	A	319	MPG	O4-CX3-CXD-O2
5	A	313	D10	C5-C6-C7-C8

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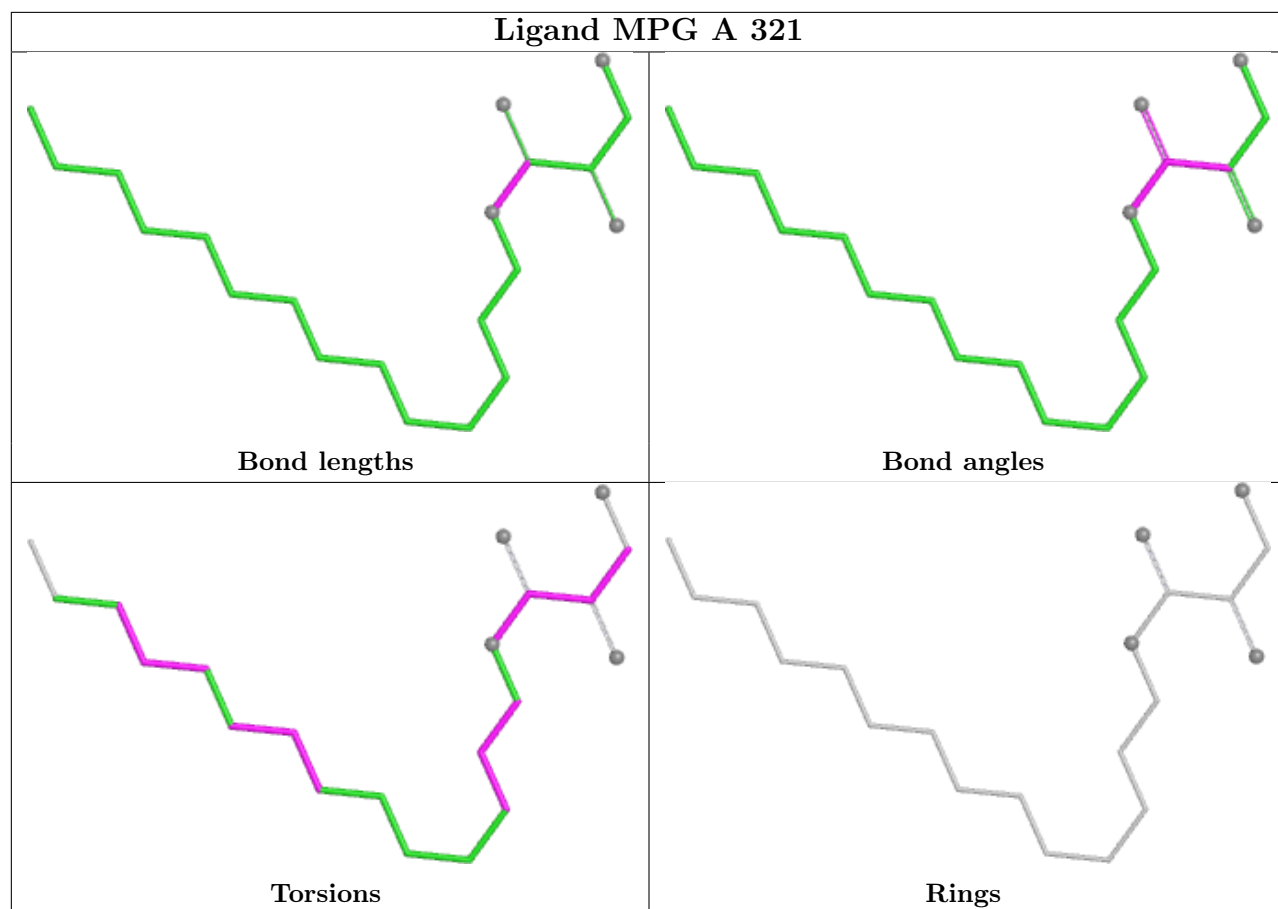
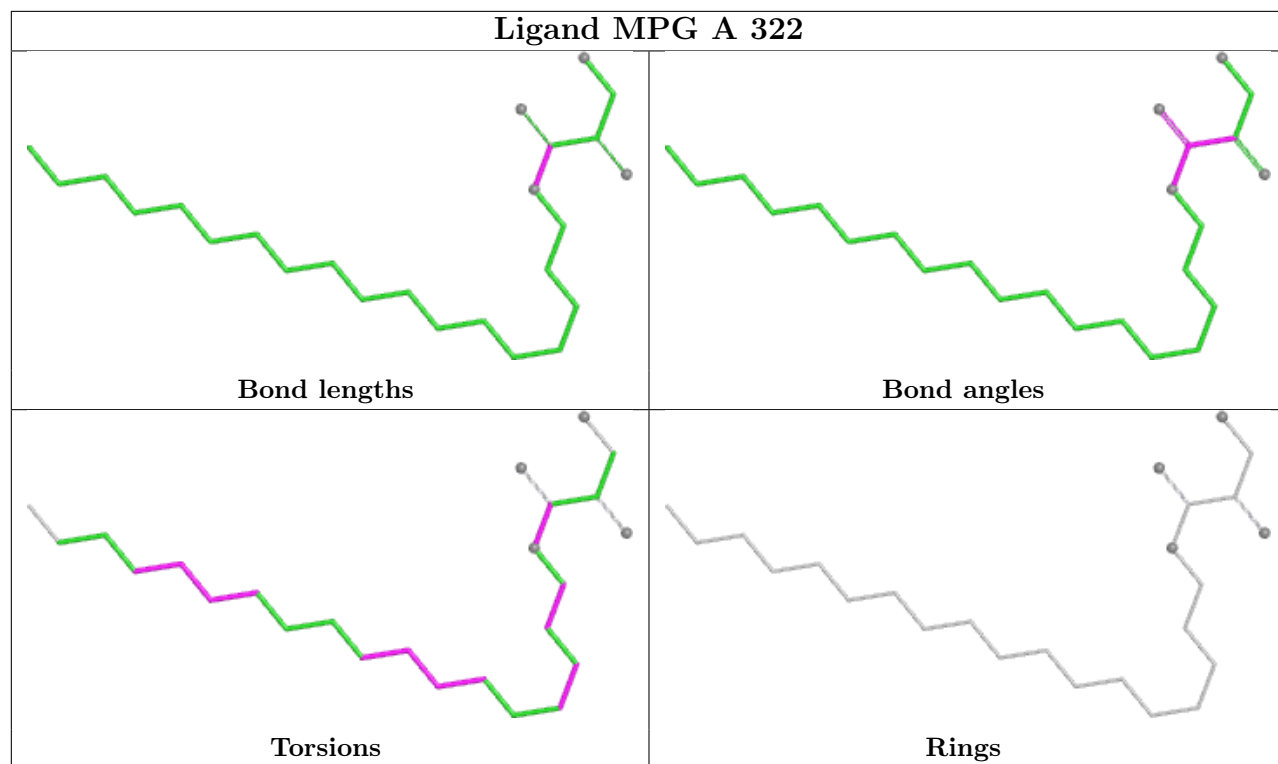
Mol	Chain	Res	Type	Atoms
6	A	322	MPG	C2-C3-C4-C5
5	A	305	D10	C4-C5-C6-C7
6	A	317	MPG	C7-C8-C9-C10
6	A	323	MPG	C9-C10-C11-C12
5	A	305	D10	C7-C8-C9-C10
6	A	323	MPG	C7-C8-C9-C10
6	A	321	MPG	C9-C10-C11-C12
5	A	304	D10	C2-C3-C4-C5
6	A	325	MPG	O4-CX3-CXD-O2
6	A	322	MPG	C12-C13-C14-C15
4	A	309	UND	C1-C2-C3-C4
6	A	325	MPG	O4-CX3-O1-C1
4	A	309	UND	C4-C5-C6-C7
6	A	324	MPG	C3-C4-C5-C6
4	A	309	UND	C3-C4-C5-C6
6	A	319	MPG	O1-CX3-CXD-O2
6	A	321	MPG	C7-C8-C9-C10
6	A	324	MPG	C7-C8-C9-C10
6	A	317	MPG	C3-C4-C5-C6

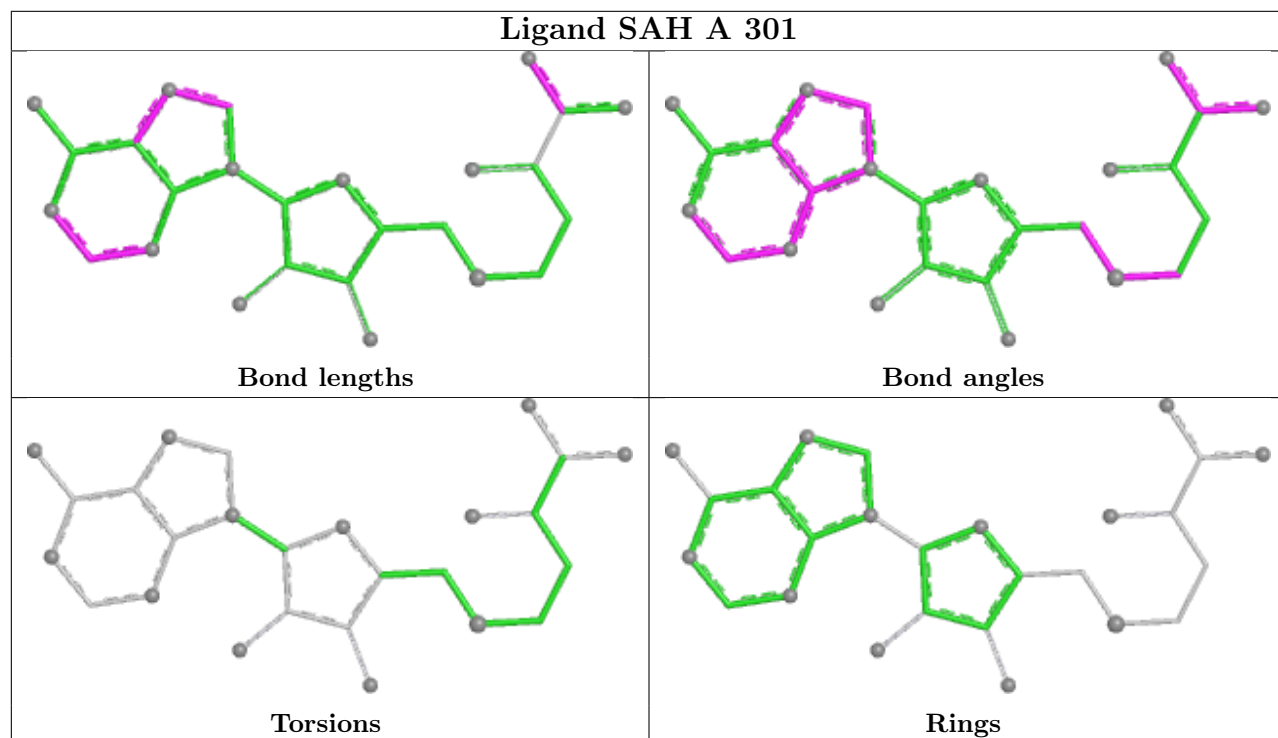
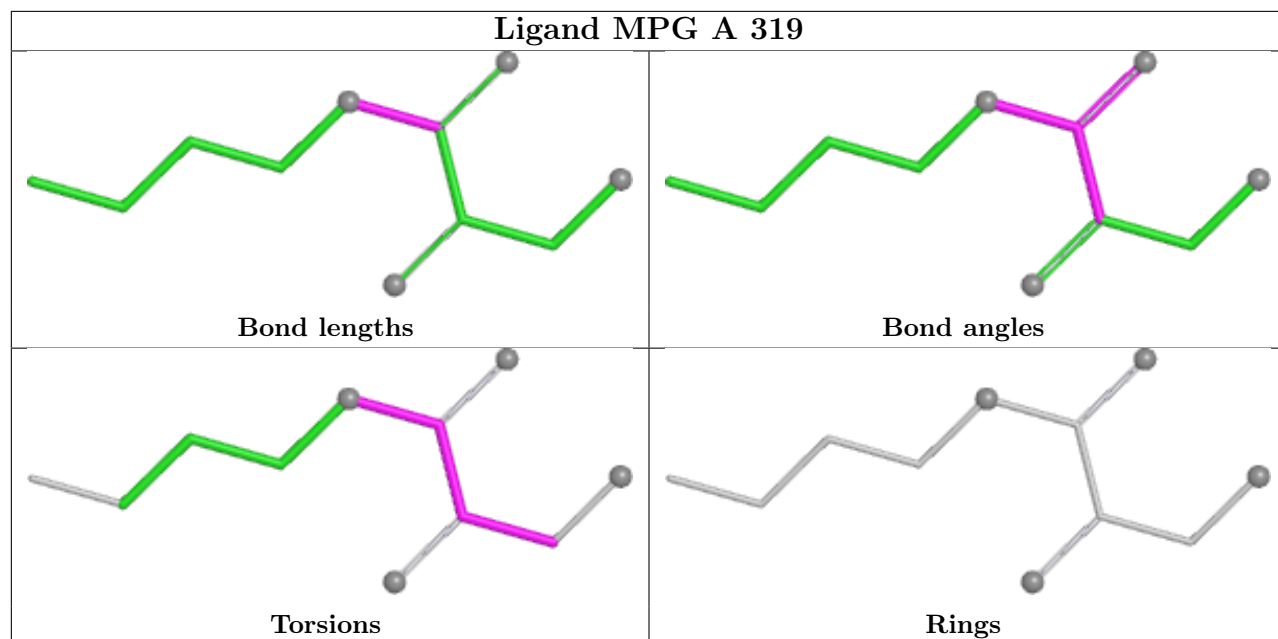
There are no ring outliers.

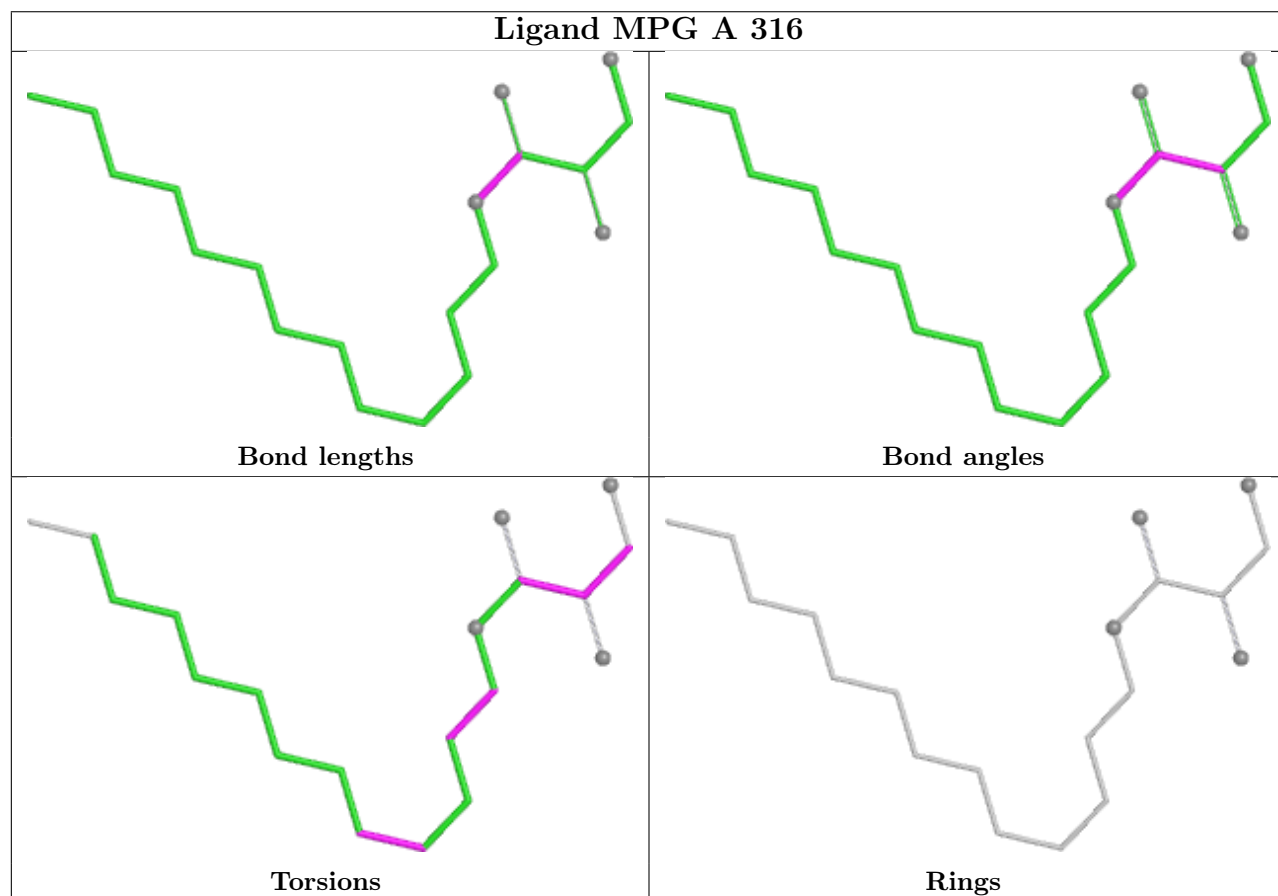
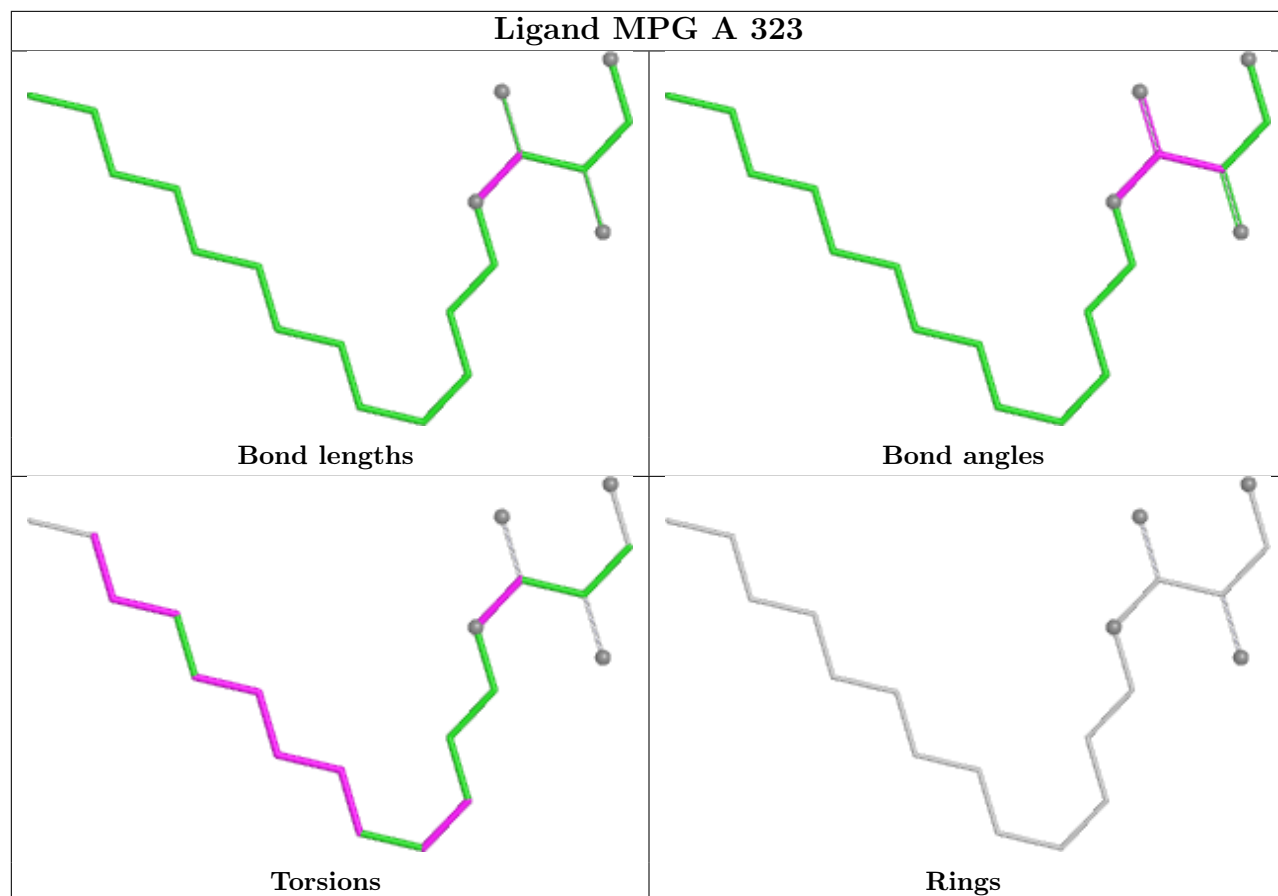
3 monomers are involved in 5 short contacts:

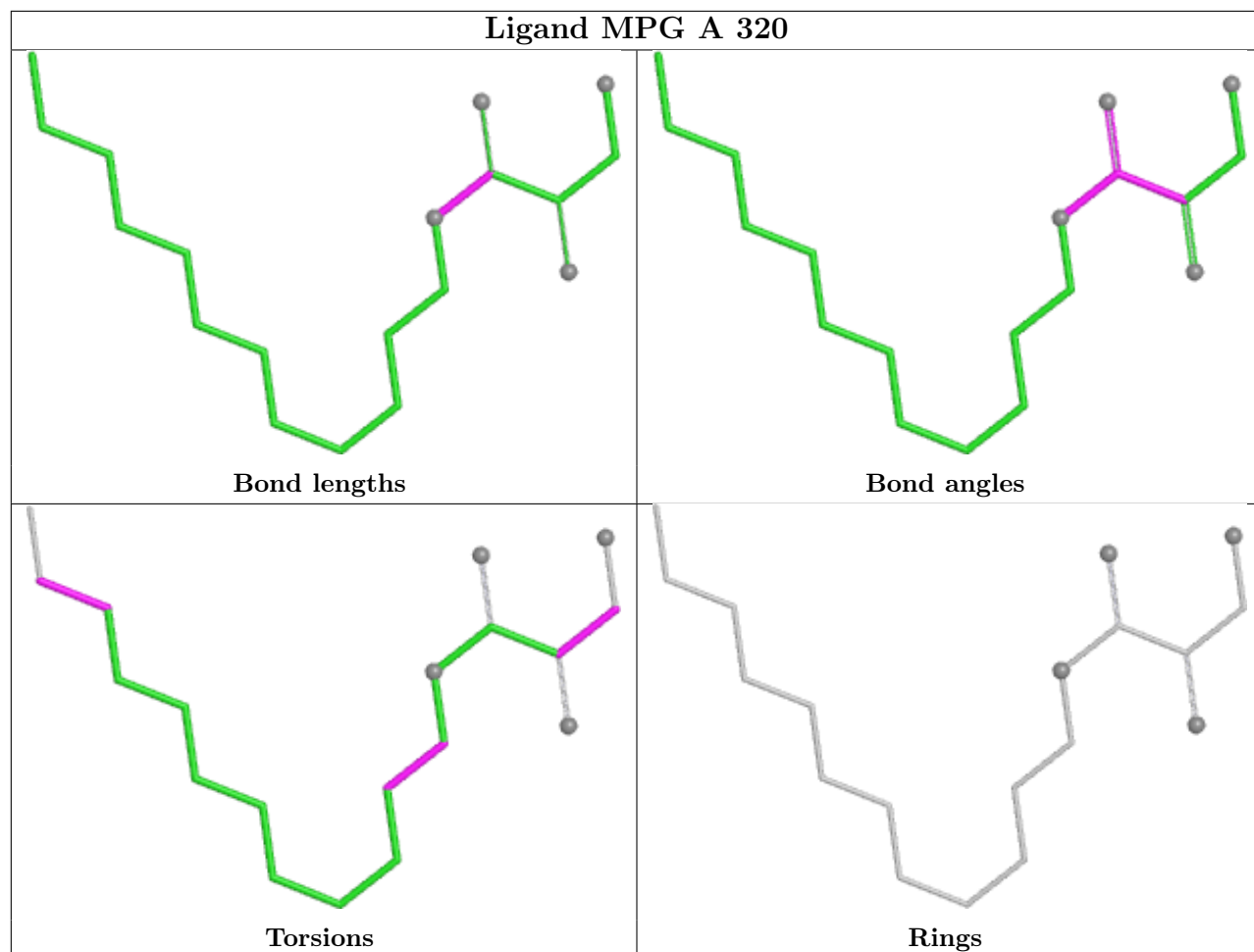
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	SAH	1	0
6	A	324	MPG	1	0
6	A	325	MPG	3	0

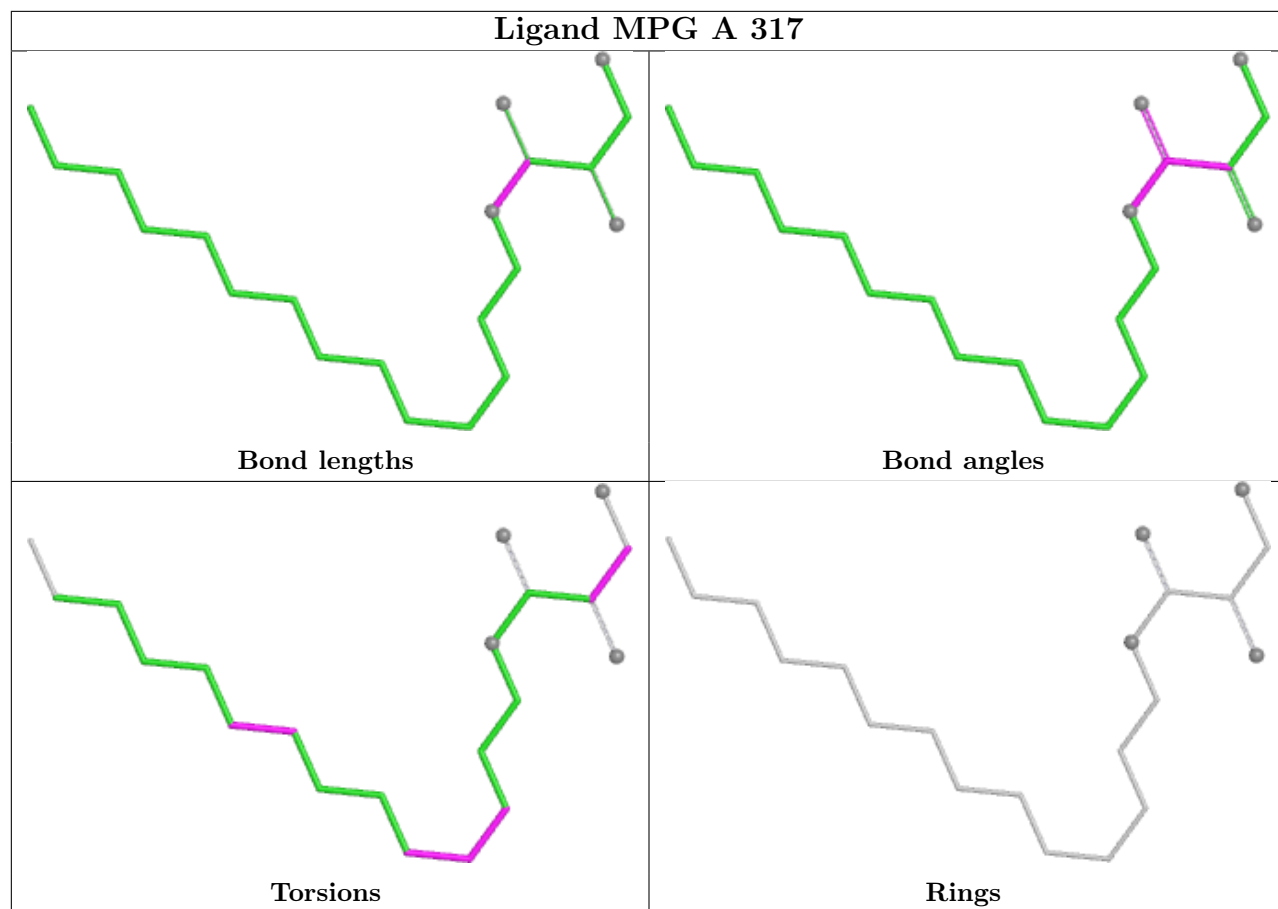
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

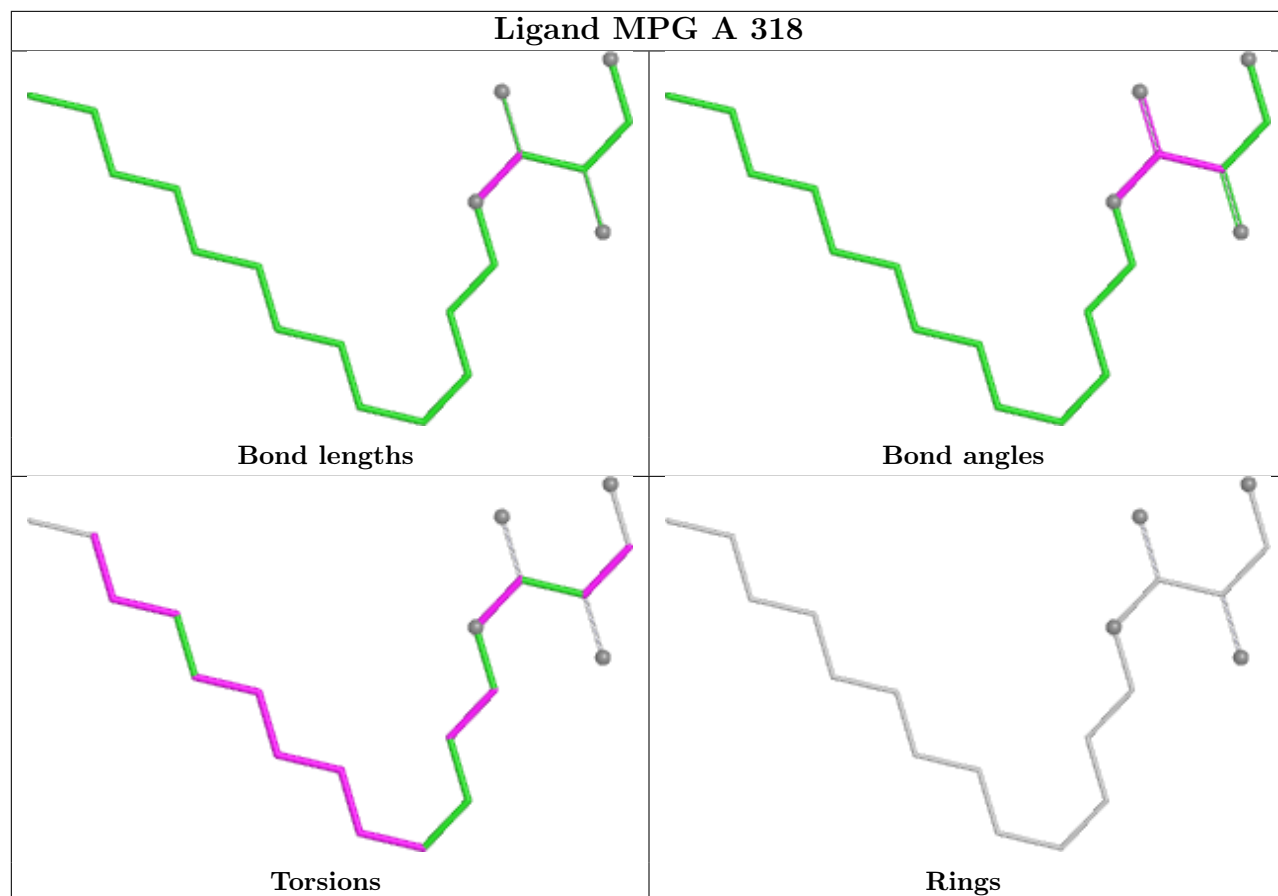


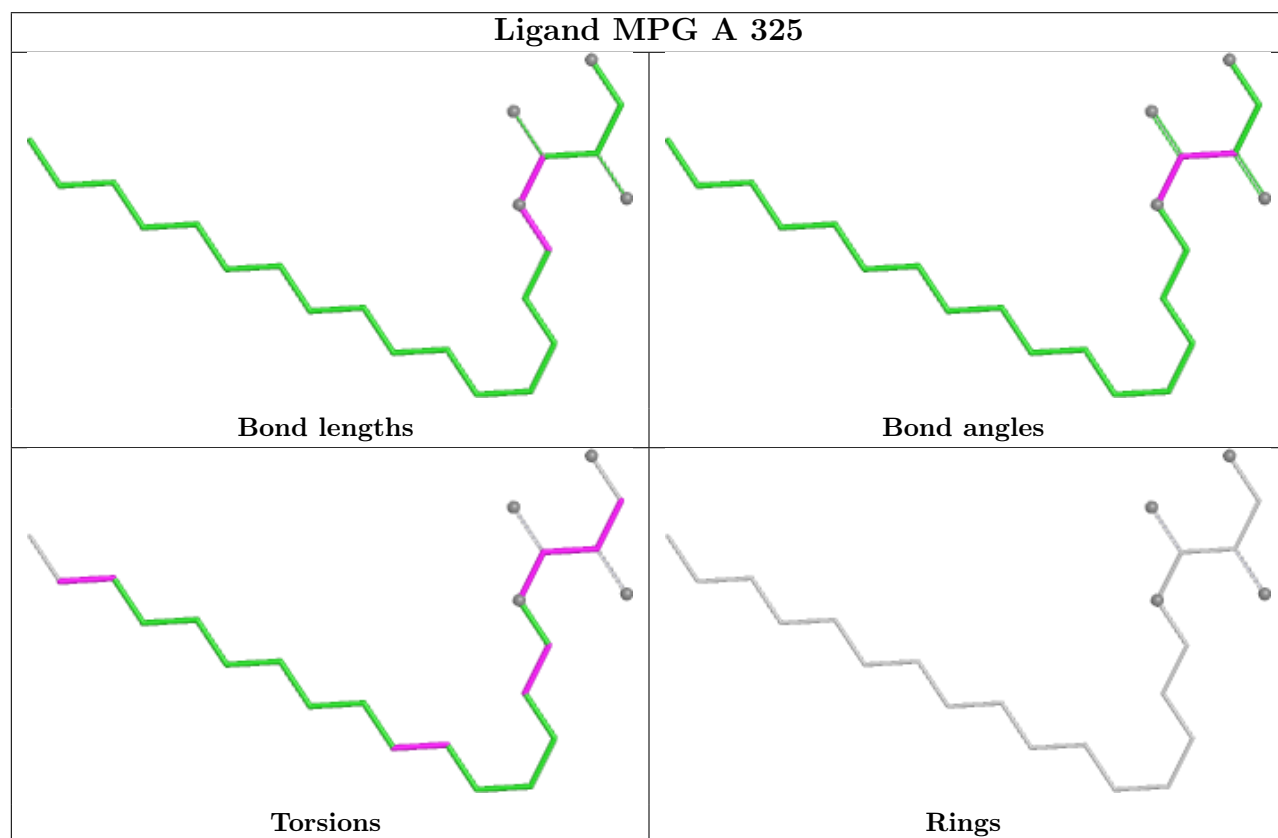
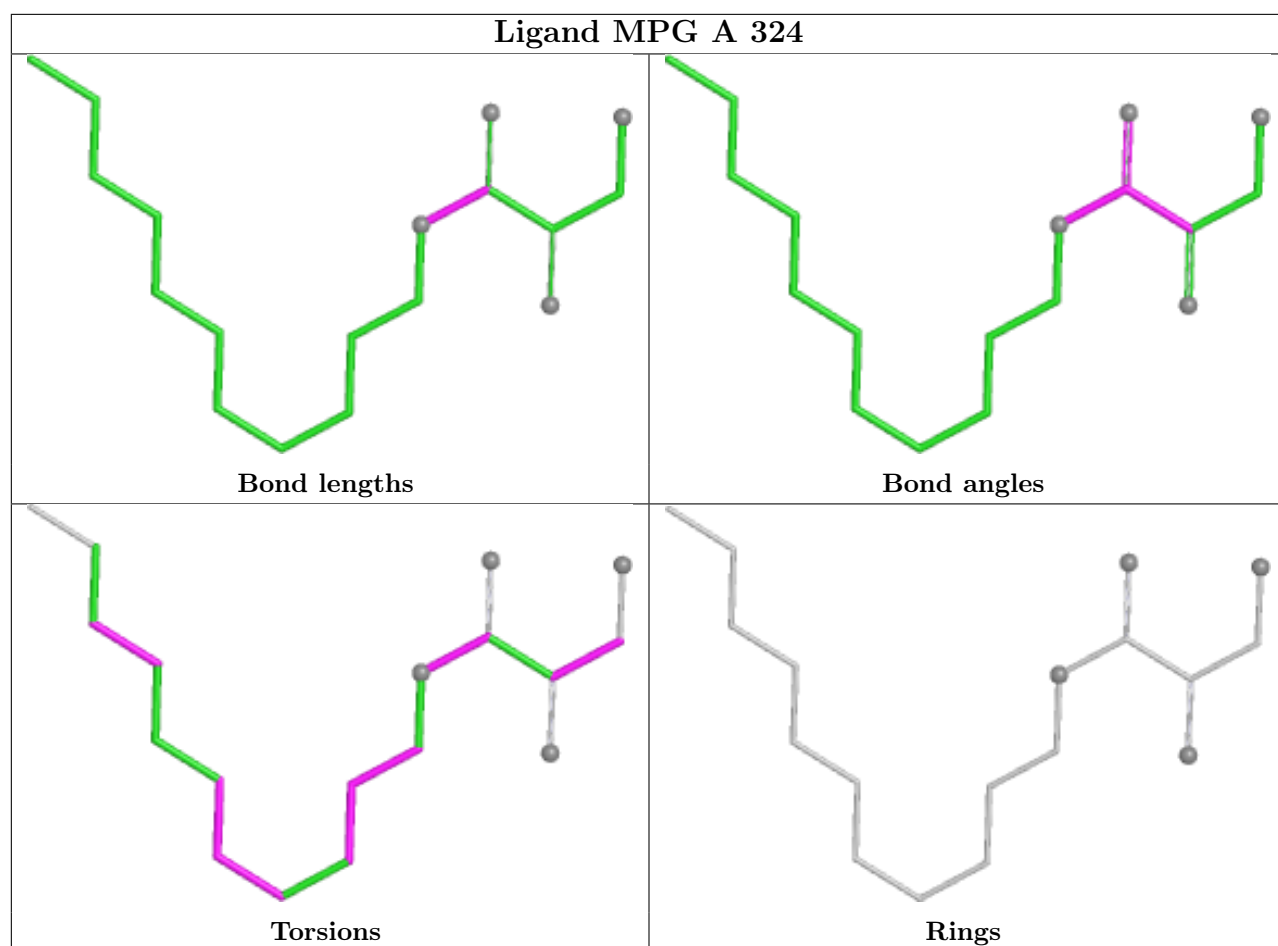












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/288 (97%)	0.13	8 (2%) 53 56	18, 30, 49, 72	4 (1%)
2	D	95/95 (100%)	0.39	3 (3%) 50 52	21, 35, 67, 103	1 (1%)
All	All	375/383 (97%)	0.19	11 (2%) 53 56	18, 31, 53, 103	5 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	0	ALA	3.9
1	A	126	ASN	3.1
1	A	127	HIS	2.6
1	A	30	TYR	2.6
1	A	281	ILE	2.5
1	A	91	ILE	2.4
1	A	29	TYR	2.3
1	A	124	VAL	2.2
2	D	87	PRO	2.1
1	A	116	LYS	2.0
2	D	14	THR	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

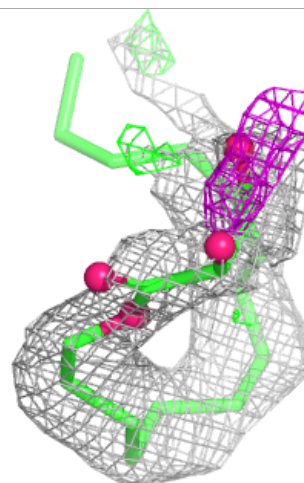
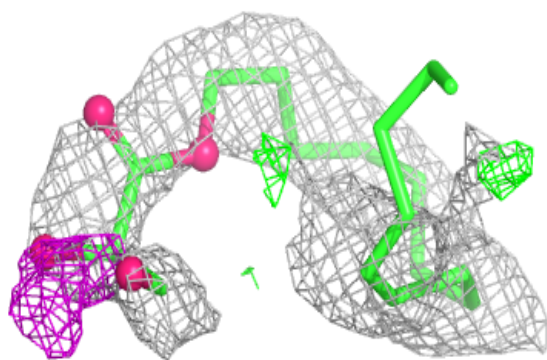
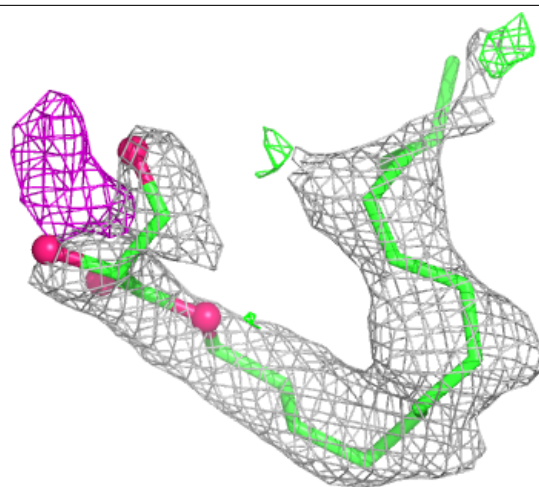
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	D10	A	306	6/10	0.60	0.27	47,57,59,61	0
5	D10	A	312	5/10	0.61	0.30	51,58,66,75	0
6	MPG	A	317	21/25	0.63	0.23	46,56,68,80	0
6	MPG	A	322	25/25	0.63	0.21	56,63,76,83	0
5	D10	A	304	9/10	0.65	0.26	45,57,59,63	0
6	MPG	A	321	21/25	0.66	0.19	38,60,77,81	0
5	D10	A	315	8/10	0.66	0.22	50,66,73,75	0
6	MPG	A	318	20/25	0.67	0.23	48,63,82,86	0
6	MPG	A	323	20/25	0.68	0.21	43,63,81,83	0
4	UND	A	302	11/11	0.70	0.22	34,50,59,60	0
4	UND	A	309	11/11	0.71	0.18	35,49,57,66	0
6	MPG	A	320	19/25	0.72	0.19	40,56,82,89	0
6	MPG	A	319	11/25	0.73	0.17	52,64,74,80	0
6	MPG	A	316	20/25	0.74	0.20	36,56,80,83	0
5	D10	A	311	8/10	0.74	0.23	50,51,58,64	0
5	D10	A	313	10/10	0.76	0.23	54,61,77,80	0
6	MPG	A	324	18/25	0.77	0.18	58,62,71,75	0
6	MPG	A	325	23/25	0.78	0.30	51,59,70,73	0
5	D10	A	314	8/10	0.80	0.23	43,55,65,66	0
5	D10	A	310	9/10	0.80	0.19	38,51,54,64	0
5	D10	A	307	6/10	0.81	0.18	40,43,47,56	0
5	D10	A	308	9/10	0.84	0.19	32,35,43,48	0
5	D10	A	305	10/10	0.85	0.16	22,38,44,45	0
4	UND	A	303	11/11	0.86	0.12	33,42,50,51	0
3	SAH	A	301	26/26	0.96	0.07	15,22,28,33	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.

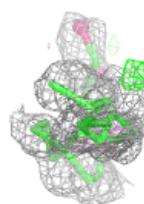
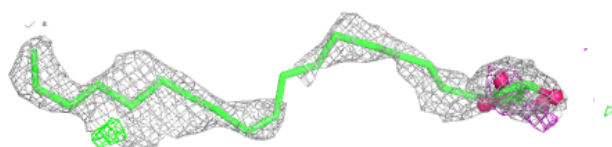
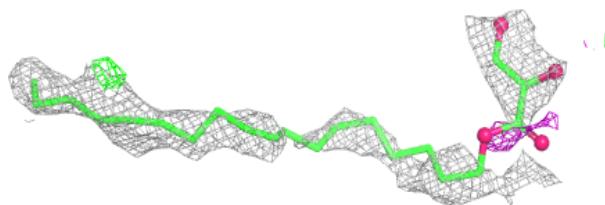
Electron density around MPG A 317:

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

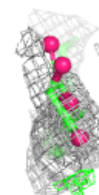
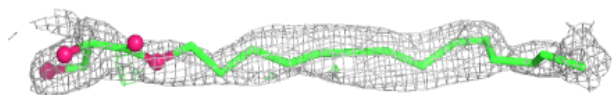
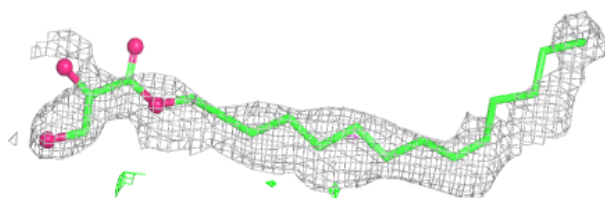


Electron density around MPG A 322:

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

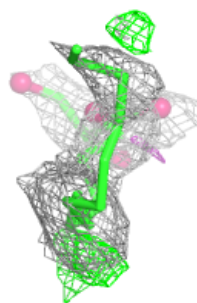
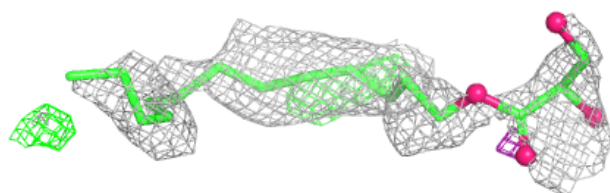
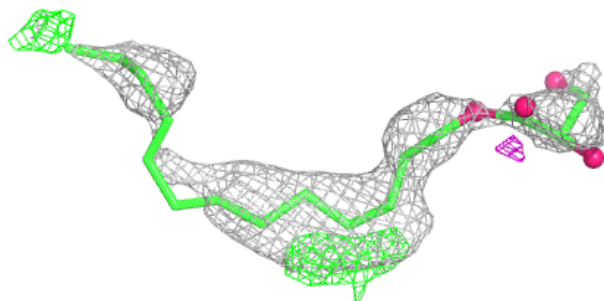
**Electron density around MPG A 321:**

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

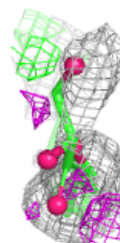
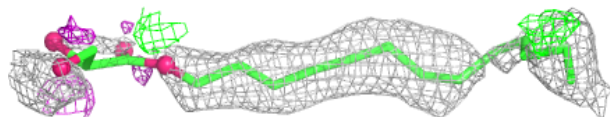
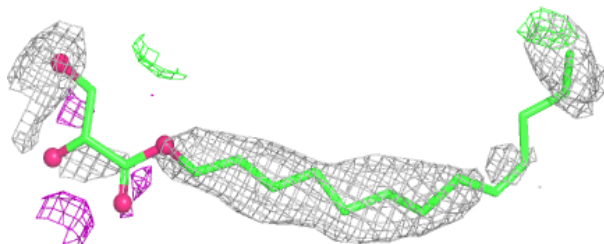


Electron density around MPG A 318:

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

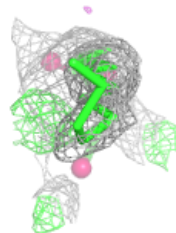
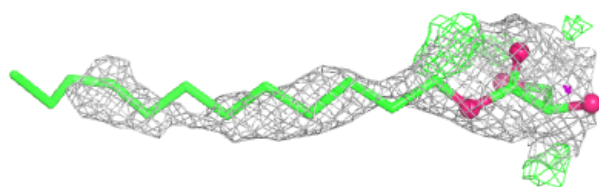
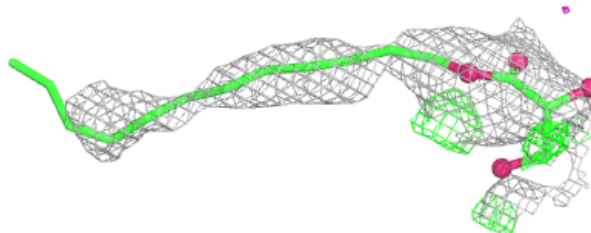
**Electron density around MPG A 323:**

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

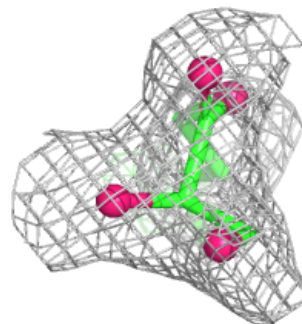
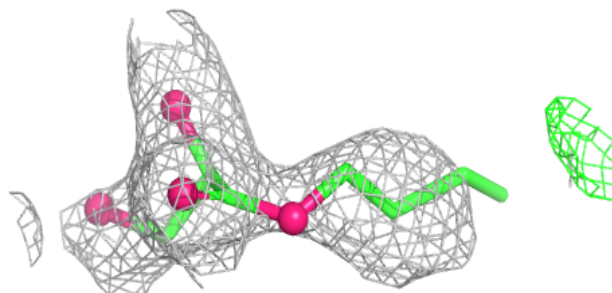
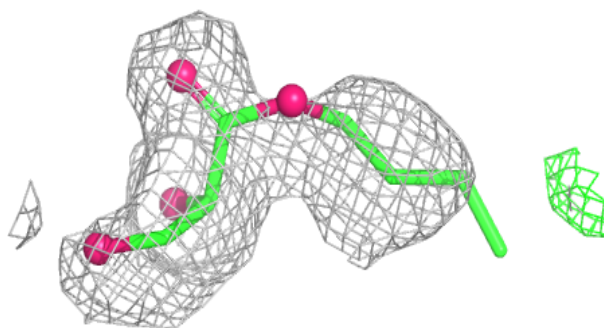


Electron density around MPG A 320:

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

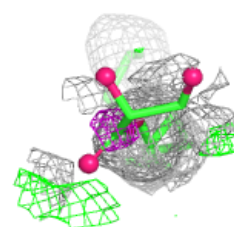
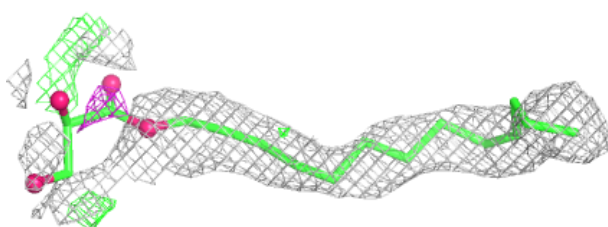
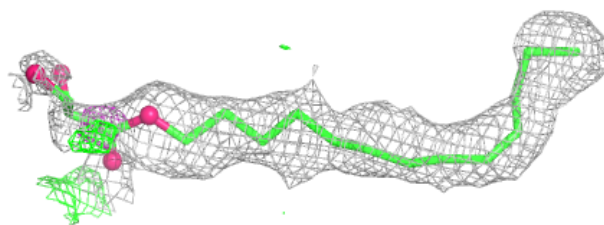
**Electron density around MPG A 319:**

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

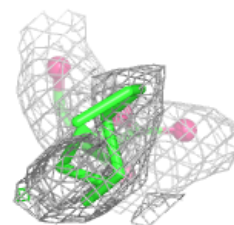
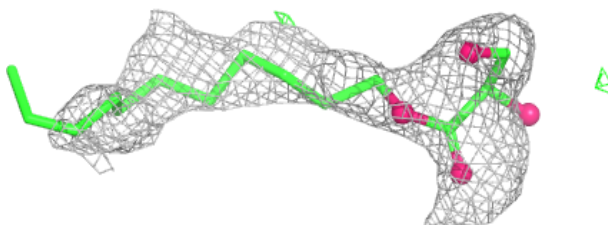
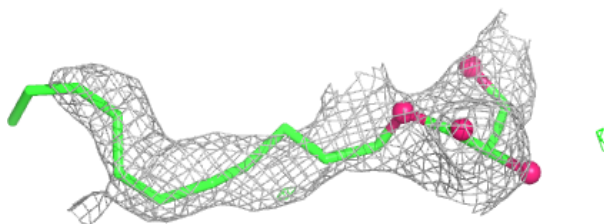


Electron density around MPG A 316:

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

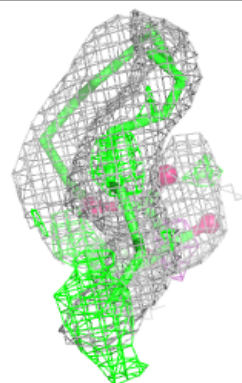
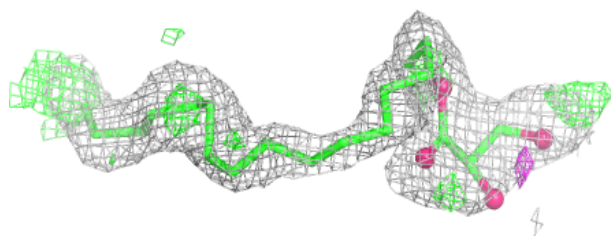
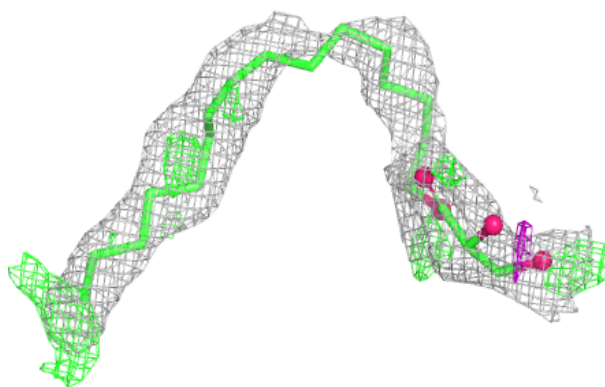
**Electron density around MPG A 324:**

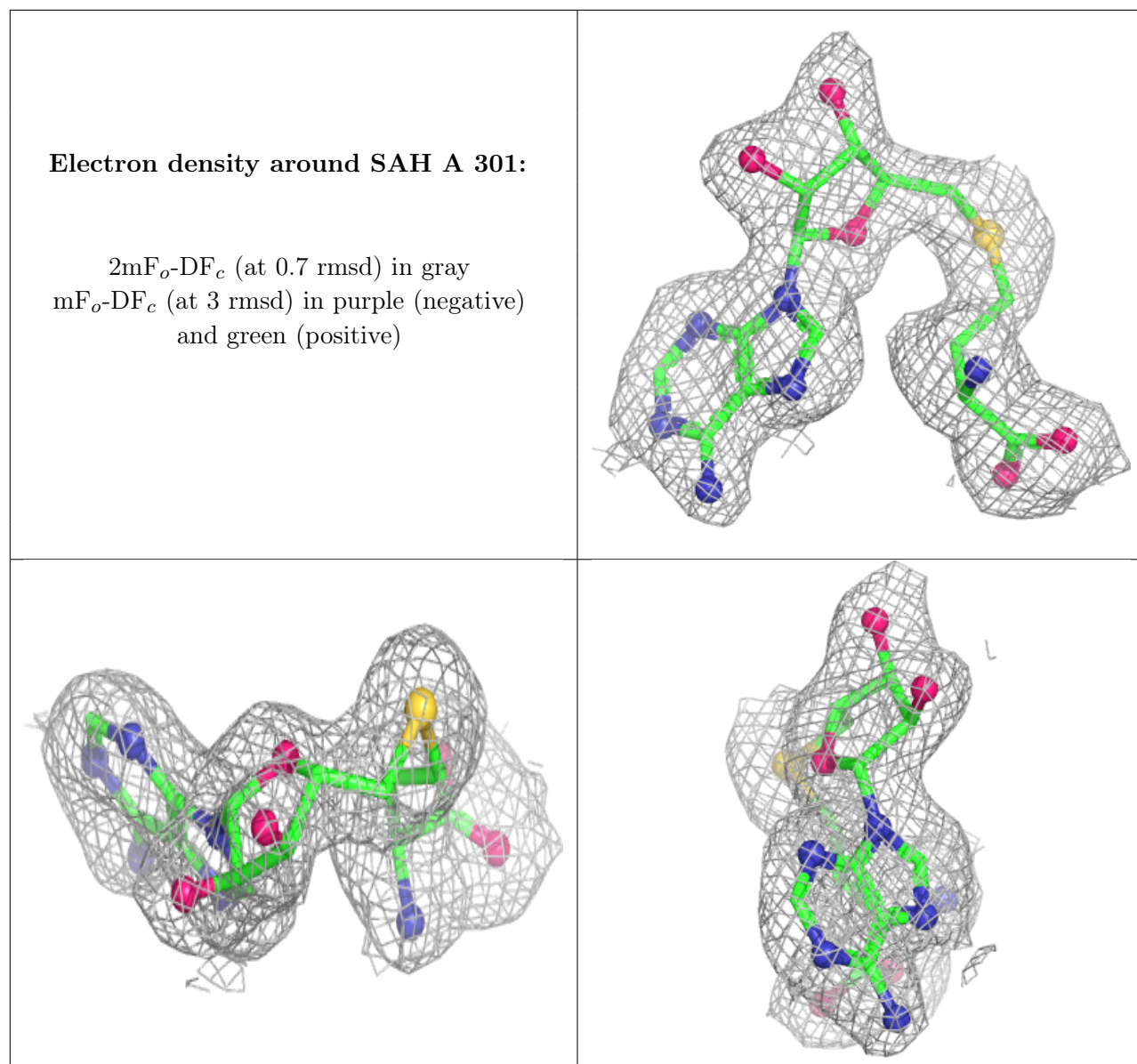
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MPG A 325:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.