



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 01:20 AM EDT

PDB ID : 2GUF  
Title : In meso crystal structure of the cobalamin transporter, BtuB  
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Deposited on : 2006-04-29  
Resolution : 1.95 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

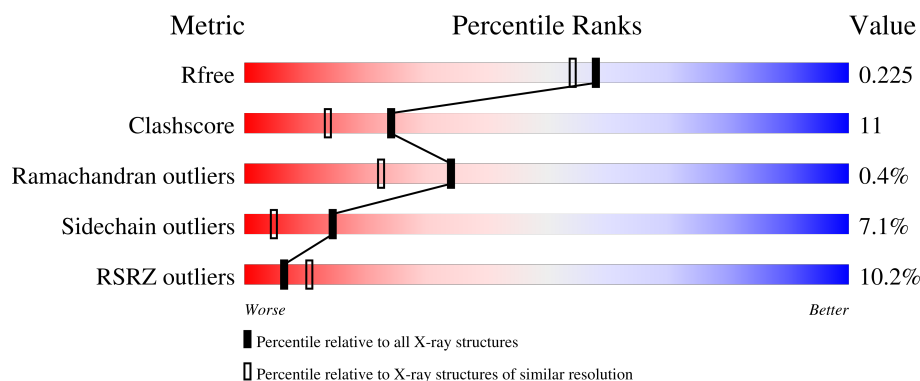
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	594	<div> <div>9%</div> <div>71%</div> <div>19%</div> <div>• 7%</div> </div>

## 2 Entry composition [i](#)

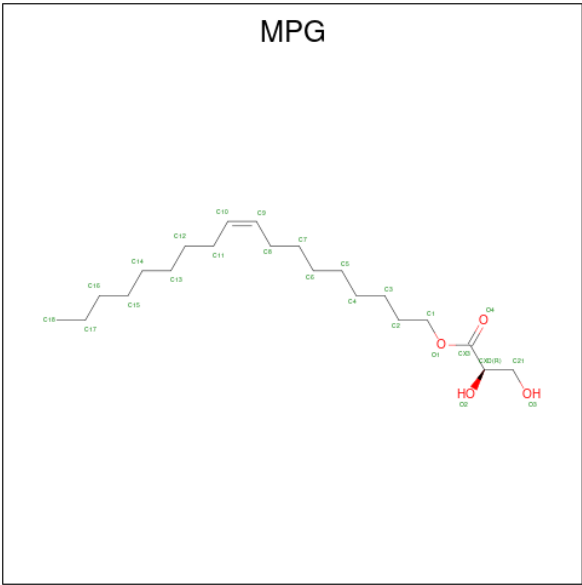
There are 5 unique types of molecules in this entry. The entry contains 5054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Vitamin B12 transporter btuB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	14	0
			4458	2814	771	871	2			

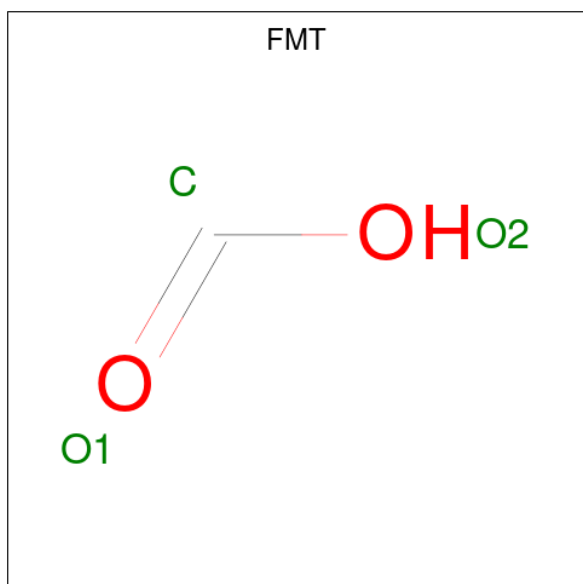
- Molecule 2 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	21	3		
2	A	1	Total	C	O	0	0
			24	21	3		
2	A	1	Total	C	O	0	0
			24	21	3		
2	A	1	Total	C	O	0	0
			24	21	3		
2	A	1	Total	C	O	0	0
			24	21	3		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $\text{C}_6\text{H}_{14}\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

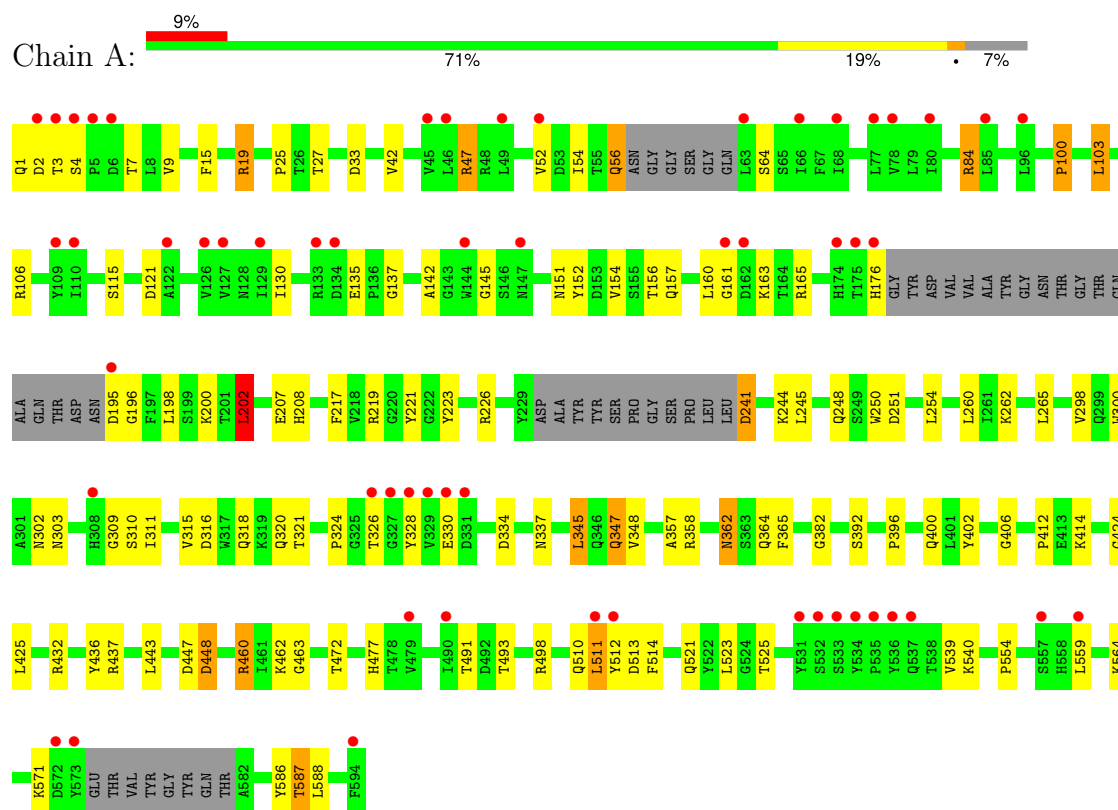
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total	O	0	0
			297	297		

### 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: Vitamin B12 transporter btuB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.61Å 80.88Å 118.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.44 – 1.95 40.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.44-1.95) 98.8 (40.44-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.225 0.190 , 0.225	Depositor DCC
$R_{free}$ test set	2592 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, FMT, MPG

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	0.93	3/4623 (0.1%)	0.96	7/6285 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	LYS	CD-CE	5.85	1.65	1.51
1	A	42	VAL	CB-CG1	-5.22	1.41	1.52
1	A	262	LYS	CE-NZ	5.03	1.61	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	47	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	202	LEU	CB-CG-CD1	5.64	120.59	111.00
1	A	202	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	84	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	498	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	447	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	241	ASP	Peptide

## 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	4458	0	4220	99	0
2	A	264	0	440	26	0
3	A	3	0	1	0	0
4	A	32	0	56	5	0
5	A	297	0	0	13	0
All	All	5054	0	4717	104	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 11.

All (104) 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:432[A]:ARG:NH2	5:A:957:HOH:O	1.78	1.15
1:A:84:ARG:HE	1:A:318:GLN:HE22	1.11	0.96
1:A:311:ILE:HD12	2:A:705:MPG:H182	1.51	0.91
1:A:248:GLN:HE22	2:A:708:MPG:H183	1.40	0.86
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.60	0.82
1:A:154[B]:VAL:HG23	2:A:702:MPG:H62C	1.63	0.81
1:A:248:GLN:HE22	2:A:708:MPG:C18	1.95	0.79
1:A:248:GLN:NE2	2:A:708:MPG:H181	1.98	0.78
1:A:248:GLN:NE2	2:A:708:MPG:C18	2.47	0.77
1:A:135:GLU:H	1:A:157:GLN:NE2	1.83	0.77
1:A:221:TYR:OH	5:A:1032:HOH:O	1.98	0.75
1:A:84:ARG:NE	1:A:318:GLN:HE22	1.82	0.75
1:A:326:THR:HB	1:A:328:TYR:HD1	1.53	0.73
1:A:135:GLU:H	1:A:157:GLN:HE22	1.35	0.72
1:A:200:LYS:HB3	2:A:702:MPG:H141	1.71	0.72
1:A:25:PRO:HG3	1:A:432[A]:ARG:NH2	2.05	0.72
1:A:347:GLN:HG2	5:A:1052:HOH:O	1.90	0.71
1:A:337:ASN:HB3	4:A:902:MPD:HM3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLN:NE2	1:A:27:THR:HG23	2.10	0.67
1:A:564[A]:LYS:HE2	1:A:587:THR:HG23	1.76	0.66
1:A:3:THR:HA	1:A:19[B]:ARG:HH12	1.62	0.64
1:A:302:ASN:ND2	2:A:704:MPG:H183	2.13	0.63
1:A:7:THR:O	1:A:19[B]:ARG:HG3	1.99	0.62
1:A:326:THR:HB	1:A:328:TYR:CD1	2.33	0.61
1:A:472:THR:OG1	1:A:477:HIS:HE1	1.84	0.60
1:A:226:ARG:HD3	1:A:244:LYS:HE2	1.83	0.60
1:A:1:GLN:HA	1:A:33:ASP:OD1	2.01	0.59
1:A:221:TYR:HA	2:A:708:MPG:H172	1.86	0.58
1:A:302:ASN:HD22	2:A:704:MPG:H183	1.68	0.57
1:A:364[A]:GLN:NE2	1:A:402:TYR:OH	2.30	0.56
1:A:357:ALA:HB1	2:A:704:MPG:H31C	1.87	0.56
1:A:460:ARG:HD2	1:A:462:LYS:HE3	1.87	0.55
1:A:362:ASN:HD22	1:A:365:PHE:H	1.55	0.55
1:A:564[B]:LYS:HE3	5:A:1132:HOH:O	2.07	0.54
1:A:47:ARG:NH2	5:A:941:HOH:O	2.40	0.53
1:A:163:LYS:NZ	2:A:709:MPG:HXD	2.23	0.53
1:A:2:ASP:O	1:A:19[B]:ARG:NH1	2.43	0.52
1:A:491:THR:OG1	1:A:493:THR:HG23	2.08	0.52
1:A:154[A]:VAL:HG13	2:A:708:MPG:H72C	1.92	0.52
2:A:705:MPG:H121	2:A:711:MPG:H161	1.93	0.51
1:A:200:LYS:O	1:A:223:TYR:HA	2.12	0.50
1:A:303:ASN:HD21	1:A:310:SER:HB2	1.76	0.50
1:A:437:ARG:CZ	1:A:460:ARG:HH11	2.24	0.50
1:A:250:TRP:HB3	2:A:706:MPG:H111	1.93	0.50
1:A:25:PRO:HG3	1:A:432[A]:ARG:CZ	2.42	0.49
1:A:115:SER:HB2	1:A:392:SER:HA	1.95	0.49
1:A:52:VAL:HG12	1:A:54:ILE:HG13	1.94	0.48
1:A:396:PRO:HD3	1:A:412:PRO:HA	1.95	0.48
1:A:510:GLN:HA	1:A:514:PHE:O	2.14	0.48
1:A:165[A]:ARG:NH2	1:A:207:GLU:OE1	2.47	0.48
1:A:84:ARG:HE	1:A:318:GLN:NE2	1.95	0.48
1:A:337:ASN:CB	4:A:902:MPD:HM3	2.42	0.47
1:A:248:GLN:HE21	2:A:708:MPG:H181	1.73	0.47
1:A:300:TRP:CE2	2:A:703:MPG:H132	2.49	0.47
1:A:202:LEU:HD13	2:A:702:MPG:H121	1.96	0.47
1:A:382:GLY:O	1:A:424:GLY:HA2	2.14	0.47
1:A:254:LEU:HG	2:A:709:MPG:H161	1.96	0.47
1:A:364[B]:GLN:HG2	1:A:365:PHE:CE1	2.49	0.47
1:A:448:ASP:OD1	1:A:448:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:NE2	5:A:919:HOH:O	2.48	0.46
1:A:315:VAL:HG13	2:A:703:MPG:H62C	1.97	0.46
1:A:84:ARG:NE	1:A:318:GLN:NE2	2.59	0.46
1:A:436:TYR:CZ	1:A:463:GLY:HA3	2.51	0.46
1:A:100:PRO:HG2	1:A:103:LEU:HD22	1.98	0.46
1:A:219[A]:ARG:NH2	5:A:1149:HOH:O	2.48	0.46
1:A:142:ALA:HA	1:A:151:ASN:O	2.17	0.45
1:A:298:VAL:HG12	2:A:703:MPG:H72C	1.97	0.45
1:A:511:LEU:HB3	5:A:1178:HOH:O	2.16	0.45
4:A:902:MPD:HM1	5:A:1167:HOH:O	2.17	0.45
1:A:165[A]:ARG:CZ	1:A:207:GLU:OE1	2.64	0.45
1:A:437:ARG:NH2	1:A:460:ARG:NH1	2.65	0.45
1:A:165[A]:ARG:NE	1:A:207:GLU:OE1	2.49	0.44
1:A:512:TYR:O	1:A:513:ASP:HB2	2.15	0.44
1:A:163:LYS:HE2	1:A:208:HIS:CE1	2.53	0.44
2:A:706:MPG:H152	2:A:706:MPG:H122	1.77	0.44
1:A:163:LYS:HZ2	2:A:709:MPG:HXD	1.82	0.44
1:A:154[B]:VAL:CG2	2:A:702:MPG:H62C	2.41	0.43
1:A:176:HIS:HA	1:A:196:GLY:HA3	2.00	0.43
1:A:9:VAL:HG13	1:A:19[B]:ARG:HG2	1.99	0.43
1:A:226:ARG:HG2	1:A:226:ARG:HH21	1.83	0.43
1:A:217:PHE:CD1	1:A:217:PHE:C	2.92	0.42
1:A:400:GLN:O	1:A:406:GLY:HA3	2.19	0.42
1:A:137:GLY:O	1:A:156:THR:HA	2.18	0.42
1:A:152:TYR:HB3	2:A:702:MPG:H51C	2.02	0.42
4:A:901:MPD:HM1	4:A:901:MPD:H4	1.84	0.42
1:A:432[A]:ARG:HD3	5:A:1009:HOH:O	2.19	0.42
1:A:521:GLN:NE2	5:A:996:HOH:O	2.48	0.42
1:A:321:THR:HG22	1:A:334:ASP:HB2	2.00	0.42
1:A:564[B]:LYS:CE	5:A:1132:HOH:O	2.65	0.42
1:A:309:GLY:HA3	1:A:345:LEU:O	2.19	0.42
4:A:904:MPD:O4	4:A:904:MPD:O2	2.26	0.42
1:A:1:GLN:HE22	1:A:27:THR:HG23	1.81	0.42
1:A:161:GLY:HA3	2:A:709:MPG:H212	2.01	0.42
1:A:15:PHE:CD1	1:A:303:ASN:HB2	2.55	0.41
1:A:145:GLY:HA2	1:A:586[A]:TYR:CE2	2.56	0.41
1:A:19[A]:ARG:NH2	5:A:1023:HOH:O	2.49	0.40
1:A:115:SER:O	1:A:358:ARG:HD3	2.20	0.40
1:A:56:GLN:HE21	1:A:56:GLN:HB2	1.51	0.40
1:A:106:ARG:HB3	1:A:130:ILE:HB	2.03	0.40
1:A:437:ARG:CZ	1:A:460:ARG:NH1	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PRO:O	1:A:554:PRO:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	555/594 (93%)	544 (98%)	9 (2%)	2 (0%)	34 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO
1	A	121	ASP

### 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	477/495 (96%)	443 (93%)	34 (7%)	14 5

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER

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Mol	Chain	Res	Type
1	A	19[A]	ARG
1	A	19[B]	ARG
1	A	56	GLN
1	A	100	PRO
1	A	103	LEU
1	A	160	LEU
1	A	195	ASP
1	A	198	LEU
1	A	202	LEU
1	A	241	ASP
1	A	245	LEU
1	A	251	ASP
1	A	260	LEU
1	A	265	LEU
1	A	316	ASP
1	A	330	GLU
1	A	345	LEU
1	A	347	GLN
1	A	348	VAL
1	A	362	ASN
1	A	425	LEU
1	A	443	LEU
1	A	448	ASP
1	A	460	ARG
1	A	511	LEU
1	A	523	LEU
1	A	525	THR
1	A	539	VAL
1	A	540	LYS
1	A	559	LEU
1	A	571	LYS
1	A	587	THR
1	A	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	157	GLN
1	A	158	GLN
1	A	176	HIS
1	A	225	ASN

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Mol	Chain	Res	Type
1	A	248	GLN
1	A	295	GLN
1	A	303	ASN
1	A	318	GLN
1	A	320	GLN
1	A	335	GLN
1	A	362	ASN
1	A	477	HIS
1	A	558	HIS

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

16 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	$\# Z  > 2$
2	MPG	A	711	-	23,23,24	0.46	0	23,23,25	0.50	0
2	MPG	A	701	-	23,23,24	0.32	0	23,23,25	0.87	1 (4%)
4	MPD	A	902	-	7,7,7	0.49	0	9,10,10	0.93	0
4	MPD	A	903	-	7,7,7	0.47	0	9,10,10	0.62	0
2	MPG	A	709	-	23,23,24	0.40	0	23,23,25	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MPD	A	901	-	7,7,7	0.35	0	9,10,10	0.83	0
2	MPG	A	705	-	23,23,24	0.35	0	23,23,25	0.91	1 (4%)
2	MPG	A	707	-	23,23,24	0.54	0	23,23,25	0.53	0
3	FMT	A	801	-	2,2,2	0.71	0	1,1,1	0.14	0
2	MPG	A	704	-	23,23,24	0.45	0	23,23,25	1.32	2 (8%)
2	MPG	A	703	-	23,23,24	0.53	0	23,23,25	0.56	0
2	MPG	A	708	-	23,23,24	0.53	0	23,23,25	0.35	0
2	MPG	A	702	-	23,23,24	0.42	0	23,23,25	0.60	0
4	MPD	A	904	-	7,7,7	0.51	0	9,10,10	1.05	1 (11%)
2	MPG	A	710	-	23,23,24	0.43	0	23,23,25	0.49	0
2	MPG	A	706	-	23,23,24	0.48	0	23,23,25	0.52	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
2	MPG	A	711	-	-	10/22/22/25	-
2	MPG	A	701	-	-	10/22/22/25	-
4	MPD	A	902	-	-	1/5/5/5	-
4	MPD	A	903	-	-	4/5/5/5	-
2	MPG	A	709	-	-	15/22/22/25	-
4	MPD	A	901	-	-	2/5/5/5	-
2	MPG	A	705	-	-	10/22/22/25	-
2	MPG	A	707	-	-	8/22/22/25	-
2	MPG	A	704	-	-	7/22/22/25	-
2	MPG	A	703	-	-	11/22/22/25	-
2	MPG	A	708	-	-	9/22/22/25	-
2	MPG	A	702	-	-	15/22/22/25	-
4	MPD	A	904	-	-	2/5/5/5	-
2	MPG	A	710	-	-	14/22/22/25	-
2	MPG	A	706	-	-	15/22/22/25	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	MPG	C1-O1-CX3	-3.42	98.53	113.58
2	A	705	MPG	C3-C2-C1	-2.47	102.75	113.47
2	A	704	MPG	C7-C6-C5	-2.27	102.88	114.37
4	A	904	MPD	O4-C4-C3	-2.26	102.38	111.35
2	A	701	MPG	C13-C12-C11	-2.18	103.39	113.86

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	MPG	O1-CX3-CXD-C21
2	A	703	MPG	O3-C21-CXD-CX3
2	A	709	MPG	O3-C21-CXD-CX3
2	A	709	MPG	O1-CX3-CXD-O2
2	A	710	MPG	O1-CX3-CXD-C21
2	A	711	MPG	O1-CX3-CXD-O2
4	A	901	MPD	C2-C3-C4-O4
4	A	903	MPD	C2-C3-C4-O4
4	A	903	MPD	C2-C3-C4-C5
2	A	706	MPG	C12-C13-C14-C15
2	A	702	MPG	O1-CX3-CXD-O2
2	A	708	MPG	O1-CX3-CXD-O2
2	A	711	MPG	C12-C13-C14-C15
2	A	703	MPG	O3-C21-CXD-O2
2	A	706	MPG	O1-C1-C2-C3
2	A	709	MPG	O1-C1-C2-C3
2	A	707	MPG	O1-CX3-CXD-O2
2	A	710	MPG	O1-CX3-CXD-O2
2	A	705	MPG	C4-C5-C6-C7
2	A	707	MPG	O1-C1-C2-C3
2	A	707	MPG	O1-CX3-CXD-C21
2	A	708	MPG	O1-CX3-CXD-C21
2	A	709	MPG	O1-CX3-CXD-C21
2	A	711	MPG	O1-CX3-CXD-C21
2	A	710	MPG	O1-C1-C2-C3
2	A	708	MPG	C13-C14-C15-C16
2	A	702	MPG	C2-C3-C4-C5
2	A	710	MPG	C14-C15-C16-C17
2	A	709	MPG	O3-C21-CXD-O2
2	A	709	MPG	C13-C14-C15-C16
2	A	705	MPG	C10-C11-C12-C13
2	A	707	MPG	C2-C3-C4-C5
2	A	706	MPG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	A	710	MPG	C11-C12-C13-C14
2	A	711	MPG	C5-C6-C7-C8
2	A	702	MPG	C11-C12-C13-C14
2	A	702	MPG	C13-C14-C15-C16
2	A	710	MPG	C5-C6-C7-C8
2	A	711	MPG	C1-C2-C3-C4
2	A	702	MPG	C10-C11-C12-C13
2	A	709	MPG	C11-C12-C13-C14
2	A	701	MPG	C13-C14-C15-C16
2	A	706	MPG	C3-C4-C5-C6
2	A	709	MPG	C2-C1-O1-CX3
2	A	702	MPG	C12-C13-C14-C15
2	A	710	MPG	C9-C10-C11-C12
2	A	707	MPG	C6-C7-C8-C9
2	A	710	MPG	C10-C11-C12-C13
2	A	703	MPG	C3-C4-C5-C6
2	A	701	MPG	CXD-CX3-O1-C1
2	A	709	MPG	C10-C11-C12-C13
2	A	703	MPG	C10-C11-C12-C13
2	A	705	MPG	C6-C7-C8-C9
2	A	709	MPG	C6-C7-C8-C9
2	A	711	MPG	C10-C11-C12-C13
2	A	701	MPG	C12-C13-C14-C15
2	A	708	MPG	C1-C2-C3-C4
2	A	703	MPG	C2-C3-C4-C5
2	A	711	MPG	C6-C7-C8-C9
2	A	702	MPG	C4-C5-C6-C7
2	A	701	MPG	C2-C3-C4-C5
2	A	711	MPG	C4-C5-C6-C7
2	A	709	MPG	C2-C3-C4-C5
2	A	705	MPG	CXD-CX3-O1-C1
2	A	703	MPG	C5-C6-C7-C8
2	A	701	MPG	C4-C5-C6-C7
2	A	704	MPG	O1-C1-C2-C3
2	A	705	MPG	C13-C14-C15-C16
2	A	711	MPG	C15-C16-C17-C18
2	A	701	MPG	C14-C15-C16-C17
2	A	708	MPG	C15-C16-C17-C18
2	A	706	MPG	CXD-CX3-O1-C1
2	A	703	MPG	C4-C5-C6-C7
2	A	702	MPG	C15-C16-C17-C18
2	A	704	MPG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	A	702	MPG	CXD-CX3-O1-C1
2	A	707	MPG	C13-C14-C15-C16
2	A	705	MPG	C15-C16-C17-C18
2	A	702	MPG	O3-C21-CXD-O2
2	A	706	MPG	O3-C21-CXD-O2
2	A	704	MPG	C3-C4-C5-C6
2	A	701	MPG	C2-C1-O1-CX3
2	A	704	MPG	C2-C1-O1-CX3
2	A	710	MPG	C2-C1-O1-CX3
2	A	706	MPG	C1-C2-C3-C4
2	A	711	MPG	C2-C1-O1-CX3
4	A	903	MPD	CM-C2-C3-C4
2	A	705	MPG	C14-C15-C16-C17
2	A	705	MPG	C7-C8-C9-C10
2	A	709	MPG	C14-C15-C16-C17
4	A	901	MPD	C2-C3-C4-C5
4	A	902	MPD	C2-C3-C4-C5
2	A	706	MPG	C2-C1-O1-CX3
2	A	706	MPG	C4-C5-C6-C7
2	A	702	MPG	C7-C8-C9-C10
2	A	710	MPG	C13-C14-C15-C16
2	A	706	MPG	C14-C15-C16-C17
2	A	701	MPG	C10-C11-C12-C13
2	A	701	MPG	C6-C7-C8-C9
2	A	706	MPG	C6-C7-C8-C9
2	A	708	MPG	O1-C1-C2-C3
2	A	708	MPG	C10-C11-C12-C13
2	A	704	MPG	C13-C14-C15-C16
2	A	707	MPG	CXD-CX3-O1-C1
2	A	706	MPG	O3-C21-CXD-CX3
2	A	708	MPG	O3-C21-CXD-CX3
2	A	710	MPG	C1-C2-C3-C4
2	A	710	MPG	C12-C13-C14-C15
2	A	706	MPG	C13-C14-C15-C16
2	A	706	MPG	C9-C10-C11-C12
2	A	704	MPG	C9-C10-C11-C12
2	A	709	MPG	C4-C5-C6-C7
2	A	707	MPG	C12-C13-C14-C15
2	A	703	MPG	C7-C8-C9-C10
2	A	703	MPG	C9-C10-C11-C12
2	A	706	MPG	C7-C8-C9-C10
2	A	709	MPG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	709	MPG	C9-C10-C11-C12
2	A	710	MPG	C4-C5-C6-C7
2	A	703	MPG	C2-C1-O1-CX3
2	A	705	MPG	C5-C6-C7-C8
2	A	705	MPG	C2-C3-C4-C5
2	A	702	MPG	C9-C10-C11-C12
2	A	702	MPG	C2-C1-O1-CX3
2	A	701	MPG	O1-C1-C2-C3
2	A	708	MPG	C2-C3-C4-C5
2	A	703	MPG	C14-C15-C16-C17
4	A	903	MPD	C1-C2-C3-C4
4	A	904	MPD	C1-C2-C3-C4
4	A	904	MPD	CM-C2-C3-C4
2	A	702	MPG	C1-C2-C3-C4
2	A	710	MPG	C3-C4-C5-C6
2	A	704	MPG	C7-C8-C9-C10

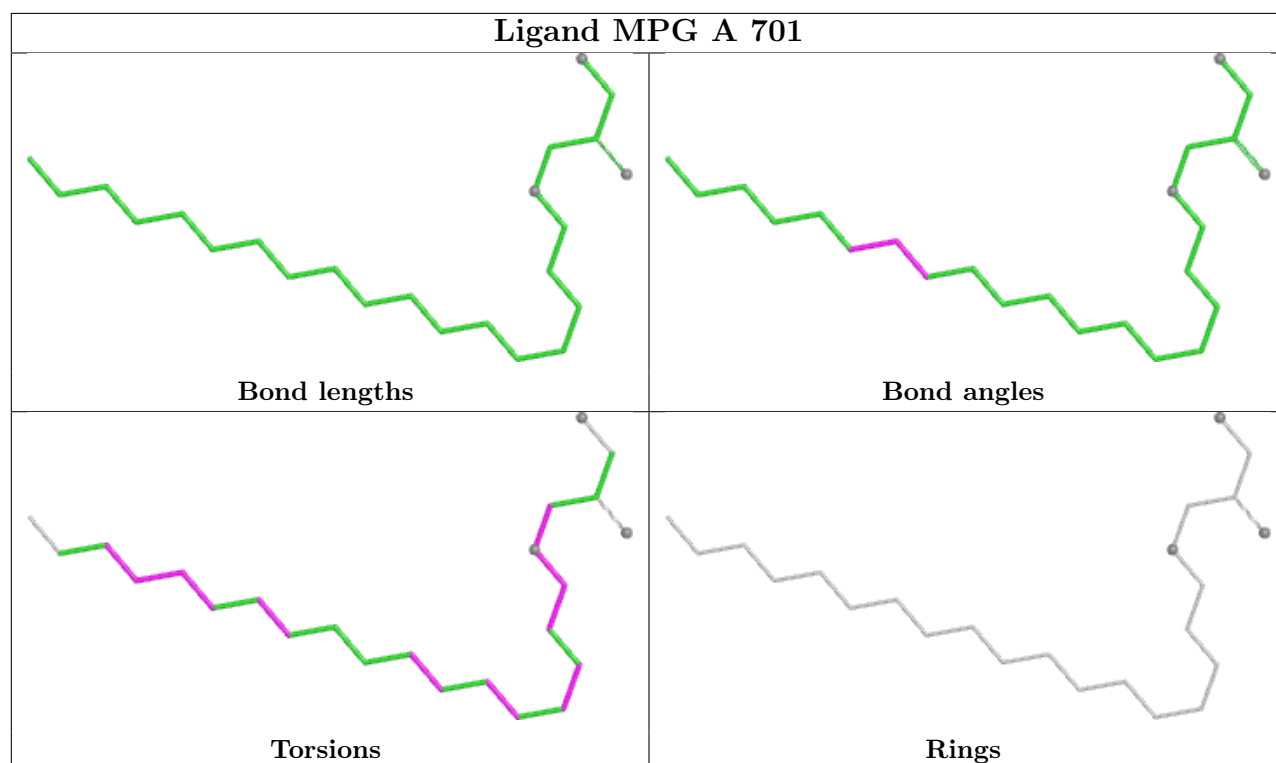
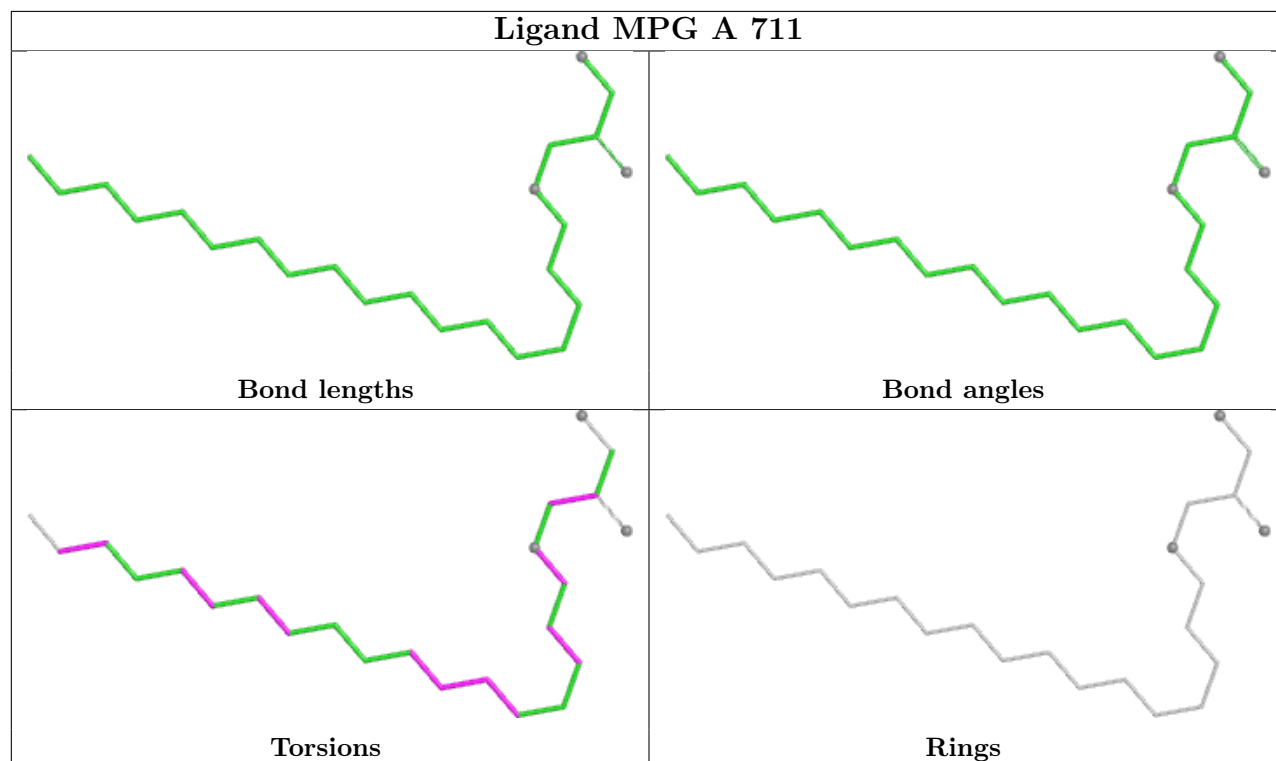
There are no ring outliers.

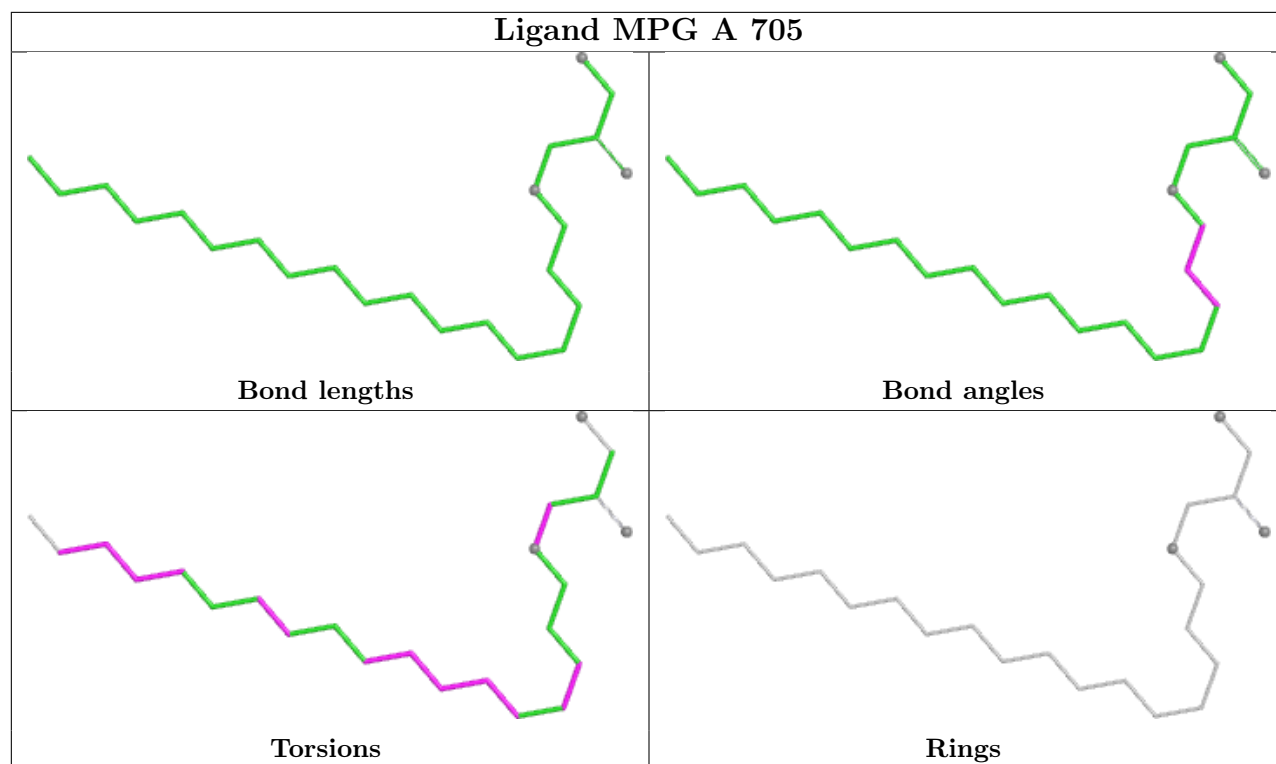
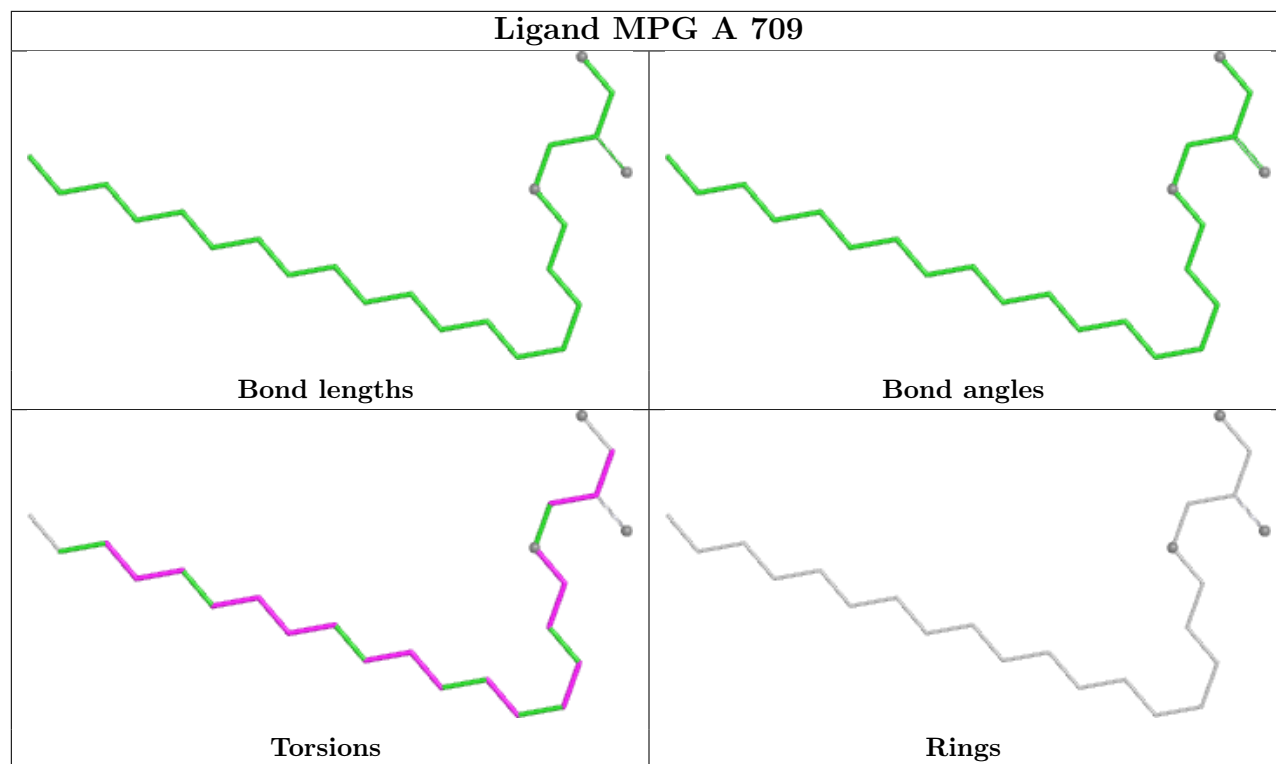
11 monomers are involved in 31 short contacts:

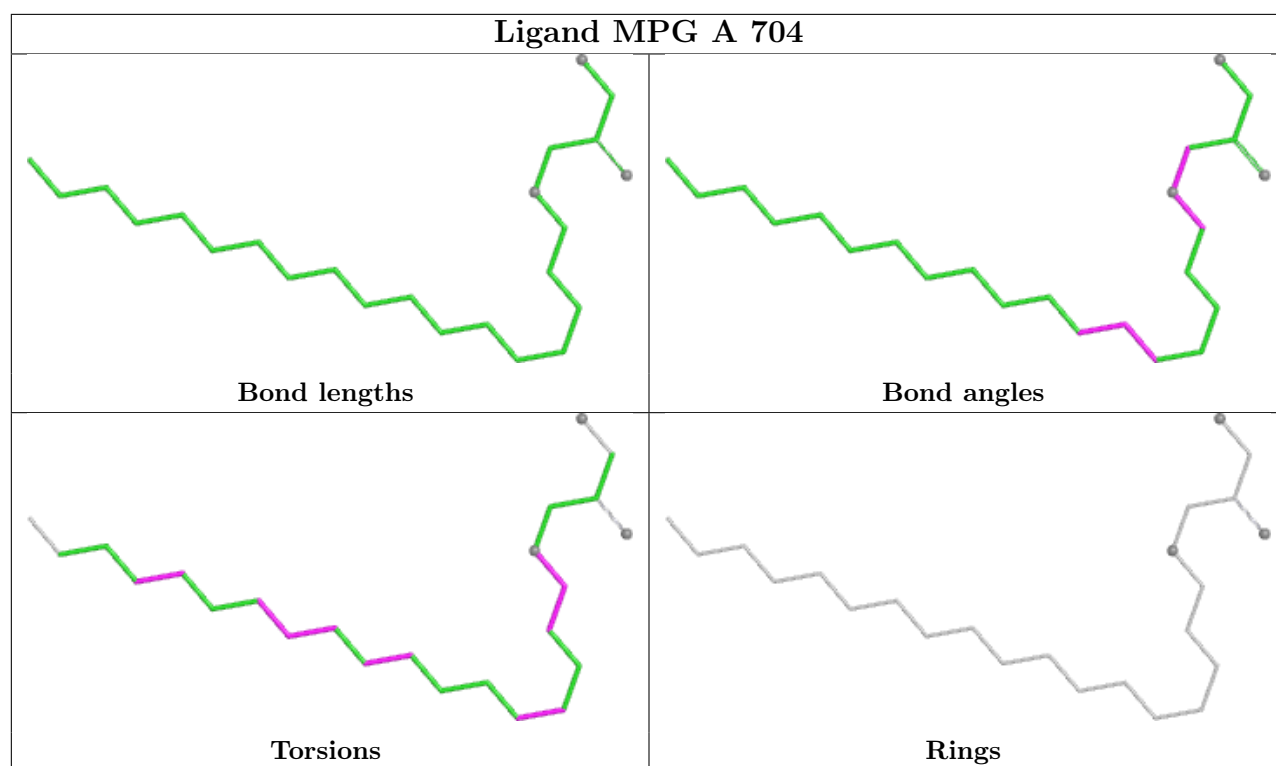
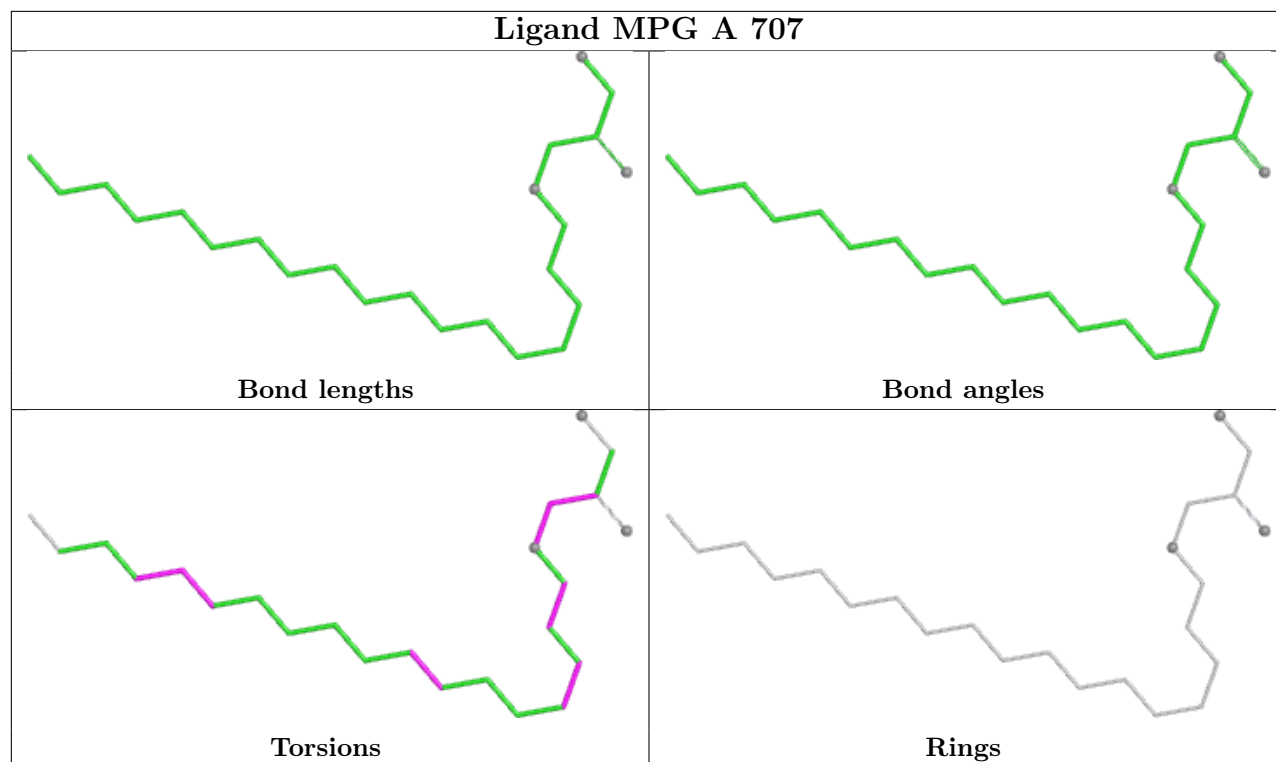
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	711	MPG	1	0
4	A	902	MPD	3	0
2	A	709	MPG	4	0
4	A	901	MPD	1	0
2	A	705	MPG	2	0
2	A	704	MPG	3	0
2	A	703	MPG	3	0
2	A	708	MPG	7	0
2	A	702	MPG	5	0
4	A	904	MPD	1	0
2	A	706	MPG	2	0

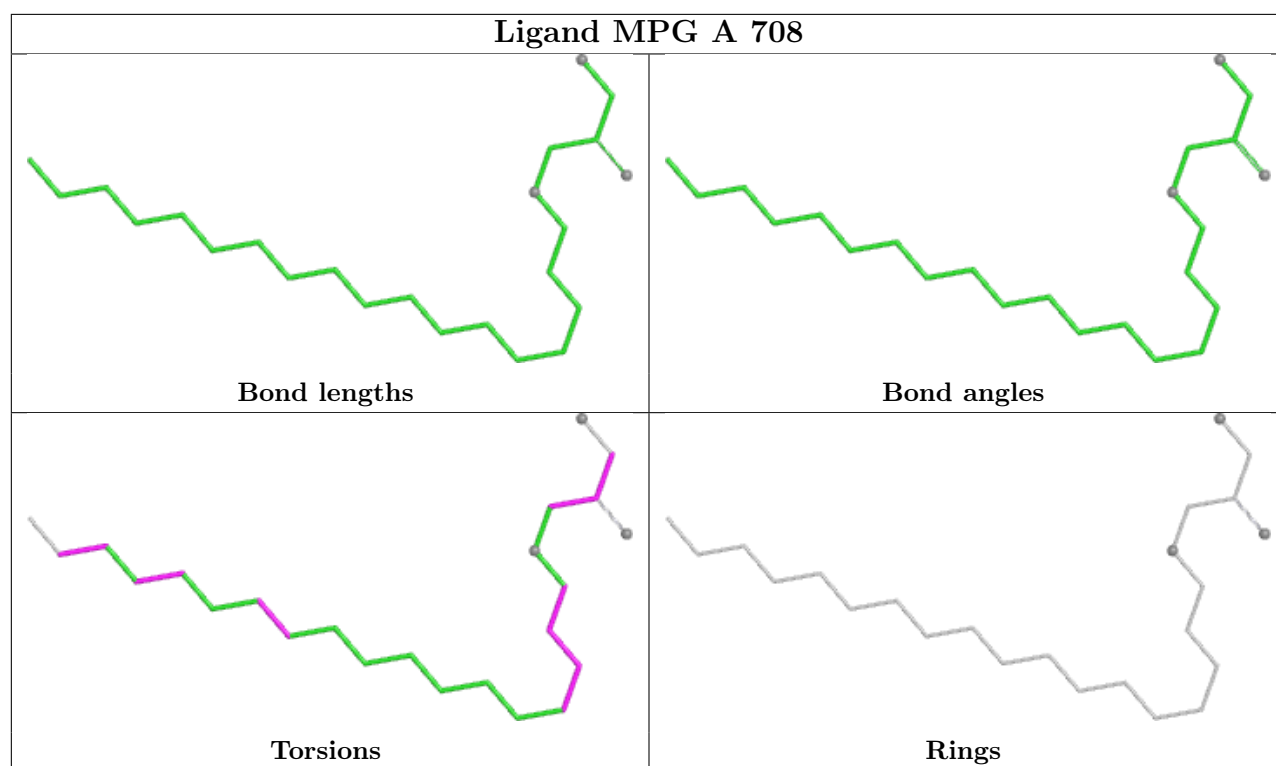
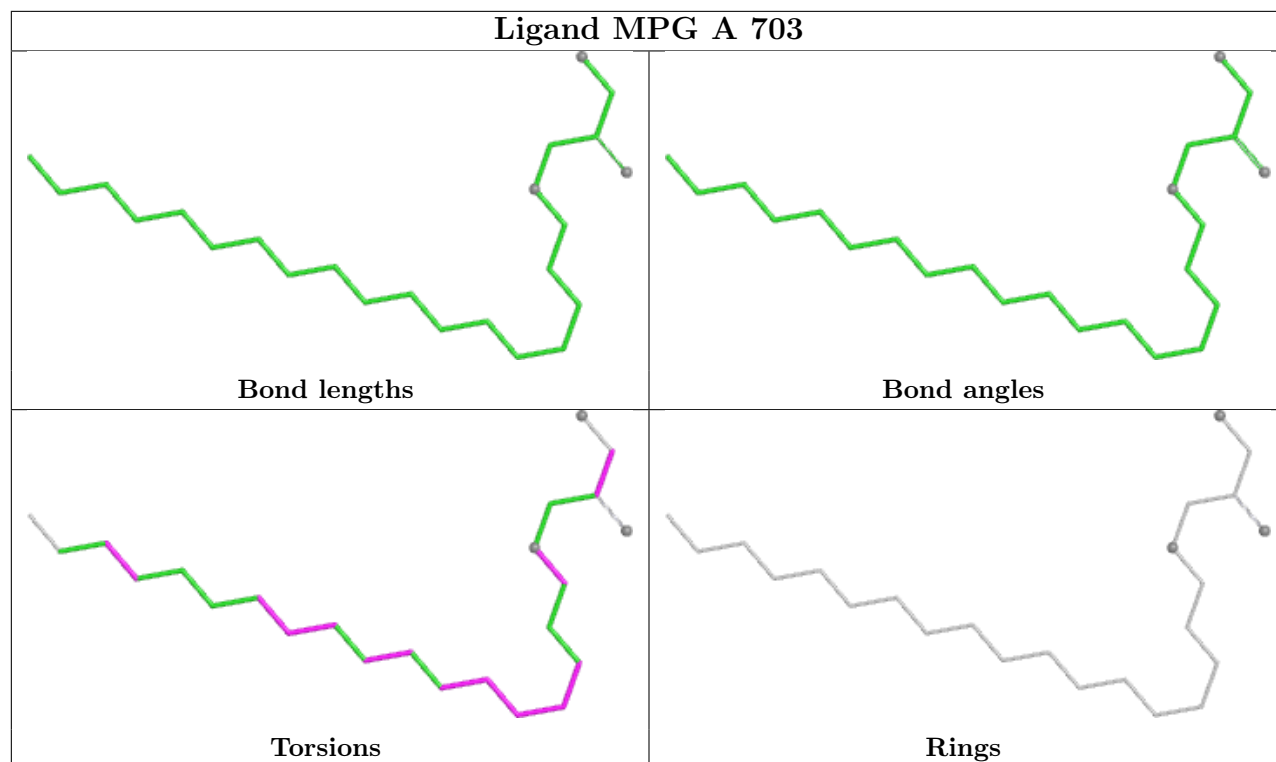
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

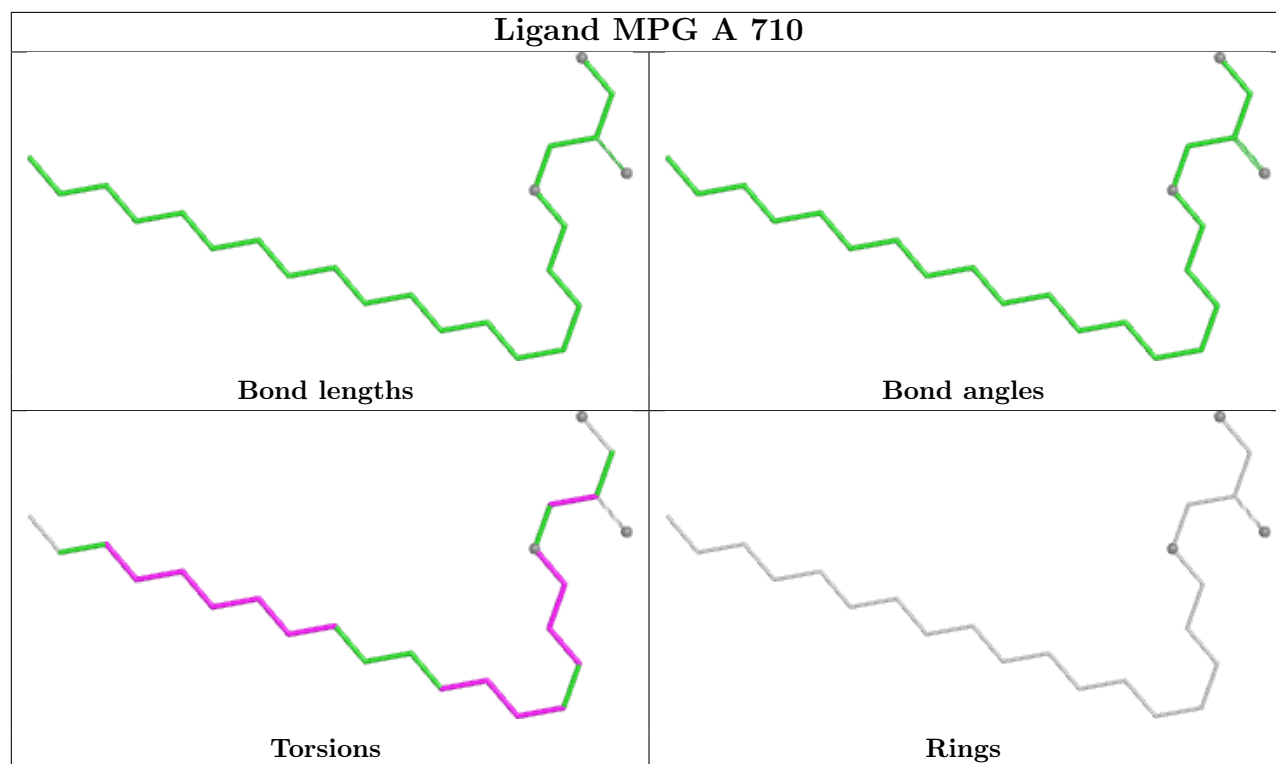
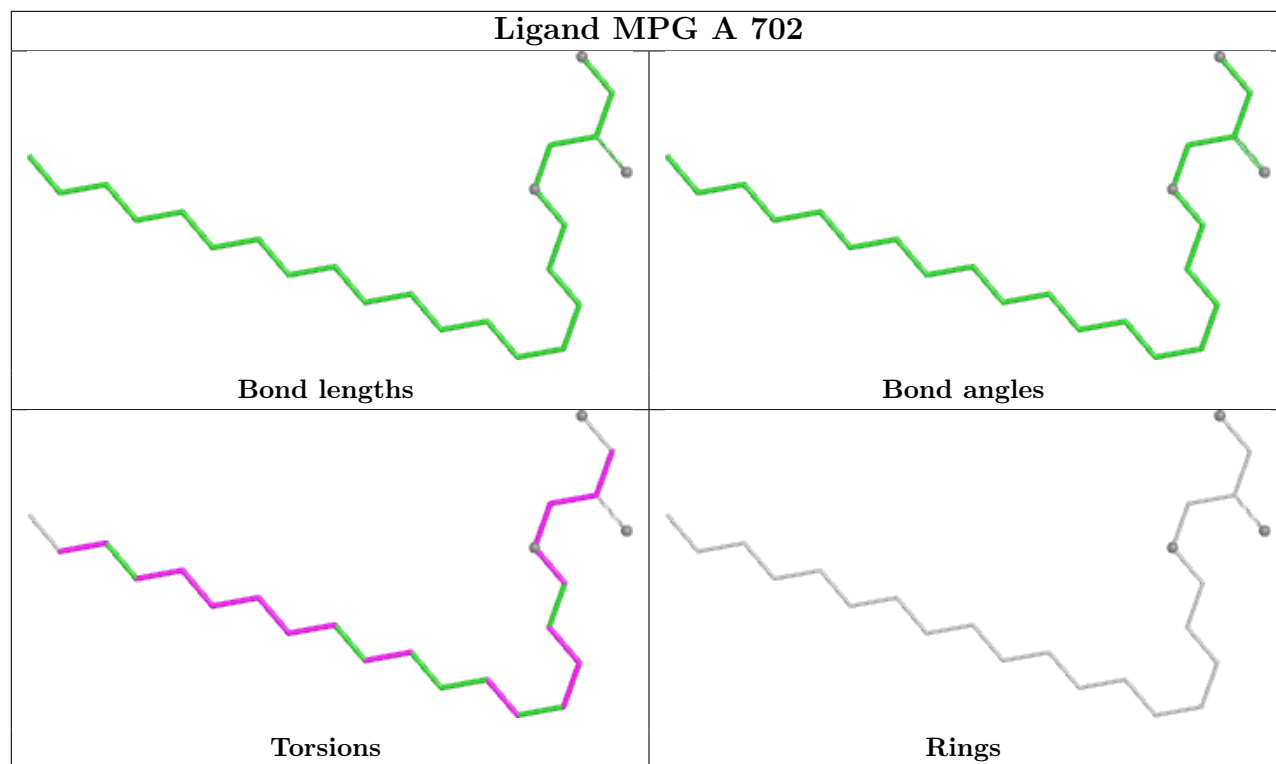
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



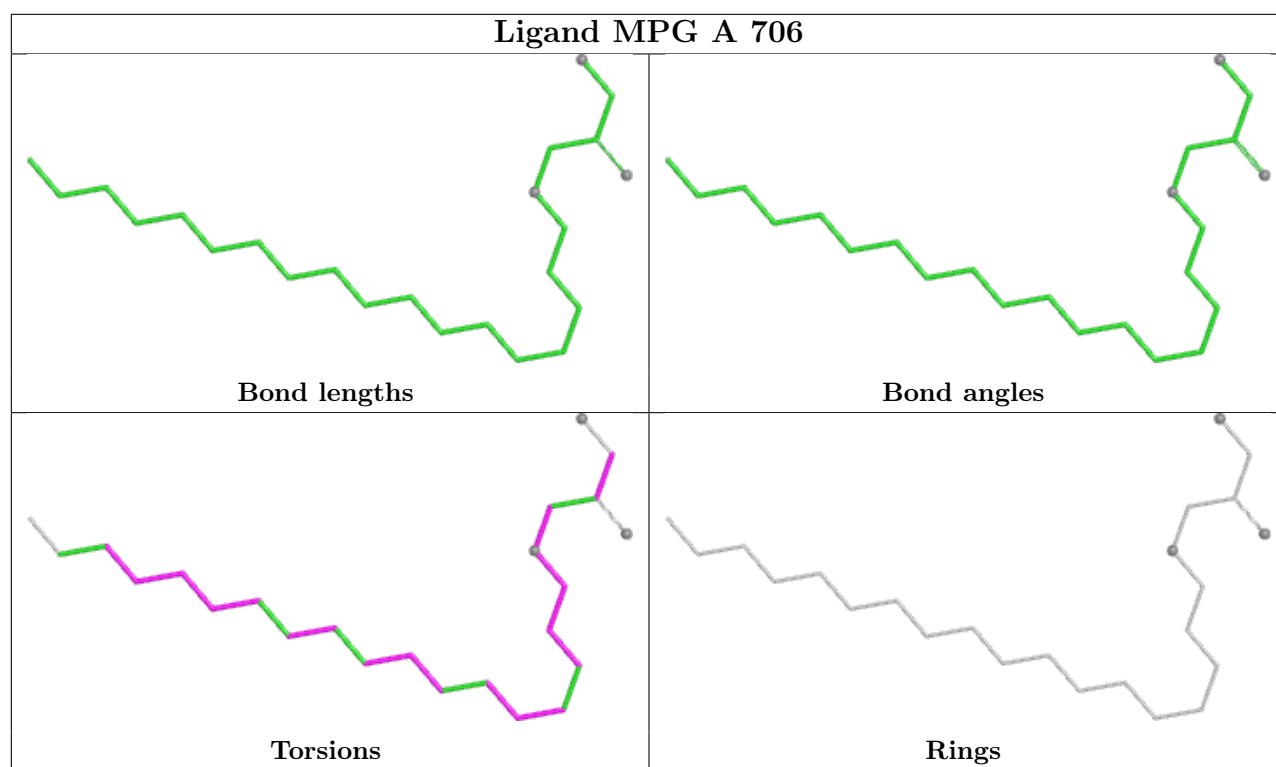












## 5.7 Other polymers i

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/594 (92%)	0.53	56 (10%) <b>6</b> <b>11</b>	21, 32, 52, 66	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	TYR	6.3
1	A	533	SER	5.2
1	A	6	ASP	5.2
1	A	536	TYR	5.2
1	A	3	THR	4.9
1	A	329	VAL	4.2
1	A	195	ASP	4.2
1	A	572	ASP	3.8
1	A	512	TYR	3.8
1	A	4	SER	3.8
1	A	144	TRP	3.8
1	A	162	ASP	3.7
1	A	535	PRO	3.7
1	A	532	SER	3.7
1	A	330	GLU	3.6
1	A	557	SER	3.5
1	A	127	VAL	3.5
1	A	134	ASP	3.3
1	A	52	VAL	3.3
1	A	326	THR	3.2
1	A	126	VAL	3.2
1	A	46	LEU	3.1
1	A	328	TYR	3.1
1	A	161	GLY	3.1
1	A	531	TYR	2.9
1	A	49	LEU	2.9
1	A	129	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	176	HIS	2.8
1	A	77	LEU	2.7
1	A	511	LEU	2.7
1	A	490	ILE	2.7
1	A	327	GLY	2.7
1	A	85	LEU	2.7
1	A	66	ILE	2.6
1	A	175	THR	2.6
1	A	96	LEU	2.6
1	A	110	ILE	2.5
1	A	45	VAL	2.4
1	A	147	ASN	2.4
1	A	63	LEU	2.4
1	A	594	PHE	2.4
1	A	78	VAL	2.4
1	A	308	HIS	2.4
1	A	537	GLN	2.4
1	A	479[A]	VAL	2.3
1	A	559	LEU	2.3
1	A	5	PRO	2.2
1	A	80	ILE	2.1
1	A	68	ILE	2.1
1	A	122	ALA	2.1
1	A	573	TYR	2.1
1	A	109	TYR	2.1
1	A	2	ASP	2.1
1	A	331	ASP	2.1
1	A	133	ARG	2.0
1	A	174	HIS	2.0

## 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

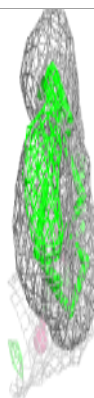
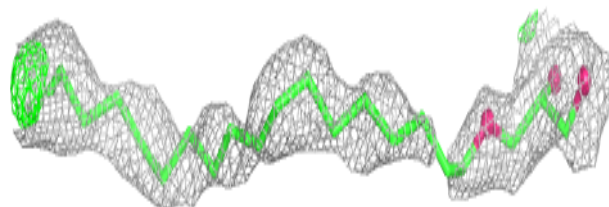
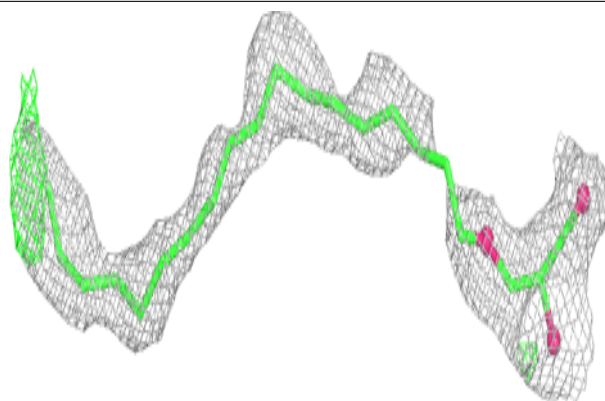
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MPG	A	708	24/25	0.61	0.24	59,72,85,86	0
2	MPG	A	709	24/25	0.69	0.28	44,73,90,90	0
2	MPG	A	711	24/25	0.72	0.26	43,74,78,79	0
2	MPG	A	707	24/25	0.78	0.22	54,60,63,64	0
2	MPG	A	706	24/25	0.79	0.26	49,60,68,70	0
2	MPG	A	702	24/25	0.80	0.24	49,61,72,73	0
2	MPG	A	710	24/25	0.84	0.21	42,61,68,69	0
4	MPD	A	904	8/8	0.85	0.22	55,59,61,61	0
4	MPD	A	902	8/8	0.86	0.22	53,55,59,60	0
2	MPG	A	703	24/25	0.87	0.16	37,50,55,59	0
2	MPG	A	705	24/25	0.87	0.19	46,52,70,72	0
2	MPG	A	701	24/25	0.88	0.17	32,46,71,73	0
2	MPG	A	704	24/25	0.89	0.17	28,42,49,57	0
3	FMT	A	801	3/3	0.89	0.18	57,57,58,58	0
4	MPD	A	901	8/8	0.92	0.18	38,41,43,44	0
4	MPD	A	903	8/8	0.93	0.18	56,57,62,65	0

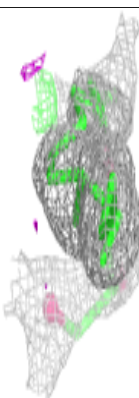
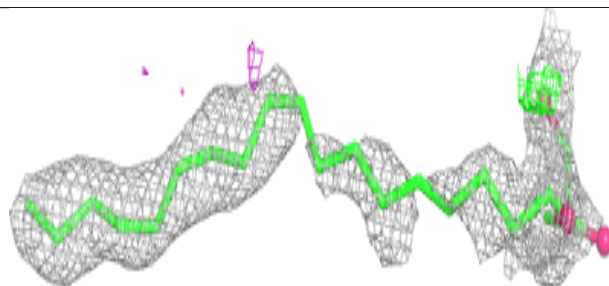
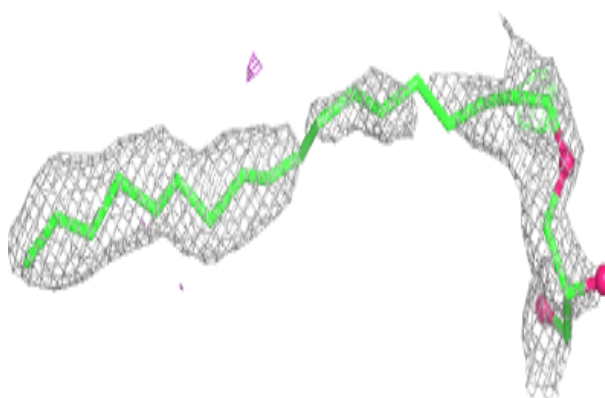
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MPG A 708:**

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

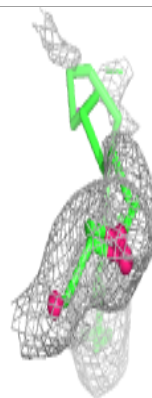
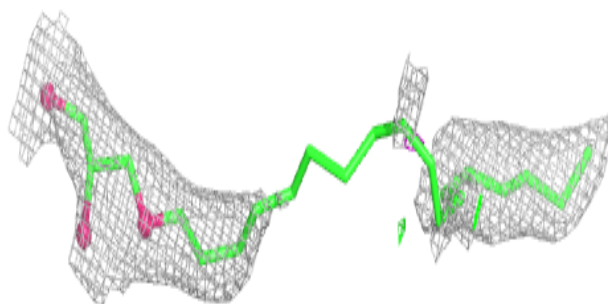
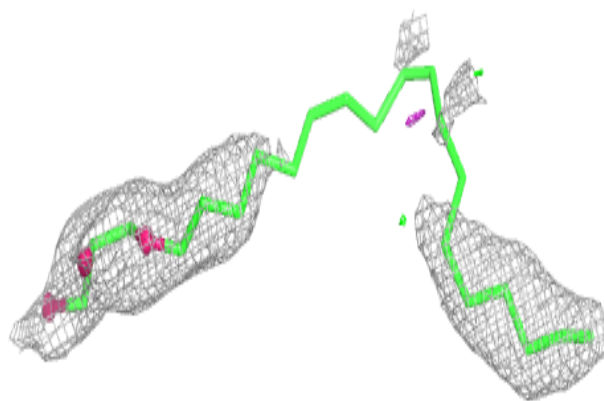
**Electron density around MPG A 709:**

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

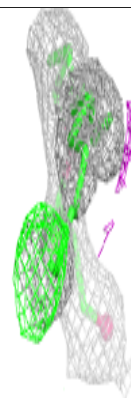
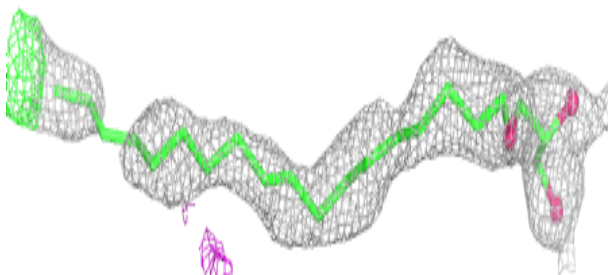
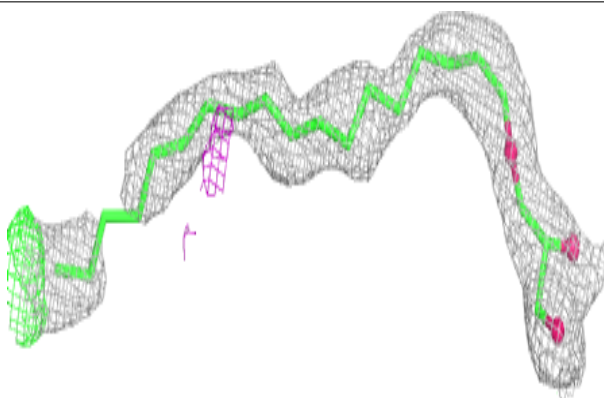


**Electron density around MPG A 711:**

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

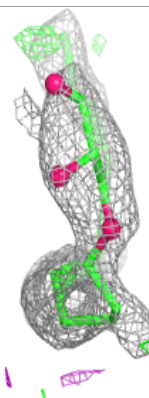
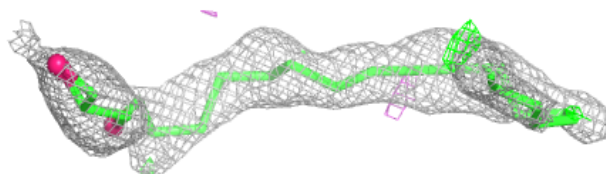
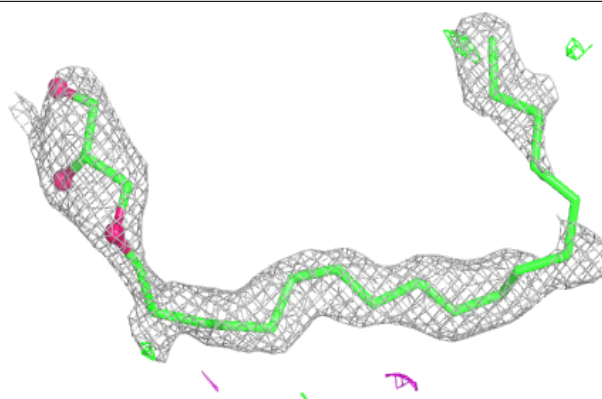
**Electron density around MPG A 707:**

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

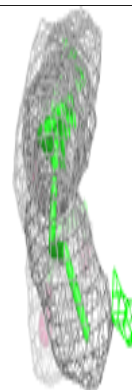
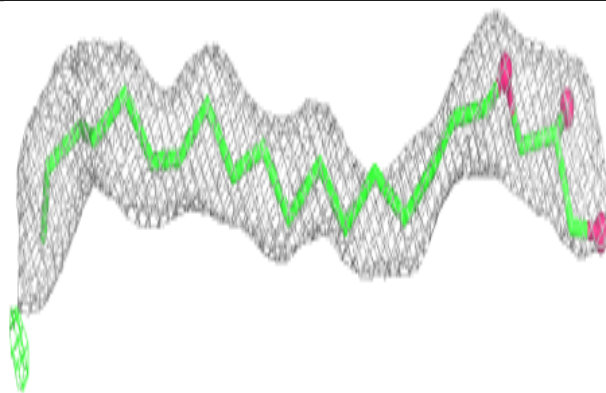
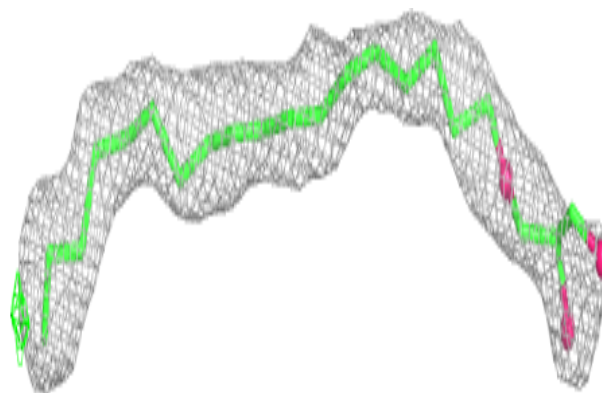


**Electron density around MPG A 706:**

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

**Electron density around MPG A 702:**

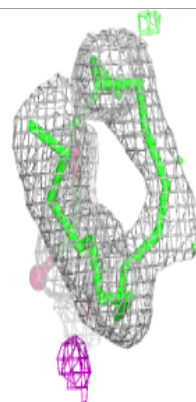
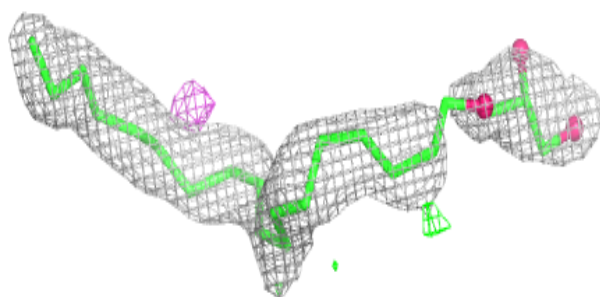
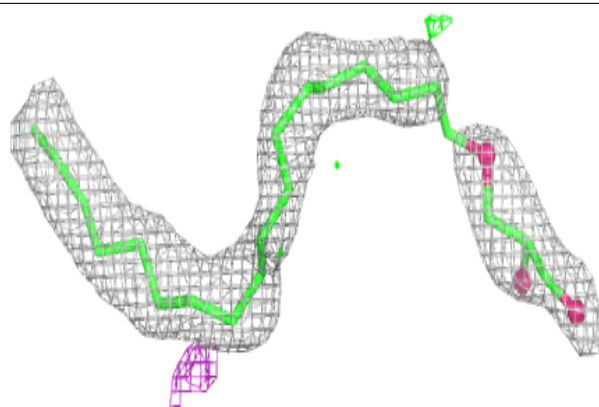
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



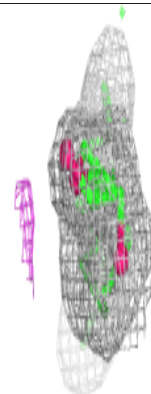
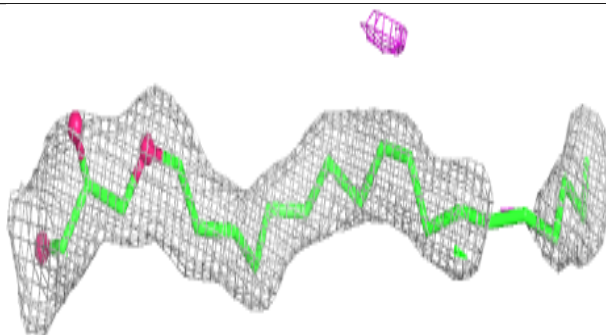
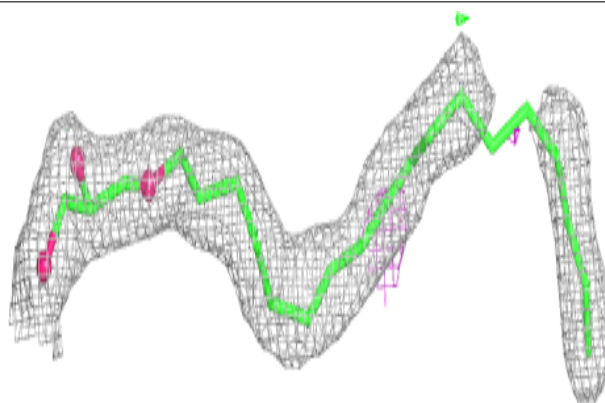


**Electron density around MPG A 710:**

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

**Electron density around MPG A 703:**

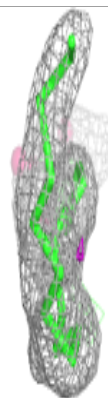
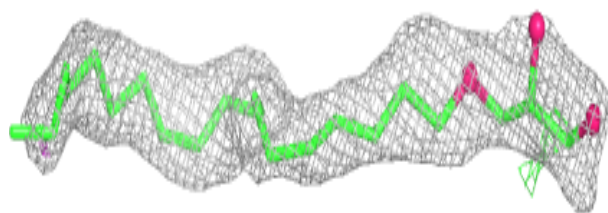
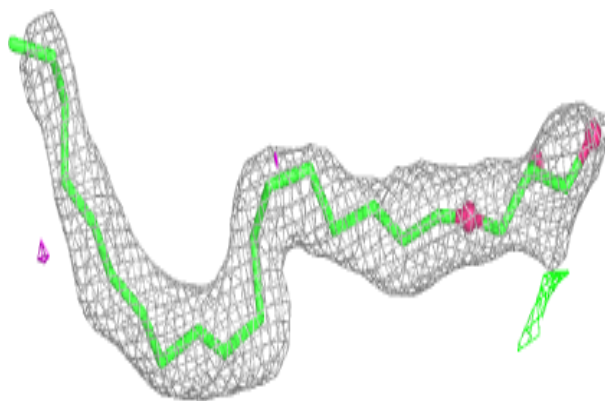
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



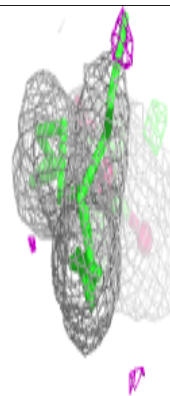
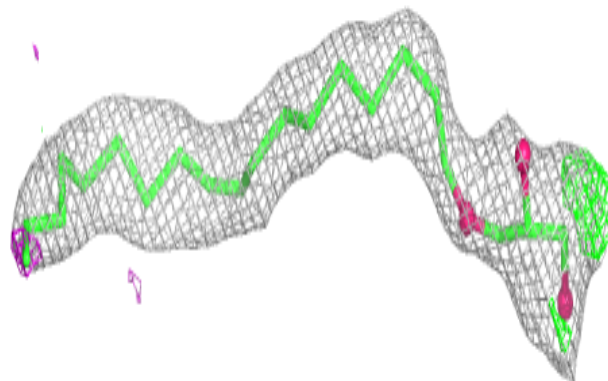
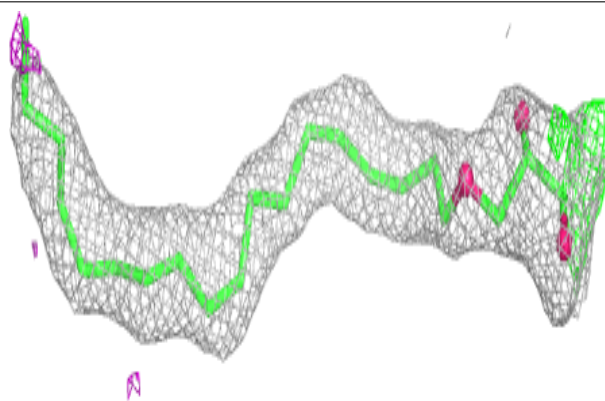


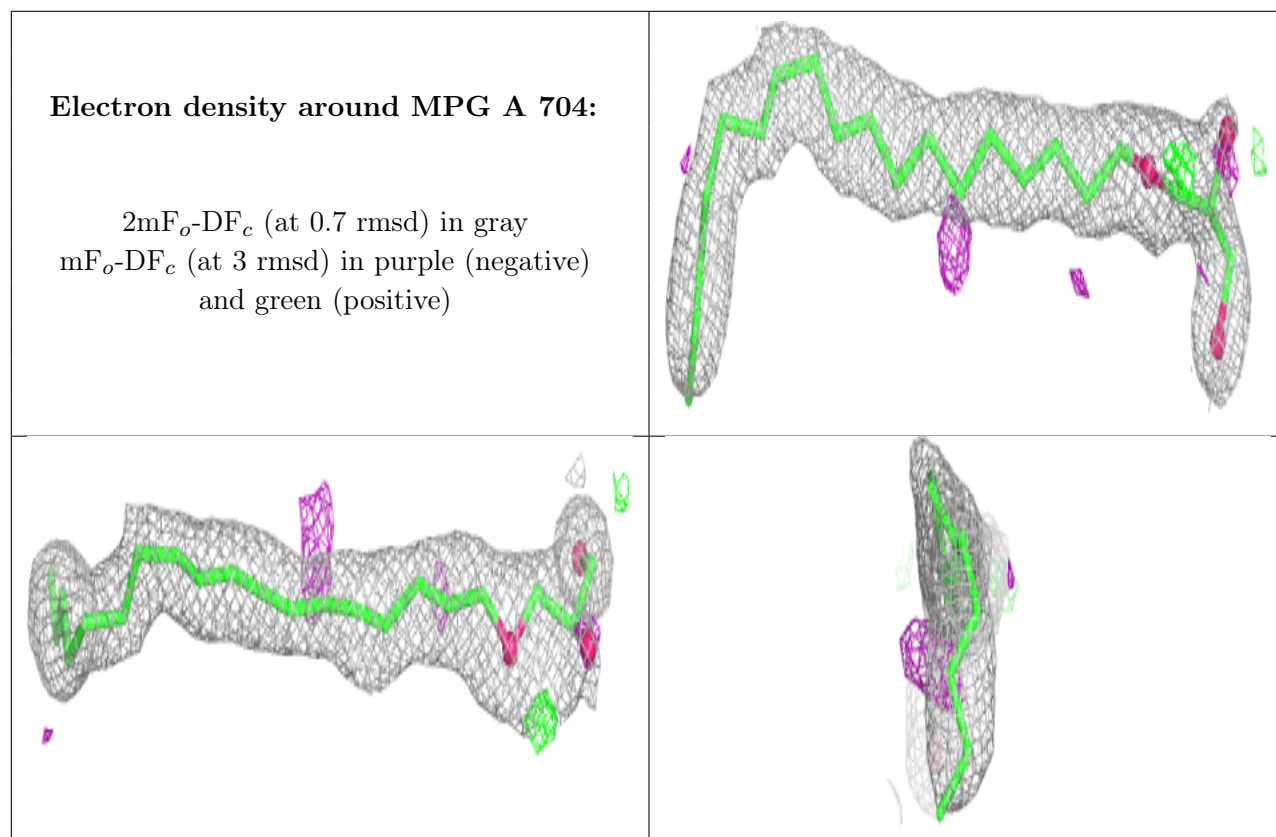
**Electron density around MPG A 705:**

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

**Electron density around MPG A 701:**

$2mF_o-DF_c$  (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.