



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2024 – 04:18 am BST

PDB ID : 7Q4J
Title : A thermostable lipase from *Thermoanaerobacter thermohydrosulfuricus* in complex a monoacylglycerol intermediate
Authors : Pinotsis, N.; Wilmanns, M.
Deposited on : 2021-10-31
Resolution : 1.91 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 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

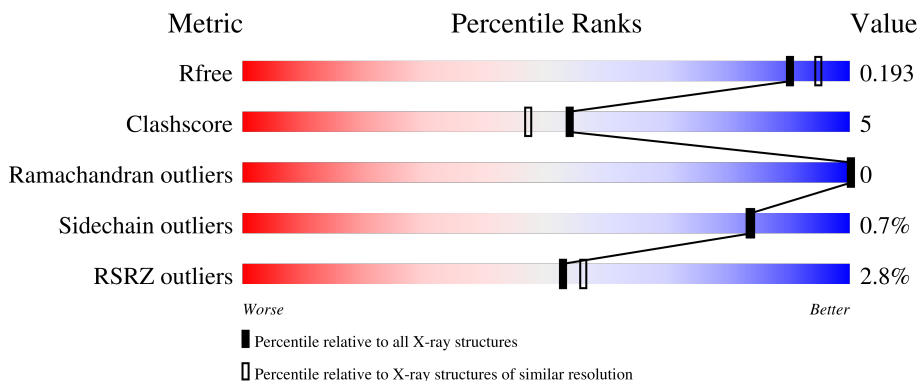
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	259	 3% 91% 9%
2	B	259	 2% 85% 14% .

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4608 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 Serine aminopeptidase S33 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	259	2086	1342	338	395	11	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ASN	HIS	variant	UNP A0A1G7VV58

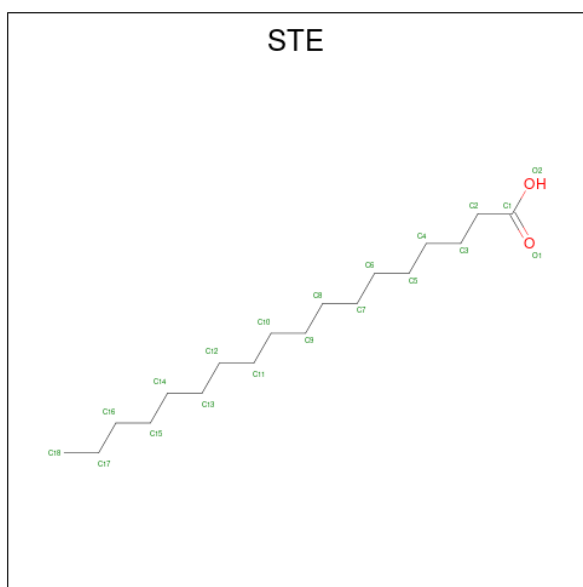
- Molecule 2 is a protein called Serine aminopeptidase S33 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	259	2099	1351	339	398	11	0	3	0

There is a discrepancy between the modelled and reference sequences:

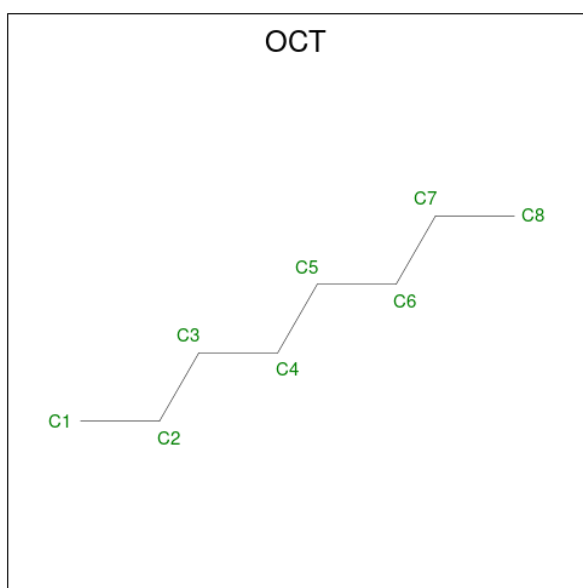
Chain	Residue	Modelled	Actual	Comment	Reference
B	148	ASN	HIS	variant	UNP A0A1G7VV58

- Molecule 3 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂) (labeled as "Ligand of Interest" by depositor).



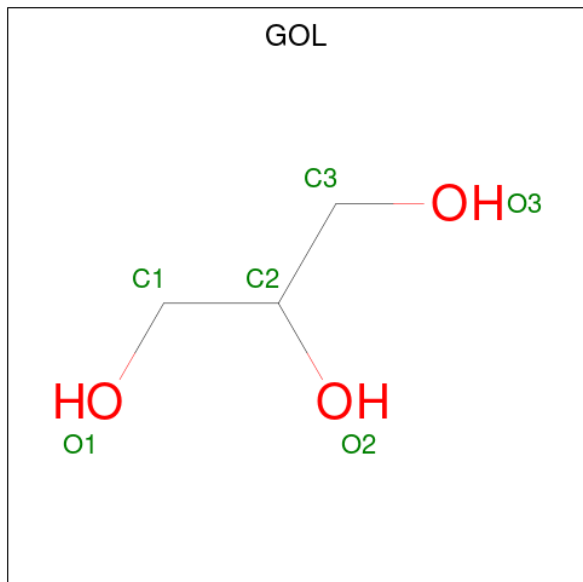
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			19	18 1		
3	B	1	Total	C O	0	0
			19	18 1		

- Molecule 4 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

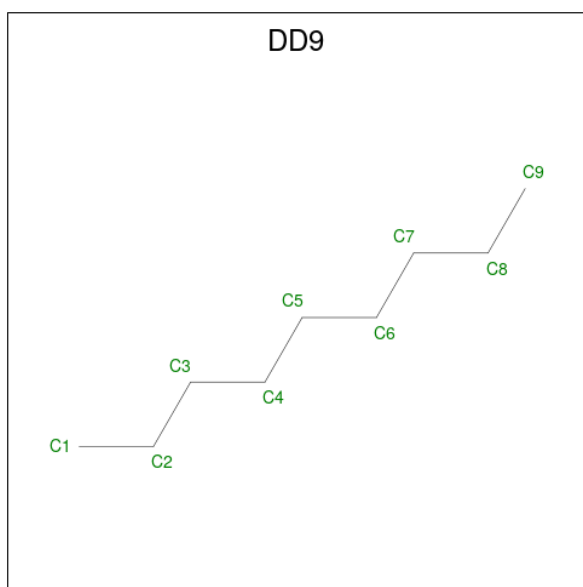


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

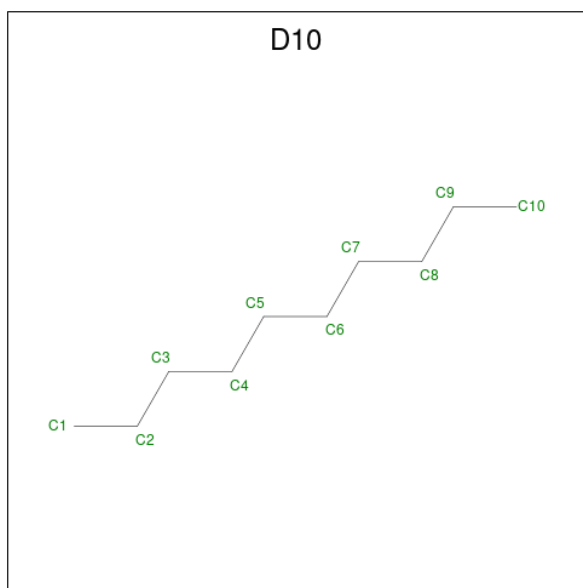
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is nonane (three-letter code: DD9) (formula: C₉H₂₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 9 9	0	0

- Molecule 9 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 10 10	0	0

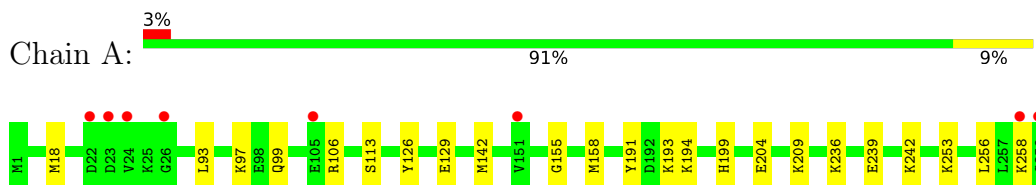
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	133	Total 133	O 133	0	0
10	B	154	Total 154	O 154	0	0

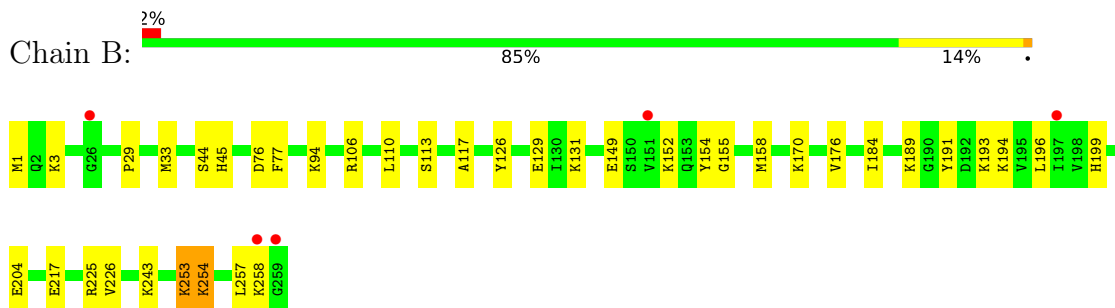
3 Residue-property plots [i](#)

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

- Molecule 1: Serine aminopeptidase S33 domain-containing protein



- Molecule 2: Serine aminopeptidase S33 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 137.53Å 67.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 1.91 19.75 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.75-1.91) 96.8 (19.75-1.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.92Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.163 , 0.194 0.163 , 0.193	Depositor DCC
R_{free} test set	1532 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtrriage
Anisotropy	0.634	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: D10, MLZ, MLY, SO4, CL, DD9, OCT, STE, GOL

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	0.29	0/1994	0.52	0/2666
2	B	0.30	0/1962	0.52	0/2621
All	All	0.29	0/3956	0.52	0/5287

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	2086	0	2085	13	0
2	B	2099	0	2099	26	0
3	A	19	0	35	7	0
3	B	19	0	35	8	0
4	A	16	0	36	2	0
5	A	18	0	24	1	0
5	B	24	0	32	9	0
6	A	20	0	0	0	0
7	A	1	0	0	0	0
8	B	9	0	20	1	0
9	B	10	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	133	0	0	2	0
10	B	154	0	0	1	0
All	All	4608	0	4388	46	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 5.

All (46) 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:113:SER:OG	3:A:301:STE:C1	2.18	0.92
2:B:225:ARG:HE	5:B:304:GOL:H12	1.40	0.84
2:B:113:SER:OG	3:B:301:STE:C1	2.30	0.79
2:B:45:HIS:H	5:B:305:GOL:H31	1.51	0.75
3:A:301:STE:H31	4:A:303:OCT:H13	1.72	0.71
1:A:18:MSE:HE1	1:A:99:GLN:HG3	1.75	0.68
2:B:155:GLY:HA2	3:B:301:STE:H161	1.75	0.68
2:B:253:MLZ:HG2	2:B:257:LEU:HD12	1.73	0.68
2:B:154:TYR:HB3	3:B:301:STE:H152	1.80	0.64
2:B:149:GLU:HB2	3:B:301:STE:H141	1.84	0.60
2:B:76:ASP:HB3	5:B:303:GOL:O1	2.02	0.59
1:A:158:MSE:HG2	3:A:301:STE:H171	1.83	0.59
1:A:239[B]:GLU:OE1	10:A:401:HOH:O	2.17	0.58
1:A:155:GLY:HA2	3:A:301:STE:H172	1.86	0.56
2:B:196:LEU:HD11	2:B:226:VAL:HG23	1.87	0.55
2:B:170:MLY:HB2	5:B:303:GOL:H12	1.92	0.51
3:B:301:STE:C1	5:B:302:GOL:O1	2.59	0.51
2:B:126:TYR:HB3	2:B:129:GLU:HG3	1.93	0.50
3:B:301:STE:C1	9:B:307:D10:H13	2.41	0.50
3:A:301:STE:C1	5:A:304:GOL:O1	2.60	0.49
2:B:254:MLZ:O	2:B:258:LYS:HG3	2.13	0.48
2:B:117:ALA:HB1	2:B:184:ILE:HD13	1.95	0.48
10:A:445:HOH:O	5:B:305:GOL:H32	2.13	0.48
1:A:97:MLY:HE2	1:A:129:GLU:OE1	2.15	0.47
2:B:1:MSE:HE1	2:B:3:MLY:HD2	1.97	0.47
2:B:77:PHE:HB3	5:B:303:GOL:H11	1.95	0.47
2:B:176:VAL:HG11	3:B:301:STE:H181	1.97	0.47
2:B:29:PRO:HG3	2:B:106:ARG:HD3	1.98	0.46
1:A:204:GLU:HA	4:A:302:OCT:H61	1.98	0.45
2:B:243:MLY:HH22	10:B:488:HOH:O	2.16	0.45
1:A:93:LEU:HG	1:A:97:MLY:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MSE:SE	3:A:301:STE:H21	2.68	0.44
1:A:106:ARG:HD3	1:A:256:LEU:O	2.18	0.43
2:B:243:MLY:HD3	2:B:243:MLY:HH23	1.73	0.43
3:B:301:STE:H102	9:B:307:D10:H72	2.01	0.43
9:B:307:D10:H22	9:B:307:D10:H51	1.86	0.43
2:B:204:GLU:HA	8:B:306:DD9:H3A	2.01	0.42
2:B:225:ARG:HH21	5:B:304:GOL:H31	1.84	0.42
2:B:189:LYS:HD2	2:B:217:GLU:O	2.20	0.42
1:A:191:TYR:CZ	1:A:193:LYS:HB2	2.55	0.42
2:B:44:SER:HA	5:B:305:GOL:H31	2.01	0.42
1:A:126:TYR:HB3	1:A:129:GLU:HG3	2.02	0.42
2:B:191:TYR:CZ	2:B:193:MLY:HB3	2.55	0.41
2:B:33:MSE:HA	2:B:110:LEU:O	2.21	0.41
1:A:113:SER:HG	3:A:301:STE:C1	2.29	0.41
2:B:158:MSE:HE3	2:B:176:VAL:HG21	2.03	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	249/259 (96%)	243 (98%)	6 (2%)	0	100	100
2	B	245/259 (95%)	240 (98%)	5 (2%)	0	100	100
All	All	494/518 (95%)	483 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	212/200 (106%)	210 (99%)	2 (1%)	78	78
2	B	210/196 (107%)	209 (100%)	1 (0%)	88	89
All	All	422/396 (107%)	419 (99%)	3 (1%)	84	83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	258	LYS
2	B	199	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

26 non-standard protein/DNA/RNA residues 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	MLY	B	3	2	9,10,11	0.60	0	6,11,13	0.53	0
2	MLY	B	236	2	9,10,11	0.56	0	6,11,13	0.70	0
2	MLY	B	127	2	9,10,11	0.53	0	6,11,13	0.82	0
1	MLY	A	97	1	9,10,11	0.58	0	6,11,13	0.90	0
1	MLY	A	94	1	9,10,11	0.55	0	6,11,13	0.82	0
1	MLY	A	127	1	9,10,11	0.55	0	6,11,13	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLZ	A	242	1	8,9,10	0.62	0	4,9,11	1.52	1 (25%)
2	MLY	B	25	2	9,10,11	0.58	0	6,11,13	0.54	0
1	MLY	A	170	1	9,10,11	0.54	0	6,11,13	0.75	0
2	MLZ	B	152	2	8,9,10	0.61	0	4,9,11	1.63	1 (25%)
1	MLZ	A	253	1	8,9,10	0.60	0	4,9,11	1.56	1 (25%)
2	MLY	B	170	2	9,10,11	0.54	0	6,11,13	0.93	0
2	MLY	B	193	2	9,10,11	0.75	0	6,11,13	0.81	0
2	MLY	B	209	2	9,10,11	0.57	0	6,11,13	0.98	0
1	MLY	A	236	1	9,10,11	0.60	0	6,11,13	0.90	1 (16%)
2	MLZ	B	131	2	8,9,10	0.66	0	4,9,11	1.60	1 (25%)
2	MLZ	B	254	2	8,9,10	0.54	0	4,9,11	1.55	1 (25%)
1	MLY	A	12	1	9,10,11	0.50	0	6,11,13	1.02	0
1	MLZ	A	209	1	8,9,10	0.59	0	4,9,11	1.37	1 (25%)
2	MLZ	B	94	2	8,9,10	0.57	0	4,9,11	1.57	1 (25%)
2	MLY	B	57	2	9,10,11	0.61	0	6,11,13	0.78	0
2	MLZ	B	194	2	8,9,10	0.67	0	4,9,11	1.57	1 (25%)
1	MLZ	A	194	1	8,9,10	0.65	0	4,9,11	1.54	1 (25%)
1	MLY	A	243	1	9,10,11	0.57	0	6,11,13	0.60	0
2	MLZ	B	253	2	8,9,10	0.55	0	4,9,11	1.64	1 (25%)
2	MLY	B	243	2	9,10,11	0.56	0	6,11,13	0.56	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	MLY	B	3	2	-	3/8/9/11	-
2	MLY	B	236	2	-	5/8/9/11	-
2	MLY	B	127	2	-	4/8/9/11	-
1	MLY	A	97	1	-	2/8/9/11	-
1	MLY	A	94	1	-	0/8/9/11	-
1	MLY	A	127	1	-	3/8/9/11	-
1	MLZ	A	242	1	-	1/7/8/10	-
2	MLY	B	25	2	-	0/8/9/11	-
1	MLY	A	170	1	-	1/8/9/11	-
2	MLZ	B	152	2	-	1/7/8/10	-
1	MLZ	A	253	1	-	5/7/8/10	-
2	MLY	B	170	2	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	193	2	-	4/8/9/11	-
2	MLY	B	209	2	-	0/8/9/11	-
1	MLY	A	236	1	-	2/8/9/11	-
2	MLZ	B	131	2	-	2/7/8/10	-
2	MLZ	B	254	2	-	3/7/8/10	-
1	MLY	A	12	1	-	3/8/9/11	-
1	MLZ	A	209	1	-	1/7/8/10	-
2	MLZ	B	94	2	-	3/7/8/10	-
2	MLY	B	57	2	-	5/8/9/11	-
2	MLZ	B	194	2	-	2/7/8/10	-
1	MLZ	A	194	1	-	1/7/8/10	-
1	MLY	A	243	1	-	1/8/9/11	-
2	MLZ	B	253	2	-	1/7/8/10	-
2	MLY	B	243	2	-	3/8/9/11	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	253	MLZ	CM-NZ-CE	3.11	120.94	111.95
2	B	254	MLZ	CM-NZ-CE	3.05	120.77	111.95
2	B	131	MLZ	CM-NZ-CE	3.05	120.75	111.95
2	B	152	MLZ	CM-NZ-CE	3.04	120.74	111.95
2	B	194	MLZ	CM-NZ-CE	3.01	120.65	111.95
1	A	194	MLZ	CM-NZ-CE	2.98	120.55	111.95
1	A	242	MLZ	CM-NZ-CE	2.93	120.42	111.95
1	A	253	MLZ	CM-NZ-CE	2.92	120.39	111.95
2	B	94	MLZ	CM-NZ-CE	2.91	120.35	111.95
1	A	209	MLZ	CM-NZ-CE	2.65	119.60	111.95
1	A	236	MLY	CD-CE-NZ	-2.03	108.28	113.79

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	194	MLZ	CD-CE-NZ-CM
1	A	253	MLZ	N-CA-CB-CG
1	A	253	MLZ	C-CA-CB-CG
1	A	253	MLZ	CD-CE-NZ-CM

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Mol	Chain	Res	Type	Atoms
2	B	3	MLY	C-CA-CB-CG
2	B	57	MLY	N-CA-CB-CG
2	B	57	MLY	O-C-CA-CB
2	B	94	MLZ	CD-CE-NZ-CM
2	B	131	MLZ	CD-CE-NZ-CM
2	B	152	MLZ	CD-CE-NZ-CM
2	B	194	MLZ	CD-CE-NZ-CM
2	B	236	MLY	N-CA-CB-CG
2	B	236	MLY	C-CA-CB-CG
2	B	253	MLZ	CD-CE-NZ-CM
2	B	94	MLZ	CG-CD-CE-NZ
1	A	12	MLY	CD-CE-NZ-CH1
1	A	12	MLY	CD-CE-NZ-CH2
1	A	127	MLY	CD-CE-NZ-CH1
2	B	193	MLY	CD-CE-NZ-CH1
2	B	193	MLY	CD-CE-NZ-CH2
2	B	243	MLY	CG-CD-CE-NZ
1	A	209	MLZ	CG-CD-CE-NZ
1	A	236	MLY	CG-CD-CE-NZ
2	B	194	MLZ	CG-CD-CE-NZ
2	B	3	MLY	CG-CD-CE-NZ
1	A	127	MLY	CD-CE-NZ-CH2
2	B	127	MLY	CD-CE-NZ-CH1
2	B	243	MLY	CD-CE-NZ-CH2
2	B	236	MLY	CG-CD-CE-NZ
2	B	254	MLZ	CA-CB-CG-CD
2	B	127	MLY	CE-CD-CG-CB
2	B	170	MLY	CE-CD-CG-CB
2	B	193	MLY	CA-CB-CG-CD
1	A	253	MLZ	CA-CB-CG-CD
2	B	57	MLY	CA-CB-CG-CD
2	B	127	MLY	CD-CE-NZ-CH2
2	B	254	MLZ	CG-CD-CE-NZ
1	A	127	MLY	CE-CD-CG-CB
2	B	127	MLY	CA-CB-CG-CD
2	B	131	MLZ	CA-CB-CG-CD
1	A	253	MLZ	CE-CD-CG-CB
1	A	243	MLY	CD-CE-NZ-CH1
2	B	3	MLY	CE-CD-CG-CB
1	A	97	MLY	CG-CD-CE-NZ
1	A	12	MLY	CE-CD-CG-CB
2	B	236	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
2	B	57	MLY	CE-CD-CG-CB
1	A	236	MLY	N-CA-CB-CG
2	B	57	MLY	C-CA-CB-CG
2	B	193	MLY	CE-CD-CG-CB
1	A	242	MLZ	CE-CD-CG-CB
1	A	170	MLY	CG-CD-CE-NZ
2	B	170	MLY	CD-CE-NZ-CH2
2	B	94	MLZ	CE-CD-CG-CB
1	A	97	MLY	CE-CD-CG-CB
2	B	254	MLZ	CD-CE-NZ-CM
2	B	243	MLY	CE-CD-CG-CB
2	B	236	MLY	CD-CE-NZ-CH2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	MLY	1	0
1	A	97	MLY	2	0
2	B	170	MLY	1	0
2	B	193	MLY	1	0
2	B	254	MLZ	1	0
2	B	253	MLZ	1	0
2	B	243	MLY	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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
9	D10	B	307	-	9,9,9	0.29	0	8,8,8	0.74	0
4	OCT	A	303	-	7,7,7	0.35	0	6,6,6	0.49	0
4	OCT	A	302	-	7,7,7	0.31	0	6,6,6	0.54	0
6	SO4	A	307	-	4,4,4	0.15	0	6,6,6	0.08	0
6	SO4	A	309	-	4,4,4	0.14	0	6,6,6	0.08	0
5	GOL	A	304	-	5,5,5	0.93	0	5,5,5	1.04	0
6	SO4	A	310	-	4,4,4	0.14	0	6,6,6	0.06	0
5	GOL	B	302	-	5,5,5	0.84	0	5,5,5	1.06	0
5	GOL	B	305	-	5,5,5	0.87	0	5,5,5	1.04	0
6	SO4	A	308	-	4,4,4	0.14	0	6,6,6	0.05	0
5	GOL	B	304	-	5,5,5	0.92	0	5,5,5	1.01	0
5	GOL	A	306	-	5,5,5	0.84	0	5,5,5	1.02	0
3	STE	B	301	-	18,18,19	0.75	1 (5%)	17,17,19	1.07	2 (11%)
8	DD9	B	306	-	8,8,8	0.33	0	7,7,7	0.56	0
3	STE	A	301	-	18,18,19	0.68	1 (5%)	17,17,19	1.21	2 (11%)
5	GOL	A	305	-	5,5,5	0.99	0	5,5,5	0.91	0
5	GOL	B	303	-	5,5,5	1.16	1 (20%)	5,5,5	1.45	1 (20%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	D10	B	307	-	-	0/7/7/7	-
4	OCT	A	303	-	-	0/5/5/5	-
4	OCT	A	302	-	-	0/5/5/5	-
5	GOL	A	304	-	-	1/4/4/4	-
5	GOL	B	302	-	-	0/4/4/4	-
5	GOL	B	305	-	-	0/4/4/4	-
5	GOL	B	304	-	-	4/4/4/4	-
5	GOL	A	306	-	-	0/4/4/4	-
3	STE	B	301	-	-	0/15/16/17	-
8	DD9	B	306	-	-	0/6/6/6	-
3	STE	A	301	-	-	0/15/16/17	-
5	GOL	A	305	-	-	4/4/4/4	-
5	GOL	B	303	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	STE	O1-C1	2.57	1.34	1.19
3	A	301	STE	O1-C1	2.38	1.33	1.19
5	B	303	GOL	O2-C2	-2.04	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	STE	C6-C5-C4	-2.57	101.38	114.42
3	A	301	STE	O1-C1-C2	-2.44	110.86	126.89
5	B	303	GOL	C3-C2-C1	-2.39	102.40	111.70
3	B	301	STE	O1-C1-C2	-2.17	112.62	126.89
3	B	301	STE	C4-C3-C2	2.06	122.76	113.79

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305	GOL	O1-C1-C2-C3
5	A	305	GOL	C1-C2-C3-O3
5	B	303	GOL	O1-C1-C2-C3
5	A	305	GOL	O1-C1-C2-O2
5	B	303	GOL	O1-C1-C2-O2
5	B	304	GOL	C1-C2-C3-O3
5	A	305	GOL	O2-C2-C3-O3
5	B	304	GOL	O1-C1-C2-O2
5	B	304	GOL	O1-C1-C2-C3
5	B	304	GOL	O2-C2-C3-O3
5	A	304	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 26 short contacts:

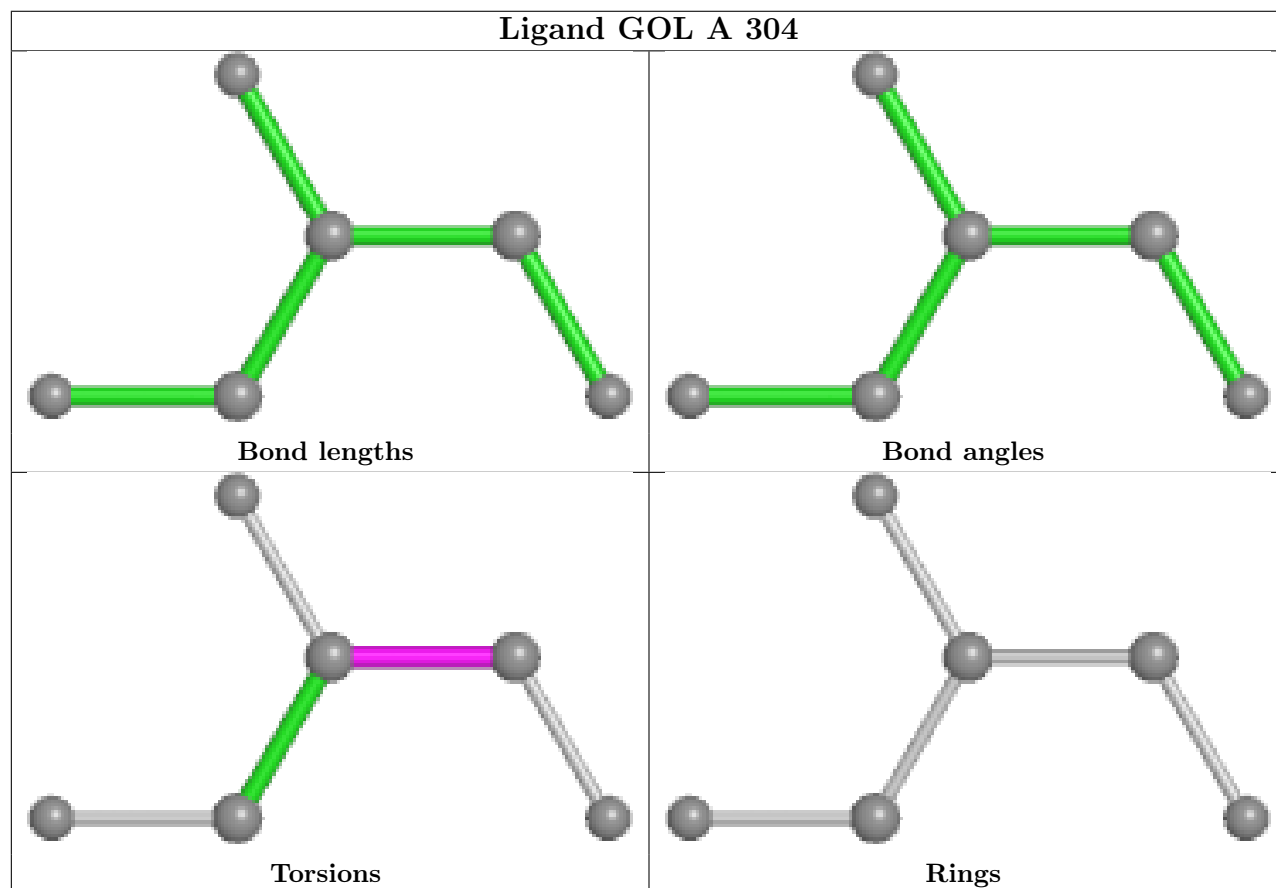
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	307	D10	3	0
4	A	303	OCT	1	0
4	A	302	OCT	1	0
5	A	304	GOL	1	0
5	B	302	GOL	1	0
5	B	305	GOL	3	0
5	B	304	GOL	2	0
3	B	301	STE	8	0
8	B	306	DD9	1	0

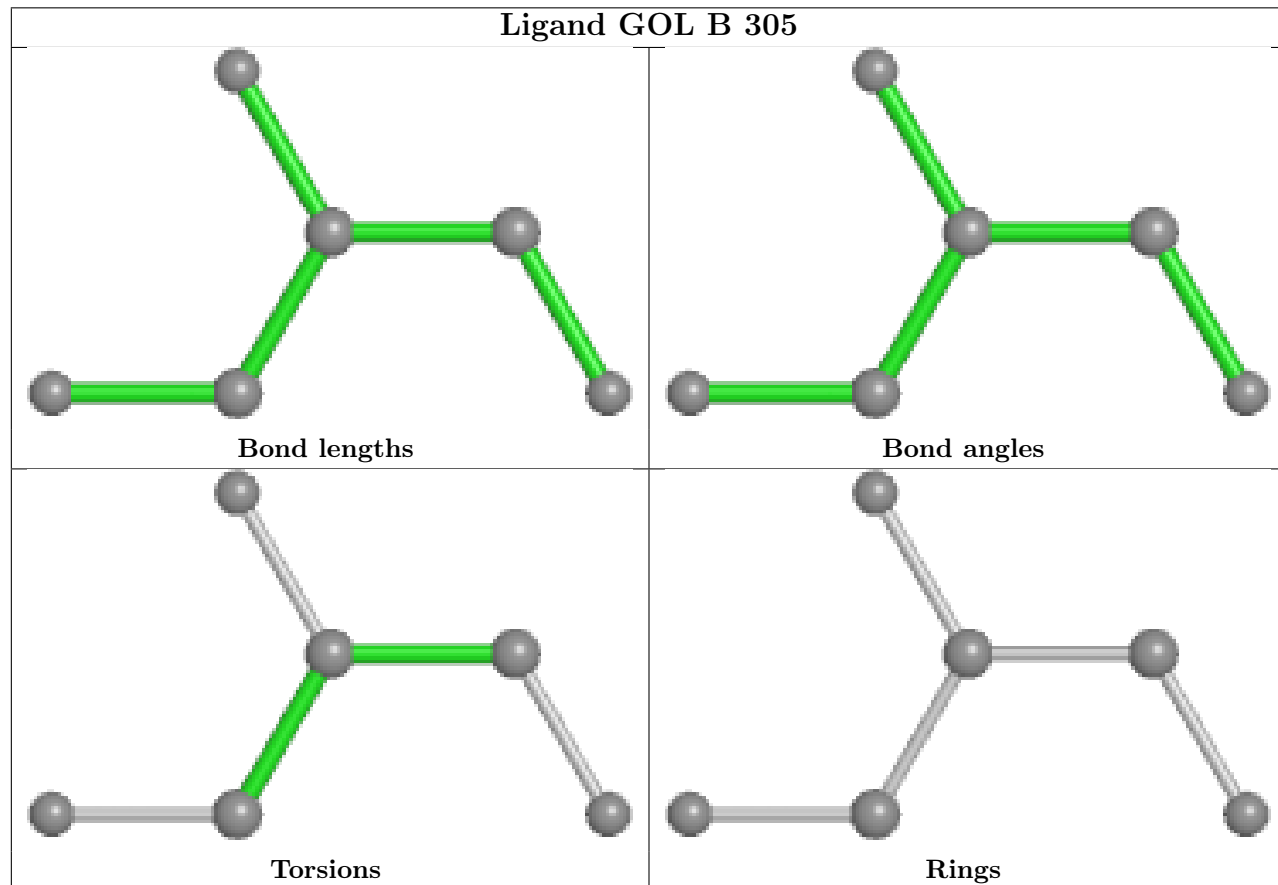
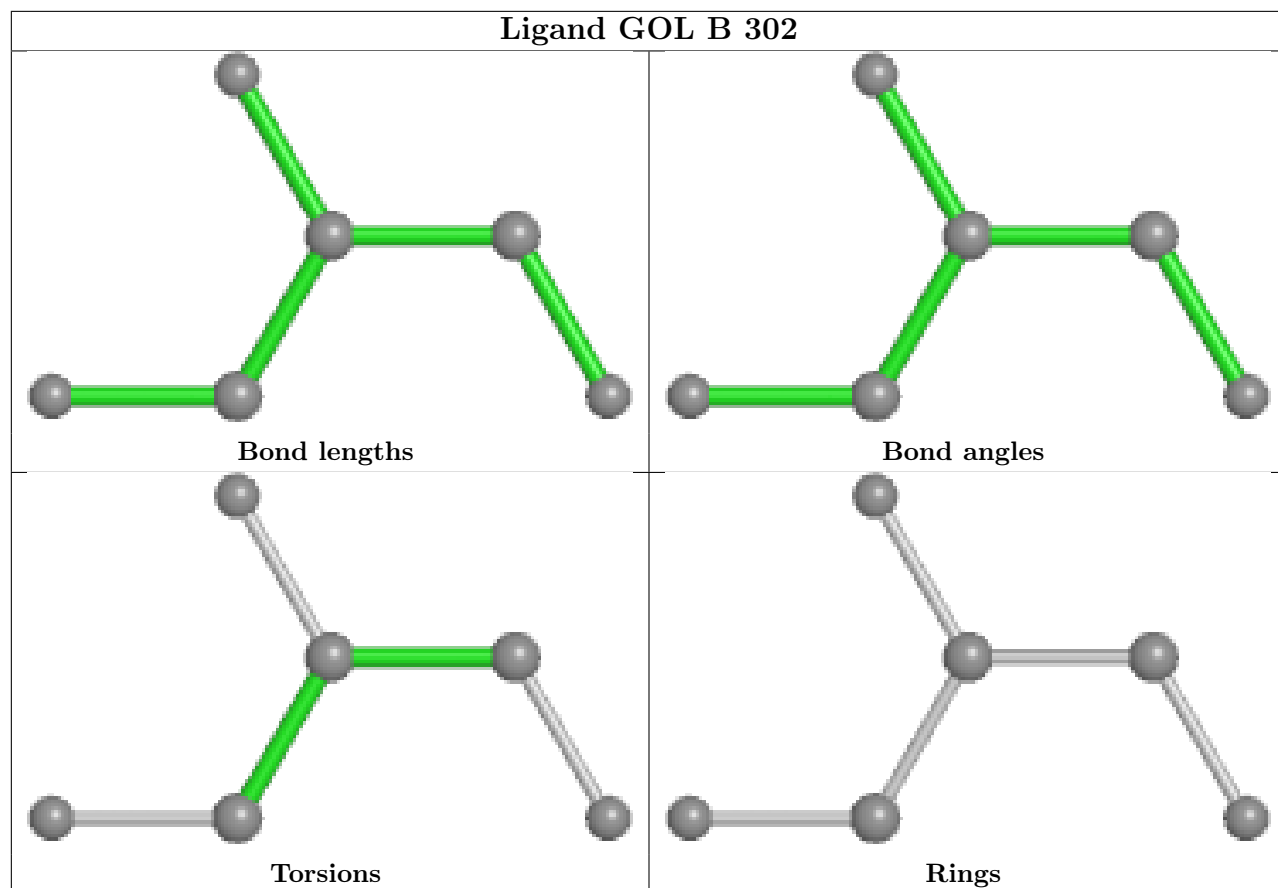
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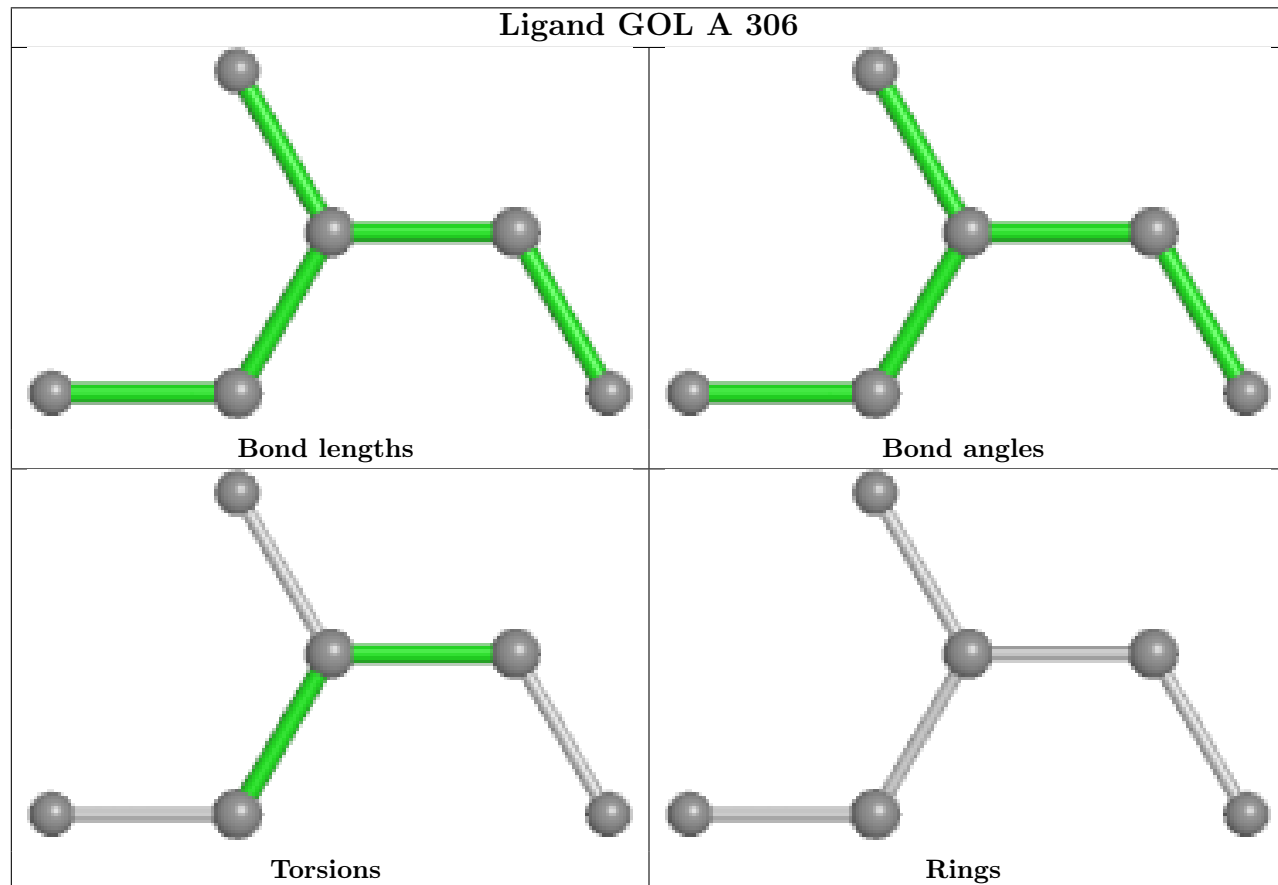
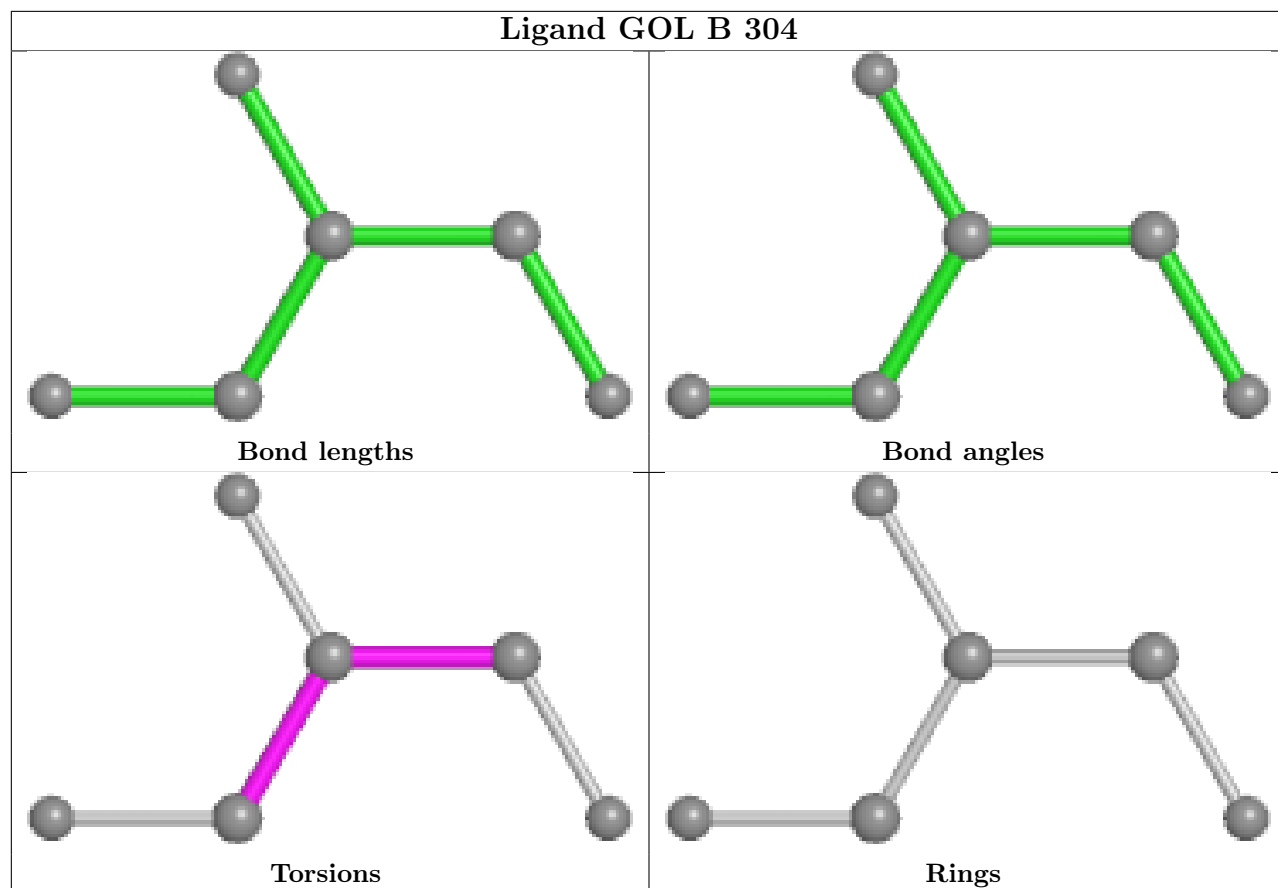
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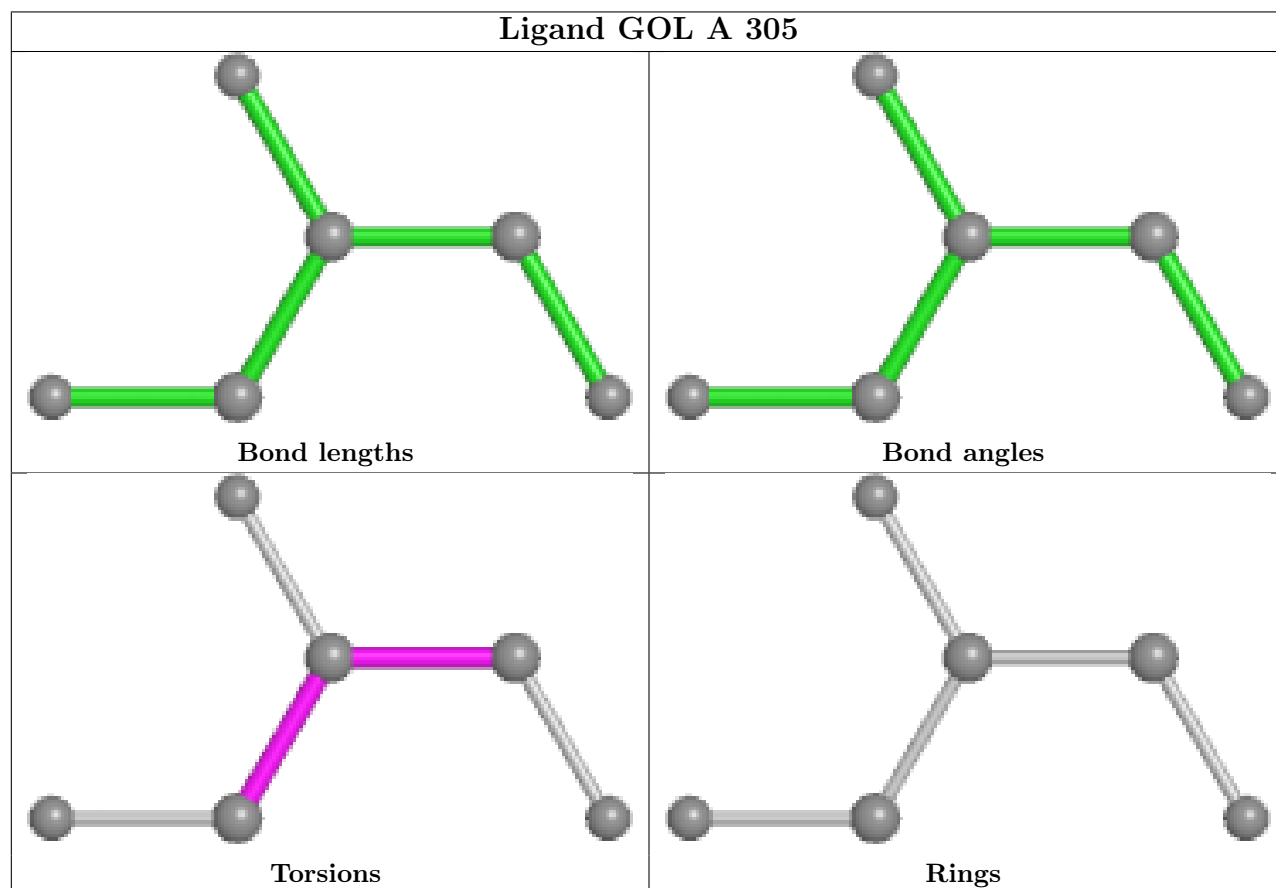
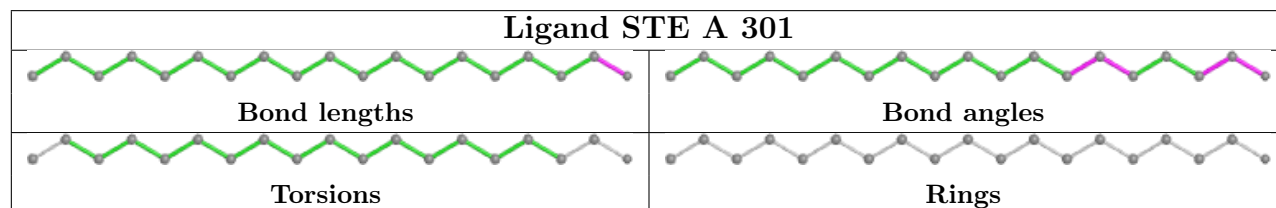
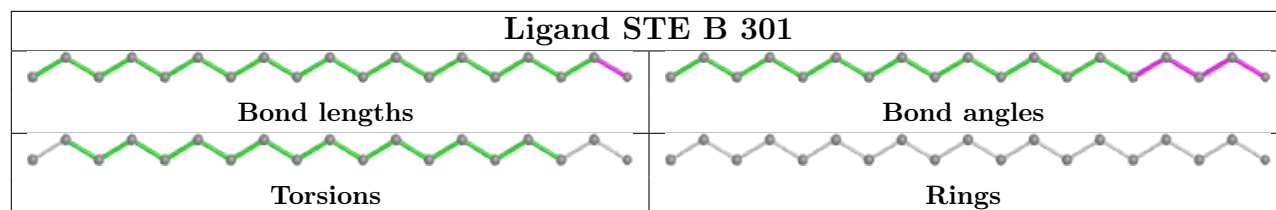
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	STE	7	0
5	B	303	GOL	3	0

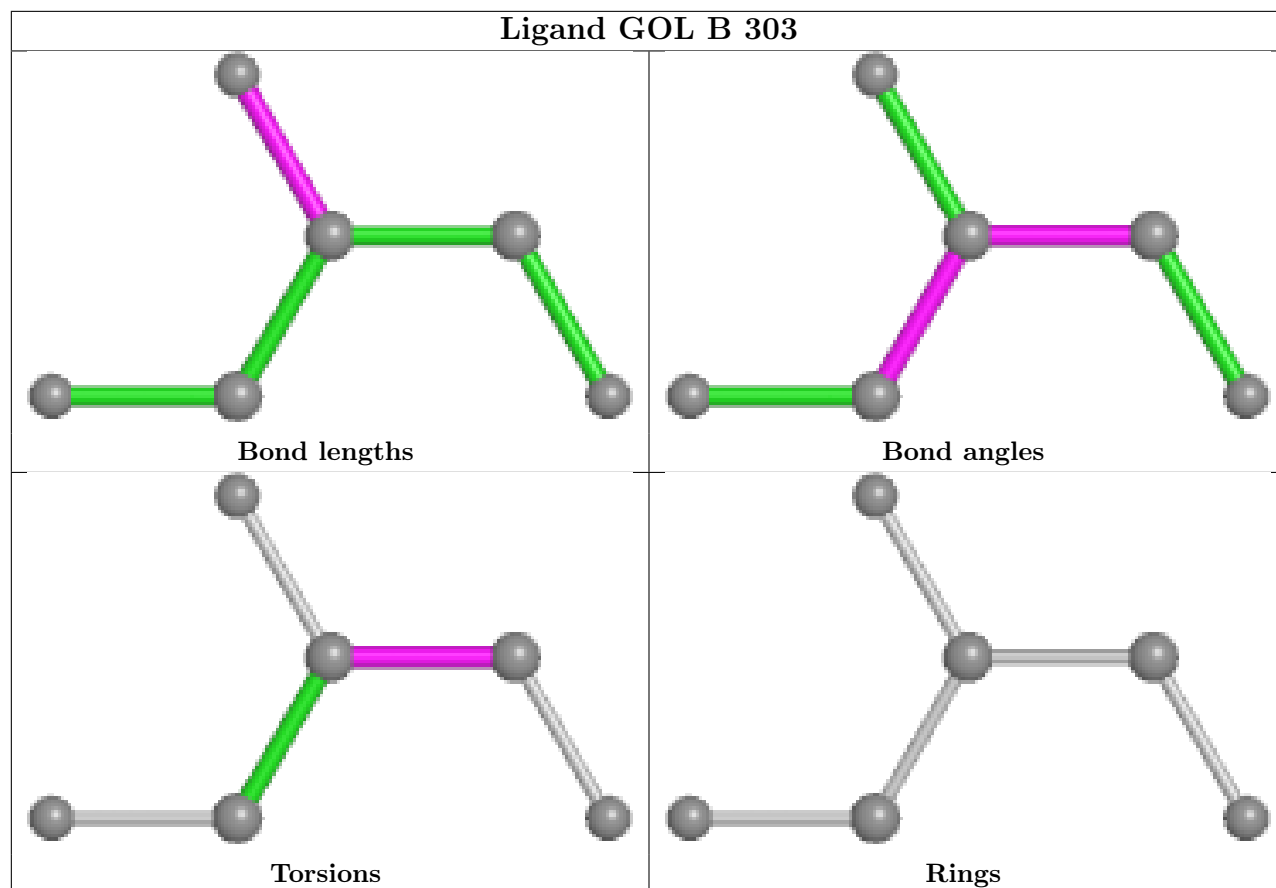
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	237/259 (91%)	0.02	8 (3%) 45 48	33, 43, 68, 103	2 (0%)
2	B	233/259 (89%)	-0.05	5 (2%) 63 66	31, 39, 57, 89	6 (2%)
All	All	470/518 (90%)	-0.02	13 (2%) 53 56	31, 41, 63, 103	8 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	259	GLY	4.5
1	A	23	ASP	4.4
1	A	259	GLY	4.4
1	A	258	LYS	4.0
2	B	151	VAL	3.9
1	A	151	VAL	3.6
1	A	26	GLY	3.1
1	A	24	VAL	2.8
2	B	197	ILE	2.6
1	A	22	ASP	2.5
2	B	26	GLY	2.1
2	B	258	LYS	2.1
1	A	105	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MLY	B	209	11/12	0.89	0.16	33,38,73,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLZ	B	152	10/11	0.90	0.17	47,50,70,71	0
2	MLY	B	236	11/12	0.91	0.14	35,39,64,67	0
2	MLY	B	25	11/12	0.92	0.18	48,54,70,73	0
1	MLY	A	236	11/12	0.92	0.13	39,46,65,67	0
2	MLZ	B	254	10/11	0.92	0.18	41,49,81,82	0
2	MLY	B	170	11/12	0.93	0.14	35,39,57,62	0
1	MLY	A	127	11/12	0.93	0.18	47,56,74,77	0
2	MLY	B	127	11/12	0.93	0.16	42,51,67,70	0
2	MLZ	B	253	10/11	0.93	0.12	37,49,78,79	0
1	MLZ	A	253	10/11	0.93	0.11	43,64,70,74	0
2	MLZ	B	194	10/11	0.94	0.12	35,41,62,65	0
2	MLZ	B	131	10/11	0.94	0.09	40,42,63,70	0
1	MLZ	A	194	10/11	0.94	0.11	45,50,70,73	0
1	MLZ	A	209	10/11	0.94	0.12	38,41,74,75	0
2	MLY	B	193	11/12	0.94	0.12	41,47,66,72	0
1	MLZ	A	242	10/11	0.95	0.11	34,42,65,66	2
2	MLZ	B	94	10/11	0.95	0.11	36,43,66,70	0
1	MLY	A	97	11/12	0.95	0.08	41,50,57,60	0
2	MLY	B	57	11/12	0.96	0.11	37,49,75,81	0
1	MLY	A	243	11/12	0.96	0.08	41,44,53,55	0
1	MLY	A	94	11/12	0.96	0.11	39,46,65,74	0
1	MLY	A	170	11/12	0.96	0.10	31,36,52,57	0
1	MLY	A	12	11/12	0.97	0.08	36,47,66,68	0
2	MLY	B	243	11/12	0.97	0.07	32,36,50,53	0
2	MLY	B	3	11/12	0.98	0.09	31,35,55,57	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
5	GOL	A	306	6/6	0.67	0.22	70,80,82,83	0
5	GOL	B	303	6/6	0.82	0.21	45,51,57,61	6
9	D10	B	307	10/10	0.82	0.25	57,66,69,69	0

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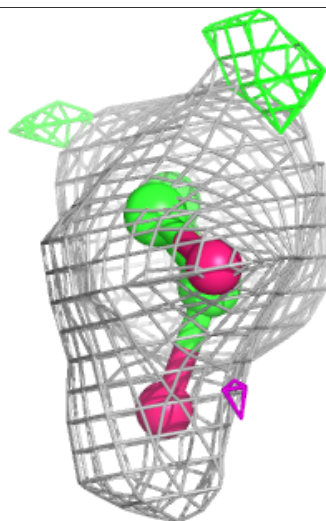
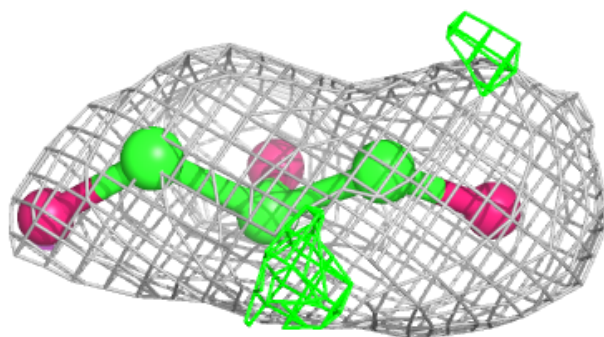
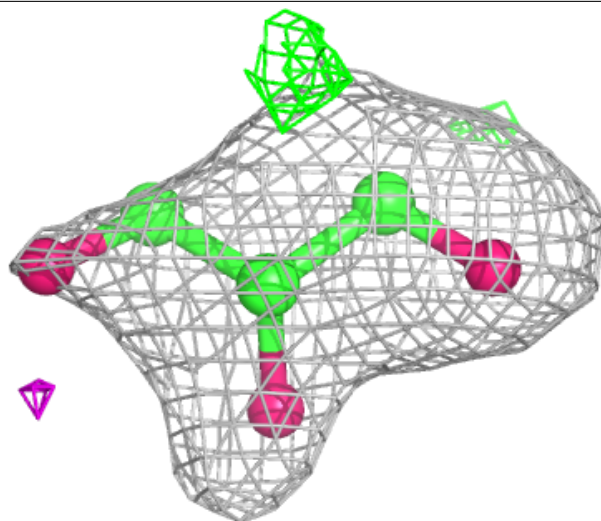
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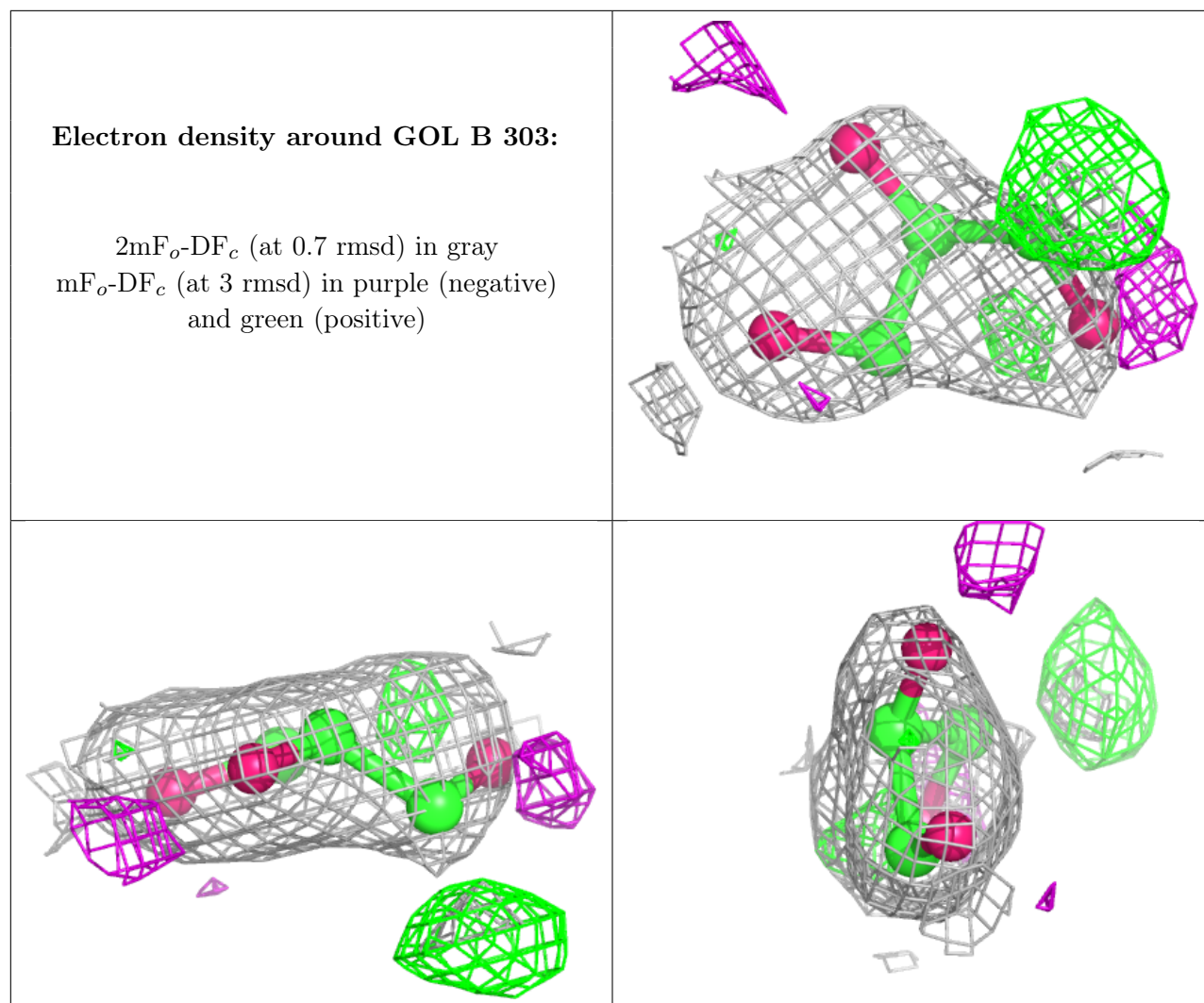
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	304	6/6	0.83	0.19	56,67,70,73	0
4	OCT	A	302	8/8	0.86	0.19	47,51,58,58	0
8	DD9	B	306	9/9	0.87	0.15	50,52,60,61	0
3	STE	A	301	19/20	0.88	0.20	28,58,63,65	0
5	GOL	B	305	6/6	0.89	0.20	44,50,66,68	0
6	SO4	A	310	5/5	0.89	0.31	88,89,92,92	5
4	OCT	A	303	8/8	0.89	0.10	54,63,66,67	0
3	STE	B	301	19/20	0.89	0.24	28,59,73,77	0
5	GOL	B	302	6/6	0.90	0.11	47,56,60,61	0
5	GOL	A	305	6/6	0.90	0.28	69,71,74,74	0
6	SO4	A	308	5/5	0.90	0.21	86,94,95,98	5
5	GOL	A	304	6/6	0.94	0.08	57,60,62,65	0
6	SO4	A	309	5/5	0.95	0.14	70,76,76,80	5
6	SO4	A	307	5/5	0.97	0.10	41,55,61,64	5
7	CL	A	311	1/1	0.99	0.05	37,37,37,37	0

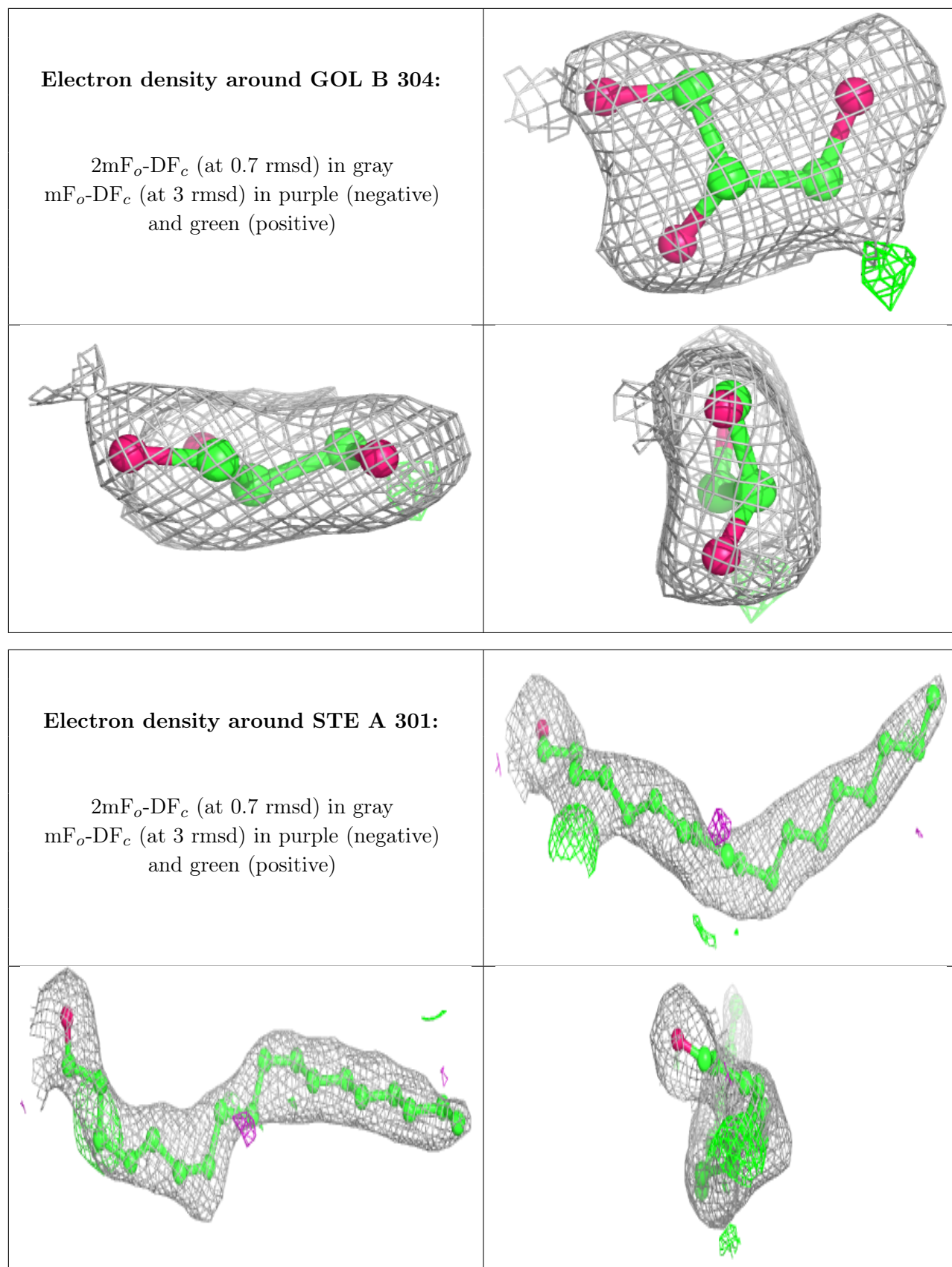
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

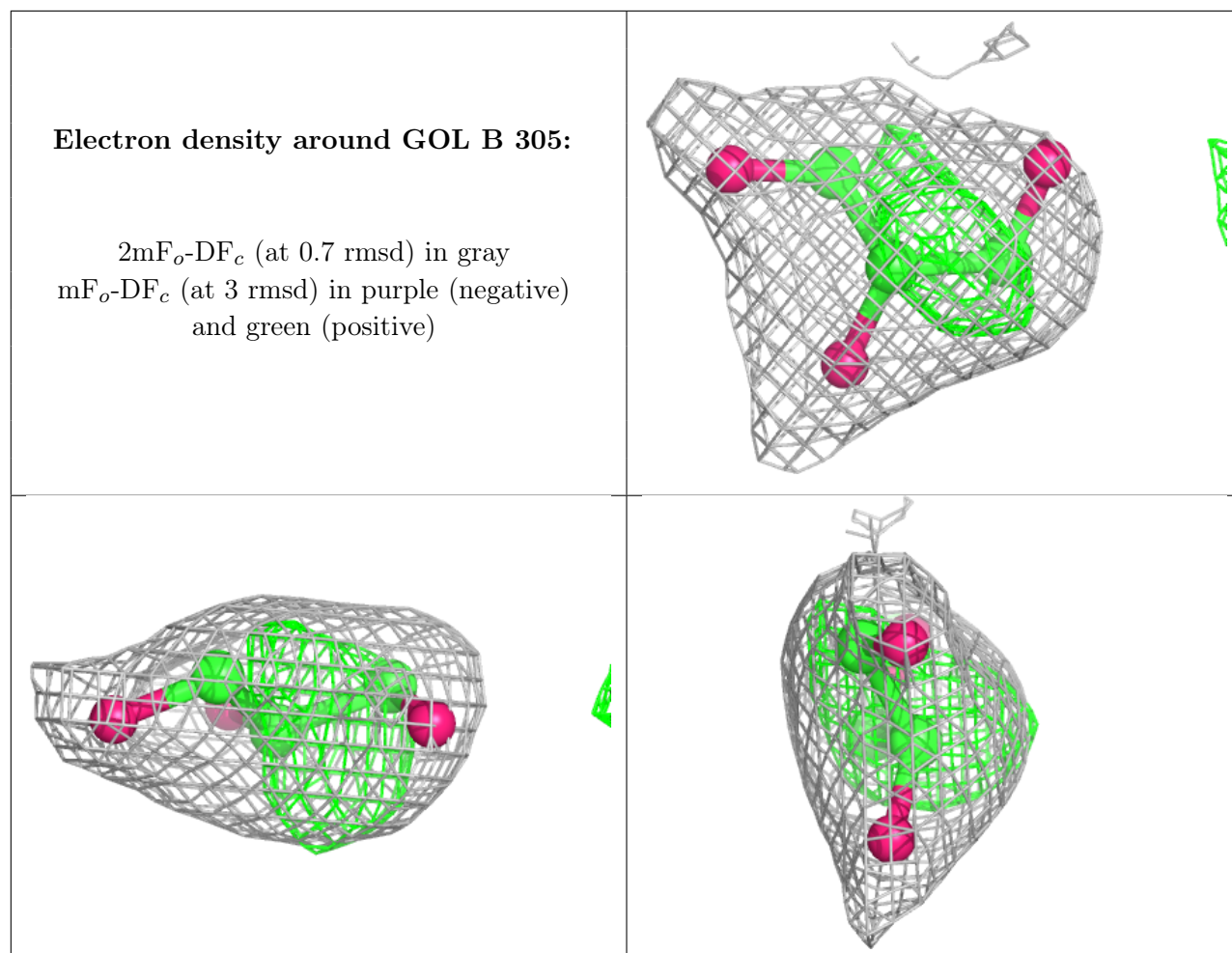
Electron density around GOL A 306:

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



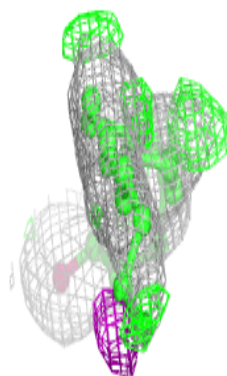
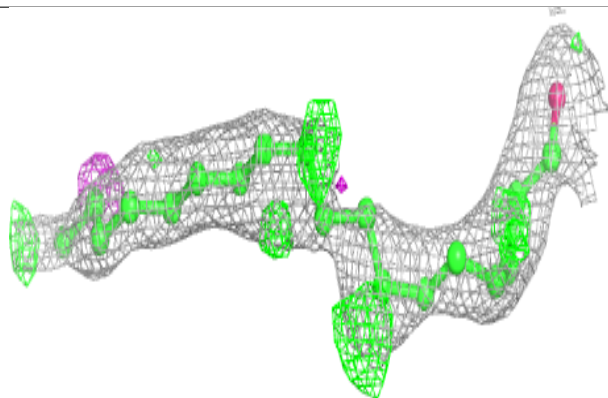
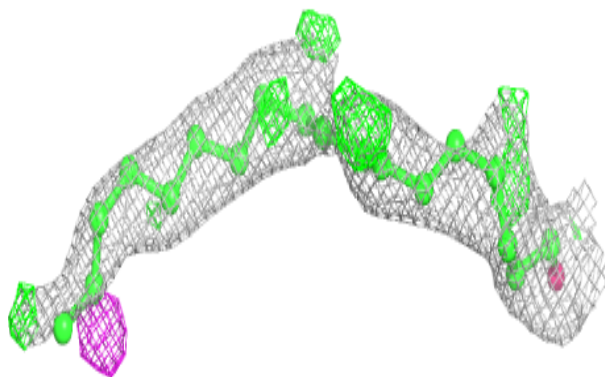




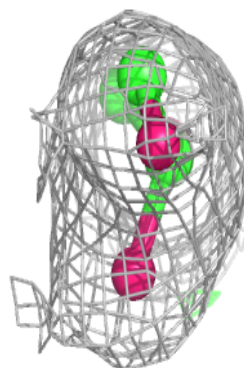
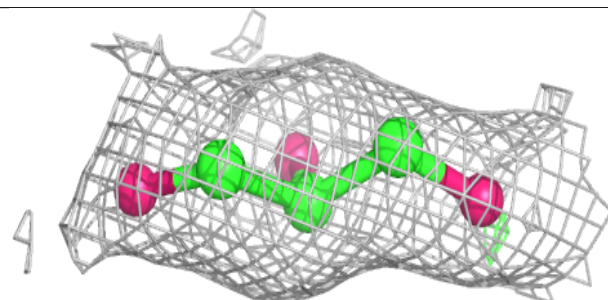
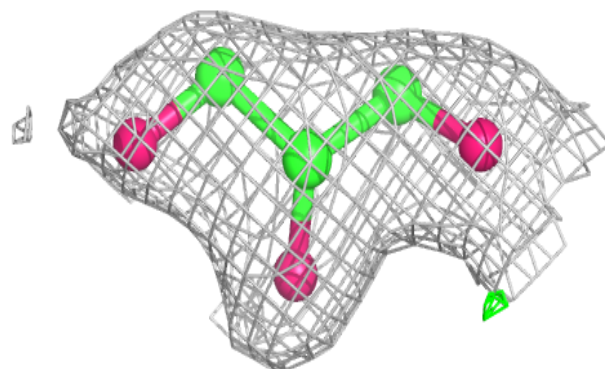


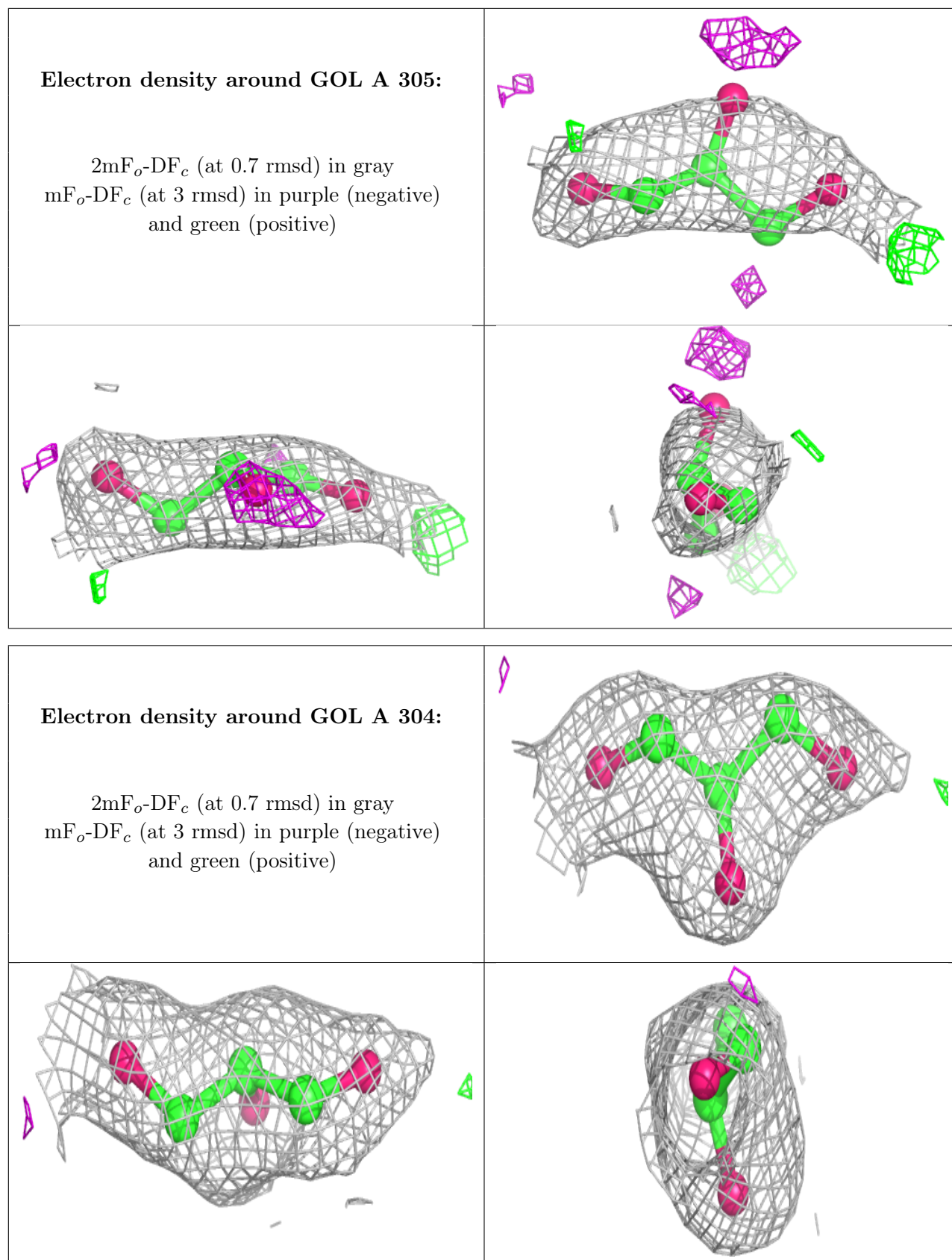
Electron density around STE B 301:

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

**Electron density around GOL B 302:**

$2mF_o-DF_c$ (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.