



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2025 – 01:09 pm BST

PDB ID : 9R0B / pdb\_00009r0b  
Title : Structure of A16/G9 (vaccinia virus) in complex with VHH D07 at pH 6.5  
Authors : Vernuccio, R.; Meola, A.; Guardado-Calvo, P.  
Deposited on : 2025-04-24  
Resolution : 2.45 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

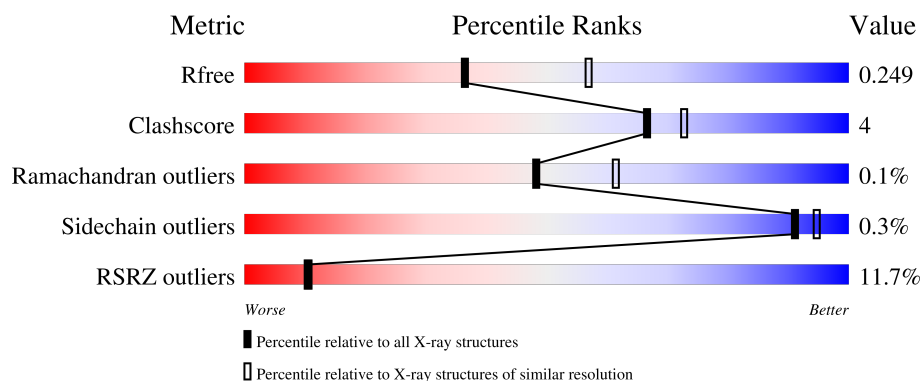
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	358	<div> <div>16%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>19%</div> </div> </div>
2	B	334	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>5%</div> <div>19%</div> </div> </div>
3	J000	154	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>•</div> <div>23%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5707 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 Virion membrane protein OPG143.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2386	1514	409	440	23			

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P16710
A	-17	LYS	-	expression tag	UNP P16710
A	-16	LEU	-	expression tag	UNP P16710
A	-15	CYS	-	expression tag	UNP P16710
A	-14	ILE	-	expression tag	UNP P16710
A	-13	LEU	-	expression tag	UNP P16710
A	-12	LEU	-	expression tag	UNP P16710
A	-11	ALA	-	expression tag	UNP P16710
A	-10	VAL	-	expression tag	UNP P16710
A	-9	VAL	-	expression tag	UNP P16710
A	-8	ALA	-	expression tag	UNP P16710
A	-7	PHE	-	expression tag	UNP P16710
A	-6	VAL	-	expression tag	UNP P16710
A	-5	GLY	-	expression tag	UNP P16710
A	-4	LEU	-	expression tag	UNP P16710
A	-3	SER	-	expression tag	UNP P16710
A	-2	LEU	-	expression tag	UNP P16710
A	-1	GLY	-	expression tag	UNP P16710
A	0	ARG	-	expression tag	UNP P16710
A	1	SER	-	expression tag	UNP P16710
A	2	ALA	-	expression tag	UNP P16710
A	296	GLY	-	expression tag	UNP P16710
A	297	SER	-	expression tag	UNP P16710
A	298	GLY	-	expression tag	UNP P16710
A	299	LEU	-	expression tag	UNP P16710
A	300	VAL	-	expression tag	UNP P16710
A	301	PRO	-	expression tag	UNP P16710

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	ARG	-	expression tag	UNP P16710
A	303	GLY	-	expression tag	UNP P16710
A	304	SER	-	expression tag	UNP P16710
A	305	GLY	-	expression tag	UNP P16710
A	306	GLY	-	expression tag	UNP P16710
A	307	SER	-	expression tag	UNP P16710
A	308	GLY	-	expression tag	UNP P16710
A	309	GLY	-	expression tag	UNP P16710
A	310	SER	-	expression tag	UNP P16710
A	311	HIS	-	expression tag	UNP P16710
A	312	HIS	-	expression tag	UNP P16710
A	313	HIS	-	expression tag	UNP P16710
A	314	HIS	-	expression tag	UNP P16710
A	315	HIS	-	expression tag	UNP P16710
A	316	HIS	-	expression tag	UNP P16710
A	317	HIS	-	expression tag	UNP P16710
A	318	HIS	-	expression tag	UNP P16710
A	319	GLY	-	expression tag	UNP P16710
A	320	GLY	-	expression tag	UNP P16710
A	321	SER	-	expression tag	UNP P16710
A	322	GLY	-	expression tag	UNP P16710
A	323	THR	-	expression tag	UNP P16710
A	324	GLY	-	expression tag	UNP P16710
A	325	GLY	-	expression tag	UNP P16710
A	326	LEU	-	expression tag	UNP P16710
A	327	ASN	-	expression tag	UNP P16710
A	328	ASP	-	expression tag	UNP P16710
A	329	ILE	-	expression tag	UNP P16710
A	330	PHE	-	expression tag	UNP P16710
A	331	GLU	-	expression tag	UNP P16710
A	332	ALA	-	expression tag	UNP P16710
A	333	GLN	-	expression tag	UNP P16710
A	334	LYS	-	expression tag	UNP P16710
A	335	ILE	-	expression tag	UNP P16710
A	336	GLU	-	expression tag	UNP P16710
A	337	TRP	-	expression tag	UNP P16710
A	338	HIS	-	expression tag	UNP P16710
A	339	GLU	-	expression tag	UNP P16710

- Molecule 2 is a protein called Entry-fusion complex protein OPG094.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	269	Total	C	N	O	S	0	0	0
			2164	1354	383	410	17			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P07611
B	-15	LYS	-	expression tag	UNP P07611
B	-14	LEU	-	expression tag	UNP P07611
B	-13	CYS	-	expression tag	UNP P07611
B	-12	ILE	-	expression tag	UNP P07611
B	-11	LEU	-	expression tag	UNP P07611
B	-10	LEU	-	expression tag	UNP P07611
B	-9	ALA	-	expression tag	UNP P07611
B	-8	VAL	-	expression tag	UNP P07611
B	-7	VAL	-	expression tag	UNP P07611
B	-6	ALA	-	expression tag	UNP P07611
B	-5	PHE	-	expression tag	UNP P07611
B	-4	VAL	-	expression tag	UNP P07611
B	-3	GLY	-	expression tag	UNP P07611
B	-2	LEU	-	expression tag	UNP P07611
B	-1	SER	-	expression tag	UNP P07611
B	0	LEU	-	expression tag	UNP P07611
B	1	GLY	-	expression tag	UNP P07611
B	2	ALA	-	expression tag	UNP P07611
B	82	ALA	ASN	conflict	UNP P07611
B	93	GLN	ASN	conflict	UNP P07611
B	156	ALA	SER	conflict	UNP P07611
B	157	ASP	ASN	conflict	UNP P07611
B	272	GLY	-	expression tag	UNP P07611
B	273	SER	-	expression tag	UNP P07611
B	274	GLY	-	expression tag	UNP P07611
B	275	LEU	-	expression tag	UNP P07611
B	276	VAL	-	expression tag	UNP P07611
B	277	PRO	-	expression tag	UNP P07611
B	278	ARG	-	expression tag	UNP P07611
B	279	GLY	-	expression tag	UNP P07611
B	280	SER	-	expression tag	UNP P07611
B	281	LEU	-	expression tag	UNP P07611
B	282	GLU	-	expression tag	UNP P07611
B	283	ASP	-	expression tag	UNP P07611
B	284	ASP	-	expression tag	UNP P07611
B	285	ASP	-	expression tag	UNP P07611

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	286	ASP	-	expression tag	UNP P07611
B	287	LYS	-	expression tag	UNP P07611
B	288	ALA	-	expression tag	UNP P07611
B	289	GLY	-	expression tag	UNP P07611
B	290	TRP	-	expression tag	UNP P07611
B	291	SER	-	expression tag	UNP P07611
B	292	HIS	-	expression tag	UNP P07611
B	293	PRO	-	expression tag	UNP P07611
B	294	GLN	-	expression tag	UNP P07611
B	295	PHE	-	expression tag	UNP P07611
B	296	GLU	-	expression tag	UNP P07611
B	297	LYS	-	expression tag	UNP P07611
B	298	GLY	-	expression tag	UNP P07611
B	299	GLY	-	expression tag	UNP P07611
B	300	GLY	-	expression tag	UNP P07611
B	301	SER	-	expression tag	UNP P07611
B	302	GLY	-	expression tag	UNP P07611
B	303	GLY	-	expression tag	UNP P07611
B	304	GLY	-	expression tag	UNP P07611
B	305	SER	-	expression tag	UNP P07611
B	306	GLY	-	expression tag	UNP P07611
B	307	GLY	-	expression tag	UNP P07611
B	308	GLY	-	expression tag	UNP P07611
B	309	SER	-	expression tag	UNP P07611
B	310	TRP	-	expression tag	UNP P07611
B	311	SER	-	expression tag	UNP P07611
B	312	HIS	-	expression tag	UNP P07611
B	313	PRO	-	expression tag	UNP P07611
B	314	GLN	-	expression tag	UNP P07611
B	315	PHE	-	expression tag	UNP P07611
B	316	GLU	-	expression tag	UNP P07611
B	317	LYS	-	expression tag	UNP P07611

- Molecule 3 is a protein called VHH D07.

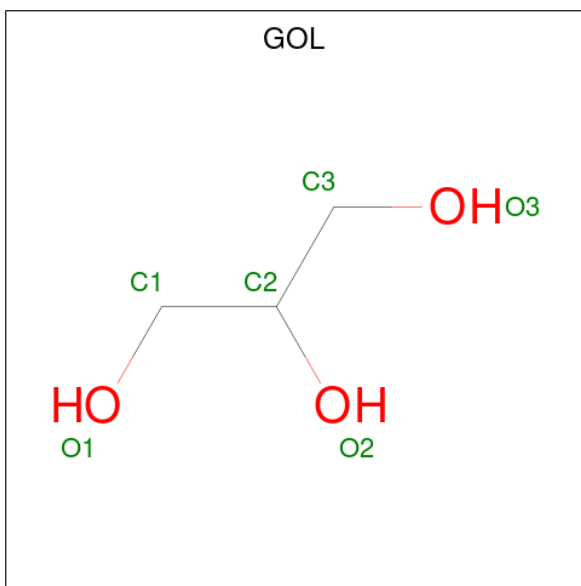
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J000	119	Total	C	N	O	S	0	0	0
			901	555	163	178	5			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is GLYCEROL (CCD ID: 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	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	J000	1	Total	C	O	0	0
			6	3	3		
5	J000	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

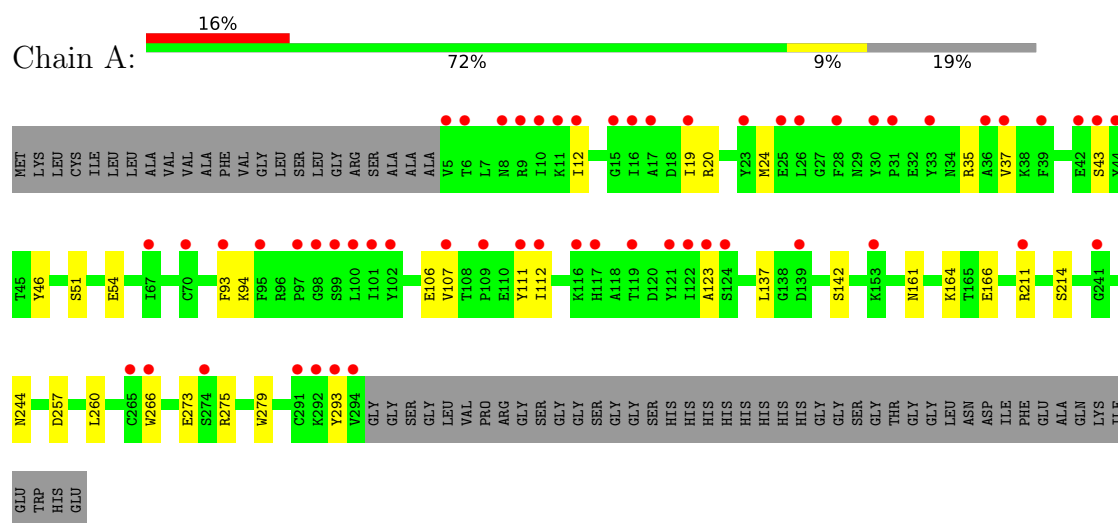
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	92	Total	O	0	0
			92	92		
6	J000	23	Total	O	0	0
			23	23		



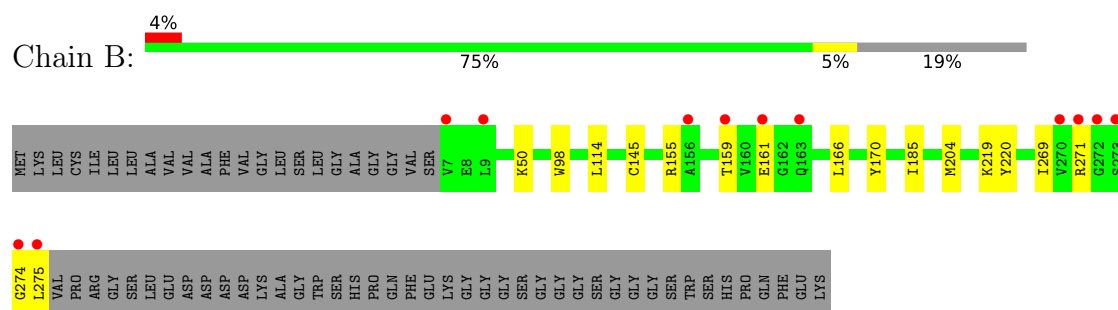
### 3 Residue-property plots [i](#)

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.

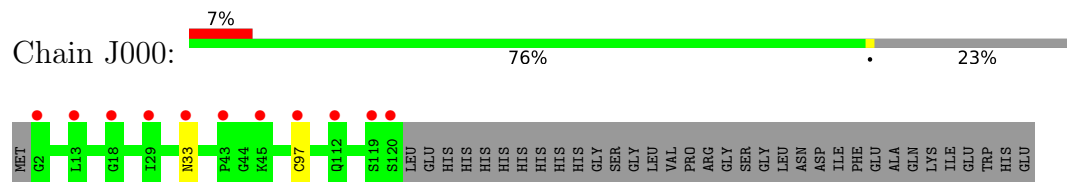
#### • Molecule 1: Virion membrane protein OPG143



#### • Molecule 2: Entry-fusion complex protein OPG094



#### • Molecule 3: VHH D07



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.46Å 146.42Å 182.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.23 – 2.45 39.23 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.23-2.45) 99.9 (39.23-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.222 , 0.249 0.222 , 0.249	Depositor DCC
$R_{free}$ test set	2402 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.3	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	0.94	EDS
Total number of atoms	5707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 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	0.11	0/2455	0.31	0/3317
2	B	0.11	0/2215	0.28	0/2997
3	J000	0.10	0/916	0.29	0/1239
All	All	0.11	0/5586	0.29	0/7553

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	2386	0	2257	21	0
2	B	2164	0	2087	12	0
3	J000	901	0	0	0	0
4	A	12	0	13	1	0
5	A	6	0	8	1	0
5	B	12	0	16	0	0
5	J000	12	0	0	0	0
6	A	99	0	0	0	0
6	B	92	0	0	0	0
6	J000	23	0	0	0	0
All	All	5707	0	4381	30	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 4.

All (30) 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:51:SER:HB2	1:A:54:GLU:HB2	1.75	0.69
1:A:35:ARG:HD2	1:A:106:GLU:HB2	1.84	0.59
1:A:214:SER:HB3	5:A:402:GOL:H11	1.89	0.55
1:A:266:TRP:HB3	2:B:275:LEU:HD13	1.89	0.53
1:A:94:LYS:HG2	1:A:123:ALA:HB2	1.92	0.51
2:B:159:THR:HG22	2:B:161:GLU:H	1.76	0.51
2:B:170:TYR:HB3	2:B:204:MET:HE1	1.93	0.51
1:A:257:ASP:HA	1:A:260:LEU:HG	1.93	0.50
1:A:111:TYR:HD2	1:A:112:ILE:HD12	1.77	0.48
2:B:145:CYS:HB3	2:B:185:ILE:HD13	1.96	0.48
1:A:273:GLU:C	1:A:275:ARG:H	2.23	0.46
2:B:219:LYS:HD3	2:B:220:TYR:CE2	2.51	0.46
1:A:161:ASN:O	1:A:164:LYS:HG3	2.16	0.46
2:B:159:THR:HG22	2:B:161:GLU:HG2	1.98	0.46
1:A:37:VAL:HA	1:A:107:VAL:HG21	1.98	0.45
2:B:155:ARG:HD2	2:B:166:LEU:HD13	1.99	0.45
1:A:260:LEU:HD13	4:A:401:MES:H82	1.99	0.44
1:A:211:ARG:H	1:A:211:ARG:CD	2.31	0.43
1:A:293:TYR:HA	2:B:269:ILE:O	2.19	0.43
2:B:269:ILE:HG23	2:B:274:GLY:H	1.84	0.43
1:A:19:ILE:HD12	1:A:19:ILE:H	1.85	0.42
1:A:137:LEU:HD22	1:A:142:SER:HB3	2.02	0.42
1:A:43:SER:HB3	1:A:46:TYR:OH	2.20	0.41
2:B:50:LYS:HD2	2:B:50:LYS:HA	1.91	0.41
1:A:12:ILE:HG12	1:A:24:MET:HE2	2.03	0.41
1:A:293:TYR:HB3	2:B:271:ARG:HG3	2.03	0.41
1:A:244:ASN:HB3	1:A:279:TRP:CD2	2.56	0.41
1:A:20:ARG:HH11	1:A:43:SER:HA	1.85	0.40
1:A:24:MET:HG3	1:A:93:PHE:CZ	2.56	0.40
2:B:98:TRP:CZ3	2:B:114:LEU:HB2	2.57	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	288/358 (80%)	267 (93%)	21 (7%)	0	100	100
2	B	267/334 (80%)	261 (98%)	6 (2%)	0	100	100
3	J000	117/154 (76%)	111 (95%)	5 (4%)	1 (1%)	14	18
All	All	672/846 (79%)	639 (95%)	32 (5%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J000	33	ASN

### 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	263/310 (85%)	262 (100%)	1 (0%)	89	94
2	B	240/286 (84%)	240 (100%)	0	100	100
3	J000	95/125 (76%)	94 (99%)	1 (1%)	70	81
All	All	598/721 (83%)	596 (100%)	2 (0%)	91	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLU
3	J000	97	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
2	B	26	ASN
2	B	122	HIS
2	B	211	GLN
2	B	218	GLN
2	B	262	ASN

### 5.3.3 RNA [i](#)

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](#)

6 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	$\# Z  > 2$
5	GOL	J000	202	-	5,5,5	0.34	0	5,5,5	0.39	0
4	MES	A	401	-	12,12,12	1.09	1 (8%)	14,16,16	0.99	2 (14%)
5	GOL	J000	201	-	5,5,5	0.32	0	5,5,5	0.31	0
5	GOL	B	402	-	5,5,5	0.32	0	5,5,5	0.39	0
5	GOL	A	402	-	5,5,5	0.33	0	5,5,5	0.24	0
5	GOL	B	401	-	5,5,5	0.34	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	J000	202	-	-	2/4/4/4	-
4	MES	A	401	-	-	1/6/14/14	0/1/1/1
5	GOL	J000	201	-	-	2/4/4/4	-
5	GOL	B	402	-	-	2/4/4/4	-
5	GOL	A	402	-	-	2/4/4/4	-
5	GOL	B	401	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	MES	C8-S	2.92	1.81	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	MES	O1S-S-C8	-2.09	104.39	106.92
4	A	401	MES	O2S-S-C8	-2.04	104.46	106.92

There are no chirality outliers.

All (10) torsion outliers are listed below:

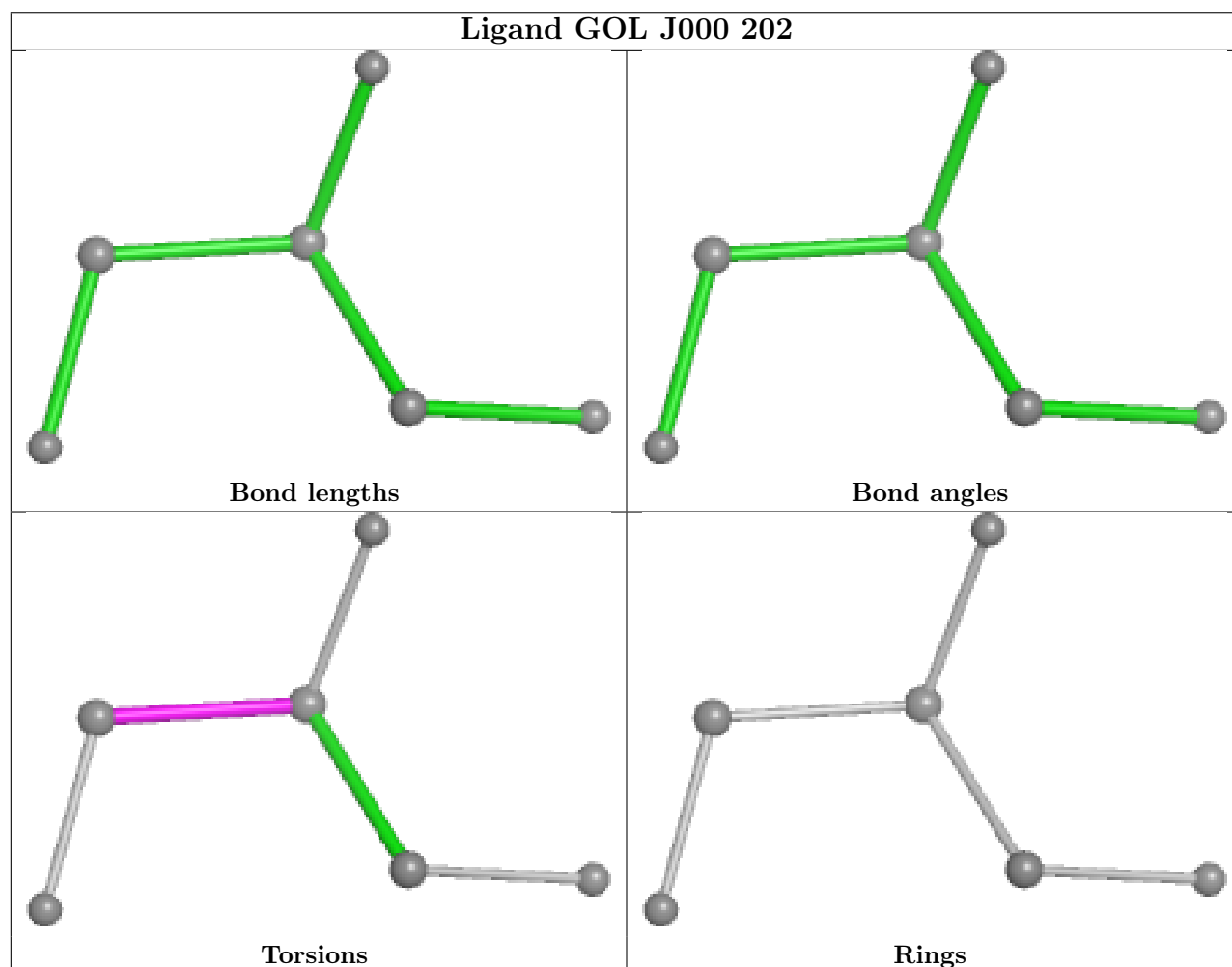
Mol	Chain	Res	Type	Atoms
4	A	401	MES	C8-C7-N4-C5
5	A	402	GOL	O1-C1-C2-C3
5	B	402	GOL	O1-C1-C2-C3
5	J000	201	GOL	C1-C2-C3-O3
5	J000	202	GOL	O1-C1-C2-C3
5	A	402	GOL	O1-C1-C2-O2
5	J000	201	GOL	O2-C2-C3-O3
5	J000	202	GOL	O1-C1-C2-O2
5	B	402	GOL	O1-C1-C2-O2
5	B	401	GOL	O2-C2-C3-O3

There are no ring outliers.

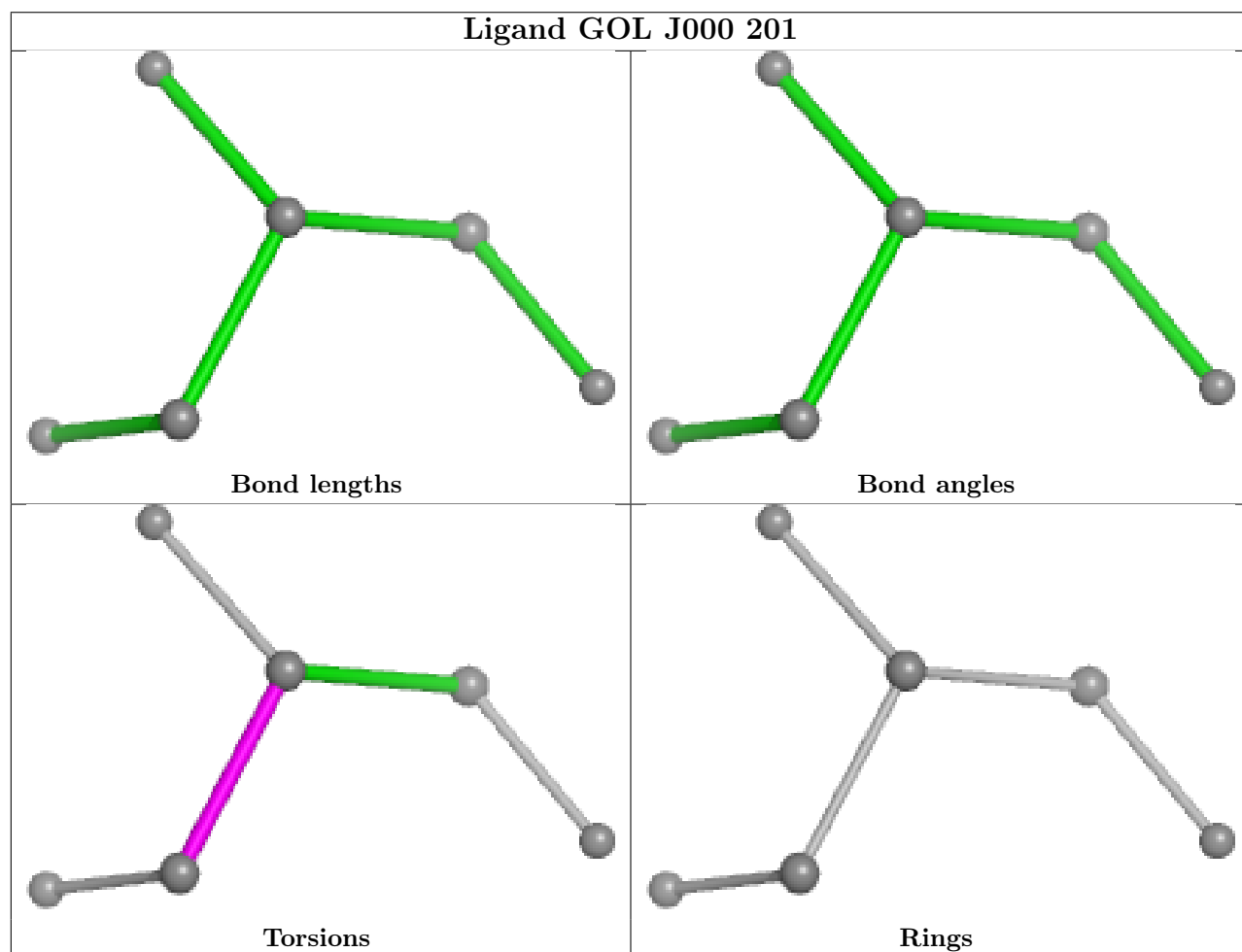
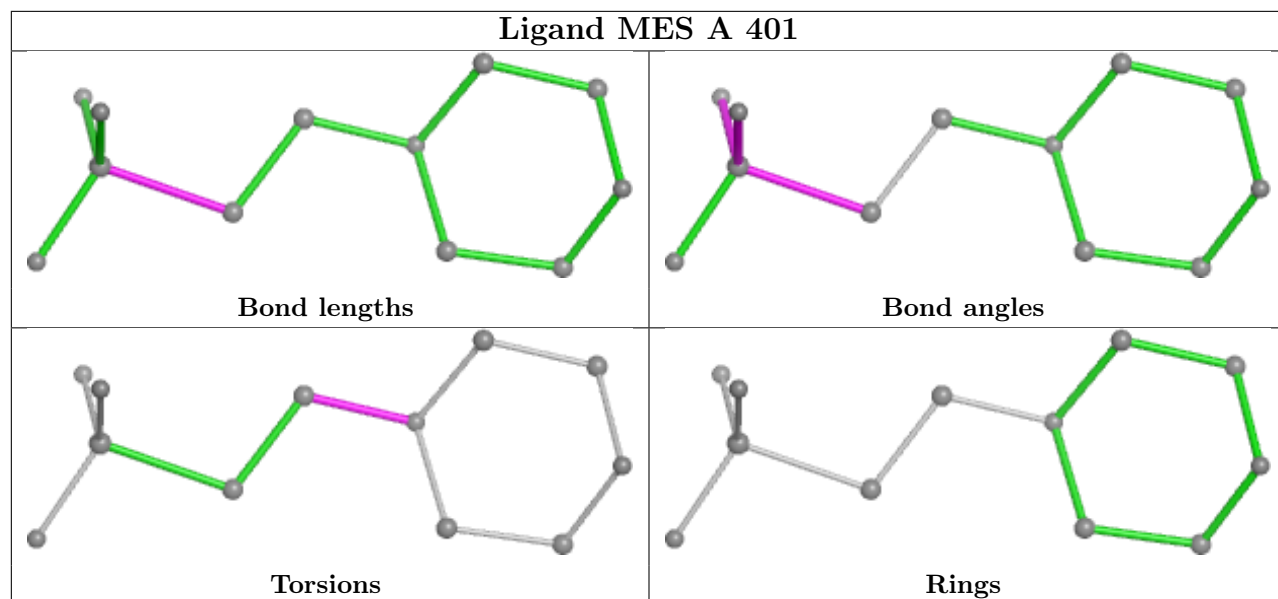
2 monomers are involved in 2 short contacts:

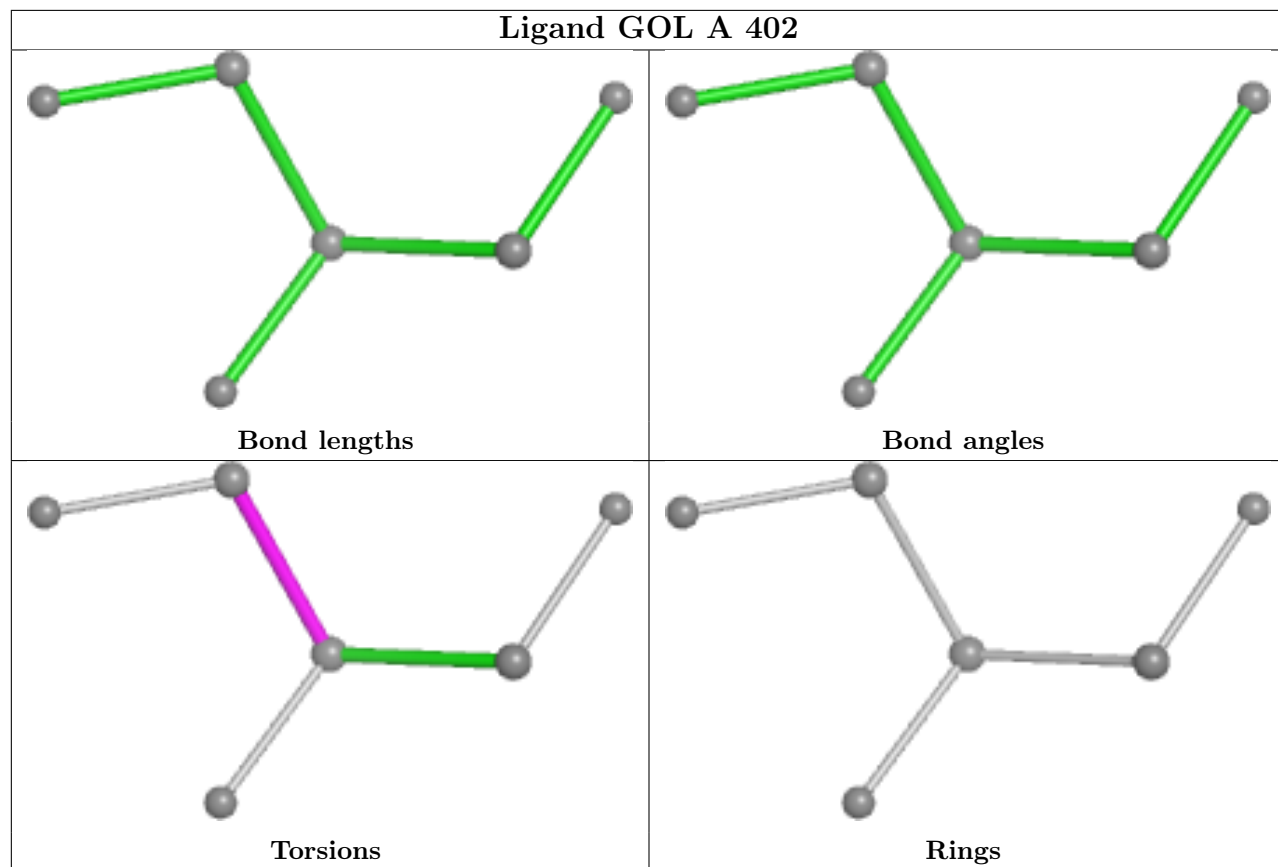
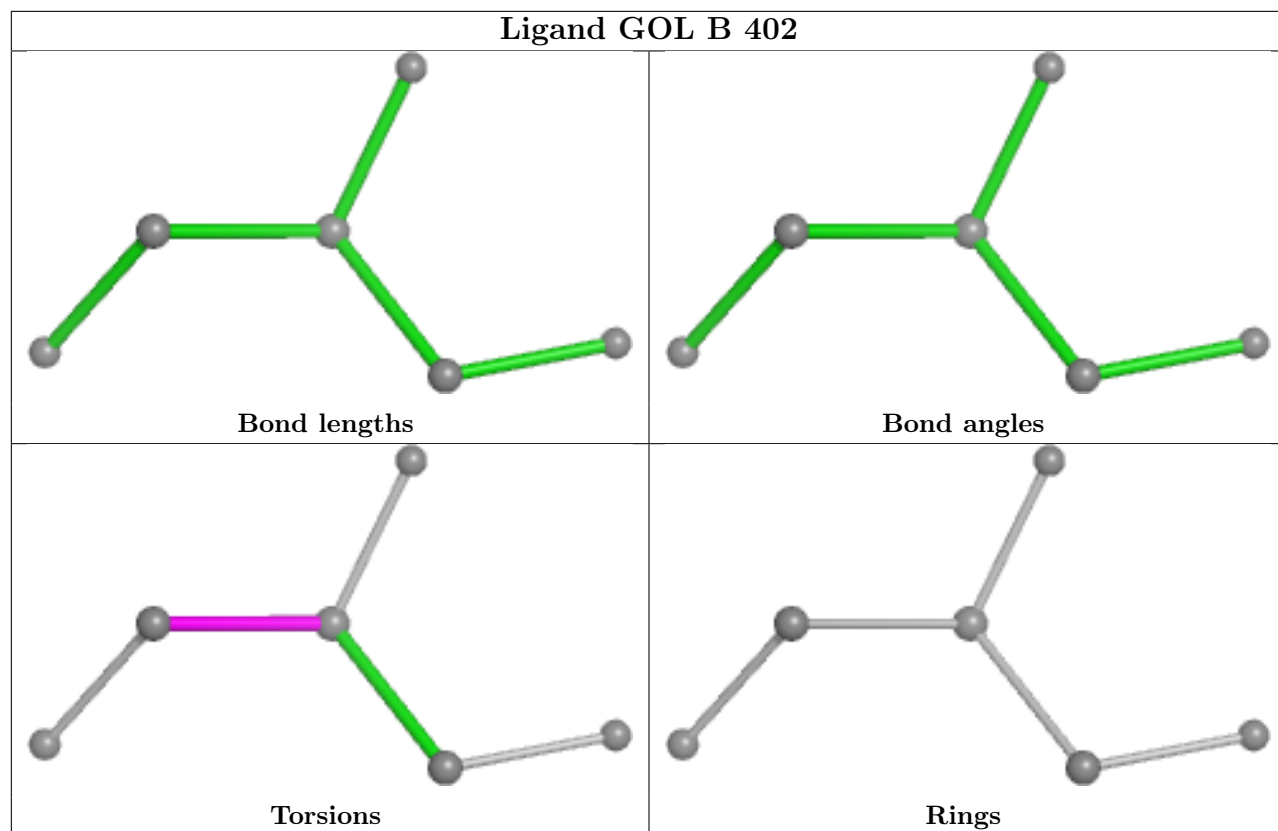
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	MES	1	0
5	A	402	GOL	1	0

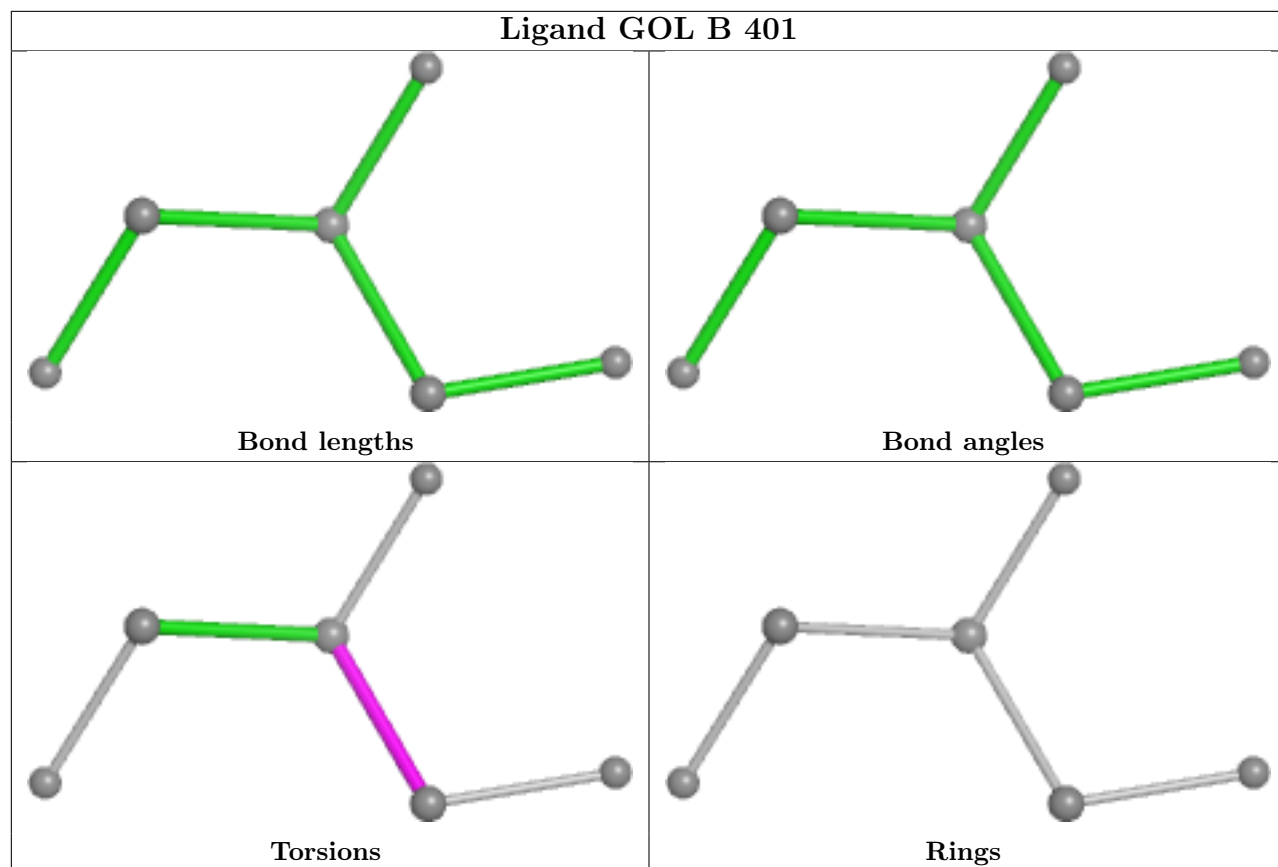
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	290/358 (81%)	0.73	56 (19%) <b>4</b> <b>3</b>	38, 62, 112, 127	0
2	B	269/334 (80%)	0.17	12 (4%) <b>39</b> <b>39</b>	39, 55, 91, 118	0
3	J000	119/154 (77%)	0.85	11 (9%) <b>16</b> <b>16</b>	53, 66, 92, 105	0
All	All	678/846 (80%)	0.53	79 (11%) <b>10</b> <b>10</b>	38, 60, 106, 127	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	275	LEU	6.5
3	J000	97	CYS	5.8
3	J000	2	GLY	5.0
2	B	7	VAL	4.6
2	B	272	GLY	4.6
1	A	43	SER	4.2
1	A	16	ILE	4.1
3	J000	120	SER	4.1
2	B	270	VAL	4.1
1	A	44	TYR	3.9
1	A	17	ALA	3.7
1	A	122	ILE	3.6
2	B	274	GLY	3.5
1	A	10	ILE	3.4
1	A	112	ILE	3.4
1	A	30	TYR	3.3
1	A	93	PHE	3.3
1	A	294	VAL	3.3
1	A	291	CYS	3.3
1	A	123	ALA	3.2
3	J000	112	GLN	3.2
1	A	121	TYR	3.1
1	A	265	CYS	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	70	CYS	3.0
3	J000	45	LYS	2.9
1	A	42	GLU	2.9
1	A	31	PRO	2.8
1	A	119	THR	2.8
1	A	293	TYR	2.8
1	A	26	LEU	2.8
1	A	6	THR	2.8
2	B	9	LEU	2.7
1	A	95	PHE	2.7
1	A	102	TYR	2.6
2	B	159	THR	2.6
1	A	97	PRO	2.6
1	A	109	PRO	2.6
3	J000	119	SER	2.6
1	A	211	ARG	2.6
1	A	241	GLY	2.5
1	A	117	HIS	2.5
1	A	100	LEU	2.5
1	A	19	ILE	2.5
1	A	274	SER	2.5
2	B	271	ARG	2.5
1	A	116	LYS	2.4
1	A	15	GLY	2.4
1	A	153	LYS	2.4
1	A	292	LYS	2.4
1	A	33	TYR	2.4
1	A	12	ILE	2.4
3	J000	29	ILE	2.4
1	A	111	TYR	2.4
1	A	98	GLY	2.4
3	J000	18	GLY	2.4
1	A	8	ASN	2.3
1	A	67	ILE	2.3
1	A	37	VAL	2.3
1	A	99	SER	2.3
1	A	124	SER	2.3
3	J000	13	LEU	2.3
1	A	25	GLU	2.3
1	A	107	VAL	2.3
2	B	156	ALA	2.3
1	A	11	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	36	ALA	2.3
1	A	139	ASP	2.2
1	A	101	ILE	2.2
1	A	5	VAL	2.2
2	B	273	SER	2.1
1	A	266	TRP	2.1
1	A	23	TYR	2.1
1	A	39	PHE	2.1
2	B	163	GLN	2.1
3	J000	33	ASN	2.1
3	J000	43	PRO	2.1
2	B	161	GLU	2.0
1	A	9	ARG	2.0
1	A	28	PHE	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.

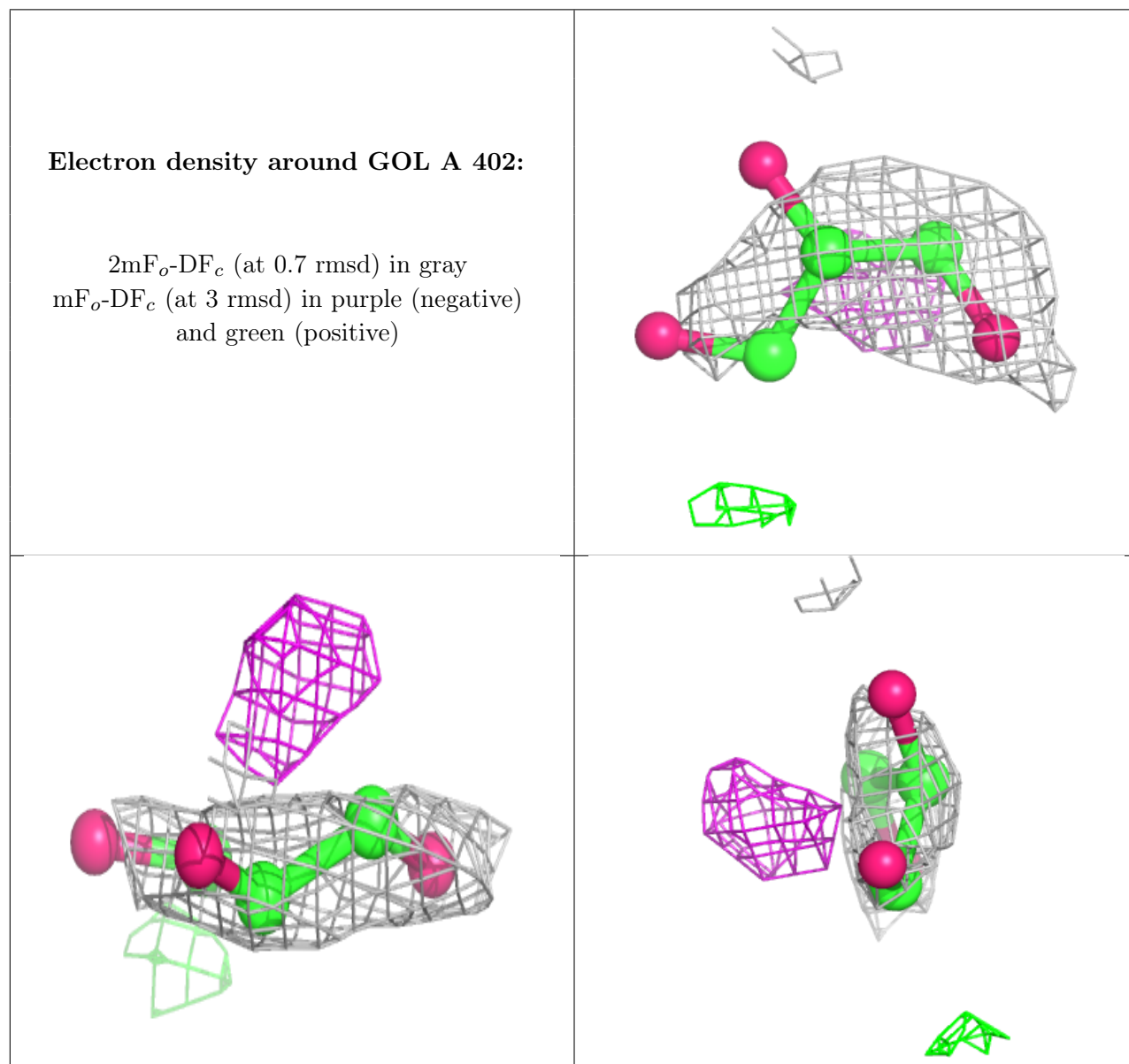
## 6.4 Ligands [i](#)

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, 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
5	GOL	A	402	6/6	0.73	0.24	75,83,94,99	0
5	GOL	J000	201	6/6	0.73	0.24	73,79,84,92	0
5	GOL	B	401	6/6	0.80	0.19	73,84,85,88	0
5	GOL	J000	202	6/6	0.87	0.16	55,73,85,94	0
5	GOL	B	402	6/6	0.94	0.17	59,63,79,92	0
4	MES	A	401	12/12	0.97	0.11	46,53,66,70	0

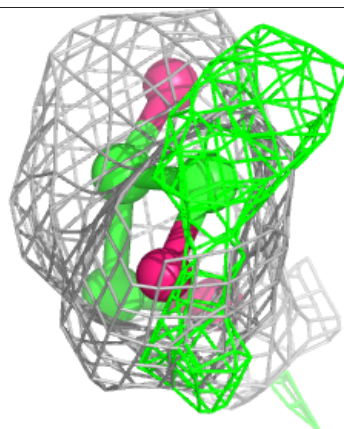
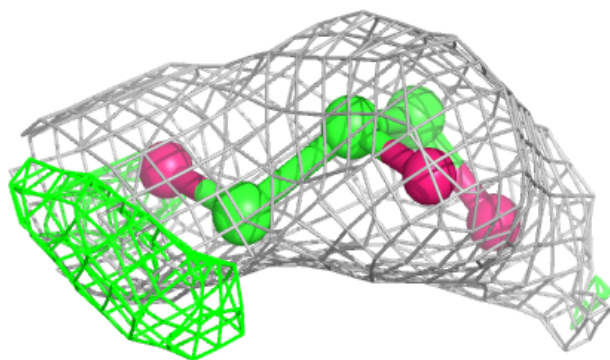
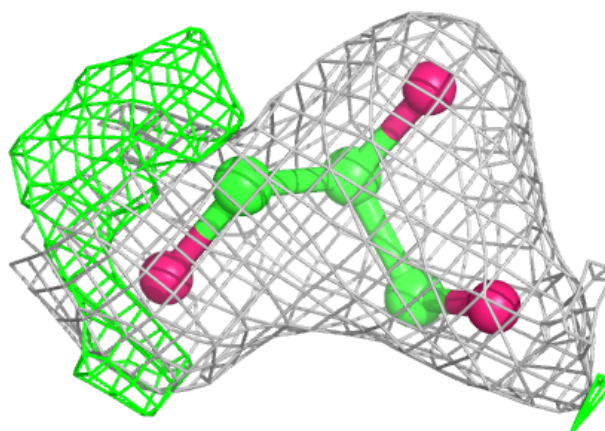
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 J000 201:**

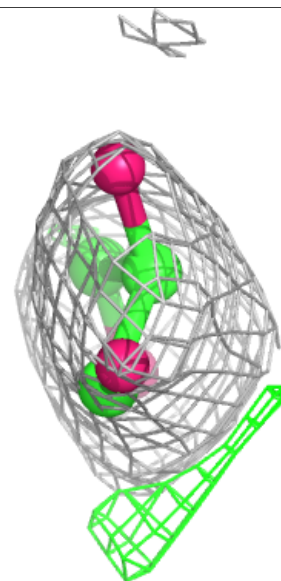
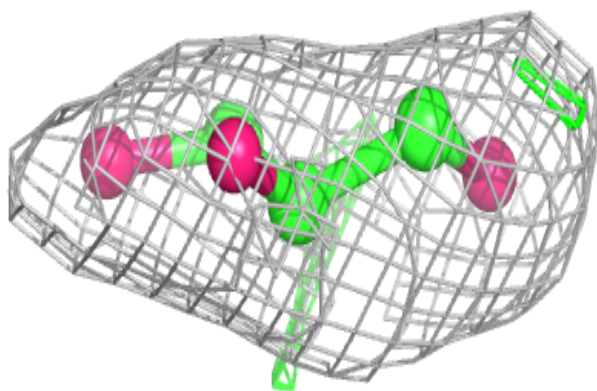
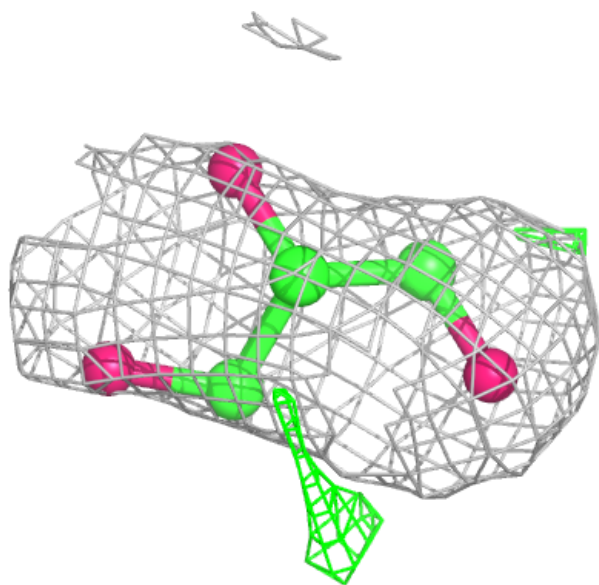
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





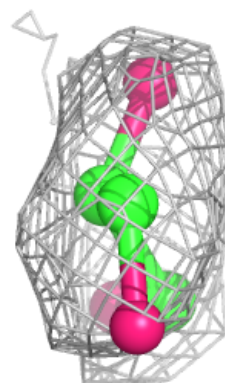
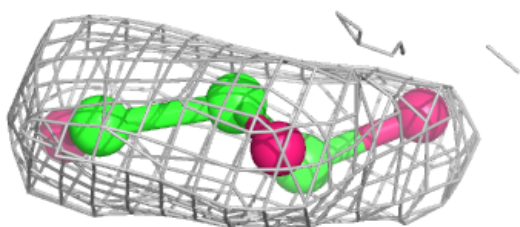
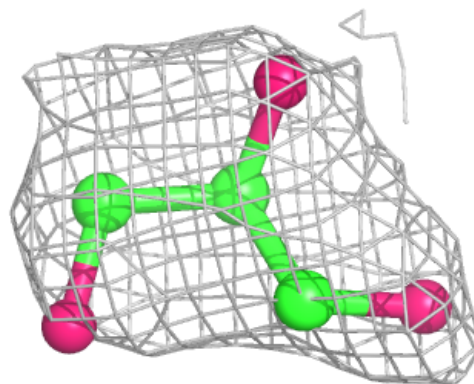
**Electron density around GOL B 401:**

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

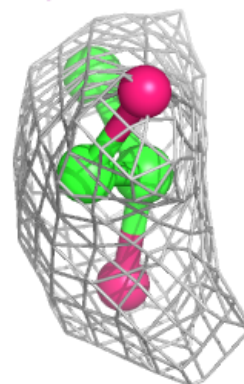
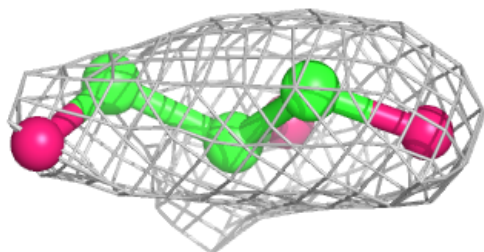
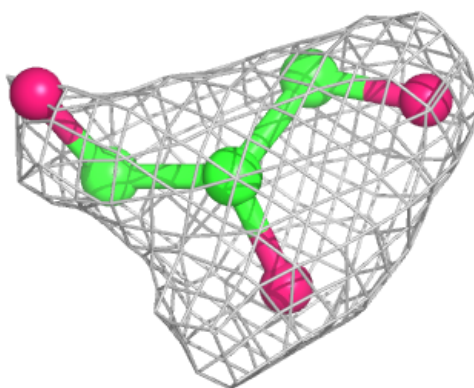


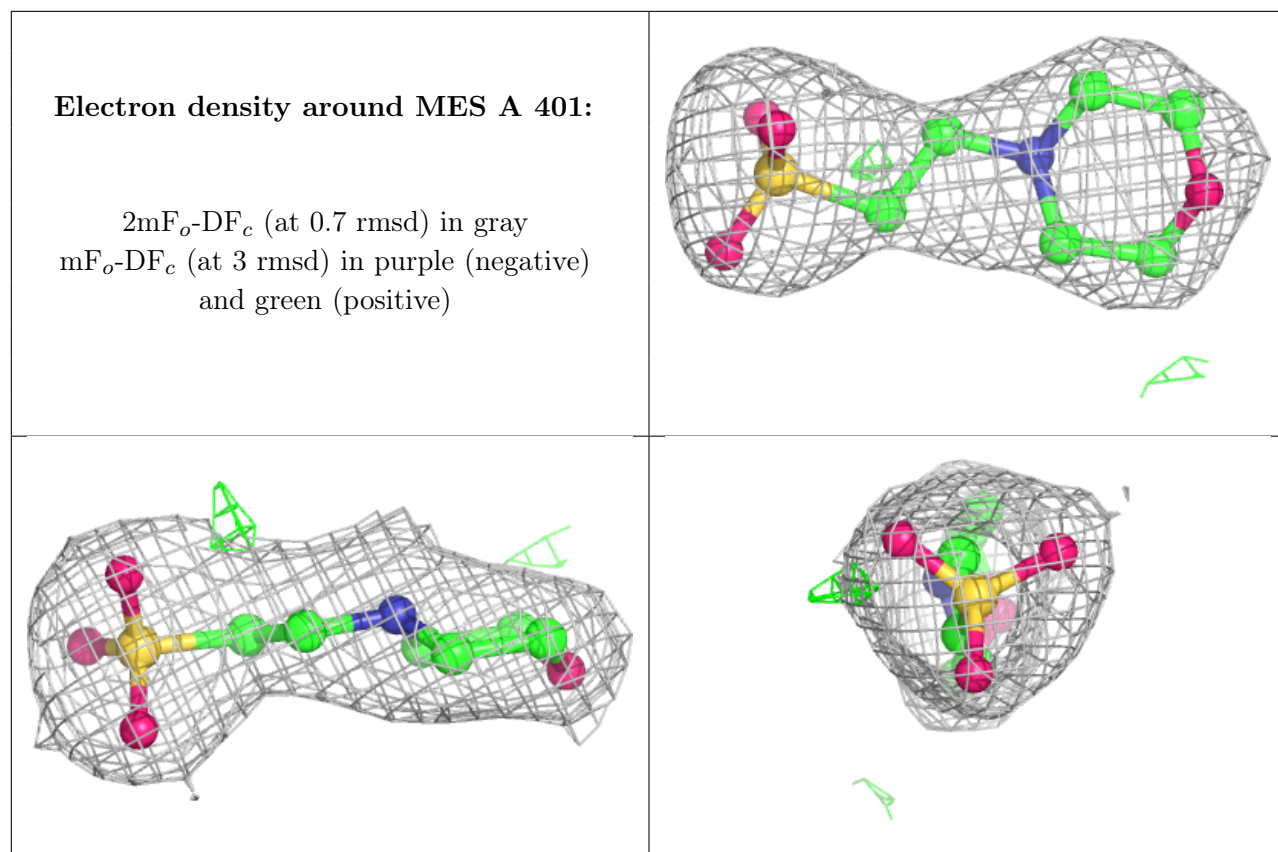
**Electron density around GOL J000 202:**

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

**Electron density around GOL B 402:**

$2mF_o-DF_c$  (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.