



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 12:18 PM JST

PDB ID : 7E9X  
Title : Trehalase of Arabidopsis thaliana acid mutant -D380A  
Authors : Taguchi, Y.; Saburi, W.; Yu, J.; Imai, R.; Yao, M.; Mori, H.  
Deposited on : 2021-03-05  
Resolution : 1.88 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
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) : 2.27

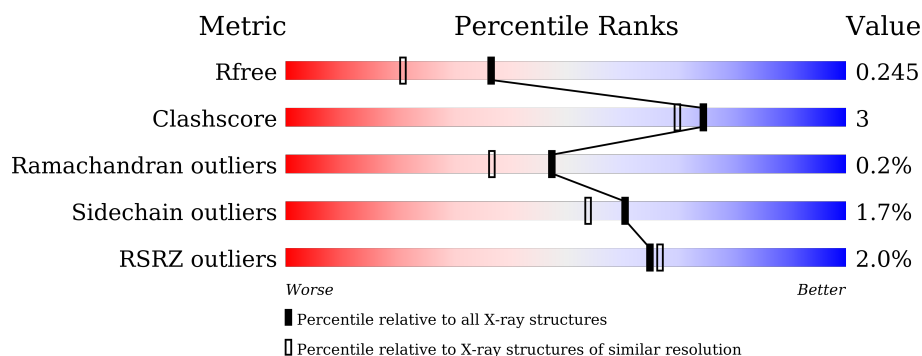
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	572	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	572	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
1	C	572	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>• 6%</div> </div> </div>
1	D	572	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18502 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 Trehalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4393	2803	738	836	16			
1	B	550	Total	C	N	O	S	0	0	0
			4398	2805	739	838	16			
1	C	540	Total	C	N	O	S	0	0	0
			4327	2766	726	819	16			
1	D	548	Total	C	N	O	S	0	0	0
			4378	2793	735	834	16			

There are 40 discrepancies between the modelled and reference sequences:

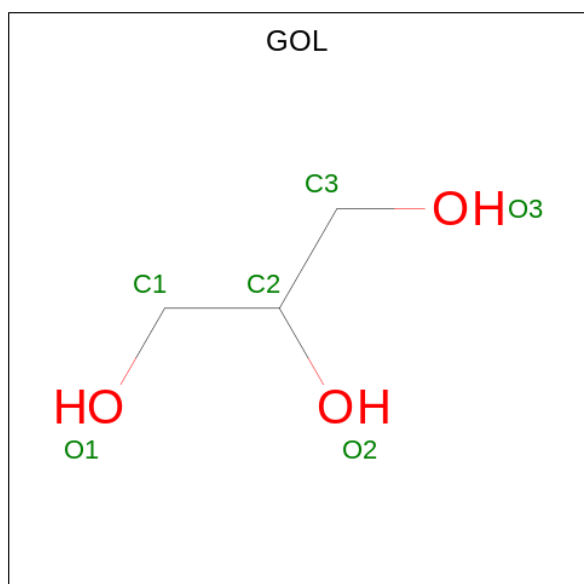
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP Q9SU50
A	380	ALA	ASP	engineered mutation	UNP Q9SU50
A	627	LEU	-	expression tag	UNP Q9SU50
A	628	GLU	-	expression tag	UNP Q9SU50
A	629	HIS	-	expression tag	UNP Q9SU50
A	630	HIS	-	expression tag	UNP Q9SU50
A	631	HIS	-	expression tag	UNP Q9SU50
A	632	HIS	-	expression tag	UNP Q9SU50
A	633	HIS	-	expression tag	UNP Q9SU50
A	634	HIS	-	expression tag	UNP Q9SU50
B	63	MET	-	initiating methionine	UNP Q9SU50
B	380	ALA	ASP	engineered mutation	UNP Q9SU50
B	627	LEU	-	expression tag	UNP Q9SU50
B	628	GLU	-	expression tag	UNP Q9SU50
B	629	HIS	-	expression tag	UNP Q9SU50
B	630	HIS	-	expression tag	UNP Q9SU50
B	631	HIS	-	expression tag	UNP Q9SU50
B	632	HIS	-	expression tag	UNP Q9SU50
B	633	HIS	-	expression tag	UNP Q9SU50
B	634	HIS	-	expression tag	UNP Q9SU50
C	63	MET	-	initiating methionine	UNP Q9SU50

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Chain	Residue	Modelled	Actual	Comment	Reference
C	380	ALA	ASP	engineered mutation	UNP Q9SU50
C	627	LEU	-	expression tag	UNP Q9SU50
C	628	GLU	-	expression tag	UNP Q9SU50
C	629	HIS	-	expression tag	UNP Q9SU50
C	630	HIS	-	expression tag	UNP Q9SU50
C	631	HIS	-	expression tag	UNP Q9SU50
C	632	HIS	-	expression tag	UNP Q9SU50
C	633	HIS	-	expression tag	UNP Q9SU50
C	634	HIS	-	expression tag	UNP Q9SU50
D	63	MET	-	initiating methionine	UNP Q9SU50
D	380	ALA	ASP	engineered mutation	UNP Q9SU50
D	627	LEU	-	expression tag	UNP Q9SU50
D	628	GLU	-	expression tag	UNP Q9SU50
D	629	HIS	-	expression tag	UNP Q9SU50
D	630	HIS	-	expression tag	UNP Q9SU50
D	631	HIS	-	expression tag	UNP Q9SU50
D	632	HIS	-	expression tag	UNP Q9SU50
D	633	HIS	-	expression tag	UNP Q9SU50
D	634	HIS	-	expression tag	UNP Q9SU50

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

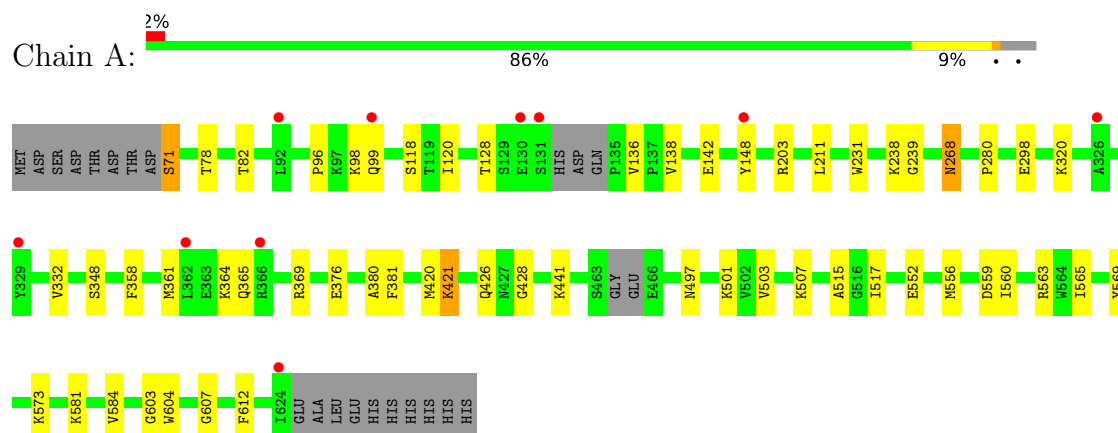
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	319	Total O 319 319	0	0
3	B	259	Total O 259 259	0	0
3	C	212	Total O 212 212	0	0
3	D	168	Total O 168 168	0	0

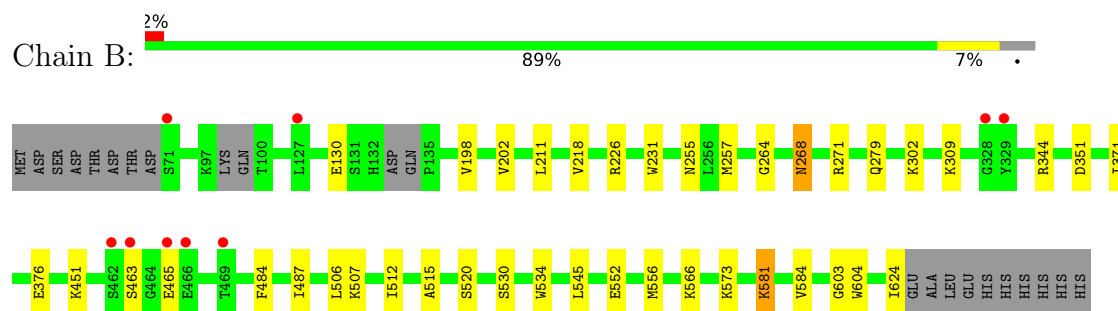
### 3 Residue-property plots [i](#)

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.

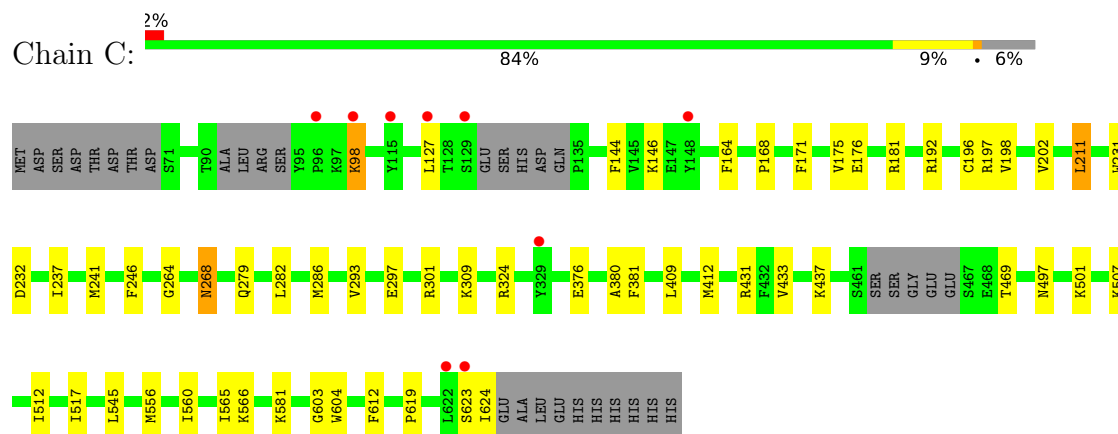
#### • Molecule 1: Trehalase



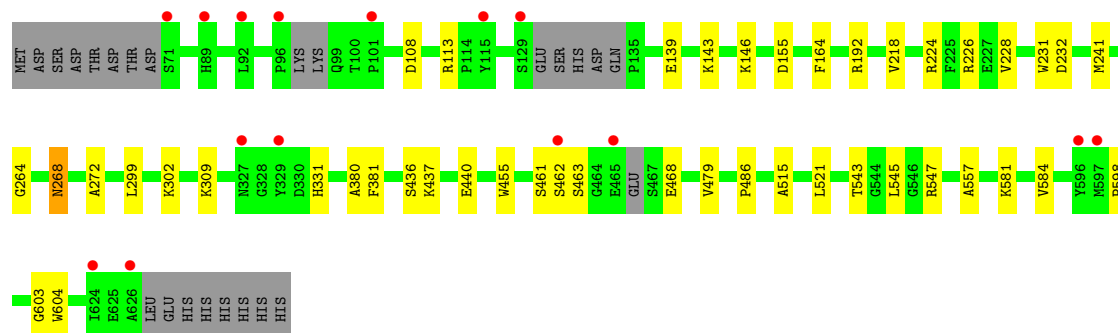
#### • Molecule 1: Trehalase



#### • Molecule 1: Trehalase



Chain D:  3% 88% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.66Å 129.65Å 151.14Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	41.55 – 1.88 49.20 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.55-1.88) 99.8 (49.20-1.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.193 , 0.245 0.194 , 0.245	Depositor DCC
$R_{free}$ test set	2000 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: 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	0.40	0/4507	0.54	0/6117
1	B	0.40	0/4513	0.54	0/6126
1	C	0.37	0/4440	0.52	0/6026
1	D	0.36	0/4491	0.50	0/6096
All	All	0.38	0/17951	0.53	0/24365

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	4393	0	4279	28	0
1	B	4398	0	4274	25	0
1	C	4327	0	4217	29	0
1	D	4378	0	4255	27	0
2	A	12	0	16	0	0
2	B	12	0	16	0	0
2	C	12	0	16	2	0
2	D	12	0	16	3	0
3	A	319	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	259	0	0	1	0
3	C	212	0	0	1	0
3	D	168	0	0	5	0
All	All	18502	0	17089	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (112) 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:B:506:LEU:HG	1:B:512:ILE:HD11	1.67	0.76
2:D:702:GOL:H32	3:D:955:HOH:O	1.85	0.75
1:A:71:SER:HB3	1:A:369:ARG:HH21	1.51	0.75
1:B:344:ARG:HD3	1:B:351:ASP:OD2	1.89	0.73
1:D:108:ASP:OD2	1:D:226:ARG:NH1	2.24	0.70
1:B:451:LYS:NZ	3:B:801:HOH:O	2.23	0.70
1:D:299:LEU:HA	1:D:302:LYS:HE2	1.73	0.70
1:D:218:VAL:HB	1:D:228:VAL:HG11	1.75	0.69
1:B:451:LYS:HE2	1:B:451:LYS:H	1.58	0.68
1:C:566:LYS:HE2	1:C:624:ILE:HG23	1.76	0.67
1:D:232:ASP:HB3	2:D:702:GOL:H11	1.79	0.64
1:A:507:LYS:NZ	1:A:552:GLU:OE2	2.25	0.62
1:A:507:LYS:HE3	1:A:556:MET:HE2	1.81	0.61
1:A:503:VAL:HG13	1:A:556:MET:HE1	1.83	0.60
1:B:264:GLY:HA2	1:B:309:LYS:HE3	1.83	0.59
1:C:565:ILE:HD11	1:C:612:PHE:HB3	1.86	0.58
1:C:324:ARG:HB3	1:C:469:THR:HG22	1.85	0.58
1:C:98:LYS:HD2	1:C:98:LYS:H	1.70	0.57
1:C:168:PRO:HB2	1:C:171:PHE:HB2	1.87	0.57
1:D:437:LYS:NZ	3:D:807:HOH:O	2.38	0.57
1:A:120:ILE:HG12	1:A:148:TYR:HB3	1.86	0.57
1:B:451:LYS:H	1:B:451:LYS:CE	2.19	0.56
2:C:702:GOL:H31	3:C:833:HOH:O	2.05	0.56
1:D:299:LEU:HA	1:D:302:LYS:CE	2.35	0.55
1:C:198:VAL:HG13	1:C:202:VAL:HB	1.87	0.55
1:D:515:ALA:HB3	1:D:584:VAL:HA	1.87	0.55
1:B:515:ALA:HB3	1:B:584:VAL:HA	1.88	0.55
1:C:433:VAL:O	1:C:437:LYS:HG3	2.07	0.54
1:A:515:ALA:HB3	1:A:584:VAL:HA	1.90	0.54
1:A:503:VAL:HG13	1:A:556:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:TYR:CE2	1:A:573:LYS:HD2	2.43	0.53
1:A:420:MET:SD	1:A:428:GLY:HA3	2.49	0.52
1:D:331:HIS:ND1	3:D:805:HOH:O	2.33	0.52
1:C:198:VAL:HG22	1:C:211:LEU:HD13	1.92	0.51
1:C:237:ILE:O	1:C:241:MET:HG3	2.10	0.51
2:D:702:GOL:H2	3:D:814:HOH:O	2.10	0.51
1:A:298:GLU:HG2	3:A:1097:HOH:O	2.09	0.51
1:B:198:VAL:HG13	1:B:202:VAL:HB	1.93	0.51
1:A:268:ASN:C	1:A:268:ASN:HD22	2.15	0.50
1:C:433:VAL:HG12	1:C:437:LYS:HE2	1.93	0.50
1:D:139:GLU:OE2	1:D:139:GLU:N	2.31	0.50
1:C:176:GLU:HB2	1:C:619:PRO:HA	1.94	0.50
1:B:257:MET:HE1	1:B:302:LYS:HB3	1.94	0.50
1:C:517:ILE:HD11	1:C:560:ILE:HD13	1.94	0.50
1:B:507:LYS:HE3	1:B:552:GLU:OE2	2.12	0.49
1:A:421:LYS:HE3	1:A:426:GLN:OE1	2.12	0.49
1:C:268:ASN:HD22	1:C:268:ASN:C	2.17	0.48
1:C:566:LYS:HG3	1:C:624:ILE:HG23	1.95	0.47
1:D:545:LEU:HB2	1:D:557:ALA:HB2	1.96	0.47
1:A:565:ILE:HD11	1:A:612:PHE:HB3	1.95	0.47
1:B:268:ASN:C	1:B:268:ASN:HD22	2.18	0.47
1:D:268:ASN:C	1:D:268:ASN:HD22	2.18	0.47
1:B:520:SER:O	1:B:530:SER:HB2	2.14	0.47
1:C:127:LEU:HD12	1:C:144:PHE:CD1	2.50	0.47
1:B:344:ARG:HD2	1:B:371:ILE:HG22	1.96	0.46
1:A:96:PRO:HB2	1:A:98:LYS:HG2	1.96	0.46
1:B:302:LYS:HB3	1:B:302:LYS:HE2	1.68	0.46
1:C:232:ASP:OD2	2:C:702:GOL:H32	2.15	0.46
1:D:264:GLY:HA2	1:D:309:LYS:HE3	1.98	0.46
1:A:98:LYS:HG3	1:A:99:GLN:HG2	1.97	0.46
1:A:517:ILE:HD11	1:A:560:ILE:HD13	1.97	0.46
1:C:175:VAL:HB	1:C:181:ARG:HG3	1.98	0.45
1:C:297:GLU:O	1:C:301:ARG:HG3	2.15	0.45
1:D:380:ALA:HA	1:D:381:PHE:HA	1.70	0.45
1:A:380:ALA:HA	1:A:381:PHE:HA	1.73	0.45
1:C:409:LEU:HD23	1:C:412:MET:HE3	1.97	0.45
1:D:164:PHE:CE2	1:D:192:ARG:HD2	2.51	0.45
1:D:224:ARG:NH1	1:D:598:PRO:O	2.50	0.45
1:C:380:ALA:HA	1:C:381:PHE:HA	1.78	0.45
1:C:545:LEU:HD13	1:C:556:MET:HE3	1.99	0.45
1:D:455:TRP:CD2	1:D:486:PRO:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:O	1:A:82:THR:HG23	2.17	0.45
1:A:358:PHE:O	1:A:364:LYS:NZ	2.49	0.44
1:D:479:VAL:HB	1:D:521:LEU:HD12	1.98	0.44
1:A:497:ASN:O	1:A:501:LYS:HG3	2.17	0.44
1:B:198:VAL:CG1	1:B:202:VAL:HB	2.48	0.44
1:C:282:LEU:O	1:C:286:MET:HG3	2.18	0.44
1:D:146:LYS:HD3	1:D:146:LYS:HA	1.66	0.44
1:A:559:ASP:OD2	1:A:563:ARG:NH2	2.46	0.43
1:A:138:VAL:O	1:A:142:GLU:HG3	2.19	0.43
1:B:226:ARG:HG3	1:B:271:ARG:HH21	1.83	0.43
1:C:246:PHE:CZ	1:C:293:VAL:HG11	2.54	0.43
1:C:497:ASN:O	1:C:501:LYS:HG3	2.18	0.43
1:D:241:MET:HA	1:D:241:MET:HE2	2.00	0.43
1:D:143:LYS:HD2	1:D:143:LYS:HA	1.90	0.43
1:D:461:SER:H	1:D:468:GLU:CD	2.23	0.43
1:B:279:GLN:HA	1:B:376:GLU:O	2.19	0.43
1:B:566:LYS:HA	1:B:624:ILE:HD11	2.00	0.42
1:A:361:MET:O	1:A:365:GLN:HG3	2.19	0.42
1:A:280:PRO:HD3	1:A:376:GLU:O	2.18	0.42
1:B:218:VAL:HG12	1:B:255:ASN:ND2	2.35	0.42
1:B:463:SER:OG	1:B:465:GLU:HG3	2.20	0.42
1:D:436:SER:O	1:D:440:GLU:HG3	2.18	0.42
1:C:164:PHE:CE2	1:C:192:ARG:HD2	2.54	0.42
1:B:484:PHE:O	1:B:487:ILE:HG22	2.20	0.42
1:D:543:THR:O	1:D:547:ARG:HG3	2.19	0.42
1:A:320:LYS:HE3	1:A:332:VAL:HG13	2.03	0.41
1:D:272:ALA:HB2	3:D:921:HOH:O	2.19	0.41
1:C:198:VAL:CG1	1:C:202:VAL:HB	2.51	0.41
1:C:279:GLN:HA	1:C:376:GLU:O	2.21	0.41
1:A:239:GLY:HA3	1:A:607:GLY:HA2	2.02	0.41
1:B:573:LYS:HD3	1:B:573:LYS:HA	1.89	0.41
1:C:264:GLY:HA2	1:C:309:LYS:HE2	2.01	0.41
1:D:462:SER:OG	1:D:463:SER:N	2.51	0.41
1:B:130:GLU:H	1:B:130:GLU:HG2	1.64	0.40
1:A:238:LYS:HD2	1:A:238:LYS:HA	1.90	0.40
1:B:534:TRP:CH2	1:B:581:LYS:HD2	2.56	0.40
1:A:128:THR:HG22	1:A:136:VAL:HG21	2.03	0.40
1:C:507:LYS:HA	1:C:512:ILE:HD12	2.04	0.40
1:D:299:LEU:CA	1:D:302:LYS:HE2	2.47	0.40
1:B:545:LEU:CD1	1:B:556:MET:HE3	2.52	0.40
1:D:155:ASP:OD1	1:D:155:ASP:N	2.52	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	543/572 (95%)	525 (97%)	17 (3%)	1 (0%)	47	37
1	B	544/572 (95%)	524 (96%)	19 (4%)	1 (0%)	47	37
1	C	532/572 (93%)	515 (97%)	16 (3%)	1 (0%)	47	37
1	D	540/572 (94%)	524 (97%)	15 (3%)	1 (0%)	47	37
All	All	2159/2288 (94%)	2088 (97%)	67 (3%)	4 (0%)	47	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	603	GLY
1	D	603	GLY
1	C	603	GLY
1	B	603	GLY

### 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	481/502 (96%)	470 (98%)	11 (2%)	50	41
1	B	481/502 (96%)	476 (99%)	5 (1%)	76	73
1	C	473/502 (94%)	462 (98%)	11 (2%)	50	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	478/502 (95%)	473 (99%)	5 (1%)	76	73
All	All	1913/2008 (95%)	1881 (98%)	32 (2%)	60	54

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	118	SER
1	A	203	ARG
1	A	211	LEU
1	A	231	TRP
1	A	268	ASN
1	A	348	SER
1	A	421	LYS
1	A	441	LYS
1	A	581	LYS
1	A	604	TRP
1	B	211	LEU
1	B	231	TRP
1	B	268	ASN
1	B	581	LYS
1	B	604	TRP
1	C	98	LYS
1	C	146	LYS
1	C	196	CYS
1	C	197	ARG
1	C	211	LEU
1	C	231	TRP
1	C	268	ASN
1	C	431	ARG
1	C	581	LYS
1	C	604	TRP
1	C	623	SER
1	D	113	ARG
1	D	231	TRP
1	D	268	ASN
1	D	581	LYS
1	D	604	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	ASN
1	D	474	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 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	GOL	D	702	-	5,5,5	0.97	0	5,5,5	1.24	0
2	GOL	C	702	-	5,5,5	0.78	0	5,5,5	1.34	1 (20%)
2	GOL	B	702	-	5,5,5	1.12	0	5,5,5	0.64	0
2	GOL	D	701	-	5,5,5	0.88	0	5,5,5	1.08	0
2	GOL	A	701	-	5,5,5	1.05	0	5,5,5	0.86	0
2	GOL	B	701	-	5,5,5	1.38	1 (20%)	5,5,5	1.13	0
2	GOL	C	701	-	5,5,5	0.64	0	5,5,5	0.72	0
2	GOL	A	702	-	5,5,5	0.83	0	5,5,5	0.81	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	GOL	D	702	-	-	1/4/4/4	-
2	GOL	C	702	-	-	0/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	D	701	-	-	2/4/4/4	-
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	B	701	-	-	4/4/4/4	-
2	GOL	C	701	-	-	2/4/4/4	-
2	GOL	A	702	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GOL	C3-C2	2.24	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	GOL	C3-C2-C1	-2.21	103.11	111.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	GOL	C1-C2-C3-O3
2	C	701	GOL	O1-C1-C2-C3
2	D	701	GOL	C1-C2-C3-O3
2	A	702	GOL	O1-C1-C2-O2
2	C	701	GOL	O1-C1-C2-O2
2	A	702	GOL	O1-C1-C2-C3
2	B	701	GOL	O1-C1-C2-C3
2	B	702	GOL	O1-C1-C2-C3
2	B	701	GOL	O2-C2-C3-O3
2	D	701	GOL	O2-C2-C3-O3
2	B	701	GOL	O1-C1-C2-O2
2	B	702	GOL	O1-C1-C2-O2
2	D	702	GOL	C1-C2-C3-O3

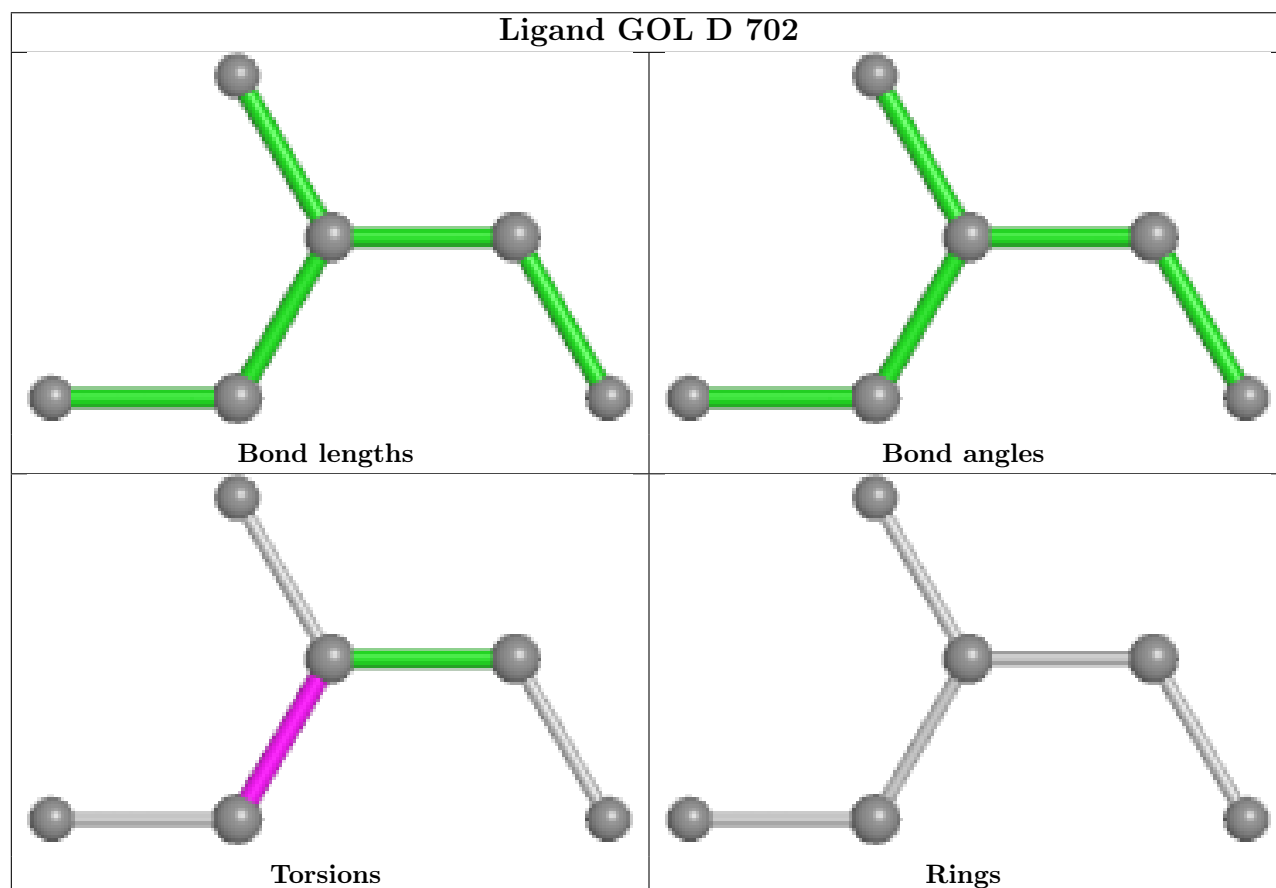
There are no ring outliers.

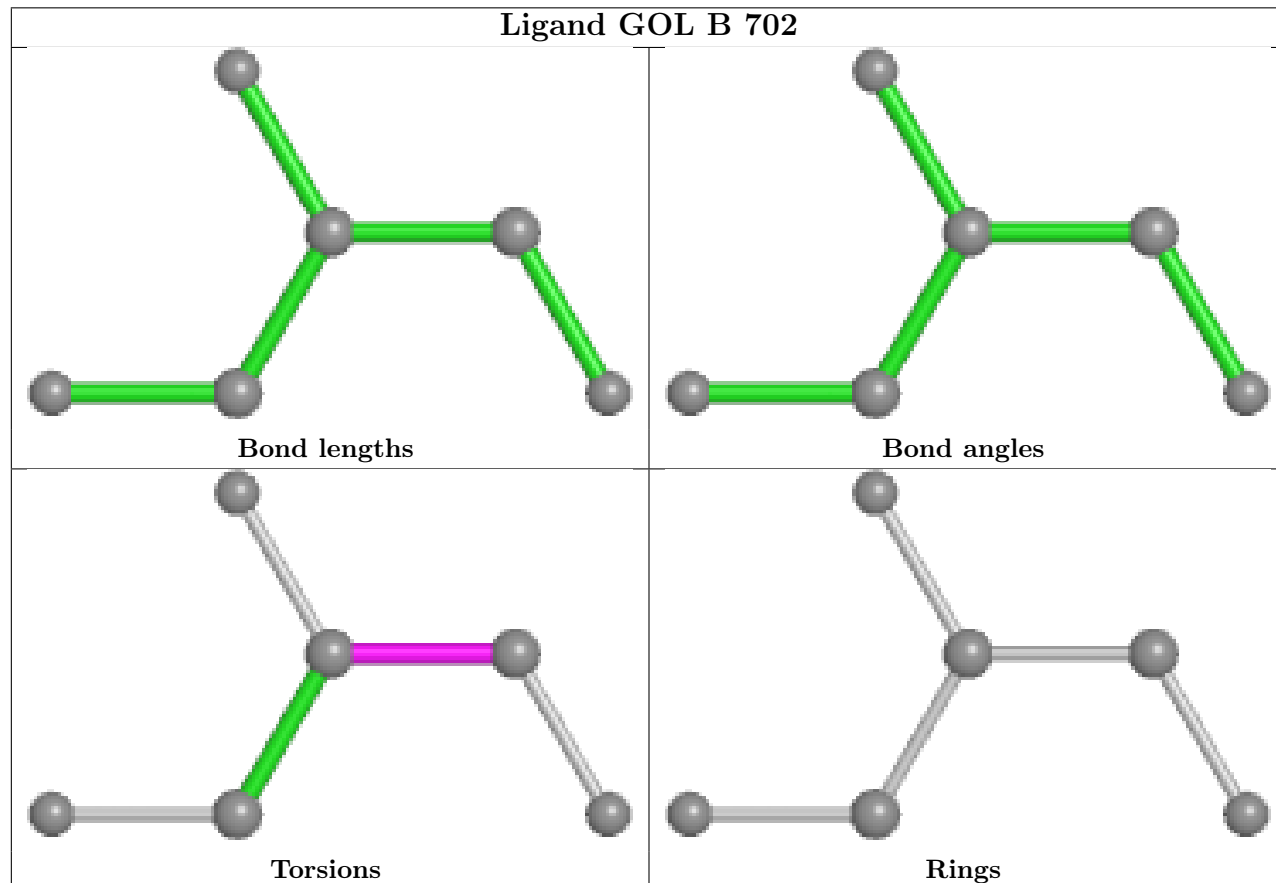
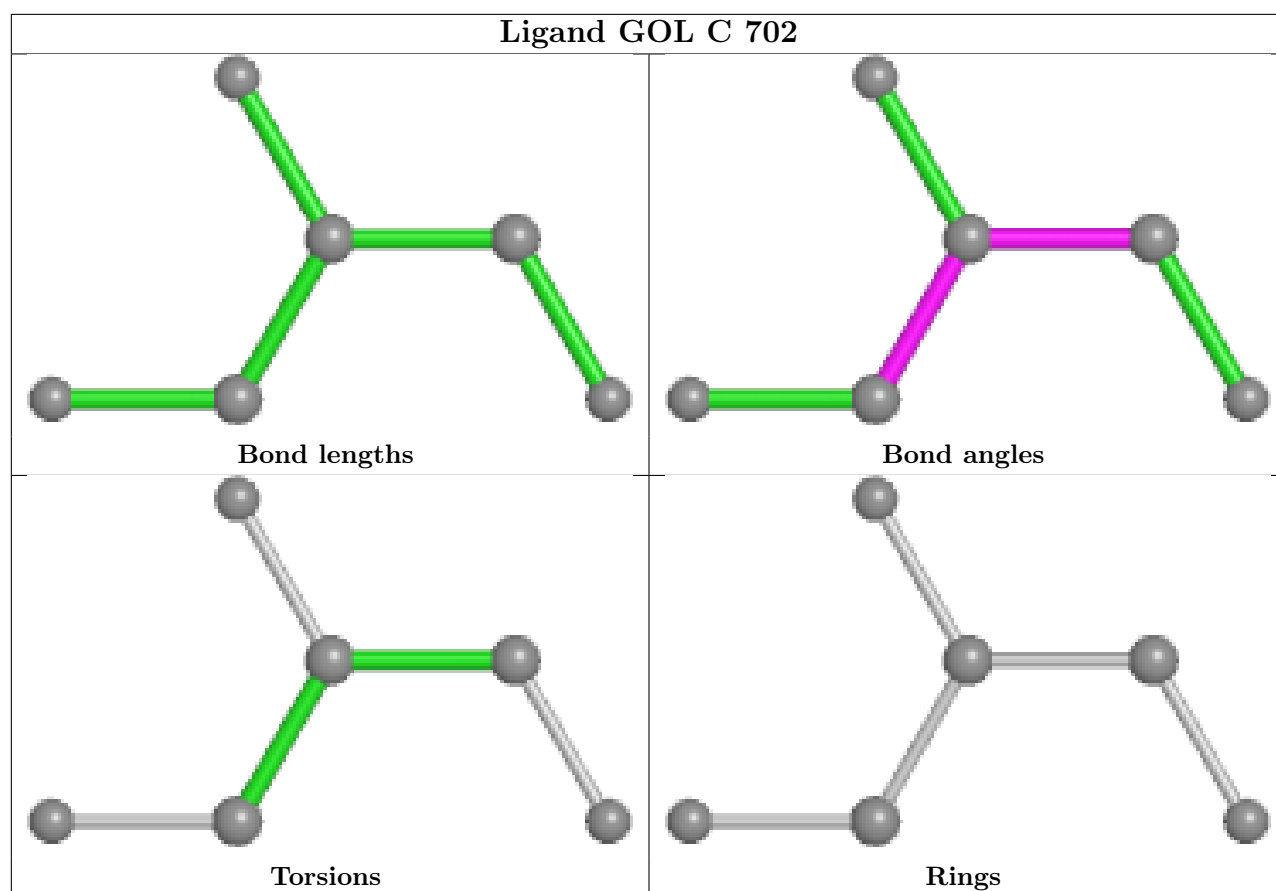
2 monomers are involved in 5 short contacts:

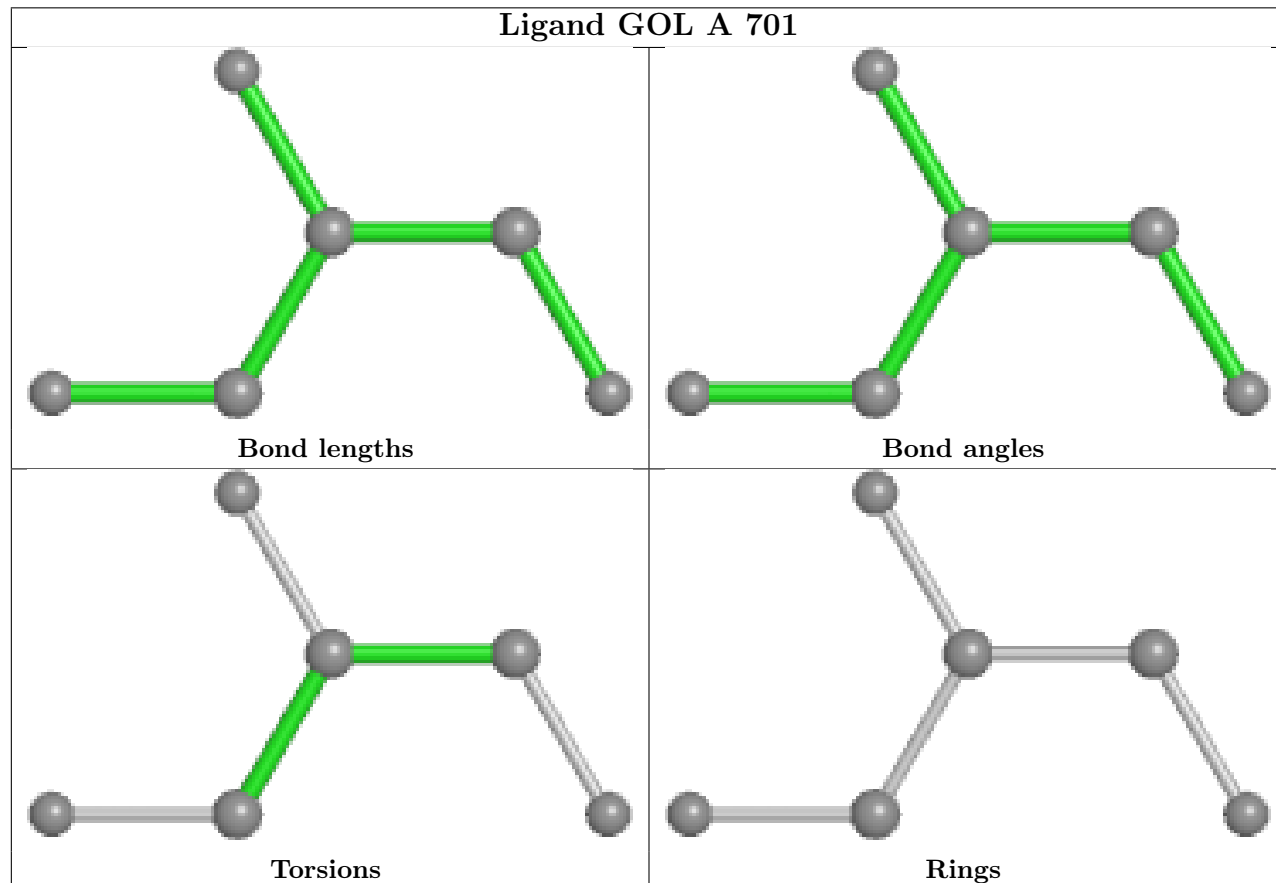
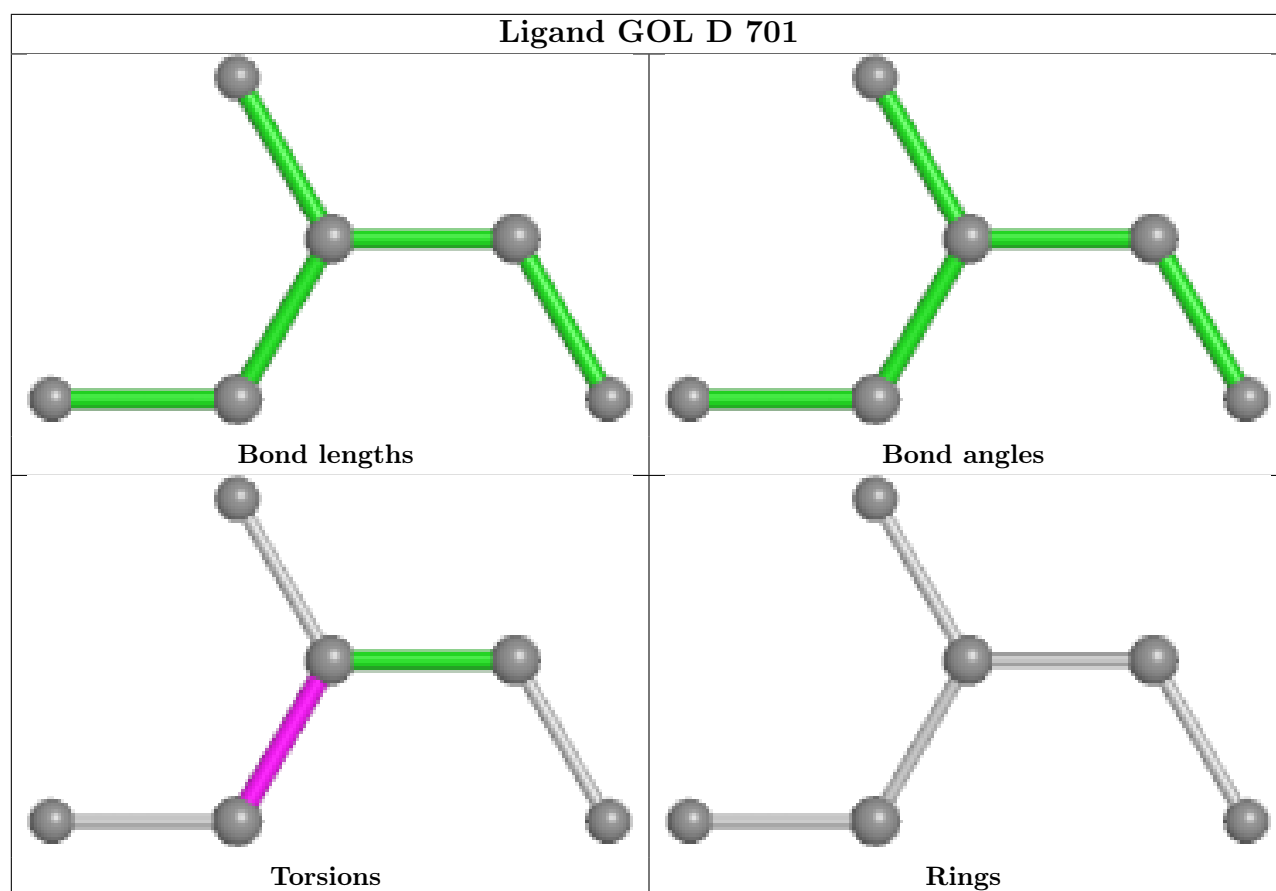


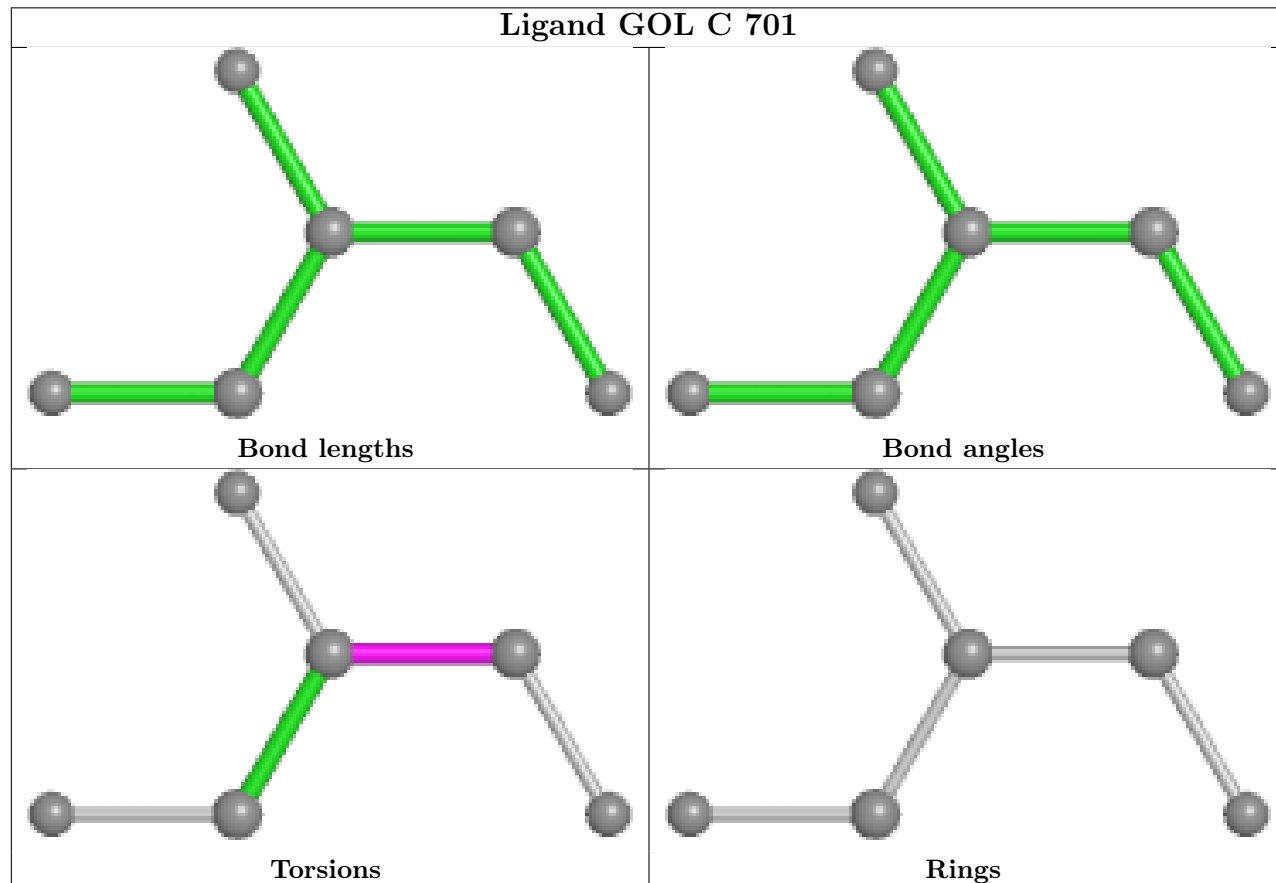
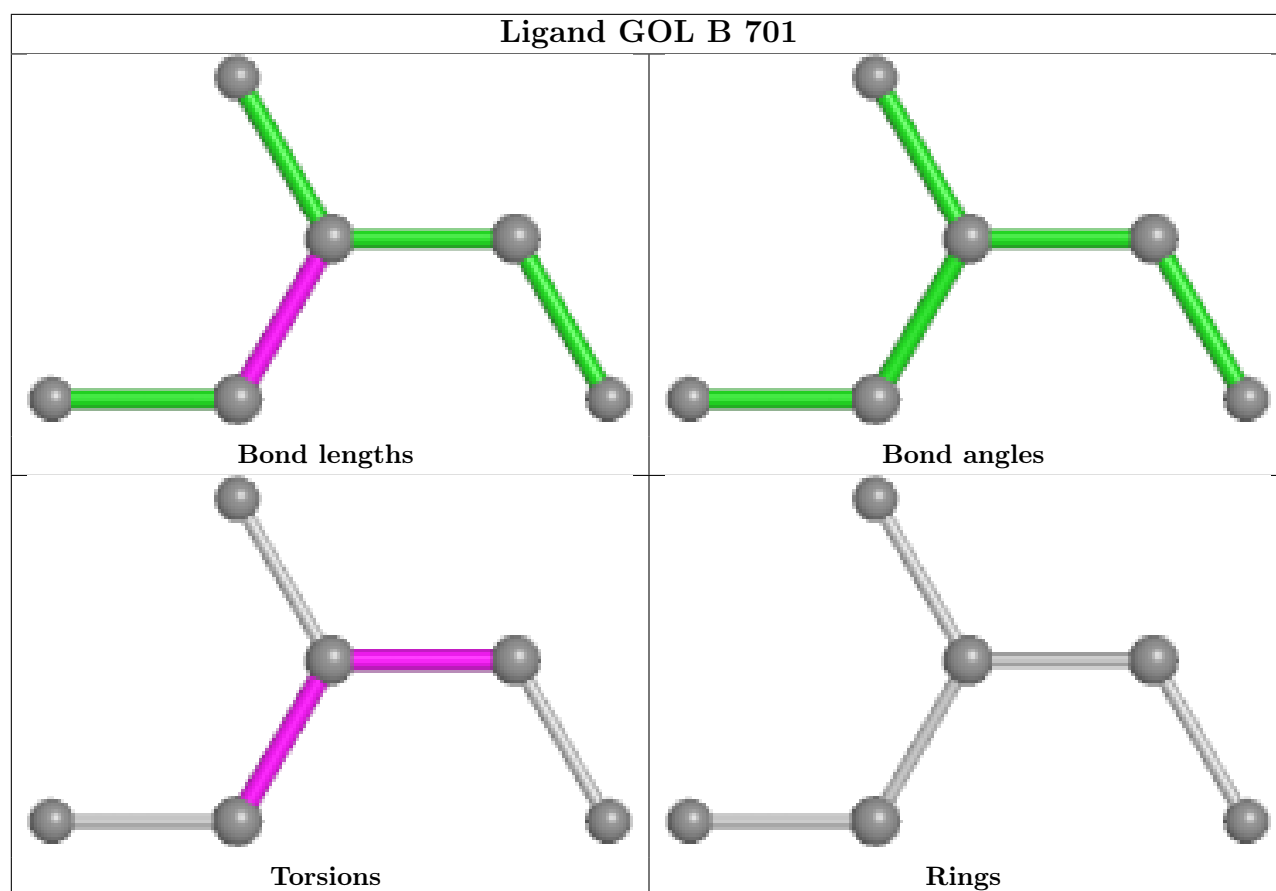
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	GOL	3	0
2	C	702	GOL	2	0

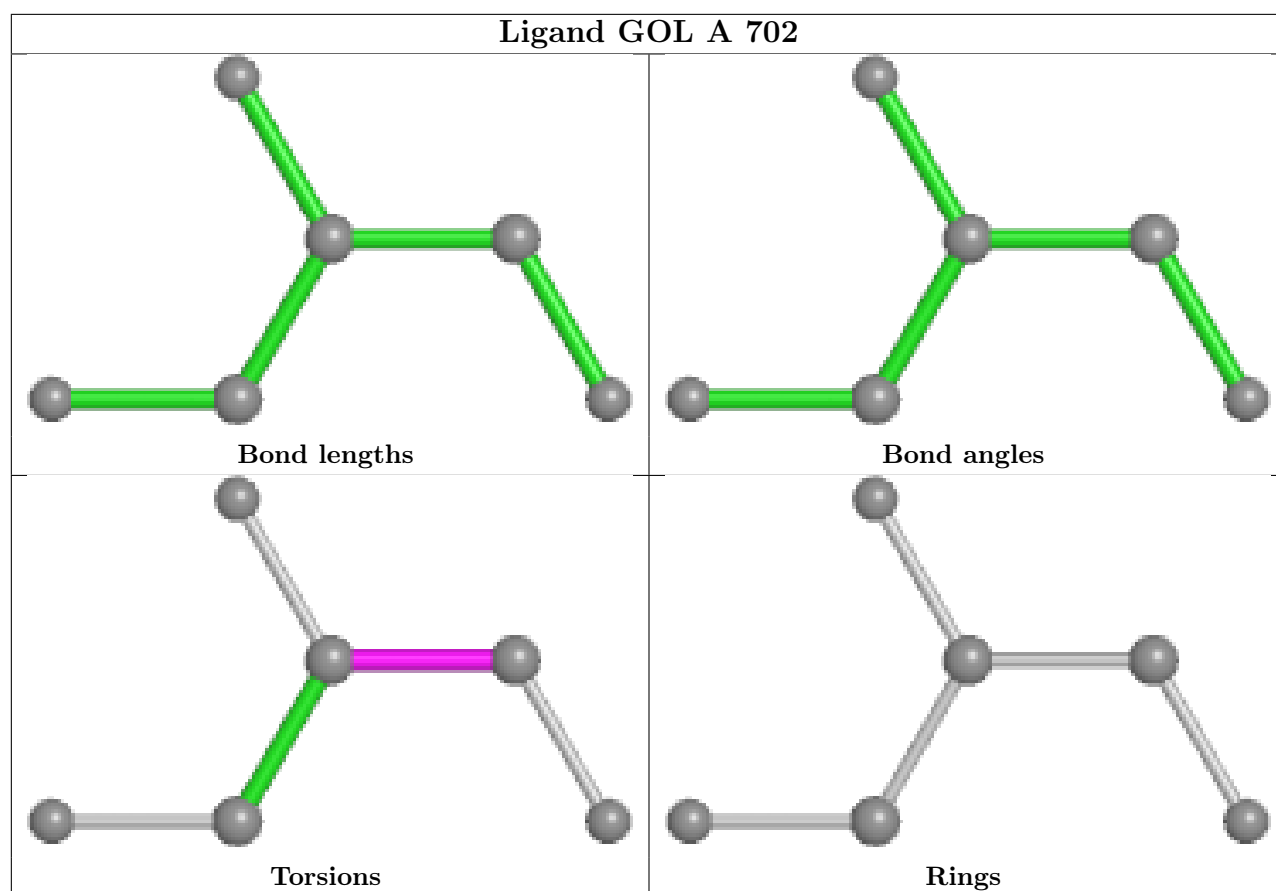
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	549/572 (95%)	-0.03	10 (1%) 68 70	21, 30, 52, 73	0
1	B	550/572 (96%)	-0.01	9 (1%) 72 74	21, 32, 49, 65	0
1	C	540/572 (94%)	0.04	9 (1%) 70 72	24, 34, 53, 75	0
1	D	548/572 (95%)	0.15	15 (2%) 54 56	24, 37, 56, 67	0
All	All	2187/2288 (95%)	0.04	43 (1%) 65 67	21, 33, 53, 75	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	4.8
1	D	329	TYR	4.1
1	B	71	SER	4.0
1	D	462	SER	3.7
1	B	329	TYR	3.7
1	D	596	TYR	3.7
1	D	129	SER	3.3
1	D	71	SER	3.2
1	B	466	GLU	3.2
1	C	148	TYR	3.2
1	A	624	ILE	3.1
1	C	98	LYS	3.1
1	C	115	TYR	3.0
1	A	99	GLN	3.0
1	C	622	LEU	2.9
1	C	127	LEU	2.9
1	D	626	ALA	2.9
1	B	463	SER	2.9
1	A	326	ALA	2.9
1	D	465	GLU	2.8
1	C	329	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	328	GLY	2.7
1	B	462	SER	2.6
1	A	130	GLU	2.5
1	D	92	LEU	2.5
1	A	131	SER	2.5
1	C	129	SER	2.5
1	A	329	TYR	2.4
1	B	127	LEU	2.4
1	B	465	GLU	2.4
1	D	115	TYR	2.3
1	D	96	PRO	2.3
1	D	597	MET	2.3
1	D	624	ILE	2.2
1	A	148	TYR	2.1
1	B	469	THR	2.1
1	C	96	PRO	2.1
1	A	362	LEU	2.1
1	D	89	HIS	2.0
1	D	101	PRO	2.0
1	A	366	ARG	2.0
1	D	327	ASN	2.0
1	C	623	SER	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 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, 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.

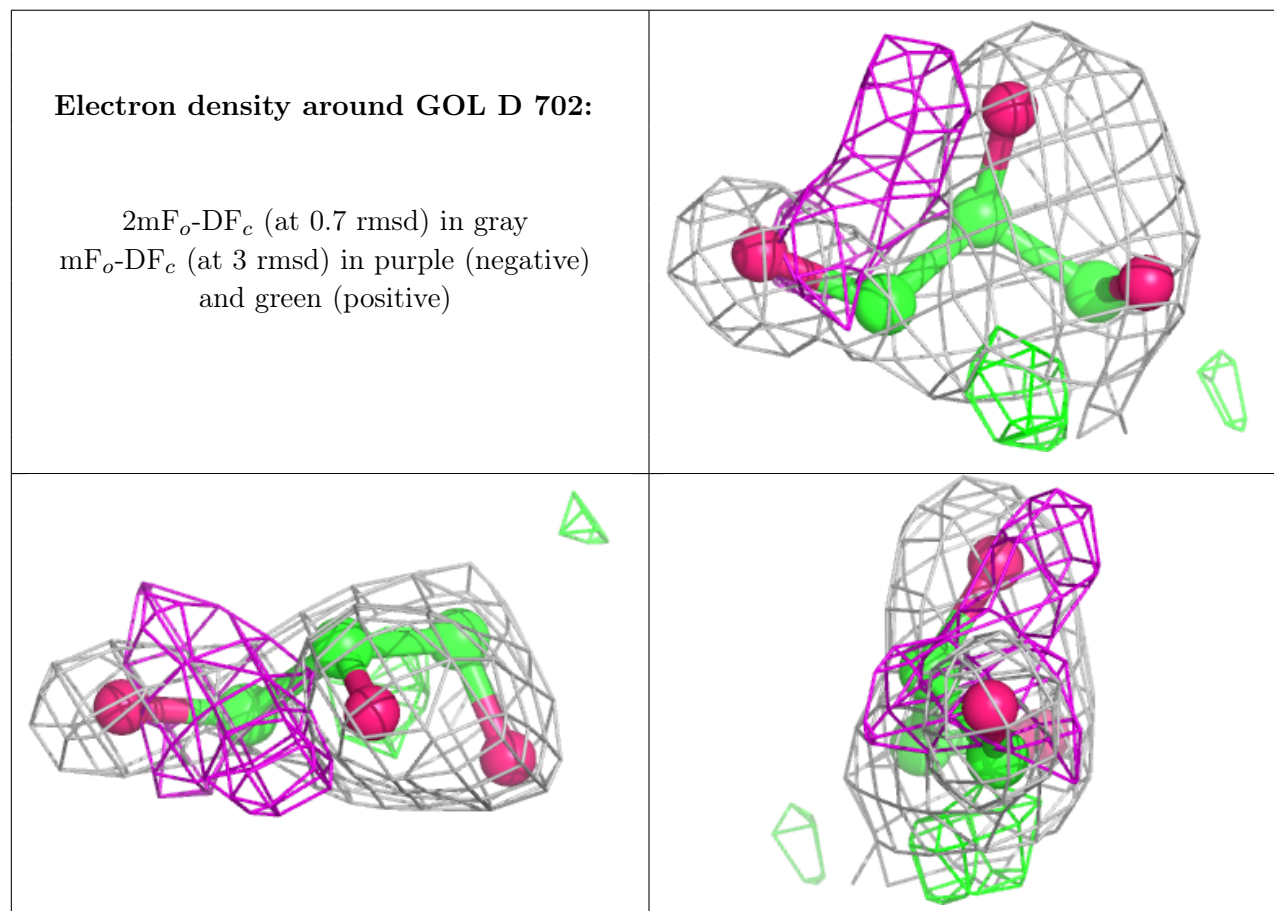
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	D	702	6/6	0.74	0.27	31,38,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	701	6/6	0.76	0.21	28,32,34,38	0
2	GOL	D	701	6/6	0.84	0.17	33,37,39,42	0
2	GOL	C	702	6/6	0.87	0.19	28,31,37,38	0
2	GOL	B	702	6/6	0.92	0.10	31,34,36,43	0
2	GOL	A	702	6/6	0.93	0.21	31,36,37,44	0
2	GOL	C	701	6/6	0.96	0.13	30,33,37,39	0
2	GOL	A	701	6/6	0.97	0.09	25,25,28,35	0

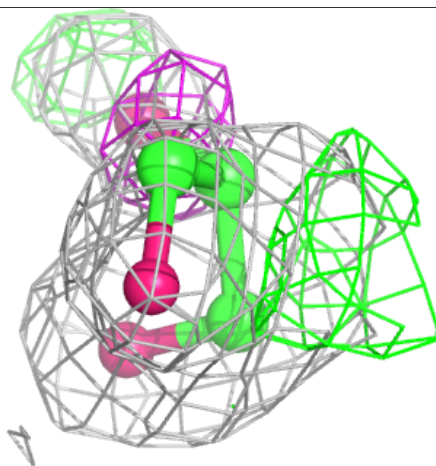
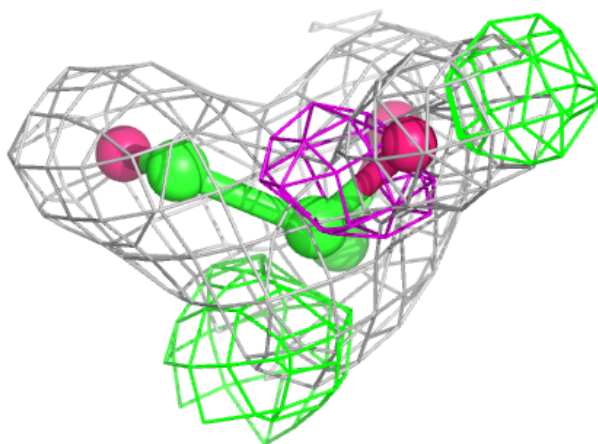
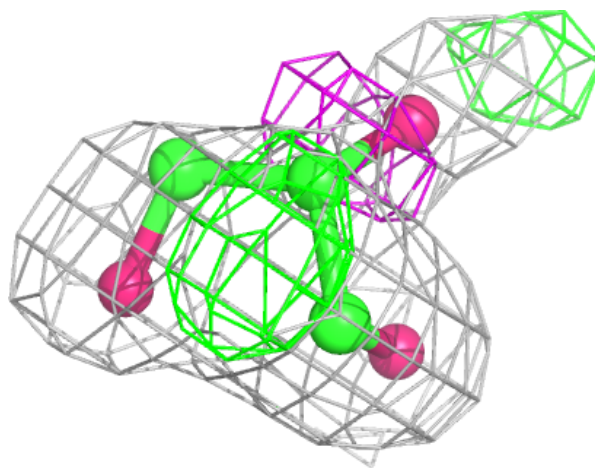
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





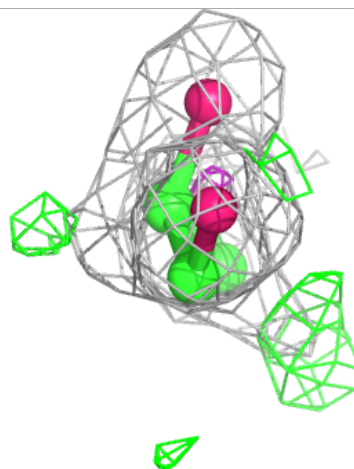
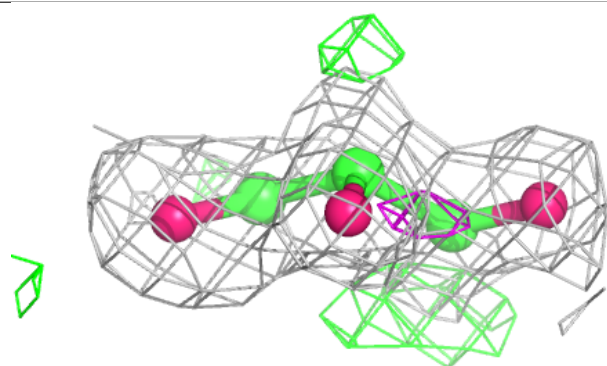
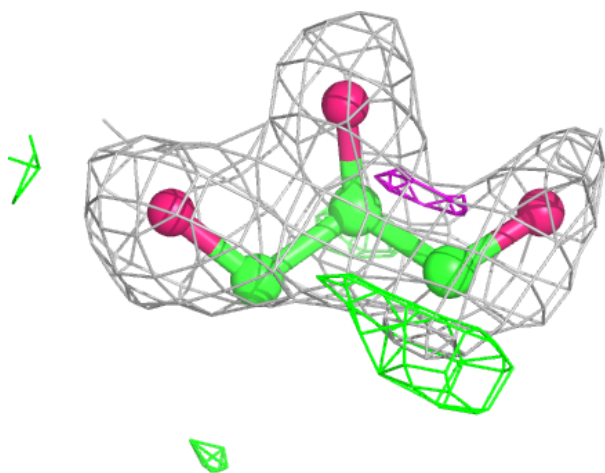
**Electron density around GOL B 701:**

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



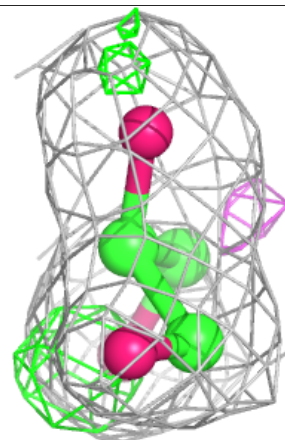
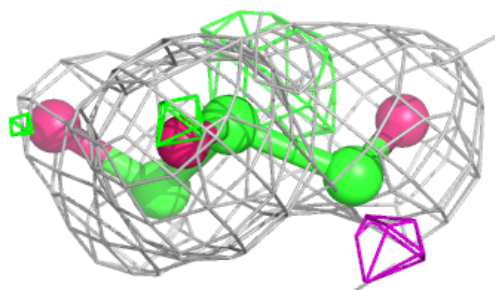
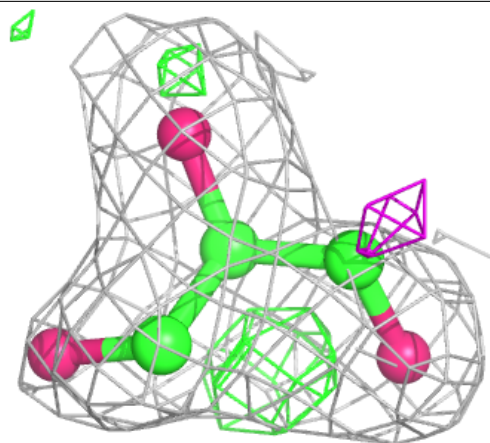
**Electron density around GOL D 701:**

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



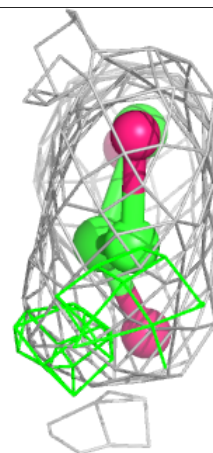
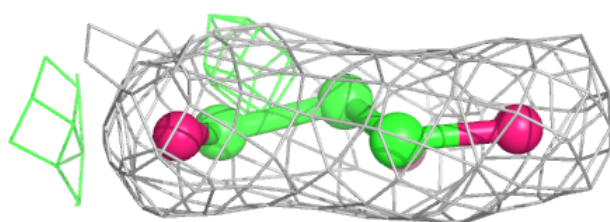
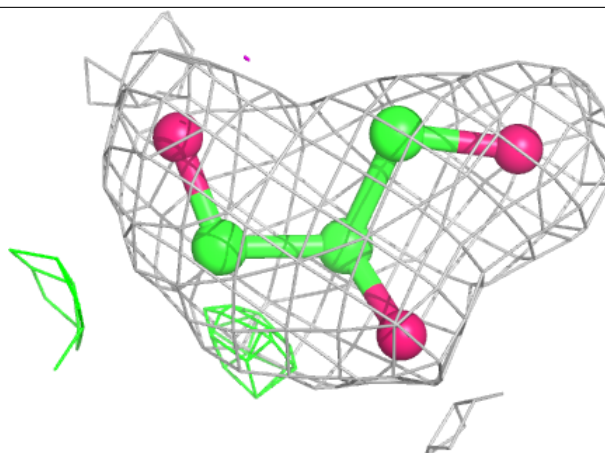
**Electron density around GOL C 702:**

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

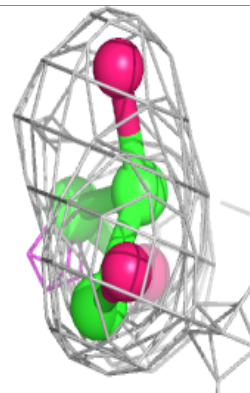
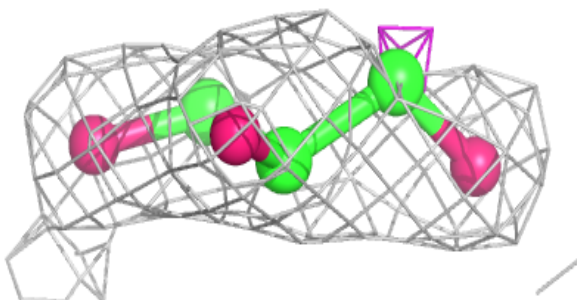
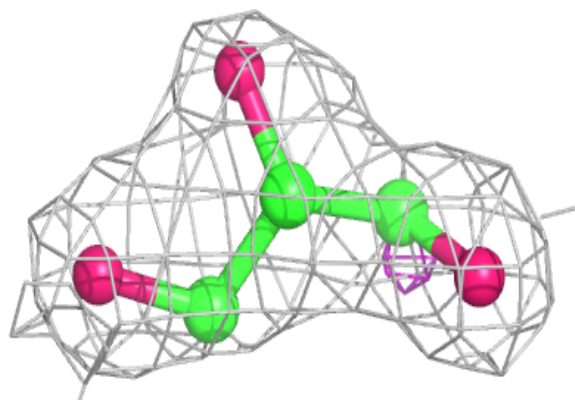


**Electron density around GOL B 702:**

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

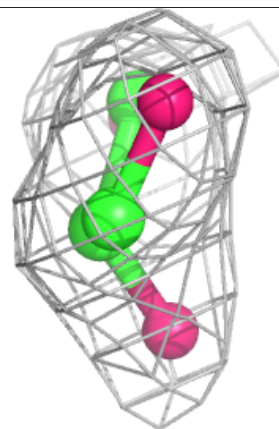
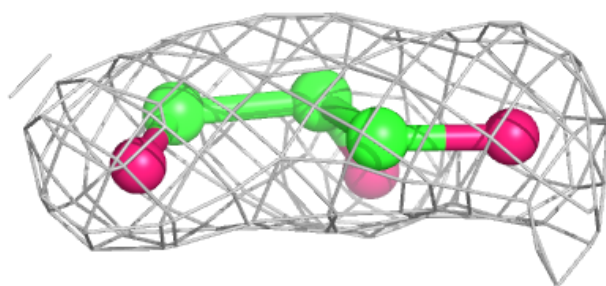
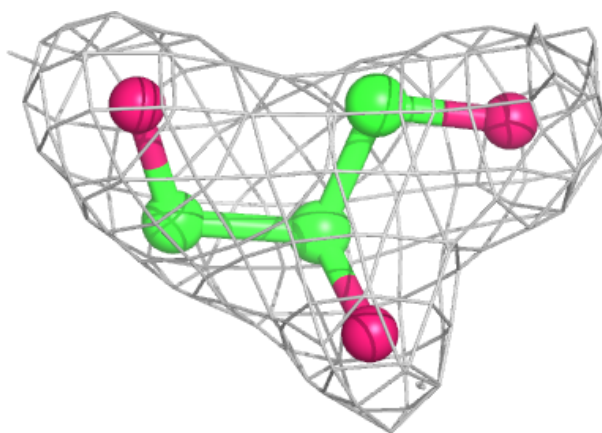
**Electron density around GOL A 702:**

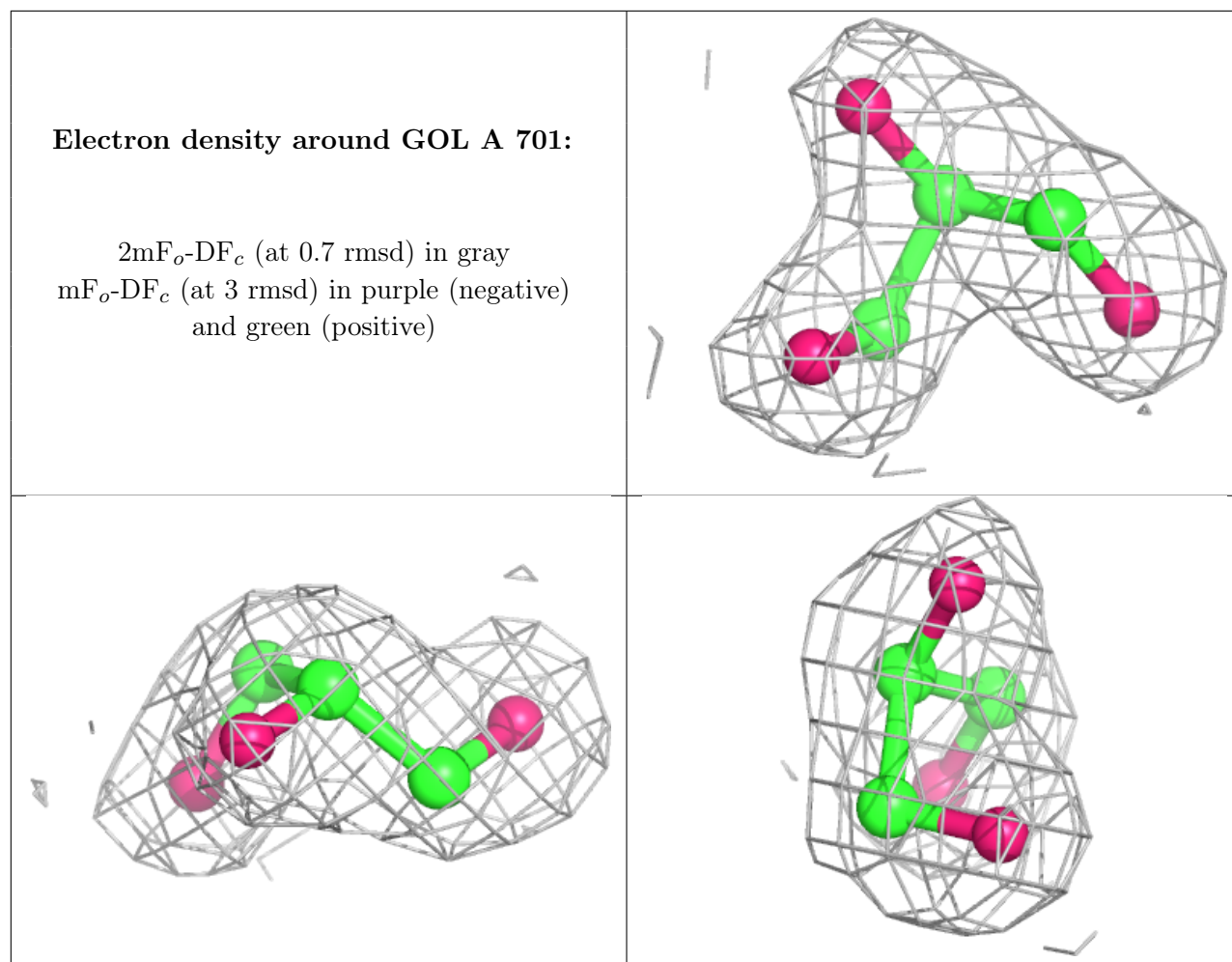
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GOL C 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.