



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2020 – 02:15 PM JST

PDB ID : 6ID4  
Title : Defining the structural basis for human alloantibody binding to human leukocyte antigen allele HLA-A\*11:01  
Authors : Lescar, J.; Wong, Y.H.; Liew, C.W.; Gu, Y.; MacAry, P.A.  
Deposited on : 2018-09-08  
Resolution : 2.40 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:

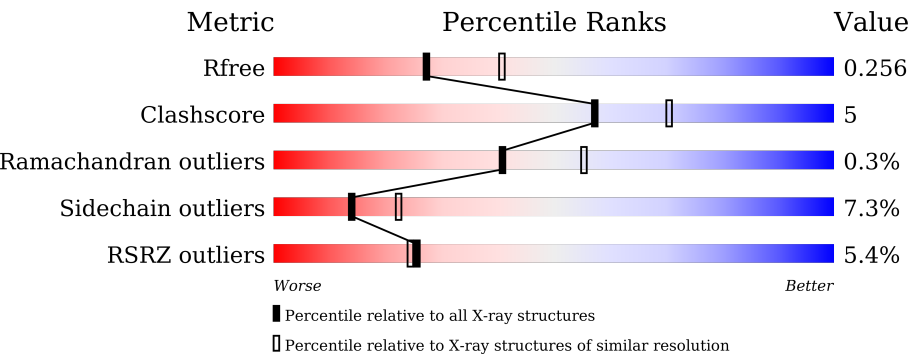
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	276	<div><div>4%</div><div>83%</div><div>15%</div><div>..</div></div>
1	E	276	<div><div>7%</div><div>82%</div><div>17%</div><div>.</div></div>
2	B	100	<div><div>3%</div><div>85%</div><div>13%</div><div>..</div></div>
2	F	100	<div><div>3%</div><div>84%</div><div>14%</div><div>..</div></div>
3	C	222	<div><div>2%</div><div>83%</div><div>12%</div><div>..</div></div>
3	H	222	<div><div>2%</div><div>84%</div><div>12%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
4	D	221	
4	L	221	
5	T	9	
5	U	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	D	601	-	-	X	-
7	PEG	E	401	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13673 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			
1	E	275	Total	C	N	O	S	0	3	0
			2267	1408	415	435	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP F6IQY1
E	0	MET	-	initiating methionine	UNP F6IQY1

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	F	99	Total	C	N	O	S	0	1	0
			837	533	143	158	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1622	1029	269	316	8			
3	H	216	Total	C	N	O	S	0	0	0
			1622	1029	269	316	8			

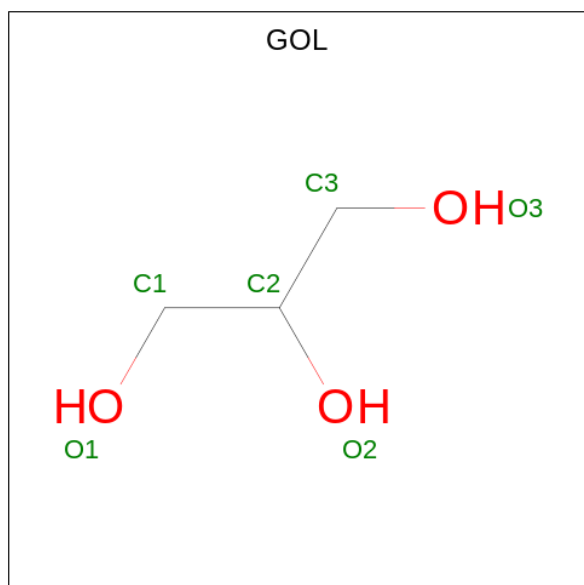
- Molecule 4 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	215	Total	C	N	O	S	0	1	0
			1619	1024	268	321	6			
4	L	216	Total	C	N	O	S	0	5	0
			1634	1034	269	325	6			

- Molecule 5 is a protein called peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	9	Total	C	N	O	S	0	0	0
			70	44	11	14	1			
5	U	9	Total	C	N	O	S	0	0	0
			70	44	11	14	1			

- Molecule 6 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 author).



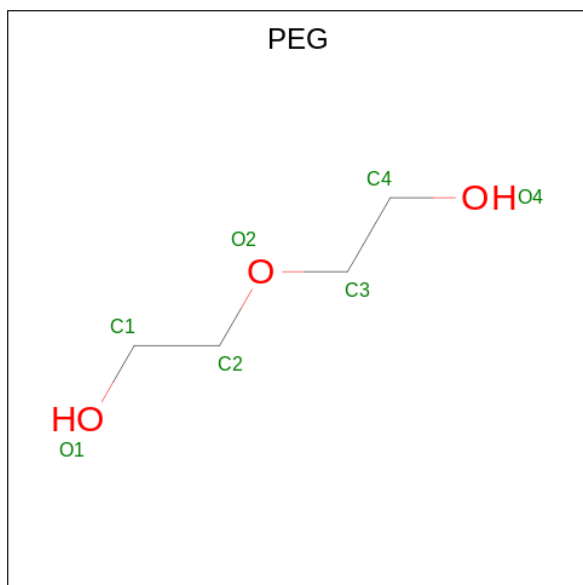
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	185	Total	O	0	0
			185	185		
8	B	70	Total	O	0	0
			70	70		
8	C	84	Total	O	0	0
			84	84		

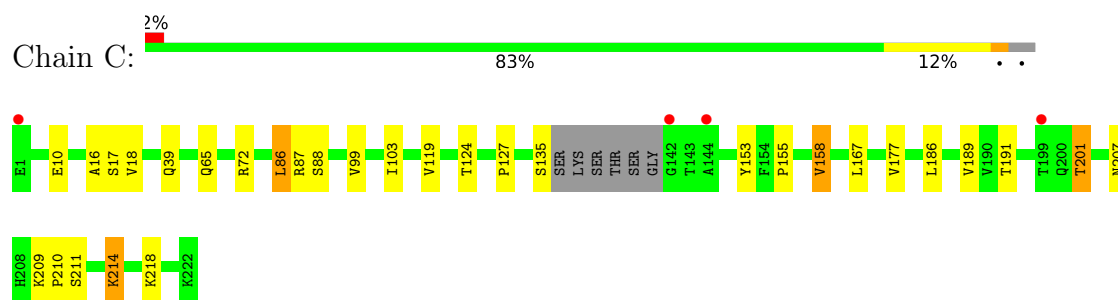
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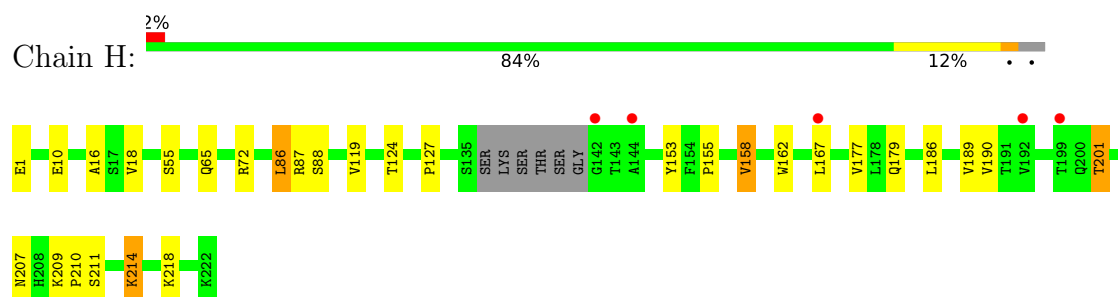
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	73	Total 73	O 73	0	0
8	E	142	Total 142	O 142	0	0
8	F	51	Total 51	O 51	0	0
8	H	98	Total 98	O 98	0	0
8	L	88	Total 88	O 88	0	0
8	T	6	Total 6	O 6	0	0
8	U	6	Total 6	O 6	0	0



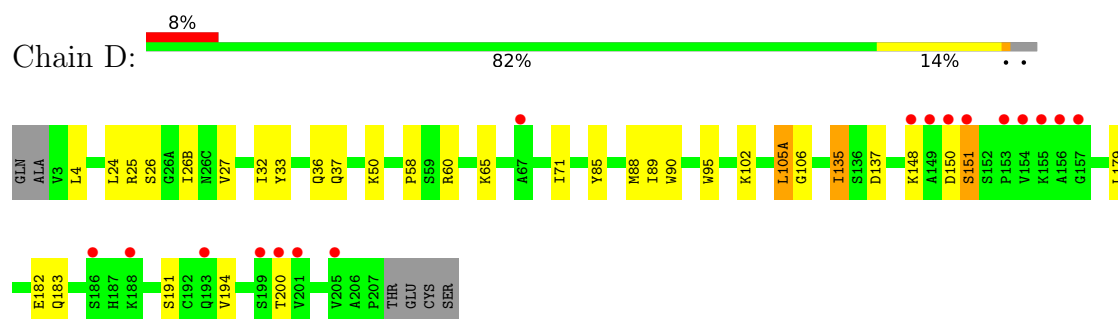




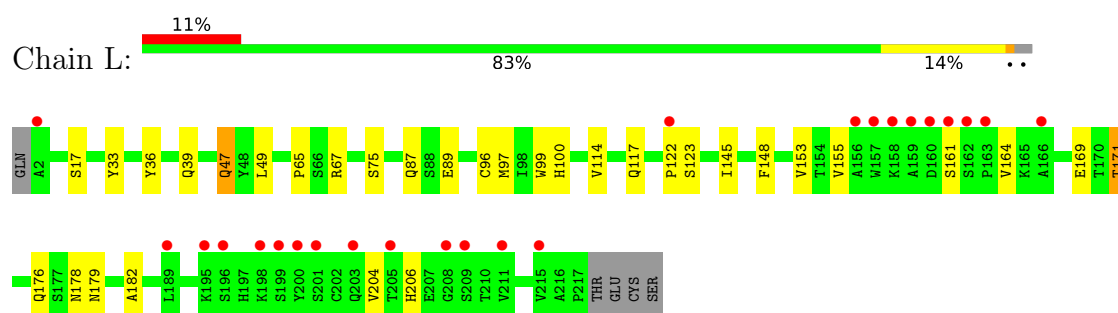
- Molecule 3: Heavy chain



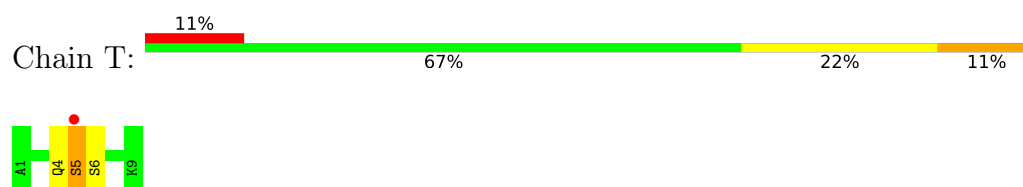
- Molecule 4: Light chain



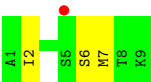
- Molecule 4: Light chain



- Molecule 5: peptide



- Molecule 5: peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.56Å 215.33Å 80.98Å 90.00° 92.96° 90.00°	Depositor
Resolution (Å)	45.78 – 2.40 45.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.78-2.40) 96.5 (45.78-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.197 , 0.246 0.203 , 0.256	Depositor DCC
$R_{free}$ test set	3997 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.004 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.047 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG

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	0.54	0/2296	0.78	0/3117
1	E	0.53	0/2337	0.78	1/3169 (0.0%)
2	B	0.50	0/852	0.78	0/1152
2	F	0.47	0/863	0.77	0/1166
3	C	0.49	0/1663	0.76	0/2269
3	H	0.49	0/1663	0.75	0/2269
4	D	0.48	0/1668	0.72	0/2280
4	L	0.54	0/1699	0.77	0/2322
5	T	0.70	0/70	0.89	0/90
5	U	0.82	0/70	1.04	0/90
All	All	0.51	0/13181	0.77	1/17924 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	100	GLY	C-N-CA	5.49	135.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	101	CYS	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2235	0	2087	24	0
1	E	2267	0	2127	31	0
2	B	829	0	794	8	0
2	F	837	0	807	6	0
3	C	1622	0	1593	13	0
3	H	1622	0	1593	14	0
4	D	1619	0	1562	18	0
4	L	1634	0	1577	17	0
5	T	70	0	74	1	0
5	U	70	0	74	1	0
6	A	12	0	16	1	0
6	B	6	0	8	2	0
6	D	6	0	8	7	0
6	E	6	0	8	0	0
7	A	7	0	10	0	0
7	B	7	0	10	0	0
7	E	14	0	20	8	0
7	F	7	0	10	0	0
8	A	185	0	0	3	0
8	B	70	0	0	0	0
8	C	84	0	0	0	0
8	D	73	0	0	0	0
8	E	142	0	0	3	0
8	F	51	0	0	0	0
8	H	98	0	0	0	0
8	L	88	0	0	1	0
8	T	6	0	0	0	0
8	U	6	0	0	0	0
All	All	13673	0	12378	124	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 (124) 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)
6:D:601:GOL:H2	1:E:90:ASP:HB2	1.43	0.98
4:D:33:TYR:HE1	6:D:601:GOL:H11	1.35	0.91
3:C:103:ILE:HG21	7:E:401:PEG:H31	1.53	0.90
1:A:138:MET:HG2	8:A:519:HOH:O	1.71	0.89
1:E:93:HIS:HE1	8:E:540:HOH:O	1.72	0.73
2:B:4:THR:HA	2:B:86:THR:HG21	1.70	0.72
3:C:39:GLN:HE22	4:D:37:GLN:HE22	1.38	0.70
1:A:93:HIS:HE1	8:A:523:HOH:O	1.75	0.70
2:F:4:THR:HA	2:F:86:THR:HG21	1.72	0.69
1:E:92:SER:N	7:E:401:PEG:H32	2.08	0.69
4:D:25:ARG:HB3	4:D:26(B):ILE:HD12	1.74	0.68
1:A:115:GLN:HG2	8:A:636:HOH:O	1.96	0.66
1:E:92:SER:H	7:E:401:PEG:H32	1.60	0.66
4:D:33:TYR:CE1	6:D:601:GOL:H11	2.25	0.66
1:A:178:THR:O	1:A:181:ARG:HD2	1.96	0.65
4:D:33:TYR:HB2	4:D:88:MET:HG3	1.78	0.65
4:L:47:GLN:HG2	8:L:309:HOH:O	1.97	0.65
1:E:17:ARG:NH1	7:E:401:PEG:H12	2.14	0.62
2:F:84:HIS:ND1	2:F:86:THR:HB	2.14	0.61
1:A:189:MET:HE3	1:A:272:LEU:HB3	1.83	0.61
2:B:84:HIS:ND1	2:B:86:THR:HB	2.16	0.60
3:H:177:VAL:HG11	4:L:169:GLU:HB3	1.85	0.59
1:E:93:HIS:HD2	1:E:119:ASP:OD2	1.85	0.59
1:A:234:ARG:HH11	2:B:8:GLN:NE2	2.00	0.58
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.87	0.58
2:F:17:ASN:ND2	2:F:97:ARG:HH22	2.01	0.57
4:L:87:GLN:O	4:L:114:VAL:HG21	2.05	0.57
1:A:178:THR:O	1:A:181:ARG:CD	2.53	0.56
4:L:145:ILE:HG12	4:L:204:VAL:HG21	1.89	0.53
2:B:4:THR:HG23	2:B:86:THR:CG2	2.39	0.53
3:C:103:ILE:CG2	7:E:401:PEG:H31	2.33	0.53
4:D:36:GLN:HG3	4:D:85:TYR:CE2	2.44	0.53
1:E:190:THR:CG2	1:E:204:TRP:HE1	2.22	0.53
4:L:122:PRO:HB3	4:L:148:PHE:HB3	1.90	0.52
4:L:36:TYR:HB2	4:L:97:MET:HG3	1.92	0.52
1:A:190:THR:CG2	1:A:204:TRP:HE1	2.23	0.52
3:C:124:THR:HG22	3:C:211:SER:HB3	1.91	0.51
6:D:601:GOL:H2	1:E:90:ASP:CB	2.29	0.51
4:D:24:LEU:HD13	4:D:27:VAL:HG23	1.93	0.51
3:H:124:THR:HG22	3:H:211:SER:HB3	1.91	0.51
1:E:5:MET:HB2	1:E:168:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PRO:O	7:E:401:PEG:H11	2.11	0.51
4:L:155:VAL:HG12	4:L:204:VAL:HG22	1.93	0.51
4:L:176:GLN:OE1	4:L:182:ALA:HB2	2.12	0.50
4:L:33:TYR:OH	4:L:100:HIS:HD2	1.95	0.50
1:E:203:CYS:HG	1:E:259:CYS:HG	1.60	0.50
4:L:153:VAL:HG12	4:L:206:HIS:HB2	1.93	0.50
1:A:5:MET:HB2	1:A:168:LEU:HG	1.93	0.49
2:F:17:ASN:HD21	2:F:97:ARG:NH2	2.09	0.49
2:B:99:MET:HB2	6:B:102:GOL:H12	1.93	0.49
1:E:266:LEU:HD22	1:E:270:LEU:HG	1.94	0.49
4:D:90:TRP:CB	6:D:601:GOL:H32	2.43	0.48
4:L:145:ILE:HG21	4:L:204:VAL:HG11	1.96	0.48
4:L:36:TYR:O	4:L:96:CYS:HA	2.13	0.48
4:D:58:PRO:HB2	4:D:60:ARG:HG2	1.96	0.48
1:E:49:ALA:O	1:E:52:ILE:HG22	2.14	0.48
3:H:167:LEU:HD21	3:H:190:VAL:HG21	1.96	0.48
1:E:267:PRO:HB2	1:E:268:LYS:HE3	1.96	0.47
1:E:66:ASN:HD21	5:T:4:GLN:HE21	1.62	0.47
4:D:50:LYS:HD2	8:E:513:HOH:O	2.14	0.47
1:A:190:THR:HG23	1:A:192:HIS:CE1	2.49	0.47
4:D:148:LYS:HB2	4:D:191:SER:HB2	1.96	0.47
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.96	0.47
3:H:201:THR:HB	3:H:218:LYS:HE3	1.97	0.47
4:D:135:ILE:HD12	4:D:194:VAL:HG21	1.97	0.47
1:A:49:ALA:O	1:A:52:ILE:HG22	2.15	0.47
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.97	0.47
3:C:88:SER:HA	3:C:119:VAL:HB	1.96	0.47
1:E:193:PRO:HA	1:E:199:ALA:HA	1.97	0.46
3:H:88:SER:HA	3:H:119:VAL:HB	1.97	0.46
3:C:201:THR:HB	3:C:218:LYS:HE3	1.97	0.46
1:E:190:THR:HG23	1:E:192:HIS:CE1	2.50	0.46
4:D:4:LEU:HD11	4:D:89:ILE:HG12	1.98	0.46
1:A:88:SER:HB2	6:A:401:GOL:O3	2.16	0.46
3:H:158:VAL:HG23	3:H:186:LEU:HD21	1.98	0.46
3:C:158:VAL:HG23	3:C:186:LEU:HD21	1.97	0.46
6:D:601:GOL:C2	1:E:90:ASP:HB2	2.32	0.45
1:A:187:THR:HA	1:A:204:TRP:O	2.16	0.45
1:A:16:GLY:HA2	4:L:99:TRP:CZ3	2.51	0.45
4:L:39:GLN:HB2	4:L:49:LEU:HD11	1.97	0.45
1:E:20:PRO:HG2	1:E:75:ARG:HG2	1.98	0.45
1:A:20:PRO:HG2	1:A:75:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:PRO:HB3	3:C:153:TYR:HB3	1.98	0.45
4:L:117:GLN:NE2	4:L:179:ASN:HB3	2.31	0.45
3:H:127:PRO:HB3	3:H:153:TYR:HB3	1.98	0.45
2:B:4:THR:HG23	2:B:86:THR:HG23	1.97	0.45
1:A:66:ASN:HB3	5:U:2:ILE:HD11	1.99	0.44
4:D:105(A):LEU:HA	4:D:106:GLY:HA3	1.79	0.44
1:E:187:THR:HA	1:E:204:TRP:O	2.17	0.44
2:F:17:ASN:ND2	2:F:97:ARG:NH2	2.66	0.44
1:E:272:LEU:HD11	8:E:565:HOH:O	2.17	0.44
3:C:155:PRO:HD2	3:C:210:PRO:CB	2.47	0.44
3:H:155:PRO:HD2	3:H:210:PRO:CB	2.47	0.43
1:E:17:ARG:HH11	7:E:401:PEG:H12	1.83	0.43
1:A:190:THR:HG22	1:A:204:TRP:HE1	1.83	0.43
3:C:99:VAL:CG1	1:E:17:ARG:HG2	2.48	0.43
4:D:95:TRP:CH2	6:D:601:GOL:H31	2.53	0.43
1:E:266:LEU:HD13	1:E:269:PRO:HA	2.01	0.43
1:A:202:ARG:HD2	1:A:204:TRP:CZ2	2.54	0.43
1:E:190:THR:HG22	1:E:204:TRP:HE1	1.82	0.43
1:A:190:THR:HG22	1:A:202:ARG:HB3	2.01	0.43
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.54	0.42
3:H:16:ALA:O	3:H:86:LEU:HB2	2.20	0.42
4:L:65:PRO:HB2	4:L:67:ARG:HG2	2.01	0.42
3:H:10:GLU:HG2	3:H:18:VAL:HG23	2.01	0.42
1:E:201:LEU:HD22	1:E:249:VAL:HG11	2.01	0.42
3:C:10:GLU:HG2	3:C:18:VAL:HG23	2.02	0.42
1:E:202:ARG:HD2	1:E:204:TRP:CZ2	2.55	0.42
3:C:16:ALA:O	3:C:86:LEU:HB2	2.20	0.42
1:E:190:THR:HG22	1:E:202:ARG:HB3	2.01	0.42
1:A:33:PHE:O	1:A:52:ILE:HG21	2.20	0.42
4:D:27:VAL:HG22	4:D:65:LYS:HD3	2.02	0.42
3:C:207:ASN:HB2	3:C:214:LYS:HE3	2.03	0.41
1:E:33:PHE:O	1:E:52:ILE:HG21	2.21	0.41
1:A:249:VAL:HG21	1:A:254:GLU:HG3	2.03	0.41
4:D:90:TRP:CZ3	1:E:16:GLY:HA2	2.56	0.41
2:B:99:MET:CB	6:B:102:GOL:H12	2.51	0.41
3:H:162:TRP:HB3	3:H:167:LEU:HD23	2.03	0.41
4:D:148:LYS:HD2	4:D:151:SER:HA	2.03	0.40
1:E:92:SER:HB2	7:E:401:PEG:H21	2.03	0.40
1:A:41:ALA:HA	3:H:55:SER:HA	2.03	0.40
3:H:207:ASN:HB2	3:H:214:LYS:HE3	2.04	0.40
3:H:179:GLN:HE21	3:H:179:GLN:HB2	1.74	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	272/276 (99%)	265 (97%)	6 (2%)	1 (0%)	34	48
1	E	276/276 (100%)	267 (97%)	8 (3%)	1 (0%)	34	48
2	B	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
2	F	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	212/222 (96%)	202 (95%)	10 (5%)	0	100	100
3	H	212/222 (96%)	202 (95%)	10 (5%)	0	100	100
4	D	214/221 (97%)	208 (97%)	5 (2%)	1 (0%)	29	41
4	L	219/221 (99%)	214 (98%)	4 (2%)	1 (0%)	29	41
5	T	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
5	U	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	1614/1656 (98%)	1558 (96%)	51 (3%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	T	5	SER
4	D	151	SER
1	A	251	SER
1	E	251	SER
4	L	178	ASN

### 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	231/233 (99%)	213 (92%)	18 (8%)	12	19
1	E	235/233 (101%)	216 (92%)	19 (8%)	11	18
2	B	94/95 (99%)	86 (92%)	8 (8%)	10	16
2	F	95/95 (100%)	86 (90%)	9 (10%)	8	12
3	C	182/187 (97%)	168 (92%)	14 (8%)	13	20
3	H	182/187 (97%)	172 (94%)	10 (6%)	21	35
4	D	179/185 (97%)	167 (93%)	12 (7%)	16	26
4	L	183/185 (99%)	175 (96%)	8 (4%)	28	45
5	T	8/8 (100%)	6 (75%)	2 (25%)	0	0
5	U	8/8 (100%)	6 (75%)	2 (25%)	0	0
All	All	1397/1416 (99%)	1295 (93%)	102 (7%)	14	22

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	35	ARG
1	A	78	LEU
1	A	81	LEU
1	A	94	THR
1	A	115	GLN
1	A	116	ASP
1	A	128	GLU
1	A	141	GLN
1	A	163	ARG
1	A	168	LEU
1	A	177	GLU
1	A	181	ARG
1	A	212	GLU
1	A	222	GLU
1	A	226	GLN
1	A	255	GLN
1	A	268	LYS
2	B	27	VAL
2	B	40	LEU
2	B	48	LYS
2	B	64	LEU

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Mol	Chain	Res	Type
2	B	70	PHE
2	B	71	THR
2	B	75	LYS
2	B	86	THR
3	C	17	SER
3	C	65	GLN
3	C	72	ARG
3	C	86	LEU
3	C	87	ARG
3	C	135	SER
3	C	158	VAL
3	C	167	LEU
3	C	177	VAL
3	C	189	VAL
3	C	191	THR
3	C	201	THR
3	C	209	LYS
3	C	214	LYS
4	D	26	SER
4	D	32	ILE
4	D	71	ILE
4	D	102	LYS
4	D	105(A)	LEU
4	D	135	ILE
4	D	137	ASP
4	D	150	ASP
4	D	179	LEU
4	D	182	GLU
4	D	183	GLN
4	D	200	THR
1	E	19	GLU
1	E	35	ARG
1	E	78	LEU
1	E	94	THR
1	E	128	GLU
1	E	141	GLN
1	E	163	ARG
1	E	168	LEU
1	E	181[A]	ARG
1	E	181[B]	ARG
1	E	183	ASP
1	E	189	MET

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Mol	Chain	Res	Type
1	E	197	HIS
1	E	212	GLU
1	E	230	LEU
1	E	255	GLN
1	E	258	THR
1	E	266	LEU
1	E	268	LYS
2	F	1	ILE
2	F	2	GLN
2	F	27	VAL
2	F	40	LEU
2	F	58	LYS
2	F	70	PHE
2	F	75	LYS
2	F	86	THR
2	F	99	MET
3	H	1	GLU
3	H	65	GLN
3	H	72	ARG
3	H	86	LEU
3	H	87	ARG
3	H	158	VAL
3	H	189	VAL
3	H	201	THR
3	H	209	LYS
3	H	214	LYS
4	L	17	SER
4	L	47	GLN
4	L	75	SER
4	L	89	GLU
4	L	123	SER
4	L	161	SER
4	L	164	VAL
4	L	171	THR
5	T	5	SER
5	T	6	SER
5	U	6	SER
5	U	7	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	86	ASN
1	A	87	GLN
1	A	93	HIS
1	A	96	GLN
1	A	127	ASN
1	A	155	GLN
1	A	156	GLN
1	A	192	HIS
1	A	260	HIS
2	B	8	GLN
2	B	17	ASN
2	B	24	ASN
3	C	212	ASN
4	D	26(C)	ASN
4	D	37	GLN
4	D	91	HIS
4	D	183	GLN
4	D	187	HIS
1	E	43	GLN
1	E	87	GLN
1	E	93	HIS
1	E	96	GLN
1	E	155	GLN
1	E	192	HIS
1	E	260	HIS
2	F	17	ASN
2	F	24	ASN
3	H	172	HIS
3	H	179	GLN
4	L	100	HIS
4	L	117	GLN
4	L	178	ASN
5	T	4	GLN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
7	PEG	A	402	-	6,6,6	0.53	0	5,5,5	0.29	0
7	PEG	F	801	-	6,6,6	0.42	0	5,5,5	0.44	0
6	GOL	A	403	-	5,5,5	0.46	0	5,5,5	0.48	0
7	PEG	B	101	-	6,6,6	0.31	0	5,5,5	1.22	1 (20%)
7	PEG	E	401	-	6,6,6	0.51	0	5,5,5	1.55	1 (20%)
6	GOL	B	102	-	5,5,5	0.81	0	5,5,5	0.69	0
6	GOL	E	402	-	5,5,5	0.39	0	5,5,5	0.43	0
6	GOL	A	401	-	5,5,5	0.19	0	5,5,5	0.30	0
6	GOL	D	601	-	5,5,5	0.59	0	5,5,5	0.49	0
7	PEG	E	403	-	6,6,6	0.82	0	5,5,5	0.87	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
7	PEG	A	402	-	-	1/4/4/4	-
7	PEG	F	801	-	-	1/4/4/4	-
6	GOL	A	403	-	-	4/4/4/4	-
7	PEG	B	101	-	-	2/4/4/4	-
7	PEG	E	401	-	-	3/4/4/4	-
6	GOL	B	102	-	-	2/4/4/4	-
6	GOL	E	402	-	-	4/4/4/4	-
6	GOL	A	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	601	-	-	2/4/4/4	-
7	PEG	E	403	-	-	3/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	401	PEG	C3-O2-C2	-2.78	101.25	113.29
7	B	101	PEG	C3-O2-C2	-2.30	103.34	113.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

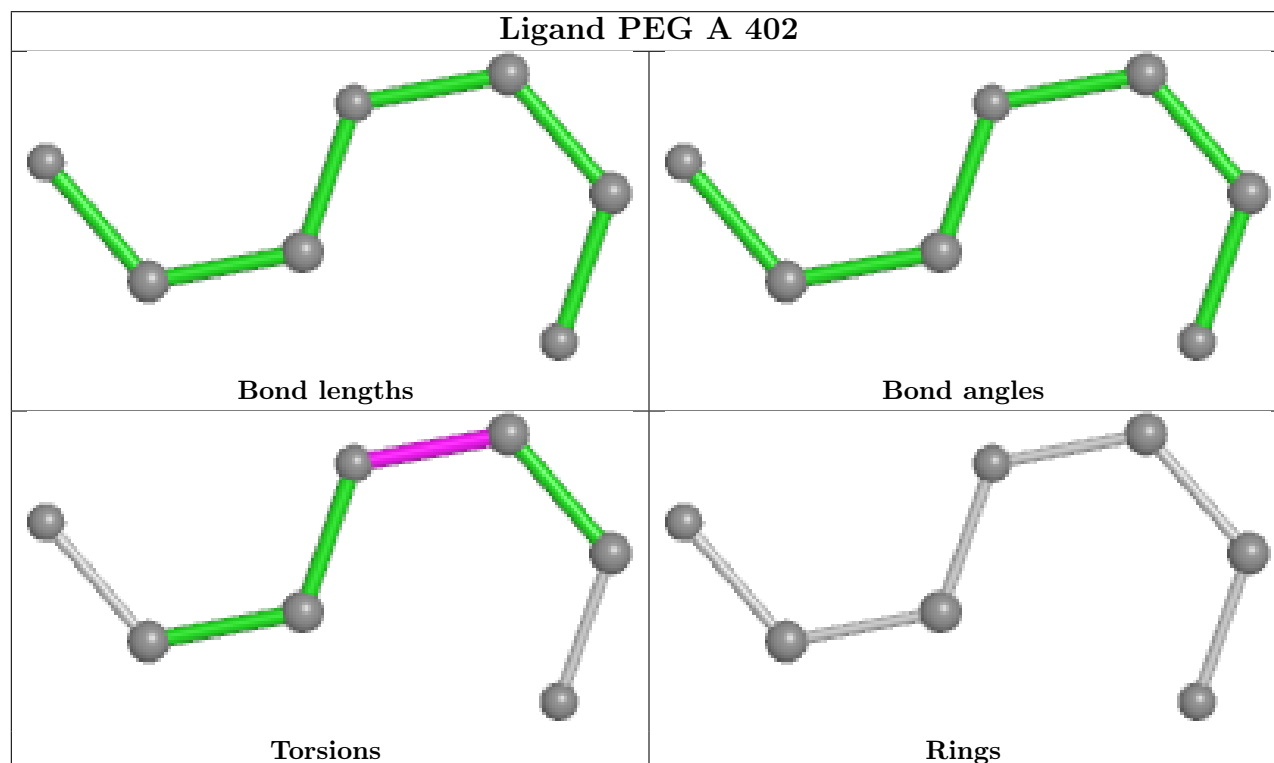
Mol	Chain	Res	Type	Atoms
6	A	403	GOL	C1-C2-C3-O3
6	B	102	GOL	O2-C2-C3-O3
6	E	402	GOL	O1-C1-C2-C3
6	E	402	GOL	C1-C2-C3-O3
6	A	401	GOL	O1-C1-C2-C3
6	D	601	GOL	O1-C1-C2-O2
6	D	601	GOL	O1-C1-C2-C3
6	A	403	GOL	O1-C1-C2-O2
6	E	402	GOL	O2-C2-C3-O3
7	F	801	PEG	O2-C3-C4-O4
7	B	101	PEG	O1-C1-C2-O2
7	E	403	PEG	O1-C1-C2-O2
6	A	403	GOL	O1-C1-C2-C3
6	B	102	GOL	C1-C2-C3-O3
6	A	403	GOL	O2-C2-C3-O3
7	E	401	PEG	O1-C1-C2-O2
7	E	403	PEG	O2-C3-C4-O4
6	E	402	GOL	O1-C1-C2-O2
7	B	101	PEG	C1-C2-O2-C3
7	A	402	PEG	C4-C3-O2-C2
7	E	403	PEG	C4-C3-O2-C2
7	E	401	PEG	C1-C2-O2-C3
6	A	401	GOL	O1-C1-C2-O2
7	E	401	PEG	O2-C3-C4-O4

There are no ring outliers.

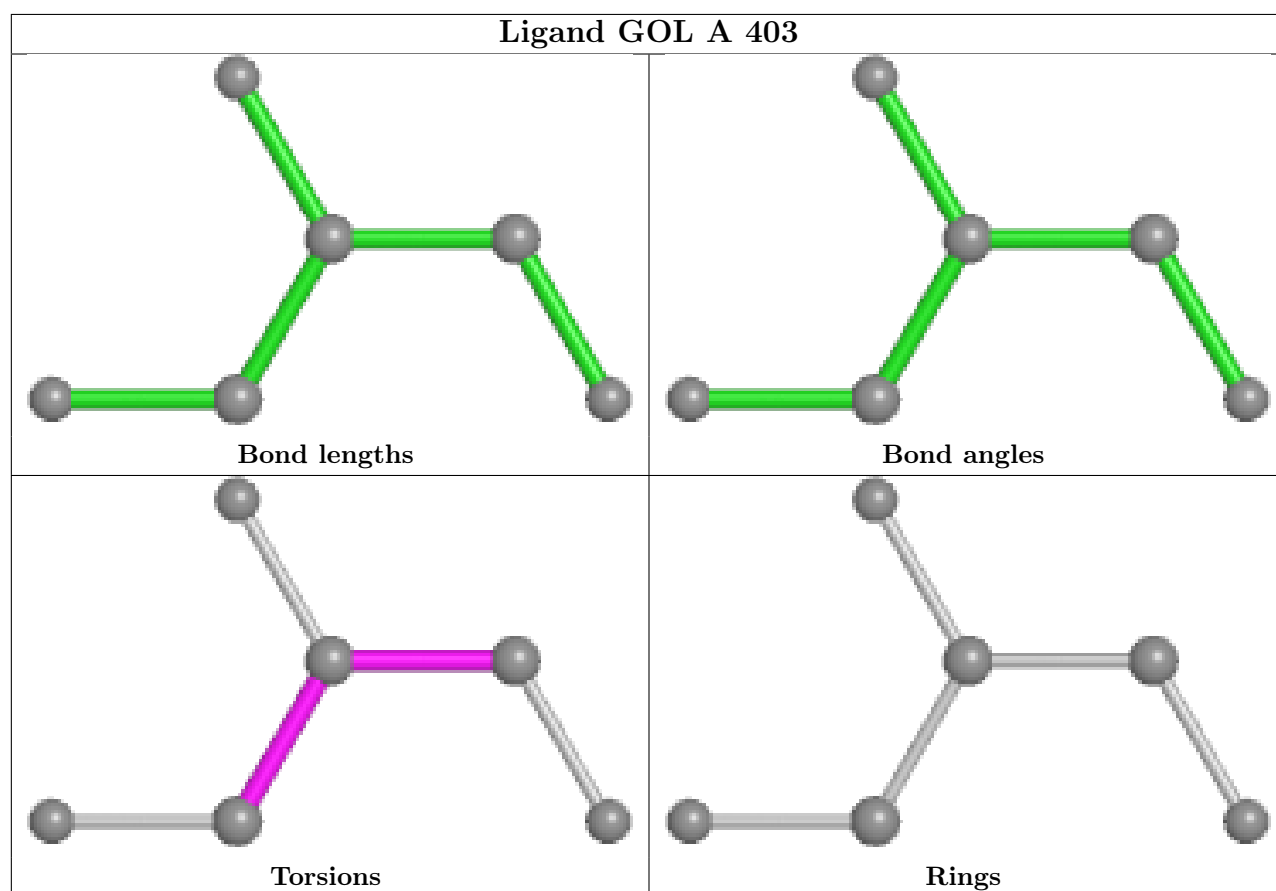
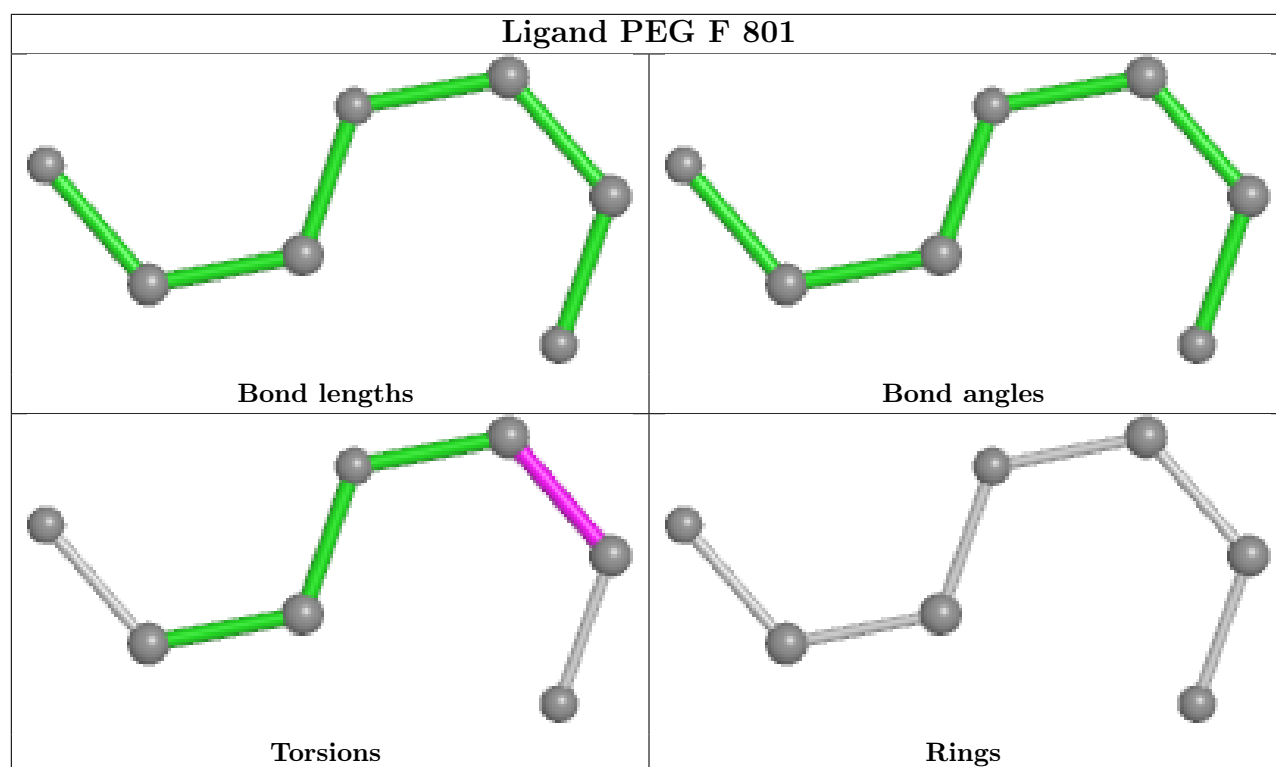
4 monomers are involved in 18 short contacts:

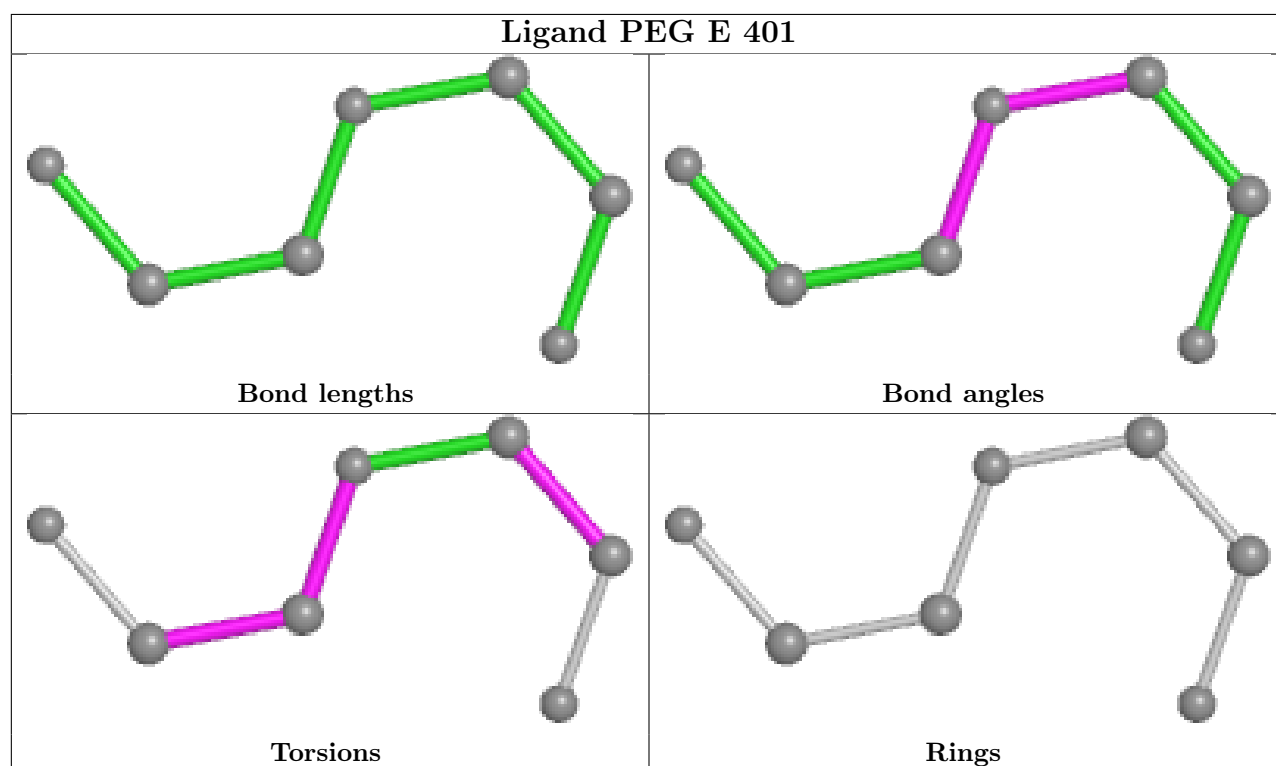
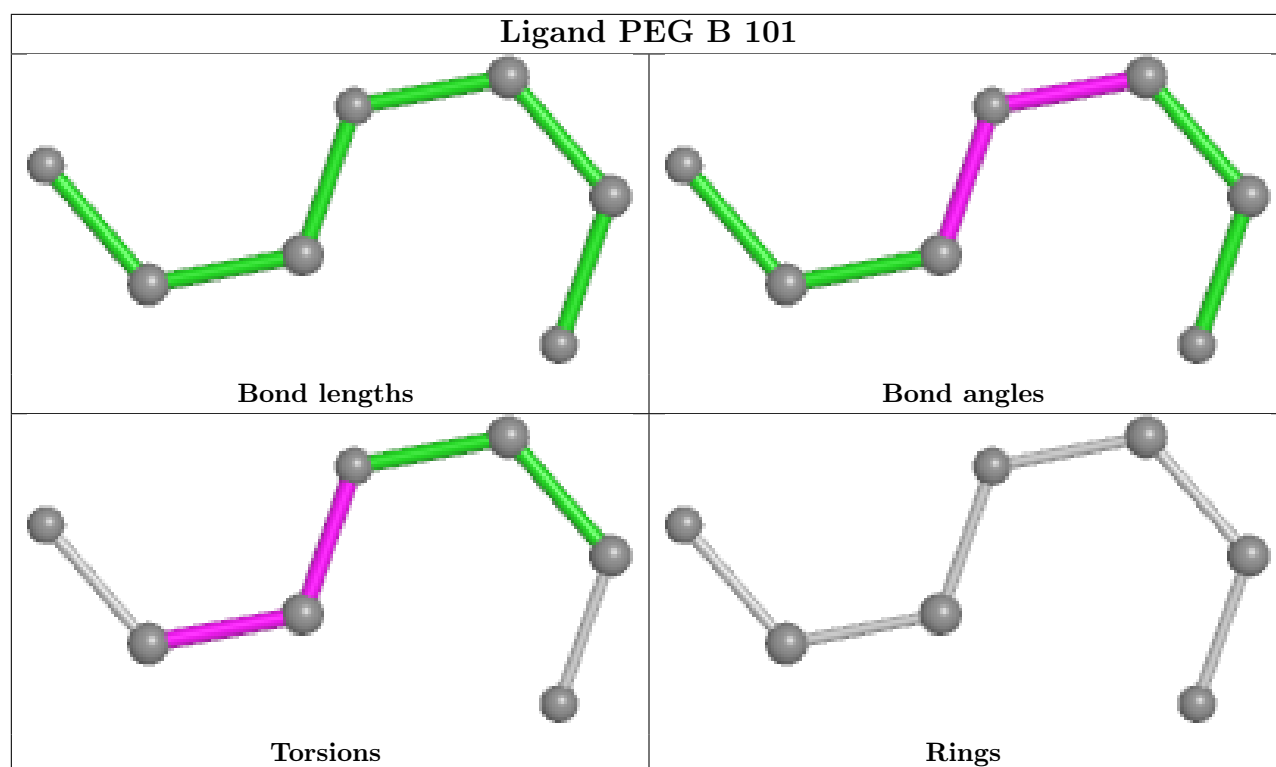
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	401	PEG	8	0
6	B	102	GOL	2	0
6	A	401	GOL	1	0
6	D	601	GOL	7	0

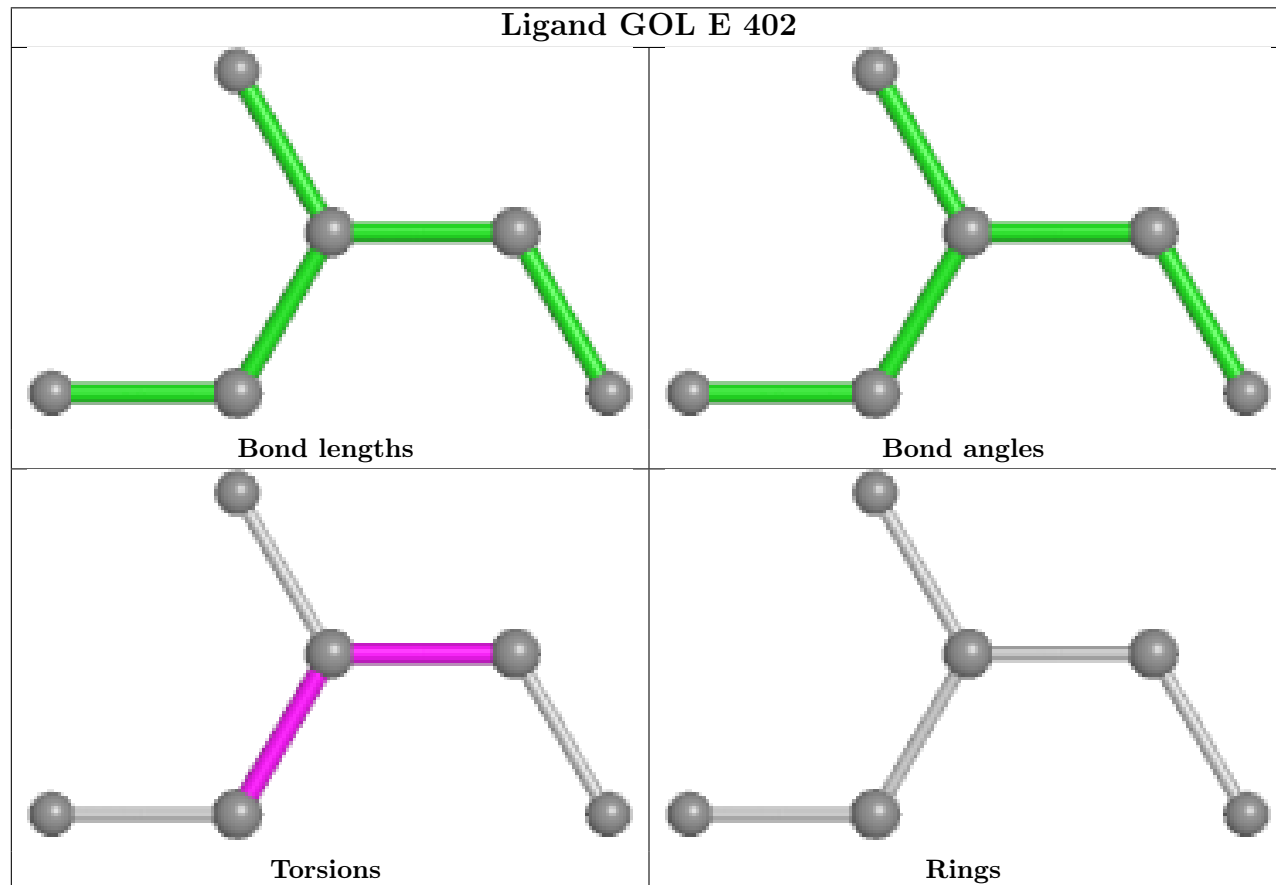
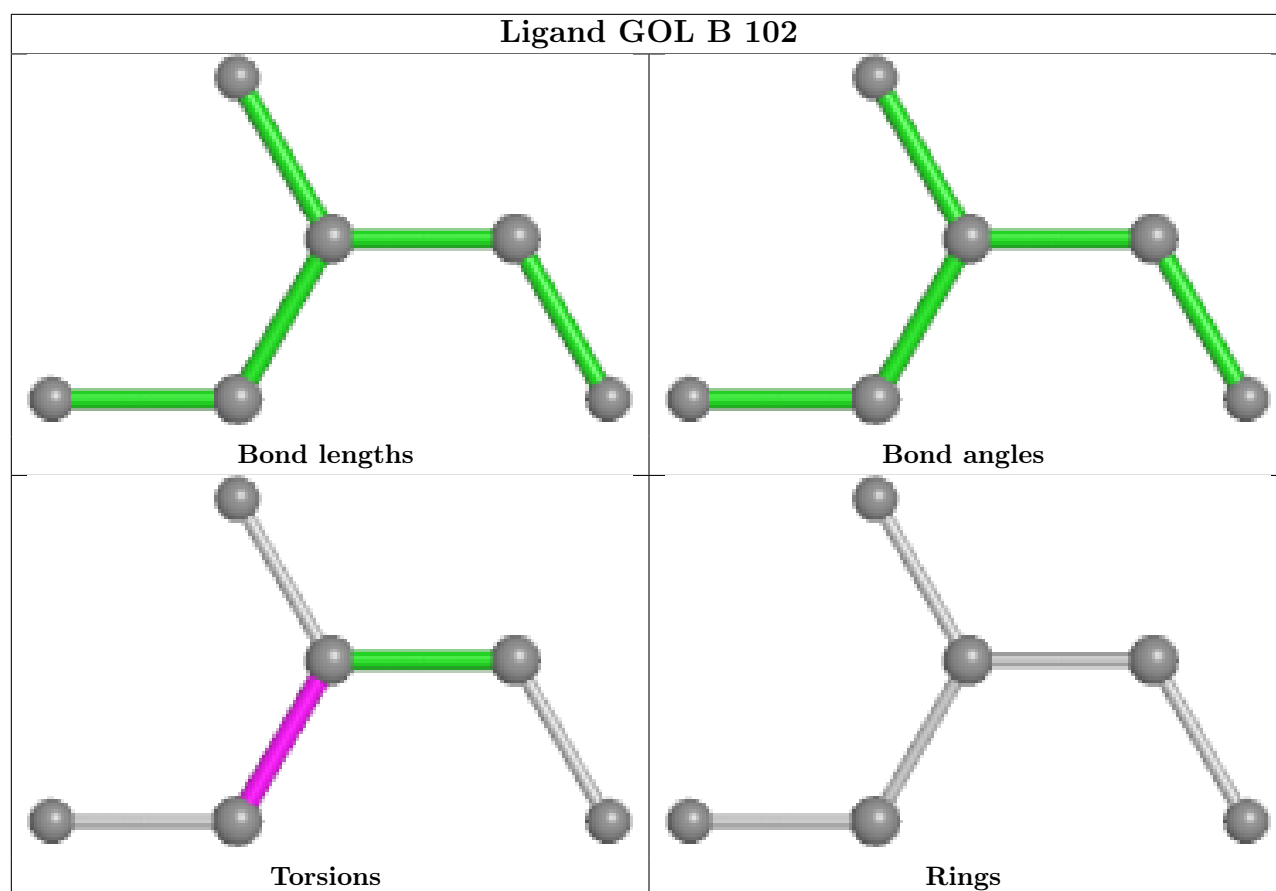
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

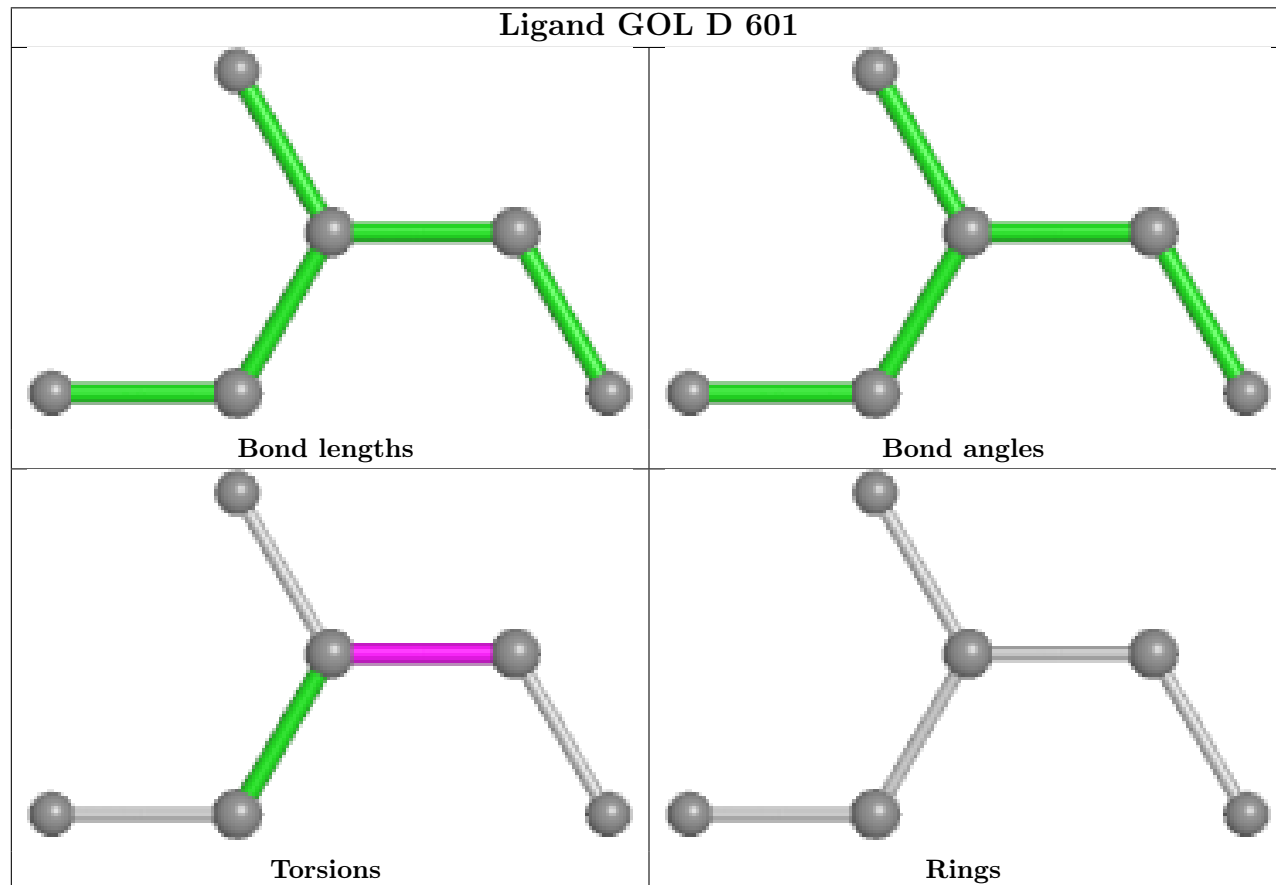
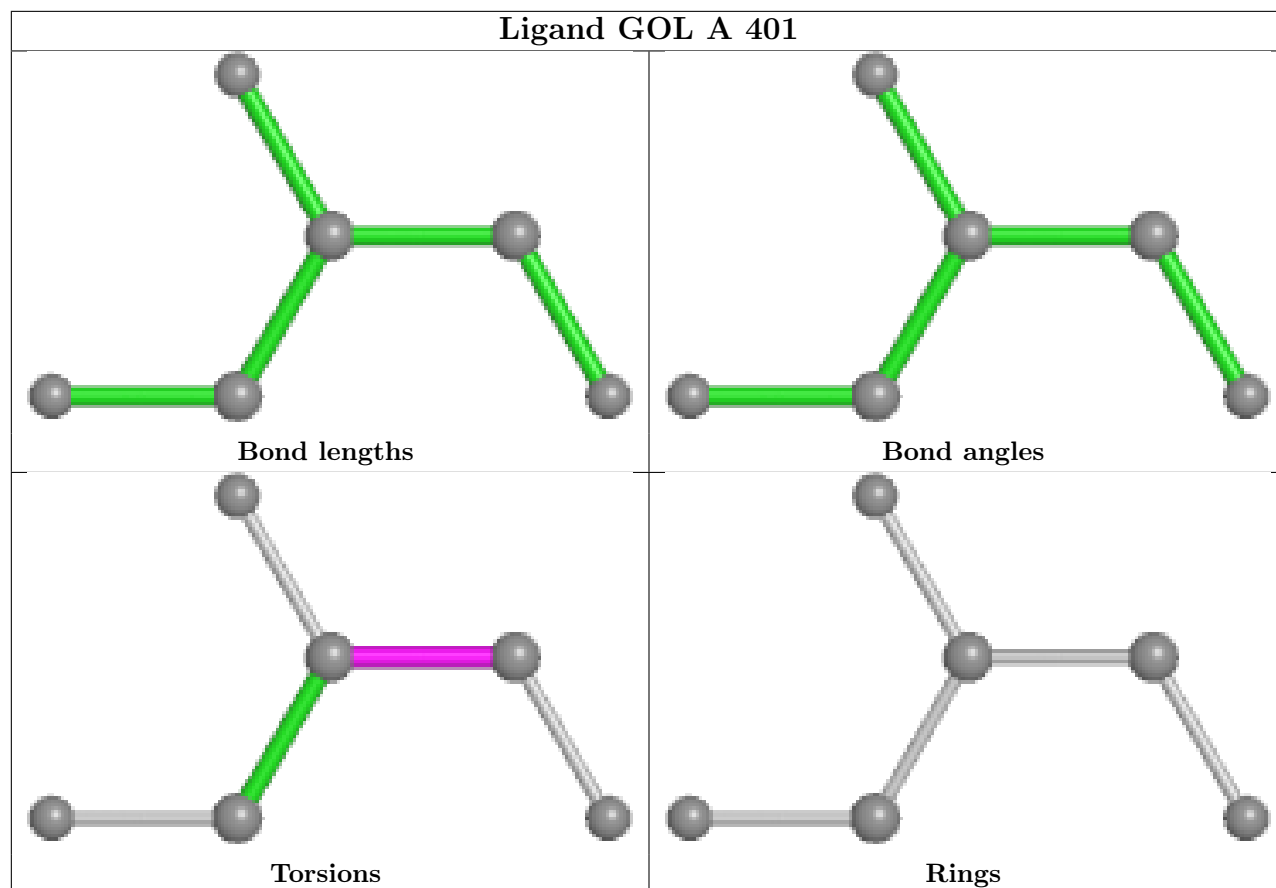


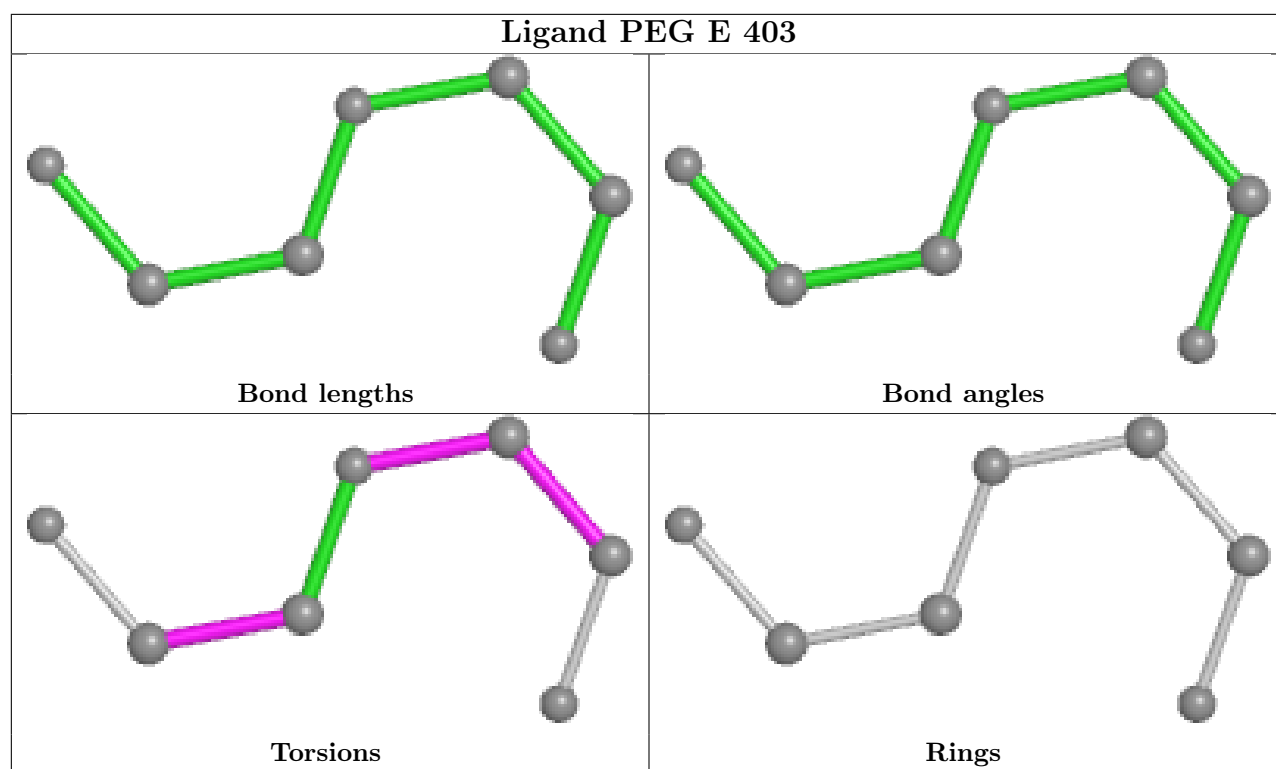












## 5.7 Other polymers [i](#)

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	274/276 (99%)	0.24	11 (4%) 38 37	31, 48, 94, 117	0
1	E	275/276 (99%)	0.35	19 (6%) 16 15	36, 54, 104, 136	0
2	B	99/100 (99%)	0.54	3 (3%) 50 49	35, 55, 85, 96	0
2	F	99/100 (99%)	0.42	3 (3%) 50 49	41, 60, 90, 105	0
3	C	216/222 (97%)	0.05	4 (1%) 66 64	38, 58, 90, 120	0
3	H	216/222 (97%)	0.16	5 (2%) 60 58	35, 60, 96, 118	0
4	D	215/221 (97%)	0.31	17 (7%) 12 11	40, 70, 101, 110	0
4	L	216/221 (97%)	0.54	24 (11%) 5 4	33, 67, 107, 120	0
5	T	9/9 (100%)	0.53	1 (11%) 5 4	39, 55, 79, 84	0
5	U	9/9 (100%)	0.68	1 (11%) 5 4	37, 49, 80, 81	0
All	All	1628/1656 (98%)	0.31	88 (5%) 25 24	31, 59, 99, 136	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	195	SER	5.6
4	L	158	LYS	5.5
2	B	1	ILE	5.3
1	A	197	HIS	5.2
4	D	149	ALA	4.7
4	D	188	LYS	4.6
1	A	196	ASP	4.5
1	A	251	SER	4.5
1	E	199	ALA	4.5
1	E	267	PRO	4.4
4	L	199	SER	4.3
5	U	5	SER	4.2
1	E	266	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	L	159	ALA	4.1
3	H	144	ALA	4.0
4	L	200	TYR	4.0
1	E	194	ILE	3.9
4	L	198	LYS	3.9
1	A	194	ILE	3.8
2	F	1	ILE	3.7
4	L	211	VAL	3.7
4	L	156	ALA	3.6
1	E	249	VAL	3.4
4	D	193	GLN	3.4
4	D	148	LYS	3.3
1	A	267	PRO	3.2
4	L	195	LYS	3.2
1	E	250	PRO	3.2
4	L	215	VAL	3.2
4	L	160	ASP	3.2
1	A	195	SER	3.1
4	L	205	THR	3.1
3	C	199	THR	3.0
1	E	196	ASP	3.0
4	L	203	GLN	2.9
4	D	199	SER	2.9
4	L	161	SER	2.8
4	D	153	PRO	2.8
4	D	201	VAL	2.8
4	L	162	SER	2.8
4	L	209	SER	2.8
1	E	197	HIS	2.8
4	D	154	VAL	2.7
3	C	144	ALA	2.7
1	A	220	ASP	2.6
4	D	200	THR	2.6
4	L	166	ALA	2.6
3	H	199	THR	2.5
4	L	196	SER	2.5
1	A	250	PRO	2.4
1	E	253	GLU	2.4
4	D	156	ALA	2.4
4	L	201	SER	2.4
1	E	108	ARG	2.4
2	B	35	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	44	GLU	2.4
4	L	189	LEU	2.4
1	E	184	PRO	2.3
1	A	1	GLY	2.3
3	H	142	GLY	2.3
4	L	157	TRP	2.3
4	D	67	ALA	2.3
4	L	208	GLY	2.3
1	E	255	GLN	2.3
4	L	163	PRO	2.2
1	E	105	PRO	2.2
1	E	1	GLY	2.2
5	T	5	SER	2.2
3	H	167	LEU	2.2
2	B	21	ASN	2.2
4	D	151	SER	2.2
1	E	268	LYS	2.1
4	D	157	GLY	2.1
3	H	192	VAL	2.1
4	L	2	ALA	2.1
1	A	253	GLU	2.1
1	E	274	TRP	2.1
2	F	3[A]	ARG	2.1
4	D	186	SER	2.1
1	E	275	GLU	2.1
3	C	142	GLY	2.1
4	L	122	PRO	2.0
4	D	205	VAL	2.0
4	D	155	LYS	2.0
4	D	150	ASP	2.0
1	E	181[A]	ARG	2.0
1	A	221	GLY	2.0
3	C	1	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands

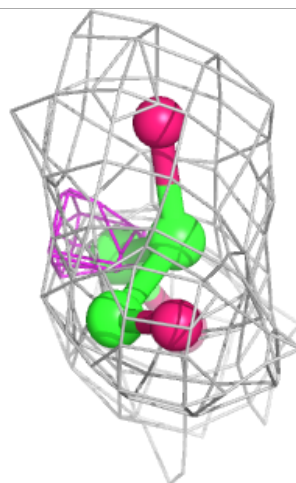
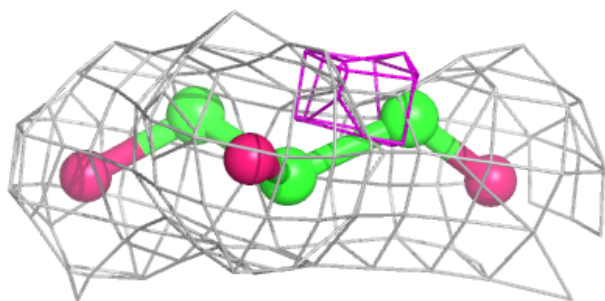
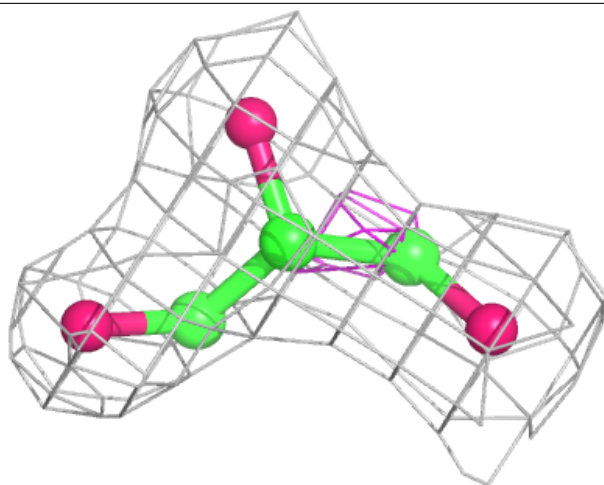
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	B	102	6/6	0.77	0.20	58,60,64,65	0
7	PEG	E	401	7/7	0.82	0.30	52,53,56,57	0
7	PEG	E	403	7/7	0.85	0.20	58,60,73,73	0
6	GOL	D	601	6/6	0.90	0.22	59,60,63,63	0
6	GOL	A	403	6/6	0.90	0.24	61,63,64,66	0
6	GOL	E	402	6/6	0.91	0.18	53,58,63,65	0
7	PEG	B	101	7/7	0.94	0.22	51,52,54,57	0
7	PEG	A	402	7/7	0.96	0.16	52,53,54,54	0
7	PEG	F	801	7/7	0.97	0.18	41,44,47,51	0
6	GOL	A	401	6/6	0.97	0.16	55,60,64,66	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.

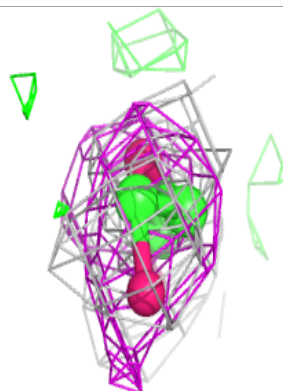
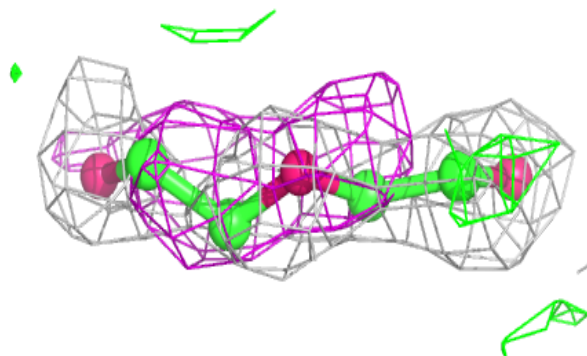
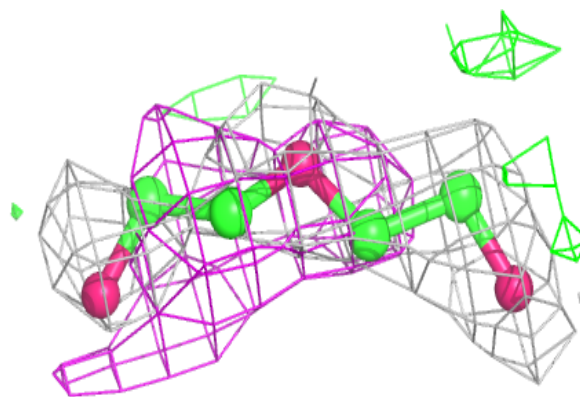
**Electron density around GOL B 102:**

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



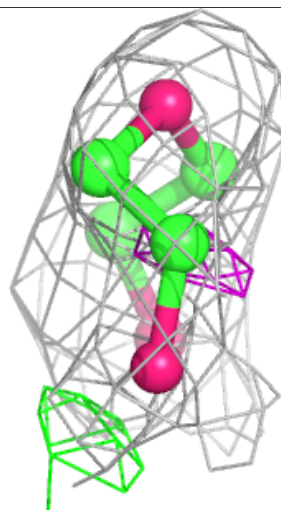
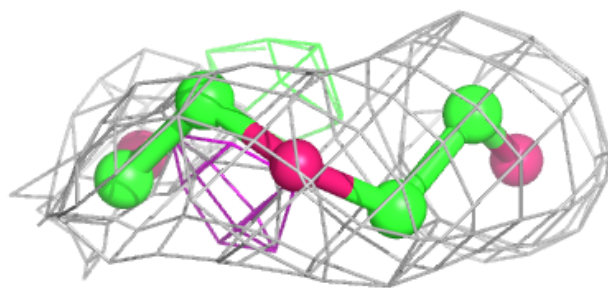
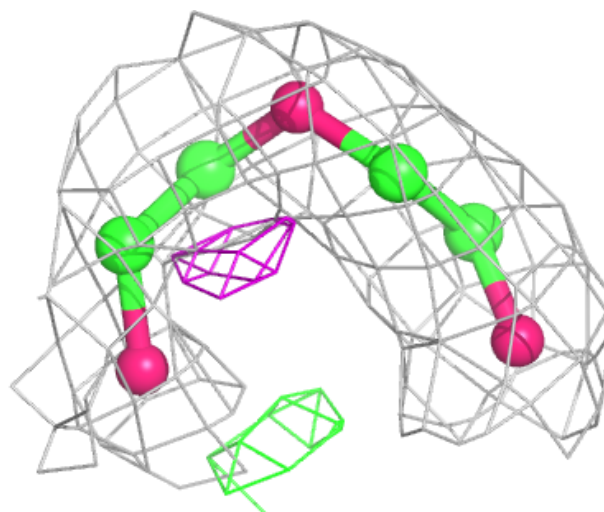
**Electron density around PEG E 401:**

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



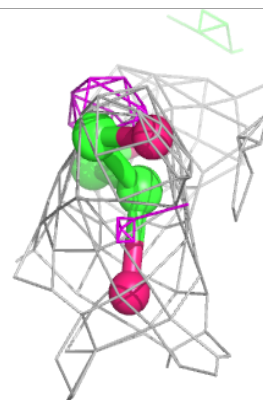
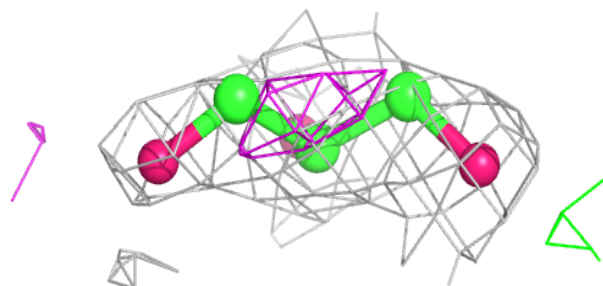
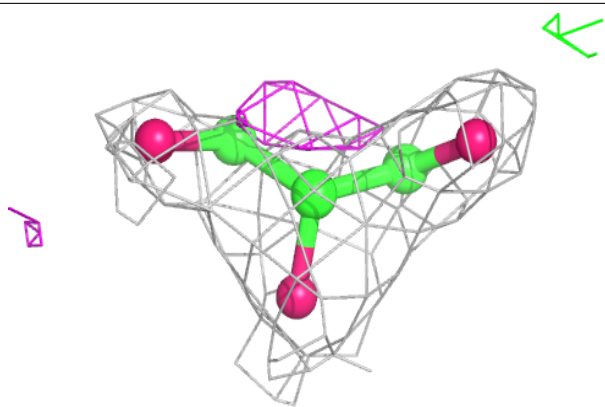
**Electron density around PEG E 403:**

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



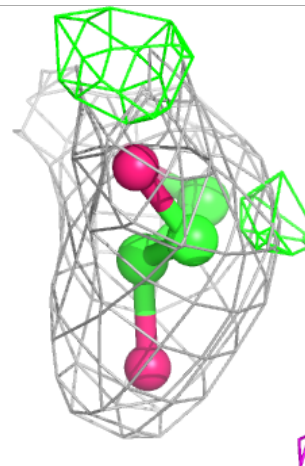
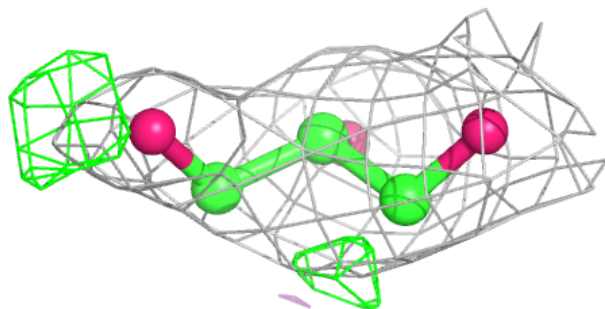
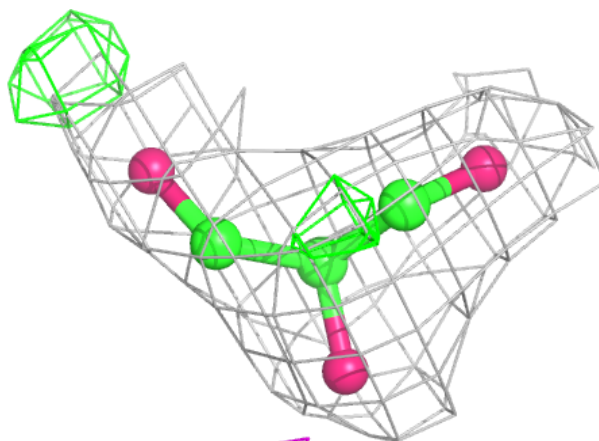
**Electron density around GOL D 601:**

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



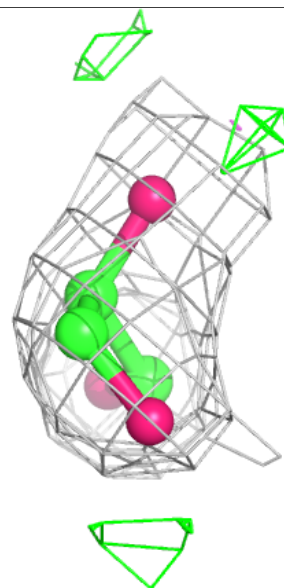
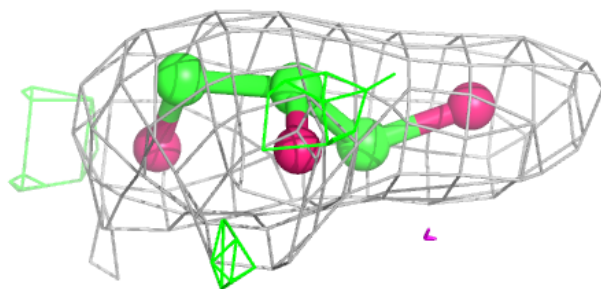
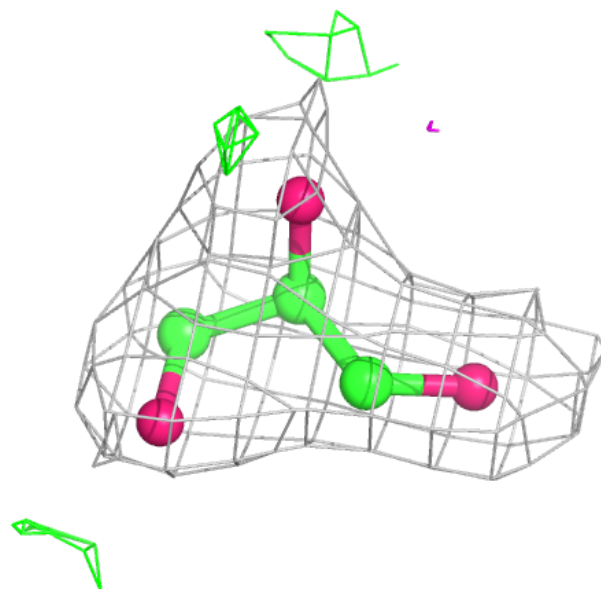
**Electron density around GOL A 403:**

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



**Electron density around GOL E 402:**

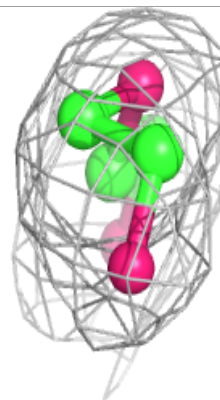
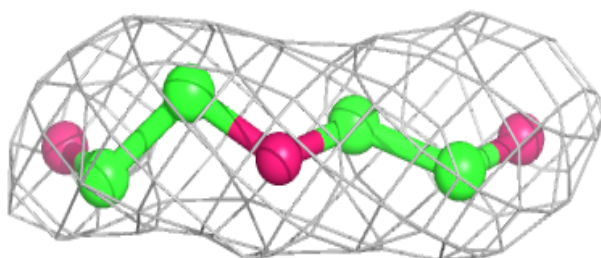
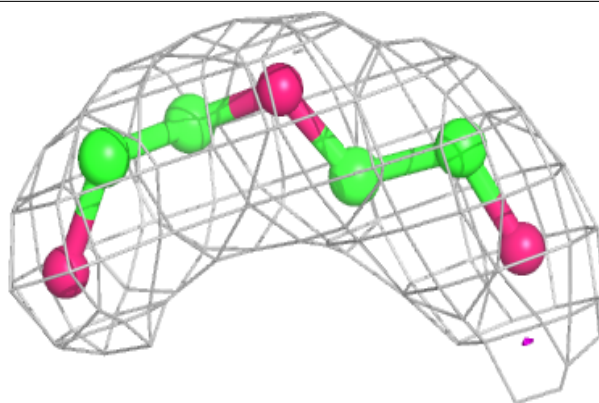
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



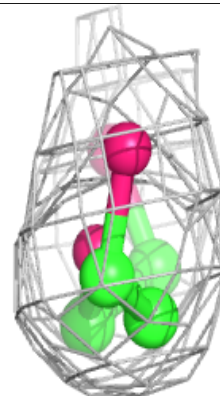
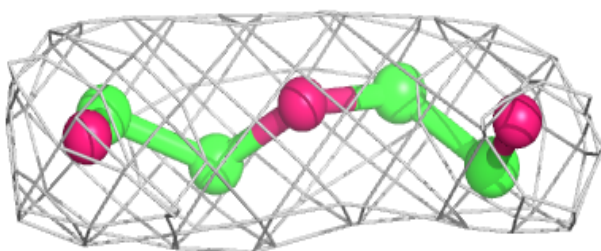
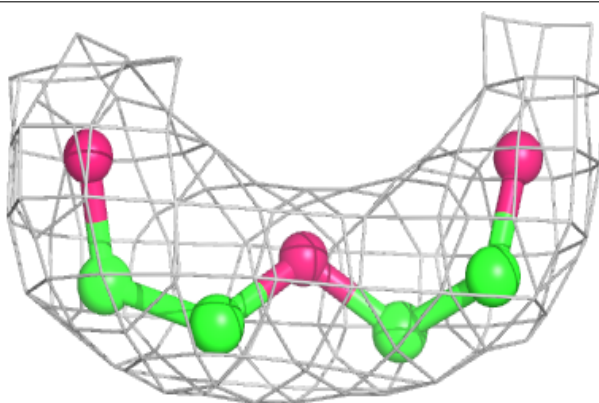


**Electron density around PEG B 101:**

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

**Electron density around PEG A 402:**

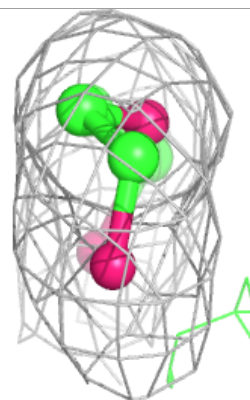
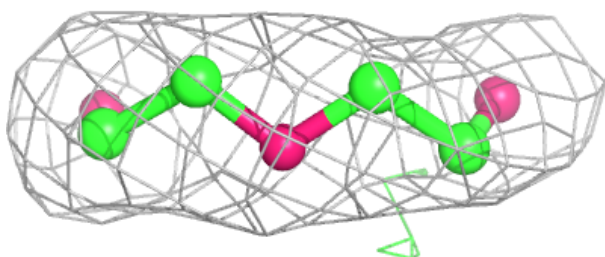
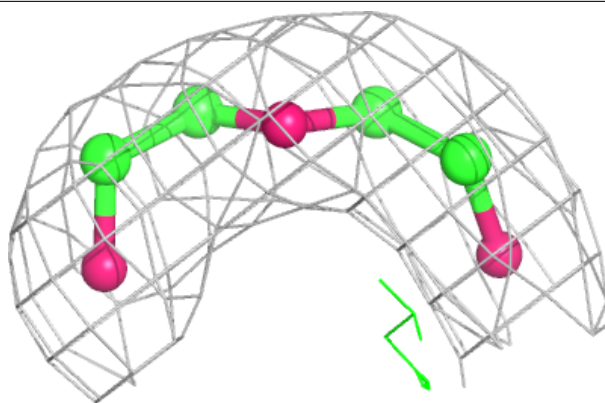
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

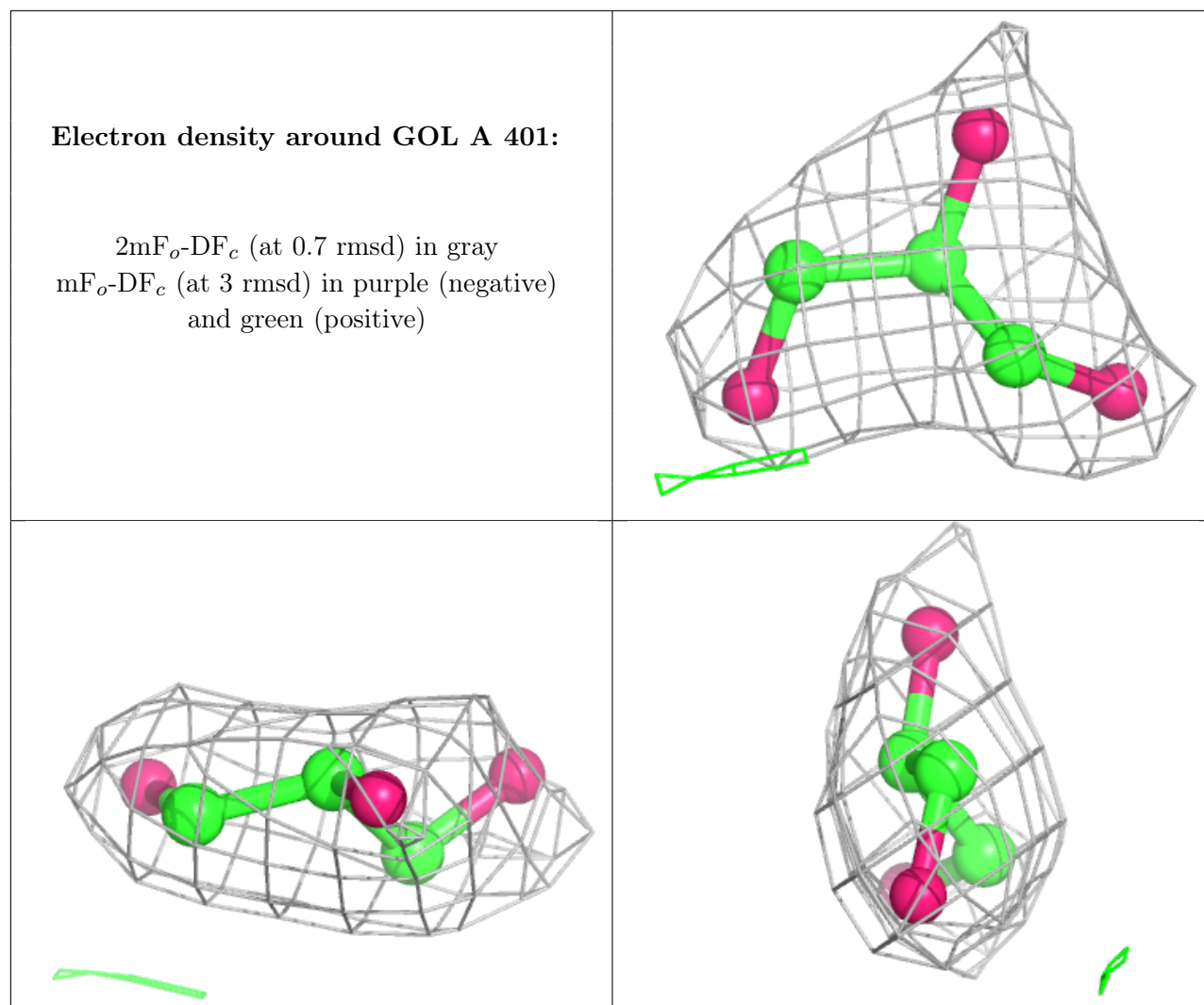




**Electron density around PEG F 801:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.