



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:09 AM UTC

PDB ID : 8E7T / pdb_00008e7t
Title : Crystal structure of Middle East respiratory syndrome coronavirus (MERS-CoV) 3CL protease inactive mutant C148A
Authors : Shaqra, A.M.; Zvornicanin, S.N.; Schiffer, C.A.
Deposited on : 2022-08-24
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

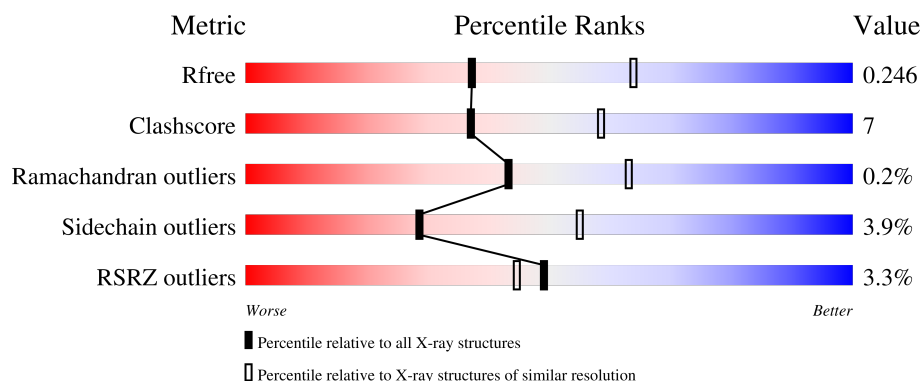
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	2% 83% 16% .
1	B	306	% 86% 12% ..
1	C	306	85% 14% .
1	D	306	10% 74% 23% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9989 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 3C-Like Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	15	0
			2424	1540	398	458	28			
1	B	303	Total	C	N	O	S	9	9	0
			2330	1485	381	439	25			
1	C	303	Total	C	N	O	S	9	9	0
			2349	1493	386	444	26			
1	D	306	Total	C	N	O	S	0	7	0
			2274	1437	375	439	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	CYS	engineered mutation	UNP W6A941
B	148	ALA	CYS	engineered mutation	UNP W6A941
C	148	ALA	CYS	engineered mutation	UNP W6A941
D	148	ALA	CYS	engineered mutation	UNP W6A941

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Na	0	0
			3	3		
3	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Na 1	0	0

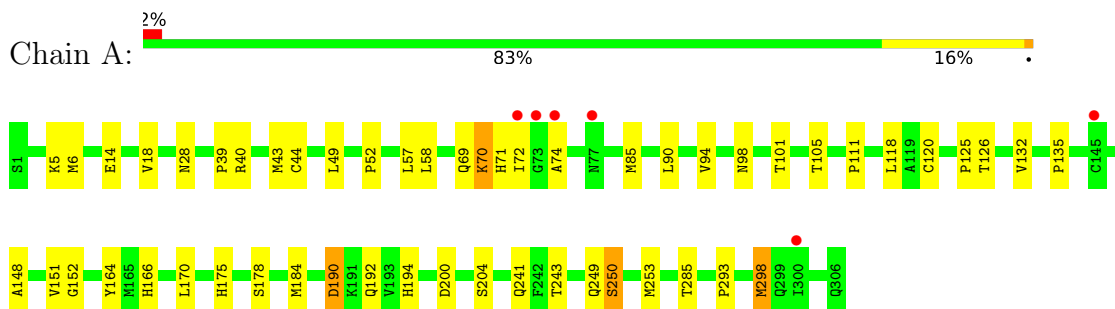
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total 192	O 192	0	0
4	B	110	Total 110	O 110	0	0
4	C	165	Total 165	O 165	0	0
4	D	86	Total 86	O 86	0	0

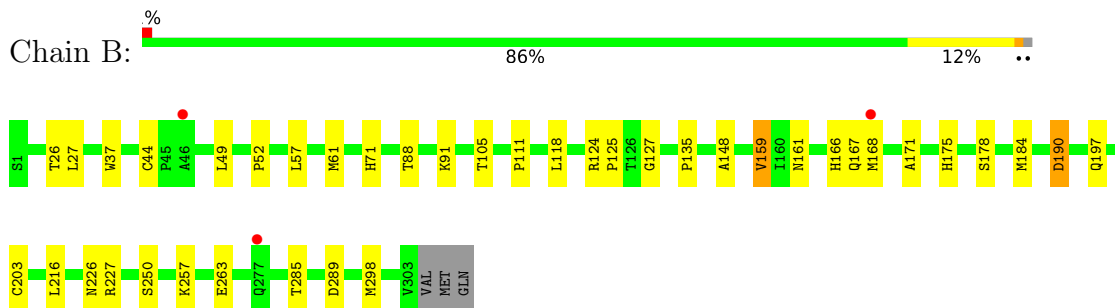
3 Residue-property plots

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.

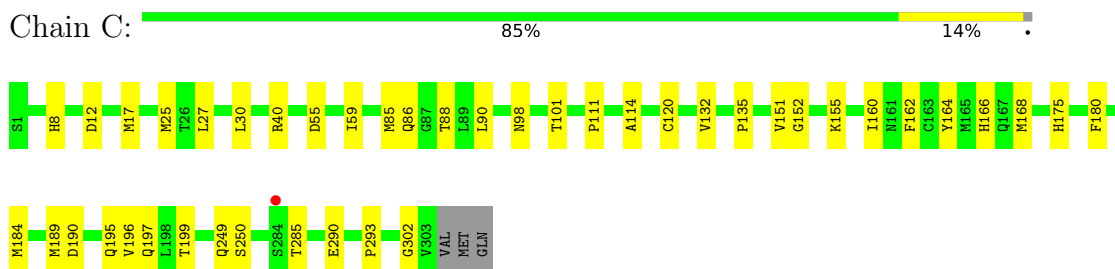
- Molecule 1: 3C-Like Protease



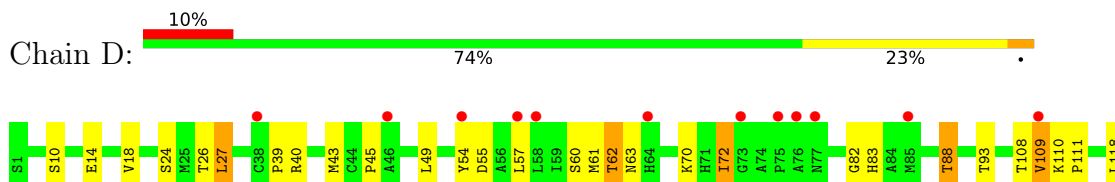
- Molecule 1: 3C-Like Protease

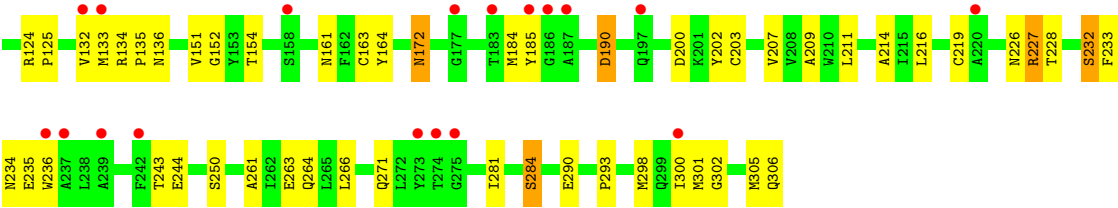


- Molecule 1: 3C-Like Protease



- Molecule 1: 3C-Like Protease





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.41Å 90.01Å 120.52Å 90.00° 108.33° 90.00°	Depositor
Resolution (Å)	24.93 – 2.50 24.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.93-2.50) 99.9 (24.93-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.244 0.187 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9989	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.19	0/2481	0.33	0/3378
1	B	0.12	0/2388	0.27	0/3259
1	C	0.13	0/2405	0.27	0/3276
1	D	0.24	0/2330	0.49	4/3185 (0.1%)
All	All	0.18	0/9604	0.35	4/13098 (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	D	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	GLU	CA-C-N	5.61	132.25	121.54
1	D	235	GLU	C-N-CA	5.61	132.25	121.54
1	D	284	SER	N-CA-C	5.31	117.93	109.81
1	D	281	ILE	N-CA-C	-5.03	100.65	107.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	232	SER	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	2424	0	2315	36	0
1	B	2330	0	2199	28	0
1	C	2349	0	2259	22	0
1	D	2274	0	2036	52	0
2	A	18	0	24	1	0
2	B	6	0	8	0	0
2	C	30	0	40	5	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	192	0	0	2	0
4	B	110	0	0	0	0
4	C	165	0	0	0	0
4	D	86	0	0	2	0
All	All	9989	0	8881	130	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 7.

All (130) 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:18:VAL:HG12	1:A:70:LYS:HG2	1.77	0.67
1:C:30:LEU:HD13	1:C:151:VAL:HG21	1.77	0.66
1:A:285:THR:HG1	1:B:285:THR:HG1	1.33	0.65
1:B:168:MET:HE1	1:B:190:ASP:HA	1.79	0.64
1:D:216:LEU:HD13	1:D:300:ILE:HD13	1.80	0.63
1:B:167:GLN:HB3	1:B:168:MET:HE3	1.81	0.63
1:A:126[A]:THR:HG22	1:B:298:MET:CE	2.28	0.63
1:A:105:THR:HA	2:A:402:GOL:H12	1.82	0.62
1:C:293:PRO:HD2	2:C:402:GOL:H11	1.82	0.61
1:D:172[B]:ASN:ND2	4:D:506:HOH:O	2.34	0.60
1:D:233[B]:PHE:CD2	1:D:266:LEU:HD22	2.38	0.59
1:C:302:GLY:HA3	2:C:405:GOL:H31	1.84	0.58
1:D:57:LEU:O	1:D:61:MET:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:OD1	1:A:190:ASP:N	2.32	0.58
1:C:168:MET:HE2	1:C:184:MET:HE3	1.84	0.58
1:D:161:ASN:ND2	4:D:507:HOH:O	2.37	0.57
1:D:233[A]:PHE:CD2	1:D:266:LEU:HD22	2.39	0.57
1:B:190:ASP:OD1	1:B:190:ASP:N	2.33	0.57
1:C:114:ALA:H	2:C:404:GOL:H2	1.70	0.56
1:A:166:HIS:HE1	1:A:175:HIS:HB3	1.70	0.56
1:D:27:LEU:HD13	1:D:39:PRO:HD2	1.88	0.56
1:A:249:GLN:O	1:A:253:MET:HG3	2.06	0.55
1:D:40:ARG:NE	1:D:88:THR:HA	2.21	0.55
1:A:40:ARG:HA	1:A:90:LEU:HG	1.88	0.55
1:C:12:ASP:HB2	1:C:160:ILE:HD11	1.90	0.55
1:B:118:LEU:HD11	1:B:125:PRO:HB3	1.90	0.54
1:D:300:ILE:HG13	1:D:301:MET:N	2.22	0.54
1:A:298[A]:MET:O	1:A:298[A]:MET:HE2	2.08	0.53
1:C:152:GLY:HA3	1:C:164:TYR:HB3	1.89	0.53
1:C:293:PRO:HG2	2:C:402:GOL:H32	1.91	0.53
1:C:111:PRO:HB3	1:C:135:PRO:HA	1.92	0.52
1:D:83:HIS:O	1:D:83:HIS:ND1	2.43	0.52
1:C:166:HIS:HE1	1:C:175:HIS:HB3	1.75	0.51
1:B:111:PRO:HB3	1:B:135:PRO:HA	1.93	0.51
1:B:105:THR:OG1	1:B:161:ASN:OD1	2.27	0.51
1:A:298[A]:MET:CE	4:A:617:HOH:O	2.59	0.51
1:B:166:HIS:HE1	1:B:175:HIS:HB3	1.76	0.50
1:D:214:ALA:HB1	1:D:219:CYS:HB3	1.92	0.50
1:B:178:SER:HA	1:B:184:MET:HA	1.92	0.50
1:C:40:ARG:HA	1:C:90:LEU:HG	1.94	0.50
1:D:54:TYR:OH	1:D:190:ASP:O	2.28	0.50
1:D:62:THR:OG1	1:D:63:ASN:N	2.44	0.50
1:C:190:ASP:OD1	1:C:190:ASP:N	2.44	0.50
1:B:105:THR:HG23	1:B:159:VAL:HG21	1.94	0.50
1:A:126[A]:THR:CG2	1:B:298:MET:CE	2.90	0.50
1:A:49:LEU:HD22	1:D:305:MET:HG3	1.94	0.49
1:A:241:GLN:HE21	1:A:241:GLN:HA	1.78	0.49
1:B:216:LEU:HD21	1:B:257:LYS:HG2	1.95	0.49
1:D:124:ARG:HH11	1:D:124:ARG:HG3	1.76	0.49
1:D:55:ASP:OD1	1:D:55:ASP:N	2.45	0.49
1:D:209:ALA:HB2	1:D:293:PRO:HG3	1.95	0.48
1:D:118:LEU:HD11	1:D:125:PRO:HB3	1.95	0.48
1:D:261:ALA:HB3	1:D:264[A]:GLN:HG3	1.95	0.48
1:A:118:LEU:HD11	1:A:125:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:MET:SD	1:D:61:MET:HG3	2.54	0.48
1:D:261:ALA:HB3	1:D:264[B]:GLN:HG3	1.95	0.48
1:D:40:ARG:NH1	1:D:54:TYR:CD2	2.82	0.47
1:D:202:TYR:O	1:D:243:THR:HG23	2.13	0.47
1:C:17:MET:HG3	1:C:120:CYS:SG	2.54	0.47
1:C:88:THR:HG21	1:C:184:MET:HE2	1.95	0.47
1:D:111:PRO:HB3	1:D:135:PRO:HA	1.95	0.47
1:D:152:GLY:HA3	1:D:164:TYR:HB3	1.96	0.47
1:D:228:THR:HG23	1:D:232:SER:HB3	1.96	0.47
1:A:5[B]:LYS:NZ	4:A:510:HOH:O	2.44	0.47
1:A:111:PRO:HB3	1:A:135:PRO:HA	1.98	0.46
1:D:134:ARG:HE	1:D:134:ARG:HB3	1.58	0.46
1:A:44:CYS:SG	1:A:52:PRO:HB3	2.56	0.46
2:C:403:GOL:H32	1:D:298:MET:O	2.16	0.46
1:D:110:LYS:HD2	1:D:110:LYS:C	2.41	0.46
1:D:190:ASP:OD1	1:D:190:ASP:N	2.31	0.46
1:B:171:ALA:HB2	1:B:197:GLN:HE22	1.81	0.45
1:D:227:ARG:HB2	1:D:263:GLU:HB3	1.98	0.45
1:D:203:CYS:O	1:D:207:VAL:HG23	2.16	0.45
1:B:57:LEU:O	1:B:61:MET:HG2	2.17	0.45
1:D:250:SER:HB2	1:D:293:PRO:HB2	1.97	0.45
1:C:55:ASP:O	1:C:59:ILE:HG13	2.17	0.45
1:C:162:PHE:HB3	1:C:180:PHE:CE1	2.53	0.44
1:C:189:MET:O	1:C:195:GLN:NE2	2.47	0.44
1:A:250[B]:SER:HB3	1:A:293:PRO:HB2	1.99	0.44
1:D:72:ILE:HG12	1:D:125:PRO:HD2	2.00	0.44
1:A:250[A]:SER:HB3	1:A:293:PRO:HB2	1.99	0.44
1:A:126[A]:THR:HG22	1:B:298:MET:HE3	2.00	0.43
1:B:168:MET:HB3	1:B:168:MET:HE2	1.45	0.43
1:D:108:THR:HG23	1:D:185:TYR:HE1	1.84	0.43
1:D:136:ASN:ND2	1:D:200:ASP:HB2	2.33	0.43
1:D:216:LEU:HD13	1:D:300:ILE:CD1	2.48	0.43
1:D:271:GLN:HE21	1:D:271:GLN:HB3	1.63	0.43
1:A:135:PRO:HD2	1:A:200:ASP:OD1	2.18	0.43
1:C:98:ASN:HB3	1:C:101:THR:OG1	2.18	0.43
1:C:132:VAL:HG21	1:C:290:GLU:HA	2.01	0.43
1:A:39:PRO:HG2	1:A:148:ALA:HB1	2.01	0.43
1:A:166:HIS:NE2	1:D:306:GLN:OE1	2.40	0.43
1:D:18:VAL:HG12	1:D:70:LYS:HB2	2.01	0.43
1:D:234:ASN:ND2	1:D:244:GLU:HG3	2.34	0.43
1:B:203:CYS:HB2	1:B:289:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASN:OD1	1:B:226:ASN:N	2.52	0.42
1:A:98:ASN:HB3	1:A:101:THR:OG1	2.20	0.42
1:A:152:GLY:HA3	1:A:164:TYR:HB3	2.00	0.42
1:B:71:HIS:HB3	1:B:124:ARG:NH2	2.35	0.42
1:B:27:LEU:HD22	1:B:148:ALA:HB3	2.02	0.42
1:D:45:PRO:O	1:D:49:LEU:HG	2.20	0.42
1:D:27:LEU:CD1	1:D:39:PRO:HD2	2.49	0.42
1:A:43:MET:HE3	1:A:57:LEU:HB3	2.01	0.42
1:B:37[A]:TRP:CH2	1:B:91:LYS:HD2	2.55	0.42
1:A:28:ASN:ND2	1:A:120:CYS:O	2.53	0.42
1:B:184:MET:HE2	1:B:184:MET:HB2	1.90	0.42
1:B:44:CYS:SG	1:B:52:PRO:HB3	2.60	0.41
1:B:88:THR:HG21	1:B:184:MET:HE2	2.02	0.41
1:D:10:SER:OG	1:D:14:GLU:OE2	2.29	0.41
1:A:6[A]:MET:HE2	1:B:127:GLY:HA3	2.03	0.41
1:C:8:HIS:ND1	1:C:155:LYS:HB2	2.36	0.41
1:C:25:MET:HE3	1:C:25:MET:HB3	1.98	0.41
1:C:40:ARG:HD2	1:C:85:MET:SD	2.60	0.41
1:D:133:MET:HE1	1:D:185:TYR:CG	2.56	0.41
1:D:233[B]:PHE:CG	1:D:266:LEU:HD22	2.56	0.41
1:A:69:GLN:HB3	1:A:71:HIS:CE1	2.55	0.41
1:A:166:HIS:CE1	1:A:175:HIS:HB3	2.54	0.41
1:D:82:GLY:O	1:D:93:THR:N	2.50	0.41
1:A:58:LEU:HD22	1:A:85:MET:HB3	2.02	0.41
1:A:204[A]:SER:OG	1:A:243:THR:O	2.38	0.41
1:D:132:VAL:HG21	1:D:290:GLU:HA	2.03	0.41
1:D:109:VAL:HG22	1:D:163:CYS:HB2	2.01	0.41
1:A:194:HIS:HA	1:D:302:GLY:HA2	2.03	0.40
1:D:184:MET:HE2	1:D:184:MET:HB2	1.89	0.40
1:B:26:THR:O	1:B:27:LEU:HD23	2.21	0.40
1:B:227:ARG:HB3	1:B:263:GLU:HB3	2.02	0.40
1:A:14:GLU:HG2	1:A:125:PRO:HG2	2.02	0.40
1:A:178:SER:HA	1:A:184[A]:MET:HA	2.03	0.40
1:A:178:SER:HA	1:A:184[B]:MET:HA	2.03	0.40
1:D:134:ARG:HB3	1:D:200:ASP:OD1	2.22	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	319/306 (104%)	310 (97%)	7 (2%)	2 (1%)	21	38
1	B	310/306 (101%)	305 (98%)	5 (2%)	0	100	100
1	C	310/306 (101%)	303 (98%)	7 (2%)	0	100	100
1	D	311/306 (102%)	297 (96%)	13 (4%)	1 (0%)	36	55
All	All	1250/1224 (102%)	1215 (97%)	32 (3%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	236	TRP
1	A	72	ILE
1	A	74	ALA

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	260/256 (102%)	248 (95%)	12 (5%)	24	48
1	B	245/256 (96%)	241 (98%)	4 (2%)	55	79
1	C	254/256 (99%)	246 (97%)	8 (3%)	35	62
1	D	223/256 (87%)	206 (92%)	17 (8%)	12	26
All	All	982/1024 (96%)	941 (96%)	41 (4%)	28	52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	94	VAL
1	A	132	VAL
1	A	151	VAL
1	A	170[A]	LEU
1	A	170[B]	LEU
1	A	190	ASP
1	A	192	GLN
1	A	250[A]	SER
1	A	250[B]	SER
1	A	298[A]	MET
1	A	298[B]	MET
1	B	49	LEU
1	B	159	VAL
1	B	190	ASP
1	B	250	SER
1	C	27	LEU
1	C	86	GLN
1	C	196	VAL
1	C	197	GLN
1	C	199	THR
1	C	249	GLN
1	C	250	SER
1	C	285	THR
1	D	24	SER
1	D	26	THR
1	D	27	LEU
1	D	60	SER
1	D	62	THR
1	D	72	ILE
1	D	88	THR
1	D	109	VAL
1	D	151	VAL
1	D	154	THR
1	D	172[A]	ASN
1	D	172[B]	ASN
1	D	190	ASP
1	D	211	LEU
1	D	226	ASN
1	D	227	ARG
1	D	284	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	172	ASN
1	A	240	ASN
1	B	69	GLN
1	B	71	HIS
1	B	77	ASN
1	B	197	GLN
1	B	240	ASN
1	B	271	GLN
1	C	240	ASN
1	D	249	GLN

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](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	401	-	5,5,5	0.98	0	5,5,5	1.04	0
2	GOL	A	401	-	5,5,5	0.91	0	5,5,5	1.11	0
2	GOL	C	403	-	5,5,5	0.96	0	5,5,5	1.05	0
2	GOL	C	405	-	5,5,5	0.95	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	402	-	5,5,5	0.94	0	5,5,5	1.05	0
2	GOL	C	404	-	5,5,5	0.95	0	5,5,5	1.04	0
2	GOL	C	401	-	5,5,5	0.99	0	5,5,5	1.03	0
2	GOL	A	403	-	5,5,5	0.94	0	5,5,5	1.08	0
2	GOL	C	402	-	5,5,5	0.97	0	5,5,5	1.00	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	B	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	C	403	-	-	0/4/4/4	-
2	GOL	C	405	-	-	0/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	C	404	-	-	4/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	A	403	-	-	0/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	C	401	GOL	C1-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	C	402	GOL	O1-C1-C2-C3
2	C	404	GOL	O1-C1-C2-O2
2	C	404	GOL	C1-C2-C3-O3
2	C	404	GOL	O2-C2-C3-O3
2	A	402	GOL	C1-C2-C3-O3
2	C	402	GOL	C1-C2-C3-O3
2	C	404	GOL	O1-C1-C2-C3
2	A	401	GOL	O1-C1-C2-O2

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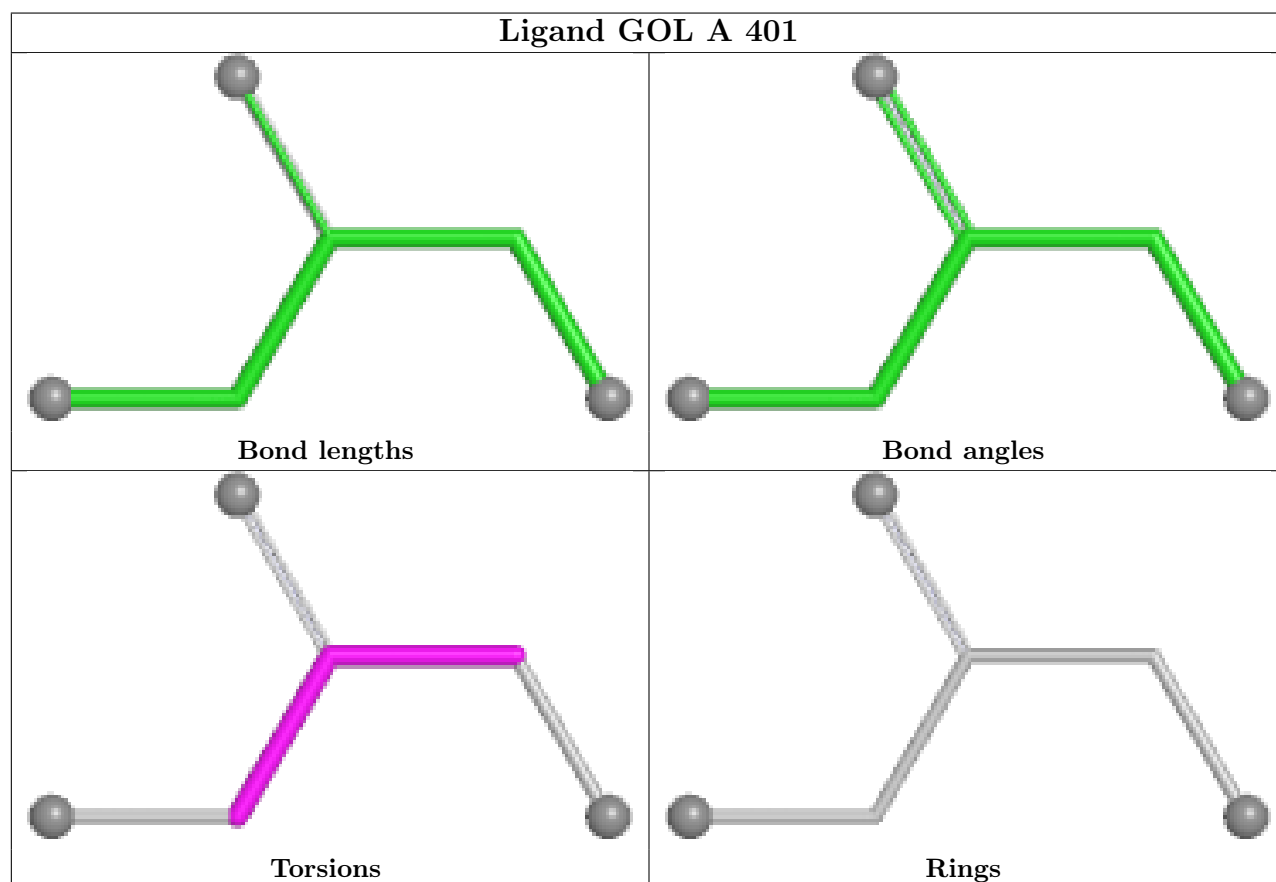
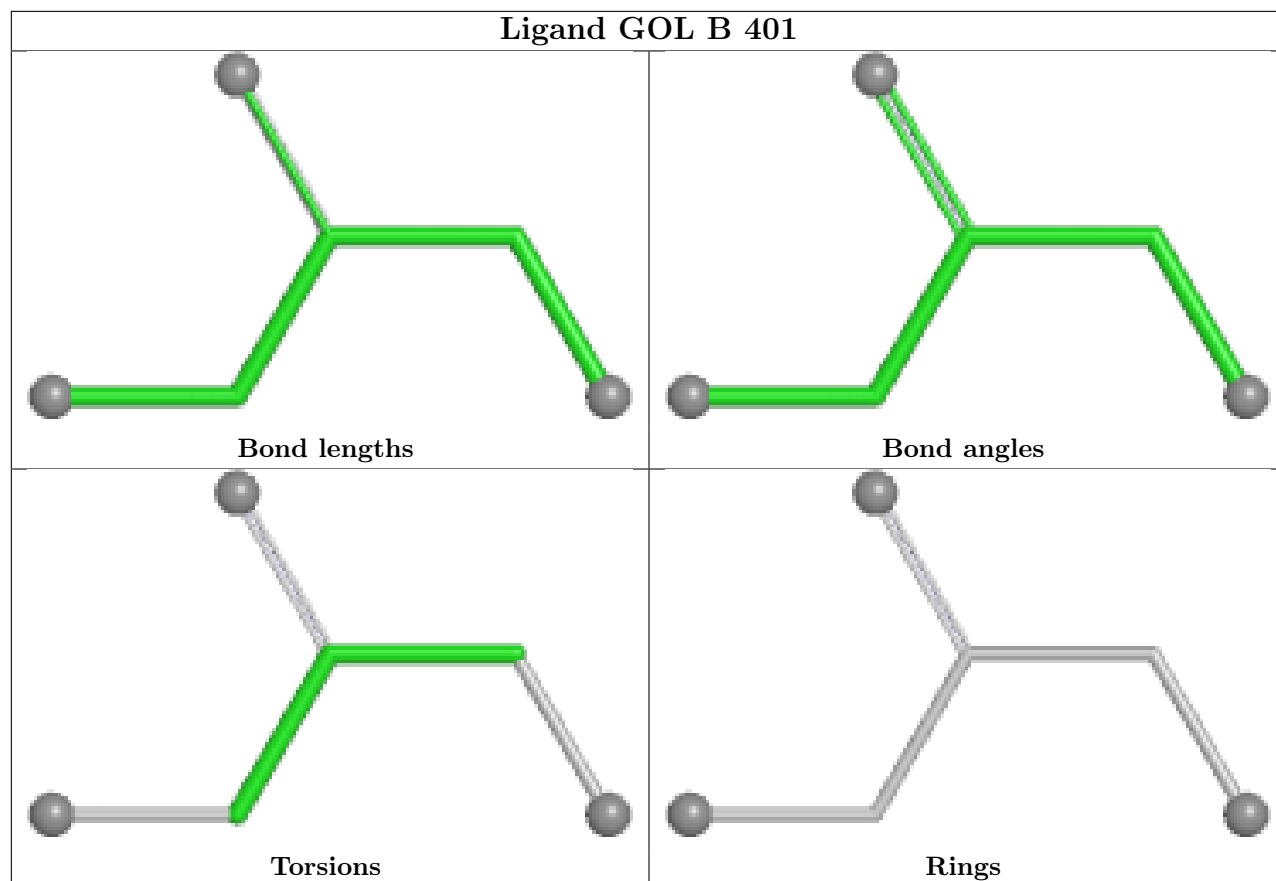
Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O2-C2-C3-O3
2	C	402	GOL	O1-C1-C2-O2
2	C	402	GOL	O2-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3

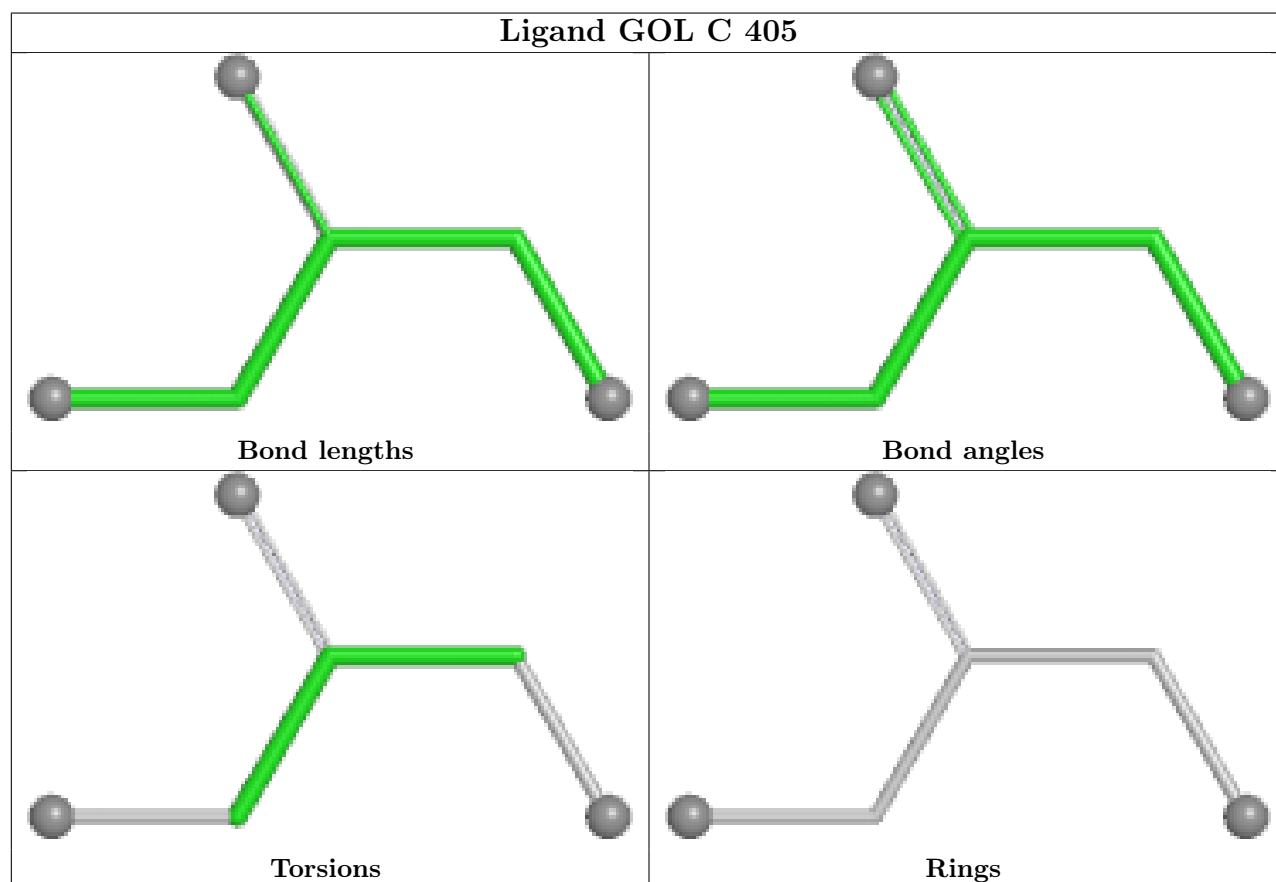
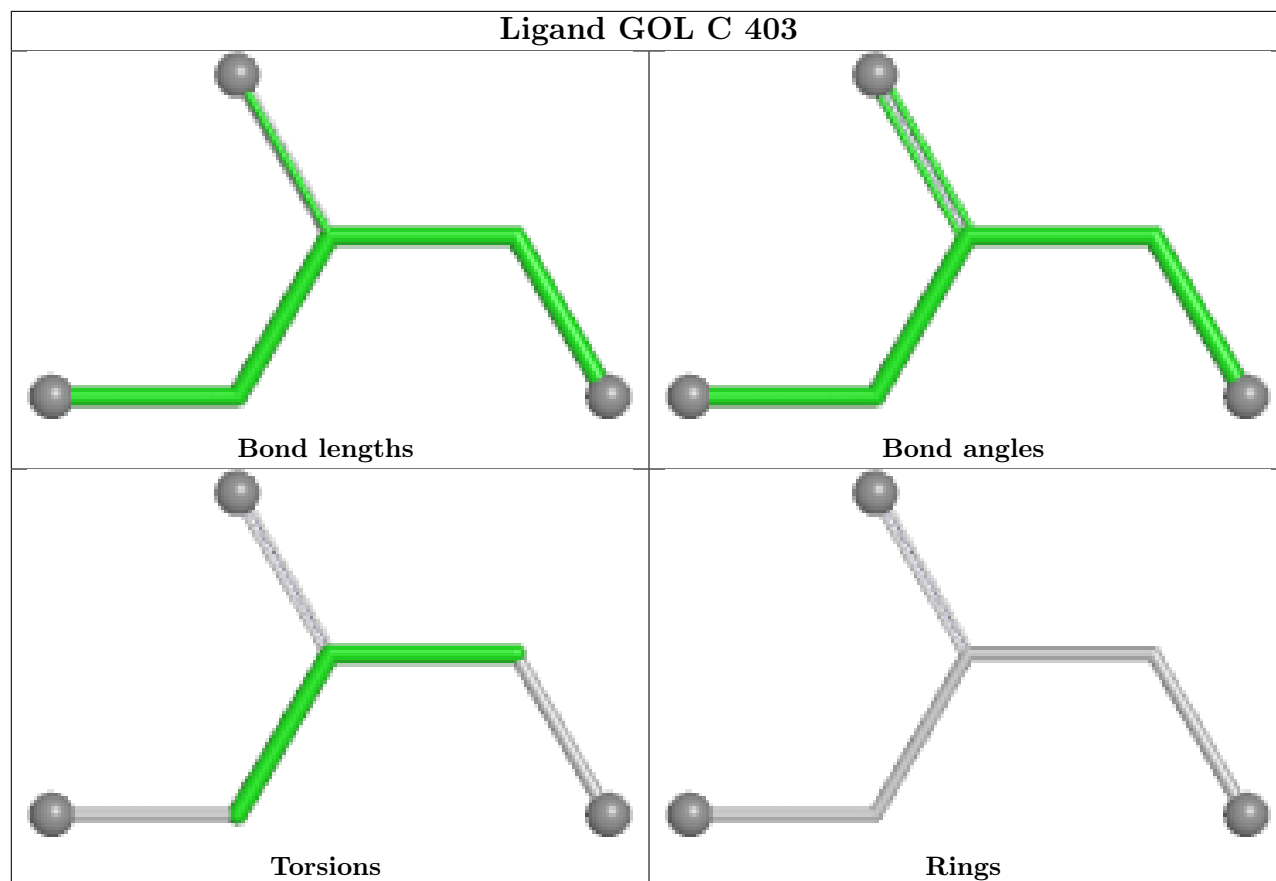
There are no ring outliers.

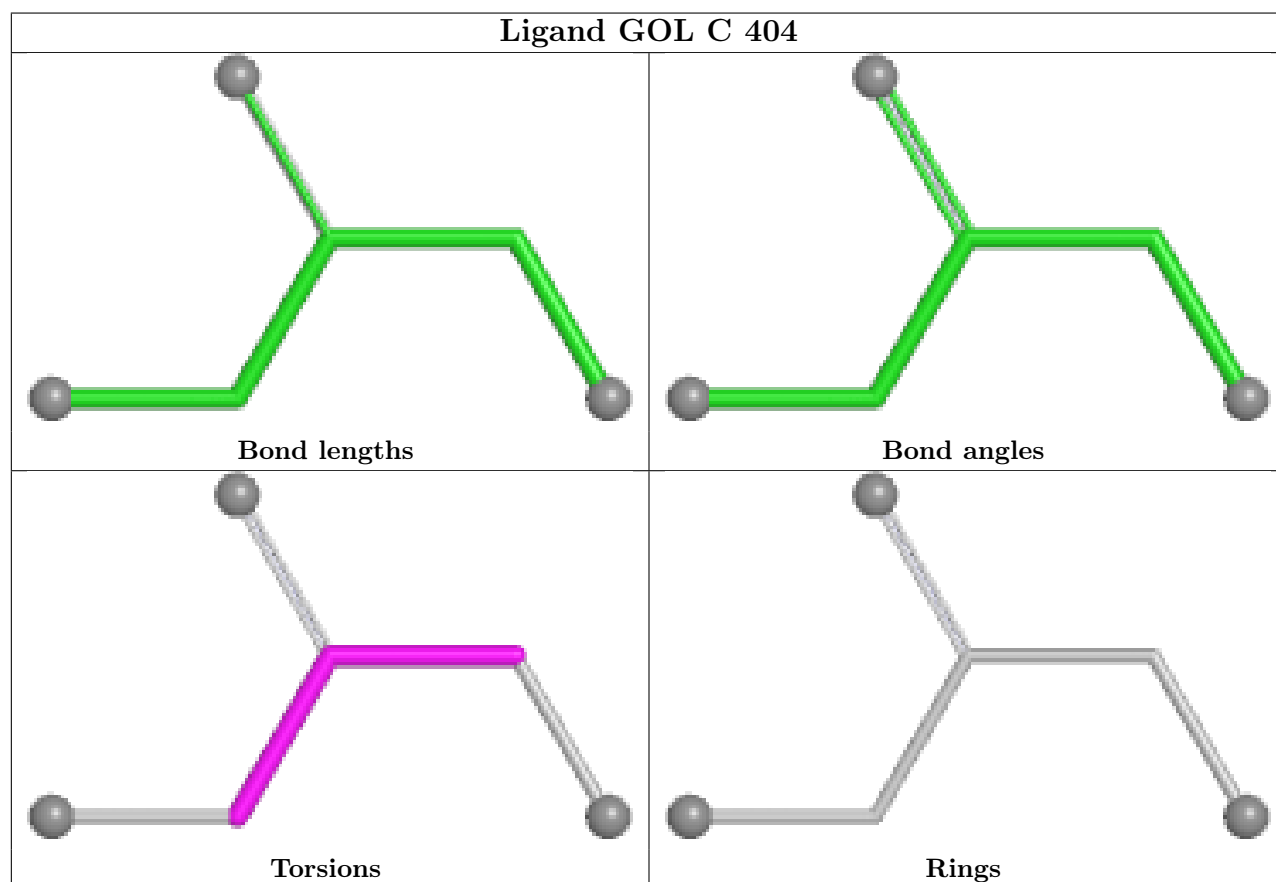
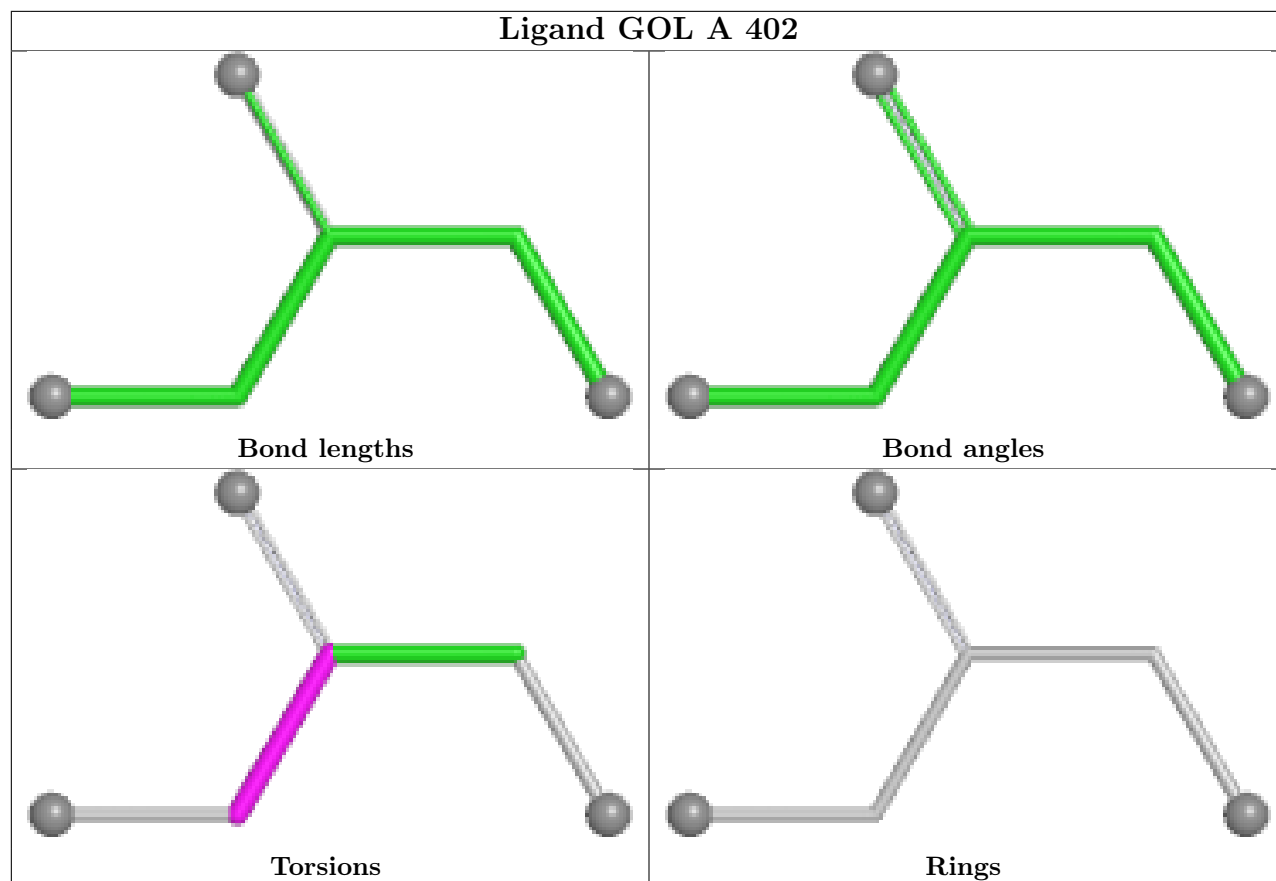
5 monomers are involved in 6 short contacts:

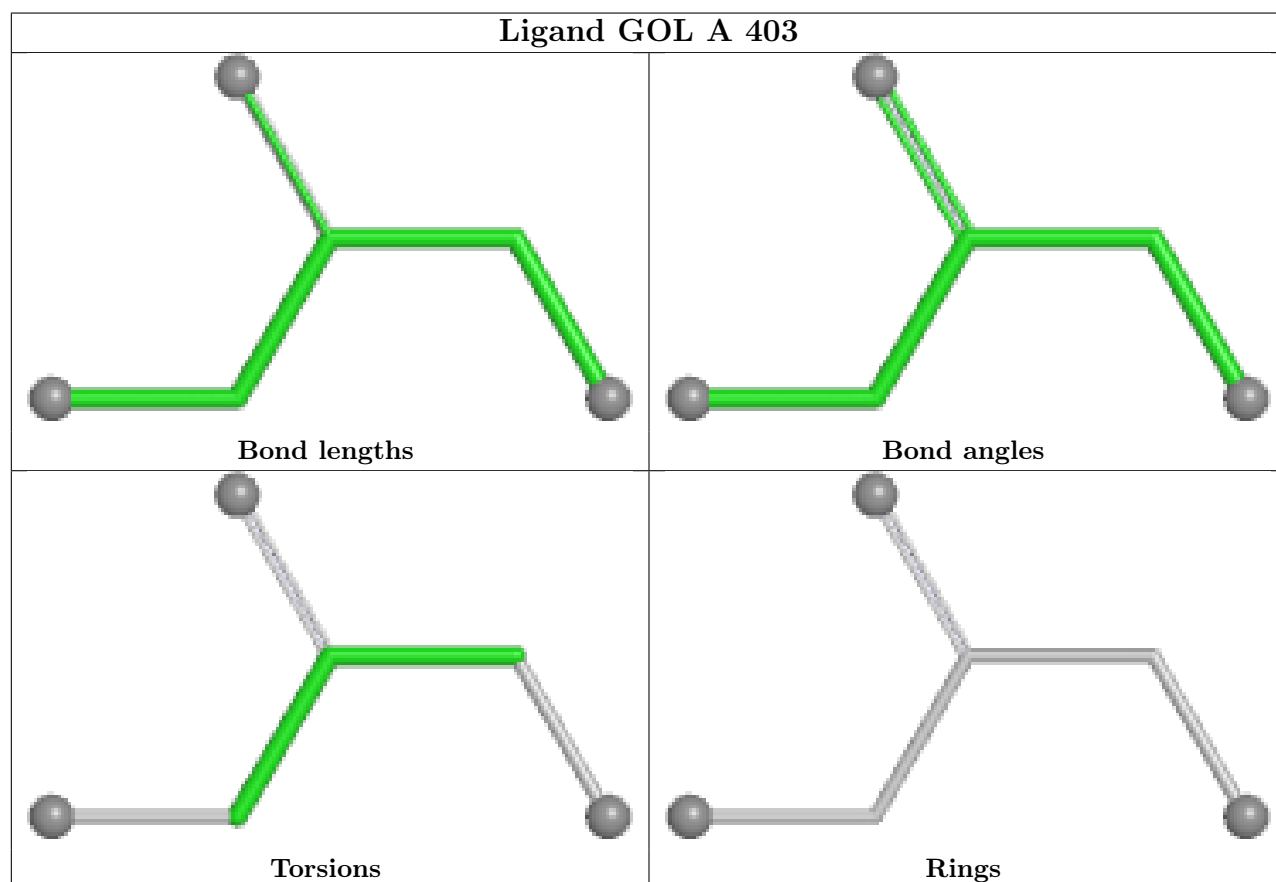
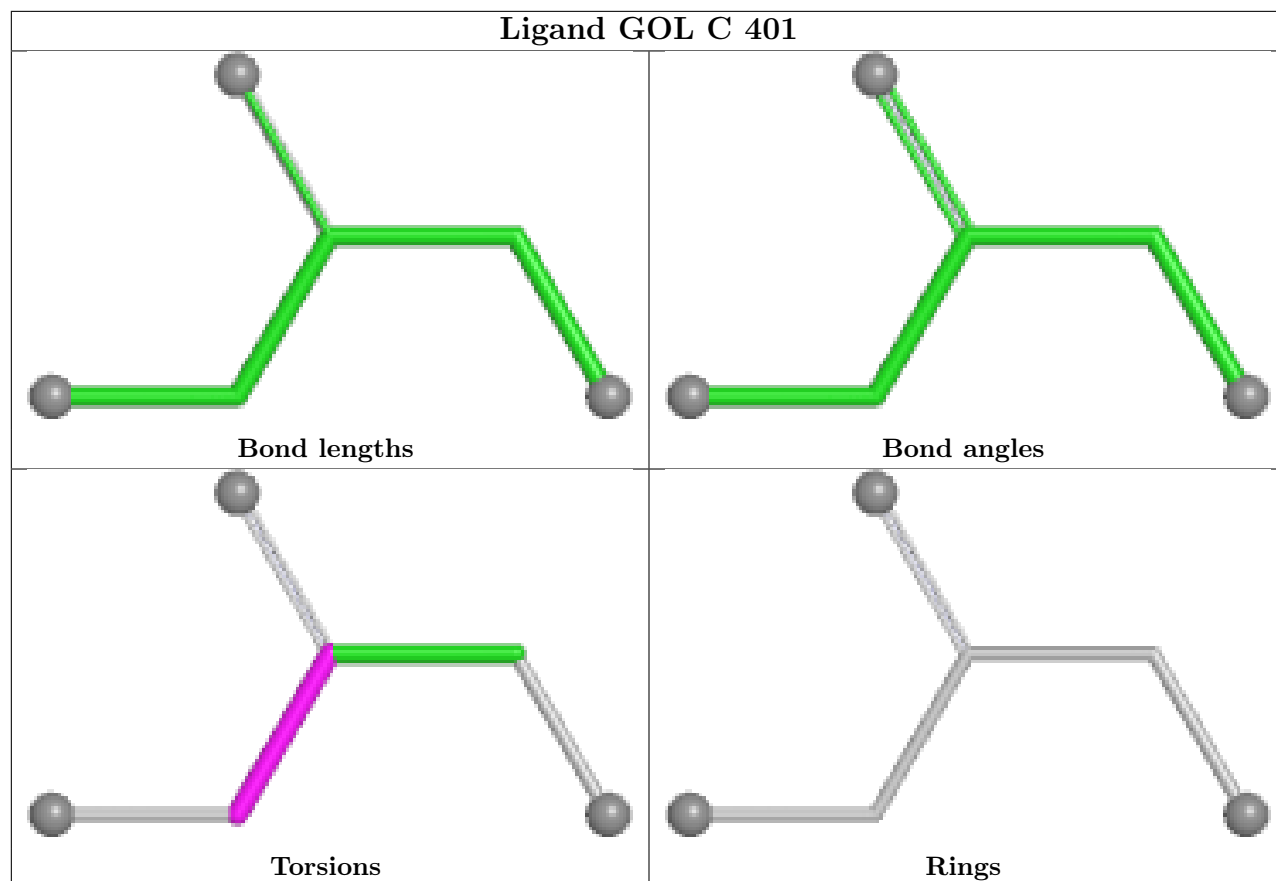
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	GOL	1	0
2	C	405	GOL	1	0
2	A	402	GOL	1	0
2	C	404	GOL	1	0
2	C	402	GOL	2	0

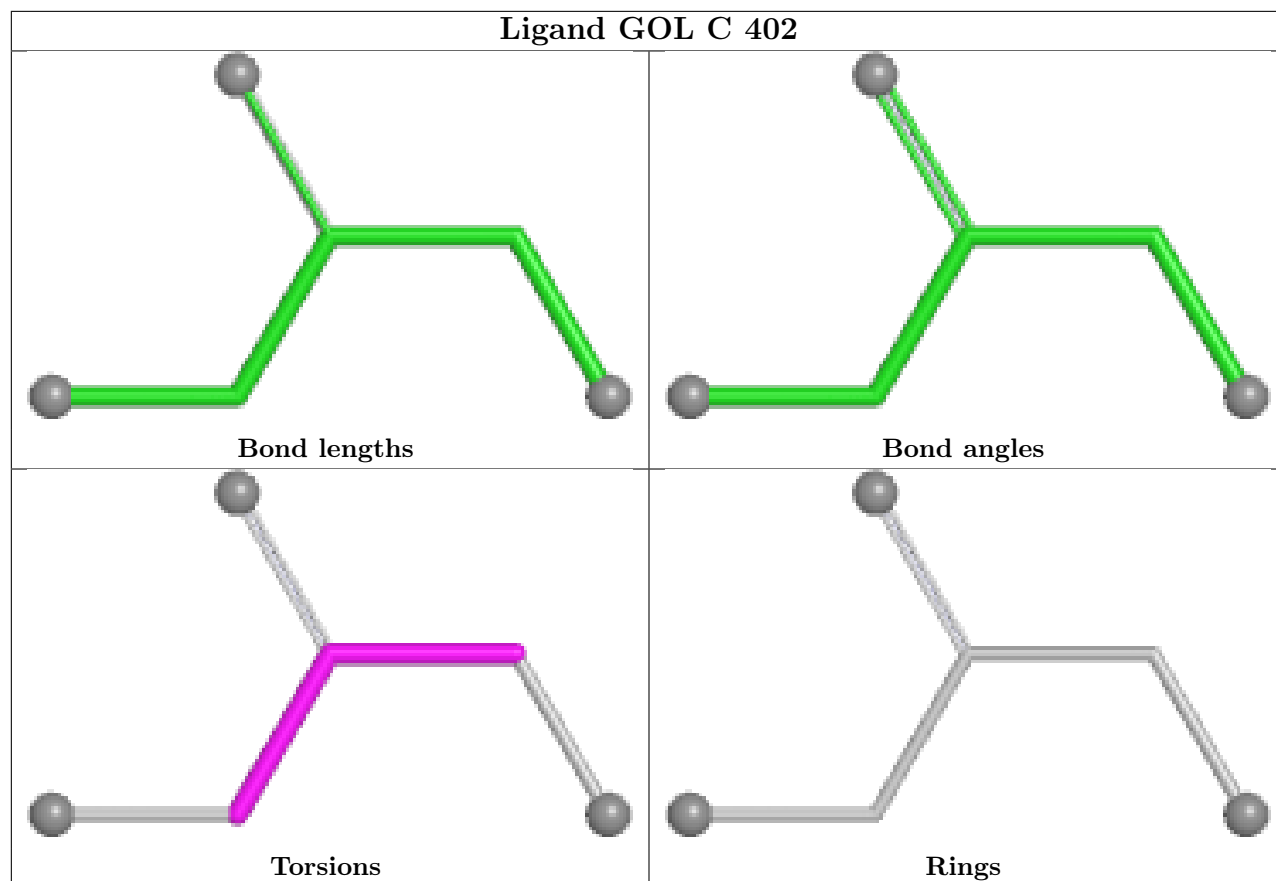
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	306/306 (100%)	-0.34	6 (1%) 65 61	9, 24, 50, 111	16 (5%)
1	B	303/306 (99%)	0.02	3 (0%) 79 76	13, 37, 58, 82	9 (2%)
1	C	302/306 (98%)	-0.42	1 (0%) 90 87	11, 25, 47, 71	10 (3%)
1	D	306/306 (100%)	0.74	30 (9%) 13 11	11, 49, 76, 87	7 (2%)
All	All	1217/1224 (99%)	0.00	40 (3%) 49 45	9, 32, 67, 111	42 (3%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	GLY	5.2
1	A	72	ILE	3.9
1	D	197	GLN	3.7
1	B	277	GLN	3.0
1	B	46	ALA	3.0
1	A	74	ALA	2.9
1	D	186	GLY	2.7
1	D	73	GLY	2.7
1	A	77	ASN	2.7
1	C	284[A]	SER	2.7
1	D	220	ALA	2.7
1	D	58	LEU	2.6
1	D	185	TYR	2.6
1	D	239	ALA	2.6
1	D	187	ALA	2.6
1	D	275	GLY	2.5
1	D	64	HIS	2.5
1	D	38	CYS	2.5
1	D	300	ILE	2.5
1	D	236	TRP	2.5
1	D	76	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	57	LEU	2.4
1	A	145	CYS	2.4
1	D	77	ASN	2.4
1	D	237	ALA	2.4
1	D	274	THR	2.3
1	D	242	PHE	2.3
1	D	46	ALA	2.2
1	D	132	VAL	2.2
1	D	133	MET	2.2
1	D	158	SER	2.2
1	D	183	THR	2.2
1	D	75	PRO	2.2
1	D	109	VAL	2.1
1	A	300	ILE	2.1
1	B	168	MET	2.1
1	D	85	MET	2.1
1	D	177	GLY	2.1
1	D	54	TYR	2.1
1	D	273	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

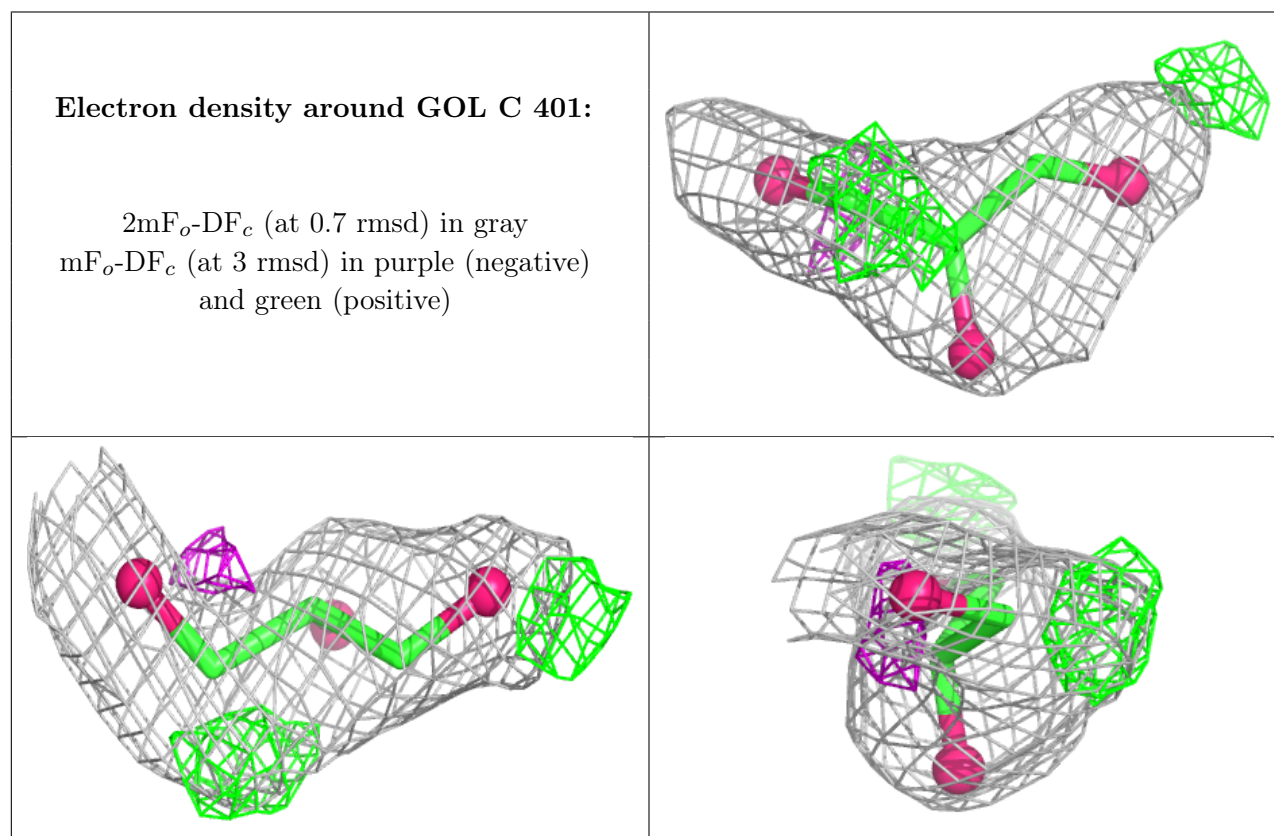
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	401	6/6	0.70	0.17	38,46,48,48	0
2	GOL	C	402	6/6	0.74	0.20	36,49,54,62	0
3	NA	D	401	1/1	0.77	0.17	64,64,64,64	0
2	GOL	C	405	6/6	0.81	0.13	46,61,72,73	0

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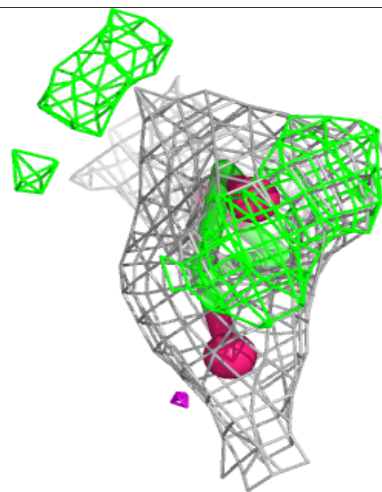
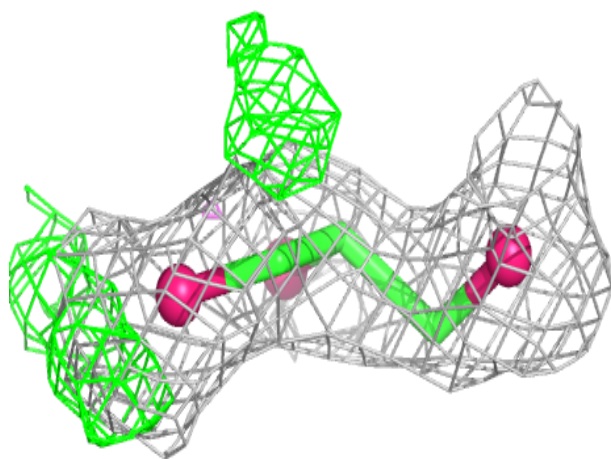
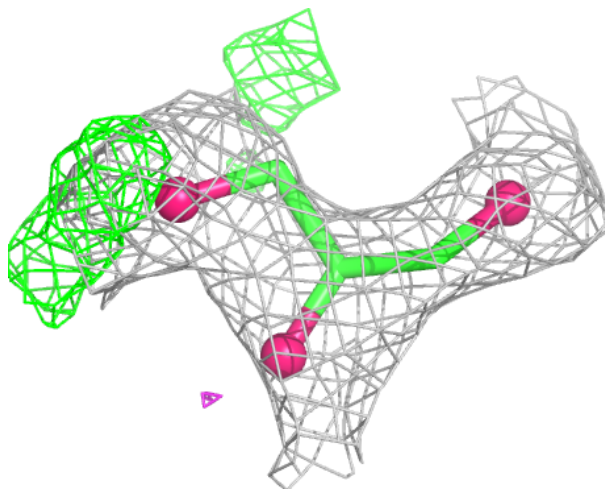
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	403	1/1	0.83	0.20	59,59,59,59	0
2	GOL	A	403	6/6	0.87	0.13	35,47,55,57	0
2	GOL	C	403	6/6	0.87	0.14	45,51,62,65	0
2	GOL	C	404	6/6	0.87	0.18	36,41,59,60	0
2	GOL	A	402	6/6	0.88	0.12	40,41,44,62	0
3	NA	B	404	1/1	0.89	0.07	52,52,52,52	0
3	NA	B	402	1/1	0.89	0.09	53,53,53,53	0
2	GOL	B	401	6/6	0.90	0.14	25,33,39,47	0
2	GOL	A	401	6/6	0.91	0.12	25,49,54,58	0
3	NA	C	406	1/1	0.94	0.12	53,53,53,53	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.



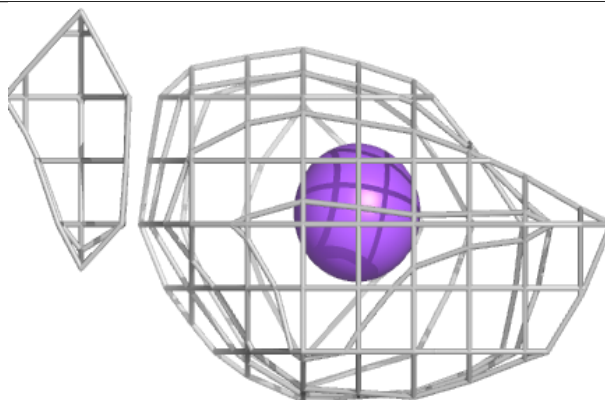
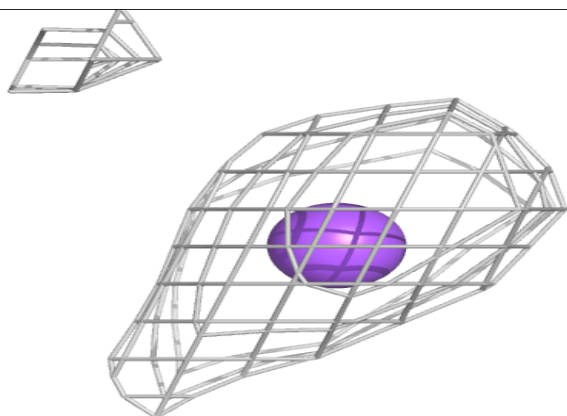
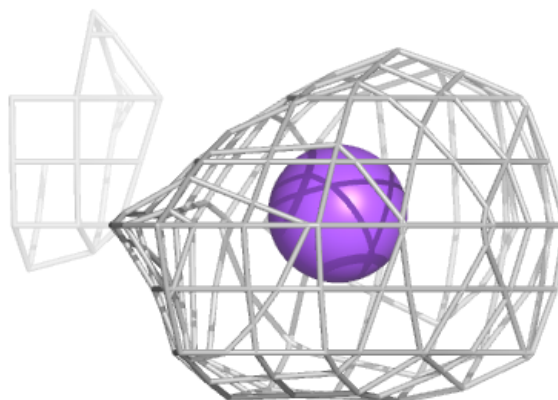
Electron density around GOL C 402:

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

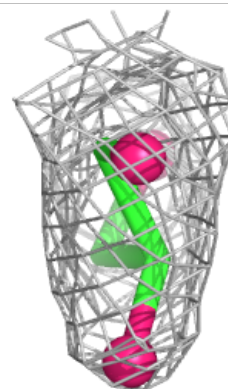
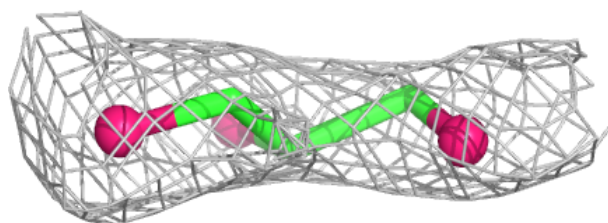
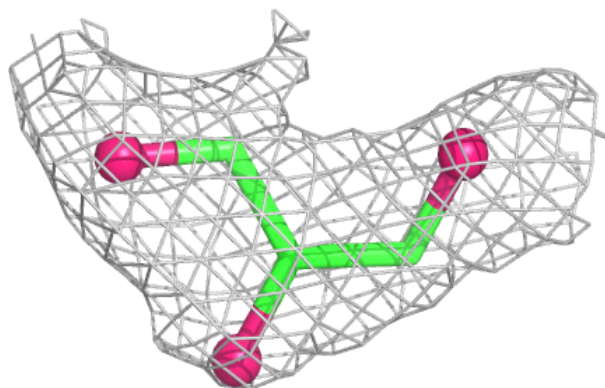


Electron density around NA D 401:

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

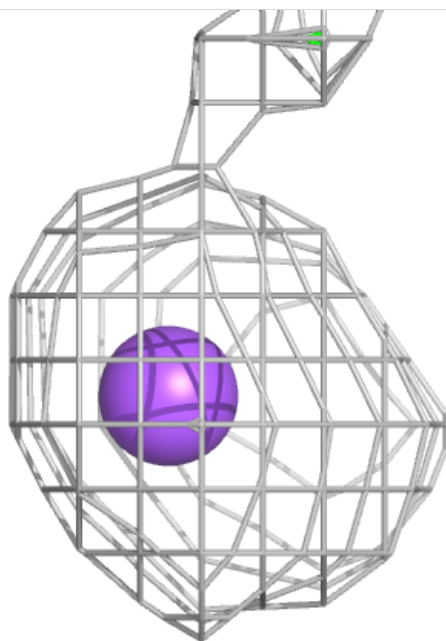
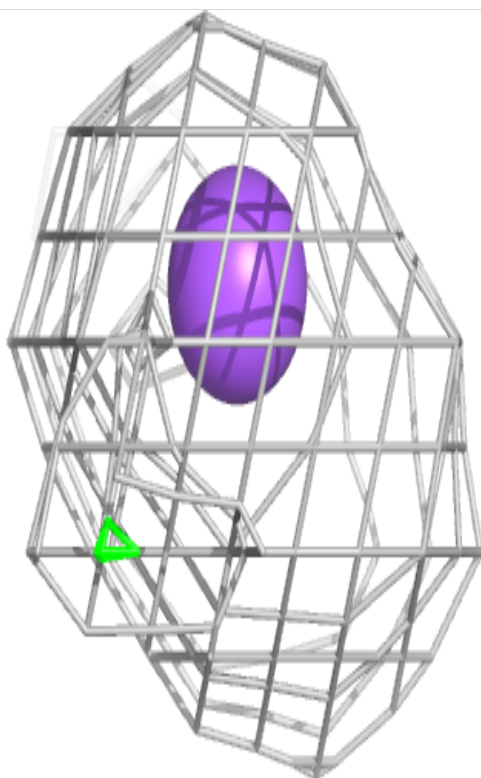
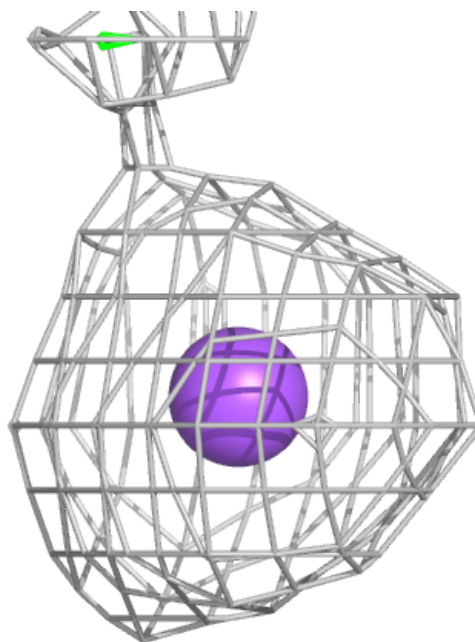
**Electron density around GOL C 405:**

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



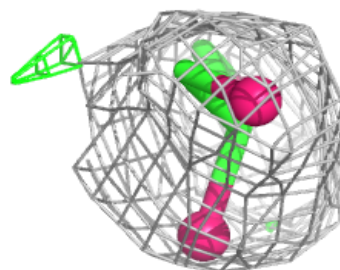
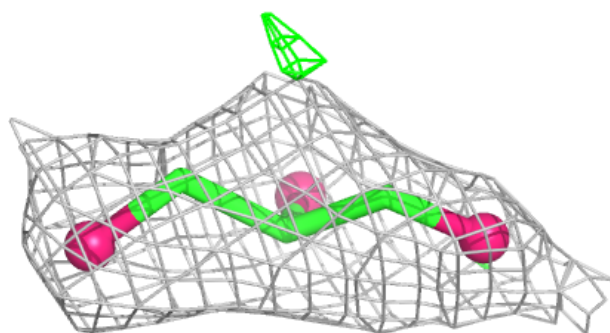
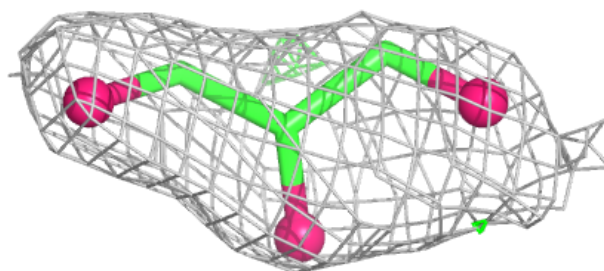
Electron density around NA B 403:

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and green (positive)

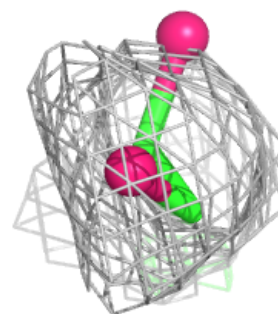
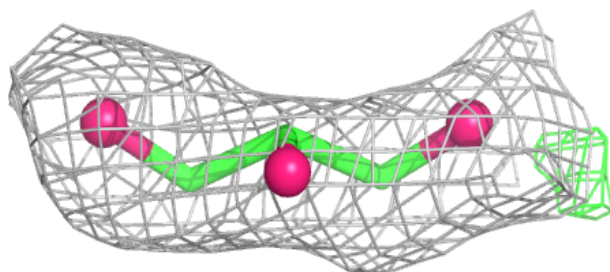
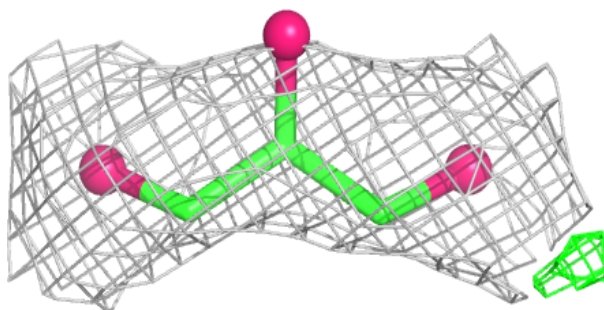


Electron density around GOL A 403:

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and green (positive)

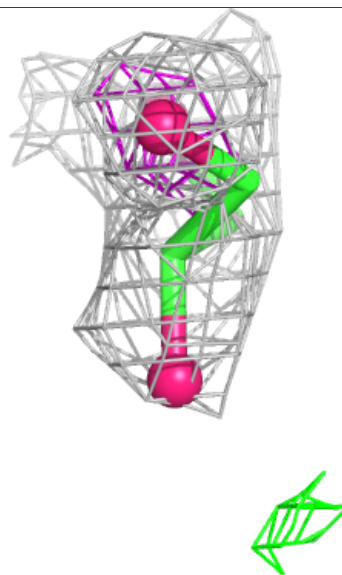
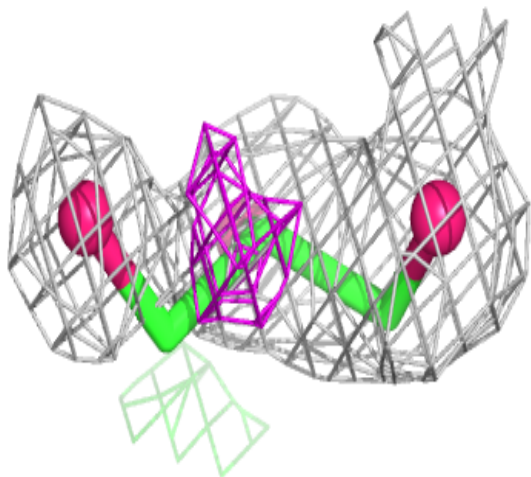
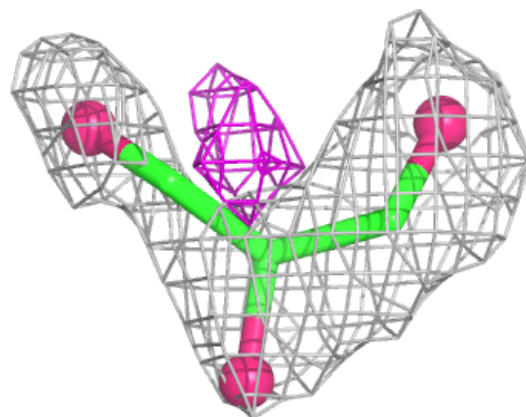
**Electron density around GOL C 403:**

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



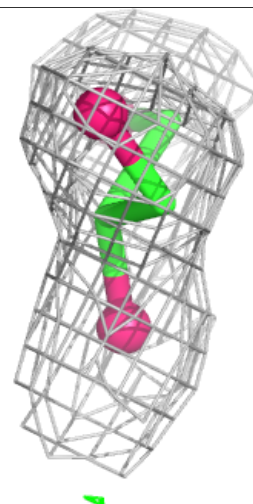
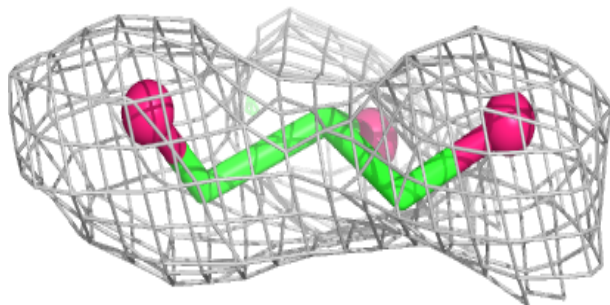
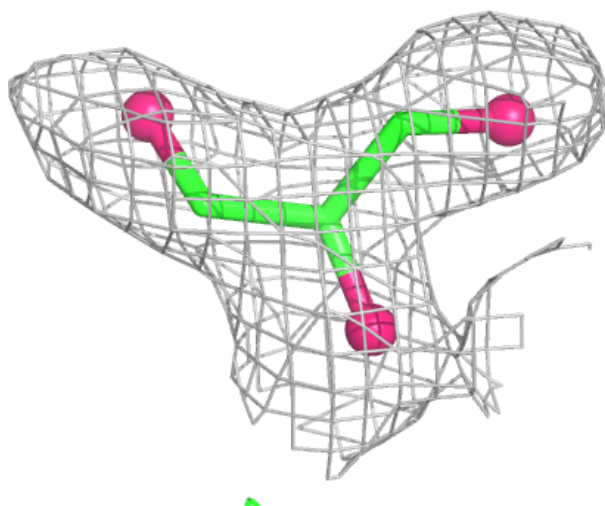
Electron density around GOL C 404:

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



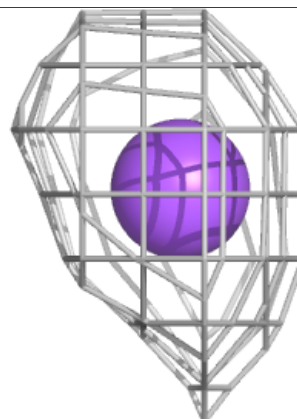
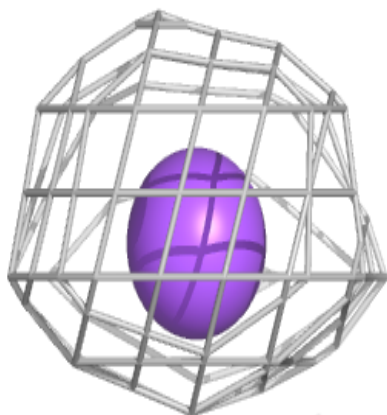
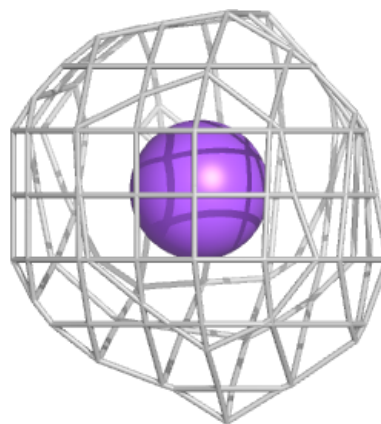
Electron density around GOL A 402:

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



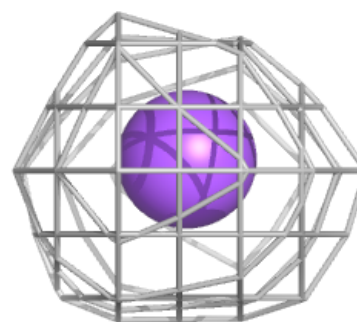
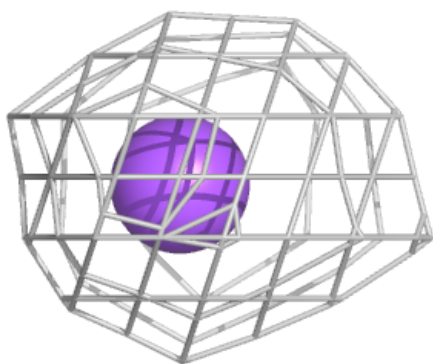
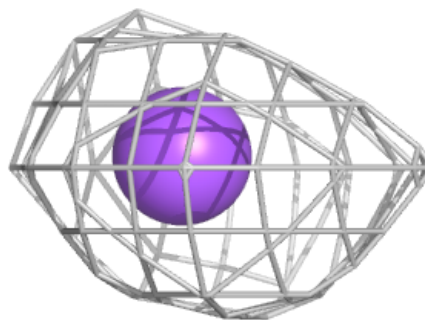
Electron density around NA B 404:

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

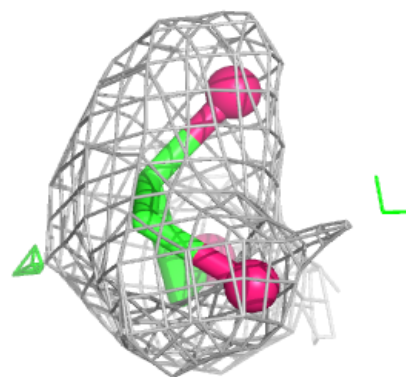
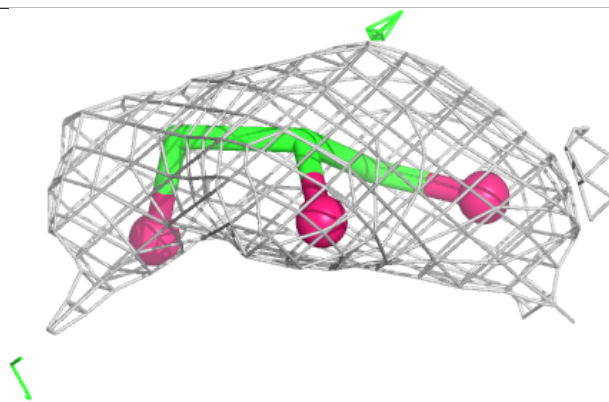
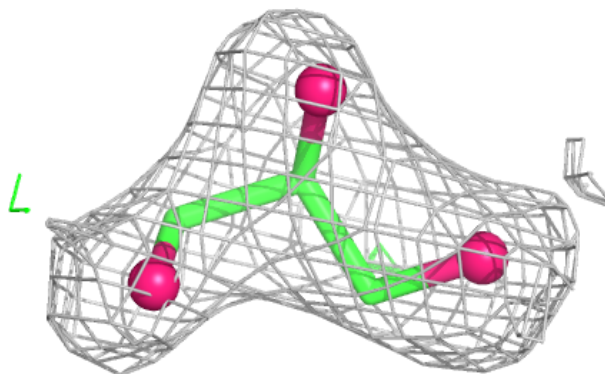


Electron density around NA B 402:

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

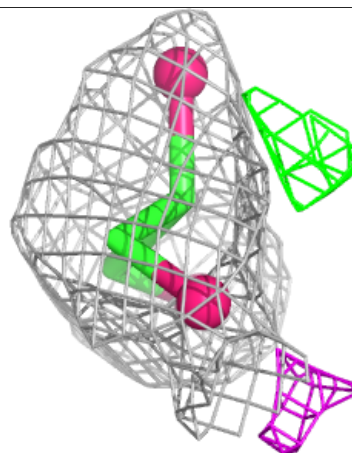
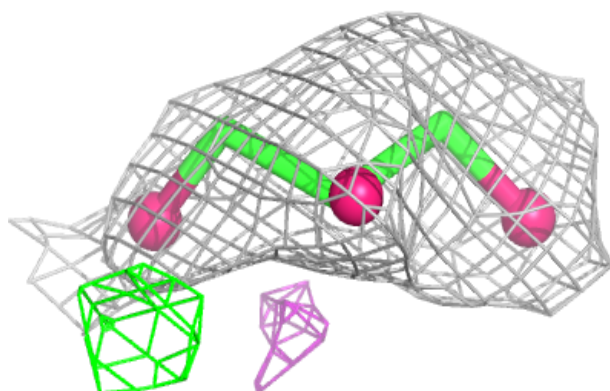
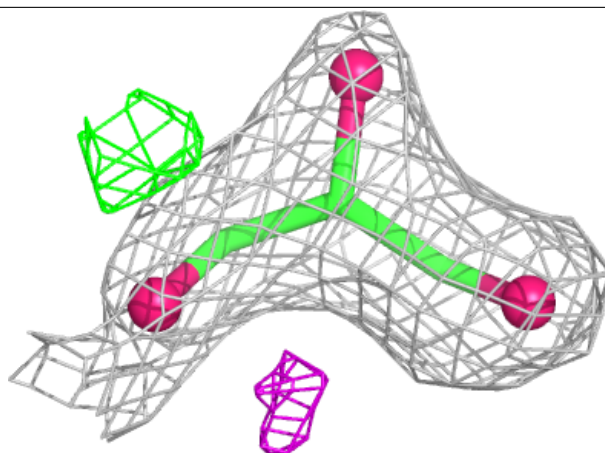
**Electron density around GOL B 401:**

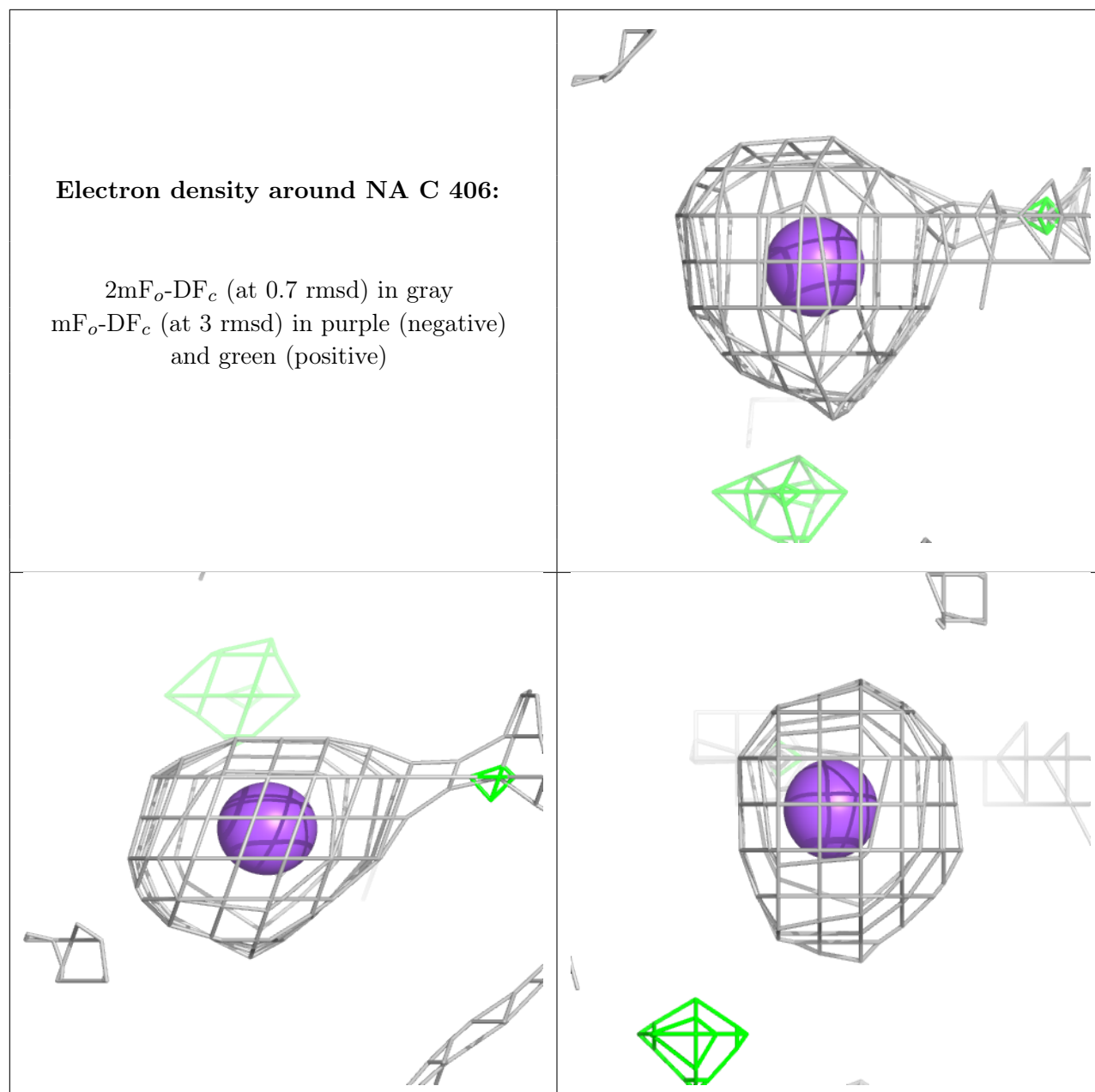
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL A 401:

$2mF_o-DF_c$ (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.