



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:24 PM UTC

PDB ID : 9LEI / pdb_00009lei
Title : Nitrile synthetase ArtA
Authors : Ma, H.L.; Zhang, K.K.
Deposited on : 2025-01-07
Resolution : 1.90 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

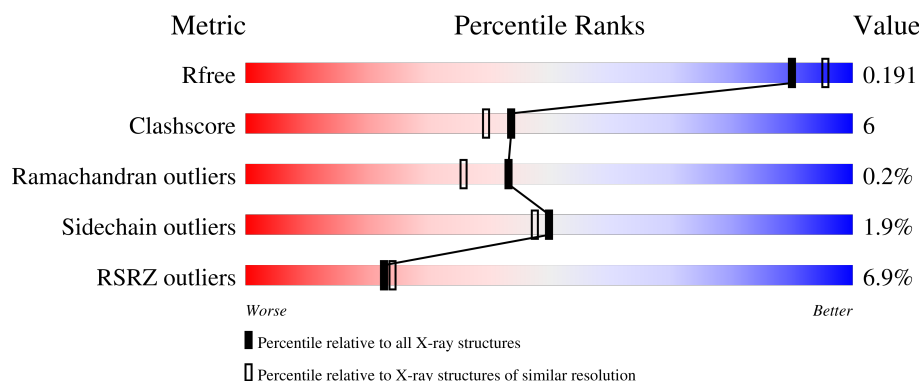
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	435	5% 75% 10% • 13%
1	B	435	3% 78% 8% • 14%
1	C	435	5% 75% 8% • 15%
1	D	435	10% 72% 14% • 13%

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
2	GOL	A	502	-	-	X	-

2 Entry composition [i](#)

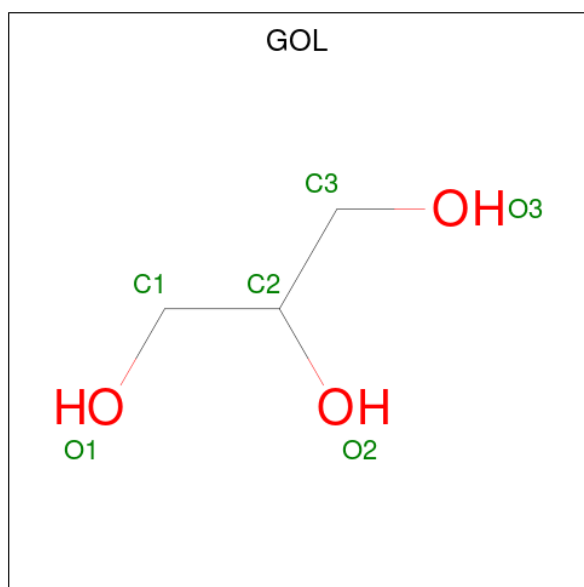
There are 3 unique types of molecules in this entry. The entry contains 13213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrile synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2946	1865	506	565	10			
1	B	376	Total	C	N	O	S	0	0	0
			2937	1861	504	562	10			
1	C	368	Total	C	N	O	S	0	0	0
			2861	1814	491	546	10			
1	D	379	Total	C	N	O	S	0	0	0
			2961	1874	508	569	10			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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		

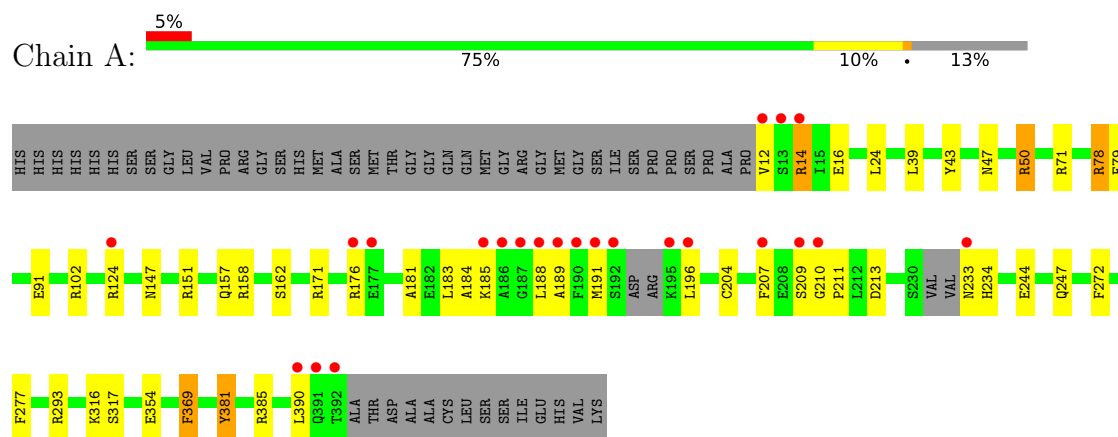
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	379	Total	O	0	0
			379	379		
3	B	439	Total	O	0	0
			439	439		
3	C	325	Total	O	0	0
			325	325		
3	D	329	Total	O	0	0
			329	329		

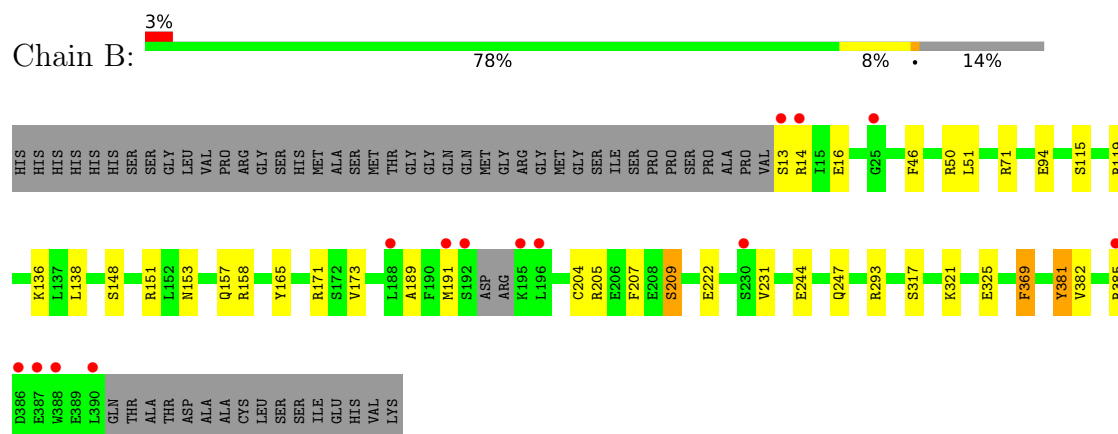
3 Residue-property plots [i](#)

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.

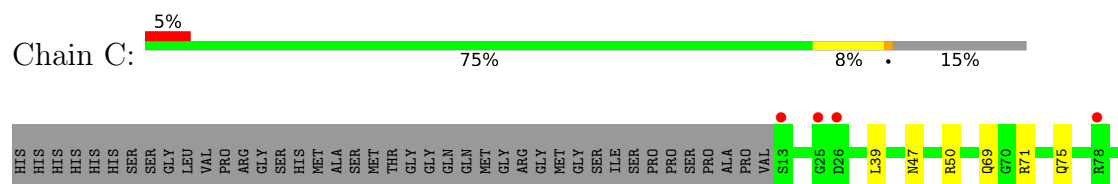
• Molecule 1: Nitrile synthetase

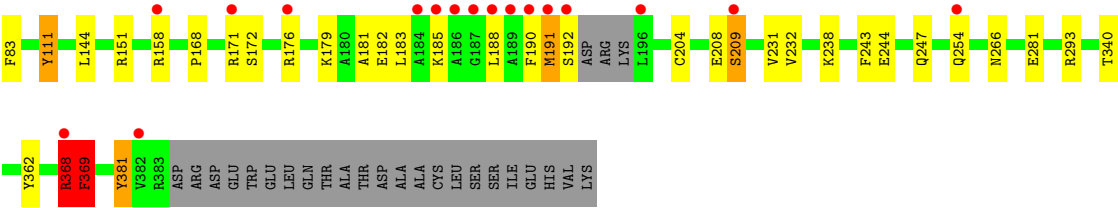


• Molecule 1: Nitrile synthetase

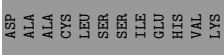
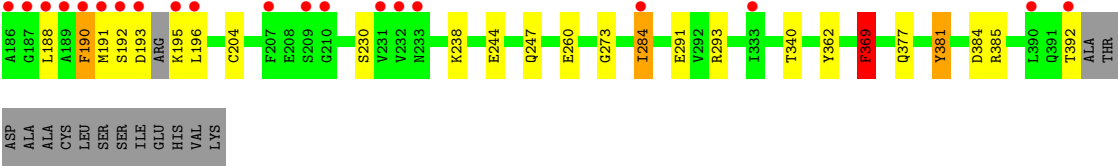
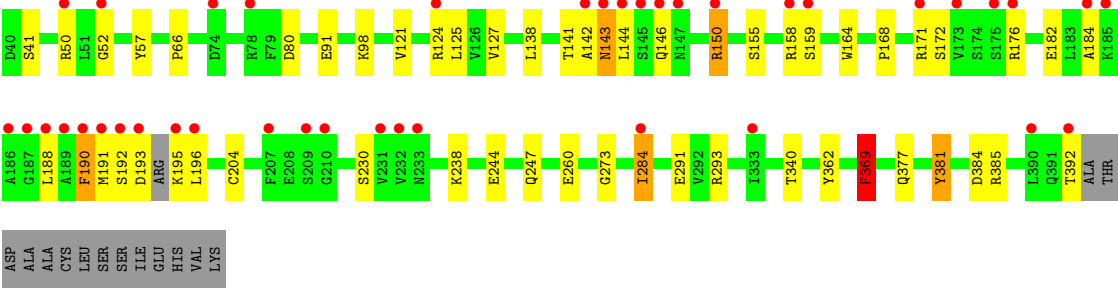
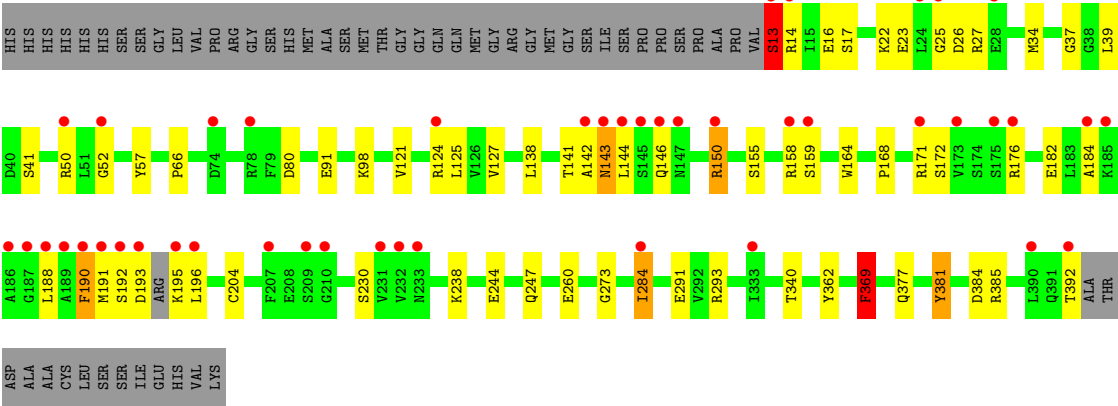


• Molecule 1: Nitrile synthetase





● Molecule 1: Nitrile synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.18Å 106.76Å 94.63Å 90.00° 108.68° 90.00°	Depositor
Resolution (Å)	44.82 – 1.90 44.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.82-1.90) 98.2 (44.82-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.163 , 0.190 0.163 , 0.191	Depositor DCC
R_{free} test set	6756 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13213	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/3006	0.75	4/4073 (0.1%)
1	B	0.35	0/2998	0.66	1/4064 (0.0%)
1	C	0.38	1/2920 (0.0%)	0.80	10/3959 (0.3%)
1	D	0.37	0/3022	0.74	4/4097 (0.1%)
All	All	0.37	1/11946 (0.0%)	0.74	19/16193 (0.1%)

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	A	0	1
1	B	0	2
1	C	0	5
1	D	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	ARG	CG-CD	5.93	1.70	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	MET	CA-CB-CG	-11.40	91.30	114.10
1	C	171	ARG	CA-CB-CG	9.59	133.28	114.10
1	C	368	ARG	CB-CA-C	-9.18	90.10	111.95
1	C	171	ARG	CB-CG-CD	-8.76	91.16	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	ARG	CA-CB-CG	8.26	130.62	114.10
1	C	368	ARG	N-CA-CB	7.51	123.75	111.21
1	D	150	ARG	CA-CB-CG	7.16	128.42	114.10
1	D	150	ARG	CB-CG-CD	7.13	127.71	111.30
1	D	13	SER	N-CA-C	-7.06	91.24	111.00
1	C	368	ARG	CB-CG-CD	6.71	126.74	111.30
1	A	14	ARG	CG-CD-NE	6.24	125.73	112.00
1	C	369	PHE	CB-CA-C	6.21	120.94	109.70
1	A	78	ARG	CB-CG-CD	-6.02	97.45	111.30
1	D	369	PHE	CB-CA-C	5.90	120.51	109.71
1	A	369	PHE	CB-CA-C	5.65	120.04	109.71
1	C	191	MET	CG-SD-CE	-5.60	88.59	100.90
1	B	369	PHE	CB-CA-C	5.54	119.84	109.71
1	A	14	ARG	CB-CA-C	5.28	118.41	109.50
1	C	191	MET	CB-CG-SD	5.04	127.84	112.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	TYR	Sidechain
1	B	209	SER	Mainchain
1	B	381	TYR	Sidechain
1	C	111	TYR	Sidechain
1	C	208	GLU	Peptide
1	C	209	SER	Mainchain
1	C	369	PHE	Sidechain
1	C	381	TYR	Sidechain
1	D	369	PHE	Sidechain
1	D	381	TYR	Sidechain

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	2946	0	2913	33	0
1	B	2937	0	2908	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2861	0	2841	30	0
1	D	2961	0	2927	57	0
2	A	12	0	15	7	0
2	B	12	0	16	1	0
2	C	12	0	16	1	0
3	A	379	0	0	8	0
3	B	439	0	0	10	0
3	C	325	0	0	13	1
3	D	329	0	0	18	1
All	All	13213	0	11636	143	1

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 6.

All (143) 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:D:143:ASN:ND2	3:D:502:HOH:O	1.95	0.99
1:D:25:GLY:N	3:D:501:HOH:O	1.88	0.97
1:C:266:ASN:HD22	2:C:502:GOL:H11	1.29	0.96
1:B:158:ARG:NH1	3:B:603:HOH:O	2.03	0.91
1:A:233:ASN:O	3:A:601:HOH:O	1.89	0.89
1:D:34:MET:SD	3:D:826:HOH:O	2.36	0.84
1:D:184:ALA:HB2	1:D:188:LEU:HD12	1.61	0.83
1:A:91:GLU:OE1	3:A:602:HOH:O	1.97	0.82
1:C:69:GLN:NE2	3:C:602:HOH:O	2.00	0.81
1:D:34:MET:HE3	1:D:138:LEU:HD21	1.60	0.81
2:B:501:GOL:O3	3:B:602:HOH:O	1.97	0.81
1:A:16:GLU:OE1	1:A:171:ARG:NH1	2.14	0.80
3:C:612:HOH:O	1:D:385:ARG:HG2	1.82	0.79
1:D:184:ALA:HA	1:D:188:LEU:HB2	1.65	0.78
1:B:16:GLU:OE1	1:B:171:ARG:NH1	2.17	0.78
1:D:14:ARG:NH2	3:D:511:HOH:O	2.17	0.77
1:D:143:ASN:O	3:D:503:HOH:O	2.05	0.75
1:B:222:GLU:OE2	3:B:604:HOH:O	2.06	0.73
1:A:213:ASP:OD1	2:A:502:GOL:O1	2.06	0.72
1:A:244:GLU:O	1:A:247:GLN:HG2	1.89	0.72
1:A:196:LEU:O	3:A:604:HOH:O	2.06	0.72
1:D:121:VAL:HG22	1:D:124:ARG:HH22	1.54	0.71
1:B:94:GLU:OE1	3:B:605:HOH:O	2.09	0.71
1:D:244:GLU:O	1:D:247:GLN:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLU:O	1:B:247:GLN:HG2	1.92	0.69
1:D:384:ASP:OD1	3:D:505:HOH:O	2.09	0.69
1:C:158:ARG:NH1	3:C:605:HOH:O	2.25	0.69
1:C:158:ARG:NH2	3:C:606:HOH:O	2.28	0.66
1:C:244:GLU:O	1:C:247:GLN:HG2	1.96	0.66
1:C:192:SER:OG	3:C:603:HOH:O	2.14	0.66
1:D:37:GLY:HA3	1:D:191:MET:HE2	1.77	0.65
1:A:385:ARG:HG2	3:B:651:HOH:O	1.96	0.64
1:C:232:VAL:HG22	3:C:784:HOH:O	1.96	0.64
1:C:158:ARG:NE	3:C:606:HOH:O	2.30	0.63
1:D:193:ASP:OD1	1:D:195:LYS:NZ	2.22	0.63
1:D:14:ARG:CZ	3:D:511:HOH:O	2.46	0.63
1:D:16:GLU:HB2	1:D:171:ARG:NH1	2.13	0.63
1:A:14:ARG:NH2	1:A:157:GLN:OE1	2.33	0.61
1:D:13:SER:O	3:D:509:HOH:O	2.16	0.61
1:D:23:GLU:OE1	3:D:508:HOH:O	2.16	0.60
1:B:46:PHE:CZ	1:B:50:ARG:HD2	2.37	0.60
1:D:230:SER:OG	3:D:510:HOH:O	2.17	0.59
1:B:157:GLN:HG3	3:B:688:HOH:O	2.03	0.58
1:C:368:ARG:NH2	1:D:273:GLY:O	2.28	0.58
1:C:158:ARG:CZ	3:C:606:HOH:O	2.51	0.58
1:A:39:LEU:CD2	1:A:176:ARG:HG2	2.34	0.58
1:A:102:ARG:HD3	3:A:605:HOH:O	2.05	0.57
1:C:190:PHE:CG	1:C:191:MET:N	2.73	0.57
1:A:196:LEU:HD11	1:A:207:PHE:HB3	1.86	0.56
1:A:79:PHE:CE1	1:A:188:LEU:HD13	2.42	0.54
1:C:182:GLU:HA	1:C:185:LYS:HE3	1.87	0.54
1:D:142:ALA:O	1:D:144:LEU:N	2.40	0.54
1:A:354:GLU:HG3	3:A:893:HOH:O	2.07	0.54
1:C:204:CYS:SG	1:C:293:ARG:HD3	2.48	0.54
1:D:66:PRO:HG2	3:D:567:HOH:O	2.08	0.54
1:A:204:CYS:SG	1:A:293:ARG:HD3	2.49	0.53
1:D:80:ASP:O	3:D:512:HOH:O	2.19	0.52
1:D:39:LEU:HD13	1:D:190:PHE:CD1	2.45	0.52
2:A:502:GOL:O2	1:B:382:VAL:HB	2.09	0.52
1:D:39:LEU:HD23	1:D:176:ARG:HG3	1.91	0.52
1:D:127:VAL:HG21	1:D:159:SER:OG	2.08	0.52
1:C:47:ASN:OD1	1:C:50:ARG:NH2	2.42	0.52
1:B:189:ALA:HB1	1:B:191:MET:HE3	1.92	0.52
1:C:39:LEU:CD2	1:C:176:ARG:HG3	2.40	0.51
1:C:39:LEU:HD22	1:C:176:ARG:HG3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD23	1:D:392:THR:HG22	1.92	0.51
1:C:293:ARG:NH2	3:C:601:HOH:O	1.89	0.51
1:D:27:ARG:HD3	1:D:52:GLY:HA3	1.93	0.51
1:C:69:GLN:HG2	1:C:83:PHE:HE2	1.75	0.50
1:A:184:ALA:HA	1:A:189:ALA:HA	1.93	0.50
1:C:181:ALA:O	1:C:185:LYS:HB2	2.12	0.50
1:D:155:SER:OG	1:D:158:ARG:NH1	2.45	0.49
1:D:260:GLU:HG3	3:D:596:HOH:O	2.11	0.49
2:A:502:GOL:O1	1:B:385:ARG:HG2	2.12	0.49
1:D:192:SER:OG	1:D:195:LYS:NZ	2.45	0.49
1:A:213:ASP:O	2:A:502:GOL:H32	2.12	0.49
1:D:121:VAL:HG22	1:D:124:ARG:NH2	2.25	0.49
2:A:502:GOL:C1	1:B:385:ARG:HG2	2.44	0.48
1:D:184:ALA:CB	1:D:188:LEU:HD12	2.38	0.48
1:D:26:ASP:O	3:D:513:HOH:O	2.20	0.47
1:D:377:GLN:CD	3:D:534:HOH:O	2.58	0.47
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.75	0.47
1:A:184:ALA:HA	1:A:189:ALA:CA	2.45	0.47
1:A:234:HIS:HB2	1:A:272:PHE:CE1	2.50	0.47
1:C:39:LEU:HD21	1:C:179:LYS:HB2	1.96	0.47
1:D:146:GLN:NE2	3:D:520:HOH:O	2.40	0.47
1:B:204:CYS:SG	1:B:293:ARG:HD3	2.55	0.47
1:D:17:SER:HB3	1:D:171:ARG:HB2	1.97	0.47
1:B:14:ARG:HE	1:B:153:ASN:HB3	1.79	0.47
1:A:390:LEU:HA	1:B:173:VAL:HG11	1.97	0.46
1:D:190:PHE:CD2	1:D:190:PHE:C	2.94	0.46
1:B:136:LYS:NZ	3:B:615:HOH:O	2.48	0.46
1:C:168:PRO:O	1:C:172:SER:HB2	2.15	0.46
1:D:150:ARG:NH2	1:D:284:ILE:HG12	2.31	0.46
1:D:41:SER:HA	1:D:141:THR:HG21	1.98	0.45
1:A:124:ARG:NH2	3:A:608:HOH:O	2.26	0.45
1:D:150:ARG:NH1	1:D:284:ILE:HG23	2.32	0.45
1:A:158:ARG:NH2	3:A:608:HOH:O	2.42	0.45
1:A:209:SER:OG	1:B:385:ARG:HG3	2.17	0.45
1:D:23:GLU:O	1:D:25:GLY:N	2.49	0.45
1:D:168:PRO:O	1:D:172:SER:HB2	2.17	0.44
1:C:75:GLN:NE2	3:C:613:HOH:O	2.47	0.44
1:A:39:LEU:HD23	1:A:176:ARG:HG2	1.99	0.44
1:D:25:GLY:O	1:D:27:ARG:HG3	2.18	0.44
1:B:321:LYS:O	1:B:325:GLU:HG3	2.18	0.44
1:D:291:GLU:OE1	1:D:293:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TYR:CE2	1:A:47:ASN:ND2	2.86	0.44
1:B:115:SER:OG	1:B:151:ARG:NH1	2.50	0.44
1:D:50:ARG:NH1	1:D:182:GLU:OE2	2.50	0.44
1:A:317:SER:OG	1:C:340:THR:HB	2.18	0.43
1:D:27:ARG:HE	1:D:52:GLY:H	1.65	0.43
1:D:98:LYS:NZ	3:D:519:HOH:O	2.40	0.43
1:A:181:ALA:O	1:A:185:LYS:HB2	2.19	0.43
1:B:46:PHE:CE2	1:B:50:ARG:HD2	2.53	0.43
2:A:502:GOL:H12	1:B:382:VAL:HG12	2.01	0.42
1:A:12:VAL:HG21	1:A:162:SER:O	2.19	0.42
1:C:238:LYS:HA	1:C:362:TYR:O	2.20	0.42
1:C:293:ARG:NH1	3:C:601:HOH:O	2.53	0.42
1:B:148:SER:OG	3:B:606:HOH:O	2.11	0.42
1:D:91:GLU:HG3	1:D:125:LEU:HD21	2.02	0.42
1:B:119:ARG:HG3	3:B:606:HOH:O	2.20	0.42
1:D:196:LEU:HA	3:D:530:HOH:O	2.19	0.42
1:A:210:GLY:HA3	1:A:211:PRO:HD2	1.93	0.41
1:B:317:SER:OG	1:D:340:THR:HB	2.21	0.41
1:C:231:VAL:HG22	3:C:861:HOH:O	2.19	0.41
1:D:13:SER:HB3	1:D:164:TRP:HZ3	1.85	0.41
1:A:316:LYS:HE2	1:A:316:LYS:HB2	1.57	0.41
2:A:502:GOL:H31	3:A:688:HOH:O	2.19	0.41
1:C:158:ARG:HG3	3:C:654:HOH:O	2.21	0.41
1:D:238:LYS:HA	1:D:362:TYR:O	2.21	0.41
1:D:190:PHE:C	1:D:190:PHE:HD2	2.28	0.41
1:B:71:ARG:NH2	3:B:624:HOH:O	2.53	0.41
1:B:205:ARG:NH1	1:B:207:PHE:HZ	2.19	0.41
1:D:39:LEU:HD13	1:D:190:PHE:HD1	1.84	0.41
1:B:138:LEU:O	1:B:165:TYR:HA	2.21	0.41
1:D:22:LYS:HA	1:D:27:ARG:HH22	1.86	0.41
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.92	0.41
1:A:147:ASN:O	1:A:151:ARG:HG3	2.20	0.40
1:C:151:ARG:NH2	1:C:281:GLU:OE2	2.49	0.40
1:C:183:LEU:HB3	1:C:188:LEU:O	2.22	0.40
1:A:183:LEU:HB3	1:A:188:LEU:O	2.21	0.40
1:A:50:ARG:HE	1:A:50:ARG:HB3	1.75	0.40
1:D:204:CYS:SG	1:D:293:ARG:HD3	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:857:HOH:O	3:D:781:HOH:O[2_444]	1.92	0.28

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	371/435 (85%)	364 (98%)	7 (2%)	0	100	100
1	B	372/435 (86%)	362 (97%)	9 (2%)	1 (0%)	36	29
1	C	364/435 (84%)	353 (97%)	10 (3%)	1 (0%)	36	29
1	D	375/435 (86%)	360 (96%)	14 (4%)	1 (0%)	36	29
All	All	1482/1740 (85%)	1439 (97%)	40 (3%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	SER
1	C	209	SER
1	D	143	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	324/370 (88%)	317 (98%)	7 (2%)	45	42
1	B	323/370 (87%)	319 (99%)	4 (1%)	63	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	315/370 (85%)	308 (98%)	7 (2%)	45	42
1	D	326/370 (88%)	320 (98%)	6 (2%)	51	50
All	All	1288/1480 (87%)	1264 (98%)	24 (2%)	50	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	71	ARG
1	A	78	ARG
1	A	191	MET
1	A	277	PHE
1	A	369	PHE
1	A	381	TYR
1	B	13	SER
1	B	231	VAL
1	B	369	PHE
1	B	381	TYR
1	C	71	ARG
1	C	111	TYR
1	C	243	PHE
1	C	254	GLN
1	C	368	ARG
1	C	369	PHE
1	C	381	TYR
1	D	13	SER
1	D	57	TYR
1	D	190	PHE
1	D	284	ILE
1	D	369	PHE
1	D	381	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	336	GLN
1	B	233	ASN
1	C	49	HIS
1	C	266	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	C	501	-	5,5,5	0.95	0	5,5,5	1.05	0
2	GOL	A	502	-	5,5,5	1.25	1 (20%)	5,5,5	1.12	0
2	GOL	C	502	-	5,5,5	0.70	0	5,5,5	0.92	0
2	GOL	A	501	-	5,5,5	1.28	1 (20%)	5,5,5	0.87	0
2	GOL	B	502	-	5,5,5	1.30	0	5,5,5	0.92	0
2	GOL	B	501	-	5,5,5	0.77	0	5,5,5	1.09	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	C	501	-	-	3/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	C	502	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	501	-	-	3/4/4/4	-
2	GOL	B	502	-	-	0/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GOL	O2-C2	-2.57	1.35	1.43
2	A	502	GOL	O2-C2	-2.15	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	A	502	GOL	C1-C2-C3-O3
2	A	502	GOL	O2-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2
2	C	501	GOL	O1-C1-C2-O2
2	A	501	GOL	O2-C2-C3-O3
2	B	501	GOL	O1-C1-C2-O2
2	C	501	GOL	O2-C2-C3-O3

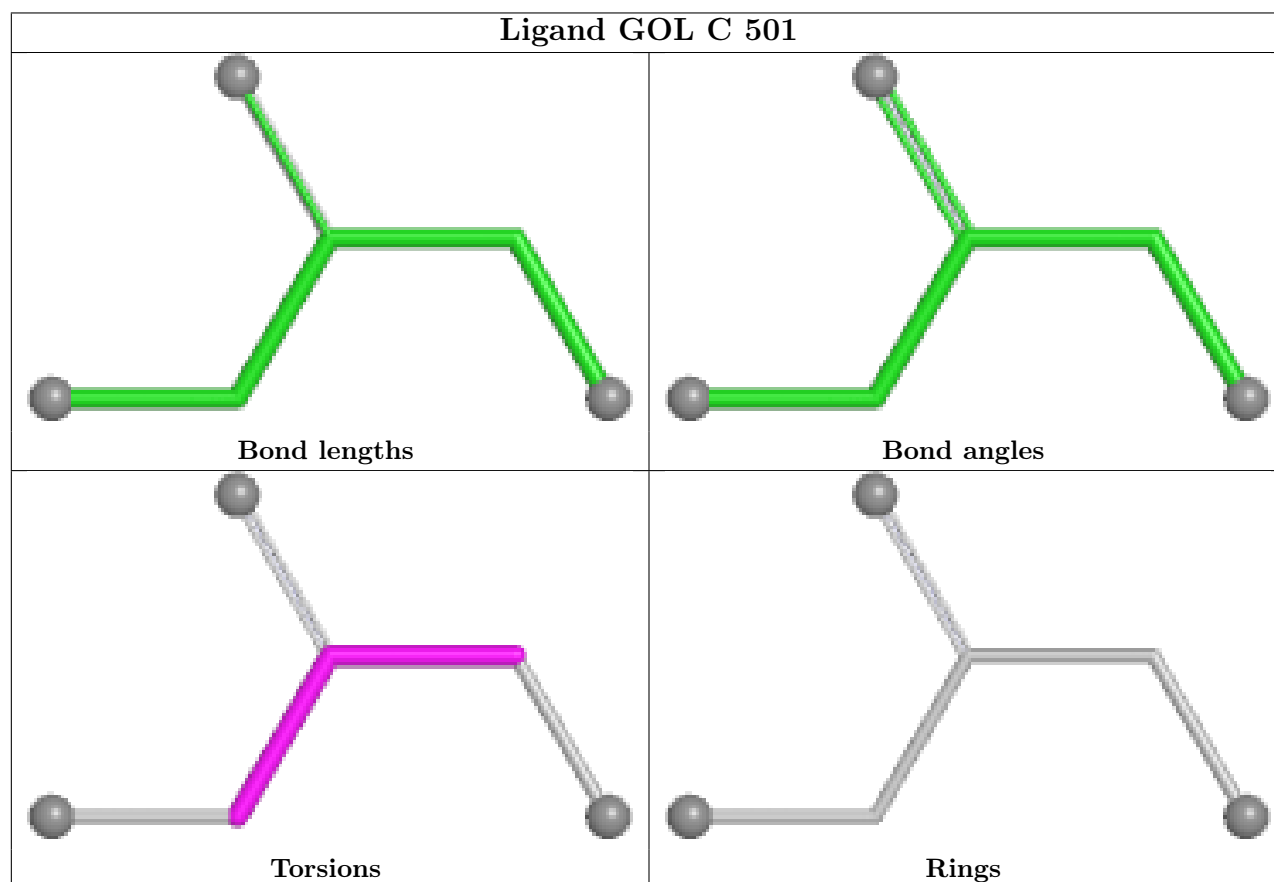
There are no ring outliers.

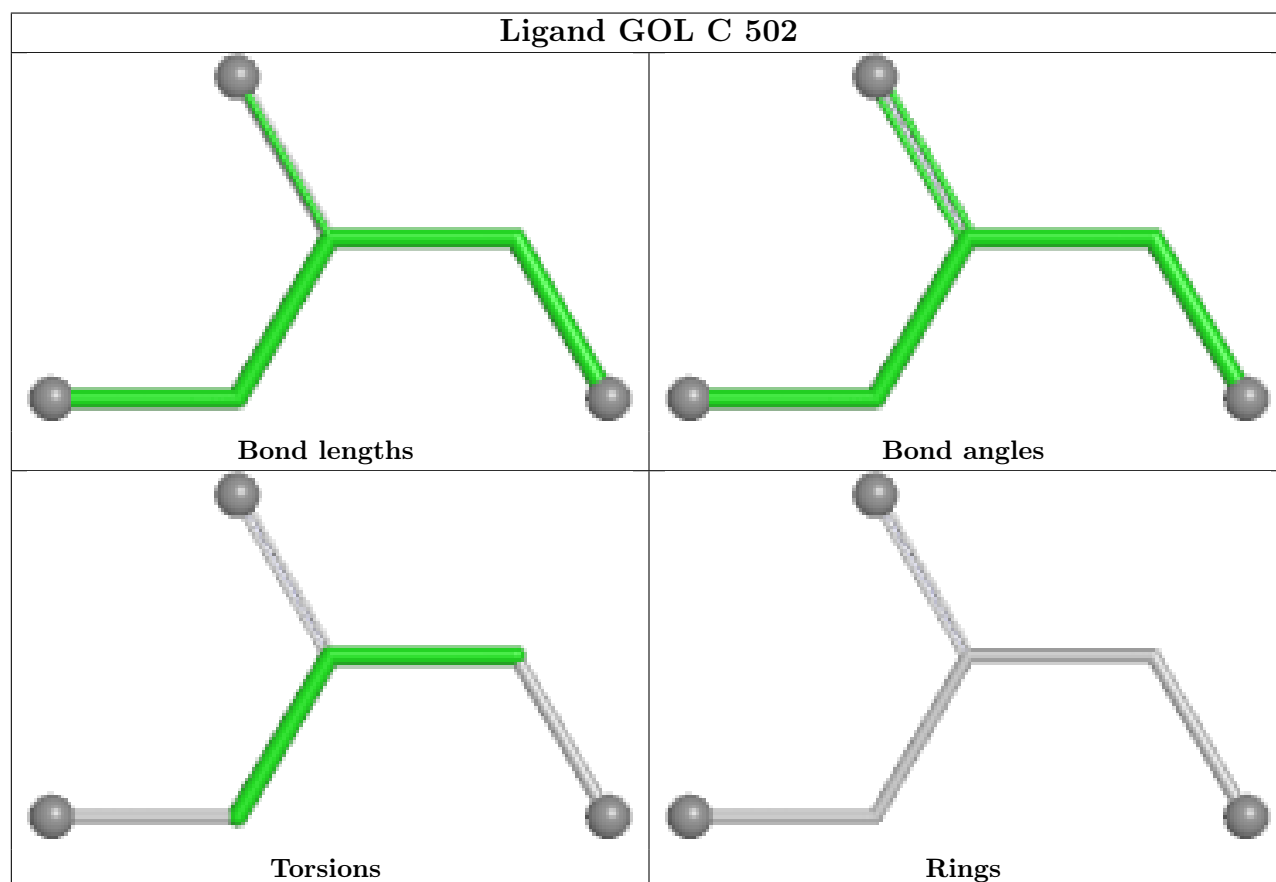
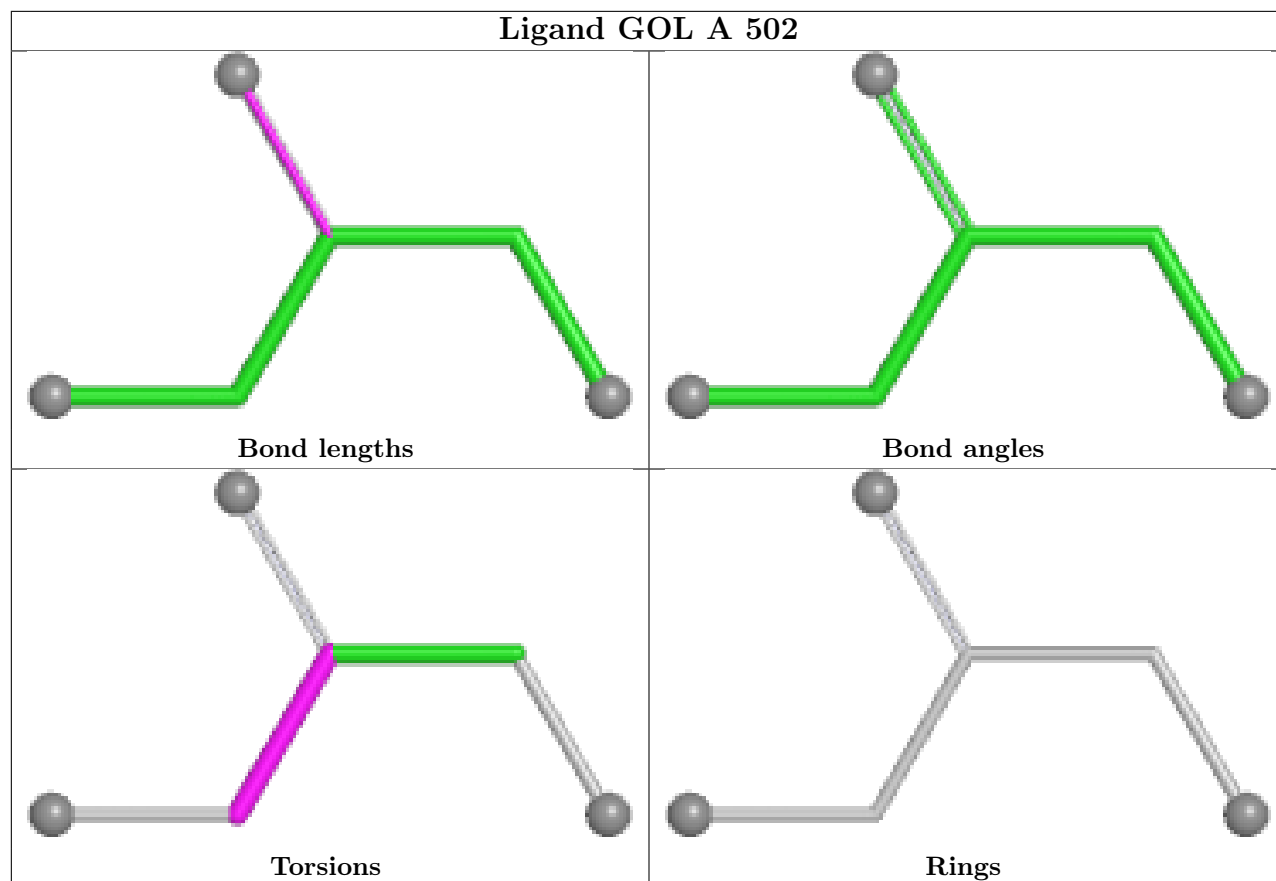
3 monomers are involved in 9 short contacts:

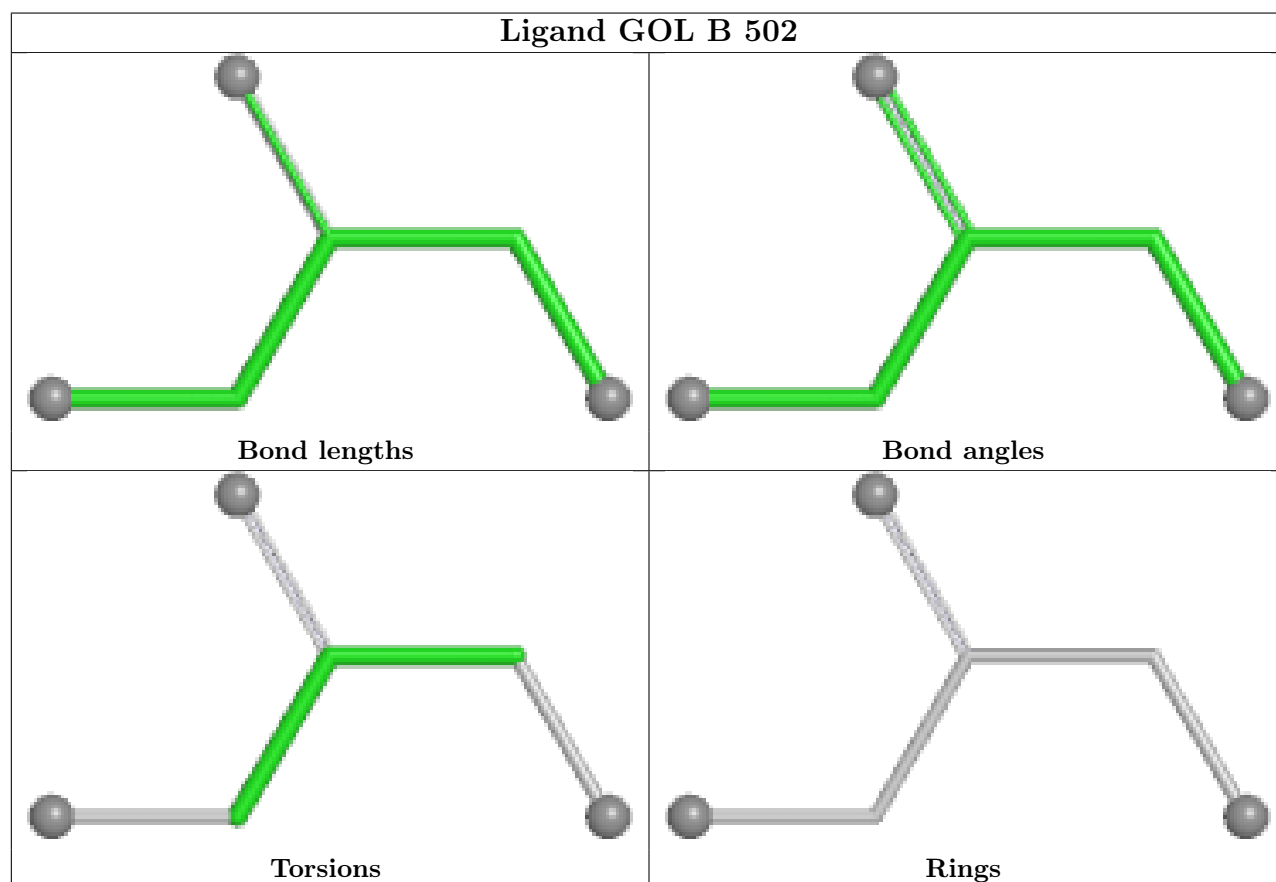
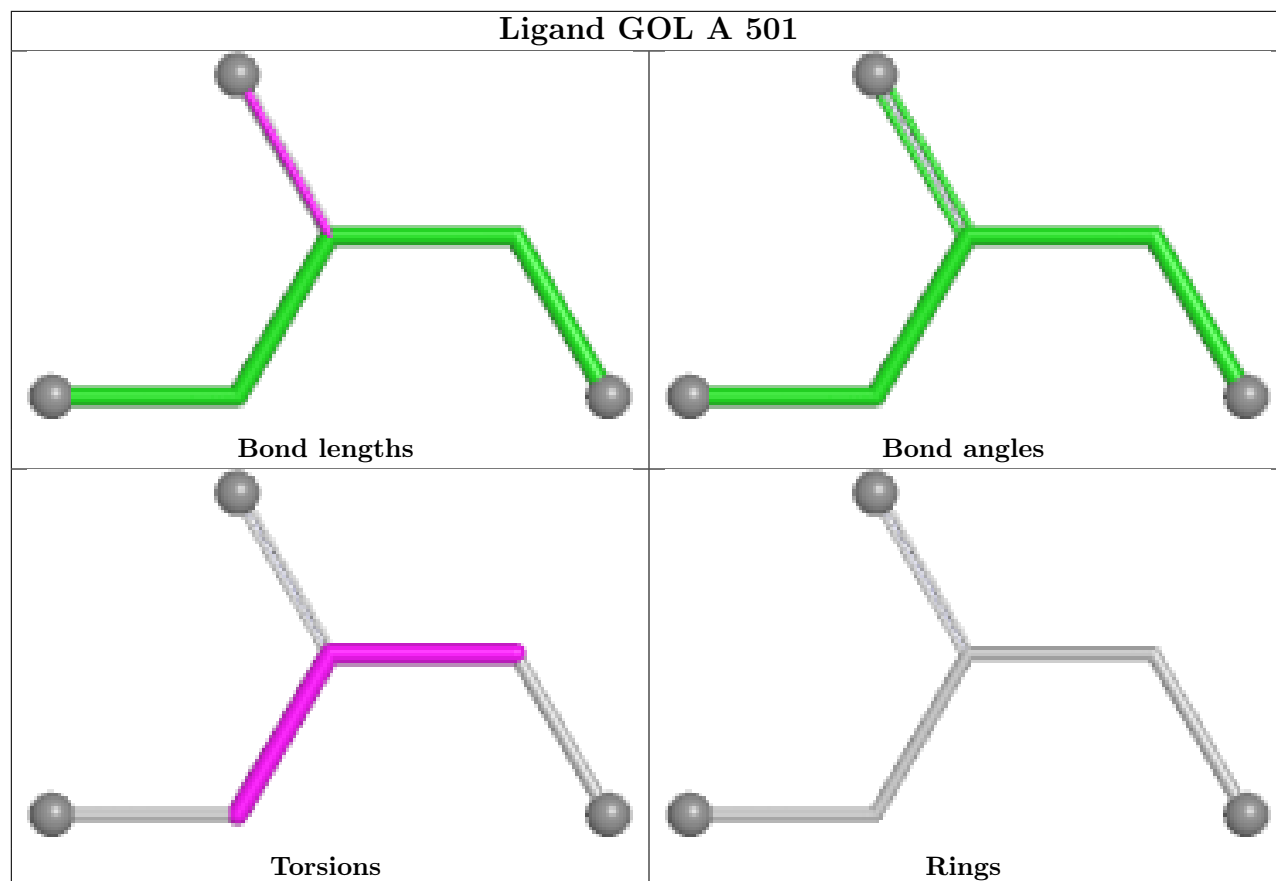
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	GOL	7	0
2	C	502	GOL	1	0
2	B	501	GOL	1	0

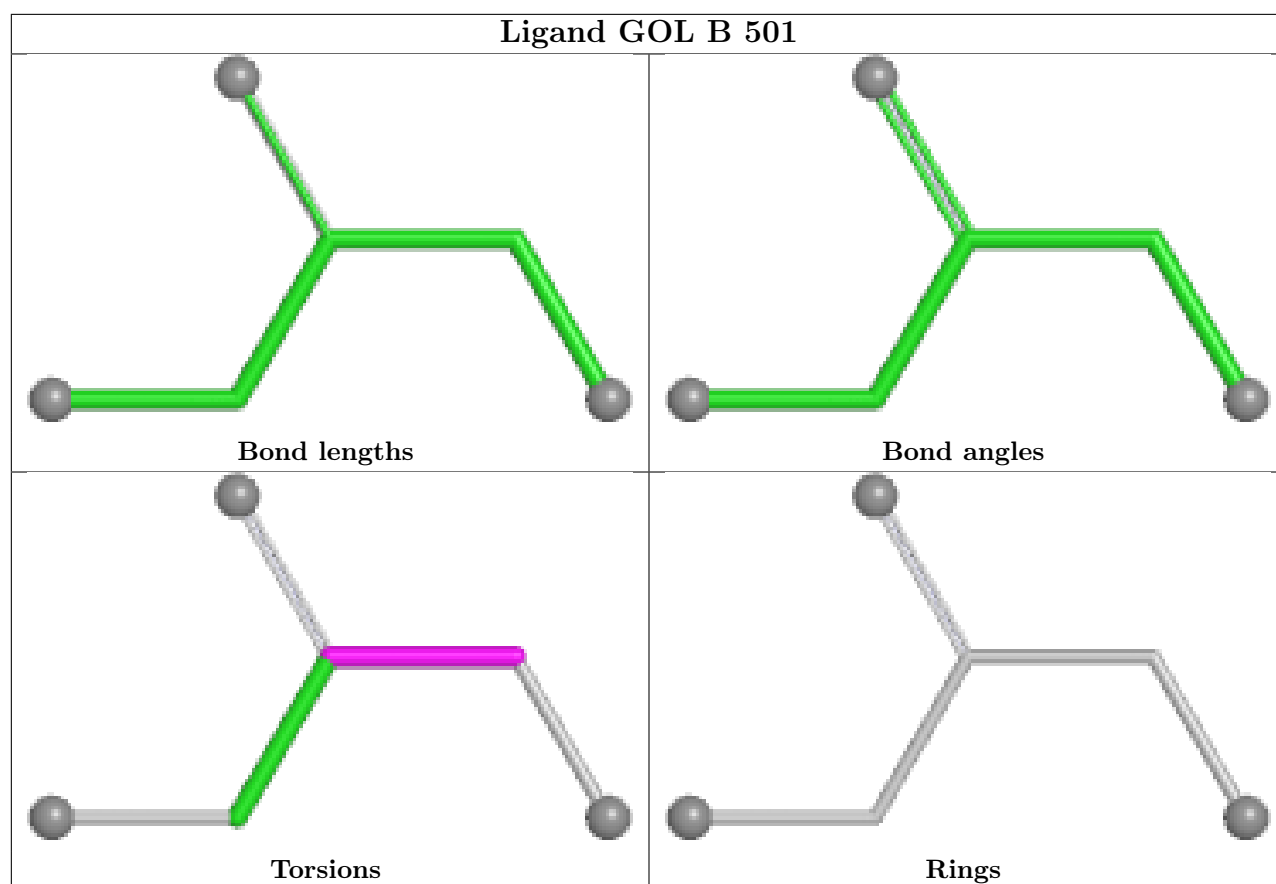
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	377/435 (86%)	-0.19	23 (6%)	27	29	9, 18, 61, 103	0
1	B	376/435 (86%)	-0.35	14 (3%)	45	48	10, 18, 45, 92	0
1	C	368/435 (84%)	-0.07	21 (5%)	29	31	12, 22, 51, 116	0
1	D	379/435 (87%)	0.30	45 (11%)	9	9	9, 24, 72, 108	0
All	All	1500/1740 (86%)	-0.07	103 (6%)	23	24	9, 20, 61, 116	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	189	ALA	10.1
1	D	188	LEU	7.7
1	D	143	ASN	7.2
1	D	190	PHE	7.0
1	D	24	LEU	6.0
1	D	144	LEU	6.0
1	A	12	VAL	5.5
1	D	142	ALA	5.5
1	C	188	LEU	5.1
1	A	13	SER	4.9
1	D	186	ALA	4.8
1	A	196	LEU	4.8
1	B	195	LYS	4.8
1	C	191	MET	4.6
1	D	231	VAL	4.6
1	D	284	ILE	4.6
1	C	158	ARG	4.5
1	B	191	MET	4.5
1	D	150	ARG	4.5
1	A	392	THR	4.4
1	D	232	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	25	GLY	4.4
1	A	188	LEU	4.3
1	A	14	ARG	4.2
1	B	390	LEU	4.2
1	D	158	ARG	4.2
1	D	187	GLY	4.1
1	B	192	SER	4.1
1	D	195	LYS	4.0
1	D	209	SER	3.8
1	D	14	ARG	3.8
1	D	25	GLY	3.7
1	D	193	ASP	3.6
1	A	195	LYS	3.6
1	D	192	SER	3.6
1	A	187	GLY	3.5
1	C	190	PHE	3.4
1	D	13	SER	3.3
1	C	196	LEU	3.3
1	D	191	MET	3.3
1	A	209	SER	3.3
1	D	333	ILE	3.3
1	A	210	GLY	3.3
1	A	233	ASN	3.3
1	C	171	ARG	3.3
1	D	173	VAL	3.2
1	A	390	LEU	3.2
1	A	190	PHE	3.2
1	A	191	MET	3.2
1	C	185	LYS	3.1
1	A	192	SER	3.1
1	D	207	PHE	3.1
1	A	185	LYS	3.1
1	D	390	LEU	3.1
1	D	124	ARG	3.1
1	B	13	SER	3.1
1	C	209	SER	3.1
1	B	385	ARG	3.0
1	D	78	ARG	3.0
1	C	189	ALA	3.0
1	B	386	ASP	3.0
1	D	184	ALA	3.0
1	D	145	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	159	SER	2.9
1	C	13	SER	2.9
1	B	387	GLU	2.9
1	D	233	ASN	2.8
1	D	392	THR	2.8
1	A	176	ARG	2.8
1	C	78	ARG	2.8
1	D	175	SER	2.8
1	A	186	ALA	2.8
1	C	192	SER	2.7
1	A	189	ALA	2.7
1	D	28	GLU	2.7
1	D	196	LEU	2.6
1	B	196	LEU	2.6
1	D	210	GLY	2.6
1	A	207	PHE	2.5
1	C	254	GLN	2.5
1	C	382	VAL	2.5
1	D	52	GLY	2.4
1	C	25	GLY	2.4
1	D	171	ARG	2.4
1	D	147	ASN	2.4
1	D	185	LYS	2.4
1	B	188	LEU	2.3
1	C	187	GLY	2.3
1	C	176	ARG	2.3
1	A	391	GLN	2.3
1	D	176	ARG	2.3
1	B	388	TRP	2.2
1	B	230	SER	2.2
1	D	50	ARG	2.2
1	D	146	GLN	2.2
1	C	26	ASP	2.1
1	C	186	ALA	2.1
1	A	124	ARG	2.1
1	C	368	ARG	2.1
1	A	177	GLU	2.1
1	C	184	ALA	2.1
1	B	14	ARG	2.0
1	D	74	ASP	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](#)

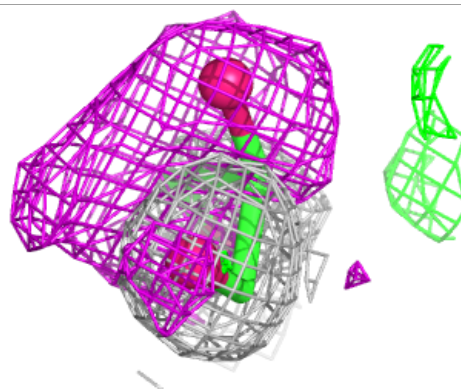
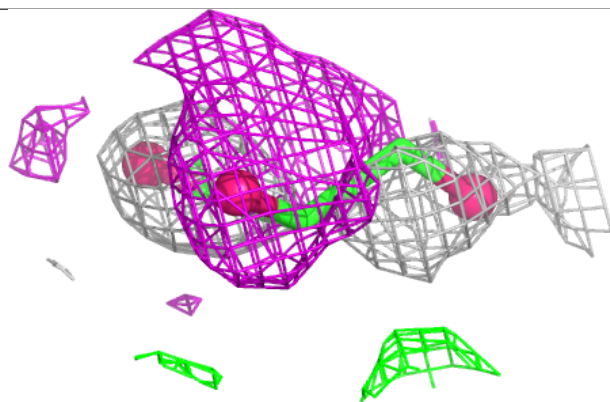
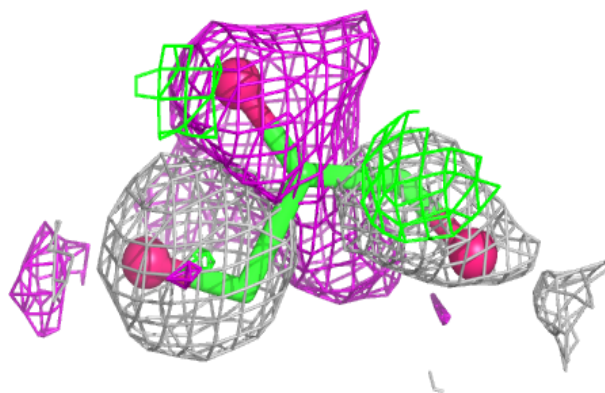
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	502	6/6	0.75	0.23	49,54,61,68	0
2	GOL	C	501	6/6	0.78	0.26	70,72,79,81	0
2	GOL	C	502	6/6	0.84	0.14	19,29,42,45	0
2	GOL	A	501	6/6	0.91	0.09	23,25,28,29	0
2	GOL	B	501	6/6	0.92	0.13	27,35,38,40	0
2	GOL	B	502	6/6	0.97	0.06	19,20,21,22	0

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

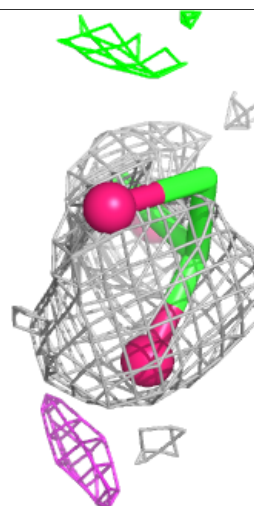
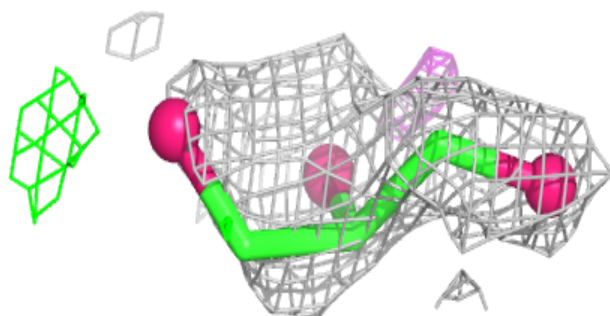
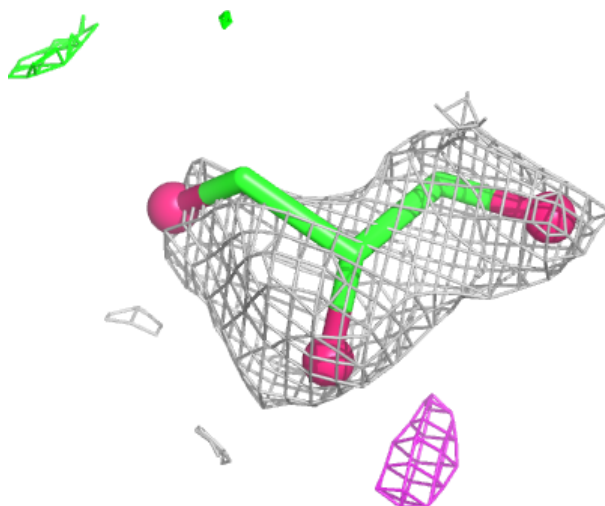
Electron density around GOL A 502:

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



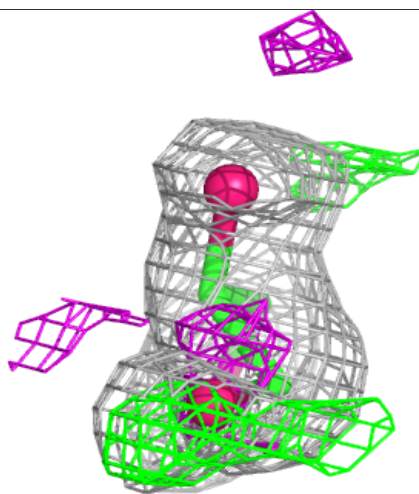
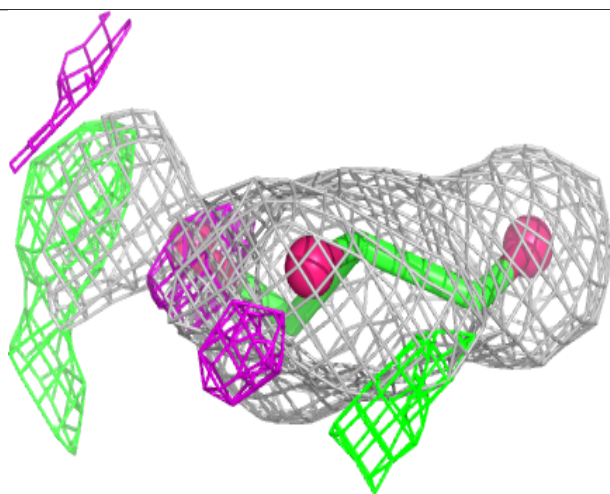
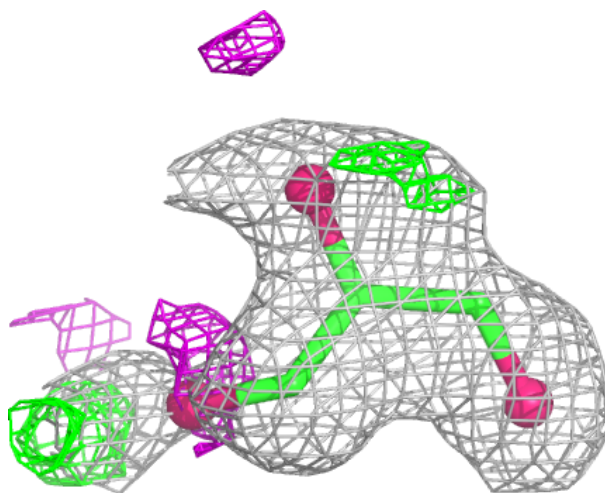
Electron density around GOL C 501:

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



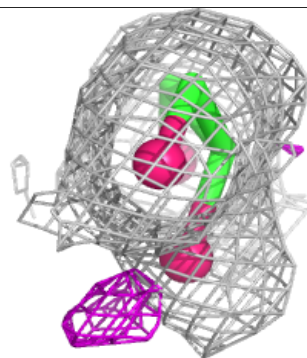
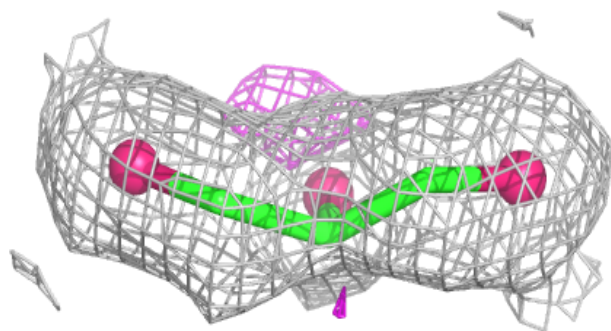
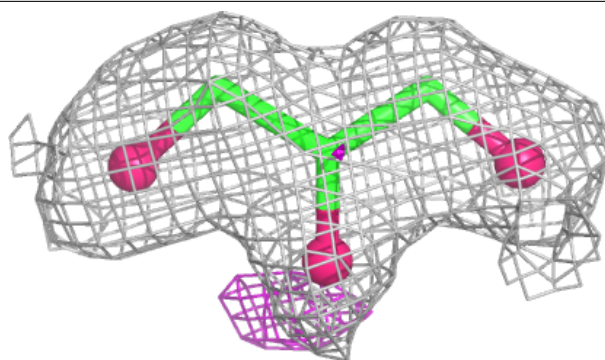
Electron density around GOL C 502:

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



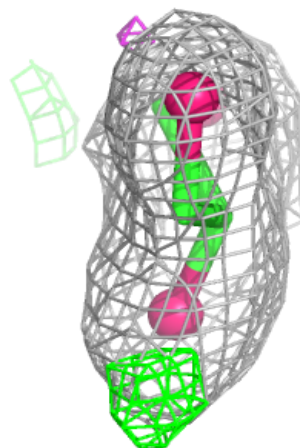
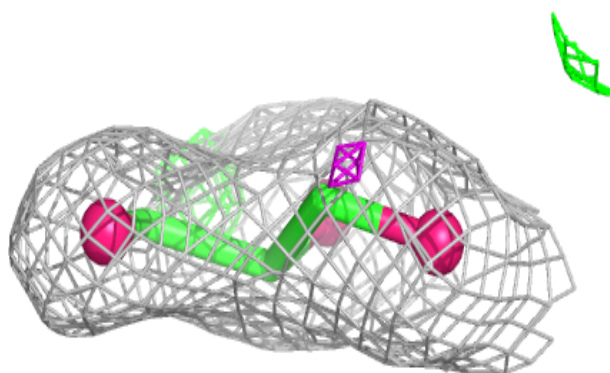
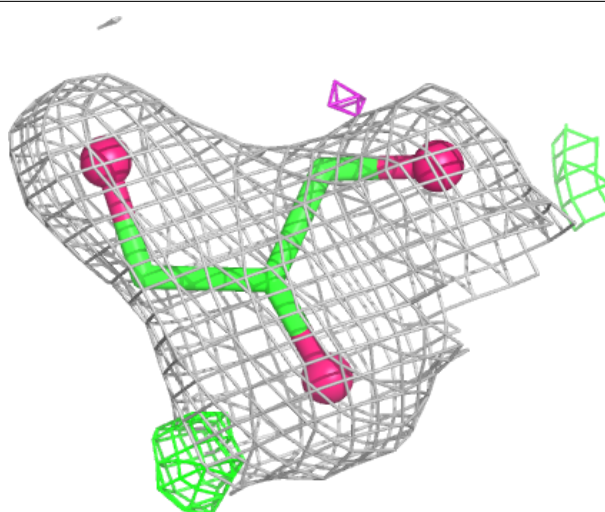
Electron density around GOL A 501:

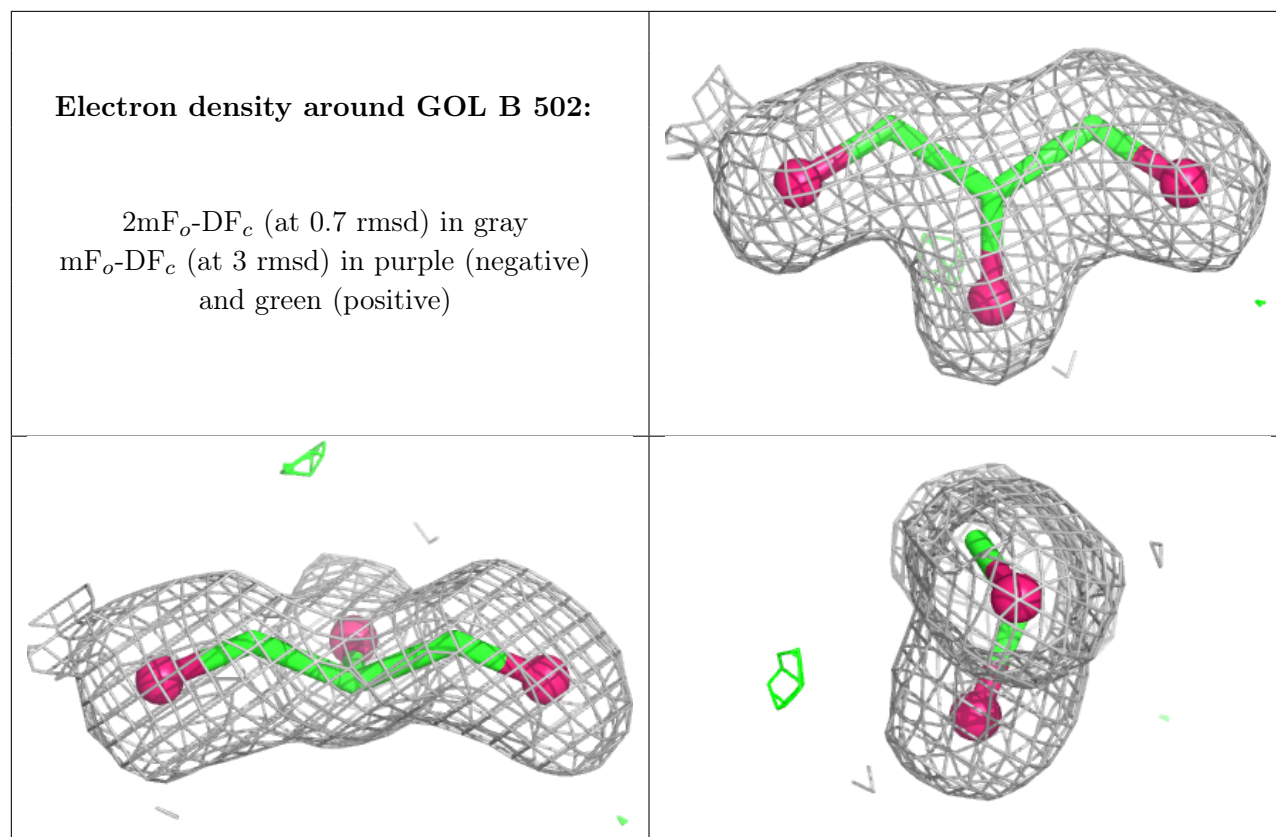
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL B 501:

$2mF_o-DF_c$ (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.