



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:42 AM UTC

PDB ID : 6ZB6 / pdb_00006zb6
Title : Crystal structure of Lolium rigidum GSTF in complex with S-(p-nitrobenzyl) glutathione
Authors : Papageorgiou, A.C.; Poudel, N.
Deposited on : 2020-06-07
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

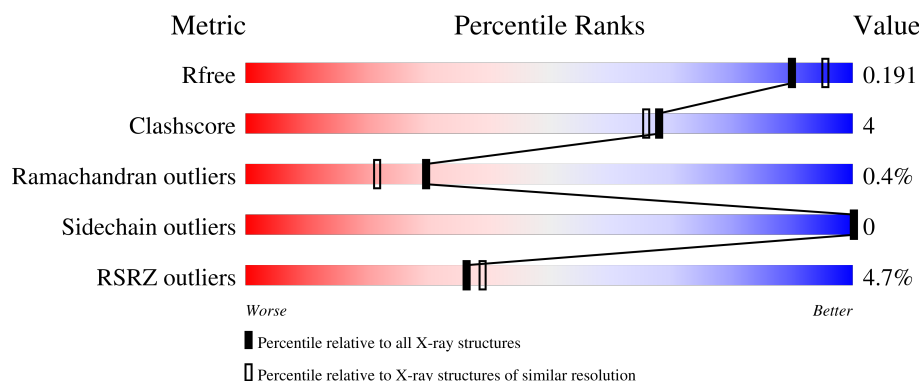
1 Overall quality at a glance

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	227	9% 87% 10% ..
1	B	227	3% 89% 6% 5%
1	C	227	4% 93% 7%
1	D	227	4% 88% 7% 5%
1	E	227	4% 89% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	227	4% 86% 9% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11820 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 Glutathione transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1777	1156	294	316	11			
1	C	227	Total	C	N	O	S	0	0	0
			1827	1186	309	321	11			
1	E	215	Total	C	N	O	S	0	0	0
			1726	1123	283	309	11			
1	B	215	Total	C	N	O	S	0	0	0
			1726	1123	283	309	11			
1	F	215	Total	C	N	O	S	0	0	0
			1726	1123	283	309	11			
1	D	215	Total	C	N	O	S	0	0	0
			1726	1123	283	309	11			

There are 48 discrepancies between the modelled and reference sequences:

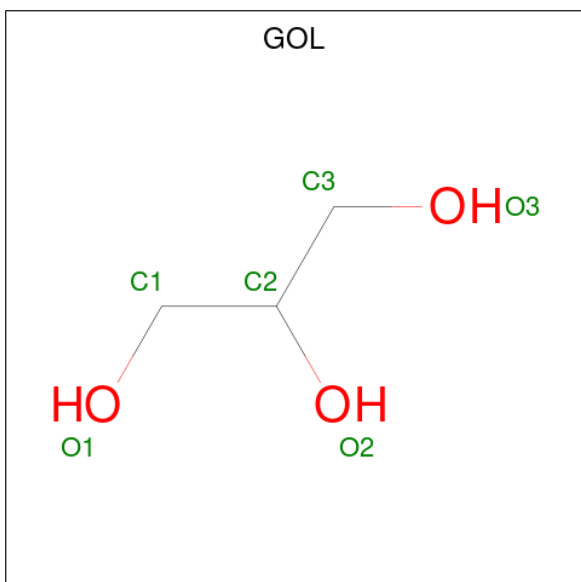
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	LYS	-	expression tag	UNP M5BPX4
A	221	GLY	-	expression tag	UNP M5BPX4
A	222	HIS	-	expression tag	UNP M5BPX4
A	223	HIS	-	expression tag	UNP M5BPX4
A	224	HIS	-	expression tag	UNP M5BPX4
A	225	HIS	-	expression tag	UNP M5BPX4
A	226	HIS	-	expression tag	UNP M5BPX4
A	227	HIS	-	expression tag	UNP M5BPX4
C	220	LYS	-	expression tag	UNP M5BPX4
C	221	GLY	-	expression tag	UNP M5BPX4
C	222	HIS	-	expression tag	UNP M5BPX4
C	223	HIS	-	expression tag	UNP M5BPX4
C	224	HIS	-	expression tag	UNP M5BPX4
C	225	HIS	-	expression tag	UNP M5BPX4
C	226	HIS	-	expression tag	UNP M5BPX4
C	227	HIS	-	expression tag	UNP M5BPX4
E	220	LYS	-	expression tag	UNP M5BPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	221	GLY	-	expression tag	UNP M5BPX4
E	222	HIS	-	expression tag	UNP M5BPX4
E	223	HIS	-	expression tag	UNP M5BPX4
E	224	HIS	-	expression tag	UNP M5BPX4
E	225	HIS	-	expression tag	UNP M5BPX4
E	226	HIS	-	expression tag	UNP M5BPX4
E	227	HIS	-	expression tag	UNP M5BPX4
B	220	LYS	-	expression tag	UNP M5BPX4
B	221	GLY	-	expression tag	UNP M5BPX4
B	222	HIS	-	expression tag	UNP M5BPX4
B	223	HIS	-	expression tag	UNP M5BPX4
B	224	HIS	-	expression tag	UNP M5BPX4
B	225	HIS	-	expression tag	UNP M5BPX4
B	226	HIS	-	expression tag	UNP M5BPX4
B	227	HIS	-	expression tag	UNP M5BPX4
F	220	LYS	-	expression tag	UNP M5BPX4
F	221	GLY	-	expression tag	UNP M5BPX4
F	222	HIS	-	expression tag	UNP M5BPX4
F	223	HIS	-	expression tag	UNP M5BPX4
F	224	HIS	-	expression tag	UNP M5BPX4
F	225	HIS	-	expression tag	UNP M5BPX4
F	226	HIS	-	expression tag	UNP M5BPX4
F	227	HIS	-	expression tag	UNP M5BPX4
D	220	LYS	-	expression tag	UNP M5BPX4
D	221	GLY	-	expression tag	UNP M5BPX4
D	222	HIS	-	expression tag	UNP M5BPX4
D	223	HIS	-	expression tag	UNP M5BPX4
D	224	HIS	-	expression tag	UNP M5BPX4
D	225	HIS	-	expression tag	UNP M5BPX4
D	226	HIS	-	expression tag	UNP M5BPX4
D	227	HIS	-	expression tag	UNP M5BPX4

- Molecule 2 is S-(P-NITROBENZYL)GLUTATHIONE (CCD ID: GTB) (formula: C₁₇H₂₂N₄O₈S) (labeled as "Ligand of Interest" by depositor).

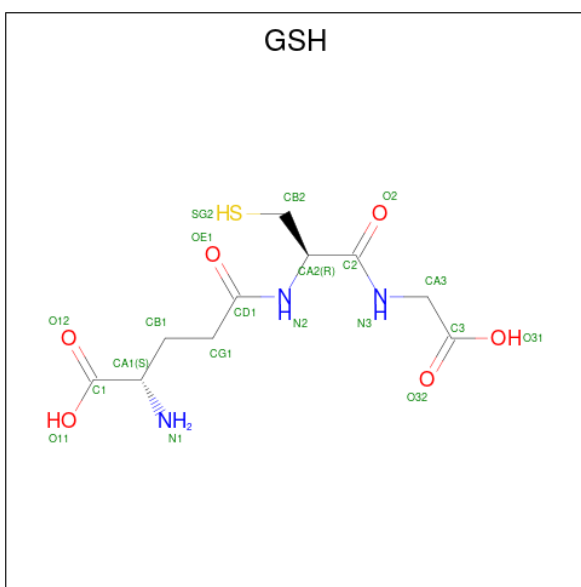


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Na 3 3	0	0
4	C	1	Total Na 1 1	0	0
4	B	2	Total Na 2 2	0	0
4	F	2	Total Na 2 2	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

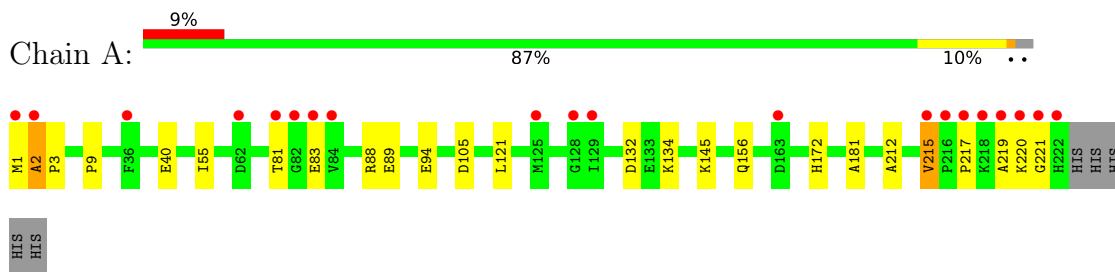
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	177	Total	O	0	0
			177	177		
6	C	185	Total	O	0	0
			185	185		
6	E	183	Total	O	0	0
			183	183		
6	B	188	Total	O	0	0
			188	188		
6	F	153	Total	O	0	0
			153	153		
6	D	187	Total	O	0	0
			187	187		

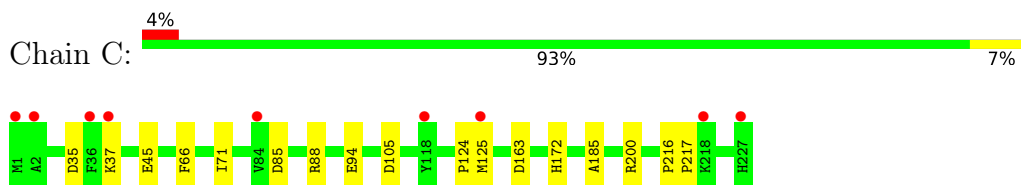
3 Residue-property plots

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.

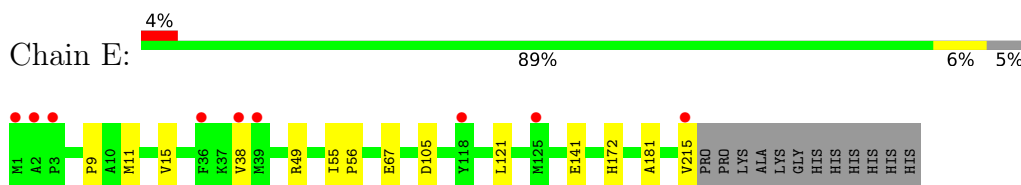
- Molecule 1: Glutathione transferase



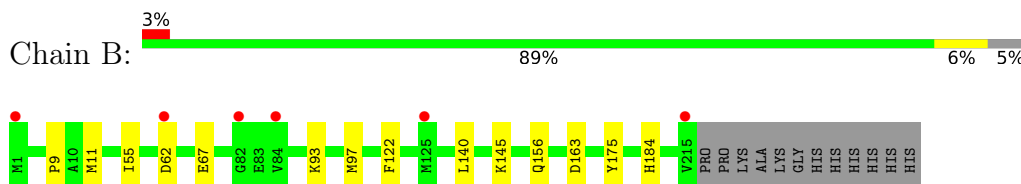
- Molecule 1: Glutathione transferase



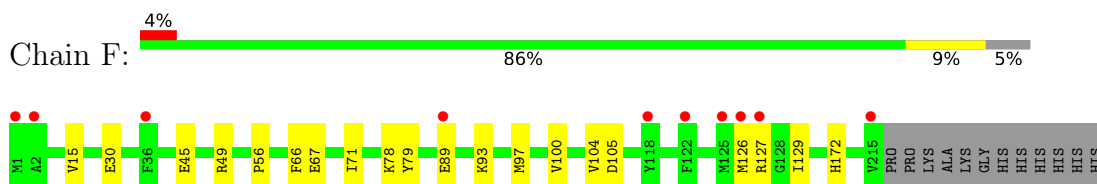
- Molecule 1: Glutathione transferase



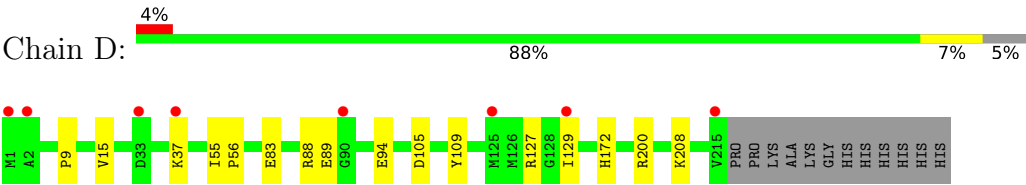
- Molecule 1: Glutathione transferase



- Molecule 1: Glutathione transferase



● Molecule 1: Glutathione transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.56Å 98.50Å 95.90Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	66.68 – 1.90 66.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (66.68-1.90) 91.3 (66.68-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.164 , 0.203 (Not available) , 0.191	Depositor DCC
R_{free} test set	1833 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11820	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 4.01% 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, GSH, NA, GTB

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	0.29	0/1828	0.50	1/2480 (0.0%)
1	B	0.32	0/1774	0.48	0/2407
1	C	0.29	0/1883	0.48	0/2555
1	D	0.29	0/1774	0.47	0/2407
1	E	0.28	0/1774	0.46	0/2407
1	F	0.26	0/1774	0.45	0/2407
All	All	0.29	0/10807	0.48	1/14663 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ALA	CB-CA-C	-5.15	110.23	117.23

There are no chirality outliers.

There are no planarity outliers.

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	1777	0	1769	20	0
1	B	1726	0	1714	12	0
1	C	1827	0	1804	13	0
1	D	1726	0	1714	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1726	0	1714	8	0
1	F	1726	0	1714	14	0
2	A	30	0	20	0	0
2	B	30	0	20	2	0
2	C	30	0	20	0	0
2	E	30	0	20	0	0
2	F	30	0	20	0	0
3	A	12	0	16	0	0
3	B	24	0	31	1	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
5	D	20	0	15	0	0
6	A	177	0	0	8	0
6	B	188	0	0	6	0
6	C	185	0	0	4	0
6	D	187	0	0	3	0
6	E	183	0	0	2	0
6	F	153	0	0	6	0
All	All	11820	0	10623	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:OD2	6:B:401:HOH:O	1.91	0.86
1:C:163:ASP:OD1	6:C:401:HOH:O	1.95	0.84
1:F:127:ARG:NH2	6:F:402:HOH:O	2.14	0.81
1:D:208:LYS:NZ	6:D:402:HOH:O	2.15	0.80
1:B:62:ASP:OD1	6:B:402:HOH:O	2.01	0.78
1:C:85:ASP:OD1	6:C:402:HOH:O	2.02	0.77
1:C:200:ARG:NH2	6:C:404:HOH:O	2.19	0.76
1:B:145:LYS:NZ	6:B:404:HOH:O	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:GLU:OE1	6:F:401:HOH:O	2.06	0.73
1:C:185:ALA:O	6:C:403:HOH:O	2.08	0.72
1:A:156:GLN:NE2	6:A:403:HOH:O	2.22	0.72
1:B:163:ASP:OD1	6:B:403:HOH:O	2.10	0.70
1:C:124:PRO:HB2	1:C:125:MET:HE1	1.76	0.68
1:A:40:GLU:OE2	6:A:401:HOH:O	2.10	0.68
1:D:89:GLU:OE2	6:D:401:HOH:O	2.11	0.67
1:B:156:GLN:NE2	6:B:405:HOH:O	2.29	0.66
1:E:141:GLU:OE1	6:E:401:HOH:O	2.15	0.64
1:F:45:GLU:OE1	6:F:403:HOH:O	2.16	0.60
1:F:93:LYS:NZ	6:F:406:HOH:O	2.35	0.59
1:E:11:MET:HB3	1:E:215:VAL:HG23	1.86	0.57
1:F:49:ARG:HD3	6:F:464:HOH:O	2.03	0.57
1:A:1:MET:SD	6:A:441:HOH:O	2.58	0.57
1:A:9:PRO:HD2	1:A:55:ILE:HD13	1.87	0.56
1:D:200:ARG:NH2	6:D:403:HOH:O	2.28	0.55
1:E:49:ARG:HD3	6:E:478:HOH:O	2.06	0.55
1:D:9:PRO:HD2	1:D:55:ILE:HD13	1.90	0.54
1:C:125:MET:N	1:C:125:MET:SD	2.81	0.52
1:F:129:ILE:H	1:F:129:ILE:HD12	1.73	0.52
1:D:15:VAL:HG22	1:D:56:PRO:HB3	1.92	0.52
1:C:124:PRO:HB2	1:C:125:MET:CE	2.39	0.52
1:F:15:VAL:HG22	1:F:56:PRO:HB3	1.92	0.51
1:F:78:LYS:HD3	1:F:79:TYR:CE2	2.45	0.51
1:C:35:ASP:OD1	1:C:37:LYS:HG2	2.11	0.51
1:B:9:PRO:HD2	1:B:55:ILE:HD13	1.93	0.50
1:B:11:MET:HE3	3:B:303:GOL:H11	1.94	0.50
1:E:121:LEU:HD11	1:E:181:ALA:HB3	1.95	0.49
1:F:97:MET:HE1	6:F:518:HOH:O	2.13	0.48
1:A:220:LYS:HD3	1:D:83:GLU:HG3	1.95	0.48
1:A:212:ALA:O	1:A:215:VAL:HG13	2.14	0.48
1:A:105:ASP:HB2	1:A:172:HIS:CE1	2.48	0.48
1:F:105:ASP:HB2	1:F:172:HIS:CE1	2.50	0.47
1:A:156:GLN:OE1	6:A:402:HOH:O	2.20	0.46
1:A:217:PRO:HG2	6:A:517:HOH:O	2.15	0.46
1:B:97:MET:HE3	1:B:97:MET:HA	1.98	0.46
1:E:38:VAL:HG22	1:E:38:VAL:O	2.16	0.45
1:C:88:ARG:HD2	1:C:94:GLU:OE1	2.17	0.45
1:D:127:ARG:HB3	1:D:129:ILE:HD12	1.98	0.45
1:A:81:THR:HG22	1:A:83:GLU:H	1.82	0.45
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLN:NE2	6:A:405:HOH:O	2.31	0.45
1:B:175:TYR:CE2	2:B:301:GTB:H5'	2.51	0.44
1:A:220:LYS:HD3	1:D:83:GLU:CG	2.48	0.44
1:C:45:GLU:H	1:C:45:GLU:CD	2.25	0.44
1:E:105:ASP:HB2	1:E:172:HIS:CE1	2.53	0.44
1:F:126:MET:HE3	1:F:126:MET:HB3	1.92	0.44
1:A:88:ARG:HD2	1:A:94:GLU:OE1	2.18	0.44
1:D:88:ARG:HD2	1:D:94:GLU:OE1	2.18	0.43
1:E:9:PRO:HD2	1:E:55:ILE:HD13	2.01	0.42
1:B:93:LYS:HG3	6:B:530:HOH:O	2.18	0.42
1:F:89:GLU:HA	1:F:89:GLU:OE1	2.19	0.42
1:A:81:THR:HG21	1:A:83:GLU:HB3	2.00	0.42
1:A:145:LYS:NZ	6:A:418:HOH:O	2.52	0.42
1:E:15:VAL:HG22	1:E:56:PRO:HB3	2.01	0.41
1:F:66:PHE:HA	1:F:71:ILE:HD11	2.01	0.41
1:C:105:ASP:HB2	1:C:172:HIS:CE1	2.55	0.41
1:C:216:PRO:HA	1:C:217:PRO:HD3	1.96	0.41
1:A:2:ALA:HA	1:A:3:PRO:HD3	1.97	0.41
1:A:132:ASP:OD2	1:A:134:LYS:NZ	2.53	0.41
1:A:181:ALA:HA	1:A:221:GLY:H	1.86	0.41
1:B:122:PHE:HB2	2:B:301:GTB:O42	2.21	0.41
1:B:140:LEU:HD11	1:B:184:HIS:CE1	2.56	0.41
1:D:37:LYS:HE2	1:D:37:LYS:H	1.85	0.41
1:D:105:ASP:HA	1:D:109:TYR:HB3	2.02	0.41
1:A:89:GLU:OE2	6:A:404:HOH:O	2.22	0.40
1:D:105:ASP:HB2	1:D:172:HIS:CE1	2.57	0.40
1:C:66:PHE:HA	1:C:71:ILE:HD11	2.03	0.40
1:F:100:VAL:O	1:F:104:VAL:HG23	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	220/227 (97%)	209 (95%)	9 (4%)	2 (1%)	14	6
1	B	213/227 (94%)	209 (98%)	3 (1%)	1 (0%)	24	16
1	C	225/227 (99%)	217 (96%)	8 (4%)	0	100	100
1	D	213/227 (94%)	206 (97%)	7 (3%)	0	100	100
1	E	213/227 (94%)	207 (97%)	5 (2%)	1 (0%)	24	16
1	F	213/227 (94%)	205 (96%)	7 (3%)	1 (0%)	24	16
All	All	1297/1362 (95%)	1253 (97%)	39 (3%)	5 (0%)	30	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	VAL
1	A	2	ALA
1	E	67	GLU
1	B	67	GLU
1	F	67	GLU

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	189/194 (97%)	189 (100%)	0	100	100
1	B	184/194 (95%)	184 (100%)	0	100	100
1	C	194/194 (100%)	194 (100%)	0	100	100
1	D	184/194 (95%)	184 (100%)	0	100	100
1	E	184/194 (95%)	184 (100%)	0	100	100
1	F	184/194 (95%)	184 (100%)	0	100	100
All	All	1119/1164 (96%)	1119 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	157	HIS
1	C	226	HIS
1	F	110	ASN
1	D	156	GLN
1	D	184	HIS

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 ⓘ

Of 25 ligands modelled in this entry, 9 are monoatomic - leaving 16 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	GTB	E	301	-	29,30,30	1.65	3 (10%)	34,39,39	1.31	4 (11%)
3	GOL	B	302	-	5,5,5	1.37	1 (20%)	5,5,5	0.74	0
3	GOL	E	302	-	5,5,5	0.99	0	5,5,5	0.93	0
3	GOL	C	302	-	5,5,5	0.93	0	5,5,5	0.92	0
3	GOL	A	303	-	5,5,5	0.92	0	5,5,5	1.01	0
3	GOL	B	305	-	5,5,5	1.33	1 (20%)	5,5,5	1.13	0
2	GTB	F	301	-	29,30,30	1.65	4 (13%)	34,39,39	1.37	4 (11%)
2	GTB	A	301	-	29,30,30	1.60	3 (10%)	34,39,39	1.30	5 (14%)
3	GOL	A	302	-	5,5,5	1.09	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTB	B	301	-	29,30,30	1.65	4 (13%)	34,39,39	1.46	6 (17%)
3	GOL	F	302	-	5,5,5	1.16	0	5,5,5	0.92	0
3	GOL	D	302	-	5,5,5	1.21	0	5,5,5	0.93	0
5	GSH	D	301	-	18,19,19	1.99	4 (22%)	21,24,24	1.49	3 (14%)
3	GOL	B	304	-	5,5,5	0.96	0	5,5,5	0.93	0
3	GOL	B	303	-	5,5,5	0.89	0	5,5,5	1.06	0
2	GTB	C	301	-	29,30,30	1.65	3 (10%)	34,39,39	1.55	7 (20%)

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	GTB	E	301	-	-	3/30/32/32	0/1/1/1
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	E	302	-	-	0/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	B	305	-	-	2/4/4/4	-
2	GTB	F	301	-	-	1/30/32/32	0/1/1/1
2	GTB	A	301	-	-	0/30/32/32	0/1/1/1
3	GOL	A	302	-	-	0/4/4/4	-
2	GTB	B	301	-	-	3/30/32/32	0/1/1/1
3	GOL	F	302	-	-	0/4/4/4	-
3	GOL	D	302	-	-	0/4/4/4	-
5	GSH	D	301	-	-	0/24/24/24	-
3	GOL	B	304	-	-	2/4/4/4	-
3	GOL	B	303	-	-	0/4/4/4	-
2	GTB	C	301	-	-	0/30/32/32	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	GTB	CD1-N2	5.24	1.45	1.34
2	F	301	GTB	CD1-N2	5.24	1.45	1.34
5	D	301	GSH	CD1-N2	5.14	1.44	1.34
2	E	301	GTB	C2-N3	5.06	1.45	1.33
2	F	301	GTB	C2-N3	5.06	1.45	1.33
2	A	301	GTB	CD1-N2	5.03	1.44	1.34
2	C	301	GTB	CD1-N2	4.91	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GTB	CD1-N2	4.91	1.44	1.34
5	D	301	GSH	C2-N3	4.90	1.45	1.33
2	C	301	GTB	C2-N3	4.90	1.45	1.33
2	B	301	GTB	C2-N3	4.82	1.44	1.33
2	A	301	GTB	C2-N3	4.69	1.44	1.33
2	B	301	GTB	O42-N41	-3.11	1.17	1.22
2	A	301	GTB	O42-N41	-2.92	1.17	1.22
2	E	301	GTB	O42-N41	-2.83	1.17	1.22
2	F	301	GTB	O42-N41	-2.73	1.18	1.22
2	C	301	GTB	O42-N41	-2.66	1.18	1.22
3	B	305	GOL	O2-C2	-2.49	1.36	1.43
5	D	301	GSH	OE1-CD1	-2.37	1.18	1.23
2	B	301	GTB	O2-C2	-2.35	1.18	1.23
2	F	301	GTB	O2-C2	-2.24	1.19	1.23
5	D	301	GSH	O2-C2	-2.16	1.19	1.23
3	B	302	GOL	C1-C2	2.08	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	GTB	CB2-SG2-C'	3.75	109.08	101.24
2	C	301	GTB	CB2-SG2-C'	3.53	108.60	101.24
2	E	301	GTB	CB2-SG2-C'	3.49	108.53	101.24
2	A	301	GTB	CB2-SG2-C'	3.43	108.40	101.24
5	D	301	GSH	CG1-CB1-CA1	-3.37	106.12	113.86
2	C	301	GTB	CB2-CA2-C2	3.22	116.73	109.46
2	E	301	GTB	CG1-CB1-CA1	-3.19	106.53	113.86
2	B	301	GTB	C1'-C'-SG2	-2.93	107.09	113.97
2	C	301	GTB	CG1-CB1-CA1	-2.82	107.40	113.86
2	C	301	GTB	O2-C2-N3	-2.81	117.04	122.98
2	F	301	GTB	CG1-CB1-CA1	-2.77	107.50	113.86
2	F	301	GTB	C1'-C'-SG2	-2.59	107.90	113.97
2	B	301	GTB	CA2-CB2-SG2	-2.54	103.98	113.92
2	B	301	GTB	CB2-CA2-N2	-2.51	104.50	111.06
5	D	301	GSH	OE1-CD1-N2	-2.48	118.75	122.95
5	D	301	GSH	CG1-CD1-N2	2.43	120.14	115.86
2	A	301	GTB	CG1-CB1-CA1	-2.40	108.36	113.86
2	B	301	GTB	C6'-C1'-C2'	2.39	121.79	118.23
2	C	301	GTB	C2-CA2-N2	-2.39	104.65	111.11
2	A	301	GTB	C1'-C'-SG2	-2.36	108.44	113.97
2	C	301	GTB	C1'-C'-SG2	-2.28	108.63	113.97
2	A	301	GTB	O12-C1-O11	-2.27	118.93	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	GTB	C1'-C'-SG2	-2.23	108.74	113.97
2	B	301	GTB	CA2-C2-N3	2.12	121.08	116.54
2	C	301	GTB	C3'-C4'-N41	2.06	121.14	119.34
2	F	301	GTB	CA2-C2-N3	2.06	120.95	116.54
2	B	301	GTB	CG1-CB1-CA1	-2.02	109.22	113.86
2	A	301	GTB	O32-C3-CA3	2.02	120.48	112.81
2	E	301	GTB	O12-C1-O11	-2.01	119.51	124.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	305	GOL	C1-C2-C3-O3
2	B	301	GTB	C3'-C4'-N41-O42
2	B	301	GTB	C5'-C4'-N41-O42
3	B	304	GOL	C1-C2-C3-O3
3	B	304	GOL	O2-C2-C3-O3
3	B	305	GOL	O2-C2-C3-O3
2	E	301	GTB	SG2-C'-C1'-C6'
2	E	301	GTB	SG2-C'-C1'-C2'
2	E	301	GTB	C1'-C'-SG2-CB2
2	B	301	GTB	C1'-C'-SG2-CB2
2	F	301	GTB	O12-C1-CA1-N1

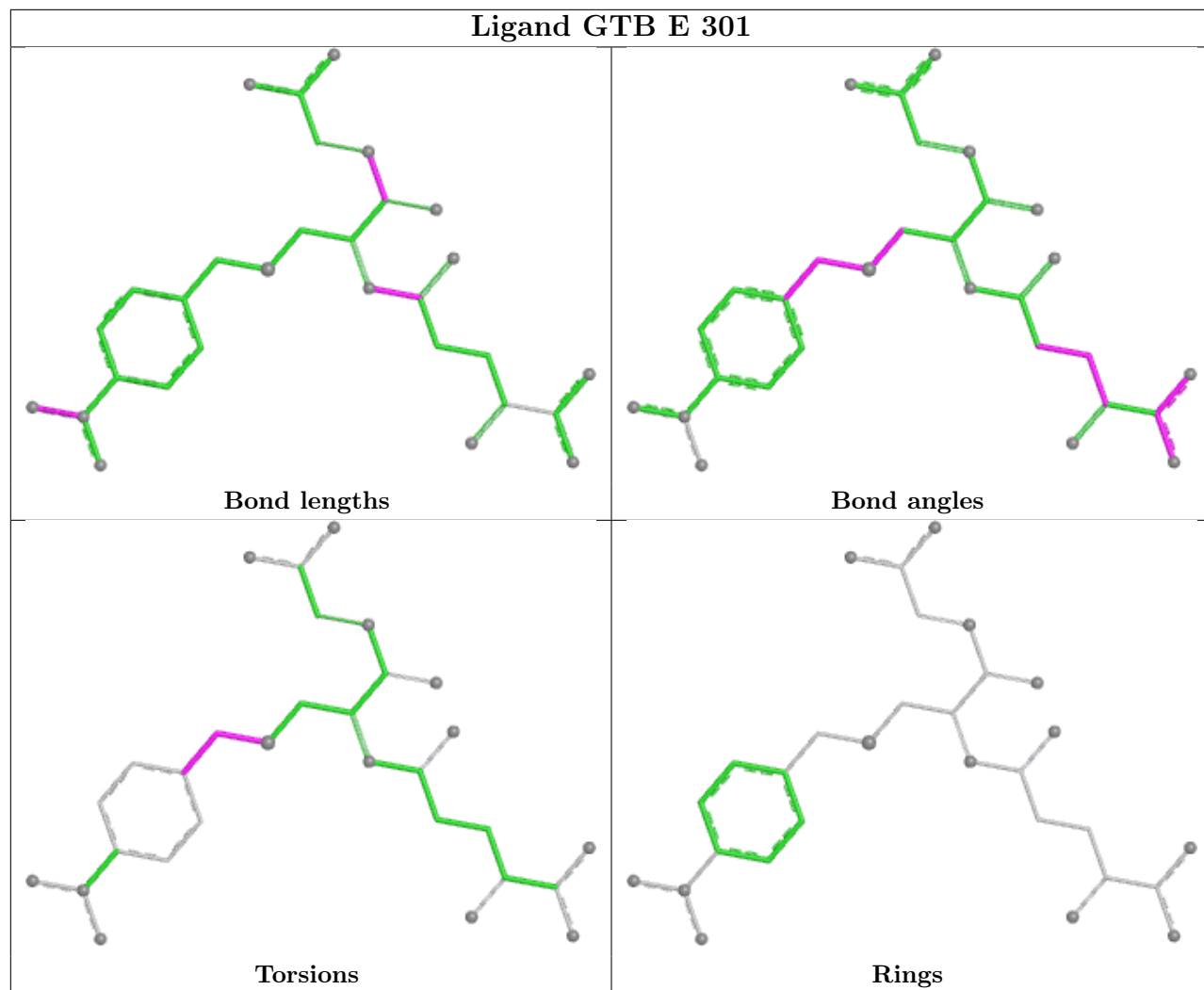
There are no ring outliers.

2 monomers are involved in 3 short contacts:

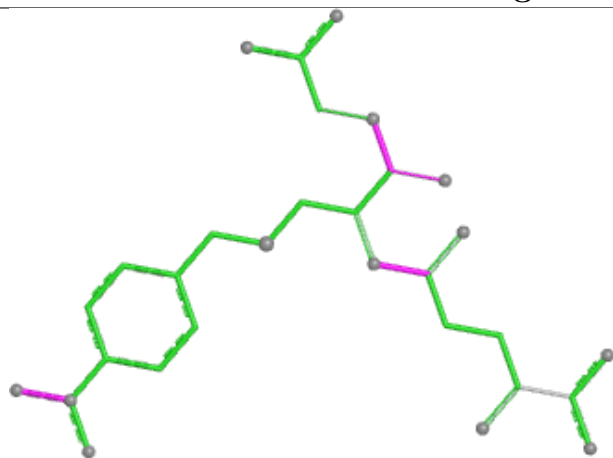
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	GTB	2	0
3	B	303	GOL	1	0

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

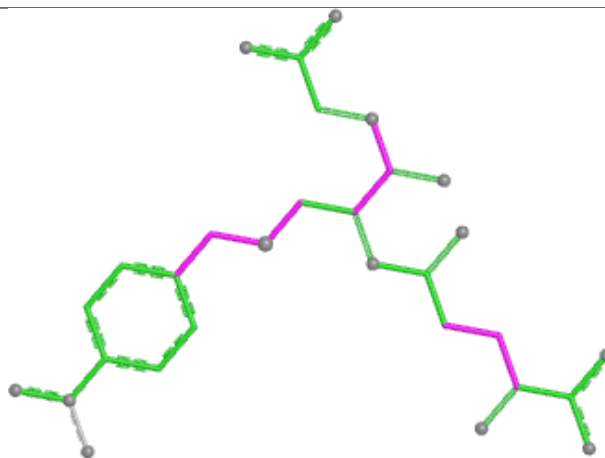
equivalents in the CSD to analyse the geometry.



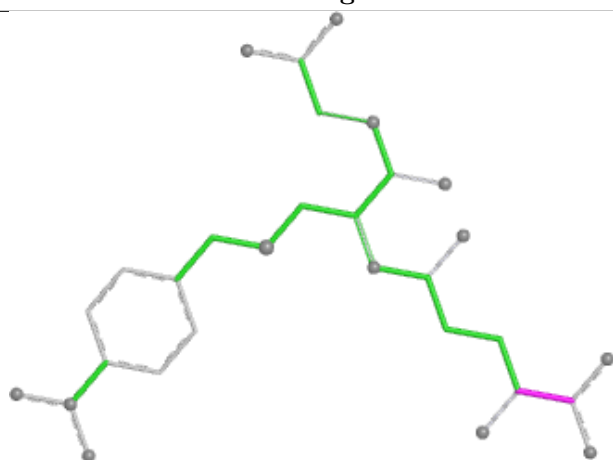
Ligand GTB F 301



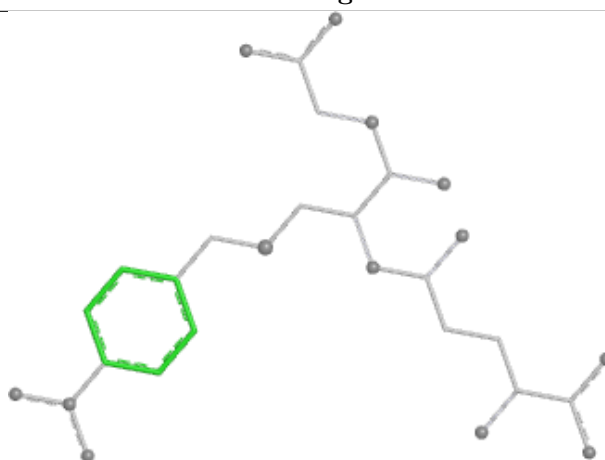
Bond lengths



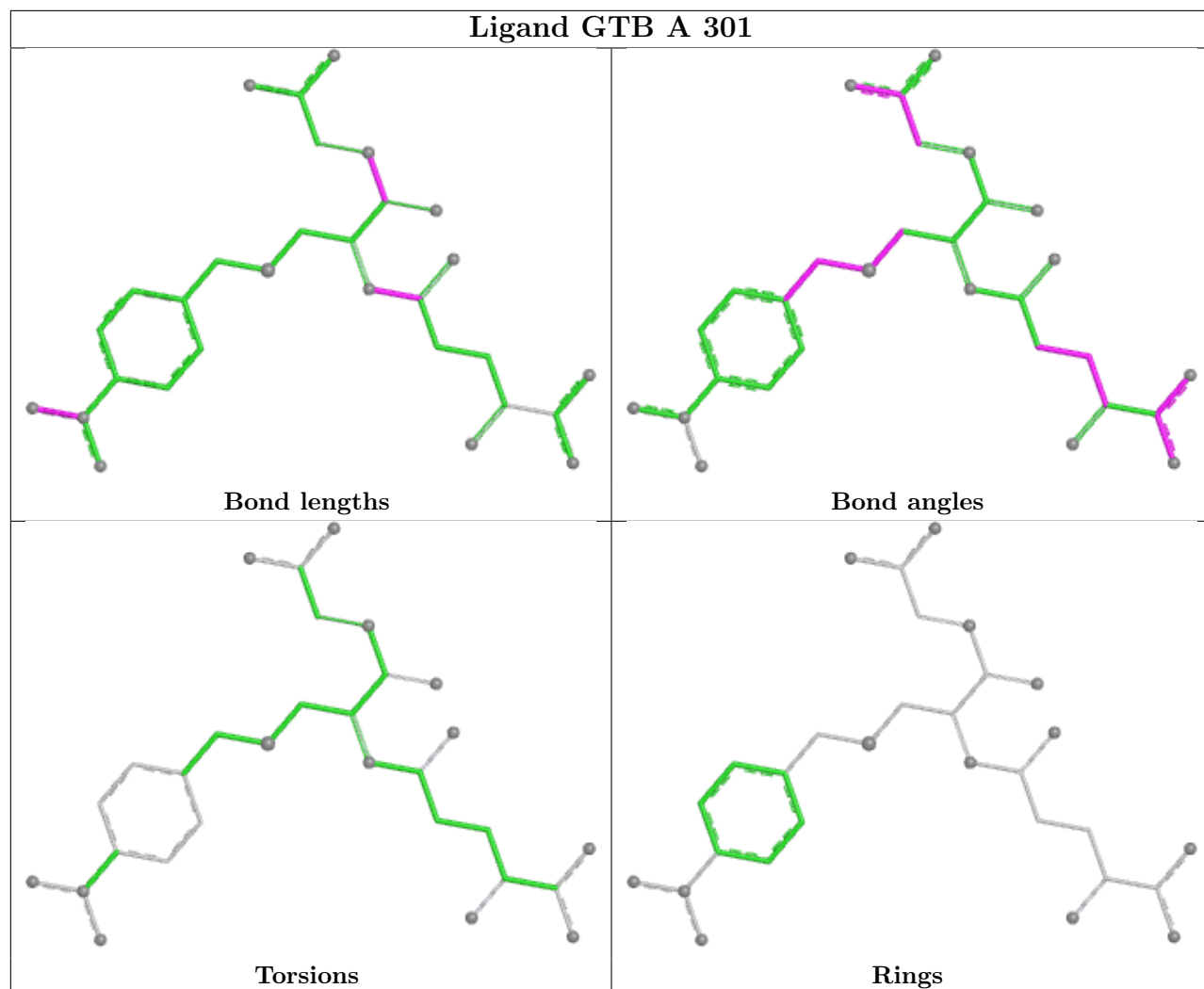
Bond angles



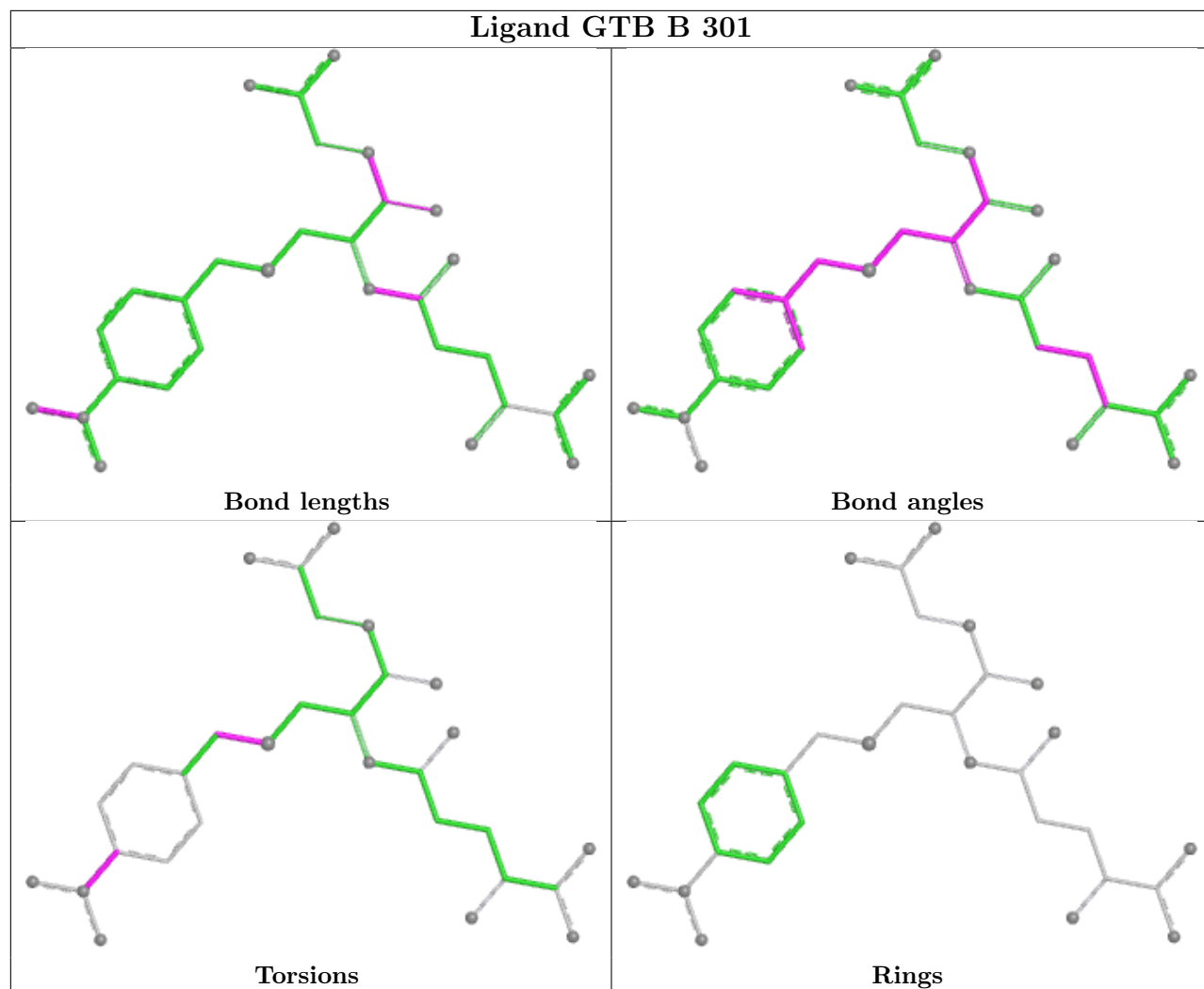
Torsions



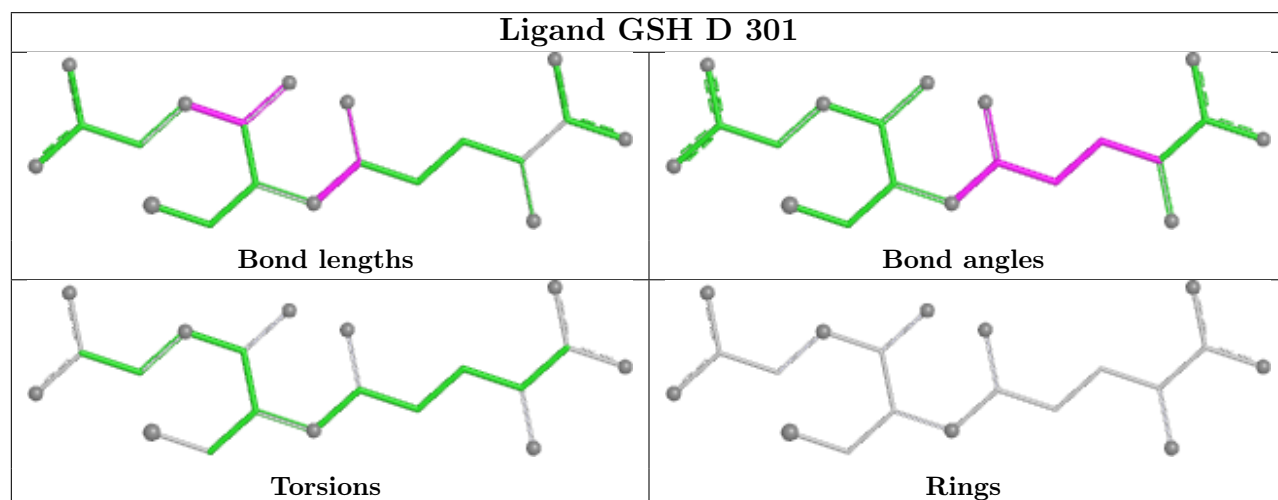
Rings

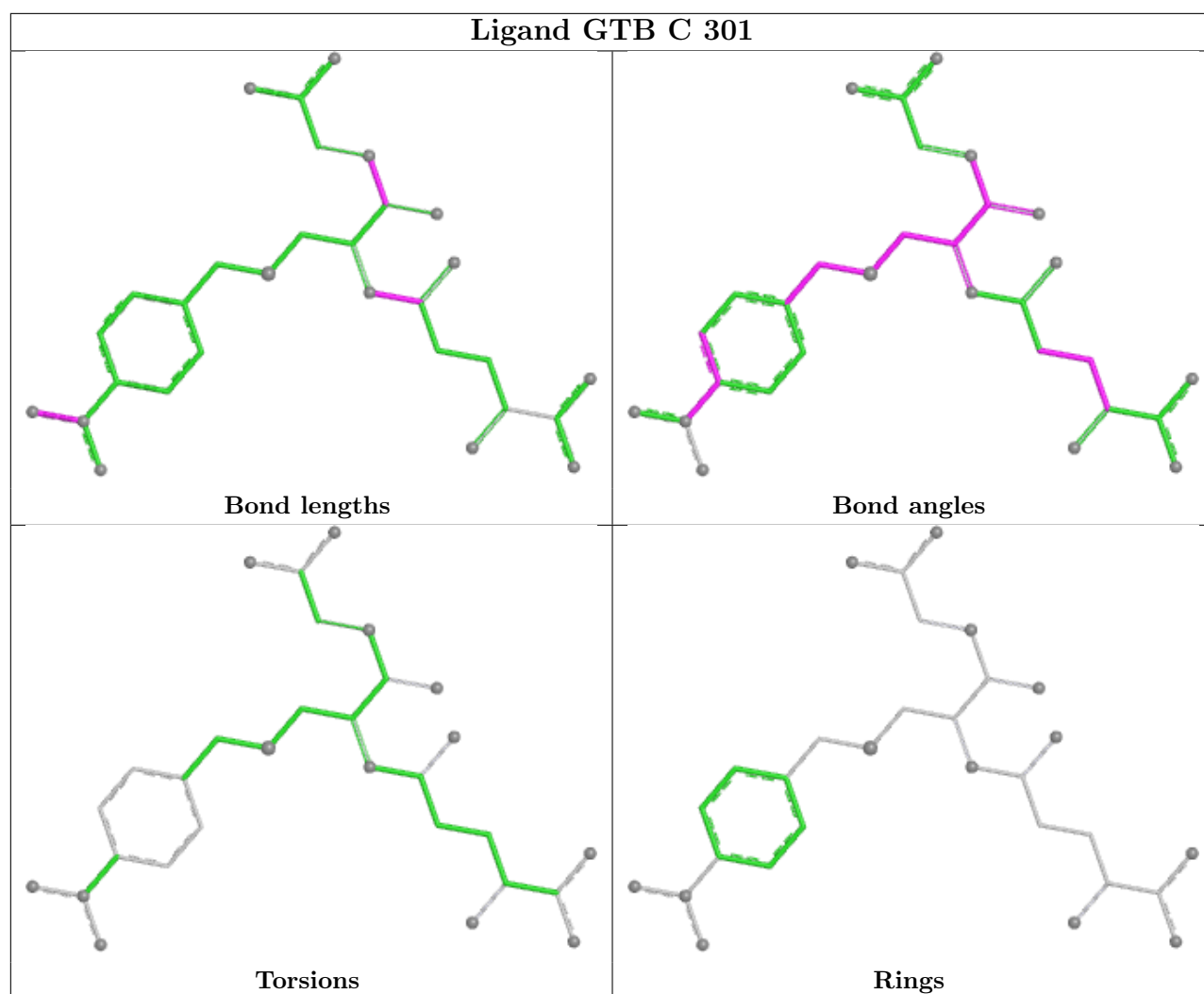


Ligand GTB B 301



Ligand GSH D 301





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	222/227 (97%)	-0.01	20 (9%) 15 16	17, 27, 79, 175	0
1	B	215/227 (94%)	-0.16	6 (2%) 55 59	18, 29, 55, 104	0
1	C	227/227 (100%)	-0.12	9 (3%) 42 45	17, 30, 60, 120	0
1	D	215/227 (94%)	-0.13	8 (3%) 45 48	18, 30, 66, 127	0
1	E	215/227 (94%)	-0.08	9 (4%) 40 43	17, 32, 71, 142	0
1	F	215/227 (94%)	-0.03	10 (4%) 36 39	16, 34, 72, 126	0
All	All	1309/1362 (96%)	-0.09	62 (4%) 36 39	16, 30, 66, 175	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	8.3
1	D	215	VAL	7.9
1	A	215	VAL	7.2
1	A	219	ALA	6.7
1	F	215	VAL	6.1
1	A	216	PRO	5.9
1	B	215	VAL	5.5
1	E	215	VAL	5.5
1	A	81	THR	5.1
1	A	217	PRO	5.0
1	A	220	LYS	4.9
1	A	222	HIS	4.7
1	E	2	ALA	4.6
1	C	1	MET	4.5
1	A	1	MET	4.5
1	E	36	PHE	4.4
1	B	1	MET	4.4
1	A	84	VAL	3.9
1	C	125	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	36	PHE	3.7
1	A	218	LYS	3.6
1	C	2	ALA	3.3
1	C	37	LYS	3.3
1	A	2	ALA	3.2
1	C	118	TYR	3.2
1	F	125	MET	3.1
1	D	1	MET	3.1
1	D	37	LYS	3.0
1	E	1	MET	3.0
1	F	1	MET	3.0
1	D	2	ALA	3.0
1	B	84	VAL	2.9
1	B	62	ASP	2.9
1	B	125	MET	2.9
1	E	39	MET	2.9
1	D	125	MET	2.8
1	E	125	MET	2.7
1	F	118	TYR	2.6
1	C	84	VAL	2.6
1	F	89	GLU	2.6
1	C	218	LYS	2.6
1	A	129	ILE	2.5
1	F	2	ALA	2.5
1	E	118	TYR	2.5
1	B	82	GLY	2.4
1	F	122	PHE	2.3
1	A	125	MET	2.3
1	F	127	ARG	2.3
1	E	3	PRO	2.3
1	A	128	GLY	2.3
1	A	163	ASP	2.2
1	E	38	VAL	2.2
1	C	227	HIS	2.2
1	D	33	ASP	2.2
1	A	82	GLY	2.2
1	D	90	GLY	2.2
1	F	126	MET	2.1
1	A	36	PHE	2.1
1	D	129	ILE	2.1
1	A	62	ASP	2.1
1	F	36	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	83	GLU	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.

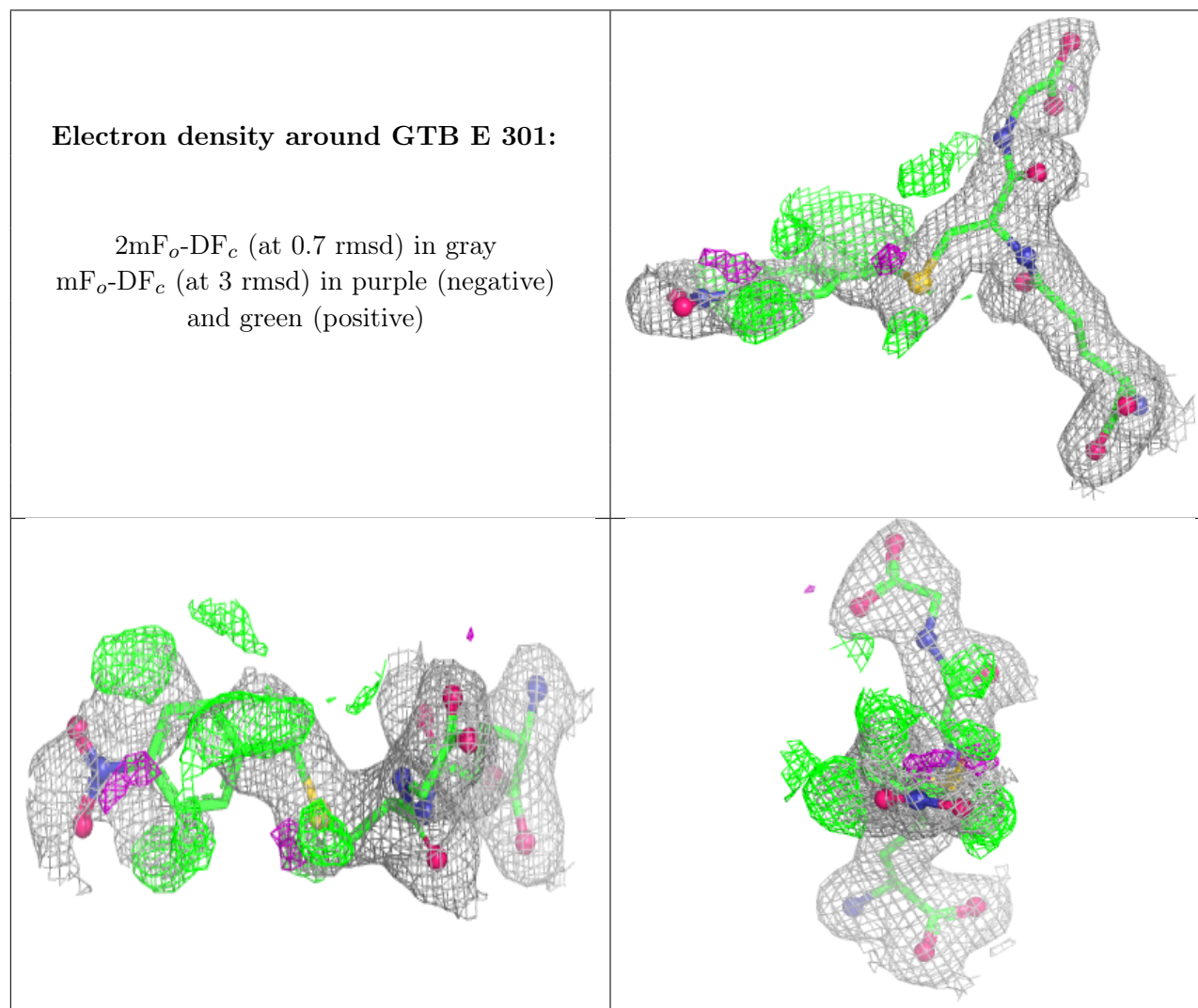
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	303	6/6	0.79	0.17	65,67,68,68	0
4	NA	B	307	1/1	0.81	0.17	64,64,64,64	0
3	GOL	B	304	6/6	0.86	0.14	47,62,69,74	0
3	GOL	B	305	6/6	0.87	0.14	35,46,50,51	0
3	GOL	A	303	6/6	0.87	0.13	48,51,54,55	0
4	NA	A	306	1/1	0.88	0.20	77,77,77,77	0
2	GTB	E	301	30/30	0.90	0.15	21,44,98,100	0
4	NA	A	305	1/1	0.90	0.09	52,52,52,52	0
4	NA	B	306	1/1	0.91	0.11	49,49,49,49	0
4	NA	F	304	1/1	0.91	0.12	64,64,64,64	0
4	NA	D	303	1/1	0.92	0.09	50,50,50,50	0
2	GTB	C	301	30/30	0.93	0.10	18,34,60,62	0
4	NA	A	304	1/1	0.93	0.16	50,50,50,50	0
2	GTB	B	301	30/30	0.94	0.10	18,30,61,68	0
4	NA	F	303	1/1	0.94	0.11	41,41,41,41	0
4	NA	C	303	1/1	0.94	0.14	54,54,54,54	0
2	GTB	F	301	30/30	0.94	0.10	24,46,75,78	0
3	GOL	C	302	6/6	0.96	0.07	26,26,28,32	0
2	GTB	A	301	30/30	0.96	0.08	18,26,58,59	0
3	GOL	F	302	6/6	0.96	0.06	27,28,30,30	0
5	GSH	D	301	20/20	0.96	0.06	20,30,50,52	0
3	GOL	A	302	6/6	0.97	0.05	20,23,26,28	0

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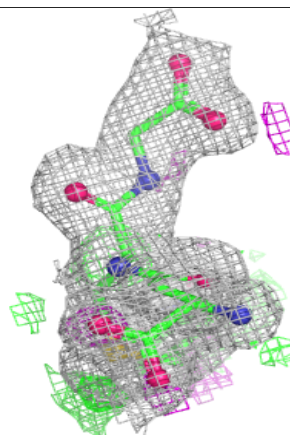
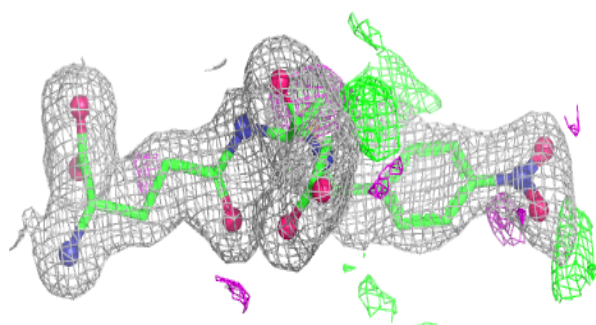
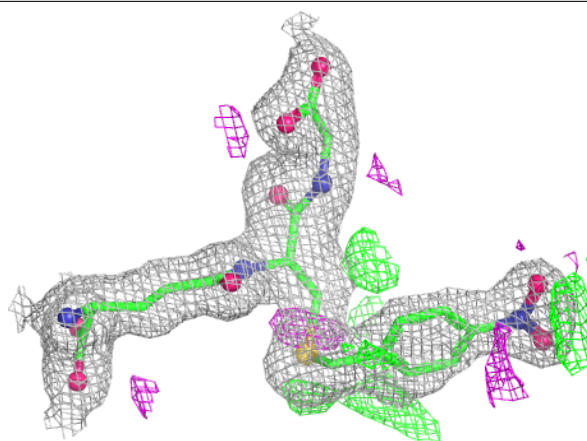
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	302	6/6	0.97	0.05	18,21,25,26	0
3	GOL	E	302	6/6	0.98	0.04	21,23,25,26	0
3	GOL	D	302	6/6	0.98	0.04	17,22,25,27	0

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.



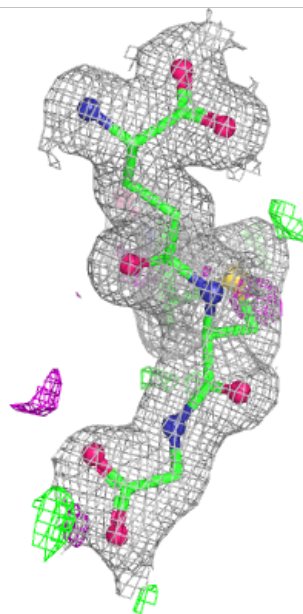
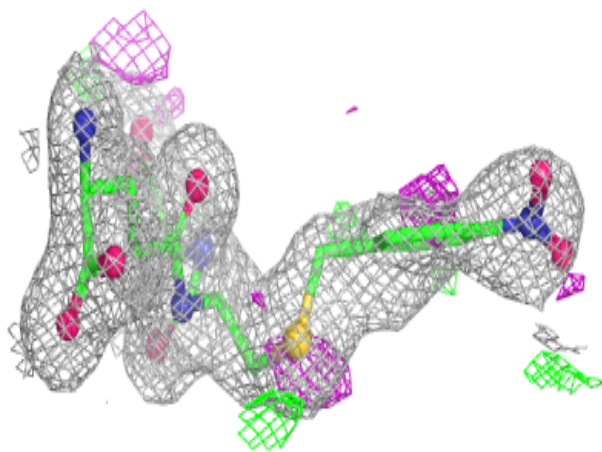
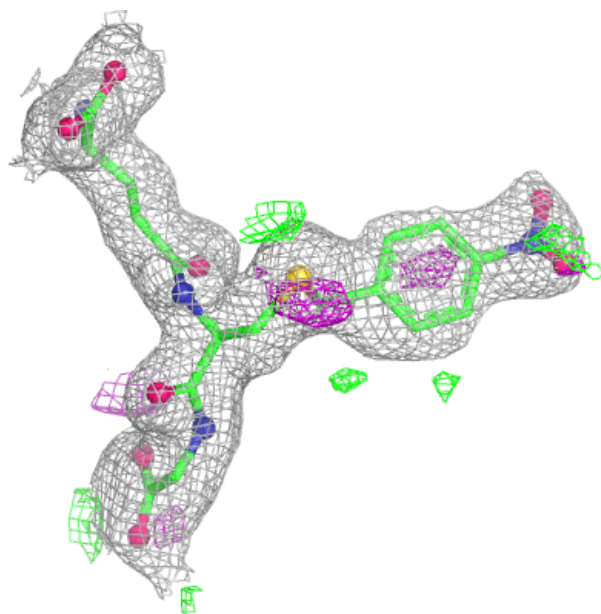
Electron density around GTB C 301:

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



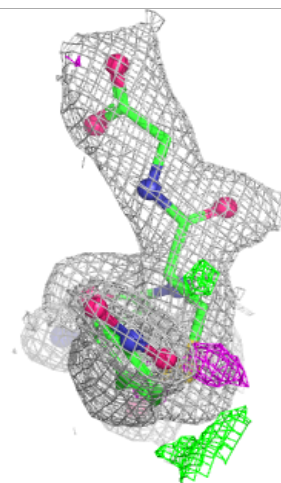
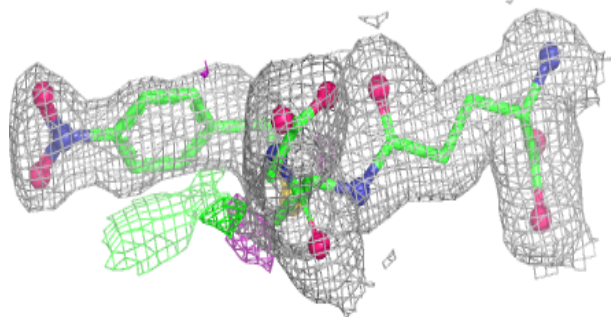
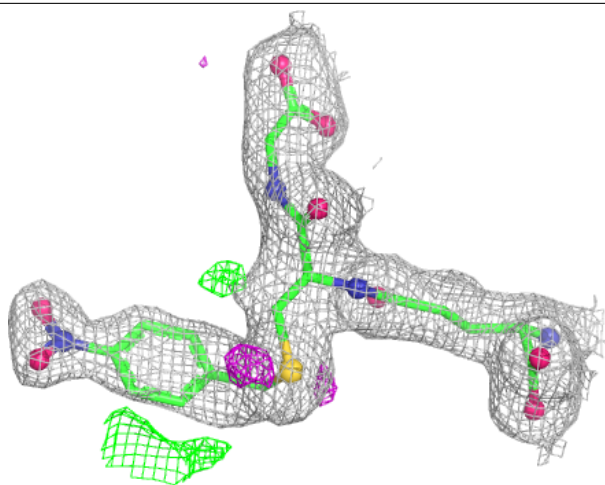
Electron density around GTB B 301:

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



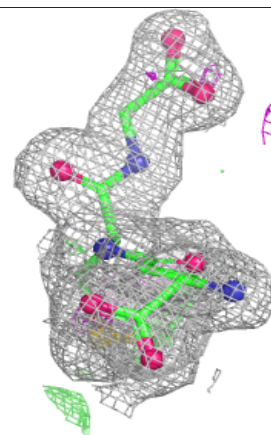
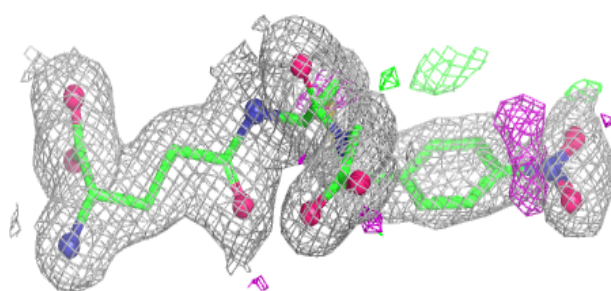
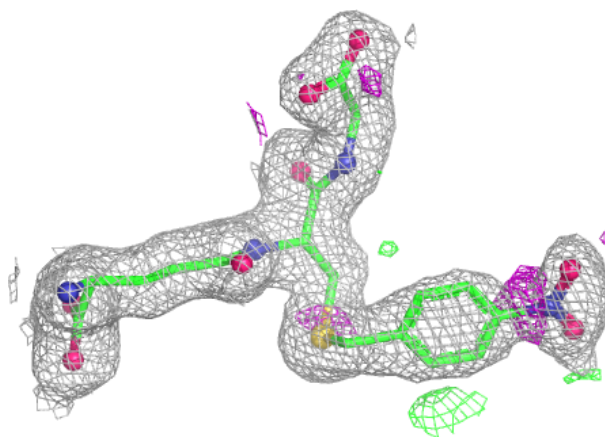
Electron density around GTB F 301:

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

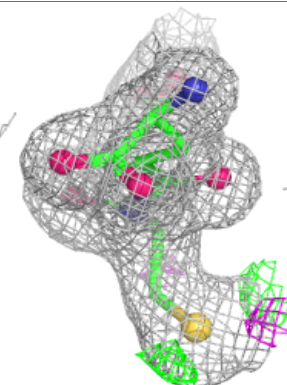
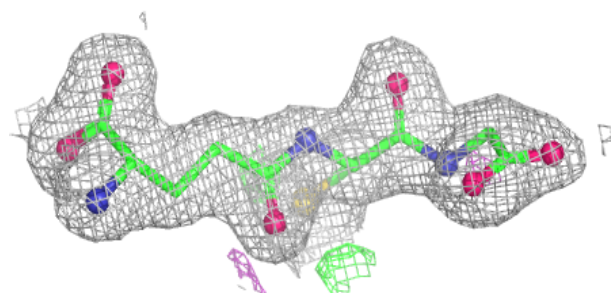
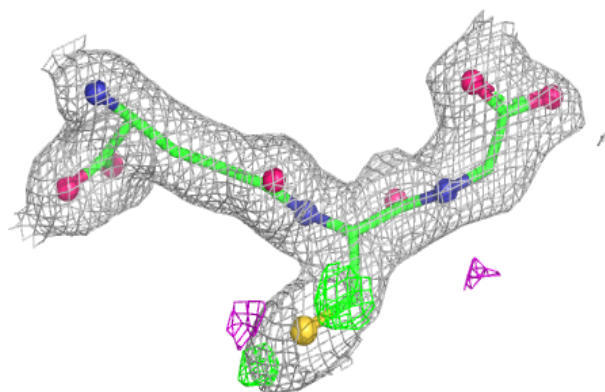


Electron density around GTB A 301:

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

**Electron density around GSH D 301:**

$2mF_o-DF_c$ (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.