



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:55 PM UTC

PDB ID : 1GTI / pdb_00001gti
Title : MODIFIED GLUTATHIONE S-TRANSFERASE (PI) COMPLEXED WITH
S (P-NITROBENZYL)GLUTATHIONE
Authors : Vega, M.C.; Coll, M.
Deposited on : 1998-01-09
Resolution : 3.00 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

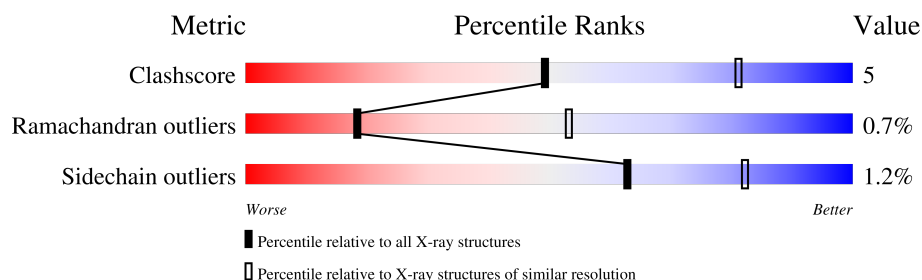
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	83% 17%
1	B	209	85% 15%
1	C	209	83% 15% .
1	D	209	81% 18% .
1	E	209	84% 16%
1	F	209	83% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10128 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.

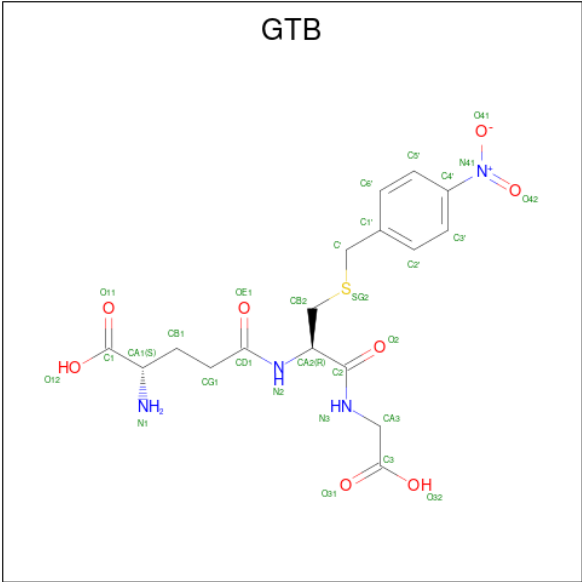
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total 1658	C 1059	N 285	O 306	S 8	111	0	0
1	B	209	Total 1658	C 1059	N 285	O 306	S 8	106	0	0
1	C	209	Total 1658	C 1059	N 285	O 306	S 8	98	0	0
1	D	209	Total 1658	C 1059	N 285	O 306	S 8	135	0	0
1	E	209	Total 1658	C 1059	N 285	O 306	S 8	114	0	0
1	F	209	Total 1658	C 1059	N 285	O 306	S 8	107	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CCS	CYS	modified residue	UNP P19157
B	47	CCS	CYS	modified residue	UNP P19157
C	47	CCS	CYS	modified residue	UNP P19157
D	47	CCS	CYS	modified residue	UNP P19157
E	47	CCS	CYS	modified residue	UNP P19157
F	47	CCS	CYS	modified residue	UNP P19157

- Molecule 2 is S-(P-NITROBENZYL)GLUTATHIONE (CCD ID: GTB) (formula: $C_{17}H_{22}N_4O_8S$).



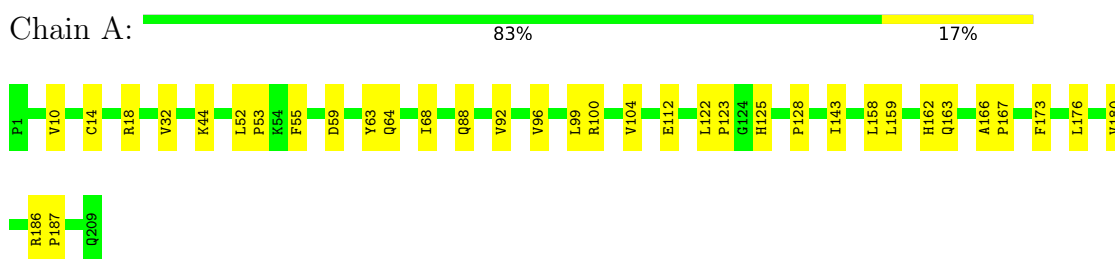
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	17	4	8	1		
2	B	1	Total	C	N	O	S	0	0
			30	17	4	8	1		
2	C	1	Total	C	N	O	S	0	0
			30	17	4	8	1		
2	D	1	Total	C	N	O	S	0	0
			30	17	4	8	1		
2	E	1	Total	C	N	O	S	0	0
			30	17	4	8	1		
2	F	1	Total	C	N	O	S	0	0
			30	17	4	8	1		

3 Residue-property plots

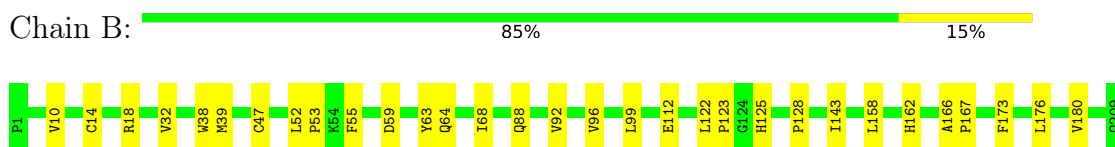
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

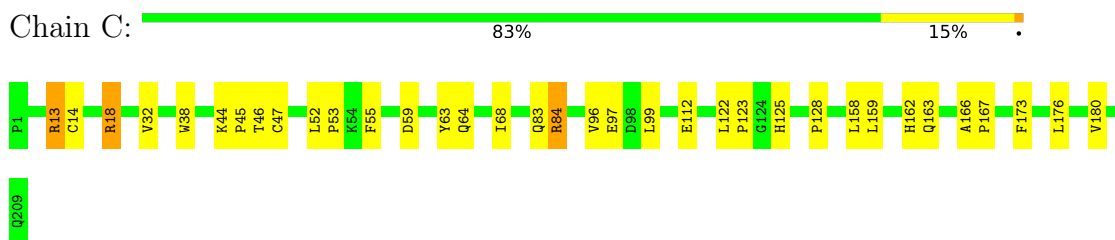
- Molecule 1: GLUTATHIONE S-TRANSFERASE



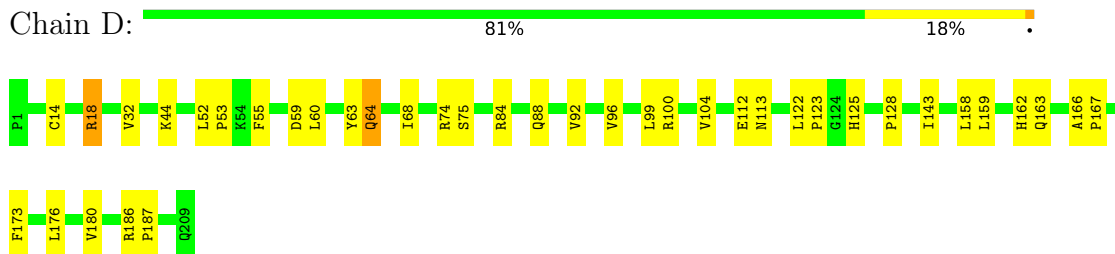
- Molecule 1: GLUTATHIONE S-TRANSFERASE



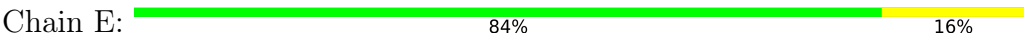
- Molecule 1: GLUTATHIONE S-TRANSFERASE



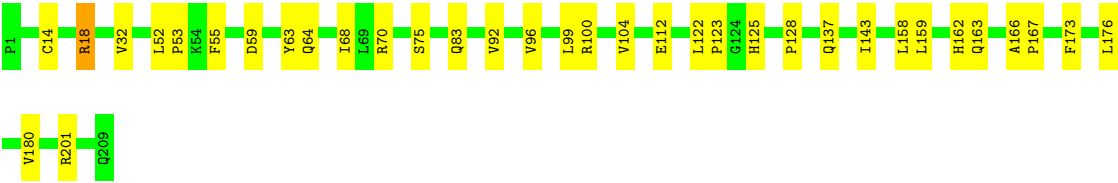
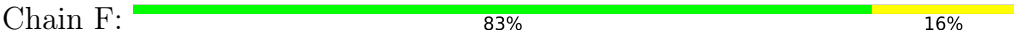
- Molecule 1: GLUTATHIONE S-TRANSFERASE



- Molecule 1: GLUTATHIONE S-TRANSFERASE



● Molecule 1: GLUTATHIONE S-TRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.45Å 132.69Å 214.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	52.5 (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.246 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10128	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.33	0/1684	0.88	8/2278 (0.4%)
1	B	0.33	0/1684	0.88	8/2278 (0.4%)
1	C	0.34	0/1684	1.02	14/2278 (0.6%)
1	D	0.34	0/1684	1.00	15/2278 (0.7%)
1	E	0.33	0/1684	0.89	8/2278 (0.4%)
1	F	0.33	0/1684	1.04	14/2278 (0.6%)
All	All	0.33	0/10104	0.95	67/13668 (0.5%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	ARG	NE-CZ-NH2	-13.74	106.83	119.20
1	D	74	ARG	NE-CZ-NH2	-13.03	107.47	119.20
1	F	70	ARG	NE-CZ-NH2	-12.81	107.67	119.20
1	F	201	ARG	NE-CZ-NH2	-11.73	108.64	119.20
1	C	13	ARG	NE-CZ-NH1	11.22	132.72	121.50
1	F	70	ARG	NE-CZ-NH1	10.94	132.44	121.50
1	D	74	ARG	NE-CZ-NH1	10.53	132.03	121.50
1	F	201	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	D	84	ARG	NE-CZ-NH2	-9.53	110.63	119.20
1	C	84	ARG	NE-CZ-NH2	-9.49	110.66	119.20
1	F	70	ARG	CD-NE-CZ	8.41	136.17	124.40
1	C	13	ARG	CD-NE-CZ	8.23	135.93	124.40
1	C	84	ARG	NE-CZ-NH1	8.18	129.68	121.50
1	D	84	ARG	NE-CZ-NH1	8.14	129.65	121.50
1	D	74	ARG	CD-NE-CZ	7.72	135.21	124.40
1	F	18	ARG	NE-CZ-NH2	-7.07	112.83	119.20
1	C	18	ARG	NE-CZ-NH2	-7.02	112.88	119.20
1	B	166	ALA	CA-C-N	6.96	128.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ALA	C-N-CA	6.96	128.54	119.84
1	E	166	ALA	CA-C-N	6.96	128.53	119.84
1	E	166	ALA	C-N-CA	6.96	128.53	119.84
1	D	18	ARG	NE-CZ-NH2	-6.92	112.98	119.20
1	F	166	ALA	CA-C-N	6.89	128.45	119.84
1	F	166	ALA	C-N-CA	6.89	128.45	119.84
1	E	173	PHE	CA-C-N	6.88	126.13	118.97
1	E	173	PHE	C-N-CA	6.88	126.13	118.97
1	C	166	ALA	CA-C-N	6.83	128.37	119.84
1	C	166	ALA	C-N-CA	6.83	128.37	119.84
1	D	166	ALA	CA-C-N	6.77	128.30	119.84
1	D	166	ALA	C-N-CA	6.77	128.30	119.84
1	A	166	ALA	CA-C-N	6.74	128.27	119.84
1	A	166	ALA	C-N-CA	6.74	128.27	119.84
1	F	201	ARG	CD-NE-CZ	6.72	133.81	124.40
1	C	173	PHE	CA-C-N	6.70	126.21	119.24
1	C	173	PHE	C-N-CA	6.70	126.21	119.24
1	D	84	ARG	CD-NE-CZ	6.61	133.66	124.40
1	D	173	PHE	CA-C-N	6.59	126.09	119.24
1	D	173	PHE	C-N-CA	6.59	126.09	119.24
1	C	84	ARG	CD-NE-CZ	6.55	133.57	124.40
1	F	173	PHE	CA-C-N	6.54	126.05	119.24
1	F	173	PHE	C-N-CA	6.54	126.05	119.24
1	B	18	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	A	18	ARG	NE-CZ-NH2	-6.44	113.41	119.20
1	C	18	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	B	173	PHE	CA-C-N	6.37	125.86	119.24
1	B	173	PHE	C-N-CA	6.37	125.86	119.24
1	F	18	ARG	NE-CZ-NH1	6.32	127.82	121.50
1	A	173	PHE	CA-C-N	6.32	125.81	119.24
1	A	173	PHE	C-N-CA	6.32	125.81	119.24
1	E	18	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	D	18	ARG	NE-CZ-NH1	6.26	127.76	121.50
1	A	18	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	E	112	GLU	N-CA-C	5.48	116.93	111.07
1	B	112	GLU	N-CA-C	5.46	116.92	110.97
1	E	18	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	D	112	GLU	N-CA-C	5.38	116.84	110.97
1	B	18	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	F	112	GLU	N-CA-C	5.36	116.80	111.07
1	A	112	GLU	N-CA-C	5.34	116.79	111.07
1	A	32	VAL	N-CA-C	5.31	116.44	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	GLU	N-CA-C	5.30	116.74	111.07
1	B	32	VAL	N-CA-C	5.24	116.33	109.21
1	E	32	VAL	N-CA-C	5.21	116.30	109.21
1	F	32	VAL	N-CA-C	5.16	116.22	109.21
1	C	32	VAL	N-CA-C	5.13	116.19	109.21
1	D	32	VAL	N-CA-C	5.07	116.10	109.21
1	D	18	ARG	CD-NE-CZ	5.04	131.46	124.40

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	1658	0	1658	16	0
1	B	1658	0	1659	15	0
1	C	1658	0	1659	16	0
1	D	1658	0	1659	20	0
1	E	1658	0	1658	16	0
1	F	1658	0	1659	18	0
2	A	30	0	20	2	0
2	B	30	0	20	3	0
2	C	30	0	20	1	0
2	D	30	0	20	1	0
2	E	30	0	20	2	0
2	F	30	0	20	1	0
All	All	10128	0	10072	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (101) 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:113:ASN:HB2	1:F:137:GLN:NE2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:GLN:HE22	1:F:75:SER:HA	1.58	0.68
1:D:96:VAL:HG13	1:D:158:LEU:HD22	1.77	0.66
1:A:96:VAL:HG13	1:A:158:LEU:HD22	1.78	0.66
1:B:96:VAL:HG13	1:B:158:LEU:HD22	1.79	0.64
1:E:96:VAL:HG13	1:E:158:LEU:HD22	1.79	0.64
1:C:96:VAL:HG13	1:C:158:LEU:HD22	1.79	0.64
1:F:96:VAL:HG13	1:F:158:LEU:HD22	1.79	0.64
1:D:52:LEU:HB3	1:D:53:PRO:HA	1.81	0.63
1:E:75:SER:HA	1:F:83:GLN:HE22	1.64	0.63
1:A:52:LEU:HB3	1:A:53:PRO:HA	1.81	0.62
1:B:52:LEU:HB3	1:B:53:PRO:HA	1.82	0.62
1:C:52:LEU:HB3	1:C:53:PRO:HA	1.82	0.62
1:F:52:LEU:HB3	1:F:53:PRO:HA	1.81	0.61
1:E:52:LEU:HB3	1:E:53:PRO:HA	1.81	0.61
1:B:10:VAL:HG21	2:B:210:GTB:H5'	1.83	0.60
1:C:99:LEU:HD23	1:C:158:LEU:HD21	1.85	0.59
1:B:99:LEU:HD23	1:B:158:LEU:HD21	1.86	0.57
1:E:99:LEU:HD23	1:E:158:LEU:HD21	1.87	0.57
1:D:99:LEU:HD23	1:D:158:LEU:HD21	1.87	0.55
1:F:99:LEU:HD23	1:F:158:LEU:HD21	1.87	0.55
1:C:38:TRP:HH2	1:C:47:CCS:SG	2.30	0.54
1:A:99:LEU:HD23	1:A:158:LEU:HD21	1.88	0.54
1:E:10:VAL:HG21	2:E:210:GTB:H5'	1.92	0.49
1:C:14:CYS:SG	1:C:53:PRO:HB3	2.52	0.49
1:B:55:PHE:HB2	1:B:68:ILE:HD13	1.95	0.49
1:D:14:CYS:SG	1:D:53:PRO:HB3	2.52	0.49
1:C:55:PHE:HB2	1:C:68:ILE:HD13	1.95	0.48
1:E:14:CYS:SG	1:E:53:PRO:HB3	2.53	0.48
1:A:14:CYS:SG	1:A:53:PRO:HB3	2.53	0.48
1:A:55:PHE:HB2	1:A:68:ILE:HD13	1.95	0.48
1:B:47:CCS:OZ2	1:B:52:LEU:HD21	2.14	0.48
1:F:14:CYS:SG	1:F:53:PRO:HB3	2.54	0.48
1:E:55:PHE:HB2	1:E:68:ILE:HD13	1.96	0.48
1:B:125:HIS:O	1:B:128:PRO:HD2	2.14	0.47
1:F:55:PHE:HB2	1:F:68:ILE:HD13	1.95	0.47
2:C:210:GTB:HB21	2:C:210:GTB:C2'	2.44	0.47
1:B:14:CYS:SG	1:B:53:PRO:HB3	2.54	0.47
1:C:125:HIS:O	1:C:128:PRO:HD2	2.14	0.47
1:D:55:PHE:HB2	1:D:68:ILE:HD13	1.96	0.47
1:E:125:HIS:O	1:E:128:PRO:HD2	2.15	0.47
1:D:125:HIS:O	1:D:128:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:N	1:A:123:PRO:HD2	2.30	0.46
1:A:125:HIS:O	1:A:128:PRO:HD2	2.16	0.46
1:D:122:LEU:N	1:D:123:PRO:HD2	2.30	0.46
1:A:159:LEU:O	1:A:163:GLN:HG3	2.16	0.46
2:B:210:GTB:HB21	2:B:210:GTB:C2'	2.44	0.46
2:E:210:GTB:C2'	2:E:210:GTB:HB21	2.45	0.46
1:D:14:CYS:O	1:D:18:ARG:HG3	2.16	0.46
1:C:159:LEU:O	1:C:163:GLN:HG3	2.15	0.46
1:E:122:LEU:N	1:E:123:PRO:HD2	2.30	0.46
2:F:210:GTB:HB21	2:F:210:GTB:C2'	2.45	0.46
1:D:113:ASN:HB2	1:F:137:GLN:CD	2.42	0.45
1:F:122:LEU:N	1:F:123:PRO:HD2	2.31	0.45
1:F:125:HIS:O	1:F:128:PRO:HD2	2.16	0.45
1:B:122:LEU:N	1:B:123:PRO:HD2	2.30	0.45
2:A:210:GTB:C2'	2:A:210:GTB:HB21	2.46	0.45
1:F:14:CYS:O	1:F:18:ARG:HG3	2.16	0.45
1:A:122:LEU:HD11	1:A:162:HIS:HD2	1.81	0.45
1:D:122:LEU:HD11	1:D:162:HIS:HD2	1.82	0.45
1:B:10:VAL:HG21	2:B:210:GTB:C5'	2.47	0.45
1:D:159:LEU:O	1:D:163:GLN:HG3	2.17	0.45
1:C:122:LEU:HD11	1:C:162:HIS:HD2	1.81	0.45
1:C:122:LEU:N	1:C:123:PRO:HD2	2.31	0.44
2:D:210:GTB:HB21	2:D:210:GTB:C2'	2.46	0.44
1:C:84:ARG:HG3	1:D:60:LEU:HD13	2.00	0.44
1:F:159:LEU:O	1:F:163:GLN:HG3	2.17	0.44
1:B:176:LEU:O	1:B:180:VAL:HG23	2.16	0.44
1:C:14:CYS:O	1:C:18:ARG:HG3	2.17	0.44
1:B:122:LEU:HD11	1:B:162:HIS:HD2	1.82	0.44
1:A:10:VAL:HG21	2:A:210:GTB:H5'	1.98	0.44
1:C:63:TYR:O	1:C:64:GLN:HB2	2.19	0.43
1:F:176:LEU:O	1:F:180:VAL:HG23	2.17	0.43
1:E:63:TYR:O	1:E:64:GLN:HB2	2.18	0.43
1:E:122:LEU:HD11	1:E:162:HIS:HD2	1.82	0.43
1:E:176:LEU:O	1:E:180:VAL:HG23	2.18	0.43
1:F:100:ARG:O	1:F:104:VAL:HG23	2.19	0.43
1:F:122:LEU:HD11	1:F:162:HIS:HD2	1.82	0.43
1:D:176:LEU:O	1:D:180:VAL:HG23	2.18	0.43
1:A:176:LEU:O	1:A:180:VAL:HG23	2.18	0.42
1:B:63:TYR:O	1:B:64:GLN:HB2	2.20	0.42
1:D:92:VAL:HG11	1:D:143:ILE:HG12	2.02	0.42
1:E:47:CCS:HD2	1:E:47:CCS:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:GLN:O	1:E:92:VAL:HG23	2.19	0.42
1:A:63:TYR:O	1:A:64:GLN:HB2	2.19	0.42
1:B:88:GLN:O	1:B:92:VAL:HG23	2.19	0.42
1:C:176:LEU:O	1:C:180:VAL:HG23	2.18	0.42
1:D:88:GLN:O	1:D:92:VAL:HG23	2.20	0.42
1:F:92:VAL:HG11	1:F:143:ILE:HG12	2.02	0.42
1:D:63:TYR:O	1:D:64:GLN:HB2	2.19	0.42
1:E:100:ARG:O	1:E:104:VAL:HG23	2.20	0.41
1:A:186:ARG:HA	1:A:187:PRO:HD2	1.87	0.41
1:F:63:TYR:O	1:F:64:GLN:HB2	2.19	0.41
1:D:186:ARG:HA	1:D:187:PRO:HD2	1.87	0.41
1:A:92:VAL:HG11	1:A:143:ILE:HG12	2.03	0.41
1:C:13:ARG:HH22	1:C:97:GLU:CD	2.29	0.41
1:C:83:GLN:HE22	1:D:75:SER:HA	1.86	0.41
1:A:100:ARG:O	1:A:104:VAL:HG23	2.21	0.40
1:D:100:ARG:O	1:D:104:VAL:HG23	2.21	0.40
1:A:88:GLN:O	1:A:92:VAL:HG23	2.21	0.40
1:B:92:VAL:HG11	1:B:143:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	60
1	B	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	12	45
1	C	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	12	45
1	D	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	12	45
1	E	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12	45
1	F	206/209 (99%)	192 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1236/1254 (99%)	1149 (93%)	78 (6%)	9 (1%)	18	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	LYS
1	A	44	LYS
1	B	38	TRP
1	B	39	MET
1	C	45	PRO
1	C	46	THR
1	E	44	LYS
1	E	41	GLY
1	D	64	GLN

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	177/177 (100%)	175 (99%)	2 (1%)	65	83
1	B	177/177 (100%)	175 (99%)	2 (1%)	65	83
1	C	177/177 (100%)	174 (98%)	3 (2%)	53	78
1	D	177/177 (100%)	175 (99%)	2 (1%)	65	83
1	E	177/177 (100%)	175 (99%)	2 (1%)	65	83
1	F	177/177 (100%)	175 (99%)	2 (1%)	65	83
All	All	1062/1062 (100%)	1049 (99%)	13 (1%)	63	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	167	PRO
1	B	59	ASP

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Mol	Chain	Res	Type
1	B	167	PRO
1	C	44	LYS
1	C	59	ASP
1	C	167	PRO
1	D	59	ASP
1	D	167	PRO
1	E	59	ASP
1	E	167	PRO
1	F	59	ASP
1	F	167	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	204	ASN
1	B	83	GLN
1	B	154	ASN
1	B	204	ASN
1	C	83	GLN
1	C	154	ASN
1	D	83	GLN
1	D	154	ASN
1	D	204	ASN
1	E	83	GLN
1	E	154	ASN
1	E	204	ASN
1	F	83	GLN
1	F	137	GLN
1	F	154	ASN
1	F	204	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CCS	B	47	1	8,9,10	0.83	0	7,10,12	1.01	0
1	CCS	F	47	1	8,9,10	0.87	0	7,10,12	0.88	0
1	CCS	C	47	1	8,9,10	0.83	0	7,10,12	0.88	0
1	CCS	D	47	1	8,9,10	0.80	0	7,10,12	0.89	0
1	CCS	A	47	1	8,9,10	0.79	0	7,10,12	0.92	0
1	CCS	E	47	1	8,9,10	0.84	0	7,10,12	0.90	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
1	CCS	B	47	1	-	2/6/8/10	-
1	CCS	F	47	1	-	3/6/8/10	-
1	CCS	C	47	1	-	3/6/8/10	-
1	CCS	D	47	1	-	4/6/8/10	-
1	CCS	A	47	1	-	2/6/8/10	-
1	CCS	E	47	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	47	CCS	N-CA-CB-SG
1	A	47	CCS	C-CA-CB-SG
1	B	47	CCS	C-CA-CB-SG
1	D	47	CCS	N-CA-CB-SG
1	D	47	CCS	C-CA-CB-SG
1	F	47	CCS	N-CA-CB-SG
1	F	47	CCS	C-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	C	47	CCS	CE-CD-SG-CB
1	F	47	CCS	CE-CD-SG-CB
1	B	47	CCS	N-CA-CB-SG
1	D	47	CCS	SG-CD-CE-OZ2
1	E	47	CCS	N-CA-CB-SG
1	C	47	CCS	SG-CD-CE-OZ1
1	D	47	CCS	SG-CD-CE-OZ1
1	C	47	CCS	SG-CD-CE-OZ2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	47	CCS	1	0
1	C	47	CCS	1	0
1	E	47	CCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GTB	B	210	-	29,30,30	0.87	1 (3%)	34,39,39	0.62	0
2	GTB	D	210	-	29,30,30	0.92	2 (6%)	34,39,39	0.62	0
2	GTB	E	210	-	29,30,30	0.89	2 (6%)	34,39,39	0.66	0
2	GTB	C	210	-	29,30,30	0.89	2 (6%)	34,39,39	0.59	0
2	GTB	F	210	-	29,30,30	0.88	2 (6%)	34,39,39	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTB	A	210	-	29,30,30	0.90	2 (6%)	34,39,39	0.60	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	GTB	B	210	-	-	0/30/32/32	0/1/1/1
2	GTB	D	210	-	-	0/30/32/32	0/1/1/1
2	GTB	E	210	-	-	0/30/32/32	0/1/1/1
2	GTB	C	210	-	-	0/30/32/32	0/1/1/1
2	GTB	F	210	-	-	0/30/32/32	0/1/1/1
2	GTB	A	210	-	-	0/30/32/32	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	210	GTB	C4'-N41	2.47	1.51	1.45
2	D	210	GTB	C4'-N41	2.44	1.51	1.45
2	F	210	GTB	C4'-N41	2.16	1.50	1.45
2	B	210	GTB	O41-N41	-2.15	1.20	1.35
2	E	210	GTB	O41-N41	-2.12	1.21	1.35
2	E	210	GTB	C4'-N41	2.09	1.50	1.45
2	F	210	GTB	O41-N41	-2.08	1.21	1.35
2	D	210	GTB	O41-N41	-2.06	1.21	1.35
2	C	210	GTB	O41-N41	-2.05	1.21	1.35
2	C	210	GTB	C4'-N41	2.05	1.50	1.45
2	A	210	GTB	O41-N41	-2.02	1.21	1.35

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

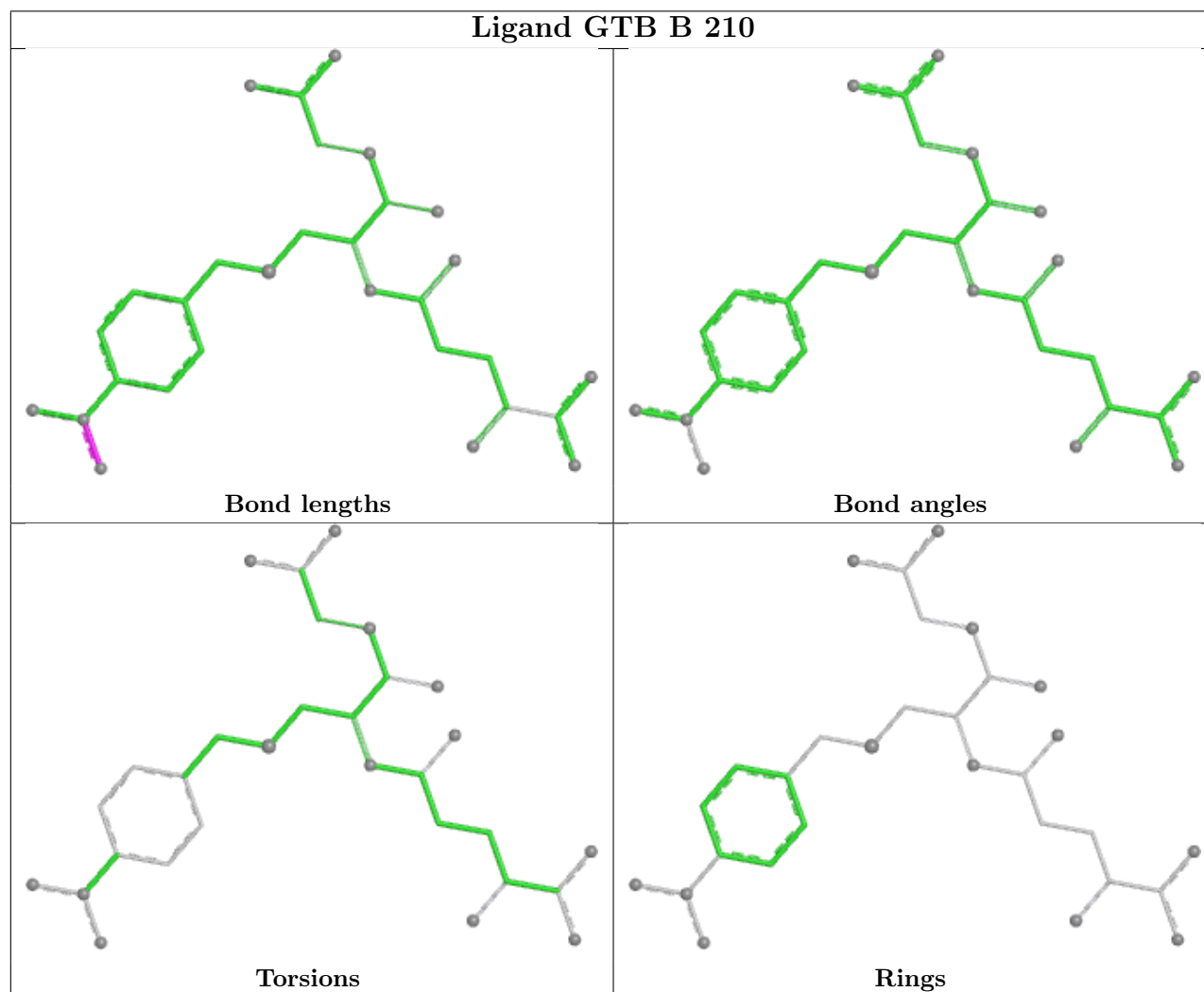
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	210	GTB	3	0
2	D	210	GTB	1	0
2	E	210	GTB	2	0

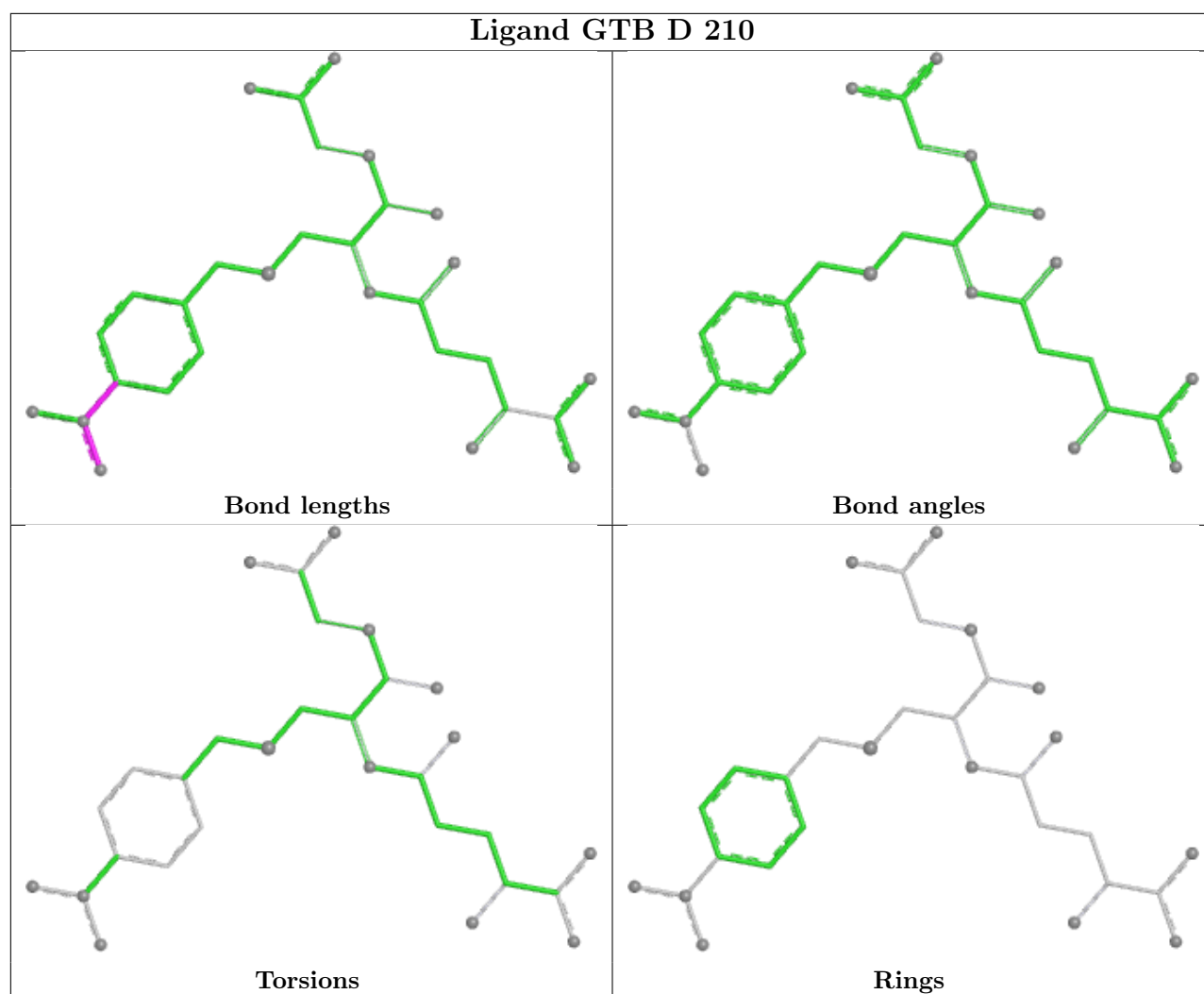
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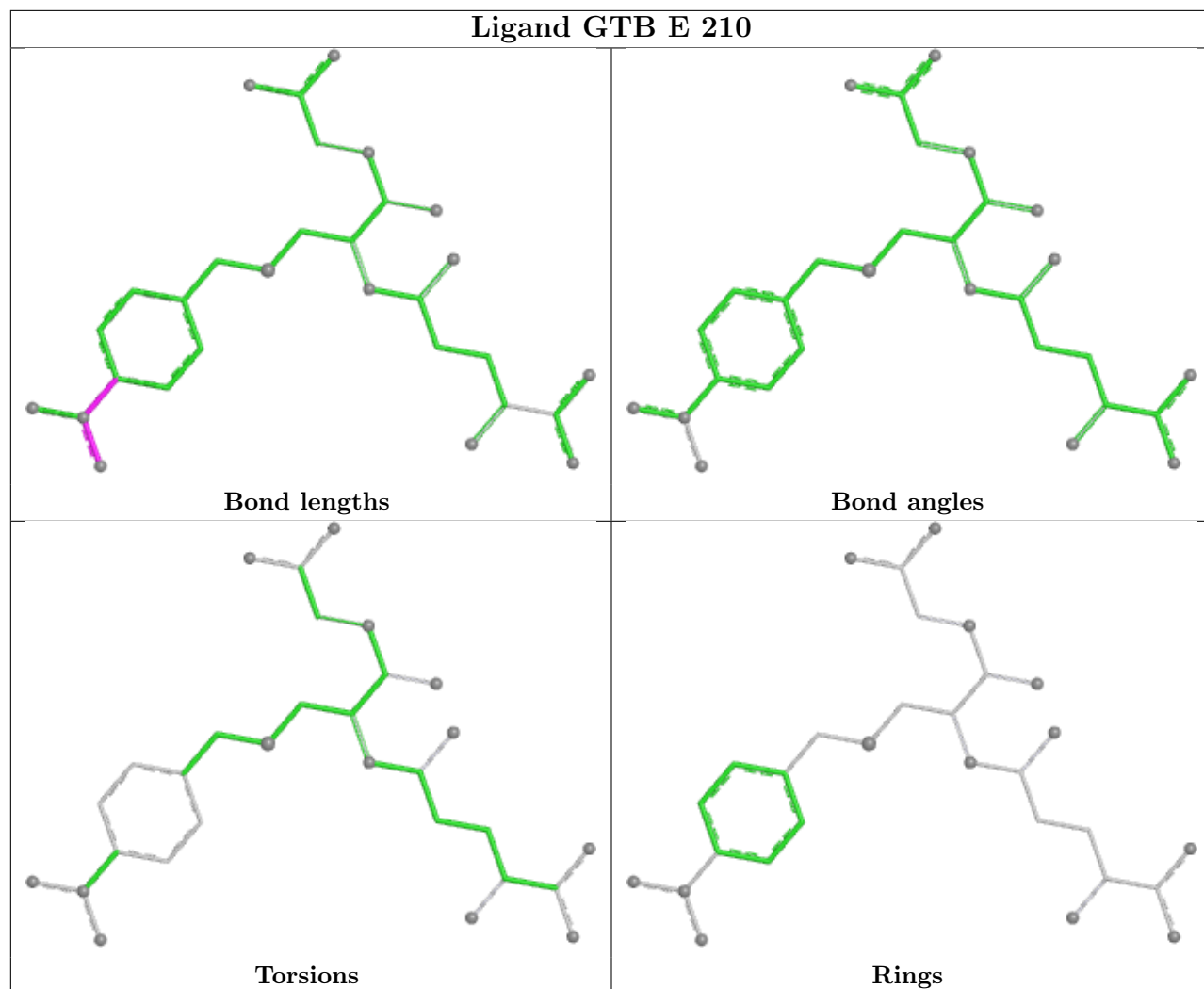
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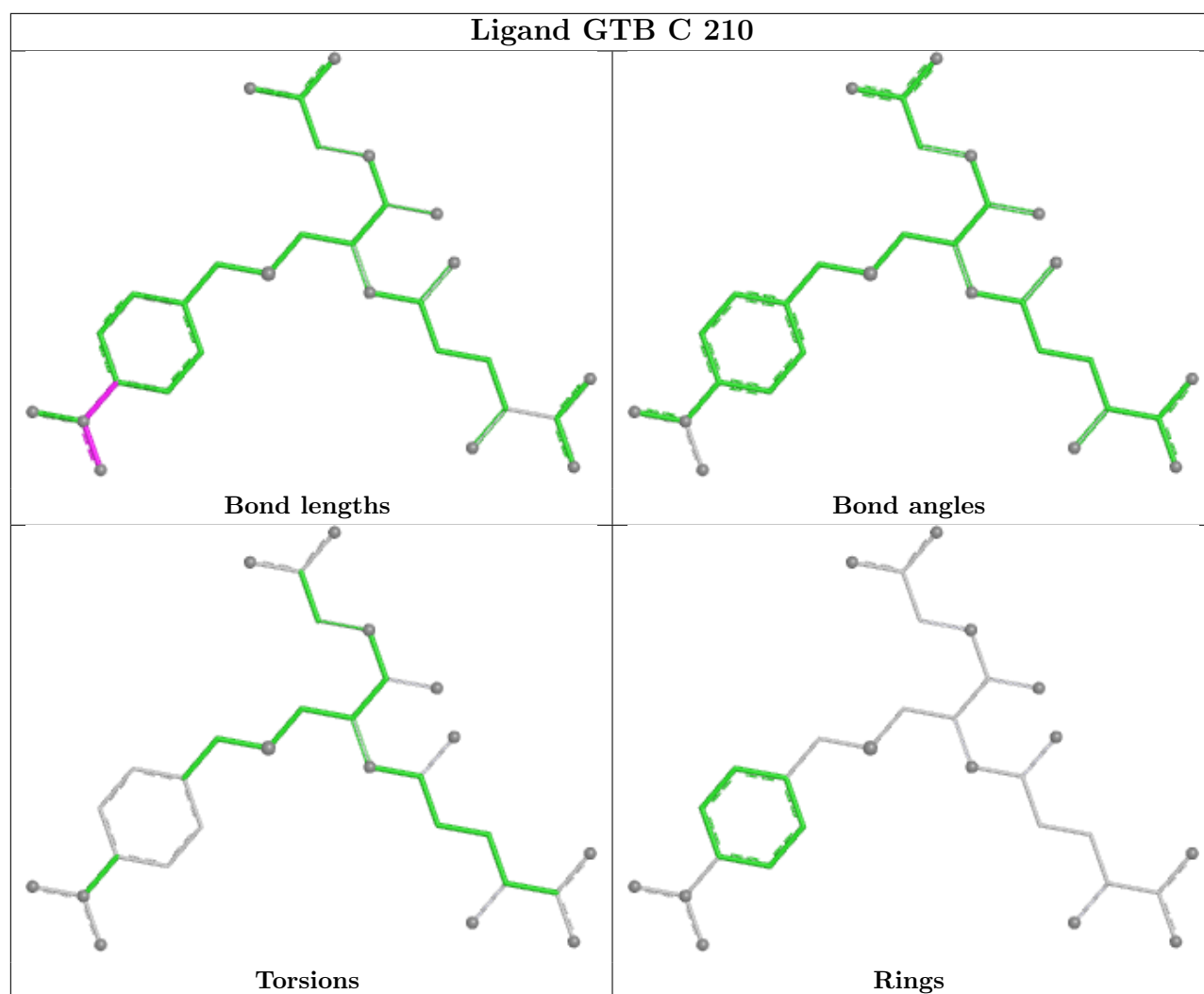
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	210	GTB	1	0
2	F	210	GTB	1	0
2	A	210	GTB	2	0

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.

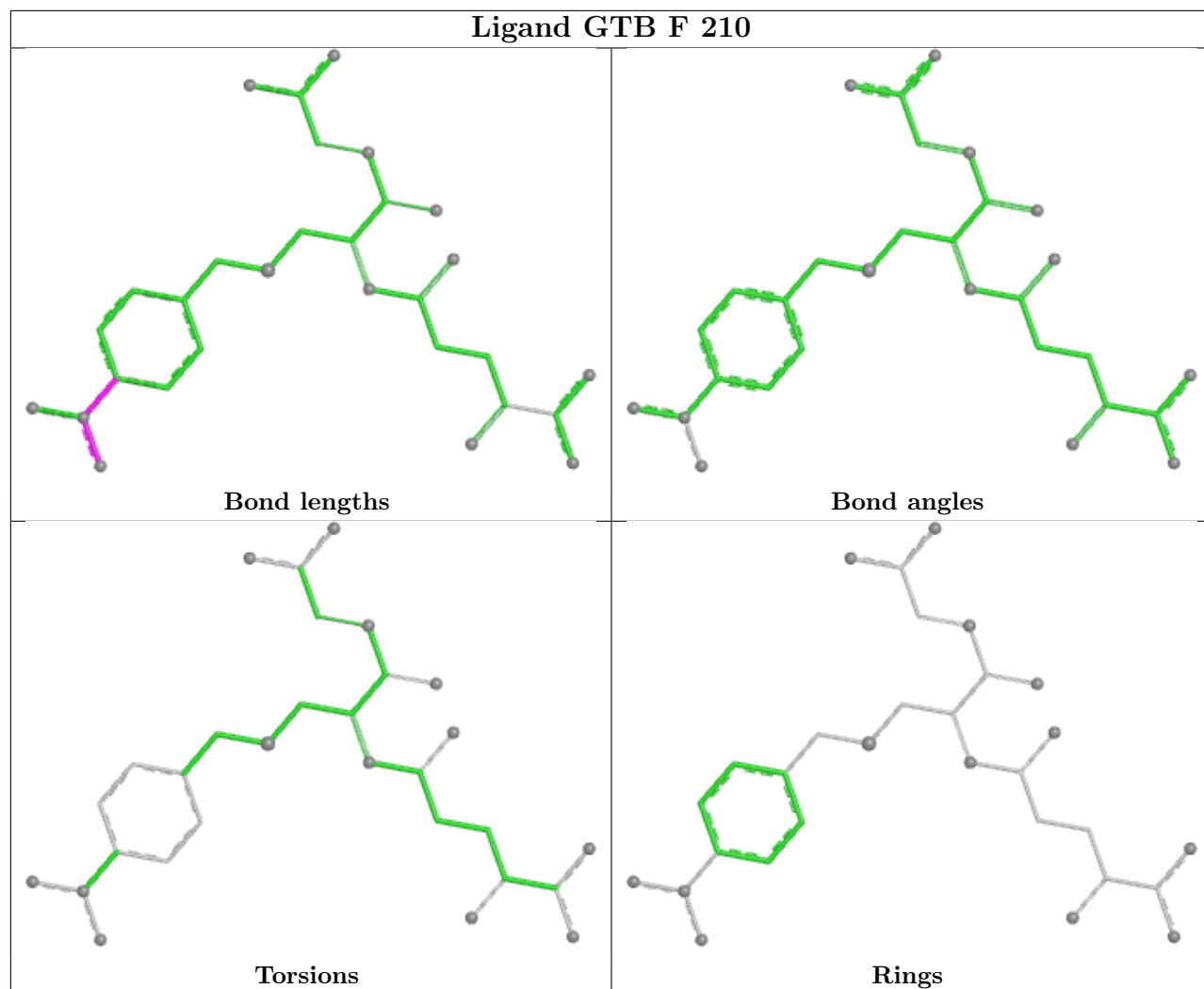


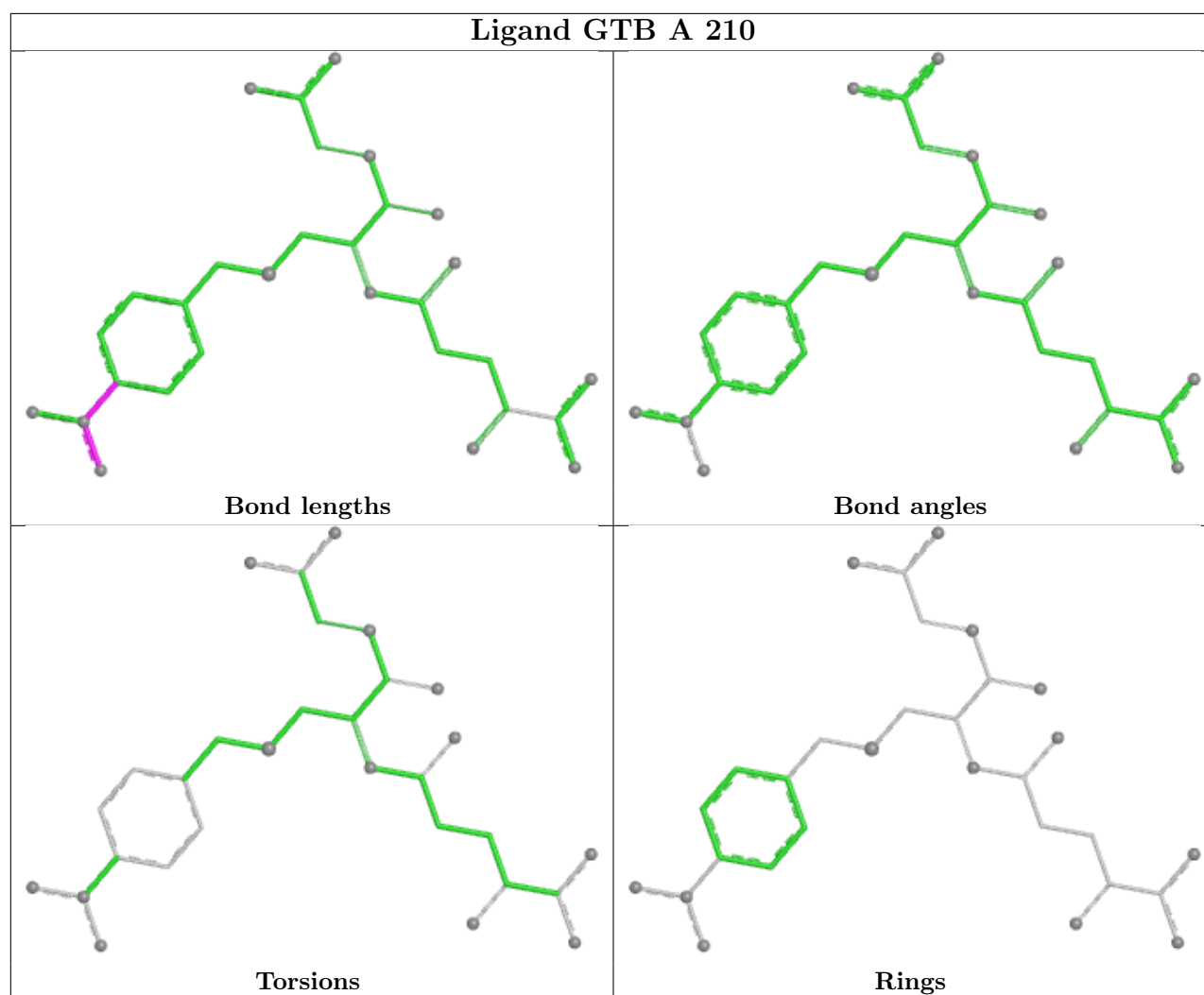






Ligand GTB F 210





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.