



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:16 AM UTC

PDB ID : 1GWC / pdb_00001gwc
Title : The structure of a tau class glutathione S-transferase from wheat, active in herbicide detoxification
Authors : Thom, R.; Cummins, I.; Dixon, D.P.; Edwards, R.; Cole, D.J.; Laphorn, A.J.
Deposited on : 2002-03-14
Resolution : 2.25 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) : **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

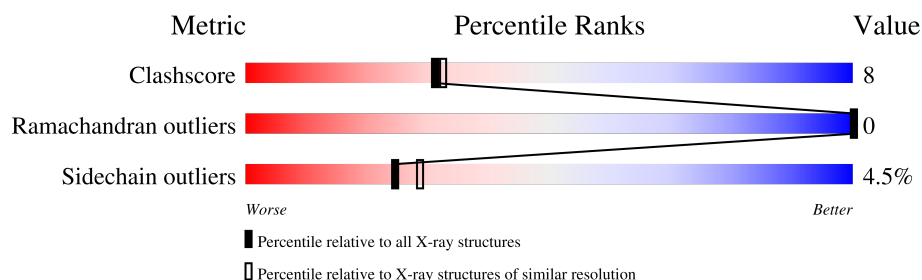
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	230	
1	B	230	
1	C	230	

2 Entry composition [i](#)

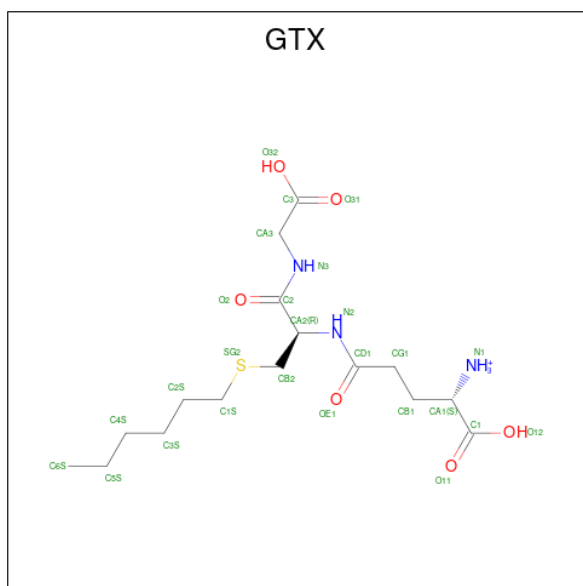
There are 4 unique types of molecules in this entry. The entry contains 5913 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TSI-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	3	0
			1705	1105	284	311	5			
1	B	221	Total	C	N	O	S	0	2	0
			1694	1098	281	311	4			
1	C	222	Total	C	N	O	S	0	4	0
			1710	1108	285	312	5			

- Molecule 2 is S-HEXYLGLUTATHIONE (CCD ID: GTX) (formula: $C_{16}H_{30}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	16	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			26	16	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			26	16	3	6	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

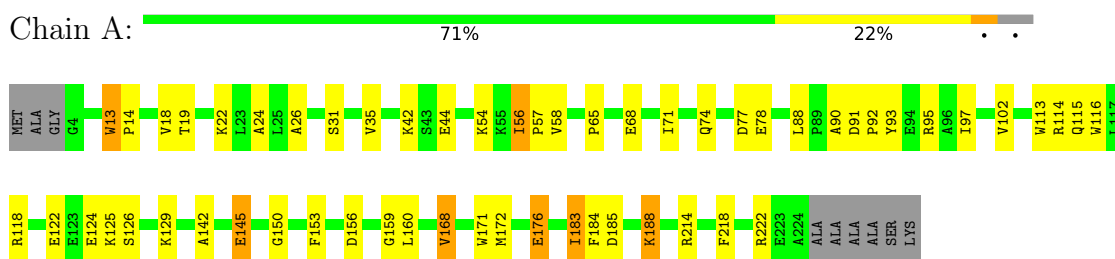
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	1
			222	222		
4	B	251	Total	O	0	3
			251	251		
4	C	238	Total	O	0	1
			238	238		

3 Residue-property plots

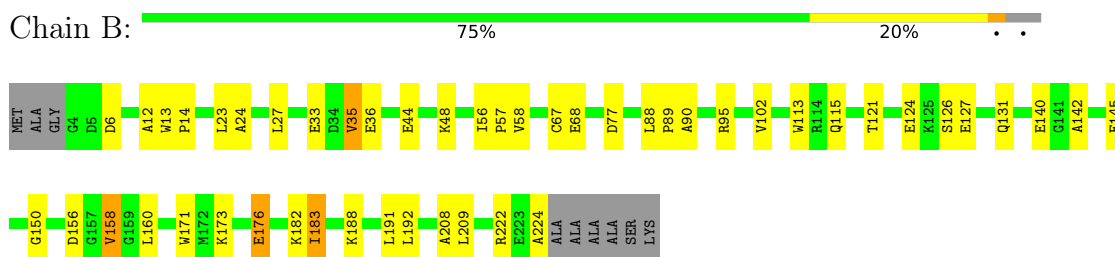
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

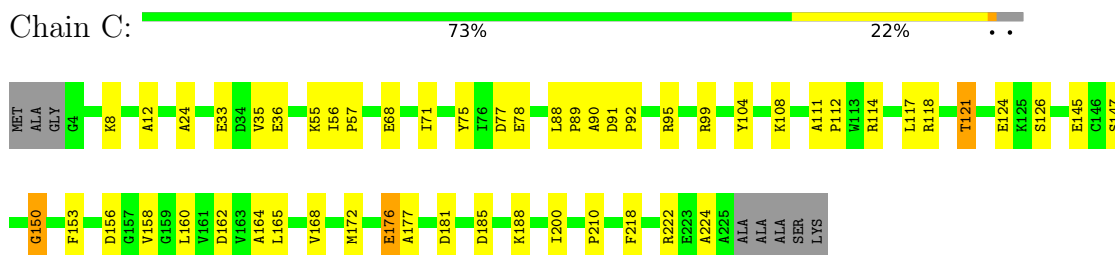
• Molecule 1: GLUTATHIONE S-TRANSFERASE TSI-1



• Molecule 1: GLUTATHIONE S-TRANSFERASE TSI-1



• Molecule 1: GLUTATHIONE S-TRANSFERASE TSI-1



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.98Å 152.39Å 146.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25	Depositor
% Data completeness (in resolution range)	90.0 (30.00-2.25)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.157 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5913	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: GTX, SO4

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	1.53	9/1758 (0.5%)	1.37	7/2381 (0.3%)
1	B	1.55	7/1744 (0.4%)	1.43	3/2364 (0.1%)
1	C	1.52	8/1768 (0.5%)	1.41	10/2395 (0.4%)
All	All	1.53	24/5270 (0.5%)	1.40	20/7140 (0.3%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	TRP	C-O	-9.22	1.16	1.24
1	A	54	LYS	CA-C	-7.80	1.43	1.53
1	B	24	ALA	CA-CB	-7.16	1.42	1.53
1	C	35	VAL	CA-CB	-6.79	1.46	1.54
1	B	158	VAL	C-O	-6.55	1.17	1.24
1	A	65	PRO	C-O	-6.54	1.16	1.23
1	B	58	VAL	CA-CB	-6.48	1.46	1.54
1	C	24	ALA	CA-CB	-6.25	1.43	1.53
1	B	209	LEU	C-O	-6.23	1.15	1.24
1	B	208	ALA	CA-CB	-6.14	1.45	1.53
1	C	162	ASP	C-O	-6.06	1.17	1.24
1	A	42	LYS	C-O	-6.04	1.16	1.23
1	B	35	VAL	CA-CB	-5.91	1.47	1.54
1	C	158	VAL	N-CA	-5.81	1.39	1.46
1	C	177	ALA	CA-CB	-5.75	1.43	1.53
1	A	24	ALA	CA-CB	-5.72	1.44	1.53
1	B	142	ALA	CA-CB	-5.66	1.44	1.53
1	A	142	ALA	CA-CB	-5.63	1.44	1.53
1	A	58	VAL	C-O	-5.63	1.18	1.24
1	A	26	ALA	CA-CB	-5.53	1.44	1.53
1	A	35	VAL	CA-CB	-5.44	1.48	1.54
1	C	150	GLY	C-O	-5.40	1.16	1.23
1	C	164	ALA	CA-CB	-5.32	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	TYR	C-O	-5.15	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	LEU	N-CA-C	6.75	119.64	111.82
1	C	145	GLU	CA-CB-CG	6.49	127.08	114.10
1	C	145	GLU	N-CA-CB	-6.49	100.32	110.44
1	B	23	LEU	CA-C-O	5.61	126.50	120.55
1	A	153	PHE	N-CA-C	-5.59	105.72	112.54
1	B	89	PRO	CB-CA-C	-5.56	103.94	111.12
1	A	176[A]	GLU	N-CA-C	-5.52	105.16	111.07
1	A	176[B]	GLU	N-CA-C	-5.52	105.16	111.07
1	C	118	ARG	N-CA-C	-5.50	104.82	112.30
1	C	224	ALA	N-CA-C	-5.45	104.37	111.02
1	C	99	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	C	153	PHE	N-CA-C	-5.41	105.49	111.71
1	A	102	VAL	N-CA-C	-5.35	105.28	110.42
1	B	102	VAL	N-CA-C	-5.35	105.32	110.72
1	C	210	PRO	CA-C-O	5.32	128.16	121.67
1	A	159	GLY	CA-C-O	5.28	127.90	121.88
1	A	145	GLU	N-CA-CB	-5.27	101.81	110.40
1	C	89	PRO	CA-C-O	5.20	128.74	122.08
1	C	147	SER	N-CA-C	5.19	116.62	111.07
1	A	19	THR	N-CA-C	-5.08	105.74	111.28

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	1705	0	1732	34	0
1	B	1694	0	1708	28	0
1	C	1710	0	1735	22	0
2	A	26	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	28	0	0
2	C	26	0	28	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
4	A	222	0	0	5	1
4	B	251	0	0	6	1
4	C	238	0	0	5	1
All	All	5913	0	5259	86	2

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 8.

All (86) 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:224:ALA:HB2	4:B:2238:HOH:O	1.33	1.24
1:A:183:ILE:HD13	1:A:183:ILE:N	1.90	0.86
1:B:88:LEU:HD21	1:B:160:LEU:HD22	1.56	0.86
1:A:90:ALA:O	1:A:95[B]:ARG:NH2	2.11	0.83
1:A:172[B]:MET:HE3	1:A:184:PHE:HD1	1.44	0.83
1:B:183:ILE:HD13	1:B:183:ILE:N	1.95	0.80
1:C:68:GLU:OE2	4:C:2109:HOH:O	2.01	0.78
1:A:88:LEU:HD21	1:A:160:LEU:HD22	1.65	0.77
1:B:90:ALA:O	1:B:95[B]:ARG:NH1	2.17	0.77
1:C:8:LYS:NZ	4:C:2008:HOH:O	2.08	0.74
1:C:88:LEU:HD21	1:C:160:LEU:HD22	1.68	0.74
3:C:1227:SO4:O3	4:C:2238:HOH:O	2.06	0.73
1:A:222:ARG:NE	4:A:2211:HOH:O	2.23	0.71
1:A:172[B]:MET:HE3	1:A:184:PHE:CD1	2.27	0.68
1:B:176[A]:GLU:OE2	1:B:182:LYS:HG2	1.96	0.66
1:A:114:ARG:HE	1:A:118:ARG:HH12	1.43	0.65
1:C:55:LYS:HE2	4:C:2237:HOH:O	1.97	0.64
1:B:115:GLN:NE2	1:B:124:GLU:O	2.31	0.61
1:B:95[B]:ARG:HH21	1:C:78:GLU:CD	2.07	0.61
1:C:90:ALA:O	1:C:95[B]:ARG:NH1	2.37	0.58
1:A:222:ARG:HG2	4:A:2213:HOH:O	2.05	0.56
1:A:145:GLU:HB2	4:A:2168:HOH:O	2.04	0.56
1:A:214:ARG:NH2	4:A:2207:HOH:O	2.38	0.55
1:A:68:GLU:OE2	4:A:2099:HOH:O	2.18	0.55
1:A:168:VAL:O	1:A:172[A]:MET:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:OD2	1:A:188:LYS:HD2	2.08	0.54
1:B:176[A]:GLU:OE2	1:B:182:LYS:CG	2.57	0.53
1:B:224:ALA:CB	4:B:2238:HOH:O	2.15	0.53
1:B:13:TRP:CG	1:B:14:PRO:HD3	2.43	0.53
1:B:140:GLU:CD	1:B:191:LEU:HB2	2.33	0.53
1:B:95[A]:ARG:NH2	4:B:2151:HOH:O	2.41	0.53
1:B:88:LEU:HD12	4:B:2151:HOH:O	2.09	0.52
1:C:121:THR:HG23	1:C:124:GLU:CD	2.35	0.51
1:C:104:TYR:CE1	1:C:108:LYS:HG3	2.45	0.51
1:A:88:LEU:HD13	1:A:95[A]:ARG:HH11	1.76	0.51
1:C:56:ILE:HB	1:C:57:PRO:HA	1.93	0.51
1:A:88:LEU:HD13	1:A:95[A]:ARG:NH1	2.27	0.50
1:A:115:GLN:NE2	1:A:124:GLU:O	2.45	0.49
1:A:218:PHE:CZ	1:A:222:ARG:HD2	2.46	0.49
1:C:218:PHE:CZ	1:C:222:ARG:HD2	2.46	0.49
1:B:33:GLU:HG2	1:B:35:VAL:HG23	1.94	0.49
3:B:1226:SO4:O3	4:B:2251:HOH:O	2.18	0.49
1:A:116:TRP:CZ2	1:A:129:LYS:HG3	2.47	0.49
1:B:127:GLU:HG3	1:B:131:GLN:OE1	2.12	0.49
1:A:74:GLN:O	1:A:78:GLU:HG3	2.13	0.48
1:A:88:LEU:CD1	1:A:95[A]:ARG:NH1	2.76	0.48
1:C:12:ALA:HA	1:C:36:GLU:OE2	2.13	0.48
1:A:13:TRP:N	1:A:14:PRO:CD	2.78	0.47
1:C:68:GLU:HB2	1:C:71:ILE:HD12	1.96	0.47
1:B:88:LEU:CD2	1:B:160:LEU:HD22	2.38	0.47
1:B:150:GLY:HA3	1:B:156:ASP:HA	1.96	0.47
1:C:168:VAL:O	1:C:172[A]:MET:HG2	2.14	0.47
1:C:111:ALA:HB3	1:C:112:PRO:HD3	1.96	0.47
1:A:18:VAL:HG12	1:A:22:LYS:HE3	1.96	0.46
2:A:1225:GTX:N3	3:A:1226:SO4:O1	2.43	0.46
1:C:165:LEU:O	1:C:168:VAL:HG22	2.16	0.46
1:A:183:ILE:HD13	1:A:183:ILE:H	1.77	0.46
1:C:33:GLU:OE2	4:C:2044:HOH:O	2.20	0.46
1:B:44:GLU:CG	1:B:48:LYS:HZ1	2.28	0.46
1:B:44:GLU:HG3	1:B:48:LYS:NZ	2.32	0.45
1:A:116:TRP:CE2	1:A:129:LYS:HG3	2.51	0.44
1:A:91:ASP:HA	1:A:92:PRO:HD3	1.86	0.44
1:C:176[A]:GLU:HG3	1:C:181:ASP:O	2.18	0.44
1:A:56:ILE:HB	1:A:57:PRO:HA	1.99	0.44
1:A:185:ASP:HB3	1:A:188:LYS:HD3	2.00	0.43
1:C:200:ILE:HG21	1:C:200:ILE:HD13	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TRP:CZ2	1:B:171:TRP:HB3	2.53	0.43
1:A:13:TRP:CG	1:A:14:PRO:HD3	2.54	0.42
1:B:56:ILE:HB	1:B:57:PRO:HA	2.02	0.42
1:B:13:TRP:N	1:B:14:PRO:CD	2.83	0.42
1:B:173:LYS:O	1:B:176[B]:GLU:HB2	2.19	0.42
1:B:6:ASP:HB2	4:B:2008:HOH:O	2.18	0.42
1:A:124:GLU:O	1:A:125:LYS:C	2.63	0.41
1:B:67:CYS:O	1:B:68:GLU:HB2	2.20	0.41
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.80	0.41
1:C:91:ASP:HA	1:C:92:PRO:HD3	1.93	0.41
1:A:150:GLY:HA3	1:A:156:ASP:HA	2.03	0.41
1:C:150:GLY:HA3	1:C:156:ASP:HA	2.01	0.41
1:A:93:TYR:CZ	1:A:97:ILE:HD11	2.56	0.40
1:A:113:TRP:CZ2	1:A:171:TRP:HB3	2.56	0.40
1:B:27:LEU:HD11	1:B:158:VAL:HG11	2.03	0.40
1:B:12:ALA:HA	1:B:36:GLU:OE2	2.20	0.40
1:C:88:LEU:HD23	1:C:88:LEU:HA	1.91	0.40
1:A:68:GLU:HB2	1:A:71:ILE:HD12	2.04	0.40
1:C:185:ASP:OD1	1:C:185:ASP:C	2.63	0.40

All (2) 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)
4:B:2240:HOH:O	4:B:2240:HOH:O[3_655]	2.00	0.20
4:A:2125:HOH:O	4:C:2137:HOH:O[5_445]	2.09	0.11

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	222/230 (96%)	217 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	221/230 (96%)	216 (98%)	5 (2%)	0	100	100
1	C	224/230 (97%)	219 (98%)	5 (2%)	0	100	100
All	All	667/690 (97%)	652 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	175/177 (99%)	166 (95%)	9 (5%)	21	23
1	B	173/177 (98%)	164 (95%)	9 (5%)	21	22
1	C	175/177 (99%)	168 (96%)	7 (4%)	28	34
All	All	523/531 (98%)	498 (95%)	25 (5%)	24	25

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	44	GLU
1	A	56	ILE
1	A	77	ASP
1	A	122	GLU
1	A	126	SER
1	A	168	VAL
1	A	183	ILE
1	A	188	LYS
1	B	77	ASP
1	B	121	THR
1	B	126	SER
1	B	145	GLU
1	B	176[A]	GLU
1	B	176[B]	GLU
1	B	183	ILE

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Mol	Chain	Res	Type
1	B	188	LYS
1	B	222	ARG
1	C	77	ASP
1	C	114	ARG
1	C	121	THR
1	C	126	SER
1	C	176[A]	GLU
1	C	176[B]	GLU
1	C	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	GTX	B	1225	-	24,25,25	1.86	3 (12%)	27,30,30	2.53	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1226	-	4,4,4	0.31	0	6,6,6	0.61	0
2	GTX	C	1226	-	24,25,25	1.94	3 (12%)	27,30,30	3.27	7 (25%)
3	SO4	C	1227	-	4,4,4	0.28	0	6,6,6	0.54	0
3	SO4	B	1226	-	4,4,4	0.31	0	6,6,6	0.77	0
2	GTX	A	1225	-	24,25,25	1.94	3 (12%)	27,30,30	3.59	9 (33%)

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	GTX	A	1225	-	-	7/30/30/30	-
2	GTX	C	1226	-	-	5/30/30/30	-
2	GTX	B	1225	-	-	1/30/30/30	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1225	GTX	OE1-CD1	6.99	1.37	1.23
2	C	1226	GTX	OE1-CD1	6.87	1.36	1.23
2	B	1225	GTX	OE1-CD1	6.38	1.35	1.23
2	C	1226	GTX	CD1-N2	5.40	1.45	1.34
2	B	1225	GTX	CD1-N2	5.01	1.44	1.34
2	A	1225	GTX	CD1-N2	4.26	1.43	1.34
2	A	1225	GTX	O12-C1	-2.47	1.22	1.30
2	C	1226	GTX	CG1-CD1	2.18	1.55	1.51
2	B	1225	GTX	O31-C3	2.07	1.28	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1225	GTX	OE1-CD1-N2	-13.83	99.53	122.95
2	C	1226	GTX	OE1-CD1-N2	-13.38	100.30	122.95
2	B	1225	GTX	OE1-CD1-N2	-10.50	105.17	122.95
2	A	1225	GTX	OE1-CD1-CG1	-8.65	106.34	122.02
2	C	1226	GTX	OE1-CD1-CG1	-7.42	108.58	122.02
2	A	1225	GTX	CG1-CD1-N2	-3.93	108.95	115.86
2	A	1225	GTX	CB1-CA1-N1	-3.51	100.98	110.12
2	A	1225	GTX	CB1-CA1-C1	3.46	119.61	110.45
2	B	1225	GTX	OE1-CD1-CG1	-3.40	115.85	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1225	GTX	CB2-CA2-C2	-2.74	103.28	109.46
2	C	1226	GTX	CG1-CD1-N2	-2.72	111.07	115.86
2	C	1226	GTX	CB1-CA1-N1	-2.72	103.04	110.12
2	C	1226	GTX	O32-C3-CA3	2.44	122.10	112.81
2	A	1225	GTX	C2S-C1S-SG2	-2.44	105.49	113.58
2	B	1225	GTX	CB1-CA1-N1	-2.43	103.79	110.12
2	B	1225	GTX	CA2-C2-N3	-2.42	111.35	116.54
2	C	1226	GTX	CA2-N2-CD1	2.41	127.73	121.68
2	B	1225	GTX	C2-CA2-N2	-2.40	104.62	111.11
2	C	1226	GTX	CB2-SG2-C1S	-2.39	95.18	102.26
2	A	1225	GTX	O12-C1-O11	-2.38	118.69	124.08
2	B	1225	GTX	O12-C1-O11	-2.23	119.02	124.08
2	B	1225	GTX	CG1-CD1-N2	2.17	119.69	115.86
2	B	1225	GTX	CA3-N3-C2	2.15	126.81	121.38
2	A	1225	GTX	CB2-SG2-C1S	-2.05	96.18	102.26

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1225	GTX	OE1-CD1-N2-CA2
2	C	1226	GTX	OE1-CD1-N2-CA2
2	B	1225	GTX	OE1-CD1-N2-CA2
2	C	1226	GTX	SG2-C1S-C2S-C3S
2	A	1225	GTX	SG2-C1S-C2S-C3S
2	A	1225	GTX	C1S-C2S-C3S-C4S
2	C	1226	GTX	C2S-C3S-C4S-C5S
2	A	1225	GTX	C3S-C4S-C5S-C6S
2	A	1225	GTX	CG1-CD1-N2-CA2
2	A	1225	GTX	C2S-C3S-C4S-C5S
2	C	1226	GTX	C3-CA3-N3-C2
2	A	1225	GTX	C2S-C1S-SG2-CB2
2	C	1226	GTX	C2S-C1S-SG2-CB2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

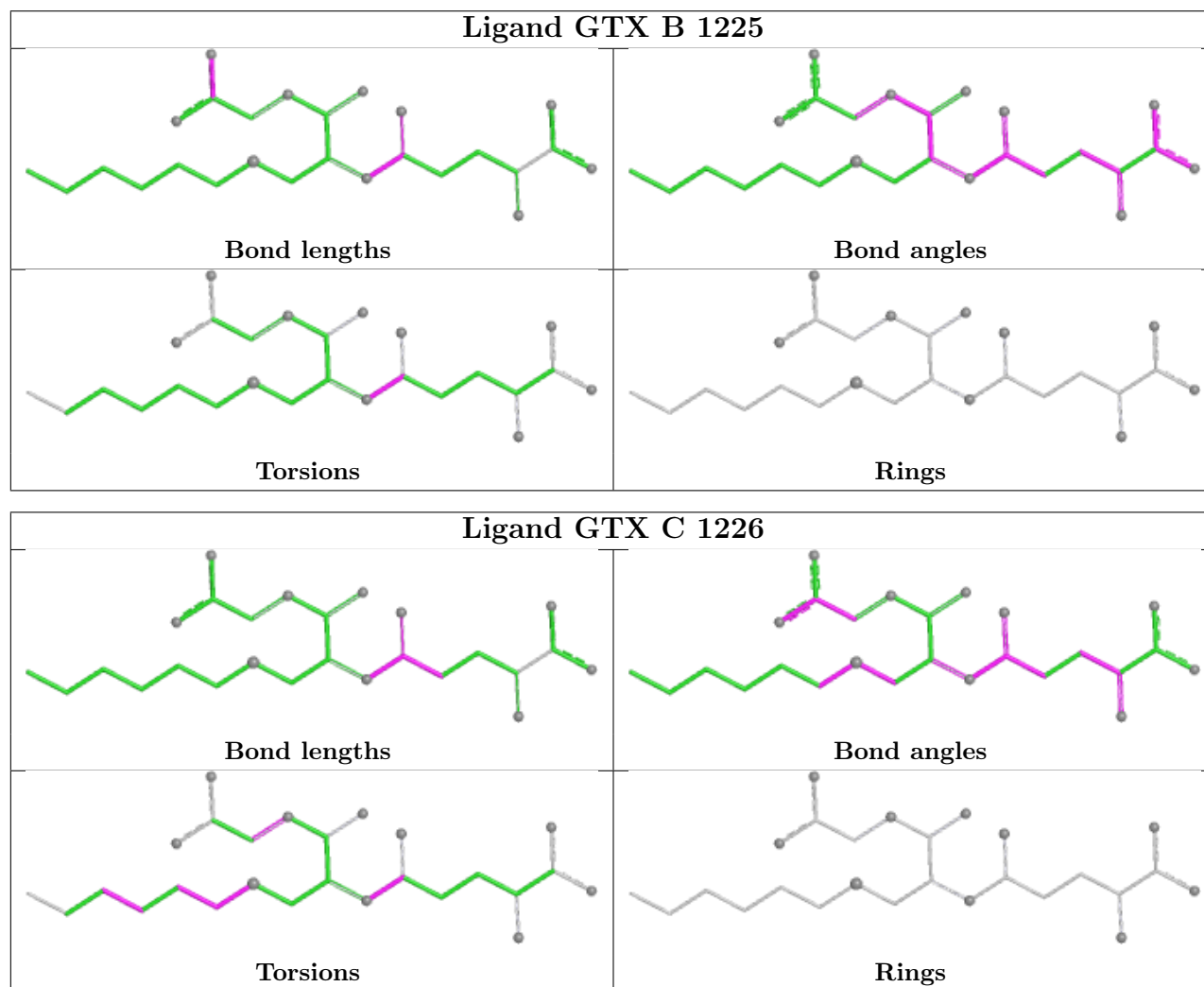
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1226	SO4	1	0
3	C	1227	SO4	1	0
3	B	1226	SO4	1	0

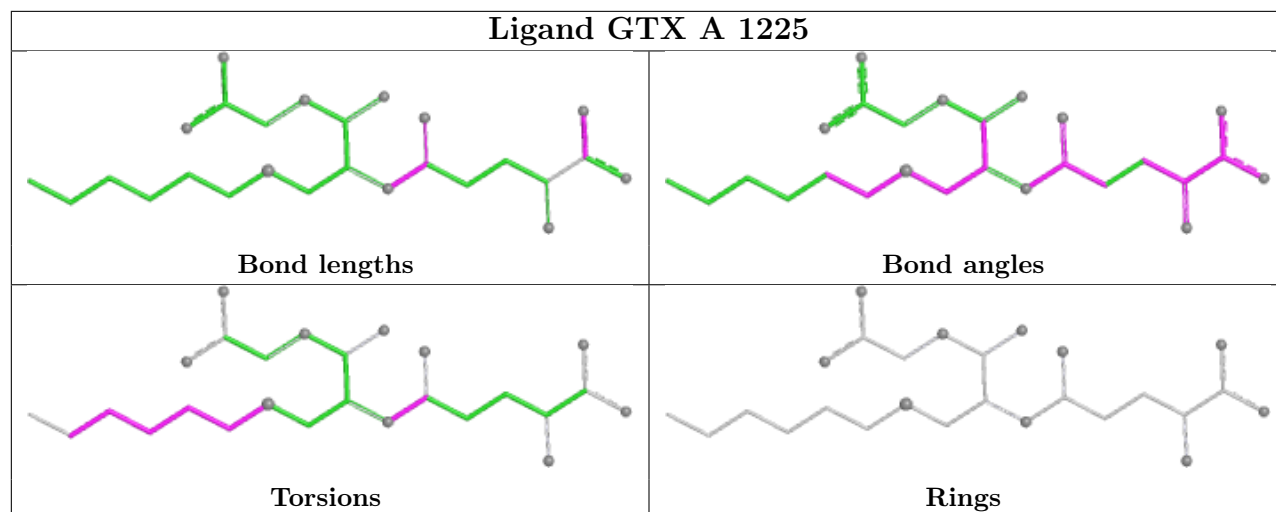
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1225	GTX	1	0

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

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.