Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:42 pm GMT

PDB ID	:	1GWC
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.; Lapthorn, 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 (i) 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 (1)) were used in the production of this report:

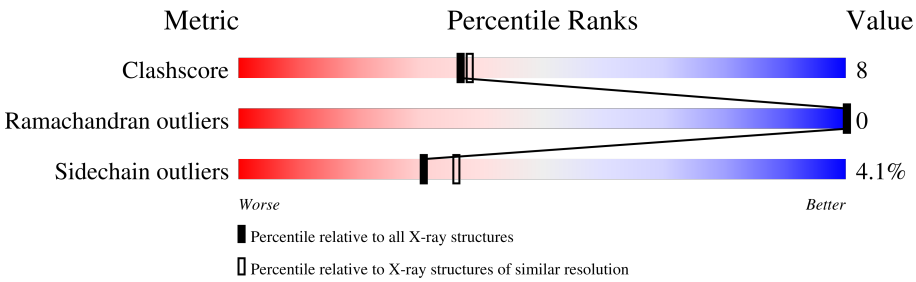
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	230	74% 19% • •
1	B	230	74% 20% • •
1	C	230	77% 18% • •

2 Entry composition (i)

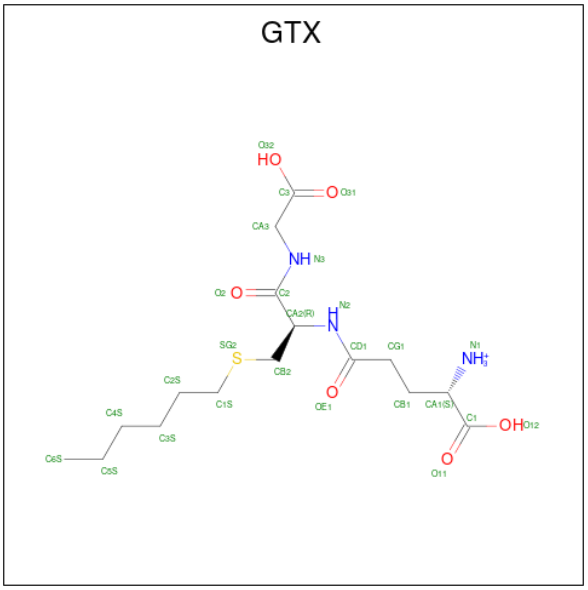
There are 4 unique types of molecules in this entry. The entry contains 5913 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

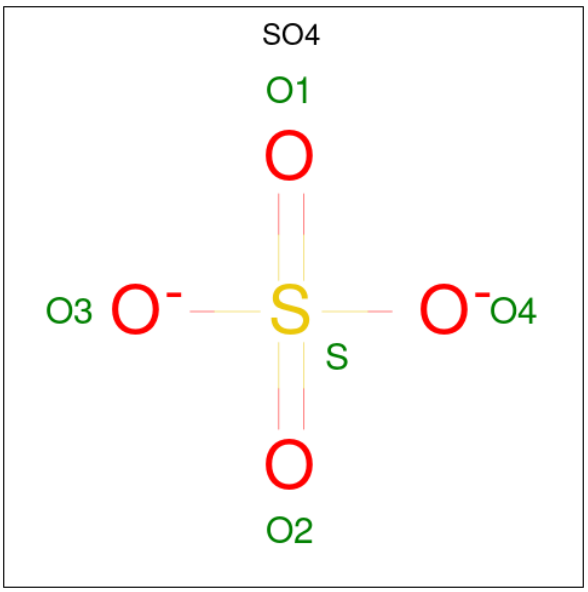
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	1705	1105	284	311	5	0	3	0
1	B	221	1694	1098	281	311	4	0	2	0
1	C	222	1710	1108	285	312	5	0	4	0

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

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

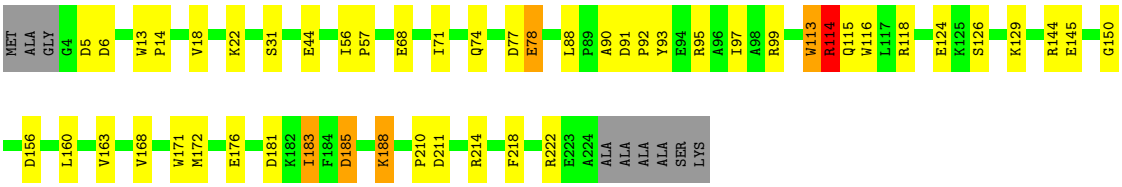
3 Residue-property plots (i)

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. 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.

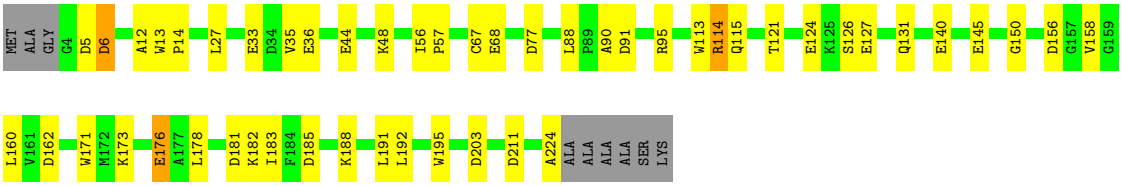
• Molecule 1: GLUTATHIONE S-TRANSFERASE TSI-1

Chain A:



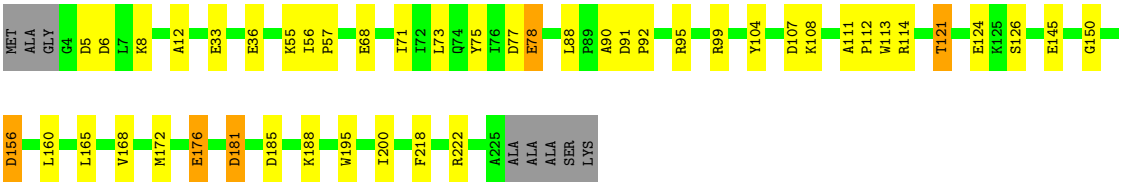
• Molecule 1: GLUTATHIONE S-TRANSFERASE TSI-1

Chain B:



• Molecule 1: GLUTATHIONE S-TRANSFERASE TSI-1

Chain C:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.19	2/1758 (0.1%)	1.21	11/2381 (0.5%)
1	B	1.23	1/1744 (0.1%)	1.26	12/2364 (0.5%)
1	C	1.18	3/1768 (0.2%)	1.25	12/2395 (0.5%)
All	All	1.20	6/5270 (0.1%)	1.24	35/7140 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	TRP	CB-CG	-5.99	1.39	1.50
1	C	113	TRP	CB-CG	-5.79	1.39	1.50
1	A	163	VAL	CB-CG2	-5.57	1.41	1.52
1	C	195	TRP	CB-CG	-5.17	1.41	1.50
1	C	75	TYR	CD2-CE2	5.10	1.47	1.39
1	A	113	TRP	CB-CG	-5.07	1.41	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ASP	CB-CG-OD2	9.40	126.76	118.30
1	C	99	ARG	NE-CZ-NH1	-8.43	116.09	120.30
1	B	91	ASP	CB-CG-OD2	7.52	125.06	118.30
1	A	5	ASP	CB-CG-OD2	7.42	124.97	118.30
1	C	5	ASP	CB-CG-OD2	7.23	124.81	118.30
1	B	6	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	5	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	99	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	181	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	73	LEU	CB-CG-CD1	6.25	121.62	111.00
1	C	145	GLU	CA-CB-CG	6.22	127.08	113.40
1	C	6	ASP	CB-CG-OD2	6.19	123.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	181	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	6	ASP	OD1-CG-OD2	-5.86	112.17	123.30
1	A	78	GLU	OE1-CD-OE2	-5.83	116.31	123.30
1	B	6	ASP	OD1-CG-OD2	-5.82	112.25	123.30
1	A	114	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	C	145	GLU	N-CA-CB	-5.71	100.32	110.60
1	B	114	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	99	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	C	185	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	107	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	181	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	78	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	B	211	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	178	LEU	CB-CG-CD2	-5.20	102.17	111.00
1	A	144	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	6	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	156	ASP	CB-CG-OD1	5.12	122.90	118.30
1	B	185	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	162	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	211	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	203	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	185	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	32	0
1	B	1694	0	1708	28	0
1	C	1710	0	1735	21	0
2	A	26	0	28	1	0
2	B	26	0	28	0	0
2	C	26	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	1
4	B	251	0	0	6	1
4	C	238	0	0	5	1
All	All	5913	0	5259	83	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 (83) 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: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: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: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:A:172[B]:MET:HE1	4:A:2182:HOH:O	1.98	0.63
1:B:115:GLN:NE2	1:B:124:GLU:O	2.31	0.61
1:C:90:ALA:O	1:C:95[B]:ARG:NH1	2.37	0.58
1:B:95[B]:ARG:HH21	1:C:78:GLU:CD	2.07	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:140:GLU:CD	1:B:191:LEU:HB2	2.33	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:C:121:THR:HG23	1:C:124:GLU:CD	2.35	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: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:C:8:LYS:NZ	4:C:2008:HOH:O	2.08	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:44:GLU:HG3	1:B:48:LYS:HZ2	1.84	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

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
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 (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	175/177 (99%)	167 (95%)	8 (5%)	27	30
1	B	173/177 (98%)	165 (95%)	8 (5%)	27	30
1	C	175/177 (99%)	168 (96%)	7 (4%)	31	37
All	All	523/531 (98%)	500 (96%)	23 (4%)	30	32

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	44	GLU
1	A	77	ASP
1	A	114	ARG
1	A	126	SER
1	A	183	ILE
1	A	188	LYS
1	A	210	PRO
1	B	77	ASP
1	B	114	ARG
1	B	121	THR
1	B	126	SER
1	B	145	GLU
1	B	176[A]	GLU
1	B	176[B]	GLU
1	B	188	LYS
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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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	GTX	B	1225	-	24,25,25	1.83	3 (12%)	29,30,30	2.49	9 (31%)
3	SO4	C	1227	-	4,4,4	0.18	0	6,6,6	0.56	0
2	GTX	C	1226	-	24,25,25	1.92	3 (12%)	29,30,30	3.22	10 (34%)
2	GTX	A	1225	-	24,25,25	1.90	3 (12%)	29,30,30	3.50	10 (34%)
3	SO4	B	1226	-	4,4,4	0.20	0	6,6,6	0.77	0
3	SO4	A	1226	-	4,4,4	0.20	0	6,6,6	0.66	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	GTX	B	1225	-	-	1/30/30/30	-
2	GTX	A	1225	-	-	7/30/30/30	-
2	GTX	C	1226	-	-	5/30/30/30	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1225	GTX	OE1-CD1	6.82	1.37	1.23
2	C	1226	GTX	OE1-CD1	6.70	1.36	1.23
2	B	1225	GTX	OE1-CD1	6.22	1.35	1.23
2	C	1226	GTX	CD1-N2	5.37	1.45	1.34
2	B	1225	GTX	CD1-N2	4.98	1.44	1.34
2	A	1225	GTX	CD1-N2	4.23	1.43	1.34
2	A	1225	GTX	O12-C1	-2.37	1.22	1.30
2	C	1226	GTX	CG1-CD1	2.29	1.55	1.51
2	B	1225	GTX	O31-C3	2.02	1.28	1.22

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1225	GTX	OE1-CD1-N2	-13.88	99.53	122.95
2	C	1226	GTX	OE1-CD1-N2	-13.42	100.30	122.95
2	B	1225	GTX	OE1-CD1-N2	-10.54	105.17	122.95
2	A	1225	GTX	OE1-CD1-CG1	-8.57	106.34	122.02
2	C	1226	GTX	OE1-CD1-CG1	-7.35	108.58	122.02
2	A	1225	GTX	CG1-CD1-N2	-3.97	108.95	115.83
2	A	1225	GTX	CB1-CA1-C1	3.91	119.61	110.30
2	A	1225	GTX	CB1-CA1-N1	-3.50	100.98	110.17
2	B	1225	GTX	OE1-CD1-CG1	-3.37	115.85	122.02
2	A	1225	GTX	CB2-CA2-C2	-2.97	103.28	109.73
2	C	1226	GTX	CG1-CD1-N2	-2.75	111.07	115.83
2	C	1226	GTX	CB1-CA1-N1	-2.72	103.04	110.17
2	C	1226	GTX	O32-C3-CA3	2.69	122.10	112.74
2	C	1226	GTX	O12-C1-CA1	2.65	122.42	113.38
2	B	1225	GTX	CA2-C2-N3	-2.58	111.35	116.54
2	A	1225	GTX	C2S-C1S-SG2	-2.55	105.49	113.69
2	B	1225	GTX	CB1-CA1-N1	-2.43	103.79	110.17
2	B	1225	GTX	C2-CA2-N2	-2.40	104.62	111.16
2	A	1225	GTX	O12-C1-O11	-2.38	118.69	124.09
2	C	1226	GTX	CA2-N2-CD1	2.36	127.73	121.65
2	C	1226	GTX	CB2-SG2-C1S	-2.36	95.18	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1226	GTX	CB1-CA1-C1	2.28	115.74	110.30
2	B	1225	GTX	O12-C1-O11	-2.23	119.02	124.09
2	B	1225	GTX	CG1-CD1-N2	2.23	119.69	115.83
2	B	1225	GTX	CA3-N3-C2	2.19	126.81	121.37
2	B	1225	GTX	O12-C1-CA1	2.06	120.39	113.38
2	A	1225	GTX	CB2-SG2-C1S	-2.03	96.18	102.27
2	C	1226	GTX	CA2-C2-N3	-2.02	112.47	116.54
2	A	1225	GTX	O32-C3-CA3	2.02	119.76	112.74

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	CG1-CD1-N2-CA2

There are no ring outliers.

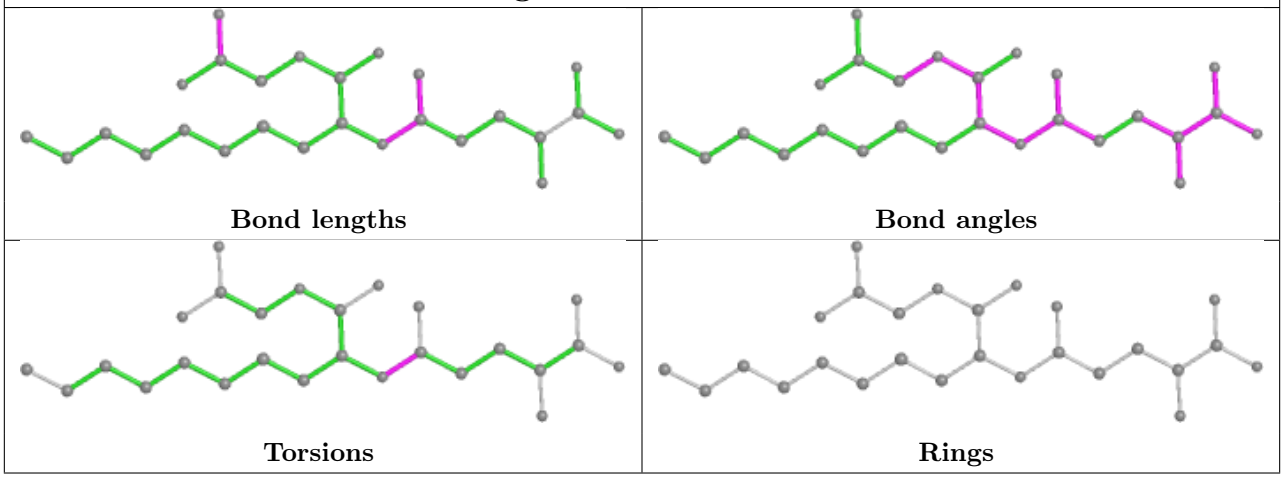
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1227	SO4	1	0
2	A	1225	GTX	1	0
3	B	1226	SO4	1	0
3	A	1226	SO4	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 then 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

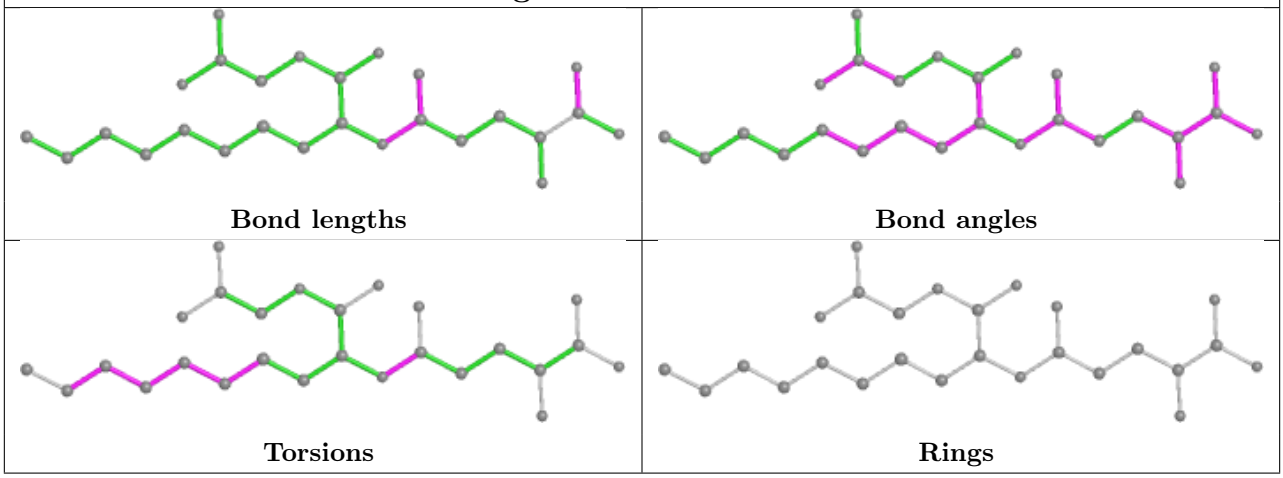
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 GTX B 1225



Ligand GTX C 1226

Ligand GTX A 1225



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.