



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:26 PM UTC

PDB ID : 1EV4 / pdb_00001ev4
Title : RAT GLUTATHIONE S-TRANSFERASE A1-1: MUTANT W21F/F220Y WITH GSO3 BOUND
Authors : Adman, E.T.; Le Trong, I.; Stenkamp, R.E.; Nieslanik, B.S.; Dietze, E.C.; Tai, G.; Ibarra, C.; Atkins, W.M.
Deposited on : 2000-04-19
Resolution : 2.20 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

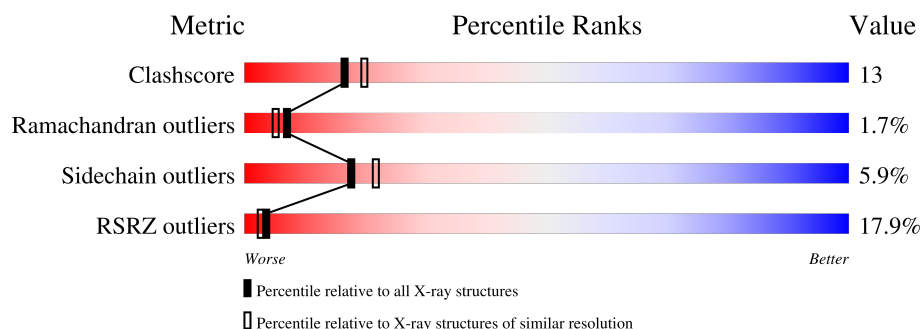
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	221	14% 64% 28% 7% .
1	C	221	22% 56% 31% 7% 6% .
1	D	221	16% 72% 23% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5599 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 A1-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1786	1152	299	324	11			
1	C	207	Total	C	N	O	S	0	0	0
			1664	1073	278	302	11			
1	D	221	Total	C	N	O	S	0	0	0
			1786	1152	299	324	11			

There are 9 discrepancies between the modelled and reference sequences:

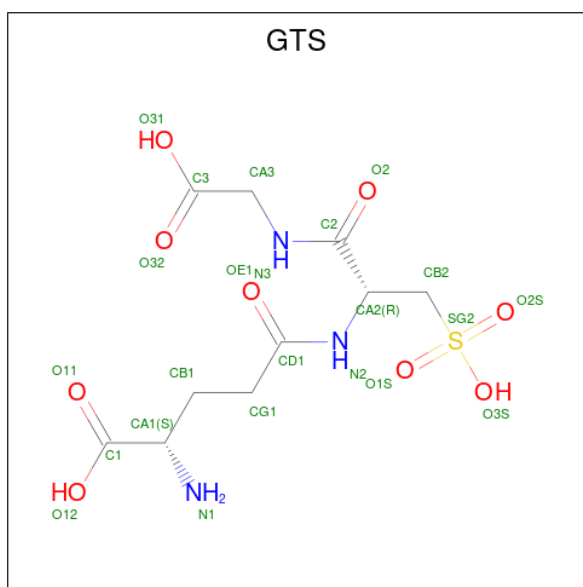
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	TRP	engineered mutation	UNP P00502
A	96	SER	THR	conflict	UNP P00502
A	220	TYR	PHE	engineered mutation	UNP P00502
C	21	PHE	TRP	engineered mutation	UNP P00502
C	96	SER	THR	conflict	UNP P00502
C	220	TYR	PHE	engineered mutation	UNP P00502
D	21	PHE	TRP	engineered mutation	UNP P00502
D	96	SER	THR	conflict	UNP P00502
D	220	TYR	PHE	engineered mutation	UNP P00502

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLUTATHIONE SULFONIC ACID (CCD ID: GTS) (formula: $C_{10}H_{17}N_3O_9S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	10	3	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			23	10	3	9	1		
3	D	1	Total	C	N	O	S	0	0
			23	10	3	9	1		

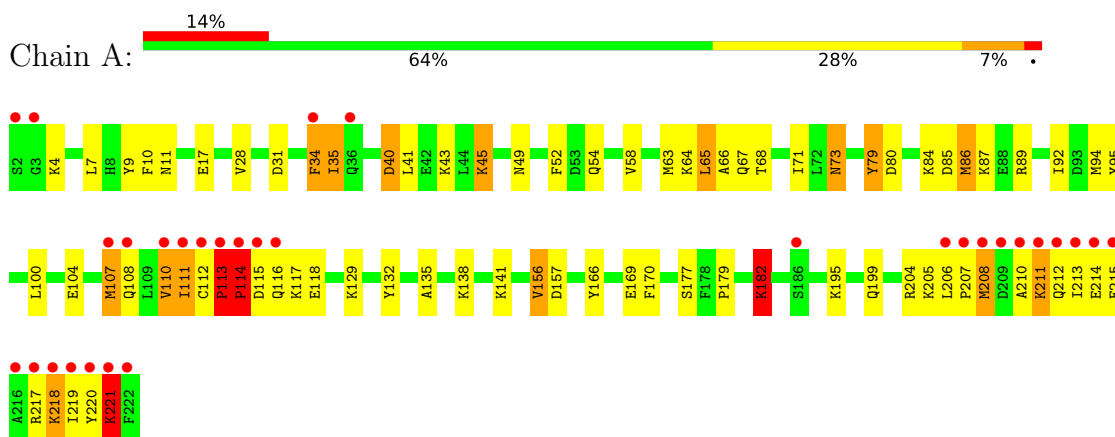
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	C	56	Total	O	0	0
			56	56		
4	D	97	Total	O	0	0
			97	97		

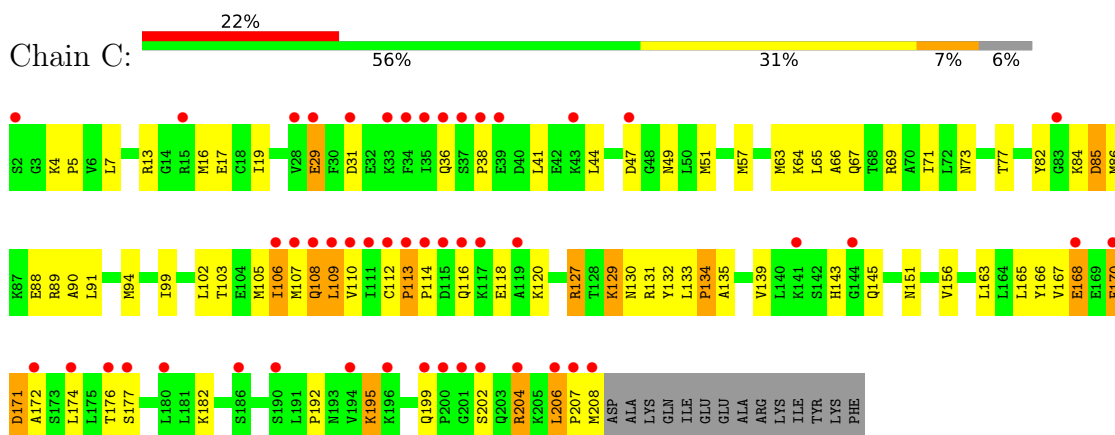
3 Residue-property plots

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.

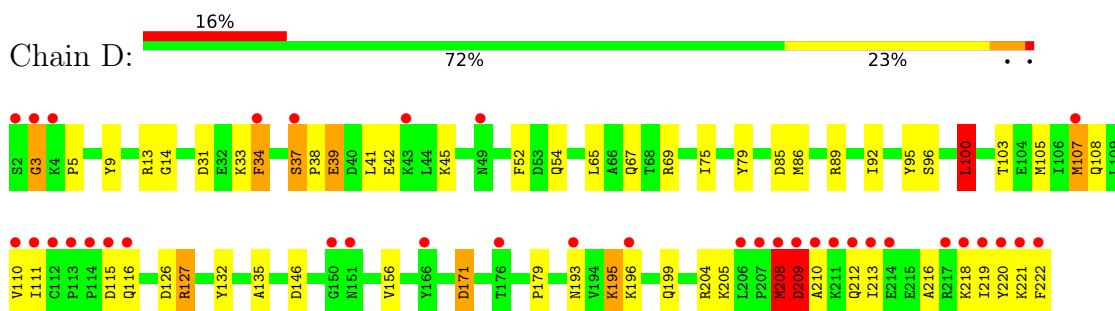
• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1



• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1



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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.60Å 275.20Å 70.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 96.1 (20.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.218 , 0.285 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5599	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GTS, 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	0.80	1/1818 (0.1%)	1.46	45/2440 (1.8%)
1	C	0.71	0/1694	1.39	15/2276 (0.7%)
1	D	0.72	0/1818	1.41	23/2440 (0.9%)
All	All	0.75	1/5330 (0.0%)	1.42	83/7156 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	MET	SD-CE	-7.85	1.59	1.79

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	ASP	CA-CB-CG	16.20	128.80	112.60
1	C	31	ASP	CA-CB-CG	14.94	127.54	112.60
1	A	31	ASP	CA-CB-CG	12.73	125.33	112.60
1	C	206	LEU	N-CA-CB	-10.36	97.05	109.59
1	D	126	ASP	CA-CB-CG	10.28	122.88	112.60
1	D	193	ASN	CA-CB-CG	-9.15	103.45	112.60
1	A	107	MET	CB-CA-C	-8.49	97.56	110.88
1	A	182	LYS	CB-CG-CD	8.27	130.32	111.30
1	A	170	PHE	N-CA-CB	-7.90	98.52	109.98
1	A	218	LYS	CB-CG-CD	7.83	129.30	111.30
1	D	222	PHE	N-CA-CB	-7.77	97.29	110.50
1	D	37	SER	N-CA-CB	-7.74	101.52	111.35
1	A	84	LYS	N-CA-CB	-7.70	99.33	110.65
1	A	129	LYS	CG-CD-CE	7.60	128.77	111.30
1	A	113	PRO	CA-C-N	7.50	129.22	119.84
1	A	113	PRO	C-N-CA	7.50	129.22	119.84
1	A	80	ASP	CA-CB-CG	-7.45	105.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ASP	CA-CB-CG	7.30	119.90	112.60
1	D	146	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	129	LYS	CB-CG-CD	-7.08	95.01	111.30
1	C	130	ASN	CA-CB-CG	-6.93	105.67	112.60
1	A	4	LYS	N-CA-CB	-6.91	99.12	109.90
1	C	85	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	40	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	4	LYS	CB-CA-C	6.77	120.35	109.51
1	C	105	MET	N-CA-CB	-6.69	100.31	110.01
1	A	73	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	34	PHE	CB-CA-C	-6.65	98.99	109.84
1	A	43	LYS	N-CA-CB	6.64	119.64	110.01
1	D	199	GLN	CB-CA-C	6.57	119.81	109.37
1	D	37	SER	CB-CA-C	6.45	119.20	110.37
1	D	107	MET	CB-CA-C	-6.39	100.81	110.90
1	A	4	LYS	CB-CG-CD	-6.39	96.61	111.30
1	A	85	ASP	CA-CB-CG	6.38	118.98	112.60
1	D	199	GLN	CA-C-N	6.33	126.35	119.89
1	D	199	GLN	C-N-CA	6.33	126.35	119.89
1	A	118	GLU	CB-CA-C	-6.29	100.40	110.84
1	D	39	GLU	N-CA-CB	6.18	119.91	110.14
1	D	196	LYS	CB-CA-C	-6.13	101.25	110.88
1	A	117	LYS	N-CA-C	6.12	117.64	110.97
1	C	36	GLN	OE1-CD-NE2	-6.09	116.50	122.60
1	C	195	LYS	CG-CD-CE	6.09	125.30	111.30
1	A	208	MET	N-CA-CB	-6.07	99.54	109.56
1	A	221	LYS	CB-CG-CD	5.94	124.95	111.30
1	A	107	MET	N-CA-CB	5.84	118.47	110.01
1	A	208	MET	CB-CA-C	5.81	118.78	109.61
1	A	114	PRO	N-CA-CB	-5.75	97.21	103.25
1	D	209	ASP	N-CA-CB	5.75	120.20	110.49
1	A	132	TYR	N-CA-C	5.74	118.65	111.24
1	D	195	LYS	N-CA-CB	-5.72	101.42	109.94
1	C	31	ASP	N-CA-CB	-5.71	101.11	110.41
1	D	34	PHE	N-CA-C	5.71	118.84	109.76
1	D	199	GLN	N-CA-CB	-5.71	103.12	109.74
1	D	209	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	171	ASP	CA-CB-CG	5.64	118.24	112.60
1	D	196	LYS	CB-CG-CD	-5.64	98.33	111.30
1	D	100	LEU	N-CA-CB	5.54	118.26	110.12
1	C	170	PHE	N-CA-CB	-5.44	101.91	110.06
1	A	86	MET	N-CA-CB	-5.43	101.84	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	LYS	CG-CD-CE	5.43	123.78	111.30
1	D	100	LEU	CB-CA-C	-5.40	101.83	110.79
1	A	63	MET	CB-CA-C	-5.38	100.40	109.50
1	A	157	ASP	CA-CB-CG	-5.35	107.25	112.60
1	A	115	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	113	PRO	CA-C-N	5.26	126.41	119.84
1	C	113	PRO	C-N-CA	5.26	126.41	119.84
1	C	129	LYS	CB-CG-CD	-5.26	99.21	111.30
1	A	65	LEU	N-CA-C	5.21	117.22	109.25
1	A	64	LYS	N-CA-C	-5.20	101.73	109.11
1	A	169	GLU	CB-CA-C	-5.15	102.09	110.85
1	A	35	ILE	CG1-CB-CG2	5.14	126.13	110.70
1	C	105	MET	CB-CA-C	5.14	118.96	110.88
1	C	118	GLU	CB-CA-C	-5.13	102.32	110.84
1	A	86	MET	N-CA-C	5.13	117.27	111.11
1	A	45	LYS	CG-CD-CE	-5.11	99.55	111.30
1	A	141	LYS	CB-CG-CD	5.08	122.99	111.30
1	A	170	PHE	CB-CA-C	5.08	118.82	110.95
1	A	87	LYS	CB-CG-CD	5.08	122.97	111.30
1	A	212	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	79	TYR	CB-CA-C	5.05	119.10	110.01
1	A	85	ASP	N-CA-C	5.05	115.00	107.88
1	C	82	TYR	N-CA-CB	-5.03	101.99	110.49
1	A	204	ARG	CB-CA-C	-5.02	102.73	110.26

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	1786	0	1852	52	0
1	C	1664	0	1726	57	0
1	D	1786	0	1852	34	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
3	A	23	0	14	1	0
3	C	23	0	14	0	0
3	D	23	0	14	1	0
4	A	126	0	0	16	0
4	C	56	0	0	11	0
4	D	97	0	0	6	0
All	All	5599	0	5472	139	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 13.

All (139) 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:A:10:PHE:HA	4:A:790:HOH:O	1.63	0.97
1:A:86:MET:HA	4:A:757:HOH:O	1.73	0.87
1:C:206:LEU:HB3	1:C:207:PRO:HD2	1.66	0.76
1:C:91:LEU:HA	4:C:735:HOH:O	1.85	0.75
1:A:73:ASN:HB3	4:A:455:HOH:O	1.87	0.75
1:A:92:ILE:HG23	1:A:156:VAL:HG22	1.68	0.73
1:C:108:GLN:HE22	1:C:112:CYS:HB3	1.53	0.72
1:A:179:PRO:O	1:A:182:LYS:HG2	1.89	0.71
1:A:179:PRO:HA	1:A:182:LYS:HE2	1.73	0.70
1:A:208:MET:N	1:A:208:MET:SD	2.63	0.70
1:D:107:MET:O	1:D:110:VAL:HG12	1.93	0.69
1:A:35:ILE:HB	4:A:790:HOH:O	1.93	0.67
1:A:210:ALA:HB3	1:A:211:LYS:NZ	2.09	0.67
1:C:29:GLU:HG2	4:C:557:HOH:O	1.94	0.67
1:C:94:MET:HE2	4:C:735:HOH:O	1.94	0.66
1:C:109:LEU:HD23	1:C:110:VAL:HG13	1.78	0.65
1:A:104:GLU:HA	1:A:107:MET:HG2	1.78	0.65
1:C:112:CYS:SG	1:C:120:LYS:HD2	2.36	0.64
1:A:49:ASN:HB2	4:A:768:HOH:O	1.97	0.64
1:D:105:MET:HE1	1:D:127:ARG:HG2	1.79	0.64
1:C:7:LEU:HB3	1:C:16:MET:HE3	1.79	0.63
1:D:110:VAL:HG11	1:D:208:MET:HG3	1.81	0.62
1:D:209:ASP:HB3	1:D:212:GLN:HB2	1.82	0.60
1:C:65:LEU:HD13	1:C:71:ILE:HA	1.82	0.60
1:C:102:LEU:HD23	1:C:163:LEU:HD21	1.84	0.59
1:A:89:ARG:HB2	4:A:757:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HB2	1:C:134:PRO:HD3	1.86	0.57
1:C:65:LEU:HB3	1:C:71:ILE:HG12	1.85	0.57
1:C:176:THR:HA	1:C:182:LYS:NZ	2.20	0.56
1:C:49:ASN:HB2	4:C:733:HOH:O	2.05	0.56
1:D:38:PRO:HD3	1:D:220:TYR:O	2.05	0.56
1:A:73:ASN:ND2	4:A:651:HOH:O	2.38	0.56
1:A:41:LEU:HD23	1:A:221:LYS:HG2	1.87	0.55
1:A:35:ILE:CB	4:A:790:HOH:O	2.53	0.55
1:A:177:SER:N	4:A:774:HOH:O	2.40	0.55
1:D:34:PHE:CZ	1:D:205:LYS:HE3	2.42	0.54
1:C:167:VAL:HG13	1:C:174:LEU:HD12	1.89	0.54
1:C:134:PRO:HD2	4:C:783:HOH:O	2.06	0.54
1:C:38:PRO:O	1:C:41:LEU:HB3	2.07	0.54
1:A:35:ILE:HG23	1:A:40:ASP:HB2	1.89	0.54
1:A:220:TYR:O	1:A:221:LYS:HB2	2.06	0.54
1:D:39:GLU:N	4:D:775:HOH:O	2.42	0.53
1:C:13:ARG:HH21	1:C:204:ARG:NH1	2.07	0.52
1:D:96:SER:O	1:D:100:LEU:HD22	2.09	0.52
1:A:207:PRO:HD2	4:A:570:HOH:O	2.08	0.52
1:A:195:LYS:HE3	4:A:699:HOH:O	2.09	0.51
1:C:108:GLN:NE2	1:C:112:CYS:HB3	2.25	0.51
1:D:218:LYS:HA	1:D:221:LYS:HD2	1.92	0.51
1:A:220:TYR:O	3:A:230:GTS:HA32	2.10	0.51
1:A:66:ALA:O	1:A:67:GLN:HB2	2.11	0.51
1:C:47:ASP:HB2	4:C:733:HOH:O	2.10	0.51
1:D:3:GLY:O	1:D:5:PRO:HD3	2.11	0.51
1:A:210:ALA:C	1:A:213:ILE:HG22	2.36	0.51
1:A:215:GLU:O	1:A:218:LYS:HG3	2.10	0.51
1:C:106:ILE:O	1:C:109:LEU:HD22	2.10	0.51
1:A:210:ALA:O	1:A:213:ILE:HG22	2.11	0.50
1:C:73:ASN:HB2	4:C:601:HOH:O	2.11	0.50
1:C:63:MET:C	1:C:64:LYS:HD2	2.36	0.50
1:A:34:PHE:CZ	1:A:205:LYS:HE3	2.47	0.50
1:A:41:LEU:HD23	1:A:219:ILE:O	2.11	0.50
1:C:103:THR:O	1:C:107:MET:HG2	2.12	0.50
1:D:92:ILE:HG23	1:D:156:VAL:HG13	1.94	0.50
1:C:145:GLN:HB3	1:C:151:ASN:OD1	2.11	0.49
1:C:131:ARG:N	4:C:783:HOH:O	2.43	0.49
1:D:216:ALA:HA	1:D:219:ILE:HD12	1.94	0.49
1:A:113:PRO:HB2	1:A:116:GLN:NE2	2.28	0.49
1:A:52:PHE:O	1:A:54:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HD2	4:A:456:HOH:O	2.12	0.48
1:C:66:ALA:O	1:C:67:GLN:HB2	2.13	0.48
1:A:210:ALA:HB3	1:A:211:LYS:HZ1	1.78	0.48
1:D:9:TYR:OH	1:D:14:GLY:HA3	2.13	0.48
1:D:34:PHE:HZ	1:D:205:LYS:CE	2.27	0.48
1:C:135:ALA:O	1:C:139:VAL:HG23	2.14	0.48
1:C:13:ARG:HH21	1:C:204:ARG:HH12	1.63	0.47
1:C:113:PRO:HD2	1:C:116:GLN:OE1	2.13	0.47
1:A:110:VAL:HG23	1:A:111:ILE:HD12	1.97	0.47
1:C:4:LYS:HD2	4:C:582:HOH:O	2.14	0.47
1:A:95:TYR:HB2	1:A:156:VAL:HG11	1.97	0.47
1:D:110:VAL:HG13	1:D:111:ILE:HG13	1.97	0.47
1:C:99:ILE:HG23	1:C:163:LEU:HD22	1.97	0.47
1:C:90:ALA:HA	4:D:342:HOH:O	2.14	0.47
1:A:218:LYS:HG3	1:A:219:ILE:N	2.30	0.46
1:A:195:LYS:O	1:A:199:GLN:HG3	2.15	0.46
1:D:34:PHE:HB2	4:D:562:HOH:O	2.15	0.46
1:C:17:GLU:HG2	1:C:166:TYR:OH	2.14	0.46
1:C:163:LEU:O	1:C:167:VAL:HG23	2.15	0.46
1:D:195:LYS:HD2	4:D:734:HOH:O	2.15	0.46
1:C:69:ARG:CZ	1:D:69:ARG:NH1	2.79	0.46
1:D:179:PRO:HG3	4:D:793:HOH:O	2.15	0.46
1:C:16:MET:SD	1:C:19:ILE:HD12	2.56	0.46
1:D:34:PHE:CZ	1:D:205:LYS:CE	2.98	0.46
1:D:41:LEU:HG	1:D:45:LYS:HE3	1.97	0.46
1:D:132:TYR:O	1:D:135:ALA:HB3	2.16	0.46
1:A:135:ALA:O	1:A:138:LYS:HB3	2.16	0.46
1:A:104:GLU:O	1:A:108:GLN:HG3	2.16	0.45
1:A:218:LYS:HG3	1:A:219:ILE:H	1.81	0.45
1:D:37:SER:HA	1:D:220:TYR:O	2.16	0.45
1:C:86:MET:HA	1:C:89:ARG:HE	1.82	0.45
1:C:13:ARG:HB2	1:C:208:MET:SD	2.56	0.45
1:C:77:THR:HG21	1:D:89:ARG:HH22	1.82	0.45
1:A:35:ILE:N	4:A:790:HOH:O	2.46	0.45
1:A:68:THR:N	4:A:742:HOH:O	2.48	0.45
1:A:206:LEU:HG	4:A:591:HOH:O	2.17	0.45
1:C:94:MET:HB3	4:C:735:HOH:O	2.14	0.45
1:D:75:ILE:HG23	1:D:79:TYR:CD2	2.52	0.44
1:A:89:ARG:HB3	4:A:456:HOH:O	2.17	0.44
1:C:5:PRO:HD2	1:C:29:GLU:O	2.18	0.44
1:C:202:SER:OG	1:C:204:ARG:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HB2	1:D:208:MET:HE1	1.99	0.44
1:A:112:CYS:HA	1:A:113:PRO:HD3	1.86	0.44
1:A:58:VAL:HG23	1:A:71:ILE:HD13	2.00	0.44
1:A:17:GLU:HG2	1:A:166:TYR:OH	2.17	0.43
1:A:213:ILE:O	1:A:217:ARG:HG3	2.18	0.43
1:C:7:LEU:HD13	1:C:16:MET:SD	2.59	0.43
1:A:11:ASN:HD22	1:A:205:LYS:HE3	1.82	0.43
1:C:165:LEU:O	1:C:168:GLU:HB3	2.18	0.43
1:D:52:PHE:O	1:D:54:GLN:HG3	2.18	0.43
1:D:103:THR:O	1:D:107:MET:HG2	2.19	0.43
1:A:41:LEU:O	1:A:45:LYS:HG3	2.19	0.43
1:C:57:MET:HA	1:C:65:LEU:O	2.18	0.42
1:C:129:LYS:HB2	1:C:129:LYS:HE3	1.79	0.42
1:C:195:LYS:O	1:C:199:GLN:HG3	2.19	0.42
1:C:143:HIS:CE1	1:C:145:GLN:HB2	2.54	0.42
1:D:67:GLN:HA	3:D:250:GTS:O11	2.19	0.42
1:A:28:VAL:HG21	1:A:79:TYR:CZ	2.55	0.42
1:C:127:ARG:O	1:C:131:ARG:HB3	2.20	0.41
1:C:132:TYR:N	4:C:783:HOH:O	2.53	0.41
1:A:112:CYS:O	1:A:114:PRO:HD3	2.20	0.41
1:C:112:CYS:CB	1:C:120:LYS:HD2	2.51	0.41
1:A:215:GLU:O	1:A:219:ILE:HG13	2.20	0.41
1:D:39:GLU:HG3	4:D:775:HOH:O	2.20	0.41
1:C:77:THR:HG21	1:D:86:MET:HB3	2.01	0.41
1:C:170:PHE:O	1:C:171:ASP:HB2	2.20	0.41
1:D:110:VAL:O	1:D:213:ILE:HD12	2.21	0.41
1:A:9:TYR:CG	1:A:10:PHE:N	2.89	0.41
1:C:51:MET:HE1	1:D:95:TYR:CD1	2.56	0.40
1:C:86:MET:N	1:C:89:ARG:HH21	2.18	0.40
1:D:218:LYS:HE2	1:D:218:LYS:HB3	1.77	0.40
1:C:85:ASP:OD1	1:C:88:GLU:HG3	2.21	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	219/221 (99%)	199 (91%)	16 (7%)	4 (2%)	6	4
1	C	205/221 (93%)	186 (91%)	17 (8%)	2 (1%)	12	11
1	D	219/221 (99%)	203 (93%)	11 (5%)	5 (2%)	5	3
All	All	643/663 (97%)	588 (91%)	44 (7%)	11 (2%)	7	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	A	221	LYS
1	D	208	MET
1	C	171	ASP
1	D	210	ALA
1	D	209	ASP
1	C	172	ALA
1	D	171	ASP
1	A	110	VAL
1	A	113	PRO
1	D	3	GLY

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	195/195 (100%)	185 (95%)	10 (5%)	21	27
1	C	183/195 (94%)	169 (92%)	14 (8%)	12	13
1	D	195/195 (100%)	185 (95%)	10 (5%)	21	27
All	All	573/585 (98%)	539 (94%)	34 (6%)	18	22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	65	LEU
1	A	100	LEU
1	A	111	ILE
1	A	114	PRO
1	A	156	VAL
1	A	182	LYS
1	A	211	LYS
1	A	214	GLU
1	A	221	LYS
1	C	29	GLU
1	C	44	LEU
1	C	84	LYS
1	C	106	ILE
1	C	108	GLN
1	C	109	LEU
1	C	114	PRO
1	C	127	ARG
1	C	134	PRO
1	C	156	VAL
1	C	168	GLU
1	C	177	SER
1	C	192	PRO
1	C	204	ARG
1	D	33	LYS
1	D	42	GLU
1	D	65	LEU
1	D	100	LEU
1	D	108	GLN
1	D	115	ASP
1	D	116	GLN
1	D	127	ARG
1	D	204	ARG
1	D	208	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	54	GLN
1	A	116	GLN
1	A	199	GLN
1	A	203	GLN

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Mol	Chain	Res	Type
1	C	8	HIS
1	C	108	GLN
1	C	193	ASN
1	D	108	GLN
1	D	193	ASN
1	D	199	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 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	$\# Z > 2$
3	GTS	A	230	-	20,22,22	0.97	2 (10%)	26,30,30	1.26	3 (11%)
3	GTS	D	250	-	20,22,22	1.28	3 (15%)	26,30,30	1.28	5 (19%)
2	SO4	A	260	-	4,4,4	0.45	0	6,6,6	0.36	0
2	SO4	D	262	-	4,4,4	0.38	0	6,6,6	0.24	0
3	GTS	C	240	-	20,22,22	0.91	2 (10%)	26,30,30	1.35	3 (11%)
2	SO4	C	261	-	4,4,4	0.38	0	6,6,6	0.25	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
3	GTS	C	240	-	-	2/27/27/27	-
3	GTS	A	230	-	-	2/27/27/27	-
3	GTS	D	250	-	-	2/27/27/27	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	250	GTS	CB2-CA2	-3.20	1.51	1.53
3	D	250	GTS	O12-C1	-2.51	1.22	1.30
3	D	250	GTS	O31-C3	-2.49	1.22	1.30
3	A	230	GTS	O12-C1	-2.39	1.23	1.30
3	A	230	GTS	O31-C3	-2.36	1.23	1.30
3	C	240	GTS	O31-C3	-2.25	1.23	1.30
3	C	240	GTS	O12-C1	-2.23	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	240	GTS	CA2-CB2-SG2	3.14	118.25	113.55
3	D	250	GTS	O1S-SG2-CB2	2.95	111.16	106.76
3	C	240	GTS	O1S-SG2-CB2	2.90	111.08	106.76
3	C	240	GTS	O3S-SG2-CB2	2.89	111.55	105.97
3	A	230	GTS	O1S-SG2-CB2	2.79	110.93	106.76
3	A	230	GTS	O3S-SG2-CB2	2.77	111.33	105.97
3	D	250	GTS	O3S-SG2-CB2	2.73	111.24	105.97
3	A	230	GTS	CA2-CB2-SG2	2.56	117.39	113.55
3	D	250	GTS	CA2-CB2-SG2	2.33	117.03	113.55
3	D	250	GTS	CB2-CA2-C2	-2.04	104.93	109.56
3	D	250	GTS	CG1-CB1-CA1	-2.03	109.20	113.86

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	230	GTS	O11-C1-CA1-N1
3	D	250	GTS	O12-C1-CA1-N1
3	A	230	GTS	O12-C1-CA1-N1

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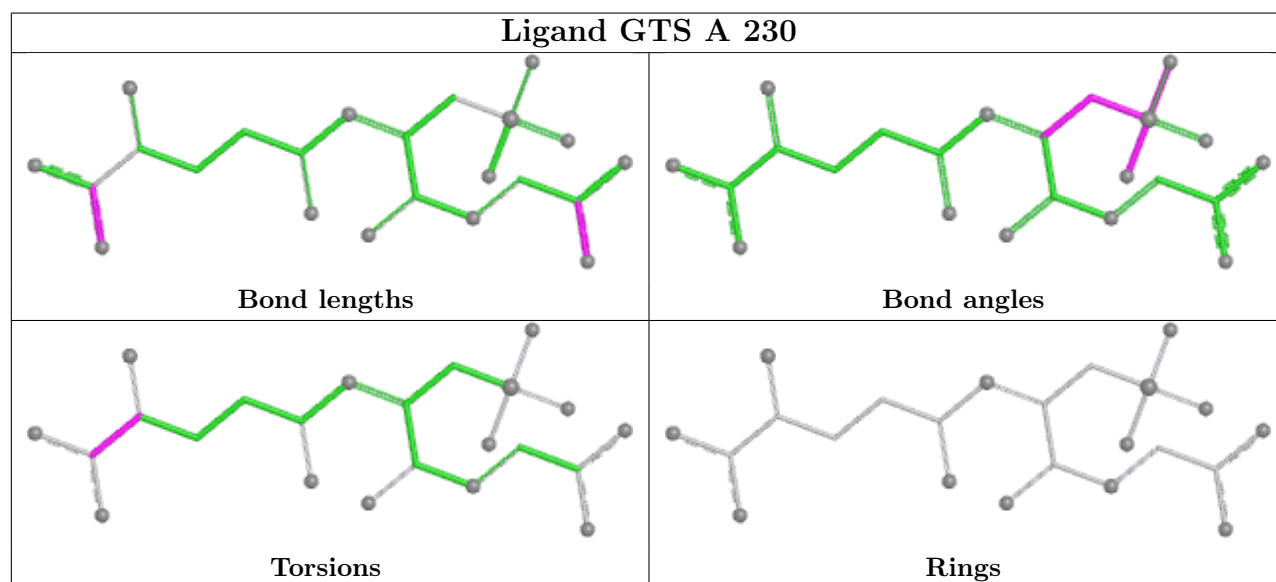
Mol	Chain	Res	Type	Atoms
3	C	240	GTS	O12-C1-CA1-N1
3	C	240	GTS	C3-CA3-N3-C2
3	D	250	GTS	C3-CA3-N3-C2

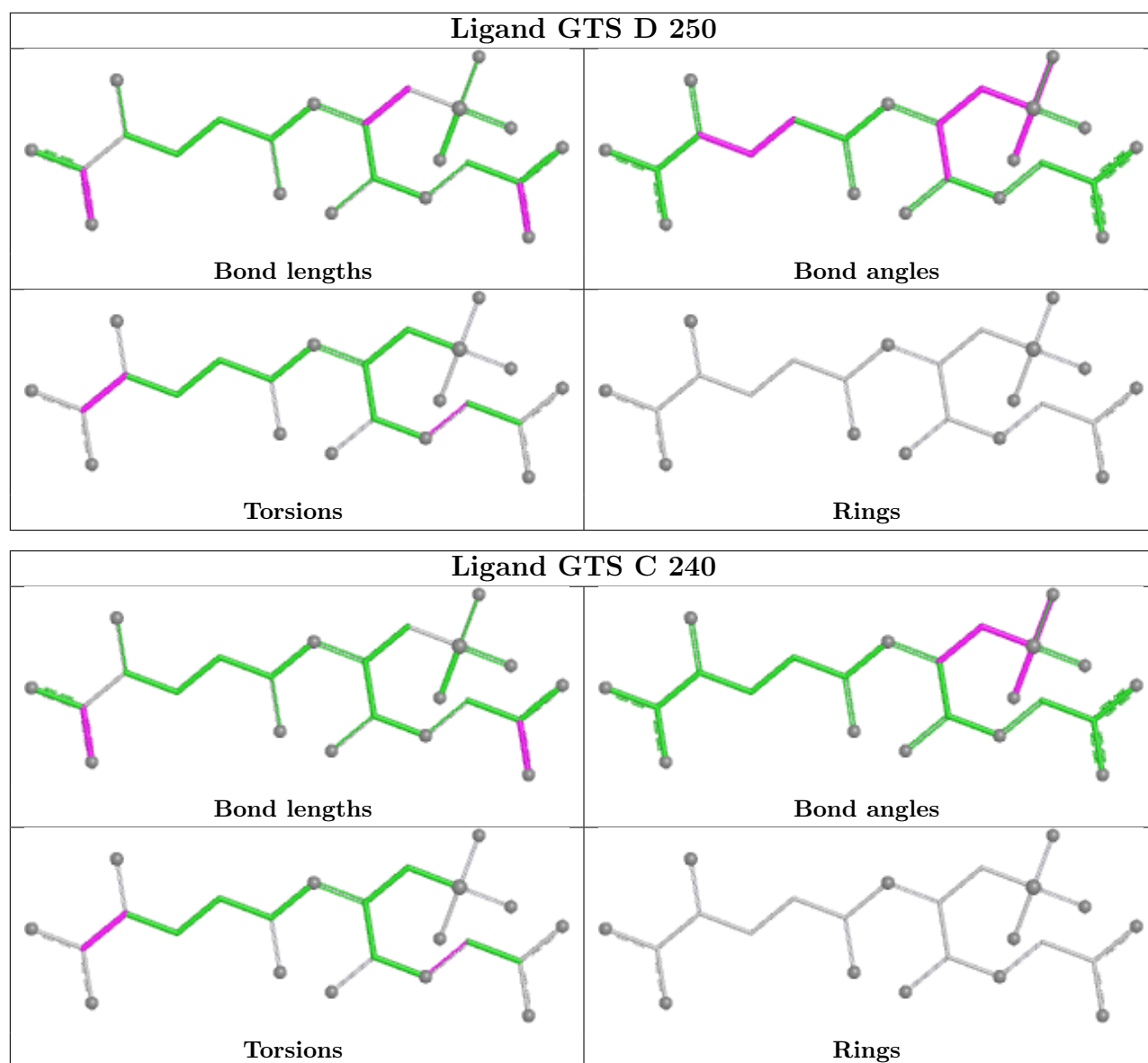
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	230	GTS	1	0
3	D	250	GTS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	221/221 (100%)	0.65	31 (14%) 6 4	16, 27, 95, 100	0
1	C	207/221 (93%)	1.35	49 (23%) 2 1	26, 47, 88, 100	0
1	D	221/221 (100%)	0.93	36 (16%) 4 3	23, 35, 81, 100	0
All	All	649/663 (97%)	0.97	116 (17%) 3 3	16, 38, 86, 100	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	11.7
1	A	213	ILE	7.0
1	A	222	PHE	6.7
1	C	112	CYS	6.1
1	A	220	TYR	6.0
1	A	219	ILE	5.9
1	C	34	PHE	5.6
1	D	222	PHE	5.4
1	C	208	MET	5.1
1	C	207	PRO	4.9
1	C	170	PHE	4.9
1	D	208	MET	4.7
1	D	206	LEU	4.6
1	D	219	ILE	4.6
1	A	210	ALA	4.6
1	A	212	GLN	4.5
1	A	206	LEU	4.4
1	A	217	ARG	4.4
1	D	166	TYR	4.3
1	A	221	LYS	4.3
1	A	208	MET	4.1
1	C	109	LEU	4.1
1	A	2	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	2	SER	4.0
1	C	201	GLY	3.9
1	A	211	LYS	3.9
1	C	114	PRO	3.9
1	D	210	ALA	3.7
1	D	207	PRO	3.7
1	C	115	ASP	3.7
1	C	206	LEU	3.6
1	C	110	VAL	3.6
1	D	2	SER	3.6
1	C	111	ILE	3.6
1	C	39	GLU	3.6
1	D	220	TYR	3.6
1	D	218	LYS	3.4
1	A	207	PRO	3.3
1	A	108	GLN	3.3
1	C	107	MET	3.3
1	A	115	ASP	3.3
1	D	114	PRO	3.3
1	C	113	PRO	3.2
1	D	209	ASP	3.2
1	C	35	ILE	3.1
1	A	214	GLU	3.1
1	A	34	PHE	3.1
1	A	116	GLN	3.1
1	D	37	SER	3.0
1	D	4	LYS	3.0
1	D	3	GLY	3.0
1	C	204	ARG	3.0
1	D	110	VAL	3.0
1	C	199	GLN	2.9
1	D	107	MET	2.9
1	D	113	PRO	2.9
1	D	43	LYS	2.9
1	C	108	GLN	2.9
1	A	113	PRO	2.9
1	A	114	PRO	2.9
1	C	172	ALA	2.9
1	D	151	ASN	2.8
1	D	116	GLN	2.8
1	D	217	ARG	2.8
1	C	202	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLU	2.8
1	C	141	LYS	2.8
1	D	193	ASN	2.8
1	A	112	CYS	2.8
1	D	49	ASN	2.7
1	C	29	GLU	2.7
1	A	107	MET	2.7
1	A	111	ILE	2.7
1	C	38	PRO	2.7
1	C	117	LYS	2.7
1	A	209	ASP	2.7
1	C	177	SER	2.7
1	C	106	ILE	2.6
1	D	34	PHE	2.6
1	C	119	ALA	2.6
1	C	37	SER	2.5
1	D	196	LYS	2.5
1	D	176	THR	2.5
1	C	116	GLN	2.5
1	C	190	SER	2.5
1	D	221	LYS	2.5
1	C	168	GLU	2.5
1	C	194	VAL	2.5
1	A	3	GLY	2.5
1	C	47	ASP	2.4
1	C	200	PRO	2.4
1	C	186	SER	2.4
1	D	112	CYS	2.4
1	D	213	ILE	2.4
1	D	111	ILE	2.3
1	C	31	ASP	2.3
1	C	144	GLY	2.3
1	A	36	GLN	2.3
1	A	110	VAL	2.3
1	C	28	VAL	2.3
1	D	212	GLN	2.2
1	C	33	LYS	2.2
1	C	43	LYS	2.2
1	A	218	LYS	2.2
1	C	176	THR	2.2
1	C	36	GLN	2.2
1	C	180	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	115	ASP	2.1
1	C	196	LYS	2.1
1	D	214	GLU	2.1
1	C	174	LEU	2.1
1	D	150	GLY	2.1
1	D	211	LYS	2.0
1	C	15	ARG	2.0
1	C	83	GLY	2.0
1	A	186	SER	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](#)

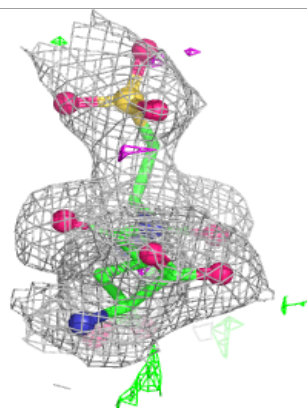
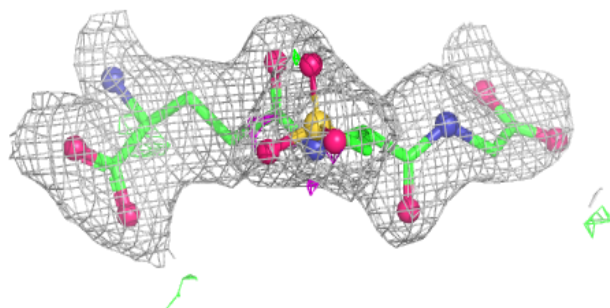
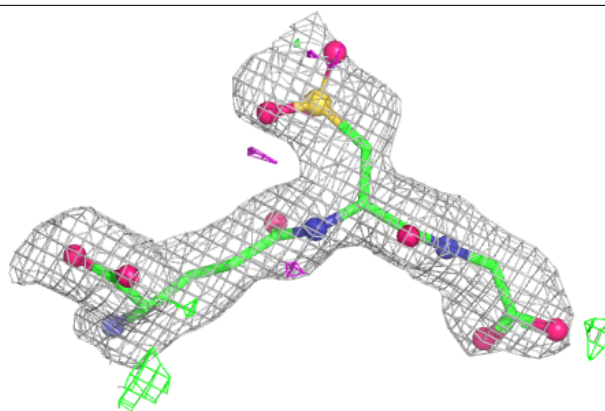
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GTS	C	240	23/23	0.85	0.16	29,60,80,83	0
2	SO4	D	262	5/5	0.86	0.17	81,81,83,85	0
3	GTS	D	250	23/23	0.89	0.11	26,39,56,58	0
3	GTS	A	230	23/23	0.90	0.12	16,33,51,59	0
2	SO4	C	261	5/5	0.91	0.13	74,74,75,77	0
2	SO4	A	260	5/5	0.92	0.11	40,42,47,49	0

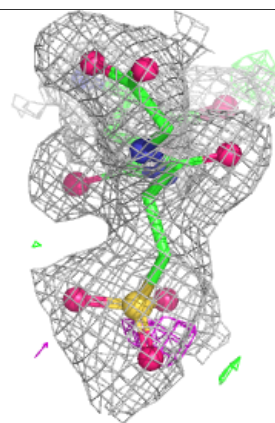
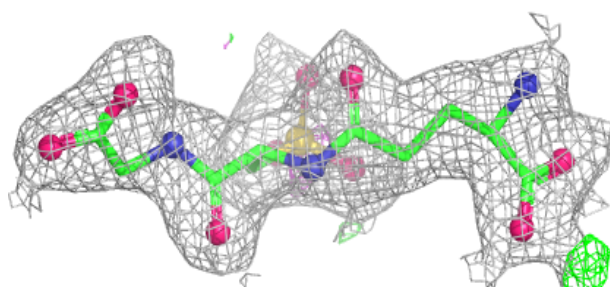
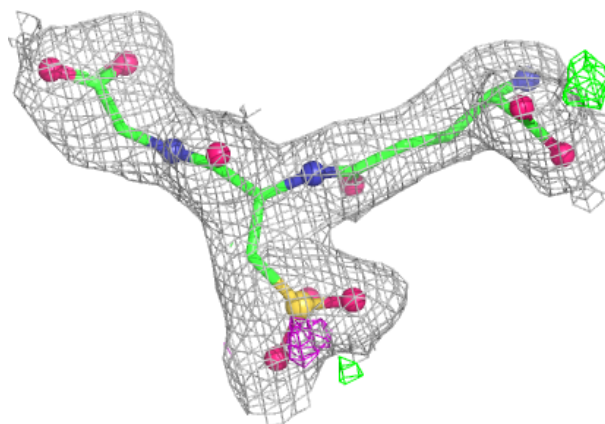
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

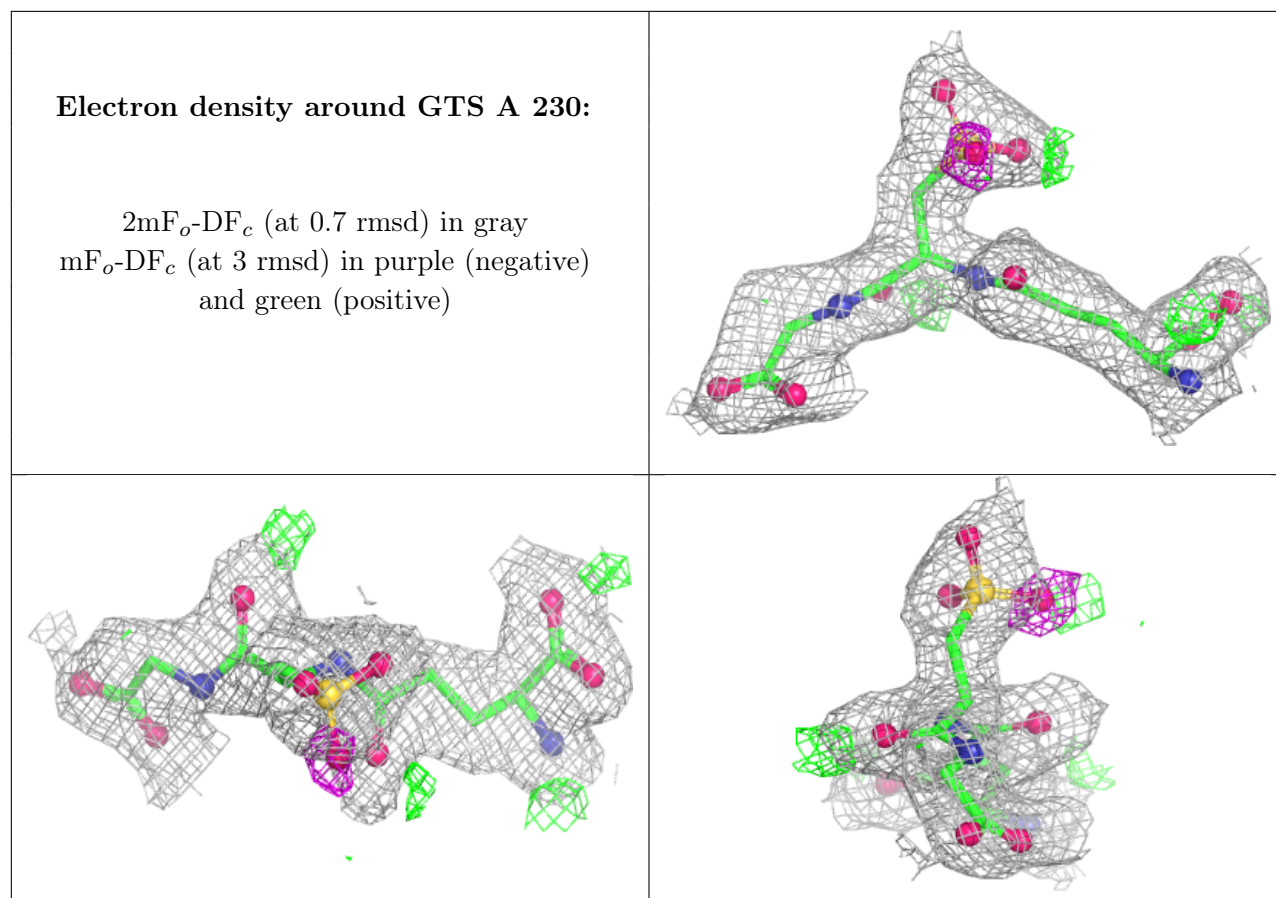
Electron density around GTS C 240:

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

**Electron density around GTS D 250:**

$2mF_o-DF_c$ (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.