



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:51 AM UTC

PDB ID : 4GST / pdb_00004gst
Title : REACTION COORDINATE MOTION IN AN SNAR REACTION CATALYZED BY GLUTATHIONE TRANSFERASE
Authors : Ji, X.; Armstrong, R.N.; Gilliland, G.L.
Deposited on : 1993-07-20
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

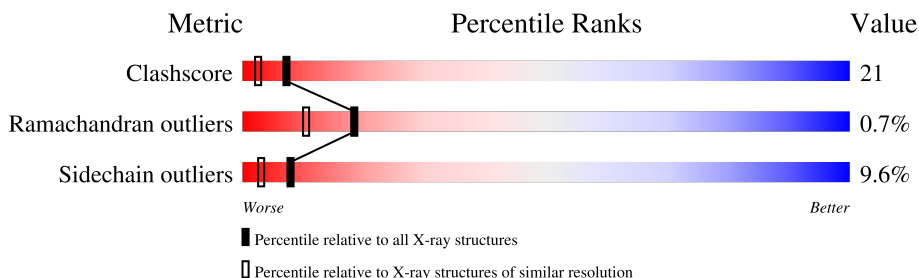
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	49% 41% 9% .
1	B	217	43% 41% 13% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	219	-	-	X	-

2 Entry composition [i](#)

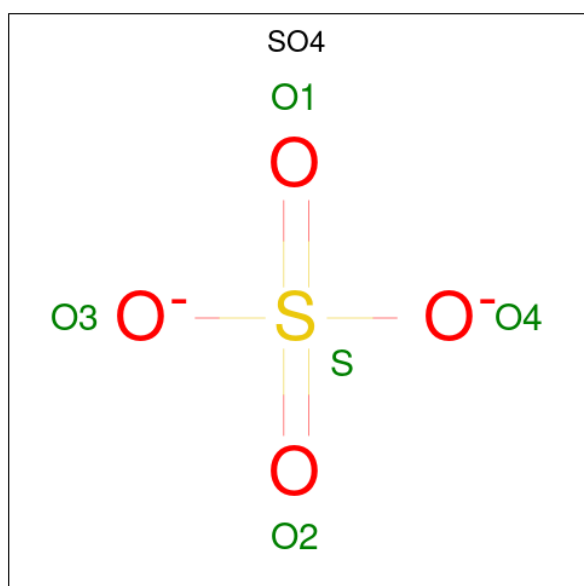
There are 4 unique types of molecules in this entry. The entry contains 4096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			
1	B	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			

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



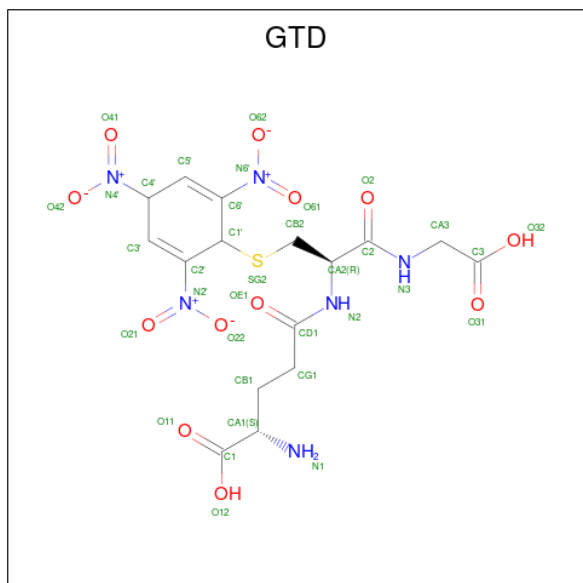
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1-(S-GLUTATHIONYL)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE (CCD ID: GTD) (formula: $C_{16}H_{20}N_6O_{12}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	16	6	12	1		
3	B	1	Total	C	N	O	S	0	0
			35	16	6	12	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total	O	0	0
			210	210		
4	B	150	Total	O	0	0
			150	150		

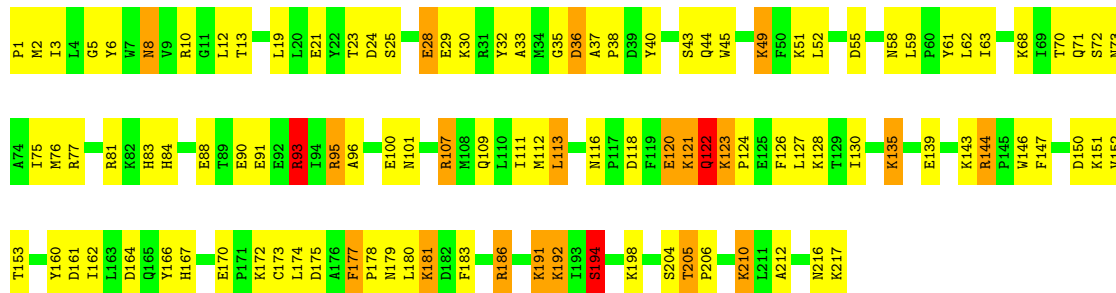
3 Residue-property plots

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.

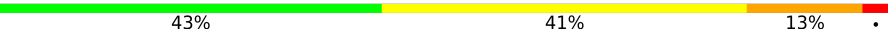
Note EDS was not executed.

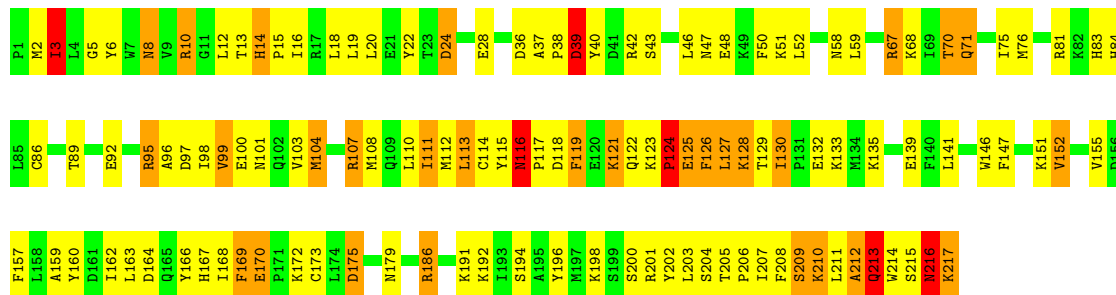
• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain A: 



• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.24Å 69.44Å 81.28Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4096	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: GTD, 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	1.27	4/1867 (0.2%)	2.18	80/2515 (3.2%)
1	B	1.34	8/1867 (0.4%)	2.26	104/2515 (4.1%)
All	All	1.30	12/3734 (0.3%)	2.22	184/5030 (3.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	LEU	CA-C	6.88	1.60	1.52
1	B	130	ILE	CA-CB	6.79	1.57	1.54
1	A	96	ALA	N-CA	6.56	1.54	1.46
1	A	130	ILE	CA-CB	6.07	1.57	1.54
1	B	100	GLU	N-CA	5.94	1.53	1.46
1	B	103	VAL	N-CA	5.77	1.53	1.46
1	B	201	ARG	N-CA	5.74	1.53	1.46
1	A	167	HIS	N-CA	5.63	1.53	1.46
1	B	163	LEU	N-CA	5.62	1.53	1.46
1	B	160	TYR	N-CA	5.33	1.52	1.46
1	B	96	ALA	N-CA	5.10	1.52	1.46
1	B	98	ILE	CA-CB	5.02	1.60	1.54

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	GLN	OE1-CD-NE2	-12.56	110.04	122.60
1	A	95	ARG	O-C-N	11.16	133.95	122.12
1	B	58	ASN	OD1-CG-ND2	-10.80	111.80	122.60
1	B	84	HIS	CA-CB-CG	-10.38	103.42	113.80
1	B	67	ARG	CD-NE-CZ	9.91	138.28	124.40
1	A	162	ILE	O-C-N	8.95	131.04	121.83
1	A	58	ASN	OD1-CG-ND2	-8.78	113.82	122.60
1	B	3	ILE	N-CA-CB	8.75	123.49	111.41
1	A	194	SER	N-CA-CB	8.58	122.74	110.12
1	B	99	VAL	O-C-N	8.42	130.16	121.91
1	B	159	ALA	CA-C-O	-8.27	111.65	120.42
1	B	107	ARG	CG-CD-NE	8.25	130.16	112.00
1	A	162	ILE	CA-C-O	-8.21	112.14	120.85
1	B	200	SER	CA-C-O	-8.08	108.77	119.11
1	A	95	ARG	CA-C-N	-7.99	110.05	120.44
1	A	95	ARG	C-N-CA	-7.99	110.05	120.44
1	B	155	VAL	CA-C-O	-7.84	112.00	120.47
1	A	166	TYR	O-C-N	7.82	131.06	122.15
1	A	70	THR	N-CA-CB	7.81	123.86	111.43
1	B	59	LEU	O-C-N	7.69	128.24	121.39
1	A	95	ARG	CA-C-O	-7.60	112.49	120.55
1	A	52	LEU	N-CA-C	7.58	122.72	113.17
1	B	159	ALA	O-C-N	7.55	130.76	122.15
1	B	71	GLN	CB-CG-CD	7.48	125.31	112.60
1	A	96	ALA	O-C-N	-7.43	114.41	122.07
1	B	100	GLU	CB-CA-C	7.30	122.49	110.81
1	A	120	GLU	CB-CG-CD	7.26	124.95	112.60
1	B	196	TYR	CA-C-O	-7.24	112.88	120.55
1	B	127	LEU	N-CA-C	-7.21	104.36	113.01
1	B	39	ASP	N-CA-C	7.19	120.16	111.82
1	B	59	LEU	CA-C-O	-7.17	112.38	119.69
1	B	200	SER	O-C-N	7.15	132.87	122.43
1	B	67	ARG	NE-CZ-NH2	-7.14	112.78	119.20
1	B	166	TYR	N-CA-C	-7.12	103.56	111.82
1	B	6	TYR	CA-C-N	7.04	131.39	120.75
1	B	6	TYR	C-N-CA	7.04	131.39	120.75
1	B	167	HIS	CA-C-N	7.02	130.78	120.74
1	B	167	HIS	C-N-CA	7.02	130.78	120.74
1	A	147	PHE	N-CA-C	7.00	118.91	111.28
1	B	101	ASN	CA-CB-CG	-6.98	105.62	112.60
1	B	201	ARG	CD-NE-CZ	6.94	134.12	124.40
1	B	70	THR	CA-C-O	-6.93	113.54	121.58
1	B	46	LEU	CB-CA-C	6.93	122.29	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	LEU	CB-CA-C	6.90	121.59	110.96
1	B	68	LYS	CA-C-O	-6.84	112.98	120.30
1	A	13	THR	CA-CB-OG1	-6.81	99.38	109.60
1	A	84	HIS	CA-CB-CG	-6.78	107.02	113.80
1	B	130	ILE	O-C-N	6.74	124.73	120.42
1	B	14	HIS	CA-C-O	6.72	124.86	118.34
1	B	89	THR	CA-CB-OG1	-6.71	99.54	109.60
1	A	175	ASP	CA-CB-CG	-6.70	105.90	112.60
1	B	111	ILE	N-CA-CB	6.70	118.84	110.47
1	A	147	PHE	CA-C-O	-6.69	113.46	120.55
1	A	183	PHE	CA-C-O	-6.66	113.36	120.42
1	B	104	MET	CB-CA-C	6.65	121.45	110.81
1	B	24	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	109	GLN	OE1-CD-NE2	-6.62	115.98	122.60
1	A	175	ASP	CB-CA-C	6.61	121.39	110.81
1	B	157	PHE	CA-C-O	6.55	127.49	120.55
1	A	29	GLU	CG-CD-OE2	-6.48	103.50	118.40
1	A	81	ARG	CD-NE-CZ	6.42	133.39	124.40
1	B	16	ILE	O-C-N	6.38	128.54	121.90
1	B	132	GLU	CB-CG-CD	6.36	123.41	112.60
1	B	164	ASP	CA-C-N	6.35	128.79	120.28
1	B	164	ASP	C-N-CA	6.35	128.79	120.28
1	B	42	ARG	CG-CD-NE	6.33	125.93	112.00
1	A	183	PHE	O-C-N	6.32	129.35	122.15
1	A	21	GLU	CA-C-N	6.30	128.72	120.28
1	A	21	GLU	C-N-CA	6.30	128.72	120.28
1	B	130	ILE	N-CA-C	6.28	120.52	112.67
1	B	101	ASN	CB-CG-ND2	6.27	125.81	116.40
1	B	18	LEU	N-CA-C	6.26	118.11	111.28
1	A	147	PHE	O-C-N	6.22	128.72	122.12
1	A	96	ALA	CA-C-O	6.20	127.33	120.82
1	B	155	VAL	O-C-N	6.20	128.80	121.80
1	B	162	ILE	CA-C-O	-6.17	114.31	120.85
1	A	70	THR	CA-C-O	-6.17	114.42	121.58
1	B	67	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	B	163	LEU	N-CA-C	-6.14	104.67	111.36
1	B	175	ASP	CB-CA-C	6.12	121.96	110.63
1	B	126	PHE	N-CA-C	-6.08	104.22	111.69
1	A	6	TYR	CA-C-N	6.04	131.08	120.87
1	A	6	TYR	C-N-CA	6.04	131.08	120.87
1	B	162	ILE	O-C-N	6.04	128.05	121.83
1	A	153	THR	CA-CB-OG1	-6.00	100.60	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	SER	N-CA-C	5.97	119.39	111.75
1	A	5	GLY	CA-C-O	-5.97	114.79	120.64
1	A	71	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	73	ASN	CA-C-N	-5.96	111.26	120.31
1	A	73	ASN	C-N-CA	-5.96	111.26	120.31
1	A	120	GLU	N-CA-C	5.94	118.54	111.71
1	A	166	TYR	CA-C-O	-5.93	114.13	120.42
1	A	101	ASN	N-CA-C	5.92	118.69	111.82
1	B	75	ILE	O-C-N	5.91	127.60	121.87
1	B	70	THR	N-CA-CB	5.90	120.81	111.43
1	B	152	VAL	N-CA-CB	5.88	119.31	110.13
1	A	83	HIS	CA-CB-CG	-5.88	107.92	113.80
1	B	83	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	52	LEU	N-CA-CB	-5.87	101.81	110.49
1	B	147	PHE	CA-C-O	-5.86	113.48	120.10
1	B	179	ASN	CA-C-O	-5.85	113.49	120.10
1	B	92	GLU	CG-CD-OE1	5.84	131.84	118.40
1	A	177	PHE	N-CA-C	5.84	119.88	108.21
1	B	70	THR	O-C-N	5.83	130.93	122.94
1	A	186	ARG	CA-CB-CG	5.82	125.73	114.10
1	A	186	ARG	N-CA-C	5.80	117.61	111.28
1	B	95	ARG	CD-NE-CZ	5.80	132.52	124.40
1	B	50	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	43	SER	N-CA-C	5.79	117.59	111.28
1	B	58	ASN	O-C-N	5.75	129.02	123.04
1	B	100	GLU	O-C-N	-5.71	116.15	122.09
1	B	179	ASN	O-C-N	5.70	128.89	122.22
1	B	10	ARG	O-C-N	5.68	127.94	122.03
1	A	58	ASN	N-CA-CB	-5.68	102.03	111.57
1	B	107	ARG	N-CA-CB	-5.64	101.83	110.01
1	A	23	THR	CA-C-O	-5.63	112.47	119.28
1	B	3	ILE	CA-C-O	-5.63	114.48	120.39
1	B	48	GLU	O-C-N	5.62	129.00	122.19
1	A	51	LYS	N-CA-C	5.62	120.83	113.30
1	B	28	GLU	CA-CB-CG	5.57	125.24	114.10
1	A	21	GLU	O-C-N	-5.55	116.35	122.07
1	B	157	PHE	O-C-N	-5.54	116.25	122.12
1	B	20	LEU	N-CA-C	-5.50	105.19	111.07
1	B	43	SER	CA-C-O	-5.49	114.06	120.20
1	A	38	PRO	N-CD-CG	-5.48	97.23	103.80
1	B	14	HIS	CA-C-N	5.47	124.92	119.24
1	B	14	HIS	C-N-CA	5.47	124.92	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASN	CB-CG-OD1	5.45	131.69	120.80
1	B	169	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	179	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	A	55	ASP	CB-CA-C	5.43	119.48	110.90
1	B	10	ARG	CA-C-O	-5.42	115.31	121.00
1	B	16	ILE	CA-C-O	-5.42	115.04	121.05
1	B	216	ASN	CA-CB-CG	-5.42	107.18	112.60
1	A	122	GLN	CB-CA-C	-5.38	100.86	110.70
1	A	172	LYS	N-CA-CB	-5.38	102.67	110.47
1	B	160	TYR	CA-C-O	5.37	126.64	120.90
1	A	173	CYS	CB-CA-C	5.37	121.53	110.31
1	B	152	VAL	O-C-N	5.36	128.45	122.61
1	A	121	LYS	CA-C-O	5.34	125.52	119.27
1	A	49	LYS	CA-C-O	5.34	126.40	120.63
1	B	28	GLU	CA-C-O	-5.33	114.87	121.11
1	B	198	LYS	CB-CA-C	-5.33	101.71	110.72
1	A	91	GLU	N-CA-CB	5.33	117.73	110.01
1	A	205	THR	CA-C-O	-5.30	115.62	120.50
1	A	179	ASN	CB-CG-ND2	-5.30	108.45	116.40
1	A	181	LYS	CA-C-N	5.29	127.37	120.28
1	A	181	LYS	C-N-CA	5.29	127.37	120.28
1	B	147	PHE	N-CA-C	5.29	117.79	111.71
1	B	68	LYS	O-C-N	5.29	129.40	123.27
1	A	113	LEU	O-C-N	5.27	127.78	122.09
1	B	81	ARG	NH1-CZ-NH2	-5.25	112.48	119.30
1	B	71	GLN	CA-CB-CG	-5.22	103.66	114.10
1	A	72	SER	O-C-N	-5.21	116.59	122.12
1	B	76	MET	O-C-N	-5.21	116.70	122.07
1	B	213	GLN	CB-CA-C	-5.21	102.58	111.02
1	B	47	ASN	CA-C-O	-5.21	114.37	120.20
1	B	116	ASN	N-CA-C	-5.20	102.46	110.32
1	B	194	SER	CA-CB-OG	-5.20	100.69	111.10
1	A	180	LEU	O-C-N	5.20	128.46	122.17
1	A	62	LEU	CA-C-O	-5.19	114.73	120.24
1	A	70	THR	O-C-N	5.19	130.05	122.94
1	B	50	PHE	CB-CA-C	5.17	119.46	110.94
1	B	141	LEU	O-C-N	5.16	127.67	122.09
1	B	48	GLU	CA-C-O	-5.15	113.40	119.48
1	A	153	THR	CA-C-O	-5.13	115.70	121.40
1	B	98	ILE	O-C-N	5.13	126.94	121.91
1	A	160	TYR	CA-C-O	5.13	126.71	121.07
1	B	52	LEU	CA-C-O	-5.12	113.32	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	GLY	CA-C-O	-5.12	116.27	120.92
1	A	75	ILE	CA-CB-CG1	-5.11	101.71	110.40
1	A	135	LYS	CA-C-O	5.11	125.97	120.55
1	A	191	LYS	CA-C-O	-5.11	115.43	120.90
1	A	95	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	B	22	TYR	CB-CA-C	5.10	118.96	110.81
1	B	97	ASP	CA-C-O	5.09	126.35	120.90
1	A	61	TYR	CA-C-O	-5.08	115.16	121.11
1	A	161	ASP	OD1-CG-OD2	-5.08	110.71	122.90
1	A	107	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	107	ARG	CD-NE-CZ	5.07	131.50	124.40
1	B	107	ARG	CB-CA-C	5.07	118.84	110.88
1	B	119	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	164	ASP	CB-CA-C	5.05	118.80	110.88
1	A	71	GLN	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	186	ARG	Sidechain

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	1818	0	1805	54	4
1	B	1818	0	1805	99	4
2	A	20	0	0	0	0
2	B	10	0	0	3	0
3	A	35	0	18	1	0
3	B	35	0	17	2	0
4	A	210	0	0	4	0
4	B	150	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4096	0	3645	153	4

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 21.

All (153) 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:123:LYS:O	1:B:127:LEU:HG	1.55	1.06
1:B:127:LEU:HA	1:B:130:ILE:HD12	1.48	0.95
1:B:125:GLU:OE1	1:B:128:LYS:HE2	1.68	0.93
1:A:107:ARG:O	1:A:111:ILE:HD12	1.69	0.90
1:A:191:LYS:HE3	1:A:192:LYS:HZ2	1.36	0.90
1:B:168:ILE:HG22	1:B:214:TRP:HZ2	1.40	0.86
1:B:111:ILE:HD11	3:B:220:GTD:O42	1.77	0.85
1:B:122:GLN:C	1:B:124:PRO:HD2	2.04	0.83
1:B:119:PHE:CE2	1:B:214:TRP:HB2	2.16	0.80
1:B:111:ILE:HG23	1:B:115:TYR:CD1	2.19	0.78
1:B:119:PHE:HB2	1:B:213:GLN:HG3	1.67	0.77
1:A:191:LYS:CE	1:A:192:LYS:HZ2	2.00	0.73
1:A:8:ASN:HD22	1:A:8:ASN:H	1.37	0.73
1:B:186:ARG:HG3	2:B:219:SO4:O1	1.90	0.72
1:A:191:LYS:HE3	1:A:192:LYS:NZ	2.05	0.71
1:B:123:LYS:HG3	1:B:169:PHE:CZ	2.26	0.71
1:A:122:GLN:NE2	1:A:122:GLN:HA	2.06	0.71
1:B:209:SER:C	1:B:211:LEU:H	1.97	0.70
1:B:24:ASP:HB2	1:B:192:LYS:NZ	2.08	0.69
1:B:209:SER:C	1:B:211:LEU:N	2.51	0.68
1:B:113:LEU:HD21	1:B:169:PHE:CZ	2.29	0.67
1:A:8:ASN:HD22	1:A:8:ASN:N	1.93	0.66
1:A:77:ARG:NH2	1:A:100:GLU:OE1	2.28	0.66
1:B:111:ILE:HG13	1:B:208:PHE:HE1	1.61	0.66
1:B:111:ILE:HG13	1:B:208:PHE:CE1	2.31	0.65
1:B:209:SER:O	1:B:211:LEU:N	2.29	0.65
1:B:207:ILE:HG13	1:B:215:SER:OG	1.97	0.65
1:A:113:LEU:HD22	1:A:126:PHE:CG	2.33	0.64
1:A:191:LYS:CE	1:A:192:LYS:NZ	2.61	0.64
1:A:90:GLU:OE1	1:A:93:ARG:NH2	2.22	0.64
1:B:108:MET:O	1:B:112:MET:HG3	1.96	0.63
1:B:135:LYS:O	1:B:139:GLU:HG3	1.98	0.63
1:B:2:MET:C	1:B:3:ILE:HD12	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:HB2	1:B:213:GLN:CG	2.29	0.61
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.36	0.61
1:B:8:ASN:HD22	1:B:8:ASN:N	1.99	0.61
1:A:1:PRO:HG2	1:A:28:GLU:HG2	1.83	0.60
1:B:107:ARG:O	1:B:111:ILE:HD12	2.02	0.60
1:B:24:ASP:CB	1:B:192:LYS:NZ	2.64	0.59
1:B:172:LYS:HD2	1:B:175:ASP:OD2	2.02	0.59
1:A:123:LYS:HD3	1:A:127:LEU:HD11	1.85	0.59
1:A:35:GLY:O	1:A:40:TYR:HA	2.03	0.58
1:B:118:ASP:O	1:B:121:LYS:HB2	2.03	0.58
1:B:123:LYS:N	1:B:124:PRO:CD	2.66	0.58
1:B:123:LYS:N	1:B:124:PRO:HD2	2.19	0.58
1:A:191:LYS:NZ	1:A:192:LYS:NZ	2.52	0.57
1:B:118:ASP:HB3	1:B:121:LYS:HB2	1.85	0.57
1:B:208:PHE:HE2	1:B:214:TRP:CZ3	2.22	0.57
1:B:3:ILE:HD12	1:B:3:ILE:N	2.20	0.56
1:B:113:LEU:HD22	1:B:126:PHE:CD2	2.39	0.56
1:A:1:PRO:CG	1:A:28:GLU:HG2	2.35	0.56
1:A:30:LYS:NZ	4:A:312:HOH:O	2.34	0.56
1:A:121:LYS:NZ	4:A:388:HOH:O	2.39	0.56
1:B:24:ASP:HB2	1:B:192:LYS:HZ1	1.71	0.55
1:B:70:THR:O	1:B:71:GLN:HB2	2.07	0.55
1:B:119:PHE:HZ	1:B:169:PHE:HE2	1.55	0.55
1:B:122:GLN:C	1:B:124:PRO:CD	2.76	0.55
1:A:194:SER:O	1:A:198:LYS:HD2	2.06	0.55
1:A:36:ASP:HB3	4:A:407:HOH:O	2.07	0.55
1:B:125:GLU:HA	1:B:128:LYS:HB2	1.89	0.55
1:B:168:ILE:HG22	1:B:214:TRP:CZ2	2.31	0.55
1:B:129:THR:OG1	1:B:133:LYS:HE2	2.06	0.54
1:B:8:ASN:HD22	1:B:8:ASN:H	1.54	0.54
1:B:118:ASP:HB3	1:B:121:LYS:HD3	1.90	0.54
1:B:186:ARG:CD	2:B:219:SO4:O1	2.55	0.54
1:A:135:LYS:NZ	1:A:139:GLU:OE2	2.30	0.54
1:B:168:ILE:CG2	1:B:214:TRP:HZ2	2.17	0.54
1:B:119:PHE:CZ	1:B:169:PHE:HE2	2.26	0.54
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.90	0.53
1:A:77:ARG:CZ	1:A:100:GLU:OE1	2.57	0.53
1:B:111:ILE:HD11	3:B:220:GTD:N4'	2.24	0.52
1:A:8:ASN:H	1:A:8:ASN:ND2	2.06	0.52
1:B:212:ALA:C	1:B:213:GLN:NE2	2.69	0.50
1:B:123:LYS:CG	1:B:169:PHE:CZ	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:OE1	1:A:151:LYS:NZ	2.45	0.50
1:B:202:TYR:CE2	1:B:204:SER:HB3	2.46	0.50
1:B:14:HIS:N	1:B:15:PRO:CD	2.75	0.49
1:B:127:LEU:CD2	1:B:169:PHE:CE1	2.95	0.49
1:B:118:ASP:CG	1:B:121:LYS:HD3	2.37	0.49
1:B:208:PHE:HE2	1:B:214:TRP:HZ3	1.61	0.49
1:A:37:ALA:HB2	1:A:40:TYR:CZ	2.48	0.49
1:A:124:PRO:O	1:A:128:LYS:HD2	2.12	0.49
1:B:146:TRP:CE2	1:B:152:VAL:HG22	2.47	0.49
1:B:125:GLU:HA	1:B:128:LYS:HD3	1.94	0.48
1:B:186:ARG:CG	2:B:219:SO4:O1	2.59	0.48
1:A:2:MET:CE	1:A:25:SER:HB3	2.43	0.48
1:B:86:CYS:O	1:B:151:LYS:HE2	2.13	0.48
1:A:122:GLN:NE2	1:A:122:GLN:CA	2.76	0.48
1:B:37:ALA:HB1	1:B:38:PRO:HA	1.95	0.48
1:B:126:PHE:C	1:B:128:LYS:N	2.70	0.48
1:B:107:ARG:O	1:B:111:ILE:CD1	2.62	0.48
1:A:146:TRP:CE2	1:A:152:VAL:HG22	2.49	0.47
1:B:12:LEU:C	1:B:12:LEU:HD12	2.39	0.47
1:B:127:LEU:HD23	1:B:169:PHE:HE1	1.80	0.47
1:A:212:ALA:HB3	1:A:216:ASN:HB3	1.95	0.47
1:A:191:LYS:NZ	1:A:192:LYS:HZ2	2.11	0.47
1:B:210:LYS:H	1:B:210:LYS:HG3	1.51	0.47
1:A:118:ASP:O	1:A:122:GLN:HB2	2.14	0.47
1:B:118:ASP:CB	1:B:121:LYS:HD3	2.45	0.46
1:B:119:PHE:CD2	1:B:213:GLN:HB2	2.50	0.46
1:B:202:TYR:CZ	1:B:204:SER:HB3	2.50	0.46
1:A:111:ILE:HD11	3:A:222:GTD:O42	2.16	0.46
1:B:130:ILE:HG21	1:B:173:CYS:HB2	1.97	0.46
1:B:168:ILE:HD13	1:B:207:ILE:HD11	1.97	0.46
1:A:107:ARG:HG2	1:A:111:ILE:CD1	2.46	0.46
1:B:119:PHE:CD2	1:B:213:GLN:O	2.69	0.46
1:B:205:THR:HB	1:B:206:PRO:HA	1.97	0.46
1:A:24:ASP:OD2	1:A:192:LYS:HE2	2.16	0.46
1:B:116:ASN:OD1	1:B:117:PRO:HD2	2.16	0.45
1:A:8:ASN:N	1:A:8:ASN:ND2	2.63	0.45
1:A:123:LYS:O	1:A:127:LEU:HG	2.16	0.45
1:B:24:ASP:CG	1:B:192:LYS:NZ	2.75	0.45
1:A:205:THR:HA	1:A:206:PRO:C	2.41	0.45
1:A:3:ILE:HD12	1:A:3:ILE:N	2.32	0.45
1:B:127:LEU:HD21	1:B:169:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:NH2	1:A:144:ARG:NE	2.64	0.45
1:A:146:TRP:CE2	1:A:152:VAL:CG2	3.00	0.45
1:B:3:ILE:N	1:B:3:ILE:CD1	2.79	0.45
1:B:127:LEU:CD2	1:B:169:PHE:HE1	2.29	0.44
1:B:111:ILE:O	1:B:111:ILE:HG22	2.16	0.44
1:A:210:LYS:HD2	4:A:386:HOH:O	2.17	0.44
1:A:116:ASN:OD1	1:A:118:ASP:N	2.37	0.44
1:B:24:ASP:CG	1:B:192:LYS:HZ3	2.25	0.44
1:B:114:CYS:HA	1:B:119:PHE:CD1	2.53	0.44
1:B:119:PHE:HE2	1:B:214:TRP:HB2	1.78	0.44
1:B:125:GLU:C	1:B:128:LYS:HB2	2.42	0.44
1:A:123:LYS:N	1:A:124:PRO:CD	2.80	0.44
1:A:76:MET:HE3	1:A:76:MET:HB3	1.86	0.43
1:A:63:ILE:HD12	1:A:68:LYS:HG2	1.99	0.43
1:B:216:ASN:HD22	1:B:216:ASN:C	2.26	0.43
1:B:130:ILE:CG2	1:B:173:CYS:HB2	2.48	0.43
1:B:39:ASP:O	1:B:40:TYR:HB2	2.18	0.43
1:B:95:ARG:O	1:B:99:VAL:HG23	2.19	0.43
1:A:30:LYS:HD3	1:A:32:TYR:CZ	2.54	0.43
1:A:10:ARG:HD2	1:A:204:SER:O	2.20	0.42
1:B:127:LEU:HD23	1:B:169:PHE:CE1	2.53	0.42
1:A:32:TYR:HD2	1:A:44:GLN:HG2	1.84	0.42
1:B:126:PHE:C	1:B:128:LYS:H	2.25	0.42
1:B:215:SER:OG	1:B:215:SER:O	2.33	0.41
1:A:33:ALA:H	1:A:44:GLN:NE2	2.19	0.41
1:B:125:GLU:O	1:B:128:LYS:HB2	2.20	0.41
1:A:1:PRO:HG2	1:A:28:GLU:CG	2.50	0.41
1:B:170:GLU:OE1	1:B:170:GLU:C	2.63	0.41
1:B:114:CYS:HA	1:B:119:PHE:CE1	2.55	0.41
1:B:127:LEU:HA	1:B:130:ILE:CD1	2.34	0.41
1:B:207:ILE:H	1:B:215:SER:HG	1.69	0.41
1:A:12:LEU:HB3	1:A:107:ARG:HD3	2.03	0.41
1:B:113:LEU:HD22	1:B:126:PHE:CE2	2.55	0.41
1:B:146:TRP:CD2	1:B:152:VAL:HG22	2.56	0.41
1:A:177:PHE:HA	1:A:178:PRO:HD2	1.84	0.40
1:B:119:PHE:CG	1:B:213:GLN:HB2	2.56	0.40
1:B:13:THR:O	1:B:13:THR:HG22	2.21	0.40
1:B:104:MET:O	1:B:108:MET:HG2	2.22	0.40

All (4) 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)
1:A:191:LYS:NZ	1:B:117:PRO:C[3_455]	1.87	0.33
1:A:88:GLU:OE2	1:B:217:LYS:NZ[3_455]	2.11	0.09
1:A:191:LYS:NZ	1:B:118:ASP:N[3_455]	2.14	0.06
1:A:191:LYS:NZ	1:B:117:PRO:O[3_455]	2.18	0.02

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	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
1	B	215/217 (99%)	202 (94%)	10 (5%)	3 (1%)	9	3
All	All	430/434 (99%)	411 (96%)	16 (4%)	3 (1%)	18	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	LYS
1	B	124	PRO
1	B	212	ALA

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	197/197 (100%)	179 (91%)	18 (9%)	9	3
1	B	197/197 (100%)	177 (90%)	20 (10%)	7	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	394/394 (100%)	356 (90%)	38 (10%)	8 3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	LEU
1	A	28	GLU
1	A	36	ASP
1	A	93	ARG
1	A	112	MET
1	A	120	GLU
1	A	122	GLN
1	A	123	LYS
1	A	143	LYS
1	A	150	ASP
1	A	170	GLU
1	A	174	LEU
1	A	181	LYS
1	A	192	LYS
1	A	194	SER
1	A	210	LYS
1	A	217	LYS
1	B	3	ILE
1	B	8	ASN
1	B	19	LEU
1	B	36	ASP
1	B	39	ASP
1	B	51	LYS
1	B	67	ARG
1	B	113	LEU
1	B	116	ASN
1	B	121	LYS
1	B	124	PRO
1	B	125	GLU
1	B	128	LYS
1	B	170	GLU
1	B	191	LYS
1	B	203	LEU
1	B	209	SER
1	B	213	GLN
1	B	216	ASN

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Mol	Chain	Res	Type
1	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	44	GLN
1	A	122	GLN
1	B	8	ASN
1	B	122	GLN
1	B	213	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](#)

8 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	SO4	A	220	-	4,4,4	0.94	0	6,6,6	0.47	0
2	SO4	A	219	-	4,4,4	0.82	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	219	-	4,4,4	1.00	0	6,6,6	0.61	0
3	GTD	A	222	-	28,35,35	2.09	5 (17%)	21,48,48	1.86	6 (28%)
3	GTD	B	220	-	28,35,35	1.83	5 (17%)	21,48,48	0.96	1 (4%)
2	SO4	A	221	-	4,4,4	0.95	0	6,6,6	0.58	0
2	SO4	B	218	-	4,4,4	0.93	0	6,6,6	0.75	0
2	SO4	A	218	-	4,4,4	0.89	0	6,6,6	0.23	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	GTD	A	222	-	-	2/31/55/55	0/1/1/1
3	GTD	B	220	-	-	2/31/55/55	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	222	GTD	CB2-SG2	-6.41	1.75	1.82
3	B	220	GTD	CB2-SG2	-5.07	1.77	1.82
3	A	222	GTD	C1'-SG2	-4.27	1.74	1.83
3	B	220	GTD	C4'-C3'	-3.98	1.39	1.50
3	B	220	GTD	C4'-C5'	-3.94	1.39	1.50
3	A	222	GTD	C4'-C5'	-3.69	1.40	1.50
3	A	222	GTD	C4'-C3'	-3.17	1.41	1.50
3	B	220	GTD	C1'-SG2	-2.74	1.78	1.83
3	B	220	GTD	OE1-CD1	2.52	1.28	1.23
3	A	222	GTD	O12-C1	2.24	1.37	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	222	GTD	CG1-CB1-CA1	-3.64	105.50	113.86
3	A	222	GTD	CB1-CA1-C1	3.34	119.31	110.45
3	A	222	GTD	O2-C2-N3	2.77	128.84	122.98
3	A	222	GTD	CG1-CD1-N2	2.74	120.69	115.86
3	A	222	GTD	O12-C1-O11	-2.41	118.61	124.08
3	A	222	GTD	OE1-CD1-N2	-2.09	119.42	122.95
3	B	220	GTD	O12-C1-O11	-2.07	119.39	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

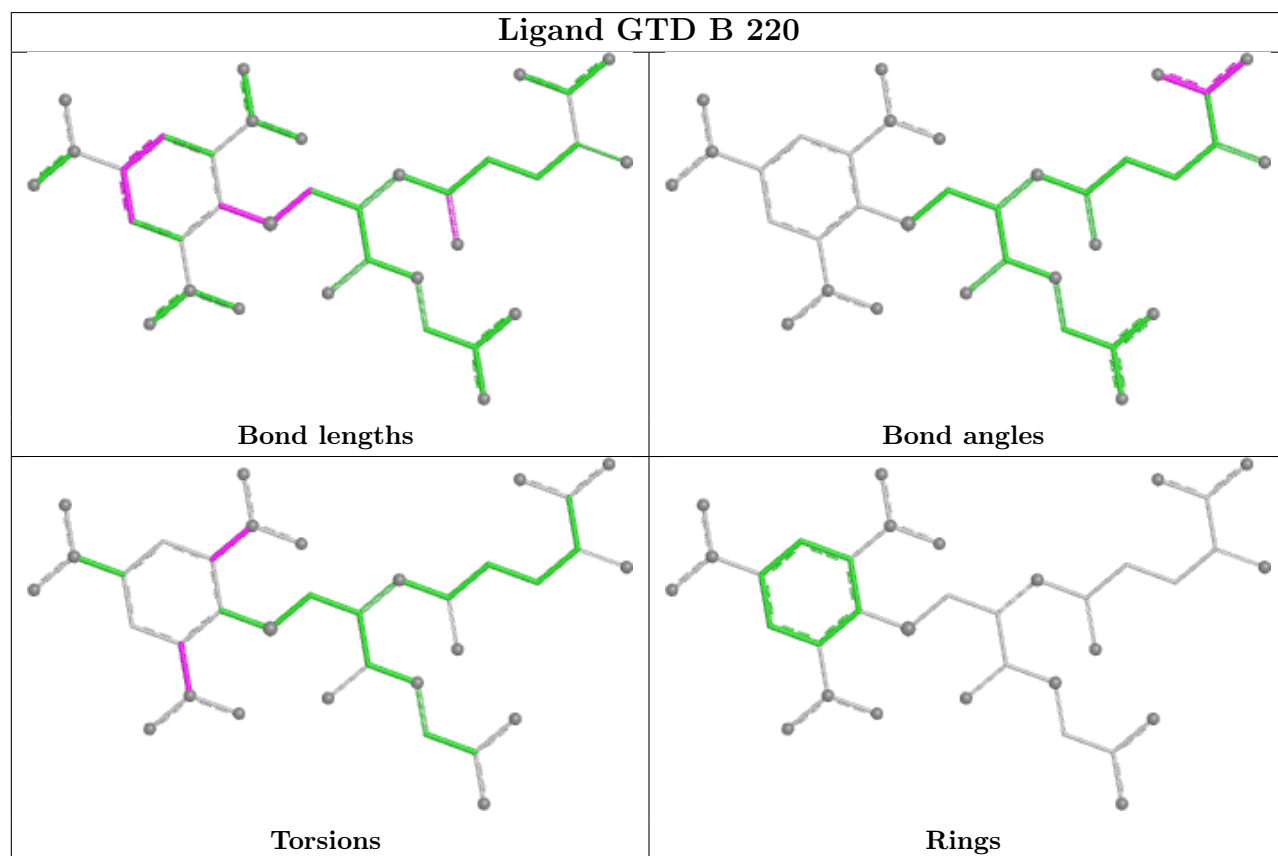
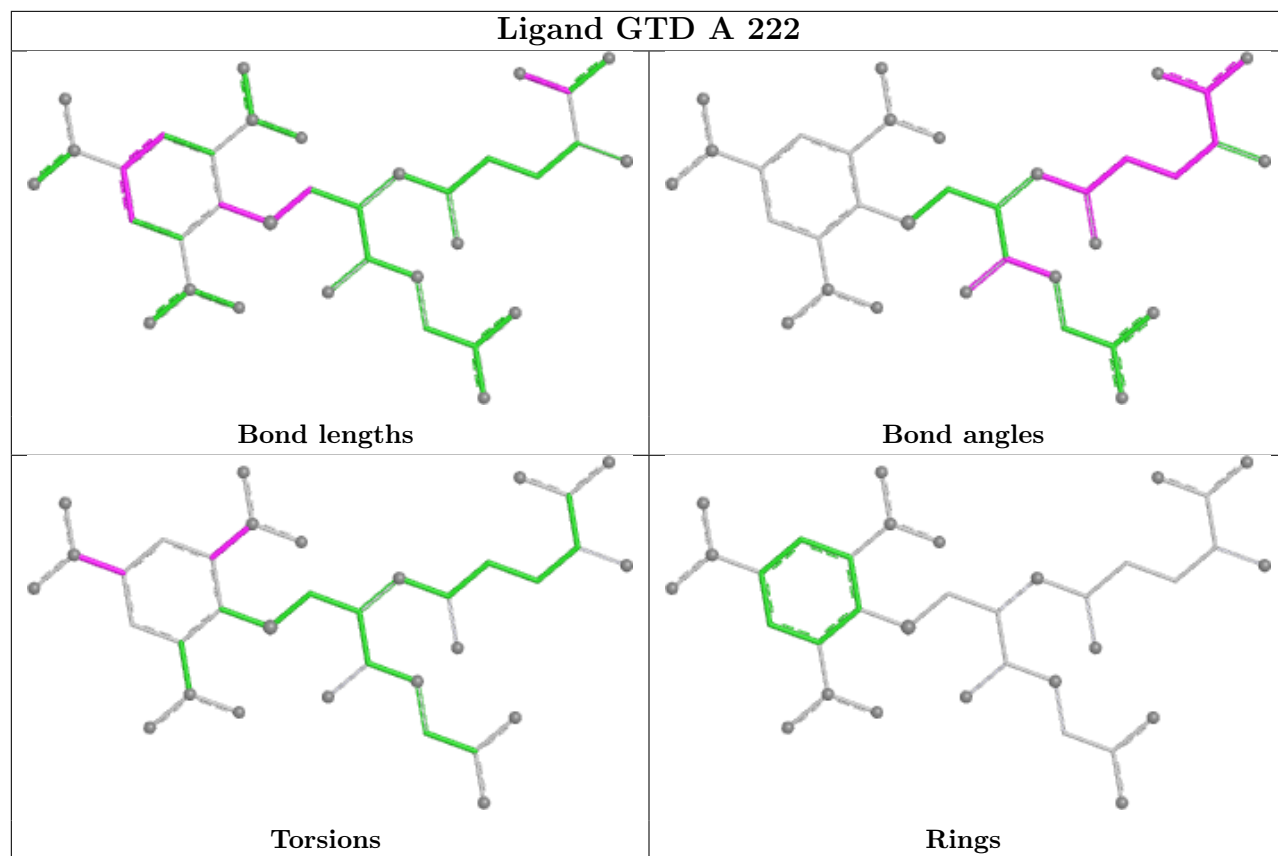
Mol	Chain	Res	Type	Atoms
3	B	220	GTD	C3'-C2'-N2'-O21
3	B	220	GTD	C5'-C6'-N6'-O61
3	A	222	GTD	C5'-C4'-N4'-O41
3	A	222	GTD	C3'-C2'-N2'-O21

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	219	SO4	3	0
3	A	222	GTD	1	0
3	B	220	GTD	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.



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.