



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:54 AM UTC

PDB ID : 5GST / pdb_00005gst
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 : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

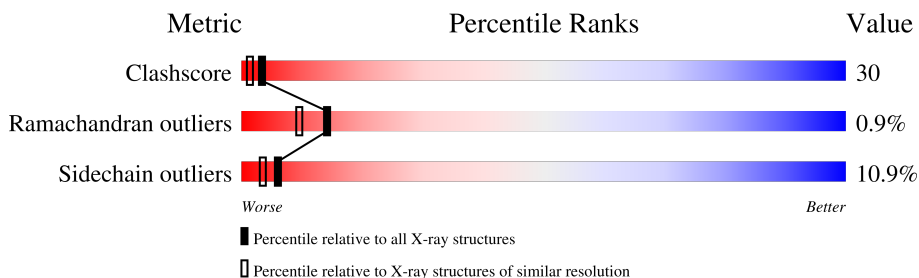
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

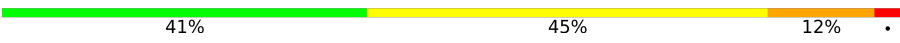
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	 41% 45% 12% .
1	B	217	 37% 41% 18% .

2 Entry composition [i](#)

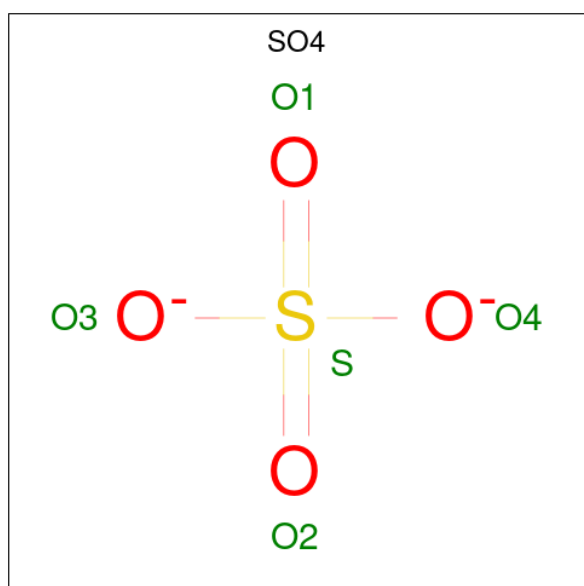
There are 4 unique types of molecules in this entry. The entry contains 4037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

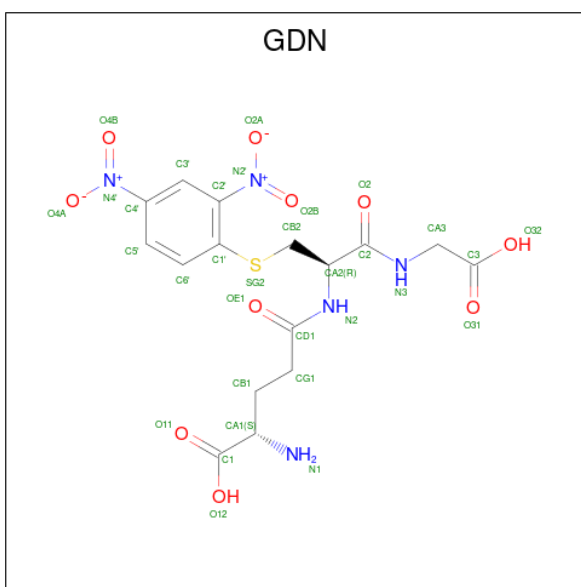
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			
1	B	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			

- 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		

- Molecule 3 is GLUTATHIONE S-(2,4 DINITROBENZENE) (CCD ID: GDN) (formula: C₁₆H₁₉N₅O₁₀S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 16	N 5	O 10	S 1	0	0
3	B	1	Total 32	C 16	N 5	O 10	S 1	0	0

- Molecule 4 is water.

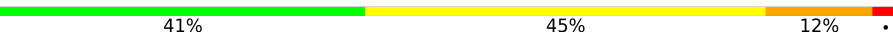
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	198	Total O 198 198	0	0
4	B	134	Total O 134 134	0	0

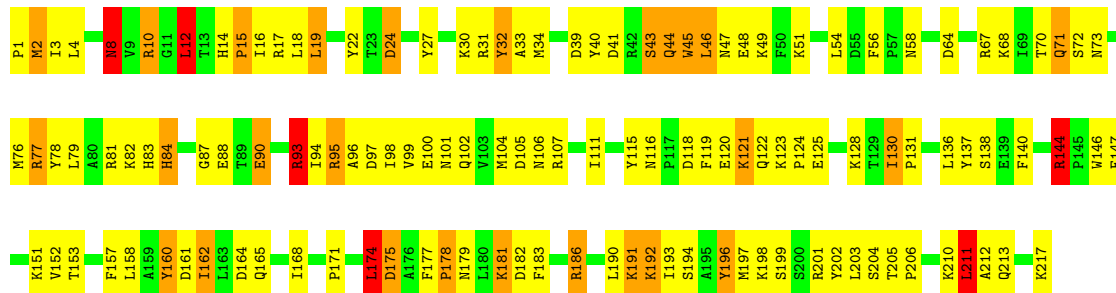
3 Residue-property plots

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.

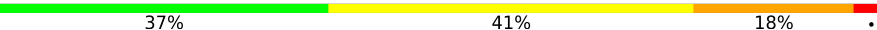
Note EDS was not executed.

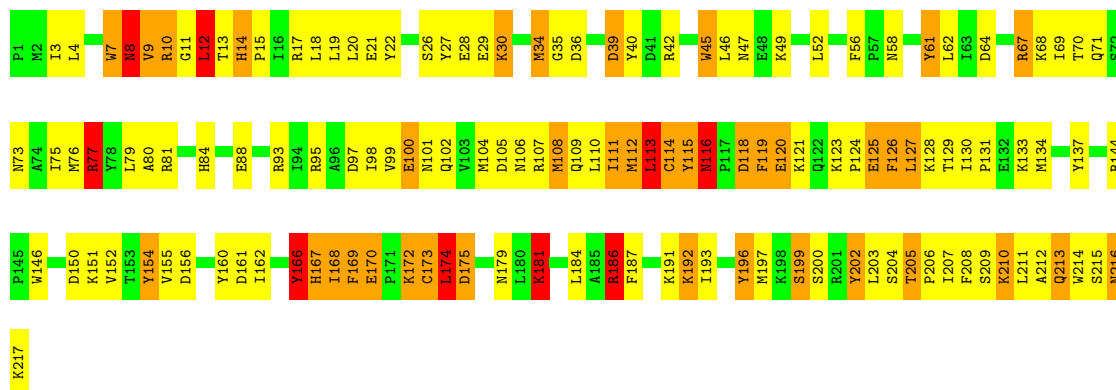
• Molecule 1: GLUTATHIONE S-TRANSFERASE

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) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4037	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: GDN, 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	1.40	8/1867 (0.4%)	2.32	105/2515 (4.2%)
1	B	1.35	7/1867 (0.4%)	2.53	125/2515 (5.0%)
All	All	1.37	15/3734 (0.4%)	2.43	230/5030 (4.6%)

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	3
All	All	0	6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ILE	CA-CB	10.80	1.59	1.54
1	B	156	ASP	N-CA	7.21	1.55	1.46
1	A	17	ARG	N-CA	6.82	1.54	1.46
1	A	136	LEU	N-CA	5.67	1.53	1.46
1	B	79	LEU	N-CA	5.56	1.53	1.46
1	A	162	ILE	C-N	-5.49	1.26	1.33
1	B	18	LEU	C-N	5.48	1.41	1.33
1	B	21	GLU	N-CA	5.47	1.53	1.46
1	B	187	PHE	N-CA	5.34	1.52	1.46
1	A	111	ILE	CA-CB	5.25	1.60	1.54
1	A	138	SER	N-CA	5.25	1.52	1.46
1	B	97	ASP	C-O	5.15	1.29	1.24
1	A	157	PHE	N-CA	5.08	1.52	1.46
1	A	16	ILE	C-N	-5.03	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	THR	CB-OG1	5.02	1.51	1.43

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ILE	CB-CG1-CD1	26.01	168.43	113.80
1	B	81	ARG	NE-CZ-NH1	19.16	140.66	121.50
1	B	93	ARG	CD-NE-CZ	17.84	149.37	124.40
1	A	71	GLN	OE1-CD-NE2	-13.19	109.41	122.60
1	B	17	ARG	NE-CZ-NH1	12.24	133.74	121.50
1	B	70	THR	CA-CB-OG1	-11.86	91.81	109.60
1	B	18	LEU	CA-C-O	11.85	133.11	120.55
1	B	58	ASN	OD1-CG-ND2	-11.73	110.87	122.60
1	A	160	TYR	CA-C-O	10.59	132.72	121.07
1	B	186	ARG	CD-NE-CZ	10.09	138.52	124.40
1	A	72	SER	O-C-N	-9.98	110.63	122.11
1	A	181	LYS	CB-CA-C	9.61	129.13	110.67
1	B	71	GLN	OE1-CD-NE2	-9.49	113.11	122.60
1	B	69	ILE	N-CA-C	9.34	121.93	108.48
1	A	43	SER	N-CA-C	9.18	122.27	111.71
1	B	20	LEU	O-C-N	9.06	131.72	122.12
1	B	26	SER	CB-CA-C	9.04	126.67	111.30
1	A	72	SER	CA-C-O	9.02	131.02	120.92
1	B	81	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	B	179	ASN	CA-C-O	-8.67	110.30	120.10
1	B	81	ARG	NH1-CZ-NH2	-8.66	108.04	119.30
1	A	196	TYR	CA-C-N	8.52	134.23	120.60
1	A	196	TYR	C-N-CA	8.52	134.23	120.60
1	A	58	ASN	OD1-CG-ND2	-8.51	114.09	122.60
1	B	101	ASN	CB-CG-ND2	8.42	129.03	116.40
1	A	107	ARG	CD-NE-CZ	8.39	136.14	124.40
1	B	160	TYR	CA-C-O	8.34	129.83	120.90
1	B	162	ILE	CA-C-O	-8.31	112.05	120.85
1	A	81	ARG	CD-NE-CZ	8.27	135.97	124.40
1	A	16	ILE	O-C-N	8.25	130.48	121.90
1	A	179	ASN	OD1-CG-ND2	8.24	130.84	122.60
1	A	73	ASN	N-CA-CB	8.23	122.35	110.16
1	B	116	ASN	O-C-N	8.14	128.23	121.31
1	A	147	PHE	N-CA-C	8.10	121.13	111.33
1	B	14	HIS	CA-C-O	7.99	126.56	118.73
1	A	174	LEU	N-CA-CB	-7.92	98.65	110.61
1	B	187	PHE	CA-C-O	7.90	128.84	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	71	GLN	CG-CD-NE2	7.75	128.02	116.40
1	B	102	GLN	O-C-N	7.74	130.45	122.09
1	B	58	ASN	CA-CB-CG	7.70	120.30	112.60
1	A	162	ILE	CA-C-N	7.69	130.92	120.38
1	A	162	ILE	C-N-CA	7.69	130.92	120.38
1	A	98	ILE	CA-C-O	7.65	129.28	121.17
1	B	97	ASP	CA-C-O	7.64	129.08	120.90
1	B	106	ASN	CA-C-O	-7.63	112.33	120.42
1	B	12	LEU	CB-CA-C	7.59	123.67	110.01
1	B	67	ARG	CA-CB-CG	7.57	129.24	114.10
1	A	77	ARG	CD-NE-CZ	-7.33	114.14	124.40
1	A	144	ARG	NE-CZ-NH1	7.31	128.81	121.50
1	A	105	ASP	O-C-N	7.26	129.55	122.07
1	A	138	SER	CA-C-O	7.16	128.34	120.82
1	B	156	ASP	N-CA-CB	-7.15	99.60	110.12
1	B	196	TYR	CA-C-N	7.15	132.05	120.60
1	B	196	TYR	C-N-CA	7.15	132.05	120.60
1	B	64	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	162	ILE	O-C-N	6.97	129.01	121.83
1	A	87	GLY	N-CA-C	-6.96	103.16	112.14
1	A	77	ARG	N-CA-CB	6.80	120.22	110.16
1	B	67	ARG	CD-NE-CZ	6.79	133.91	124.40
1	A	137	TYR	N-CA-CB	6.72	119.76	110.01
1	B	30	LYS	N-CA-CB	6.69	121.22	110.65
1	A	77	ARG	NE-CZ-NH2	6.68	125.21	119.20
1	B	154	TYR	CA-C-O	6.66	127.62	120.10
1	B	113	LEU	CA-C-O	6.65	130.26	120.42
1	A	168	ILE	CA-C-O	6.63	127.88	120.85
1	B	166	TYR	O-C-N	6.60	128.87	122.07
1	A	47	ASN	OD1-CG-ND2	6.60	129.20	122.60
1	A	160	TYR	O-C-N	-6.59	115.03	122.08
1	B	200	SER	CB-CA-C	-6.58	98.04	110.67
1	A	94	ILE	CA-C-O	6.57	127.82	120.85
1	B	169	PHE	CA-CB-CG	6.55	120.36	113.80
1	B	118	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	168	ILE	N-CA-C	-6.48	106.24	111.81
1	B	84	HIS	CB-CA-C	-6.45	102.16	112.09
1	B	62	LEU	CA-C-O	6.45	127.47	120.32
1	A	12	LEU	N-CA-CB	-6.43	100.90	110.61
1	A	165	GLN	CB-CA-C	-6.43	100.11	110.79
1	B	36	ASP	CA-CB-CG	-6.42	106.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ALA	CA-C-O	6.41	127.56	120.63
1	A	201	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	A	102	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	B	84	HIS	CA-C-N	6.39	134.06	123.25
1	B	84	HIS	C-N-CA	6.39	134.06	123.25
1	B	10	ARG	NE-CZ-NH1	-6.38	115.11	121.50
1	B	71	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	153	THR	OG1-CB-CG2	6.32	121.93	109.30
1	A	32	TYR	CA-C-O	-6.30	114.10	121.16
1	B	69	ILE	O-C-N	-6.28	116.39	123.18
1	B	58	ASN	O-C-N	6.27	129.56	123.29
1	A	177	PHE	CA-CB-CG	-6.26	107.54	113.80
1	B	100	GLU	CA-C-O	6.26	127.59	120.90
1	A	24	ASP	CA-CB-CG	-6.24	106.36	112.60
1	B	100	GLU	CB-CA-C	6.22	120.77	110.81
1	B	45	TRP	O-C-N	6.22	129.33	122.11
1	B	18	LEU	O-C-N	-6.21	115.54	122.12
1	B	106	ASN	O-C-N	6.20	129.22	122.15
1	A	174	LEU	CA-C-O	6.18	126.68	119.32
1	A	175	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	45	TRP	O-C-N	6.17	129.63	122.17
1	A	101	ASN	OD1-CG-ND2	-6.14	116.45	122.60
1	B	192	LYS	N-CA-CB	6.14	119.15	110.12
1	B	210	LYS	CA-CB-CG	6.14	126.38	114.10
1	A	17	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	B	137	TYR	N-CA-CB	6.10	118.85	110.01
1	A	194	SER	CA-C-N	6.07	128.41	120.28
1	A	194	SER	C-N-CA	6.07	128.41	120.28
1	A	90	GLU	CA-C-O	6.01	127.13	120.82
1	B	126	PHE	N-CA-C	-6.00	103.69	111.02
1	A	81	ARG	CA-C-N	6.00	128.33	120.28
1	A	81	ARG	C-N-CA	6.00	128.33	120.28
1	B	160	TYR	O-C-N	-6.00	115.85	122.09
1	A	96	ALA	N-CA-C	6.00	117.48	111.07
1	B	173	CYS	CB-CA-C	5.99	120.74	110.86
1	A	164	ASP	CB-CA-C	5.98	120.35	110.90
1	B	20	LEU	CA-C-O	-5.97	114.22	120.55
1	B	95	ARG	CA-C-N	5.97	128.60	120.54
1	B	95	ARG	C-N-CA	5.97	128.60	120.54
1	B	39	ASP	N-CA-C	5.96	119.81	112.54
1	B	161	ASP	N-CA-C	5.96	117.44	111.07
1	A	174	LEU	CB-CA-C	5.95	120.23	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASP	CB-CA-C	5.92	122.20	110.42
1	B	61	TYR	CA-C-N	5.90	131.83	122.74
1	B	61	TYR	C-N-CA	5.90	131.83	122.74
1	B	202	TYR	CB-CA-C	5.90	119.73	109.65
1	B	93	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	A	76	MET	CA-C-O	5.88	126.99	120.82
1	B	200	SER	N-CA-CB	5.87	119.37	110.28
1	B	7	TRP	N-CA-CB	5.86	118.61	110.17
1	B	109	GLN	N-CA-C	-5.86	104.90	111.28
1	A	137	TYR	O-C-N	5.85	128.10	122.07
1	A	177	PHE	N-CA-C	5.82	119.85	108.21
1	B	17	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	B	13	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	111	ILE	O-C-N	-5.80	116.23	121.91
1	A	72	SER	CB-CA-C	5.79	120.36	110.74
1	B	75	ILE	O-C-N	5.79	127.58	121.91
1	B	99	VAL	O-C-N	5.77	127.47	121.87
1	A	8	ASN	CA-CB-CG	-5.76	106.83	112.60
1	B	56	PHE	O-C-N	5.76	126.56	121.37
1	A	58	ASN	O-C-N	5.75	129.15	122.99
1	B	114	CYS	N-CA-C	-5.75	105.98	112.87
1	B	205	THR	CB-CA-C	5.73	118.85	109.97
1	A	178	PRO	N-CA-CB	-5.72	97.24	103.25
1	B	98	ILE	O-C-N	5.72	127.51	121.91
1	B	150	ASP	O-C-N	5.69	128.64	122.15
1	B	175	ASP	CA-CB-CG	-5.69	106.91	112.60
1	B	76	MET	O-C-N	-5.66	116.20	122.09
1	A	183	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	18	LEU	CD1-CG-CD2	-5.61	98.46	110.80
1	B	27	TYR	CA-C-O	5.60	127.72	121.40
1	A	45	TRP	CA-C-O	-5.58	114.58	120.55
1	B	80	ALA	CB-CA-C	5.57	120.15	110.68
1	B	125	GLU	CA-CB-CG	5.57	125.23	114.10
1	A	106	ASN	O-C-N	5.56	129.11	122.27
1	A	144	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
1	B	114	CYS	CB-CA-C	5.53	122.32	110.21
1	A	2	MET	N-CA-C	-5.53	102.70	110.50
1	A	48	GLU	CA-CB-CG	5.51	125.12	114.10
1	B	18	LEU	N-CA-C	5.51	117.29	111.28
1	B	100	GLU	O-C-N	-5.48	116.39	122.09
1	A	168	ILE	CA-C-N	5.47	128.06	120.29
1	A	168	ILE	C-N-CA	5.47	128.06	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	44	GLN	CA-C-O	5.45	126.33	120.55
1	B	47	ASN	CA-C-O	-5.45	114.78	120.55
1	A	198	LYS	CA-CB-CG	-5.44	103.21	114.10
1	A	144	ARG	CD-NE-CZ	5.44	132.01	124.40
1	A	67	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	A	186	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	B	187	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	158	LEU	N-CA-CB	-5.43	102.20	110.07
1	B	154	TYR	N-CA-C	5.42	117.95	111.71
1	B	192	LYS	CA-C-O	-5.42	114.80	120.55
1	B	205	THR	CA-C-O	-5.42	115.35	120.34
1	B	64	ASP	CB-CG-OD1	5.42	130.86	118.40
1	B	200	SER	O-C-N	5.40	128.91	122.27
1	B	17	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
1	A	15	PRO	CA-C-N	5.35	127.40	120.56
1	A	15	PRO	C-N-CA	5.35	127.40	120.56
1	A	182	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	100	GLU	CA-C-N	5.33	127.86	120.29
1	B	100	GLU	C-N-CA	5.33	127.86	120.29
1	A	4	LEU	CA-C-O	-5.32	114.61	120.30
1	B	29	GLU	CG-CD-OE1	5.31	130.60	118.40
1	A	105	ASP	CA-C-N	-5.28	112.28	120.31
1	A	105	ASP	C-N-CA	-5.28	112.28	120.31
1	A	16	ILE	CA-CB-CG2	-5.28	101.52	110.50
1	B	47	ASN	N-CA-CB	5.28	117.88	110.12
1	B	133	LYS	CA-C-O	5.28	126.02	120.42
1	A	177	PHE	CA-C-N	5.27	126.42	119.84
1	A	177	PHE	C-N-CA	5.27	126.42	119.84
1	A	70	THR	CA-CB-OG1	-5.26	101.71	109.60
1	B	73	ASN	CA-C-O	5.26	126.13	120.55
1	B	210	LYS	N-CA-C	-5.24	106.58	112.87
1	A	10	ARG	CD-NE-CZ	-5.24	117.07	124.40
1	B	181	LYS	N-CA-CB	5.23	117.81	110.12
1	A	105	ASP	N-CA-CB	5.21	117.57	110.01
1	A	192	LYS	CA-C-O	-5.21	113.97	119.97
1	A	201	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	A	183	PHE	N-CA-C	-5.17	105.64	111.28
1	B	199	SER	CA-CB-OG	-5.17	100.76	111.10
1	A	31	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	A	168	ILE	O-C-N	-5.16	116.51	121.83
1	A	153	THR	CA-C-O	-5.15	115.74	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	LEU	CB-CA-C	5.14	119.32	110.79
1	B	97	ASP	O-C-N	-5.12	116.76	122.09
1	A	78	TYR	N-CA-C	-5.12	105.70	111.28
1	B	115	TYR	N-CA-CB	5.11	118.16	110.65
1	B	77	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	B	8	ASN	OD1-CG-ND2	-5.11	117.50	122.60
1	A	19	LEU	O-C-N	5.09	127.96	122.15
1	A	93	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	B	125	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	56	PHE	O-C-N	5.07	125.93	121.32
1	B	104	MET	CA-CB-CG	-5.06	103.99	114.10
1	B	126	PHE	O-C-N	5.05	127.48	122.08
1	B	173	CYS	CA-CB-SG	5.04	126.00	114.40
1	B	104	MET	CA-C-N	5.02	126.97	120.44
1	B	104	MET	C-N-CA	5.02	126.97	120.44
1	A	190	LEU	CA-C-N	5.02	129.16	121.19
1	A	190	LEU	C-N-CA	5.02	129.16	121.19
1	B	4	LEU	O-C-N	-5.01	117.36	123.27
1	B	73	ASN	O-C-N	-5.01	116.81	122.12
1	B	179	ASN	O-C-N	5.01	128.08	122.22
1	A	179	ASN	CA-C-N	5.00	129.14	120.58
1	A	179	ASN	C-N-CA	5.00	129.14	120.58
1	A	76	MET	N-CA-CB	5.00	117.27	110.01
1	A	211	LEU	CB-CA-C	5.00	119.17	110.72
1	B	155	VAL	N-CA-CB	5.00	118.08	110.58

There are no chirality outliers.

All (6) 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	144	ARG	Sidechain
1	B	186	ARG	Sidechain
1	B	77	ARG	Sidechain

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	1818	0	1805	83	1
1	B	1818	0	1805	133	2
2	A	5	0	0	0	0
3	A	32	0	18	5	0
3	B	32	0	18	3	0
4	A	198	0	0	1	0
4	B	134	0	0	4	0
All	All	4037	0	3646	222	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 30.

All (222) 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:174:LEU:HD23	1:B:181:LYS:HG2	1.26	1.14
1:B:3:ILE:HG21	1:B:30:LYS:HE3	1.11	1.08
1:A:34:MET:HE1	1:A:211:LEU:HD23	1.35	1.07
1:B:168:ILE:HG22	1:B:214:TRP:HZ2	1.21	1.05
1:A:191:LYS:CD	1:A:191:LYS:H	1.67	1.04
1:A:95:ARG:HH12	1:A:144:ARG:HH21	1.04	1.03
1:B:127:LEU:HA	1:B:130:ILE:HG13	1.41	0.99
1:B:34:MET:HE2	1:B:40:TYR:HB3	1.44	0.99
1:B:207:ILE:HG12	1:B:215:SER:OG	1.62	0.98
1:A:8:ASN:N	1:A:8:ASN:HD22	1.59	0.97
1:B:212:ALA:HB3	1:B:216:ASN:HB3	1.43	0.97
3:B:218:GDN:O2A	3:B:218:GDN:HB21	1.64	0.97
1:B:10:ARG:HD3	1:B:207:ILE:HD12	1.48	0.96
1:A:95:ARG:NH1	1:A:144:ARG:HH21	1.62	0.96
1:A:12:LEU:HD12	1:A:12:LEU:C	1.93	0.93
1:B:116:ASN:HD22	1:B:118:ASP:H	1.14	0.92
1:B:116:ASN:ND2	1:B:118:ASP:H	1.67	0.92
1:A:34:MET:CE	1:A:40:TYR:HB3	2.00	0.92
1:A:191:LYS:H	1:A:191:LYS:HD2	1.36	0.90
1:A:34:MET:HE3	1:A:40:TYR:HB3	1.53	0.89
1:B:111:ILE:HG23	1:B:115:TYR:HD2	1.35	0.89
1:B:111:ILE:HG23	1:B:115:TYR:CD2	2.09	0.88
1:B:174:LEU:HD21	1:B:184:LEU:HD12	1.57	0.87
1:A:12:LEU:HD12	1:A:12:LEU:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:MET:HE1	1:A:211:LEU:CD2	2.05	0.86
1:A:8:ASN:HD22	1:A:8:ASN:H	1.22	0.84
1:B:123:LYS:O	1:B:127:LEU:HG	1.78	0.84
1:A:83:HIS:C	1:A:84:HIS:ND1	2.37	0.82
1:B:168:ILE:HG22	1:B:214:TRP:CZ2	2.13	0.82
1:B:193:ILE:O	1:B:197:MET:HG3	1.82	0.80
1:B:125:GLU:O	1:B:128:LYS:HB2	1.82	0.79
1:A:193:ILE:O	1:A:197:MET:HG3	1.82	0.79
1:A:191:LYS:H	1:A:191:LYS:HD3	1.48	0.78
1:A:124:PRO:O	1:A:128:LYS:HD2	1.84	0.77
3:B:218:GDN:O2A	3:B:218:GDN:CB2	2.33	0.77
1:B:123:LYS:HB3	1:B:124:PRO:HD3	1.64	0.76
1:B:197:MET:SD	4:B:269:HOH:O	2.43	0.75
1:B:116:ASN:O	1:B:213:GLN:OE1	2.03	0.75
1:B:127:LEU:HD13	1:B:170:GLU:OE1	1.85	0.75
1:B:35:GLY:O	1:B:40:TYR:HA	1.87	0.74
1:B:114:CYS:HB2	1:B:208:PHE:HE2	1.51	0.74
1:B:114:CYS:CB	1:B:208:PHE:HE2	2.01	0.73
1:B:114:CYS:O	1:B:213:GLN:HG2	1.88	0.73
1:B:127:LEU:HD23	1:B:169:PHE:CE2	2.25	0.72
1:A:8:ASN:H	1:A:8:ASN:ND2	1.88	0.71
1:A:118:ASP:O	1:A:122:GLN:HG2	1.90	0.71
1:A:140:PHE:O	1:A:144:ARG:NH2	2.23	0.71
1:B:42:ARG:HH12	1:B:45:TRP:HD1	1.37	0.71
1:B:125:GLU:O	1:B:128:LYS:CB	2.39	0.71
1:B:125:GLU:HA	1:B:128:LYS:HD2	1.72	0.70
1:A:95:ARG:HH12	1:A:144:ARG:NH2	1.84	0.70
1:B:113:LEU:HG	1:B:119:PHE:HE1	1.57	0.69
1:B:123:LYS:CG	1:B:127:LEU:HD21	2.22	0.69
1:B:216:ASN:C	1:B:216:ASN:HD22	2.01	0.68
1:B:134:MET:HE1	1:B:166:TYR:CD2	2.29	0.68
1:B:30:LYS:HD2	1:B:61:TYR:OH	1.93	0.68
1:B:205:THR:HG23	1:B:206:PRO:HA	1.76	0.67
1:B:119:PHE:CG	1:B:213:GLN:HG3	2.30	0.66
1:A:39:ASP:OD1	1:A:39:ASP:N	2.28	0.66
1:B:42:ARG:HH12	1:B:45:TRP:CD1	2.13	0.66
1:B:42:ARG:NH1	1:B:45:TRP:HD1	1.94	0.66
1:B:52:LEU:O	1:B:68:LYS:NZ	2.20	0.65
1:B:174:LEU:CD2	1:B:181:LYS:HG2	2.17	0.65
1:A:124:PRO:O	1:A:128:LYS:CD	2.44	0.65
1:A:175:ASP:OD1	1:A:181:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:HIS:ND1	1:A:84:HIS:N	2.44	0.64
1:B:173:CYS:O	1:B:175:ASP:N	2.30	0.64
1:A:24:ASP:OD2	1:A:192:LYS:HE2	1.98	0.64
1:A:34:MET:HE2	1:A:40:TYR:HB3	1.79	0.64
1:B:116:ASN:HD22	1:B:116:ASN:C	2.06	0.64
1:A:191:LYS:CD	1:A:191:LYS:N	2.49	0.63
1:B:130:ILE:O	1:B:134:MET:HE2	1.98	0.63
1:B:168:ILE:CG2	1:B:214:TRP:HZ2	2.05	0.63
1:A:144:ARG:HG3	1:A:144:ARG:HH11	1.63	0.63
1:A:30:LYS:HE2	1:A:32:TYR:CE1	2.33	0.63
1:B:119:PHE:CE2	1:B:214:TRP:HB2	2.35	0.61
1:B:123:LYS:HG2	1:B:127:LEU:HD21	1.81	0.61
1:B:172:LYS:HA	1:B:175:ASP:OD2	2.00	0.61
1:B:113:LEU:HG	1:B:119:PHE:CE1	2.34	0.61
3:A:219:GDN:C6'	3:A:219:GDN:HA2	2.30	0.61
1:B:130:ILE:N	1:B:131:PRO:CD	2.63	0.60
1:B:12:LEU:CB	1:B:107:ARG:HD3	2.33	0.59
1:A:119:PHE:HB2	1:A:213:GLN:HG3	1.85	0.58
1:B:114:CYS:HB2	1:B:208:PHE:CE2	2.36	0.58
1:A:202:TYR:CE2	1:A:204:SER:OG	2.54	0.58
1:B:40:TYR:HE1	1:B:210:LYS:HB2	1.70	0.57
1:B:146:TRP:CH2	1:B:186:ARG:HG2	2.39	0.57
1:A:95:ARG:NH1	1:A:144:ARG:NH2	2.44	0.57
1:B:8:ASN:N	1:B:8:ASN:HD22	2.02	0.57
1:A:118:ASP:OD2	1:A:122:GLN:OE1	2.22	0.57
1:B:35:GLY:C	1:B:40:TYR:HA	2.30	0.56
1:B:12:LEU:HB2	1:B:107:ARG:HD3	1.87	0.56
1:B:34:MET:CE	1:B:40:TYR:HB3	2.25	0.56
1:B:130:ILE:N	1:B:131:PRO:HD2	2.21	0.56
1:B:119:PHE:HB2	1:B:213:GLN:HG3	1.86	0.55
1:A:12:LEU:C	1:A:12:LEU:CD1	2.71	0.55
1:B:3:ILE:CG2	1:B:30:LYS:HE3	2.07	0.55
1:A:24:ASP:CG	1:A:192:LYS:HE2	2.31	0.55
1:A:146:TRP:CE2	1:A:152:VAL:HG22	2.41	0.55
1:A:95:ARG:CZ	1:A:144:ARG:HE	2.20	0.55
1:B:173:CYS:C	1:B:175:ASP:H	2.14	0.55
1:A:115:TYR:CZ	1:A:212:ALA:HB2	2.41	0.55
1:B:203:LEU:C	1:B:203:LEU:HD23	2.32	0.55
1:B:120:GLU:HA	1:B:120:GLU:OE1	2.06	0.54
1:A:191:LYS:HD2	1:A:191:LYS:N	2.16	0.54
1:B:116:ASN:HD22	1:B:118:ASP:N	1.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:CG	1:A:8:ASN:O	2.51	0.54
1:A:174:LEU:HD23	1:A:181:LYS:CG	2.37	0.54
1:B:120:GLU:O	1:B:124:PRO:HD3	2.08	0.54
1:B:45:TRP:CZ2	1:B:49:LYS:HG3	2.43	0.53
1:B:113:LEU:HD22	1:B:126:PHE:CD2	2.44	0.53
1:B:7:TRP:HZ2	1:B:42:ARG:NH1	2.07	0.53
1:A:95:ARG:NH2	1:A:144:ARG:NE	2.57	0.52
1:B:112:MET:O	1:B:116:ASN:HB2	2.08	0.52
1:B:118:ASP:OD2	1:B:121:LYS:HB2	2.08	0.52
1:B:119:PHE:CB	1:B:213:GLN:HG3	2.40	0.52
1:B:123:LYS:HG3	1:B:127:LEU:HD21	1.91	0.52
1:B:209:SER:C	1:B:211:LEU:N	2.68	0.52
1:A:14:HIS:N	1:A:15:PRO:CD	2.73	0.51
1:A:121:LYS:HD2	1:A:121:LYS:N	2.22	0.51
1:B:116:ASN:ND2	1:B:116:ASN:C	2.68	0.51
1:B:114:CYS:CB	1:B:208:PHE:CE2	2.88	0.51
1:B:209:SER:C	1:B:211:LEU:H	2.18	0.51
1:B:129:THR:C	1:B:131:PRO:HD2	2.35	0.51
1:B:8:ASN:HD22	1:B:8:ASN:H	1.59	0.51
1:B:173:CYS:C	1:B:175:ASP:N	2.69	0.51
1:A:95:ARG:CZ	1:A:144:ARG:HH21	2.23	0.51
1:B:111:ILE:HG22	1:B:112:MET:N	2.26	0.51
1:A:8:ASN:ND2	1:A:8:ASN:C	2.68	0.50
1:A:118:ASP:OD2	1:A:122:GLN:HG2	2.12	0.50
1:A:32:TYR:HD1	1:A:44:GLN:HG2	1.75	0.50
1:A:54:LEU:HD23	1:A:68:LYS:HB3	1.94	0.50
1:A:93:ARG:NH2	4:A:322:HOH:O	2.37	0.50
1:B:39:ASP:O	1:B:40:TYR:C	2.55	0.50
1:B:125:GLU:HA	1:B:128:LYS:HB2	1.94	0.49
1:B:119:PHE:O	1:B:123:LYS:HB2	2.12	0.49
1:B:7:TRP:CZ2	1:B:42:ARG:NH1	2.80	0.49
1:A:174:LEU:HD23	1:A:181:LYS:HG3	1.94	0.49
1:B:22:TYR:O	1:B:192:LYS:HD2	2.13	0.48
1:A:2:MET:CE	1:A:82:LYS:HZ2	2.26	0.48
1:A:77:ARG:NH2	1:A:97:ASP:OD1	2.47	0.48
1:A:191:LYS:HD3	1:A:191:LYS:N	2.20	0.48
1:B:196:TYR:O	1:B:199:SER:OG	2.26	0.48
1:A:196:TYR:O	1:A:199:SER:OG	2.32	0.48
1:B:40:TYR:CE1	1:B:210:LYS:HB2	2.48	0.48
1:B:110:LEU:O	1:B:111:ILE:C	2.56	0.48
1:B:111:ILE:CG2	1:B:115:TYR:HD2	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLU:C	1:B:128:LYS:HB2	2.38	0.48
1:B:203:LEU:C	1:B:203:LEU:CD2	2.87	0.48
1:B:10:ARG:HD3	1:B:207:ILE:CD1	2.34	0.48
1:B:10:ARG:O	1:B:11:GLY:C	2.57	0.47
1:A:2:MET:HE2	1:A:64:ASP:OD2	2.15	0.47
1:B:118:ASP:OD2	1:B:121:LYS:HD3	2.13	0.47
1:B:119:PHE:CD2	1:B:213:GLN:HB2	2.49	0.47
1:B:202:TYR:CE2	1:B:204:SER:HB3	2.50	0.47
1:A:99:VAL:O	1:A:100:GLU:C	2.57	0.47
1:B:10:ARG:HD2	1:B:204:SER:O	2.14	0.47
1:B:100:GLU:OE1	1:B:154:TYR:OH	2.21	0.47
1:B:113:LEU:HD22	1:B:126:PHE:CG	2.50	0.47
1:B:114:CYS:SG	1:B:119:PHE:CE1	3.04	0.47
3:B:218:GDN:O2A	3:B:218:GDN:SG2	2.72	0.47
1:A:116:ASN:C	1:A:118:ASP:H	2.24	0.46
1:B:192:LYS:HG3	4:B:263:HOH:O	2.15	0.46
1:A:193:ILE:N	1:A:193:ILE:HD12	2.30	0.46
1:B:12:LEU:HB3	1:B:107:ARG:HD3	1.97	0.46
1:B:123:LYS:CB	1:B:124:PRO:HD3	2.38	0.46
1:B:126:PHE:C	1:B:128:LYS:H	2.21	0.46
1:B:14:HIS:N	1:B:15:PRO:CD	2.79	0.45
1:B:119:PHE:CZ	1:B:169:PHE:HE1	2.35	0.45
1:A:2:MET:CE	1:A:82:LYS:NZ	2.80	0.45
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.52	0.45
1:A:202:TYR:CZ	1:A:204:SER:OG	2.70	0.45
1:A:2:MET:O	1:A:27:TYR:HA	2.17	0.44
1:B:120:GLU:O	1:B:124:PRO:CD	2.65	0.44
1:B:123:LYS:HB3	1:B:124:PRO:CD	2.43	0.44
1:B:113:LEU:C	1:B:115:TYR:N	2.73	0.44
1:A:10:ARG:HH11	1:A:10:ARG:HD2	1.58	0.44
1:A:12:LEU:O	1:A:12:LEU:CD1	2.56	0.44
1:A:24:ASP:OD2	1:A:192:LYS:CE	2.66	0.44
1:A:122:GLN:O	1:A:125:GLU:HB2	2.18	0.43
1:B:8:ASN:ND2	4:B:254:HOH:O	2.51	0.43
1:A:123:LYS:N	1:A:124:PRO:HD2	2.33	0.43
1:A:43:SER:HA	1:A:46:LEU:HB2	1.99	0.43
1:B:146:TRP:CE2	1:B:152:VAL:HG22	2.54	0.43
1:B:172:LYS:C	1:B:175:ASP:OD2	2.62	0.43
1:B:114:CYS:HB3	1:B:208:PHE:CE2	2.54	0.43
1:A:115:TYR:HE2	1:A:211:LEU:CD1	2.30	0.42
1:B:12:LEU:C	1:B:12:LEU:CD1	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HG	1:B:127:LEU:H	1.67	0.42
1:A:104:MET:HE2	1:A:104:MET:HB2	1.93	0.42
1:A:205:THR:HB	1:A:206:PRO:HA	2.01	0.42
1:B:108:MET:HE3	1:B:108:MET:HB2	1.79	0.42
1:B:7:TRP:C	1:B:9:VAL:H	2.27	0.42
1:A:130:ILE:N	1:A:131:PRO:CD	2.83	0.42
1:B:123:LYS:CB	1:B:124:PRO:CD	2.97	0.42
1:A:116:ASN:C	1:A:118:ASP:N	2.76	0.42
1:A:162:ILE:HA	1:A:162:ILE:HD12	1.74	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.87	0.42
1:B:110:LEU:O	1:B:113:LEU:HB3	2.20	0.42
1:B:152:VAL:HG23	4:B:258:HOH:O	2.19	0.42
1:B:216:ASN:ND2	1:B:217:LYS:HG2	2.35	0.42
3:A:219:GDN:HN2A	1:B:105:ASP:CG	2.27	0.41
1:B:111:ILE:O	1:B:115:TYR:N	2.53	0.41
1:B:119:PHE:HE2	1:B:214:TRP:HB2	1.83	0.41
1:B:77:ARG:CZ	1:B:100:GLU:OE1	2.69	0.41
1:A:210:LYS:H	1:A:210:LYS:HG2	1.49	0.41
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.85	0.41
1:B:167:HIS:O	1:B:167:HIS:CG	2.74	0.41
1:B:168:ILE:CG2	1:B:214:TRP:CZ2	2.91	0.41
1:A:22:TYR:HB2	1:A:193:ILE:HD11	2.03	0.41
1:A:71:GLN:OE1	3:A:219:GDN:N1	2.54	0.41
1:B:40:TYR:HE1	1:B:210:LYS:CB	2.33	0.41
1:B:113:LEU:C	1:B:115:TYR:H	2.27	0.41
1:B:172:LYS:HE2	1:B:172:LYS:HB3	1.89	0.41
1:B:216:ASN:HD22	1:B:217:LYS:N	2.18	0.41
1:A:24:ASP:OD1	1:A:192:LYS:HE2	2.21	0.41
3:A:219:GDN:HA2	3:A:219:GDN:H6'	2.01	0.40
1:A:33:ALA:H	1:A:44:GLN:NE2	2.19	0.40
1:A:205:THR:HA	1:A:206:PRO:C	2.47	0.40
1:A:160:TYR:O	1:A:161:ASP:C	2.65	0.40
3:A:219:GDN:SG2	3:A:219:GDN:O2A	2.79	0.40
1:B:118:ASP:OD2	1:B:121:LYS:CD	2.70	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)
1:B:67:ARG:NH2	1:B:67:ARG:NH2[2_555]	1.70	0.50
1:A:90:GLU:CB	1:B:67:ARG:NH1[2_555]	2.00	0.20

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	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
1	B	215/217 (99%)	196 (91%)	15 (7%)	4 (2%)	6	3
All	All	430/434 (99%)	397 (92%)	29 (7%)	4 (1%)	14	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	ILE
1	B	112	MET
1	B	174	LEU
1	B	119	PHE

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	197/197 (100%)	176 (89%)	21 (11%)	6	4
1	B	197/197 (100%)	175 (89%)	22 (11%)	6	3
All	All	394/394 (100%)	351 (89%)	43 (11%)	6	3

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	3	ILE

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Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	LEU
1	A	19	LEU
1	A	41	ASP
1	A	46	LEU
1	A	51	LYS
1	A	84	HIS
1	A	88	GLU
1	A	120	GLU
1	A	121	LYS
1	A	144	ARG
1	A	151	LYS
1	A	171	PRO
1	A	174	LEU
1	A	178	PRO
1	A	191	LYS
1	A	203	LEU
1	A	211	LEU
1	A	217	LYS
1	B	8	ASN
1	B	9	VAL
1	B	12	LEU
1	B	19	LEU
1	B	28	GLU
1	B	34	MET
1	B	88	GLU
1	B	108	MET
1	B	113	LEU
1	B	116	ASN
1	B	120	GLU
1	B	127	LEU
1	B	151	LYS
1	B	166	TYR
1	B	167	HIS
1	B	170	GLU
1	B	172	LYS
1	B	174	LEU
1	B	181	LYS
1	B	191	LYS
1	B	213	GLN
1	B	216	ASN

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	8	ASN
1	A	44	GLN
1	A	122	GLN
1	A	167	HIS
1	A	216	ASN
1	B	8	ASN
1	B	47	ASN
1	B	102	GLN
1	B	106	ASN
1	B	116	ASN
1	B	216	ASN

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](#)

3 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	218	-	4,4,4	0.79	0	6,6,6	0.32	0
3	GDN	A	219	-	31,32,32	2.24	6 (19%)	34,43,43	2.18	15 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDN	B	218	-	31,32,32	1.72	6 (19%)	34,43,43	2.22	9 (26%)

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	GDN	B	218	-	-	4/31/35/35	0/1/1/1
3	GDN	A	219	-	-	2/31/35/35	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	219	GDN	O4B-N4'	9.06	1.38	1.22
3	B	218	GDN	C1'-SG2	-5.34	1.69	1.77
3	A	219	GDN	C1'-SG2	-4.78	1.70	1.77
3	B	218	GDN	O12-C1	3.57	1.42	1.30
3	B	218	GDN	CB2-SG2	-3.29	1.74	1.81
3	B	218	GDN	C4'-N4'	-2.80	1.38	1.45
3	A	219	GDN	O12-C1	2.76	1.39	1.30
3	A	219	GDN	CB2-SG2	-2.63	1.75	1.81
3	B	218	GDN	CB1-CG1	2.33	1.59	1.52
3	A	219	GDN	O2B-N2'	2.21	1.26	1.22
3	B	218	GDN	C2-N3	-2.08	1.28	1.33
3	A	219	GDN	C2'-C1'	-2.04	1.36	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	218	GDN	CB2-SG2-C1'	7.49	118.36	102.42
3	B	218	GDN	O4B-N4'-C4'	4.76	125.37	118.82
3	B	218	GDN	C3'-C2'-C1'	-4.26	118.52	122.97
3	A	219	GDN	C3'-C2'-C1'	-4.24	118.54	122.97
3	A	219	GDN	OE1-CD1-N2	4.18	130.02	122.95
3	A	219	GDN	O32-C3-O31	-3.80	113.57	123.33
3	A	219	GDN	O2B-N2'-C2'	-3.73	112.65	119.03
3	A	219	GDN	CG1-CB1-CA1	-3.32	106.25	113.86
3	A	219	GDN	CB2-SG2-C1'	3.25	109.34	102.42
3	B	218	GDN	C6'-C1'-C2'	2.86	122.79	118.71
3	A	219	GDN	O32-C3-CA3	2.83	123.58	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	218	GDN	CG1-CB1-CA1	-2.69	107.68	113.86
3	A	219	GDN	O4B-N4'-C4'	2.52	122.28	118.82
3	A	219	GDN	C6'-C1'-C2'	2.45	122.22	118.71
3	A	219	GDN	CB1-CG1-CD1	-2.43	107.65	113.06
3	A	219	GDN	OE1-CD1-CG1	-2.43	117.62	122.02
3	B	218	GDN	CB1-CG1-CD1	-2.40	107.71	113.06
3	A	219	GDN	O2-C2-CA2	-2.38	115.49	120.48
3	B	218	GDN	C3-CA3-N3	-2.38	105.67	113.06
3	B	218	GDN	O2-C2-CA2	-2.34	115.57	120.48
3	A	219	GDN	CA2-C2-N3	2.33	121.55	116.54
3	A	219	GDN	CB1-CA1-C1	2.32	116.60	110.45
3	B	218	GDN	O12-C1-O11	-2.28	118.92	124.08
3	A	219	GDN	CG1-CD1-N2	-2.06	112.23	115.86

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	218	GDN	C6'-C1'-SG2-CB2
3	B	218	GDN	C2'-C1'-SG2-CB2
3	B	218	GDN	CA2-CB2-SG2-C1'
3	A	219	GDN	C3-CA3-N3-C2
3	A	219	GDN	O12-C1-CA1-N1
3	B	218	GDN	O11-C1-CA1-N1

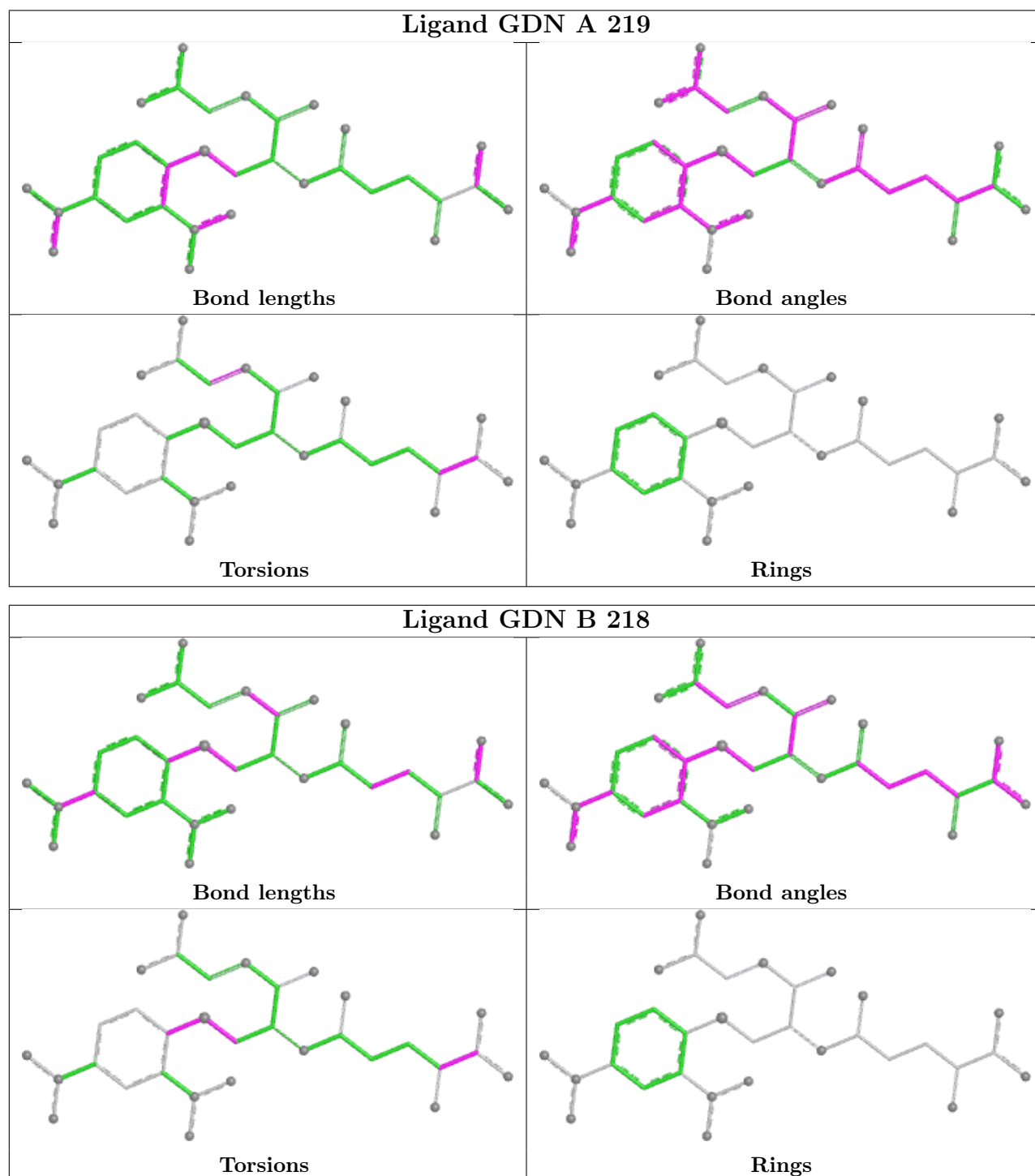
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	219	GDN	5	0
3	B	218	GDN	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.