



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:31 AM UTC

PDB ID : 6GSX / pdb_00006gsx
Title : FIRST-SPHERE AND SECOND-SPHERE ELECTROSTATIC EFFECTS IN
THE ACTIVE SITE OF A CLASS MU GLUTATHIONE TRANSFERASE
Authors : Xiao, G.; Ji, X.; Armstrong, R.N.; Gilliland, G.L.
Deposited on : 1996-01-26
Resolution : 1.91 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

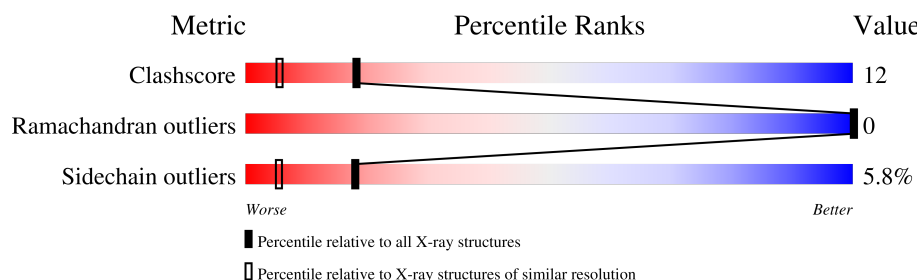
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)

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	
1	B	217	

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
3	GPS	A	221	X	-	-	-
3	GPS	B	218	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4167 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.

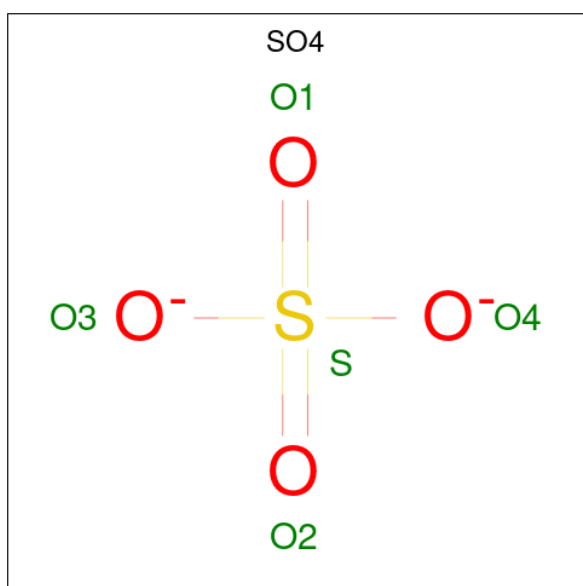
- Molecule 1 is a protein called MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1817	1177	303	326	11			
1	B	217	Total	C	N	O	S	0	0	0
			1817	1177	303	326	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	PHE	TYR	engineered mutation	UNP P04905
B	6	PHE	TYR	engineered mutation	UNP P04905

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



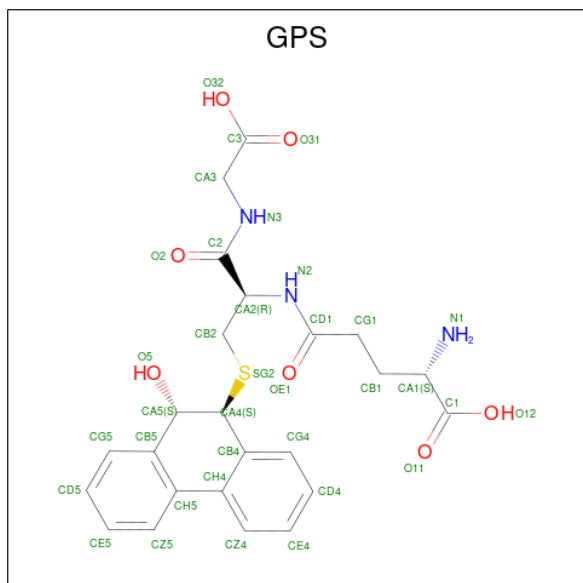
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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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		

- Molecule 3 is L-gamma-glutamyl-S-[(9S,10S)-10-hydroxy-9,10-dihydrophenanthren-9-yl]-L-cysteinyglycine (CCD ID: GPS) (formula: C₂₄H₂₇N₃O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	24	3	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	24	3	7	1		

- Molecule 4 is water.

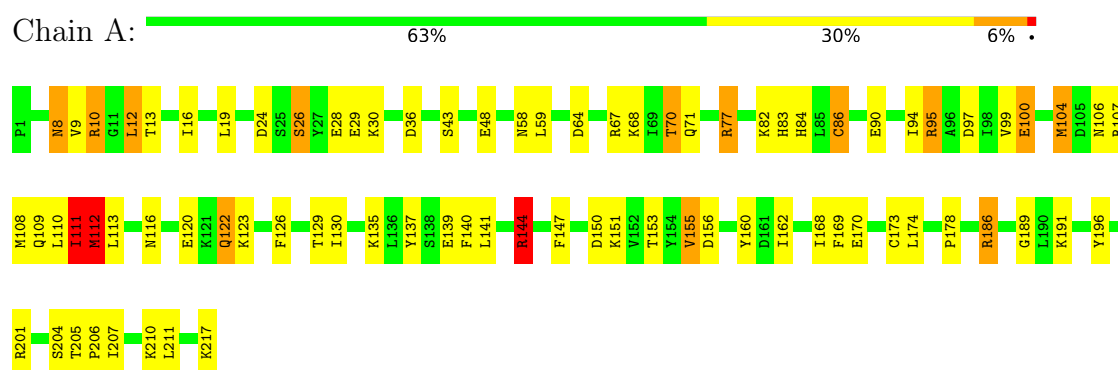
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	257	Total	O	0	0
			257	257		
4	B	191	Total	O	0	0
			191	191		

3 Residue-property plots

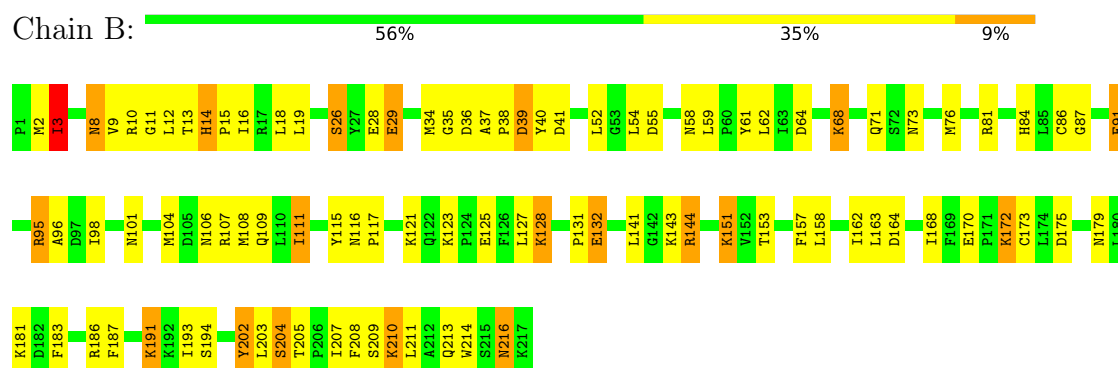
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3



• Molecule 1: MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3



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	87.84Å 69.22Å 81.32Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	6.00 – 1.91	Depositor
% Data completeness (in resolution range)	92.1 (6.00-1.91)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4167	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: GPS, 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	1.39	11/1866 (0.6%)	2.06	61/2513 (2.4%)
1	B	1.39	9/1866 (0.5%)	2.08	61/2513 (2.4%)
All	All	1.39	20/3732 (0.5%)	2.07	122/5026 (2.4%)

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	2
1	B	0	2
All	All	0	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ILE	CA-CB	7.75	1.58	1.54
1	B	98	ILE	CA-CB	7.13	1.62	1.54
1	A	94	ILE	CA-CB	6.17	1.61	1.54
1	A	160	TYR	N-CA	6.15	1.53	1.46
1	B	13	THR	CA-CB	5.86	1.63	1.53
1	B	76	MET	N-CA	5.80	1.53	1.46
1	A	10	ARG	N-CA	5.80	1.53	1.46
1	B	183	PHE	N-CA	5.65	1.53	1.46
1	B	58	ASN	CA-CB	5.64	1.62	1.53
1	B	157	PHE	N-CA	5.60	1.53	1.46
1	B	96	ALA	N-CA	5.54	1.52	1.46
1	A	59	LEU	CA-C	5.49	1.59	1.52
1	A	77	ARG	NE-CZ	5.41	1.39	1.33
1	A	100	GLU	N-CA	5.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	GLU	N-CA	5.22	1.51	1.46
1	A	196	TYR	C-O	5.17	1.30	1.24
1	B	59	LEU	CA-C	5.16	1.58	1.52
1	B	179	ASN	C-N	-5.15	1.27	1.33
1	A	16	ILE	CA-CB	5.13	1.60	1.54
1	A	70	THR	C-N	-5.13	1.26	1.33

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	CD-NE-CZ	12.78	142.29	124.40
1	B	16	ILE	O-C-N	11.07	136.45	121.84
1	B	132	GLU	CB-CG-CD	10.63	130.68	112.60
1	B	16	ILE	CA-C-O	-9.73	110.30	120.71
1	B	59	LEU	O-C-N	9.60	129.94	121.39
1	A	95	ARG	CD-NE-CZ	9.35	137.49	124.40
1	A	100	GLU	CA-C-O	9.34	130.89	120.90
1	B	186	ARG	CD-NE-CZ	9.11	137.16	124.40
1	B	71	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	A	150	ASP	CA-CB-CG	-8.59	104.01	112.60
1	A	24	ASP	CA-CB-CG	-8.48	104.12	112.60
1	A	122	GLN	OE1-CD-NE2	8.47	131.07	122.60
1	A	155	VAL	CA-C-O	-8.42	111.38	120.47
1	B	84	HIS	CA-CB-CG	-8.27	105.53	113.80
1	B	26	SER	CB-CA-C	8.24	123.96	110.78
1	A	112	MET	N-CA-CB	8.08	121.99	110.12
1	B	95	ARG	CD-NE-CZ	8.02	135.63	124.40
1	A	99	VAL	O-C-N	7.99	129.74	121.91
1	A	156	ASP	CA-CB-CG	-7.89	104.71	112.60
1	A	137	TYR	O-C-N	7.85	131.10	122.15
1	B	59	LEU	CA-C-O	-7.73	111.81	119.69
1	B	186	ARG	NE-CZ-NH1	7.69	129.19	121.50
1	B	76	MET	O-C-N	-7.59	114.20	122.09
1	A	84	HIS	CA-CB-CG	-7.47	106.33	113.80
1	A	68	LYS	O-C-N	7.46	132.00	123.27
1	B	13	THR	CA-CB-OG1	-7.36	98.56	109.60
1	A	67	ARG	CD-NE-CZ	-7.17	114.36	124.40
1	B	205	THR	CA-C-O	-7.14	113.77	120.34
1	A	12	LEU	CA-C-O	7.04	127.90	119.59
1	A	104	MET	CB-CA-C	6.99	122.00	110.81
1	A	59	LEU	O-C-N	6.99	128.23	121.66
1	B	101	ASN	CA-CB-CG	-6.96	105.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	MET	O-C-N	6.94	129.48	122.12
1	B	204	SER	CA-CB-OG	-6.83	97.45	111.10
1	A	95	ARG	O-C-N	6.76	129.04	122.07
1	B	18	LEU	O-C-N	-6.70	115.12	122.09
1	A	77	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	A	83	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	64	ASP	CB-CA-C	6.42	121.28	112.09
1	A	144	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	A	111	ILE	CA-CB-CG2	6.37	121.33	110.50
1	A	141	LEU	O-C-N	6.33	128.93	122.09
1	B	109	GLN	O-C-N	6.21	128.47	122.07
1	A	189	GLY	CA-C-O	-6.20	112.13	119.45
1	A	144	ARG	NH1-CZ-NH2	-6.19	111.26	119.30
1	B	141	LEU	O-C-N	6.15	128.73	122.09
1	B	106	ASN	CA-CB-CG	6.14	118.74	112.60
1	B	14	HIS	CA-C-O	6.12	124.26	118.63
1	B	73	ASN	CB-CG-ND2	-6.08	107.27	116.40
1	B	205	THR	O-C-N	5.92	125.97	121.65
1	A	169	PHE	O-C-N	5.90	128.88	122.15
1	A	95	ARG	CA-C-O	-5.89	114.64	120.82
1	B	64	ASP	CA-C-N	-5.86	113.80	120.42
1	B	64	ASP	C-N-CA	-5.86	113.80	120.42
1	A	162	ILE	CA-C-O	-5.86	114.64	120.85
1	A	116	ASN	O-C-N	5.81	126.25	121.31
1	A	29	GLU	CG-CD-OE2	-5.80	105.06	118.40
1	A	205	THR	CA-CB-OG1	-5.78	100.92	109.60
1	B	10	ARG	CA-C-O	-5.76	114.31	120.42
1	A	43	SER	N-CA-C	5.75	118.33	111.71
1	B	41	ASP	CA-CB-CG	-5.74	106.86	112.60
1	B	111	ILE	N-CA-CB	5.73	117.25	110.55
1	A	70	THR	O-C-N	5.71	130.76	122.94
1	A	191	LYS	CA-C-O	-5.68	114.82	121.07
1	B	202	TYR	CB-CA-C	5.68	118.97	109.89
1	B	61	TYR	CA-C-O	-5.67	114.80	121.44
1	A	173	CYS	N-CA-C	5.66	119.44	112.54
1	B	187	PHE	O-C-N	5.63	127.87	122.07
1	B	111	ILE	O-C-N	5.62	127.42	121.91
1	B	18	LEU	CA-C-N	5.61	128.25	120.29
1	B	18	LEU	C-N-CA	5.61	128.25	120.29
1	A	90	GLU	CA-C-O	5.59	126.47	120.55
1	B	86	CYS	O-C-N	5.58	129.32	122.84
1	B	158	LEU	O-C-N	5.55	128.08	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	LEU	N-CA-C	5.54	117.76	111.11
1	B	68	LYS	CA-C-O	-5.52	114.39	120.24
1	B	193	ILE	N-CA-CB	5.49	117.60	110.57
1	A	186	ARG	CA-C-N	5.47	127.55	120.44
1	A	186	ARG	C-N-CA	5.47	127.55	120.44
1	A	189	GLY	O-C-N	5.44	129.57	122.71
1	B	62	LEU	O-C-N	5.43	129.90	123.27
1	B	132	GLU	N-CA-CB	5.37	118.11	110.16
1	A	77	ARG	CD-NE-CZ	-5.36	116.89	124.40
1	B	162	ILE	CA-C-O	-5.36	115.17	120.85
1	B	28	GLU	CA-CB-CG	5.36	124.81	114.10
1	A	207	ILE	N-CA-C	-5.35	105.91	111.58
1	B	194	SER	N-CA-CB	-5.35	101.97	109.94
1	A	86	CYS	N-CA-CB	-5.34	102.19	110.46
1	B	3	ILE	O-C-N	5.33	129.01	123.26
1	A	110	LEU	CA-C-O	5.31	126.18	120.55
1	A	77	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	97	ASP	CA-C-O	5.24	126.51	120.90
1	B	13	THR	OG1-CB-CG2	-5.24	98.83	109.30
1	B	87	GLY	CA-C-O	-5.23	116.25	121.90
1	B	95	ARG	O-C-N	5.17	127.40	122.07
1	B	58	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	13	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	155	VAL	O-C-N	5.15	127.61	121.80
1	B	91	GLU	CA-CB-CG	5.13	124.37	114.10
1	B	157	PHE	CA-CB-CG	-5.12	108.68	113.80
1	B	183	PHE	N-CA-C	-5.12	105.78	111.36
1	B	163	LEU	N-CA-C	-5.09	105.62	111.07
1	B	179	ASN	CA-C-O	-5.08	114.36	120.10
1	A	28	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	100	GLU	O-C-N	-5.07	116.82	122.09
1	A	211	LEU	CA-C-O	-5.07	114.14	119.97
1	A	26	SER	CA-C-O	-5.07	115.16	120.58
1	A	112	MET	CA-C-O	-5.06	115.19	120.55
1	A	147	PHE	CA-C-O	-5.05	114.39	120.10
1	B	73	ASN	OD1-CG-ND2	5.05	127.65	122.60
1	B	28	GLU	CA-C-O	-5.04	115.22	121.11
1	B	143	LYS	CA-C-N	5.03	128.30	120.60
1	B	143	LYS	C-N-CA	5.03	128.30	120.60
1	A	58	ASN	N-CA-CB	-5.03	103.12	111.57
1	A	174	LEU	CB-CA-C	5.02	117.99	109.55
1	B	81	ARG	NE-CZ-NH2	-5.02	114.68	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	A	168	ILE	CA-C-N	5.02	127.41	120.29
1	A	168	ILE	C-N-CA	5.02	127.41	120.29
1	B	29	GLU	CG-CD-OE2	-5.01	106.88	118.40
1	A	129	THR	CA-CB-OG1	-5.01	102.09	109.60
1	B	9	VAL	CA-C-O	-5.00	116.74	121.64

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Sidechain
1	A	201	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	29	GLU	Mainchain

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	1817	0	1805	36	0
1	B	1817	0	1805	46	0
2	A	15	0	0	0	0
3	A	35	0	25	8	0
3	B	35	0	25	5	0
4	A	257	0	0	10	0
4	B	191	0	0	8	0
All	All	4167	0	3660	89	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 12.

All (89) 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)
3:A:221:GPS:HG4	3:A:221:GPS:HB2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:MET:HA	1:B:111:ILE:HD12	1.52	0.89
1:A:77:ARG:NH2	4:A:259:HOH:O	2.09	0.84
3:A:221:GPS:HB2	3:A:221:GPS:CG4	2.10	0.78
1:A:95:ARG:NH2	1:A:144:ARG:HE	1.82	0.76
1:A:111:ILE:HD11	3:A:221:GPS:CD5	2.17	0.75
4:A:450:HOH:O	3:B:218:GPS:HG5	1.87	0.74
1:B:125:GLU:HA	1:B:128:LYS:HE3	1.71	0.72
1:A:19:LEU:O	1:A:19:LEU:HD23	1.90	0.71
1:A:108:MET:O	1:A:112:MET:HG2	1.90	0.70
1:B:175:ASP:OD1	1:B:181:LYS:NZ	2.23	0.70
1:A:8:ASN:HD22	1:A:8:ASN:H	1.40	0.69
1:B:151:LYS:HE3	1:B:153:THR:HG22	1.75	0.69
1:A:107:ARG:O	1:A:111:ILE:HD12	1.92	0.68
1:A:140:PHE:O	1:A:144:ARG:NH2	2.26	0.68
1:B:213:GLN:HA	4:B:356:HOH:O	1.94	0.68
3:B:218:GPS:HE5	4:B:244:HOH:O	1.96	0.65
1:B:2:MET:HE1	4:B:270:HOH:O	1.96	0.65
1:A:135:LYS:NZ	1:A:139:GLU:OE2	2.28	0.61
3:B:218:GPS:HB2	3:B:218:GPS:CG4	2.30	0.61
1:B:170:GLU:HG3	1:B:173:CYS:HB3	1.82	0.61
1:A:95:ARG:HH22	1:A:144:ARG:HH21	1.50	0.60
3:B:218:GPS:HB2	3:B:218:GPS:HG4	1.85	0.59
1:A:111:ILE:HD11	3:A:221:GPS:CE5	2.33	0.57
1:B:95:ARG:NH2	1:B:144:ARG:HE	2.02	0.57
1:B:104:MET:O	1:B:108:MET:HG2	2.05	0.57
1:A:8:ASN:HD22	1:A:8:ASN:N	2.03	0.57
1:A:82:LYS:NZ	4:A:288:HOH:O	2.38	0.56
1:A:86:CYS:HB2	4:A:367:HOH:O	2.04	0.56
1:B:39:ASP:O	1:B:40:TYR:C	2.49	0.55
1:B:52:LEU:O	1:B:68:LYS:NZ	2.37	0.55
1:B:35:GLY:O	1:B:40:TYR:HA	2.07	0.55
3:A:221:GPS:HE5	4:A:238:HOH:O	2.08	0.54
1:A:12:LEU:HD23	3:A:221:GPS:CD5	2.38	0.54
1:A:122:GLN:HG3	4:A:376:HOH:O	2.09	0.53
1:B:34:MET:HE3	1:B:40:TYR:HB3	1.91	0.53
1:B:123:LYS:HE2	1:B:127:LEU:HD11	1.91	0.52
1:A:95:ARG:NH2	1:A:144:ARG:HH21	2.08	0.52
1:B:54:LEU:HD23	1:B:68:LYS:HB3	1.92	0.52
1:A:12:LEU:HD23	3:A:221:GPS:CG5	2.40	0.52
1:B:91:GLU:O	1:B:95:ARG:HG3	2.10	0.52
1:B:116:ASN:OD1	1:B:117:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASN:ND2	1:B:216:ASN:H	2.08	0.51
1:A:111:ILE:CD1	3:A:221:GPS:CD5	2.88	0.51
1:B:34:MET:HE1	1:B:211:LEU:CD1	2.42	0.50
1:B:128:LYS:O	1:B:131:PRO:HD2	2.11	0.50
1:A:210:LYS:HG3	4:A:280:HOH:O	2.11	0.49
1:A:217:LYS:O	1:A:217:LYS:HG3	2.13	0.49
1:B:116:ASN:O	1:B:213:GLN:HG3	2.12	0.49
1:A:123:LYS:NZ	4:A:285:HOH:O	2.46	0.49
1:A:9:VAL:HG12	1:A:206:PRO:HG2	1.94	0.49
1:B:191:LYS:HD3	1:B:191:LYS:C	2.37	0.48
1:B:3:ILE:HD12	1:B:3:ILE:N	2.28	0.48
1:B:14:HIS:N	1:B:15:PRO:CD	2.78	0.47
1:A:77:ARG:NH2	1:A:100:GLU:OE1	2.48	0.47
1:A:36:ASP:OD1	1:A:210:LYS:NZ	2.42	0.47
1:A:70:THR:O	1:A:71:GLN:HB2	2.14	0.46
1:A:109:GLN:NE2	4:A:459:HOH:O	2.18	0.46
1:B:12:LEU:HB3	1:B:107:ARG:HD3	1.98	0.46
1:B:208:PHE:HE2	1:B:214:TRP:CZ3	2.34	0.46
1:B:209:SER:OG	1:B:211:LEU:HD12	2.16	0.46
1:B:202:TYR:CZ	1:B:204:SER:HB3	2.52	0.45
1:B:55:ASP:OD2	4:B:320:HOH:O	2.21	0.45
1:B:40:TYR:N	4:B:393:HOH:O	2.50	0.44
1:A:30:LYS:NZ	1:A:48:GLU:OE2	2.45	0.44
1:B:116:ASN:HA	1:B:117:PRO:HD3	1.77	0.44
1:A:113:LEU:HD22	1:A:126:PHE:CG	2.52	0.44
1:A:8:ASN:H	1:A:8:ASN:ND2	2.12	0.44
1:B:8:ASN:HD22	1:B:8:ASN:H	1.66	0.44
1:A:10:ARG:HD2	1:A:204:SER:O	2.18	0.43
1:B:34:MET:HE1	1:B:211:LEU:HD11	1.99	0.43
1:B:107:ARG:O	1:B:111:ILE:HG13	2.19	0.43
1:A:120:GLU:HB2	4:A:366:HOH:O	2.18	0.43
1:B:11:GLY:HA2	3:B:218:GPS:HZ5	2.01	0.43
1:B:209:SER:OG	1:B:211:LEU:HB2	2.19	0.43
1:B:210:LYS:HE2	4:B:332:HOH:O	2.17	0.43
1:B:68:LYS:NZ	4:B:346:HOH:O	2.36	0.42
1:A:104:MET:O	1:A:108:MET:HG2	2.19	0.42
1:B:37:ALA:HB2	1:B:40:TYR:CZ	2.55	0.42
1:A:19:LEU:HD23	1:A:19:LEU:C	2.45	0.41
1:B:172:LYS:HD2	1:B:175:ASP:OD2	2.20	0.41
1:B:207:ILE:HD12	1:B:214:TRP:CH2	2.55	0.41
1:A:153:THR:OG1	1:A:155:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LYS:HZ2	1:B:210:LYS:HG2	1.70	0.41
1:B:151:LYS:HE3	1:B:153:THR:CG2	2.48	0.41
1:B:115:TYR:HE2	1:B:211:LEU:HB2	1.86	0.41
1:B:107:ARG:NH2	4:B:362:HOH:O	2.53	0.41
1:A:217:LYS:HE3	1:A:217:LYS:HB2	1.94	0.40
1:B:164:ASP:O	1:B:168:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

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%)	211 (98%)	4 (2%)	0	100	100
1	B	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
All	All	430/434 (99%)	418 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/197 (100%)	190 (96%)	7 (4%)	31	15
1	B	197/197 (100%)	181 (92%)	16 (8%)	11	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	394/394 (100%)	371 (94%)	23 (6%)	18 5

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	26	SER
1	A	111	ILE
1	A	112	MET
1	A	144	ARG
1	A	151	LYS
1	A	178	PRO
1	B	3	ILE
1	B	8	ASN
1	B	19	LEU
1	B	26	SER
1	B	36	ASP
1	B	38	PRO
1	B	39	ASP
1	B	121	LYS
1	B	128	LYS
1	B	132	GLU
1	B	151	LYS
1	B	172	LYS
1	B	191	LYS
1	B	203	LEU
1	B	210	LYS
1	B	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	106	ASN
1	A	122	GLN
1	B	8	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](#)

5 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	0.77	0	6,6,6	0.25	0
3	GPS	B	218	-	35,37,37	1.80	7 (20%)	46,51,51	1.82	14 (30%)
2	SO4	A	219	-	4,4,4	0.80	0	6,6,6	0.16	0
2	SO4	A	218	-	4,4,4	0.74	0	6,6,6	0.43	0
3	GPS	A	221	-	35,37,37	1.72	8 (22%)	46,51,51	1.87	15 (32%)

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	GPS	B	218	-	2/2/8/10	0/27/43/43	0/3/3/3
3	GPS	A	221	-	2/2/8/10	2/27/43/43	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	218	GPS	CA4-SG2	-5.68	1.69	1.84
3	A	221	GPS	CA4-SG2	-5.14	1.71	1.84
3	B	218	GPS	CG4-CB4	3.40	1.43	1.39
3	B	218	GPS	CZ5-CH5	3.05	1.44	1.40
3	B	218	GPS	OE1-CD1	2.61	1.28	1.23
3	B	218	GPS	C2-N3	-2.54	1.27	1.33
3	A	221	GPS	CZ5-CH5	2.51	1.43	1.40
3	A	221	GPS	OE1-CD1	2.51	1.28	1.23
3	A	221	GPS	CB5-CA5	2.42	1.55	1.51
3	B	218	GPS	CH5-CB5	-2.40	1.37	1.40
3	B	218	GPS	CG1-CD1	-2.38	1.46	1.51
3	A	221	GPS	CB1-CG1	-2.36	1.45	1.52
3	A	221	GPS	CH4-CB4	2.35	1.43	1.40
3	A	221	GPS	CB1-CA1	2.26	1.58	1.53
3	A	221	GPS	CA2-C2	2.10	1.58	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	218	GPS	O32-C3-O31	-4.79	111.01	123.33
3	A	221	GPS	CB1-CG1-CD1	3.74	121.41	113.06
3	A	221	GPS	O2-C2-N3	3.60	130.59	122.98
3	B	218	GPS	CD4-CE4-CZ4	3.59	124.66	120.24
3	A	221	GPS	O2-C2-CA2	-3.52	113.11	120.48
3	B	218	GPS	CH5-CB5-CA5	3.24	122.64	118.64
3	B	218	GPS	CZ5-CH5-CB5	3.10	121.86	118.50
3	A	221	GPS	CD5-CG5-CB5	-3.05	117.34	120.99
3	B	218	GPS	CE4-CD4-CG4	-2.88	116.69	120.24
3	A	221	GPS	CZ5-CH5-CB5	2.87	121.61	118.50
3	B	218	GPS	CH5-CH4-CB4	-2.84	115.56	119.64
3	A	221	GPS	CE5-CZ5-CH5	-2.83	115.54	120.23
3	B	218	GPS	CE5-CZ5-CH5	-2.82	115.55	120.23
3	B	218	GPS	O32-C3-CA3	2.67	122.96	112.81
3	B	218	GPS	CD5-CE5-CZ5	2.52	123.35	120.24
3	A	221	GPS	O32-C3-O31	-2.44	117.05	123.33
3	A	221	GPS	CH5-CB5-CA5	2.41	121.62	118.64
3	A	221	GPS	CH5-CH4-CB4	-2.33	116.30	119.64
3	A	221	GPS	CG5-CB5-CA5	-2.32	116.31	120.94
3	B	218	GPS	CG5-CB5-CA5	-2.24	116.48	120.94
3	B	218	GPS	O2-C2-N3	2.23	127.69	122.98
3	A	221	GPS	CG5-CB5-CH5	2.22	122.07	119.35
3	A	221	GPS	CB4-CA4-SG2	-2.20	105.29	111.02
3	B	218	GPS	O12-C1-O11	-2.14	119.22	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	221	GPS	CD5-CE5-CZ5	2.11	122.85	120.24
3	B	218	GPS	CZ5-CH5-CH4	-2.11	117.33	121.61
3	B	218	GPS	CB1-CG1-CD1	2.08	117.71	113.06
3	A	221	GPS	CA2-N2-CD1	2.07	126.87	121.68
3	A	221	GPS	O5-CA5-CA4	-2.04	103.44	109.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	221	GPS	CA5
3	A	221	GPS	CA4
3	B	218	GPS	CA5
3	B	218	GPS	CA4

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	221	GPS	C1-CA1-CB1-CG1
3	A	221	GPS	N1-CA1-CB1-CG1

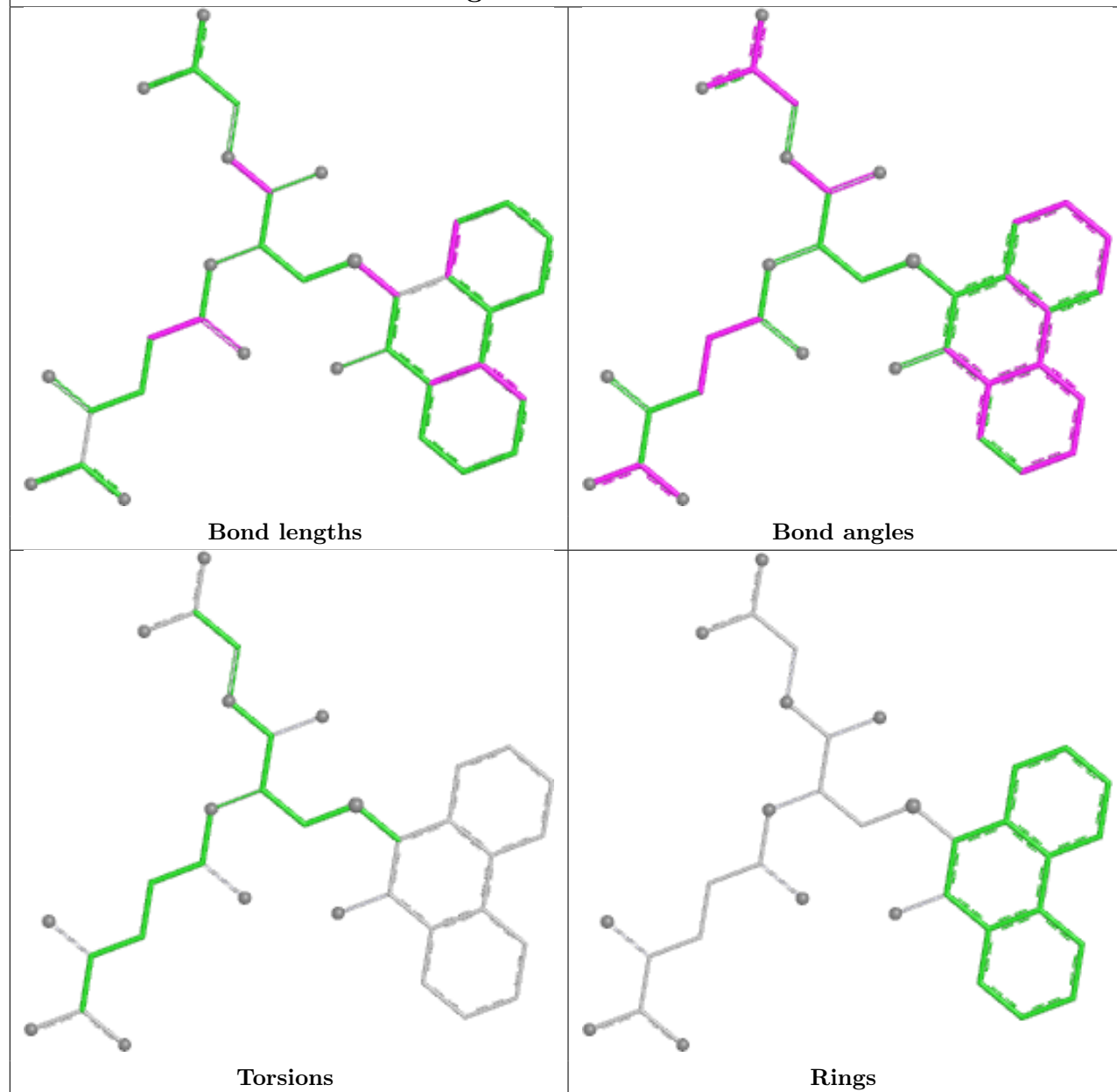
There are no ring outliers.

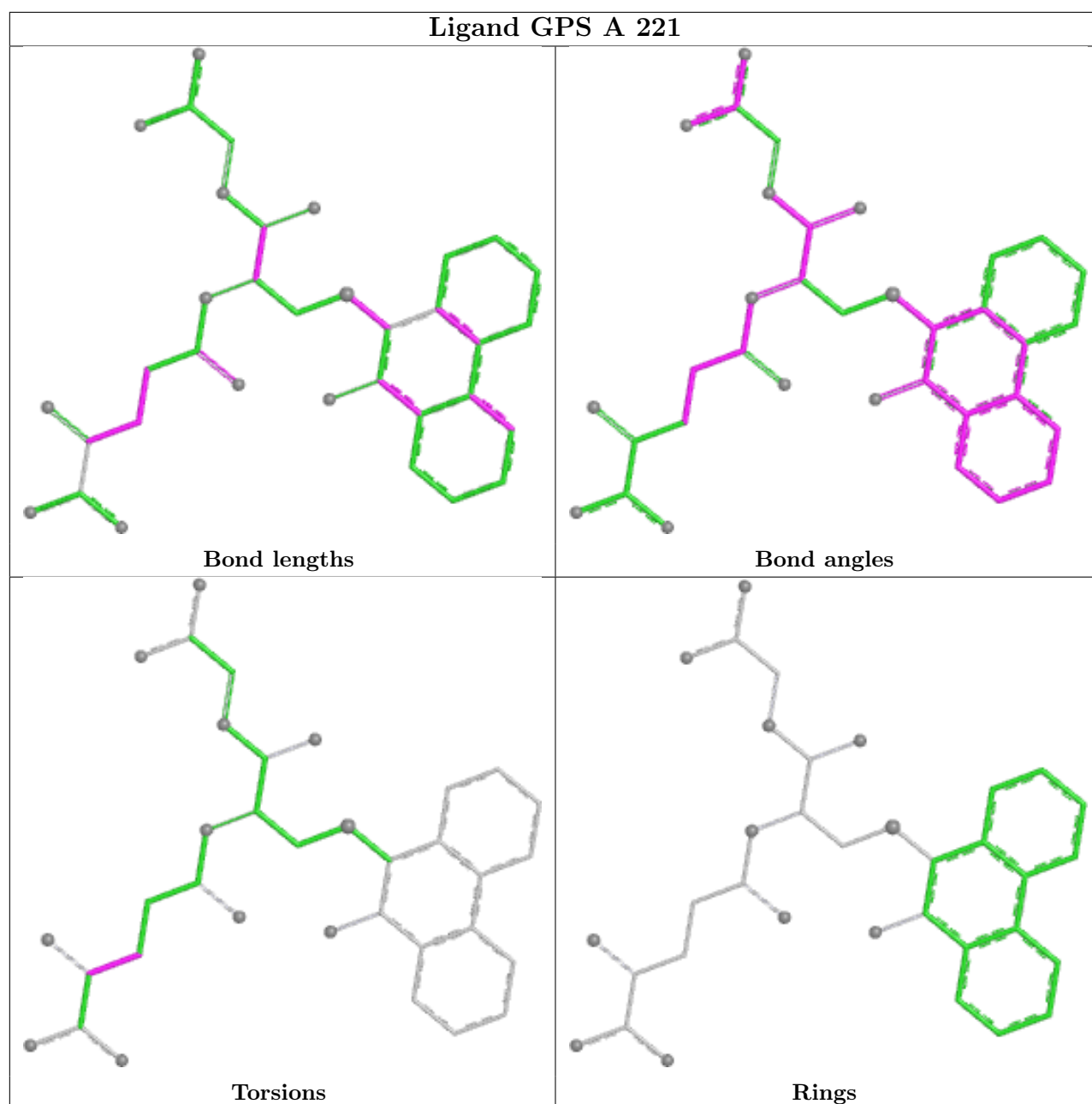
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	218	GPS	5	0
3	A	221	GPS	8	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.

Ligand GPS B 218





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.