



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:11 PM EDT

PDB ID : 6GSV  
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 : 1.75 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

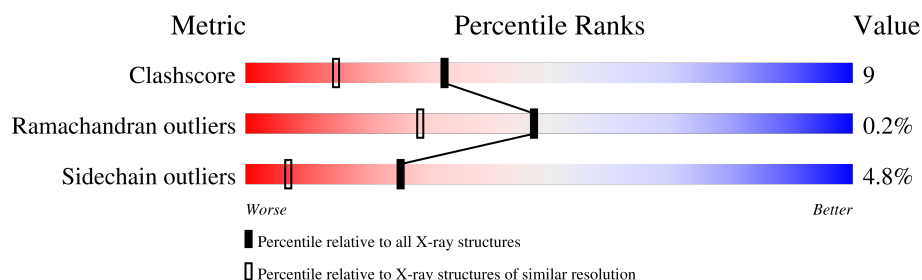
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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  $\geq 3$ , 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	220	X	-	-	-
3	GPS	B	219	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4191 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.

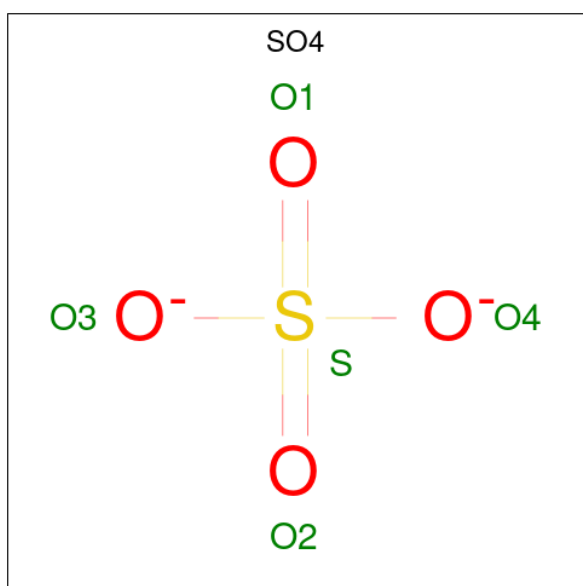
- Molecule 1 is a protein called MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1817	1176	303	327	11			
1	B	217	Total	C	N	O	S	0	0	0
			1817	1176	303	327	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	THR	engineered mutation	UNP P04905
B	13	SER	THR	engineered mutation	UNP P04905

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



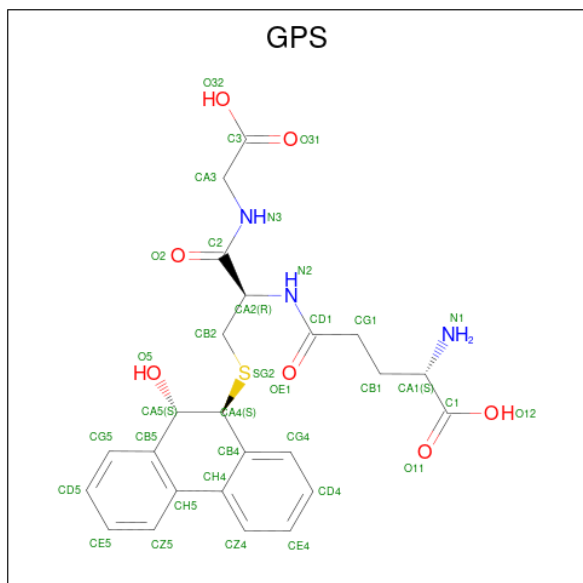
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	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 (three-letter code: GPS) (formula: C<sub>24</sub>H<sub>27</sub>N<sub>3</sub>O<sub>7</sub>S).



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	220	Total	O	0	0
			220	220		
4	B	252	Total	O	0	0
			252	252		

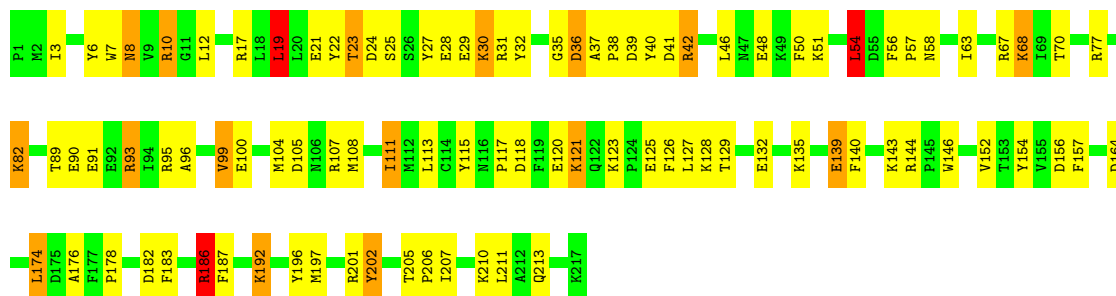
### 3 Residue-property plots

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.

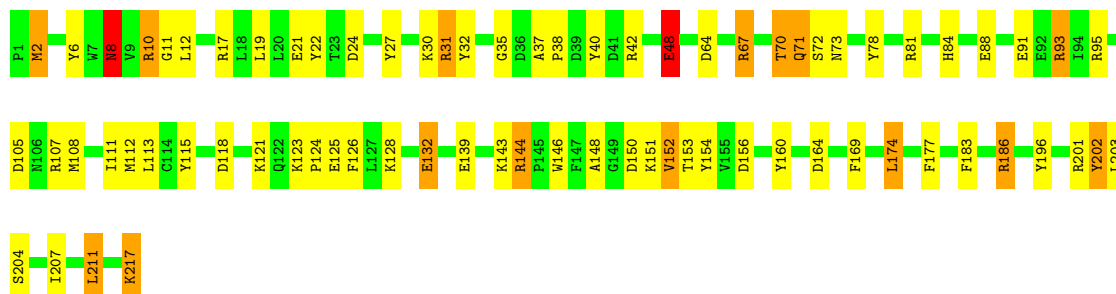
#### • Molecule 1: MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3

Chain A: 



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

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, $\alpha$ , $\beta$ , $\gamma$	86.62Å 68.54Å 80.37Å 90.00° 105.74° 90.00°	Depositor
Resolution (Å)	6.00 – 1.75	Depositor
% Data completeness (in resolution range)	94.0 (6.00-1.75)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, $R_{free}$	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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	1.13	1/1866 (0.1%)	2.15	77/2513 (3.1%)
1	B	1.17	4/1866 (0.2%)	2.07	61/2513 (2.4%)
All	All	1.15	5/3732 (0.1%)	2.11	138/5026 (2.7%)

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	2
1	B	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	GLU	CD-OE2	-7.28	1.17	1.25
1	B	72	SER	CB-OG	5.80	1.49	1.42
1	B	196	TYR	CE2-CZ	5.64	1.45	1.38
1	B	21	GLU	CD-OE1	-5.57	1.19	1.25
1	A	90	GLU	CD-OE1	-5.09	1.20	1.25

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ARG	NE-CZ-NH2	-18.83	110.88	120.30
1	A	17	ARG	NE-CZ-NH2	-17.55	111.52	120.30
1	B	144	ARG	NE-CZ-NH1	17.52	129.06	120.30
1	A	186	ARG	NE-CZ-NH1	16.97	128.79	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ARG	NE-CZ-NH1	16.46	128.53	120.30
1	A	17	ARG	NE-CZ-NH1	16.00	128.30	120.30
1	B	10	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	A	144	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	B	31	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	107	ARG	NE-CZ-NH1	13.13	126.86	120.30
1	B	31	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	A	10	ARG	NE-CZ-NH2	-12.49	114.05	120.30
1	A	202	TYR	CB-CG-CD2	-12.14	113.72	121.00
1	B	78	TYR	CB-CG-CD2	-11.82	113.91	121.00
1	B	93	ARG	CD-NE-CZ	11.78	140.10	123.60
1	A	31	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	154	TYR	CB-CG-CD1	-11.42	114.15	121.00
1	B	91	GLU	CB-CG-CD	11.07	144.08	114.20
1	A	93	ARG	NE-CZ-NH2	-10.99	114.81	120.30
1	A	186	ARG	NE-CZ-NH2	-10.89	114.85	120.30
1	A	182	ASP	CB-CG-OD2	-10.89	108.50	118.30
1	A	144	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	139	GLU	CG-CD-OE2	-10.52	97.26	118.30
1	B	93	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	B	95	ARG	CD-NE-CZ	10.41	138.18	123.60
1	A	105	ASP	CB-CG-OD1	10.27	127.54	118.30
1	B	202	TYR	CB-CG-CD1	-9.79	115.13	121.00
1	B	42	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	B	17	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	183	PHE	CB-CG-CD1	-9.04	114.47	120.80
1	A	54	LEU	CB-CG-CD2	8.68	125.75	111.00
1	A	36	ASP	CB-CG-OD1	8.59	126.03	118.30
1	A	91	GLU	CB-CG-CD	8.56	137.31	114.20
1	A	54	LEU	CB-CG-CD1	-8.54	96.48	111.00
1	B	160	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	A	182	ASP	CB-CG-OD1	8.43	125.88	118.30
1	B	148	ALA	CB-CA-C	-8.39	97.52	110.10
1	A	105	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	B	22	TYR	CB-CG-CD2	-8.31	116.01	121.00
1	B	144	ARG	CD-NE-CZ	8.24	135.13	123.60
1	A	132	GLU	OE1-CD-OE2	-8.06	113.63	123.30
1	B	105	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	186	ARG	CD-NE-CZ	7.86	134.60	123.60
1	A	107	ARG	CD-NE-CZ	7.82	134.55	123.60
1	A	24	ASP	CB-CG-OD1	7.78	125.30	118.30
1	B	24	ASP	CB-CG-OD1	7.72	125.25	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	MET	CG-SD-CE	-7.70	87.87	100.20
1	A	10	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	67	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	139	GLU	OE1-CD-OE2	7.62	132.44	123.30
1	A	6	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	B	42	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	115	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	B	107	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	B	164	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	91	GLU	CG-CD-OE1	7.45	133.20	118.30
1	A	42	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	25	SER	O-C-N	7.37	134.50	122.70
1	A	95	ARG	O-C-N	7.37	134.50	122.70
1	B	174	LEU	CB-CG-CD1	7.36	123.51	111.00
1	A	154	TYR	CB-CG-CD2	7.34	125.41	121.00
1	A	19	LEU	CB-CG-CD2	7.34	123.47	111.00
1	B	2	MET	CA-CB-CG	-7.34	100.83	113.30
1	B	48	GLU	CG-CD-OE1	-7.28	103.75	118.30
1	B	132	GLU	CB-CG-CD	7.23	133.72	114.20
1	A	8	ASN	CA-CB-CG	7.18	129.20	113.40
1	B	91	GLU	OE1-CD-OE2	-7.16	114.71	123.30
1	B	107	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	56	PHE	CB-CG-CD2	-7.03	115.88	120.80
1	B	152	VAL	CA-CB-CG2	6.91	121.27	110.90
1	A	187	PHE	CB-CG-CD1	-6.80	116.04	120.80
1	B	118	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	B	70	THR	O-C-N	6.66	133.36	122.70
1	A	32	TYR	CB-CG-CD1	6.65	124.99	121.00
1	B	107	ARG	NH1-CZ-NH2	-6.65	112.09	119.40
1	B	48	GLU	CG-CD-OE2	6.64	131.58	118.30
1	B	148	ALA	N-CA-CB	6.59	119.33	110.10
1	A	91	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	A	70	THR	CA-CB-CG2	-6.40	103.44	112.40
1	B	154	TYR	CG-CD1-CE1	-6.32	116.24	121.30
1	A	139	GLU	CG-CD-OE1	6.25	130.81	118.30
1	A	96	ALA	CB-CA-C	6.23	119.45	110.10
1	B	93	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	118	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	A	48	GLU	O-C-N	6.15	132.53	122.70
1	B	150	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	139	GLU	OE1-CD-OE2	6.11	130.63	123.30
1	A	156	ASP	CB-CG-OD2	-6.07	112.83	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	TYR	CB-CG-CD1	6.04	124.62	121.00
1	A	39	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	23	THR	O-C-N	6.03	132.35	122.70
1	A	29	GLU	CG-CD-OE2	-5.95	106.41	118.30
1	A	50	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	B	156	ASP	CB-CG-OD1	-5.92	112.98	118.30
1	A	95	ARG	CD-NE-CZ	5.82	131.75	123.60
1	B	78	TYR	CD1-CG-CD2	5.76	124.23	117.90
1	B	81	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	68	LYS	O-C-N	5.72	131.85	122.70
1	A	41	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	84	HIS	CA-CB-CG	-5.62	104.05	113.60
1	B	169	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	A	201	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	183	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	A	152	VAL	CA-CB-CG1	5.53	119.19	110.90
1	A	107	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
1	B	154	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	58	ASN	N-CA-CB	-5.50	100.70	110.60
1	A	8	ASN	CB-CG-OD1	5.49	132.57	121.60
1	B	160	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	93	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	A	213	GLN	CB-CG-CD	5.43	125.72	111.60
1	B	73	ASN	CB-CG-OD1	5.41	132.42	121.60
1	B	81	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	157	PHE	CB-CG-CD1	5.40	124.58	120.80
1	A	7	TRP	CE3-CZ3-CH2	5.39	127.13	121.20
1	A	99	VAL	O-C-N	5.39	131.32	122.70
1	A	164	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	67	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	201	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	27	TYR	CB-CG-CD1	5.32	124.19	121.00
1	B	95	ARG	O-C-N	5.29	131.16	122.70
1	B	19	LEU	O-C-N	5.24	131.09	122.70
1	A	202	TYR	CB-CG-CD1	5.23	124.14	121.00
1	A	54	LEU	CD1-CG-CD2	-5.23	94.82	110.50
1	B	177	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	A	77	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	67	ARG	CD-NE-CZ	-5.18	116.35	123.60
1	A	91	GLU	N-CA-CB	5.17	119.92	110.60
1	A	121	LYS	CA-CB-CG	5.16	124.76	113.40
1	B	186	ARG	CD-NE-CZ	5.14	130.80	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	GLU	CG-CD-OE1	5.12	128.55	118.30
1	A	120	GLU	CG-CD-OE1	5.09	128.49	118.30
1	B	6	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
1	B	22	TYR	CG-CD2-CE2	-5.06	117.25	121.30
1	B	8	ASN	CB-CA-C	5.04	120.48	110.40
1	A	99	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	A	174	LEU	O-C-N	5.03	130.74	122.70
1	A	100	GLU	CG-CD-OE1	5.01	128.32	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Sidechain
1	A	30	LYS	Mainchain
1	B	144	ARG	Sidechain
1	B	186	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	1817	0	1803	32	3
1	B	1817	0	1803	26	2
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	35	0	25	4	0
3	B	35	0	25	7	0
4	A	220	0	0	1	0
4	B	252	0	0	2	0
All	All	4191	0	3656	64	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 9.

All (64) 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:125:GLU:HA	1:B:128:LYS:HD2	1.45	0.97
3:A:220:GPS:CG4	3:A:220:GPS:HB2	2.06	0.85
3:A:220:GPS:HB2	3:A:220:GPS:HG4	1.59	0.83
1:A:63:ILE:HD12	1:A:68:LYS:HD3	1.66	0.78
1:B:151:LYS:HE2	1:B:153:THR:HG22	1.67	0.76
1:B:111:ILE:HD11	3:B:219:GPS:CD5	2.17	0.74
1:A:125:GLU:HA	1:A:128:LYS:HE3	1.80	0.63
1:B:111:ILE:HD11	3:B:219:GPS:CE5	2.32	0.60
1:B:37:ALA:HB2	1:B:40:TYR:CZ	2.40	0.57
1:B:113:LEU:HD22	1:B:126:PHE:CG	2.40	0.56
1:A:54:LEU:HD13	1:A:57:PRO:HA	1.88	0.55
1:A:125:GLU:O	1:A:129:THR:HG23	2.06	0.55
3:B:219:GPS:CG4	3:B:219:GPS:HB2	2.35	0.54
1:B:111:ILE:CD1	3:B:219:GPS:CD5	2.86	0.54
1:A:21:GLU:HG3	1:A:196:TYR:CG	2.45	0.52
1:B:202:TYR:CE2	1:B:204:SER:HB3	2.45	0.52
1:B:11:GLY:HA2	3:B:219:GPS:HZ5	1.92	0.51
1:A:54:LEU:HD13	1:A:57:PRO:CB	2.40	0.51
1:B:108:MET:O	1:B:112:MET:HG3	2.11	0.51
1:B:2:MET:HG2	1:B:64:ASP:HA	1.93	0.50
1:A:205:THR:HB	1:A:206:PRO:HA	1.93	0.50
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.93	0.50
1:A:42:ARG:HH21	1:A:46:LEU:HD21	1.74	0.50
1:B:30:LYS:HD3	1:B:32:TYR:CZ	2.46	0.50
1:B:146:TRP:CE2	1:B:152:VAL:HG22	2.47	0.50
1:B:8:ASN:CB	1:B:31:ARG:HB3	2.42	0.49
1:A:21:GLU:HG3	1:A:196:TYR:CD1	2.47	0.49
1:B:132:GLU:HB3	4:B:256:HOH:O	2.12	0.48
1:A:125:GLU:OE1	1:A:128:LYS:NZ	2.41	0.48
1:A:104:MET:O	1:A:108:MET:HG2	2.13	0.48
1:B:35:GLY:O	1:B:40:TYR:HA	2.13	0.47
1:B:217:LYS:OXT	1:B:217:LYS:HG2	2.15	0.47
1:A:35:GLY:O	1:A:40:TYR:HA	2.14	0.47
1:A:135:LYS:O	1:A:139:GLU:HG3	2.15	0.47
1:A:54:LEU:HD13	1:A:57:PRO:CA	2.44	0.47
3:B:219:GPS:HB2	3:B:219:GPS:HG4	1.97	0.46
1:A:111:ILE:HD11	3:A:220:GPS:CZ5	2.45	0.46
1:A:123:LYS:O	1:A:127:LEU:HG	2.16	0.45
1:A:22:TYR:O	1:A:192:LYS:HE3	2.17	0.45
1:A:89:THR:O	1:A:93:ARG:HG3	2.15	0.45
1:B:123:LYS:HB3	1:B:124:PRO:HD3	1.98	0.45
1:A:176:ALA:O	1:A:178:PRO:HD3	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:HG2	1:A:202:TYR:CE1	2.52	0.45
1:B:37:ALA:HB1	1:B:38:PRO:HA	2.00	0.44
1:B:8:ASN:HB3	1:B:31:ARG:HB3	2.00	0.44
1:B:115:TYR:HE2	1:B:211:LEU:HB3	1.82	0.44
1:A:19:LEU:HD22	1:A:23:THR:HG23	2.00	0.44
1:A:37:ALA:HB2	1:A:40:TYR:CZ	2.53	0.44
1:A:99:VAL:CG2	1:A:140:PHE:HE2	2.29	0.44
1:A:82:LYS:HB2	1:A:82:LYS:HZ3	1.83	0.43
1:A:54:LEU:HD13	1:A:57:PRO:HB3	1.99	0.43
1:A:37:ALA:HB1	1:A:38:PRO:HA	2.00	0.43
1:B:203:LEU:HD23	1:B:203:LEU:C	2.40	0.42
1:A:113:LEU:HD22	1:A:126:PHE:CG	2.55	0.42
1:A:192:LYS:HD3	1:A:192:LYS:H	1.85	0.42
1:B:70:THR:O	1:B:71:GLN:HB2	2.19	0.42
1:A:3:ILE:HG12	1:A:28:GLU:CG	2.50	0.41
1:A:10:ARG:HB3	1:A:207:ILE:HA	2.02	0.41
1:B:32:TYR:HE1	1:B:48:GLU:OE1	2.03	0.41
1:A:36:ASP:OD1	1:A:210:LYS:NZ	2.44	0.41
1:A:146:TRP:CH2	1:A:186:ARG:HG2	2.56	0.41
3:A:220:GPS:HA4	3:A:220:GPS:HA2	1.76	0.41
4:A:333:HOH:O	3:B:219:GPS:HG5	2.20	0.41
1:B:93:ARG:NH1	4:B:317:HOH:O	2.44	0.41

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:B:67:ARG:NH2	1:B:67:ARG:NH2[2_555]	1.58	0.62
1:A:121:LYS:NZ	1:B:143:LYS:O[3_555]	1.91	0.29
1:A:51:LYS:NZ	1:A:197:MET:O[4_546]	2.00	0.20
1:A:38:PRO:CB	1:A:211:LEU:CD1[2_656]	2.13	0.07

## 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%)	210 (98%)	5 (2%)	0	100	100
1	B	215/217 (99%)	208 (97%)	6 (3%)	1 (0%)	29	12
All	All	430/434 (99%)	418 (97%)	11 (3%)	1 (0%)	47	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLN

### 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%)	186 (94%)	11 (6%)	21	5
1	B	197/197 (100%)	189 (96%)	8 (4%)	30	10
All	All	394/394 (100%)	375 (95%)	19 (5%)	25	7

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	LEU
1	A	19	LEU
1	A	30	LYS
1	A	54	LEU
1	A	82	LYS
1	A	111	ILE
1	A	117	PRO
1	A	143	LYS
1	A	174	LEU
1	A	192	LYS
1	B	8	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	12	LEU
1	B	48	GLU
1	B	88	GLU
1	B	121	LYS
1	B	174	LEU
1	B	211	LEU
1	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	213	GLN
1	B	8	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 monosaccharides 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	218	-	4,4,4	0.61	0	6,6,6	0.39	0
3	GPS	B	219	-	29,37,37	2.03	9 (31%)	37,51,51	1.92	12 (32%)
2	SO4	A	219	-	4,4,4	0.58	0	6,6,6	0.46	0
2	SO4	B	218	-	4,4,4	0.64	0	6,6,6	0.19	0
3	GPS	A	220	-	29,37,37	1.83	7 (24%)	37,51,51	2.27	16 (43%)

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	219	-	2/2/8/10	1/21/43/43	0/3/3/3
3	GPS	A	220	-	2/2/8/10	1/21/43/43	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	219	GPS	CA4-SG2	-4.90	1.71	1.84
3	A	220	GPS	CA4-SG2	-4.45	1.72	1.84
3	A	220	GPS	CA1-N1	4.27	1.56	1.47
3	B	219	GPS	CA3-N3	4.08	1.53	1.46
3	B	219	GPS	CG4-CB4	3.97	1.44	1.39
3	B	219	GPS	CA1-N1	3.88	1.55	1.47
3	A	220	GPS	C2-N3	-3.28	1.26	1.33
3	A	220	GPS	CZ5-CH5	3.28	1.45	1.40
3	B	219	GPS	C2-N3	-2.94	1.27	1.33
3	B	219	GPS	O5-CA5	2.89	1.48	1.42
3	A	220	GPS	CA2-C2	2.51	1.59	1.52
3	A	220	GPS	CG4-CB4	2.45	1.42	1.39
3	B	219	GPS	CZ5-CH5	2.40	1.43	1.40
3	B	219	GPS	CH5-CB5	-2.38	1.37	1.40
3	B	219	GPS	CA2-C2	2.32	1.58	1.52
3	A	220	GPS	CD1-N2	2.06	1.38	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	220	GPS	CB4-CA4-SG2	-5.29	97.59	111.17
3	A	220	GPS	O2-C2-CA2	-4.51	110.96	120.45
3	B	219	GPS	O2-C2-N3	4.46	132.57	122.99

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	220	GPS	O2-C2-N3	4.10	131.80	122.99
3	B	219	GPS	O5-CA5-CB5	-4.09	102.42	110.49
3	B	219	GPS	O2-C2-CA2	-3.99	112.06	120.45
3	A	220	GPS	O5-CA5-CB5	-3.69	103.22	110.49
3	A	220	GPS	CG5-CB5-CA5	-3.36	113.52	120.87
3	A	220	GPS	CG1-CB1-CA1	-3.19	106.41	113.84
3	A	220	GPS	CH5-CB5-CA5	2.89	123.43	119.00
3	A	220	GPS	CD5-CG5-CB5	-2.88	117.35	121.01
3	A	220	GPS	CA5-CA4-SG2	-2.83	102.21	110.88
3	B	219	GPS	CH5-CH4-CB4	-2.82	115.64	119.64
3	A	220	GPS	CG5-CB5-CH5	2.78	122.98	119.32
3	B	219	GPS	CG5-CB5-CA5	-2.72	114.91	120.87
3	A	220	GPS	CD4-CE4-CZ4	2.61	124.17	120.19
3	B	219	GPS	CD5-CG5-CB5	-2.60	117.70	121.01
3	B	219	GPS	CH5-CB5-CA5	2.56	122.91	119.00
3	A	220	GPS	CZ4-CH4-CB4	-2.45	115.82	118.53
3	A	220	GPS	CG1-CD1-N2	-2.40	111.67	115.83
3	B	219	GPS	CD4-CE4-CZ4	2.35	123.77	120.19
3	A	220	GPS	CG4-CB4-CH4	2.33	122.38	119.32
3	B	219	GPS	C2-CA2-N2	-2.29	104.93	111.16
3	A	220	GPS	C2-CA2-N2	-2.23	105.09	111.16
3	A	220	GPS	CE4-CD4-CG4	-2.17	116.88	120.19
3	B	219	GPS	CG5-CB5-CH5	2.12	122.11	119.32
3	B	219	GPS	CA3-N3-C2	-2.11	119.30	122.34
3	B	219	GPS	CB4-CA4-SG2	-2.03	105.96	111.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	220	GPS	CA5
3	A	220	GPS	CA4
3	B	219	GPS	CA5
3	B	219	GPS	CA4

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	219	GPS	OE1-CD1-N2-CA2
3	A	220	GPS	OE1-CD1-N2-CA2

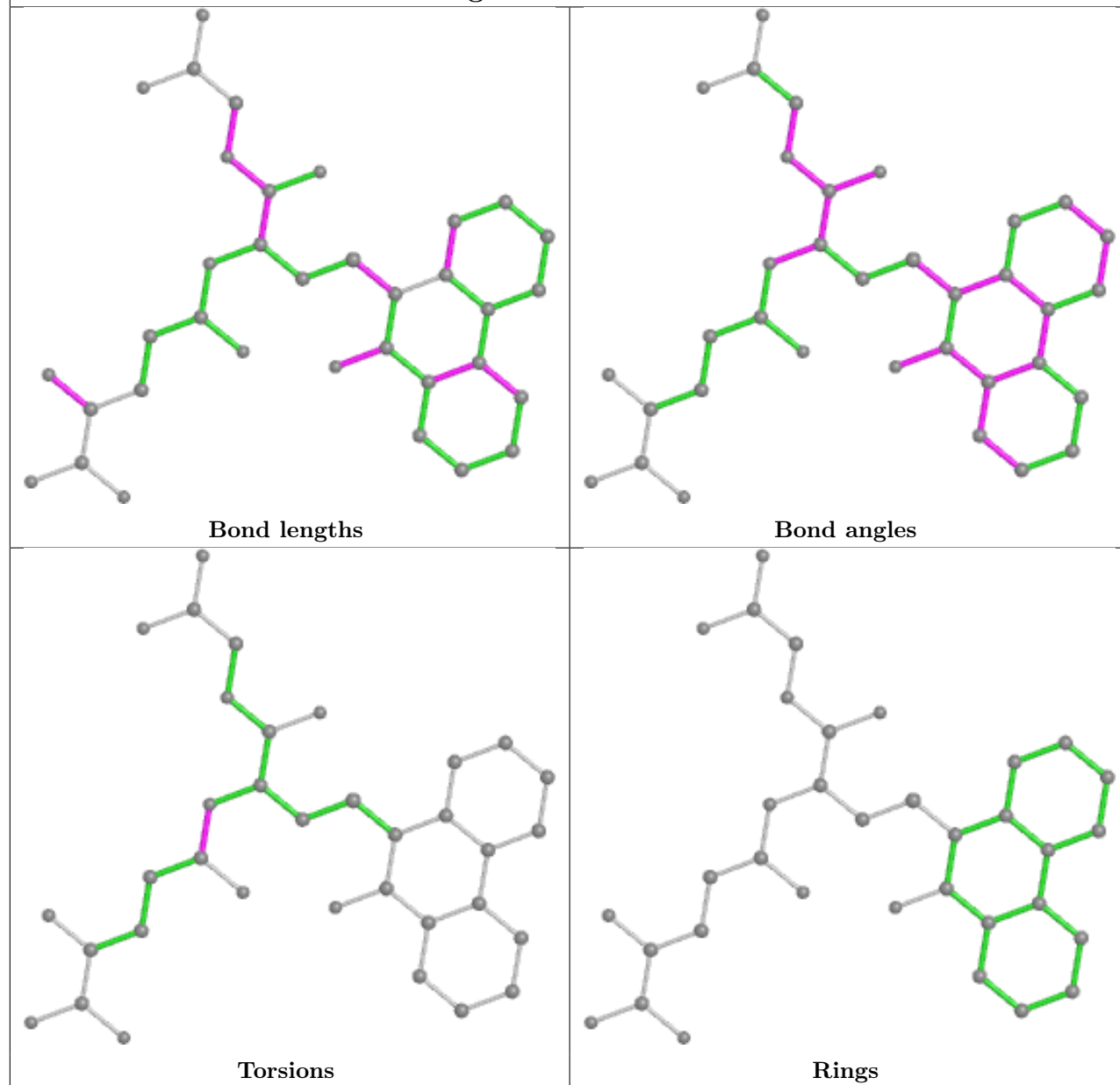
There are no ring outliers.

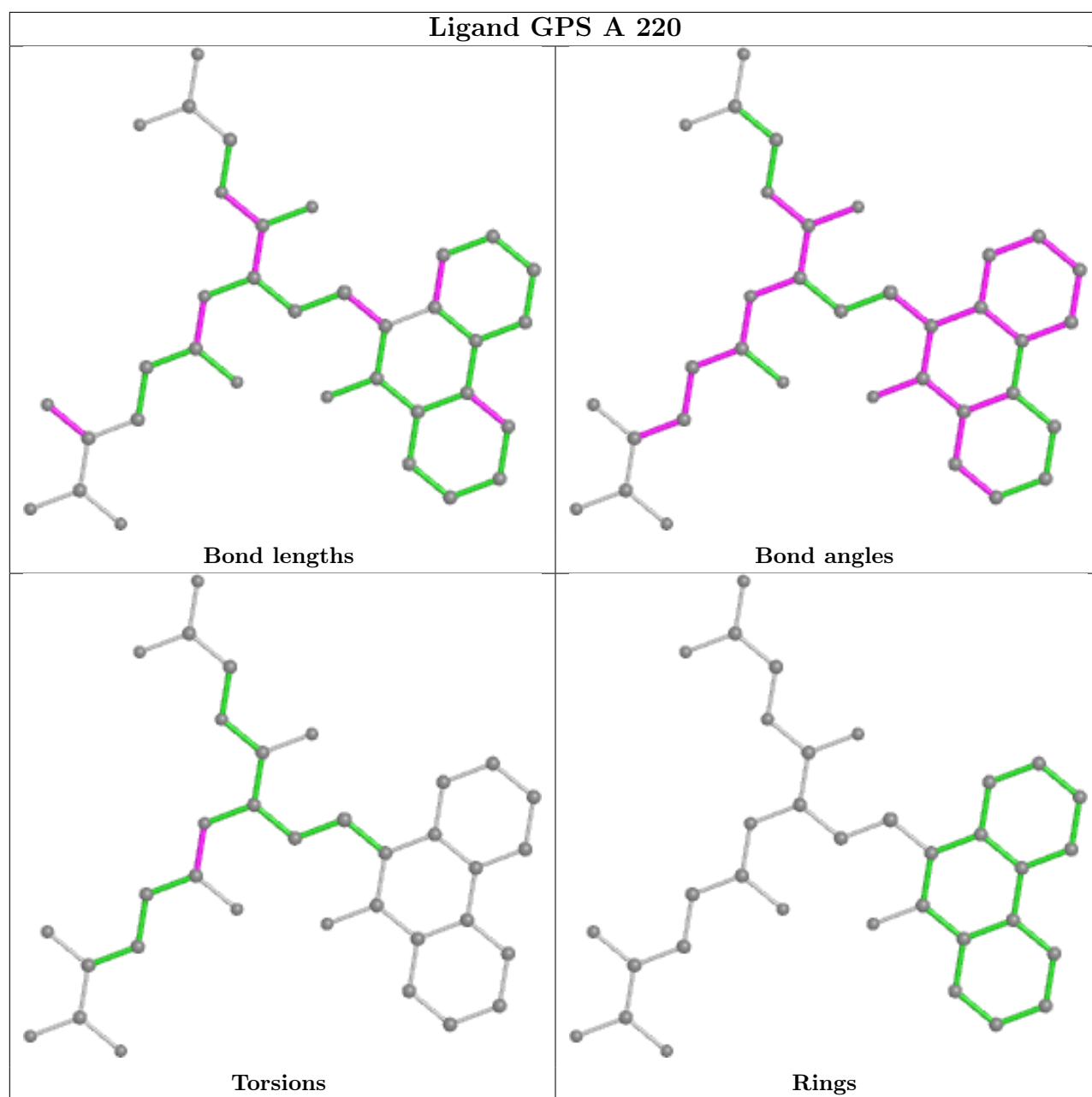
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	219	GPS	7	0
3	A	220	GPS	4	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 219





## 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.