



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 6GSV / pdb_00006gsv
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

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

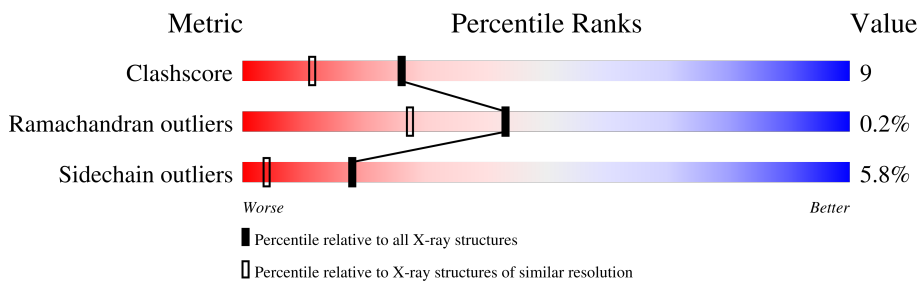
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (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 ≥ 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.

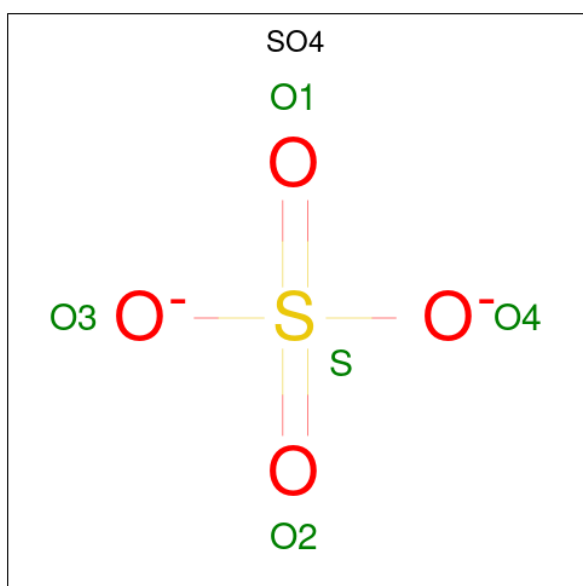
- Molecule 1 is a protein called MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3.

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 (CCD ID: SO4) (formula: O₄S).



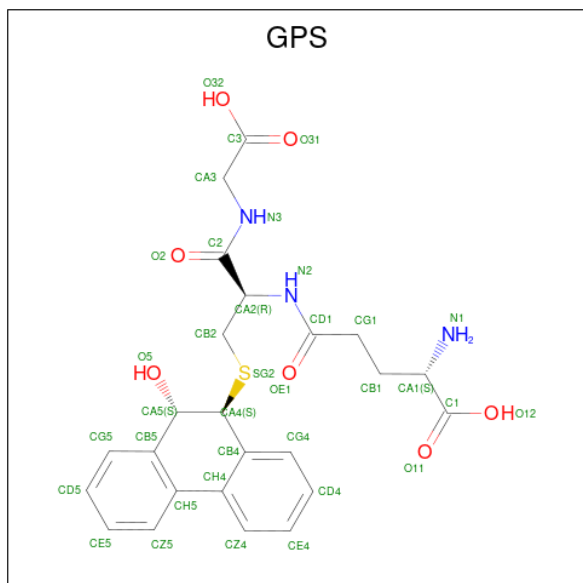
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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

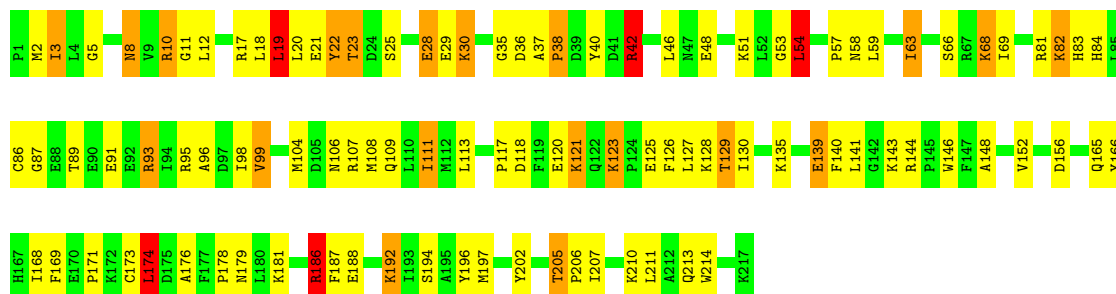
3 Residue-property plots

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.

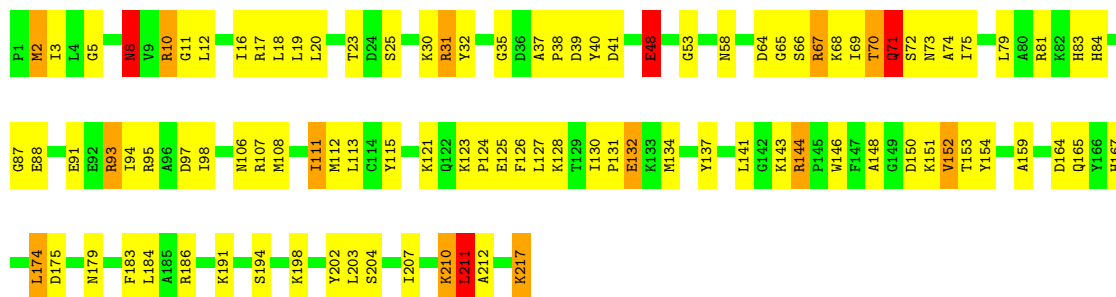
• Molecule 1: MU CLASS GLUTATHIONE S-TRANSFERASE OF ISOENZYME 3-3

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, α , β , γ	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 ²)	16.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GPS

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	1.42	9/1866 (0.5%)	2.32	102/2513 (4.1%)
1	B	1.44	5/1866 (0.3%)	2.30	108/2513 (4.3%)
All	All	1.43	14/3732 (0.4%)	2.31	210/5026 (4.2%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	LEU	CA-C	7.23	1.60	1.52
1	A	96	ALA	N-CA	7.19	1.55	1.46
1	A	87	GLY	N-CA	6.73	1.53	1.45
1	A	69	ILE	N-CA	6.21	1.53	1.46
1	B	154	TYR	C-N	6.17	1.40	1.34
1	B	130	ILE	CA-CB	5.95	1.57	1.54
1	B	5	GLY	CA-C	5.92	1.56	1.52
1	B	20	LEU	N-CA	5.90	1.53	1.46
1	B	71	GLN	N-CA	5.50	1.53	1.46
1	A	98	ILE	CA-CB	5.42	1.60	1.54
1	A	20	LEU	N-CA	5.38	1.52	1.46
1	A	166	TYR	C-N	-5.21	1.27	1.33
1	A	63	ILE	CA-CB	5.09	1.60	1.54
1	A	205	THR	CA-C	5.07	1.57	1.52

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	GLU	CB-CG-CD	18.52	144.08	112.60
1	A	8	ASN	CA-CB-CG	16.60	129.20	112.60
1	A	91	GLU	CB-CG-CD	14.54	137.31	112.60
1	B	132	GLU	CB-CG-CD	12.43	133.72	112.60
1	A	95	ARG	O-C-N	11.68	134.50	122.12
1	B	93	ARG	CD-NE-CZ	11.21	140.10	124.40
1	A	205	THR	O-C-N	10.86	128.66	121.71
1	B	8	ASN	OD1-CG-ND2	10.74	133.34	122.60
1	A	25	SER	O-C-N	9.86	134.50	122.86
1	A	8	ASN	OD1-CG-ND2	-9.86	112.75	122.60
1	B	95	ARG	CD-NE-CZ	9.84	138.18	124.40
1	B	84	HIS	CA-CB-CG	-9.75	104.05	113.80
1	A	99	VAL	O-C-N	9.61	131.32	121.91
1	B	144	ARG	NE-CZ-NH2	-9.24	110.88	119.20
1	A	139	GLU	CG-CD-OE2	-9.19	97.26	118.40
1	B	5	GLY	O-C-N	8.98	130.52	123.61
1	B	95	ARG	O-C-N	8.83	131.16	122.07
1	A	166	TYR	CA-C-N	8.77	132.04	120.28
1	A	166	TYR	C-N-CA	8.77	132.04	120.28
1	A	28	GLU	CB-CG-CD	8.54	127.11	112.60
1	A	17	ARG	NE-CZ-NH2	-8.53	111.52	119.20
1	A	141	LEU	O-C-N	8.21	130.52	122.07
1	A	5	GLY	CA-C-O	-8.06	113.17	120.75
1	B	194	SER	O-C-N	8.03	130.63	122.12
1	A	84	HIS	CA-CB-CG	-7.99	105.81	113.80
1	B	150	ASP	CA-CB-CG	7.95	120.55	112.60
1	B	73	ASN	CA-CB-CG	-7.73	104.87	112.60
1	A	118	ASP	CA-CB-CG	-7.72	104.88	112.60
1	A	213	GLN	CB-CG-CD	7.71	125.72	112.60
1	B	70	THR	O-C-N	7.70	133.36	122.74
1	B	144	ARG	CD-NE-CZ	7.67	135.13	124.40
1	B	144	ARG	NE-CZ-NH1	7.56	129.06	121.50
1	B	137	TYR	CA-C-N	7.50	130.19	120.44
1	B	137	TYR	C-N-CA	7.50	130.19	120.44
1	A	48	GLU	O-C-N	7.50	132.53	122.26
1	B	164	ASP	CA-C-O	-7.42	113.03	120.82
1	A	68	LYS	O-C-N	7.33	131.85	123.27
1	B	183	PHE	O-C-N	7.29	129.58	122.07
1	A	186	ARG	NE-CZ-NH1	7.29	128.79	121.50
1	A	186	ARG	CD-NE-CZ	7.29	134.60	124.40
1	B	10	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	A	54	LEU	CD1-CG-CD2	-7.26	94.82	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ARG	CD-NE-CZ	7.25	134.55	124.40
1	A	87	GLY	N-CA-C	-7.24	103.60	111.93
1	A	23	THR	O-C-N	7.23	132.35	122.37
1	B	184	LEU	O-C-N	7.22	129.78	122.12
1	A	95	ARG	CA-C-O	-7.19	112.93	120.55
1	A	174	LEU	O-C-N	7.13	130.74	122.25
1	B	93	ARG	NE-CZ-NH2	7.06	125.55	119.20
1	B	10	ARG	NE-CZ-NH1	7.03	128.53	121.50
1	A	173	CYS	N-CA-C	6.92	120.82	112.38
1	B	19	LEU	O-C-N	6.81	131.09	122.23
1	A	17	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	A	144	ARG	NE-CZ-NH2	-6.73	113.14	119.20
1	A	91	GLU	N-CA-CB	6.70	119.92	109.94
1	A	148	ALA	O-C-N	6.70	131.63	122.46
1	B	17	ARG	CA-C-O	6.68	127.63	120.55
1	B	87	GLY	N-CA-C	-6.67	103.53	112.14
1	A	18	LEU	CA-C-O	-6.67	113.48	120.55
1	B	5	GLY	CA-C-O	-6.66	115.12	120.91
1	B	2	MET	CA-CB-CG	-6.64	100.83	114.10
1	A	205	THR	CA-C-O	-6.63	114.40	120.50
1	A	83	HIS	CA-CB-CG	-6.59	107.21	113.80
1	A	156	ASP	O-C-N	6.54	130.31	122.27
1	A	59	LEU	O-C-N	6.50	127.18	121.39
1	A	168	ILE	CA-C-O	6.50	127.74	120.85
1	B	81	ARG	O-C-N	6.49	129.00	122.12
1	A	58	ASN	N-CA-CB	-6.47	100.70	111.57
1	B	83	HIS	O-C-N	6.46	129.94	122.25
1	B	19	LEU	CA-C-O	-6.45	113.08	120.24
1	A	91	GLU	CG-CD-OE1	6.43	133.20	118.40
1	B	152	VAL	CA-CB-CG2	6.39	121.27	110.40
1	B	48	GLU	CG-CD-OE1	-6.37	103.75	118.40
1	B	159	ALA	CA-C-O	-6.36	114.15	120.70
1	B	159	ALA	O-C-N	6.33	128.93	122.09
1	B	148	ALA	CB-CA-C	-6.30	97.52	110.38
1	B	94	ILE	CA-C-N	6.26	128.58	120.44
1	B	94	ILE	C-N-CA	6.26	128.58	120.44
1	B	131	PRO	O-C-N	6.24	129.72	122.23
1	B	141	LEU	O-C-N	6.23	129.25	122.15
1	A	95	ARG	CA-C-N	-6.21	111.47	120.29
1	A	95	ARG	C-N-CA	-6.21	111.47	120.29
1	B	179	ASN	CA-C-O	-6.20	113.98	120.55
1	A	84	HIS	CB-CA-C	-6.18	103.58	111.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ILE	CB-CG1-CD1	-6.17	100.83	113.80
1	B	150	ASP	N-CA-C	6.15	118.07	111.36
1	B	175	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	68	LYS	CA-C-N	-6.11	114.45	122.94
1	A	68	LYS	C-N-CA	-6.11	114.45	122.94
1	B	8	ASN	CB-CA-C	6.10	120.48	111.88
1	A	129	THR	CA-C-N	6.07	125.19	120.33
1	A	129	THR	C-N-CA	6.07	125.19	120.33
1	B	134	MET	O-C-N	6.05	128.53	122.12
1	B	65	GLY	CA-C-N	6.01	129.44	120.31
1	B	65	GLY	C-N-CA	6.01	129.44	120.31
1	A	179	ASN	CA-C-O	-5.99	114.20	120.55
1	A	91	GLU	O-C-N	5.97	128.30	122.09
1	A	93	ARG	CA-C-O	5.96	126.87	120.55
1	B	167	HIS	CA-C-O	5.96	126.87	120.55
1	B	53	GLY	O-C-N	5.96	129.71	122.32
1	B	2	MET	CG-SD-CE	-5.92	87.87	100.90
1	A	25	SER	CA-C-O	-5.91	115.12	121.56
1	A	86	CYS	CA-C-N	-5.91	114.49	120.10
1	A	86	CYS	C-N-CA	-5.91	114.49	120.10
1	B	210	LYS	CA-C-N	5.89	128.66	120.29
1	B	210	LYS	C-N-CA	5.89	128.66	120.29
1	A	8	ASN	CB-CG-OD1	5.89	132.57	120.80
1	B	18	LEU	CA-C-O	-5.88	114.19	120.42
1	A	3	ILE	O-C-N	5.88	129.43	123.20
1	B	148	ALA	N-CA-CB	5.86	119.33	110.30
1	B	58	ASN	N-CA-CB	-5.84	101.76	111.57
1	B	70	THR	CA-C-O	-5.83	114.73	121.49
1	B	174	LEU	O-C-N	5.81	129.28	122.24
1	B	73	ASN	CB-CG-OD1	5.81	132.42	120.80
1	A	130	ILE	N-CA-C	5.80	119.31	112.35
1	B	31	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	B	131	PRO	N-CA-C	-5.77	105.51	113.53
1	B	98	ILE	CA-C-O	-5.76	115.06	121.17
1	B	198	LYS	O-C-N	5.76	129.54	122.34
1	B	67	ARG	CD-NE-CZ	-5.75	116.35	124.40
1	B	174	LEU	N-CA-CB	-5.75	101.93	110.61
1	B	3	ILE	CA-C-O	-5.75	114.36	120.39
1	B	83	HIS	CA-CB-CG	-5.73	108.07	113.80
1	B	48	GLU	CG-CD-OE2	5.73	131.58	118.40
1	A	106	ASN	O-C-N	5.73	129.31	122.27
1	A	10	ARG	NE-CZ-NH2	-5.72	114.05	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ALA	O-C-N	5.72	129.99	122.33
1	B	75	ILE	CA-C-O	5.68	127.19	121.17
1	A	99	VAL	CA-C-O	-5.66	115.17	121.17
1	B	94	ILE	CA-C-O	-5.64	114.87	120.85
1	A	66	SER	O-C-N	5.63	129.19	122.27
1	B	19	LEU	CA-C-N	-5.62	112.75	120.28
1	B	19	LEU	C-N-CA	-5.62	112.75	120.28
1	A	169	PHE	O-C-N	5.58	128.12	122.09
1	A	120	GLU	O-C-N	5.56	128.01	122.12
1	B	79	LEU	O-C-N	5.55	128.48	122.15
1	B	107	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
1	B	23	THR	O-C-N	5.53	130.00	122.37
1	B	165	GLN	CA-C-N	-5.51	112.89	120.28
1	B	165	GLN	C-N-CA	-5.51	112.89	120.28
1	B	183	PHE	CA-C-O	-5.51	115.04	120.82
1	A	188	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	8	ASN	CB-CA-C	5.50	117.98	111.22
1	A	123	LYS	N-CA-C	5.50	121.09	113.45
1	A	194	SER	O-C-N	5.49	127.72	122.07
1	A	68	LYS	CA-C-O	-5.47	114.44	120.24
1	A	5	GLY	O-C-N	5.46	128.82	123.80
1	B	98	ILE	O-C-N	5.46	127.26	121.91
1	B	25	SER	O-C-N	5.46	129.30	122.86
1	A	187	PHE	O-C-N	5.43	127.96	122.09
1	A	81	ARG	O-C-N	5.42	127.66	122.07
1	A	19	LEU	O-C-N	5.41	128.32	122.15
1	B	97	ASP	N-CA-CB	5.41	117.99	109.94
1	A	139	GLU	CG-CD-OE1	5.40	130.81	118.40
1	B	31	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	B	16	ILE	O-C-N	5.38	128.90	121.90
1	B	107	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	130	ILE	CA-C-O	5.37	122.29	118.69
1	A	107	ARG	NE-CZ-NH1	5.37	126.86	121.50
1	A	121	LYS	CA-CB-CG	5.33	124.76	114.10
1	A	42	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	38	PRO	CA-C-N	5.28	129.66	120.68
1	A	38	PRO	C-N-CA	5.28	129.66	120.68
1	A	53	GLY	O-C-N	5.28	128.87	122.32
1	B	184	LEU	CA-C-O	-5.28	114.95	120.55
1	B	23	THR	CA-C-O	-5.28	112.89	119.28
1	A	179	ASN	OD1-CG-ND2	5.27	127.87	122.60
1	B	41	ASP	CA-C-O	-5.27	115.68	120.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	VAL	CA-C-N	-5.26	113.44	120.54
1	A	99	VAL	C-N-CA	-5.26	113.44	120.54
1	A	95	ARG	CD-NE-CZ	5.25	131.75	124.40
1	A	2	MET	CA-C-N	-5.25	116.12	123.10
1	A	2	MET	C-N-CA	-5.25	116.12	123.10
1	A	22	TYR	CA-C-O	-5.25	114.99	120.55
1	B	17	ARG	O-C-N	-5.24	116.57	122.12
1	B	67	ARG	CA-CB-CG	-5.24	103.63	114.10
1	B	53	GLY	CA-C-O	-5.23	112.64	119.44
1	A	109	GLN	CA-C-O	-5.23	114.88	120.42
1	B	3	ILE	O-C-N	5.22	128.90	123.26
1	A	29	GLU	CG-CD-OE2	-5.21	106.41	118.40
1	B	97	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	11	GLY	CA-C-O	-5.20	114.89	121.44
1	B	210	LYS	CB-CG-CD	5.19	123.23	111.30
1	A	171	PRO	O-C-N	5.18	128.20	122.24
1	A	165	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	19	LEU	CA-C-N	-5.17	113.35	120.28
1	A	19	LEU	C-N-CA	-5.17	113.35	120.28
1	A	152	VAL	CA-CB-CG1	5.17	119.19	110.40
1	A	121	LYS	CB-CG-CD	5.17	123.19	111.30
1	A	214	TRP	CA-C-O	-5.16	115.08	121.06
1	B	95	ARG	CA-C-O	-5.16	115.41	120.82
1	B	39	ASP	CA-C-O	-5.13	115.43	120.82
1	A	179	ASN	O-C-N	5.12	127.55	122.12
1	B	74	ALA	N-CA-C	-5.12	105.78	111.36
1	A	144	ARG	O-C-N	5.12	127.16	121.53
1	B	72	SER	CB-CA-C	5.08	118.93	110.81
1	A	96	ALA	CB-CA-C	5.06	119.45	110.85
1	B	68	LYS	CA-C-N	-5.05	114.65	122.69
1	B	68	LYS	C-N-CA	-5.05	114.65	122.69
1	B	48	GLU	O-C-N	5.05	127.74	122.23
1	B	69	ILE	O-C-N	5.05	128.41	123.00
1	A	10	ARG	N-CA-CB	-5.05	102.75	110.07
1	B	106	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	B	183	PHE	N-CA-C	-5.04	105.68	111.07
1	B	211	LEU	N-CA-CB	-5.04	102.71	110.16
1	B	127	LEU	O-C-N	5.03	127.46	122.12
1	B	73	ASN	CB-CG-ND2	-5.03	108.86	116.40
1	B	212	ALA	CA-C-O	5.02	127.72	121.99
1	A	54	LEU	CB-CG-CD2	5.02	125.75	110.70
1	A	98	ILE	O-C-N	5.01	126.82	121.91

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	35	3
1	B	1817	0	1803	28	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	69	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 (69) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:125:GLU:HG2	1:B:128:LYS:HZ1	1.76	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
1:B:203:LEU:HD23	1:B:203:LEU:C	2.40	0.47
1:A:174:LEU:O	1:A:181:LYS:NZ	2.23	0.46
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:B:2:MET:HE3	1:B:2:MET:HB2	1.79	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:176:ALA:C	1:A:178:PRO:HD3	2.43	0.43
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:A:36:ASP:OD1	1:A:210:LYS:NZ	2.44	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:205:THR:HA	1:A:206:PRO:C	2.46	0.41
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: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%)	24	11
All	All	430/434 (99%)	418 (97%)	11 (3%)	1 (0%)	43	27

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%)	185 (94%)	12 (6%)	17	3
1	B	197/197 (100%)	186 (94%)	11 (6%)	19	4
All	All	394/394 (100%)	371 (94%)	23 (6%)	18	4

All (23) 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	42	ARG
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
1	B	12	LEU
1	B	48	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	66	SER
1	B	88	GLU
1	B	121	LYS
1	B	174	LEU
1	B	191	LYS
1	B	210	LYS
1	B	211	LEU
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	73	ASN
1	A	106	ASN
1	A	122	GLN
1	B	8	ASN
1	B	101	ASN
1	B	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	218	-	4,4,4	0.71	0	6,6,6	0.23	0
3	GPS	B	219	-	35,37,37	1.87	9 (25%)	46,51,51	2.06	15 (32%)
2	SO4	A	218	-	4,4,4	0.68	0	6,6,6	0.37	0
2	SO4	A	219	-	4,4,4	0.65	0	6,6,6	0.49	0
3	GPS	A	220	-	35,37,37	1.63	6 (17%)	46,51,51	2.28	19 (41%)

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	1/27/43/43	0/3/3/3
3	GPS	A	220	-	2/2/8/10	1/27/43/43	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	219	GPS	CA4-SG2	-5.11	1.71	1.84
3	A	220	GPS	CA4-SG2	-4.63	1.72	1.84
3	B	219	GPS	CG4-CB4	4.25	1.44	1.39
3	B	219	GPS	CA3-N3	3.38	1.53	1.45
3	A	220	GPS	CZ5-CH5	3.37	1.45	1.40
3	A	220	GPS	C2-N3	-3.07	1.26	1.33
3	B	219	GPS	O5-CA5	2.95	1.48	1.42
3	B	219	GPS	C2-N3	-2.75	1.27	1.33
3	A	220	GPS	CG4-CB4	2.61	1.42	1.39
3	A	220	GPS	CA2-C2	2.58	1.59	1.52
3	B	219	GPS	CB1-CA1	2.50	1.58	1.53
3	B	219	GPS	CH5-CB5	-2.47	1.37	1.40
3	B	219	GPS	CZ5-CH5	2.47	1.43	1.40
3	B	219	GPS	CA2-C2	2.38	1.58	1.52
3	A	220	GPS	CD1-N2	2.07	1.38	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	220	GPS	CB4-CA4-SG2	-5.17	97.59	111.02
3	A	220	GPS	O2-C2-CA2	-4.55	110.96	120.48
3	B	219	GPS	O2-C2-N3	4.53	132.57	122.98
3	B	219	GPS	O32-C3-O31	-4.48	111.82	123.33
3	B	219	GPS	O5-CA5-CB5	-4.19	102.42	110.42
3	A	220	GPS	O2-C2-N3	4.17	131.80	122.98
3	B	219	GPS	O2-C2-CA2	-4.02	112.06	120.48
3	A	220	GPS	CH5-CB5-CA5	3.87	123.43	118.64
3	A	220	GPS	O5-CA5-CB5	-3.78	103.22	110.42
3	A	220	GPS	CG5-CB5-CA5	-3.72	113.52	120.94
3	B	219	GPS	CH5-CB5-CA5	3.45	122.91	118.64
3	A	220	GPS	O32-C3-O31	-3.32	114.80	123.33
3	A	220	GPS	CG1-CB1-CA1	-3.25	106.41	113.86
3	A	220	GPS	CD4-CE4-CZ4	3.18	124.17	120.24
3	A	220	GPS	O12-C1-O11	-3.13	116.98	124.08
3	A	220	GPS	CD5-CG5-CB5	-3.04	117.35	120.99
3	B	219	GPS	CG5-CB5-CA5	-3.02	114.91	120.94
3	A	220	GPS	CG5-CB5-CH5	2.97	122.98	119.35
3	B	219	GPS	O12-C1-O11	-2.86	117.59	124.08
3	B	219	GPS	CD4-CE4-CZ4	2.86	123.77	120.24
3	A	220	GPS	CA5-CA4-SG2	-2.83	102.21	110.88
3	B	219	GPS	CH5-CH4-CB4	-2.79	115.64	119.64
3	B	219	GPS	CD5-CG5-CB5	-2.74	117.70	120.99
3	A	220	GPS	CE4-CD4-CG4	-2.72	116.88	120.24
3	A	220	GPS	CG4-CB4-CH4	2.48	122.38	119.35
3	A	220	GPS	CZ4-CH4-CB4	-2.47	115.82	118.50
3	B	219	GPS	O32-C3-CA3	2.41	121.96	112.81
3	A	220	GPS	CG1-CD1-N2	-2.38	111.67	115.86
3	B	219	GPS	CB1-CA1-N1	-2.30	104.12	110.12
3	B	219	GPS	C2-CA2-N2	-2.28	104.93	111.11
3	B	219	GPS	CG5-CB5-CH5	2.26	122.11	119.35
3	A	220	GPS	C2-CA2-N2	-2.22	105.09	111.11
3	B	219	GPS	O5-CA5-CA4	-2.19	102.99	109.58
3	A	220	GPS	CZ4-CH4-CH5	2.03	125.72	121.61

All (4) chirality outliers are listed below:

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

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

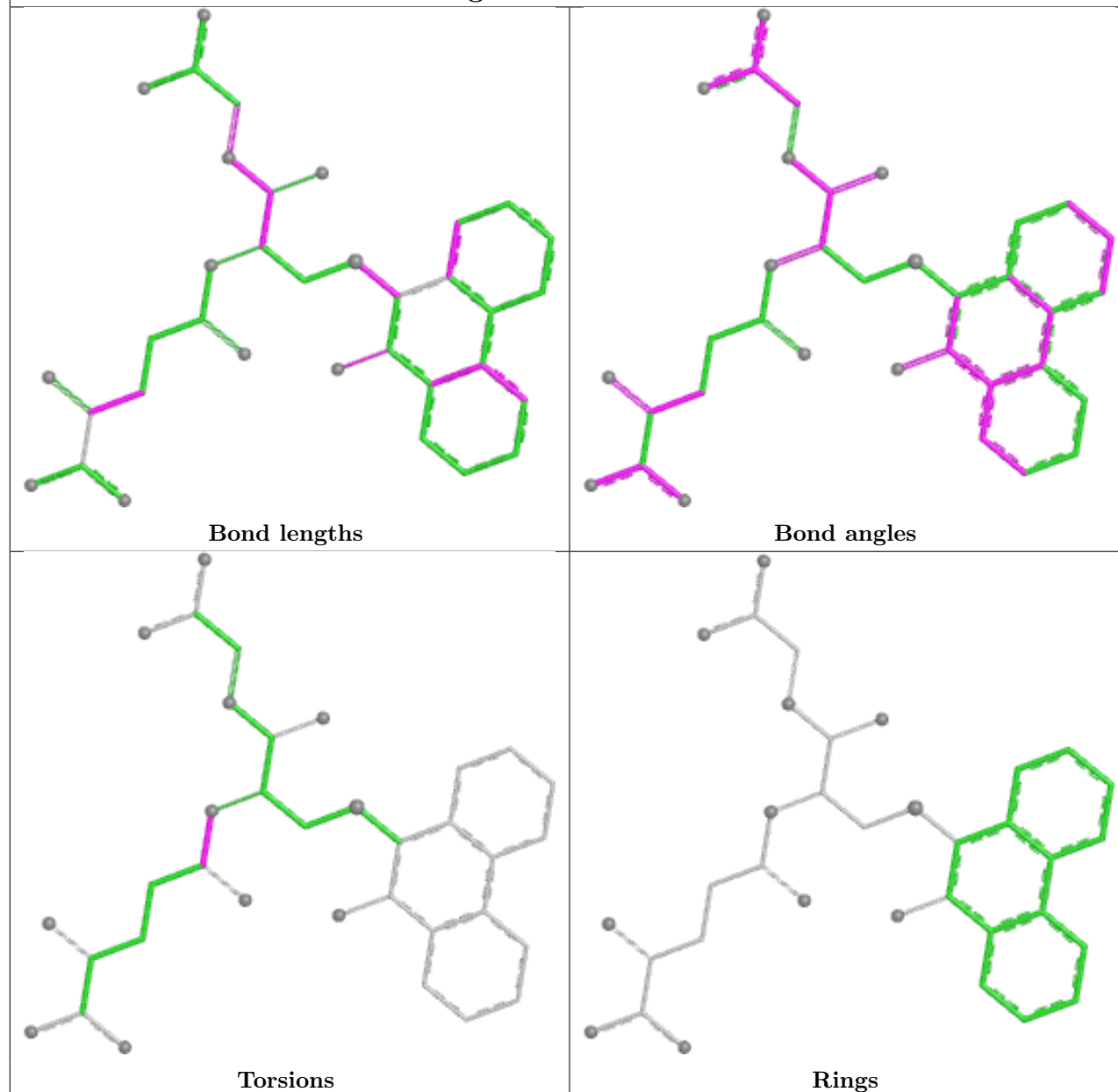
There are no ring outliers.

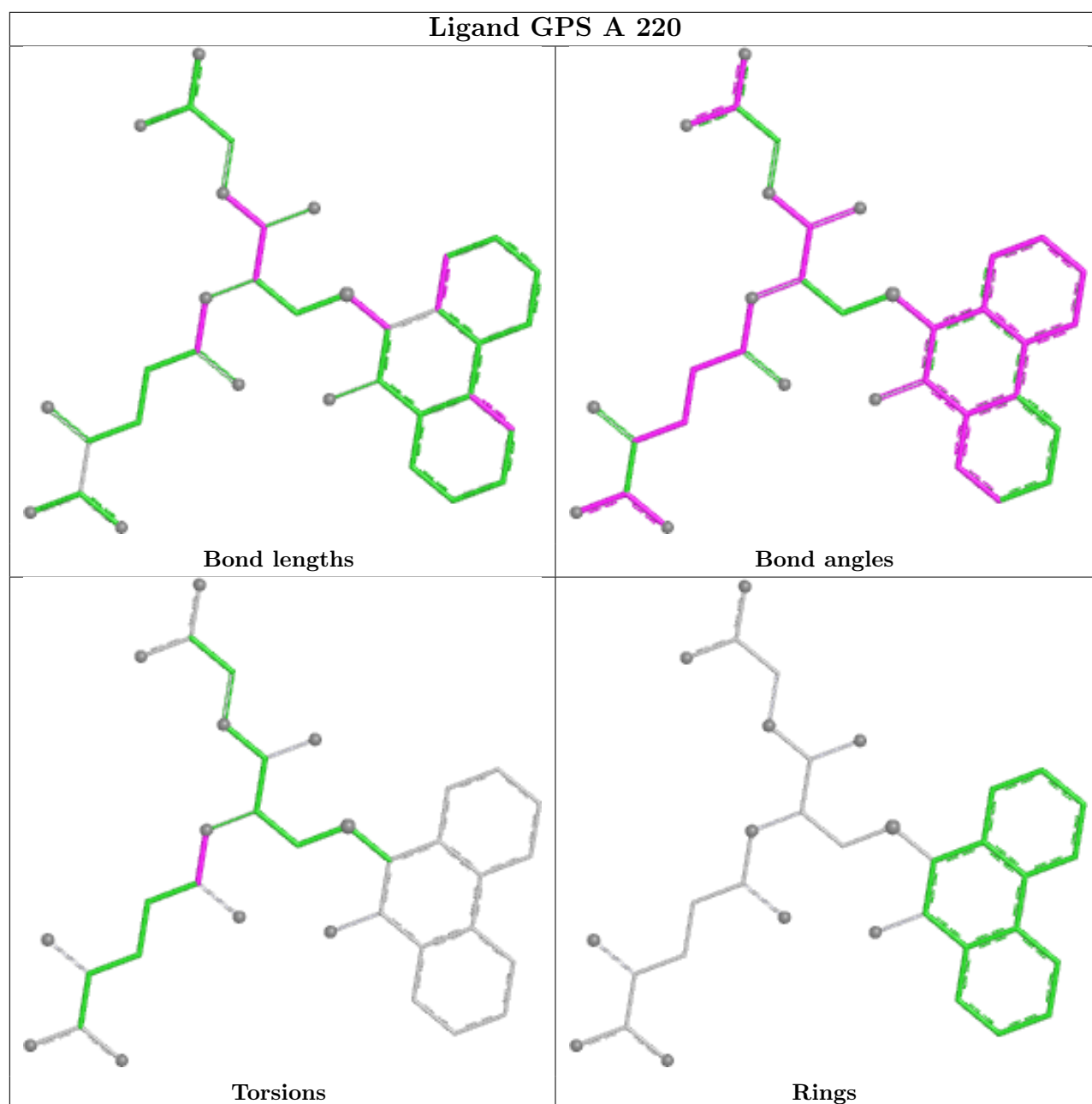
2 monomers are involved in 11 short contacts:

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.