



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:21 AM UTC

PDB ID : 1IYE / pdb_00001iye
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI BRANCHED-CHAIN
AMINO ACID AMINOTRANSFERASE
Authors : Hirotsu, K.; Goto, M.
Deposited on : 2002-08-07
Resolution : 1.82 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

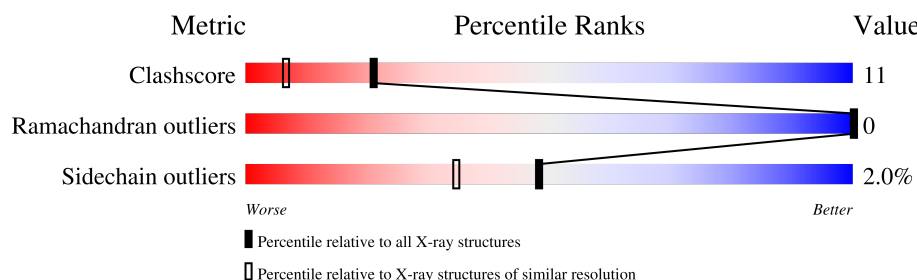
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)

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	309	
1	B	309	
1	C	309	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGU	A	513	X	X	-	-
2	PGU	B	913	X	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGU	C	1413	X	X	-	-

2 Entry composition [i](#)

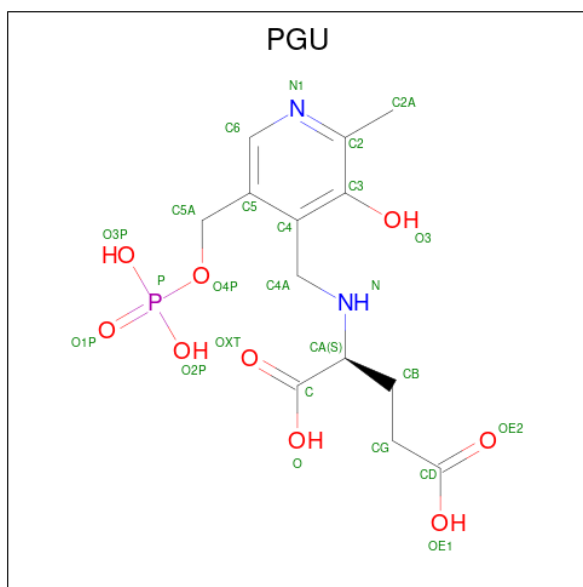
There are 3 unique types of molecules in this entry. The entry contains 7661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2362	1499	410	443	10			
1	B	304	Total	C	N	O	S	0	0	0
			2362	1499	410	443	10			
1	C	304	Total	C	N	O	S	0	0	0
			2362	1499	410	443	10			

- Molecule 2 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-glutamic acid (CCD ID: PGU) (formula: C₁₃H₁₉N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 3 is water.

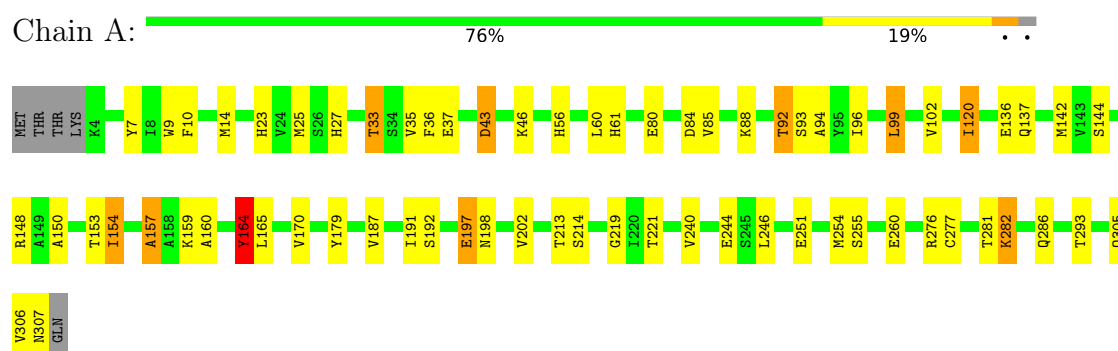
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total 150	O 150	0	0
3	B	144	Total 144	O 144	0	0
3	C	206	Total 206	O 206	0	0

3 Residue-property plots [i](#)

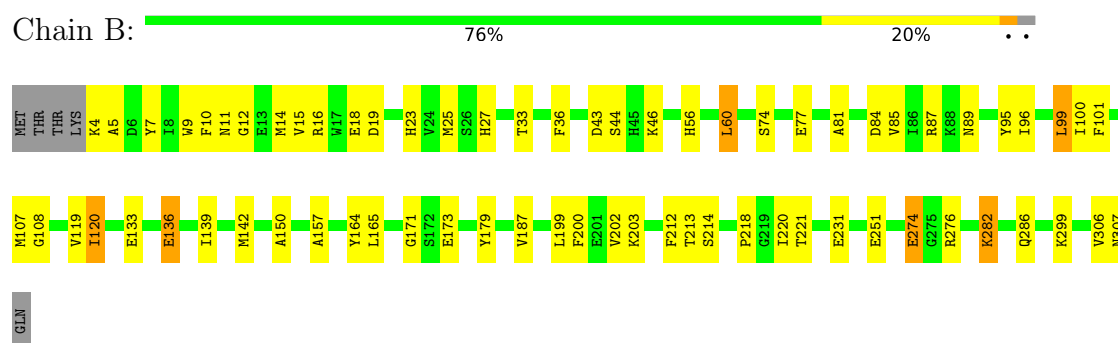
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

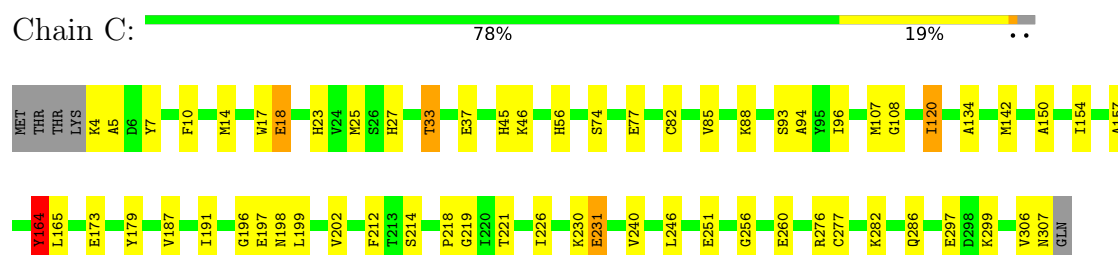
• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE



• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE



• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.60Å 98.86Å 138.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.82	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.82)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7661	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.40	0/2418	0.93	12/3279 (0.4%)
1	B	0.39	0/2418	0.91	5/3279 (0.2%)
1	C	0.42	0/2418	0.90	7/3279 (0.2%)
All	All	0.40	0/7254	0.91	24/9837 (0.2%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	TYR	N-CA-C	8.13	122.86	113.19
1	A	164	TYR	N-CA-C	8.13	122.86	113.19
1	B	164	TYR	N-CA-C	7.70	122.35	113.19
1	A	165	LEU	N-CA-C	-7.13	103.51	111.28
1	B	165	LEU	N-CA-C	-6.70	103.98	111.28
1	C	165	LEU	N-CA-C	-6.33	104.38	111.28
1	C	214	SER	N-CA-C	-6.30	105.45	112.57
1	A	214	SER	N-CA-C	-6.21	105.55	112.57
1	B	214	SER	N-CA-C	-6.04	105.75	112.57
1	A	293	THR	N-CA-C	-6.03	106.26	113.97
1	C	221	THR	N-CA-C	-5.99	104.83	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ASP	N-CA-C	-5.99	99.52	109.46
1	A	221	THR	N-CA-C	-5.96	104.86	111.36
1	C	157	ALA	N-CA-C	-5.95	105.51	112.89
1	A	92	THR	N-CA-C	-5.85	106.69	113.88
1	A	33	THR	N-CA-C	5.84	118.67	109.39
1	C	134	ALA	N-CA-C	5.76	118.05	111.02
1	A	154	ILE	N-CA-C	-5.73	100.79	107.61
1	A	153	THR	N-CA-C	-5.64	102.44	111.02
1	A	43	ASP	N-CA-C	-5.61	101.34	110.20
1	B	221	THR	N-CA-C	-5.60	104.80	111.69
1	A	157	ALA	N-CA-C	-5.56	106.45	113.18
1	A	281	THR	N-CA-C	-5.44	105.35	111.28
1	C	33	THR	N-CA-C	5.12	117.53	109.39

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	TYR	Sidechain
1	C	164	TYR	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	2362	0	2302	54	0
1	B	2362	0	2302	56	0
1	C	2362	0	2302	48	0
2	A	25	0	14	2	0
2	B	25	0	13	0	0
2	C	25	0	14	0	0
3	A	150	0	0	0	0
3	B	144	0	0	2	0
3	C	206	0	0	3	1
All	All	7661	0	6947	155	1

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 11.

All (155) 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:C:14:MET:HE2	1:C:88:LYS:HG2	1.45	0.99
1:A:46:LYS:HB3	1:A:305:GLN:HE21	1.33	0.94
1:B:16:ARG:HE	1:B:18:GLU:HB2	1.31	0.92
1:B:274:GLU:H	1:B:274:GLU:CD	1.85	0.85
1:B:16:ARG:NE	1:B:18:GLU:HB2	1.97	0.78
1:A:9:TRP:HB2	1:A:85:VAL:CG1	2.15	0.77
1:B:16:ARG:HG2	1:B:19:ASP:OD2	1.85	0.77
1:B:36:PHE:HB3	1:B:99:LEU:HD23	1.69	0.74
1:C:306:VAL:O	1:C:307:ASN:HB2	1.89	0.72
1:B:202:VAL:HB	1:B:251:GLU:HB2	1.72	0.72
1:C:276:ARG:NH1	1:C:277:CYS:H	1.88	0.72
1:A:277:CYS:SG	1:A:282:LYS:HG2	2.30	0.71
1:B:136:GLU:O	1:B:276:ARG:NH1	2.23	0.71
1:A:276:ARG:CZ	1:A:277:CYS:H	2.05	0.70
1:A:306:VAL:O	1:A:307:ASN:HB2	1.93	0.69
1:B:107:MET:HA	1:B:107:MET:HE2	1.73	0.69
1:C:297:GLU:HG2	1:C:299:LYS:HG3	1.76	0.68
1:C:231:GLU:OE2	1:C:299:LYS:HE3	1.95	0.67
1:C:276:ARG:HD2	3:C:1599:HOH:O	1.95	0.66
1:A:202:VAL:HB	1:A:251:GLU:HB2	1.77	0.66
1:A:9:TRP:HB2	1:A:85:VAL:HG11	1.77	0.65
1:A:14:MET:HE2	1:A:88:LYS:HG2	1.77	0.65
1:A:7:TYR:HB3	1:A:14:MET:HE3	1.79	0.65
1:C:18:GLU:H	1:C:18:GLU:CD	2.02	0.64
1:C:202:VAL:HB	1:C:251:GLU:HB2	1.78	0.64
1:A:282:LYS:HZ1	1:A:286:GLN:HE21	1.45	0.62
1:B:142:MET:HE1	1:B:173:GLU:HG2	1.81	0.62
1:B:23:HIS:CD2	1:B:25:MET:H	2.17	0.62
1:C:276:ARG:HH11	1:C:276:ARG:HA	1.64	0.62
1:B:133:GLU:HA	1:B:136:GLU:OE1	2.00	0.62
1:A:157:ALA:HB2	3:C:1596:HOH:O	1.99	0.61
1:B:7:TYR:HB3	1:B:14:MET:HE3	1.81	0.61
1:A:136:GLU:O	1:A:276:ARG:NH2	2.34	0.61
1:A:46:LYS:HB3	1:A:305:GLN:NE2	2.12	0.60
1:C:23:HIS:HD2	1:C:25:MET:H	1.50	0.60
1:B:96:ILE:HD12	1:B:96:ILE:N	2.16	0.60
1:A:23:HIS:HD2	1:A:25:MET:HB2	1.67	0.60
1:A:282:LYS:NZ	1:A:286:GLN:HE21	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:HIS:HB3	1:A:102:VAL:HB	1.83	0.59
1:B:16:ARG:HD2	1:B:18:GLU:OE1	2.03	0.58
1:B:15:VAL:HG12	1:B:19:ASP:HB2	1.85	0.58
1:B:81:ALA:O	1:B:85:VAL:HG23	2.03	0.58
1:C:4:LYS:HE2	1:C:17:TRP:CD1	2.38	0.58
1:B:150:ALA:HB2	1:B:187:VAL:HG11	1.86	0.58
1:B:23:HIS:HD2	1:B:25:MET:H	1.51	0.58
1:C:154:ILE:HG13	1:C:154:ILE:O	2.04	0.57
1:B:9:TRP:CZ2	1:B:12:GLY:HA2	2.40	0.56
1:A:154:ILE:O	1:A:154:ILE:HG13	2.04	0.56
1:C:4:LYS:HG2	1:C:5:ALA:N	2.20	0.56
1:A:282:LYS:O	1:A:286:GLN:HG3	2.06	0.56
1:B:84:ASP:OD1	1:B:87:ARG:NH1	2.39	0.56
1:C:198:ASN:ND2	1:C:219:GLY:HA3	2.22	0.55
1:A:96:ILE:N	1:A:96:ILE:HD12	2.21	0.55
1:C:282:LYS:O	1:C:286:GLN:HG3	2.07	0.54
1:A:36:PHE:HB3	1:A:99:LEU:HD23	1.89	0.54
1:C:23:HIS:CD2	1:C:25:MET:H	2.25	0.54
1:C:191:ILE:HD11	1:C:246:LEU:HG	1.89	0.54
1:C:74:SER:OG	1:C:77:GLU:HG3	2.06	0.54
1:A:191:ILE:HD11	1:A:246:LEU:HG	1.89	0.54
1:C:142:MET:HE1	1:C:173:GLU:HG2	1.89	0.54
1:B:171:GLY:HA3	3:B:1024:HOH:O	2.08	0.53
1:B:74:SER:OG	1:B:77:GLU:HG3	2.08	0.53
1:A:244:GLU:HG3	1:B:157:ALA:HB3	1.91	0.52
1:B:10:PHE:CD2	1:B:120:ILE:HD11	2.43	0.52
1:B:119:VAL:O	1:B:120:ILE:HD12	2.08	0.52
1:C:231:GLU:CD	1:C:299:LYS:HE3	2.35	0.52
1:A:159:LYS:NZ	2:A:513:PGU:H4A1	2.25	0.52
1:B:10:PHE:CE2	1:B:11:ASN:ND2	2.77	0.52
1:B:23:HIS:HD2	1:B:25:MET:HB2	1.75	0.52
1:C:10:PHE:CG	1:C:120:ILE:HD11	2.44	0.52
1:C:37:GLU:OE2	1:C:56:HIS:HD2	1.93	0.52
1:C:10:PHE:CD1	1:C:120:ILE:HD11	2.46	0.51
1:C:45:HIS:H	1:C:45:HIS:CD2	2.28	0.51
1:B:306:VAL:O	1:B:307:ASN:HB2	2.09	0.51
1:C:27:HIS:HD2	1:C:33:THR:OG1	1.93	0.51
1:B:10:PHE:HE2	1:B:11:ASN:ND2	2.09	0.50
1:C:276:ARG:NH1	1:C:277:CYS:N	2.57	0.50
1:B:15:VAL:CG1	1:B:19:ASP:HB2	2.41	0.50
1:B:199:LEU:C	1:B:199:LEU:HD13	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:HZ1	2:A:513:PGU:H4A1	1.77	0.50
1:A:276:ARG:NH2	1:A:277:CYS:CB	2.75	0.49
1:C:7:TYR:HB3	1:C:14:MET:HE3	1.93	0.49
1:A:276:ARG:NH2	1:A:277:CYS:HB3	2.28	0.49
1:C:142:MET:HB2	1:C:179:TYR:CG	2.48	0.49
1:A:144:SER:HB2	1:A:170:VAL:HG13	1.95	0.49
1:B:99:LEU:HD13	1:B:101:PHE:CD2	2.48	0.48
1:B:142:MET:HB2	1:B:179:TYR:CG	2.48	0.48
1:A:198:ASN:ND2	1:A:219:GLY:HA3	2.28	0.48
1:B:7:TYR:CB	1:B:14:MET:HE3	2.43	0.48
1:A:197:GLU:HG3	1:A:254:MET:HB3	1.94	0.48
1:A:27:HIS:HD2	1:A:33:THR:OG1	1.97	0.48
1:A:136:GLU:O	1:A:276:ARG:CZ	2.62	0.48
1:A:93:SER:O	1:A:94:ALA:HB2	2.14	0.48
1:B:95:TYR:C	1:B:96:ILE:HD12	2.39	0.48
1:A:213:THR:HG21	1:C:240:VAL:HG12	1.96	0.47
1:A:10:PHE:CG	1:A:120:ILE:HD11	2.50	0.47
1:A:282:LYS:NZ	1:A:286:GLN:NE2	2.63	0.47
1:C:198:ASN:HD21	1:C:219:GLY:HA3	1.79	0.47
1:C:276:ARG:NH1	1:C:276:ARG:HA	2.29	0.47
1:B:27:HIS:HE1	1:B:108:GLY:O	1.97	0.46
1:C:82:CYS:O	1:C:85:VAL:HG12	2.15	0.46
1:A:150:ALA:HB2	1:A:187:VAL:HG11	1.97	0.46
1:A:37:GLU:OE2	1:A:56:HIS:HD2	1.99	0.46
1:C:256:GLY:O	1:C:260:GLU:N	2.48	0.46
1:A:306:VAL:O	1:A:307:ASN:CB	2.63	0.46
1:A:255:SER:HA	1:A:260:GLU:O	2.17	0.45
1:B:15:VAL:HG12	1:B:16:ARG:N	2.31	0.45
1:B:199:LEU:HD13	1:B:200:PHE:N	2.30	0.45
1:B:203:LYS:NZ	3:B:1038:HOH:O	2.49	0.45
1:C:4:LYS:HG2	1:C:5:ALA:H	1.80	0.45
1:B:282:LYS:HZ3	1:B:286:GLN:CG	2.30	0.44
1:A:164:TYR:CD1	1:A:164:TYR:N	2.85	0.44
1:C:27:HIS:HE1	1:C:108:GLY:O	2.00	0.44
1:A:137:GLN:HA	1:A:276:ARG:NH1	2.33	0.44
1:C:196:GLY:O	1:C:197:GLU:HG3	2.17	0.44
1:A:137:GLN:C	1:A:276:ARG:NH1	2.75	0.44
1:C:199:LEU:C	1:C:199:LEU:HD13	2.42	0.44
1:A:36:PHE:CE1	1:A:159:LYS:HE3	2.52	0.44
1:A:144:SER:CB	1:A:170:VAL:HG13	2.48	0.44
1:C:96:ILE:HD12	1:C:96:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:CZ	1:C:277:CYS:H	2.31	0.44
1:B:282:LYS:O	1:B:282:LYS:HD3	2.18	0.43
1:A:197:GLU:HB2	1:A:255:SER:O	2.18	0.43
1:B:4:LYS:HG2	1:B:5:ALA:N	2.32	0.43
1:C:226:ILE:O	1:C:230:LYS:HG3	2.19	0.43
1:B:27:HIS:HD2	1:B:33:THR:OG1	2.02	0.43
1:C:212:PHE:CE1	1:C:218:PRO:HA	2.54	0.42
1:B:60:LEU:HD13	1:B:100:ILE:HD11	2.01	0.42
1:A:276:ARG:HA	1:A:276:ARG:HD2	1.69	0.42
1:A:142:MET:HB2	1:A:179:TYR:CG	2.55	0.42
1:A:148:ARG:HG3	1:A:192:SER:CB	2.49	0.42
1:B:23:HIS:CD2	1:B:25:MET:HB2	2.53	0.42
1:A:80:GLU:OE2	1:A:84:ASP:OD1	2.38	0.42
1:A:35:VAL:HA	1:A:160:ALA:HA	2.00	0.42
1:B:10:PHE:CE2	1:B:120:ILE:HD11	2.55	0.41
1:B:5:ALA:HB1	1:B:89:ASN:OD1	2.20	0.41
1:B:56:HIS:CD2	1:B:220:ILE:HD12	2.55	0.41
1:B:96:ILE:N	1:B:96:ILE:CD1	2.83	0.41
1:B:44:SER:C	1:B:46:LYS:H	2.28	0.41
1:C:150:ALA:HB2	1:C:187:VAL:HG11	2.02	0.41
1:C:164:TYR:CD1	1:C:164:TYR:N	2.88	0.41
1:B:23:HIS:HD2	1:B:25:MET:CB	2.33	0.41
1:B:231:GLU:OE2	1:B:299:LYS:HE3	2.21	0.41
1:C:14:MET:HE2	1:C:88:LYS:CG	2.32	0.41
1:C:56:HIS:HE1	3:C:1435:HOH:O	2.02	0.41
1:A:43:ASP:OD1	1:A:92:THR:HB	2.21	0.41
1:A:240:VAL:HG12	1:B:213:THR:HG21	2.02	0.41
1:B:212:PHE:CE1	1:B:218:PRO:HA	2.56	0.41
1:C:107:MET:HE2	1:C:107:MET:HA	2.03	0.41
1:B:142:MET:HB2	1:B:179:TYR:CD2	2.56	0.40
1:C:46:LYS:HB3	1:C:46:LYS:HE2	1.83	0.40
1:A:276:ARG:NH2	1:A:277:CYS:HB2	2.35	0.40
1:B:139:ILE:C	1:B:139:ILE:HD12	2.47	0.40
1:A:9:TRP:HB2	1:A:85:VAL:HG12	2.01	0.40
1:C:93:SER:O	1:C:94:ALA:HB2	2.20	0.40

All (1) 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)
3:C:1578:HOH:O	3:C:1578:HOH:O[4_555]	1.93	0.27

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	302/309 (98%)	295 (98%)	7 (2%)	0	100	100
1	B	302/309 (98%)	292 (97%)	10 (3%)	0	100	100
1	C	302/309 (98%)	296 (98%)	6 (2%)	0	100	100
All	All	906/927 (98%)	883 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	246/251 (98%)	240 (98%)	6 (2%)	43	27
1	B	246/251 (98%)	240 (98%)	6 (2%)	43	27
1	C	246/251 (98%)	243 (99%)	3 (1%)	63	54
All	All	738/753 (98%)	723 (98%)	15 (2%)	48	35

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	61	HIS
1	A	99	LEU
1	A	120	ILE
1	A	197	GLU

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Mol	Chain	Res	Type
1	A	282	LYS
1	B	60	LEU
1	B	99	LEU
1	B	120	ILE
1	B	136	GLU
1	B	274	GLU
1	B	282	LYS
1	C	18	GLU
1	C	120	ILE
1	C	231	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	27	HIS
1	A	56	HIS
1	A	58	GLN
1	A	137	GLN
1	A	239	GLN
1	A	286	GLN
1	A	305	GLN
1	A	307	ASN
1	B	23	HIS
1	B	27	HIS
1	B	56	HIS
1	B	58	GLN
1	B	61	HIS
1	B	163	ASN
1	B	271	GLN
1	B	286	GLN
1	B	305	GLN
1	B	307	ASN
1	C	23	HIS
1	C	27	HIS
1	C	45	HIS
1	C	56	HIS
1	C	58	GLN
1	C	61	HIS
1	C	137	GLN
1	C	307	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 ⓘ

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	PGU	A	513	-	25,25,25	2.10	8 (32%)	31,35,35	3.88	18 (58%)
2	PGU	B	913	-	25,25,25	2.17	7 (28%)	31,35,35	3.94	18 (58%)
2	PGU	C	1413	-	25,25,25	2.19	8 (32%)	31,35,35	3.86	18 (58%)

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
2	PGU	A	513	-	1/1/4/5	9/20/20/20	0/1/1/1
2	PGU	B	913	-	1/1/4/5	9/20/20/20	0/1/1/1
2	PGU	C	1413	-	1/1/4/5	8/20/20/20	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1413	PGU	C3-C2	6.38	1.47	1.41
2	B	913	PGU	C3-C2	6.12	1.47	1.41
2	A	513	PGU	C3-C2	5.58	1.46	1.41
2	C	1413	PGU	C2-N1	3.43	1.39	1.33
2	B	913	PGU	C5-C4	3.41	1.45	1.40
2	A	513	PGU	CA-N	-3.37	1.39	1.46
2	A	513	PGU	C2-N1	3.29	1.39	1.33
2	C	1413	PGU	CA-N	-3.25	1.39	1.46
2	A	513	PGU	OXT-C	3.24	1.31	1.22
2	A	513	PGU	C5-C4	3.24	1.45	1.40
2	B	913	PGU	OXT-C	3.23	1.31	1.22
2	B	913	PGU	C2-N1	3.13	1.39	1.33
2	C	1413	PGU	OXT-C	3.04	1.31	1.22
2	B	913	PGU	CA-N	-3.04	1.39	1.46
2	A	513	PGU	OE1-CD	-2.85	1.21	1.30
2	C	1413	PGU	C5-C4	2.72	1.44	1.40
2	B	913	PGU	OE1-CD	-2.65	1.22	1.30
2	C	1413	PGU	OE1-CD	-2.56	1.22	1.30
2	B	913	PGU	C4A-N	2.22	1.53	1.46
2	A	513	PGU	C4A-N	2.13	1.53	1.46
2	C	1413	PGU	C4A-N	2.10	1.53	1.46
2	C	1413	PGU	O-C	2.10	1.37	1.30
2	A	513	PGU	O-C	2.01	1.37	1.30

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1413	PGU	C6-C5-C4	11.23	126.56	118.06
2	A	513	PGU	C6-C5-C4	10.90	126.31	118.06
2	B	913	PGU	C6-C5-C4	10.90	126.31	118.06
2	A	513	PGU	C2A-C2-C3	10.50	133.08	120.80
2	B	913	PGU	C2A-C2-C3	10.37	132.93	120.80
2	C	1413	PGU	C2A-C2-C3	10.19	132.72	120.80
2	B	913	PGU	C3-C4-C5	-7.35	112.07	118.73
2	C	1413	PGU	C3-C4-C5	-7.03	112.35	118.73
2	A	513	PGU	C3-C4-C5	-6.91	112.46	118.73
2	B	913	PGU	C4A-C4-C5	5.59	125.84	119.75
2	A	513	PGU	C4A-C4-C5	5.02	125.21	119.75
2	A	513	PGU	C5A-C5-C6	-4.94	111.31	119.36
2	B	913	PGU	C5A-C5-C6	-4.84	111.47	119.36
2	B	913	PGU	C4A-N-CA	4.67	122.60	113.84
2	C	1413	PGU	C5A-C5-C6	-4.64	111.81	119.36
2	A	513	PGU	C2A-C2-N1	-4.62	108.94	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1413	PGU	C4A-C4-C5	4.59	124.75	119.75
2	B	913	PGU	C2A-C2-N1	-4.48	109.19	117.64
2	C	1413	PGU	C2A-C2-N1	-4.33	109.49	117.64
2	C	1413	PGU	C4A-N-CA	4.31	121.93	113.84
2	A	513	PGU	C4A-N-CA	3.91	121.18	113.84
2	A	513	PGU	C5-C6-N1	-3.85	117.57	123.83
2	A	513	PGU	CB-CA-C	3.77	119.30	110.35
2	C	1413	PGU	C5-C6-N1	-3.75	117.73	123.83
2	B	913	PGU	C5-C6-N1	-3.65	117.89	123.83
2	B	913	PGU	O4P-C5A-C5	3.51	115.93	109.36
2	B	913	PGU	CB-CA-C	3.34	118.29	110.35
2	A	513	PGU	O4P-C5A-C5	3.27	115.49	109.36
2	C	1413	PGU	CB-CA-C	3.26	118.09	110.35
2	C	1413	PGU	OE1-CD-OE2	2.97	130.98	123.33
2	C	1413	PGU	OE2-CD-CG	-2.91	113.85	123.09
2	C	1413	PGU	O3-C3-C2	-2.89	111.59	117.58
2	B	913	PGU	OE2-CD-CG	-2.89	113.94	123.09
2	A	513	PGU	OE2-CD-CG	-2.84	114.09	123.09
2	B	913	PGU	OE1-CD-OE2	2.76	130.44	123.33
2	A	513	PGU	OE1-CD-OE2	2.74	130.37	123.33
2	B	913	PGU	O3-C3-C2	-2.70	111.97	117.58
2	A	513	PGU	O3-C3-C2	-2.69	112.00	117.58
2	A	513	PGU	O2P-P-O1P	2.61	121.01	110.83
2	B	913	PGU	O2P-P-O1P	2.61	120.99	110.83
2	C	1413	PGU	O2P-P-O1P	2.54	120.74	110.83
2	C	1413	PGU	O4P-C5A-C5	2.54	114.11	109.36
2	C	1413	PGU	C3-C2-N1	-2.51	117.80	120.96
2	B	913	PGU	C3-C2-N1	-2.45	117.87	120.96
2	C	1413	PGU	O3-C3-C4	2.42	125.21	118.18
2	A	513	PGU	C3-C2-N1	-2.37	117.97	120.96
2	A	513	PGU	O3-C3-C4	2.36	125.04	118.18
2	B	913	PGU	C4-C3-C2	2.35	123.45	119.91
2	B	913	PGU	O3-C3-C4	2.20	124.57	118.18
2	C	1413	PGU	C4A-C4-C3	2.19	122.89	119.98
2	C	1413	PGU	C4-C3-C2	2.18	123.20	119.91
2	B	913	PGU	O4P-P-O1P	2.10	112.11	106.44
2	A	513	PGU	O4P-P-O1P	2.07	112.02	106.44
2	A	513	PGU	C4-C3-C2	2.02	122.96	119.91

All (3) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
2	A	513	PGU	CA
2	B	913	PGU	CA
2	C	1413	PGU	CA

All (26) torsion outliers are listed below:

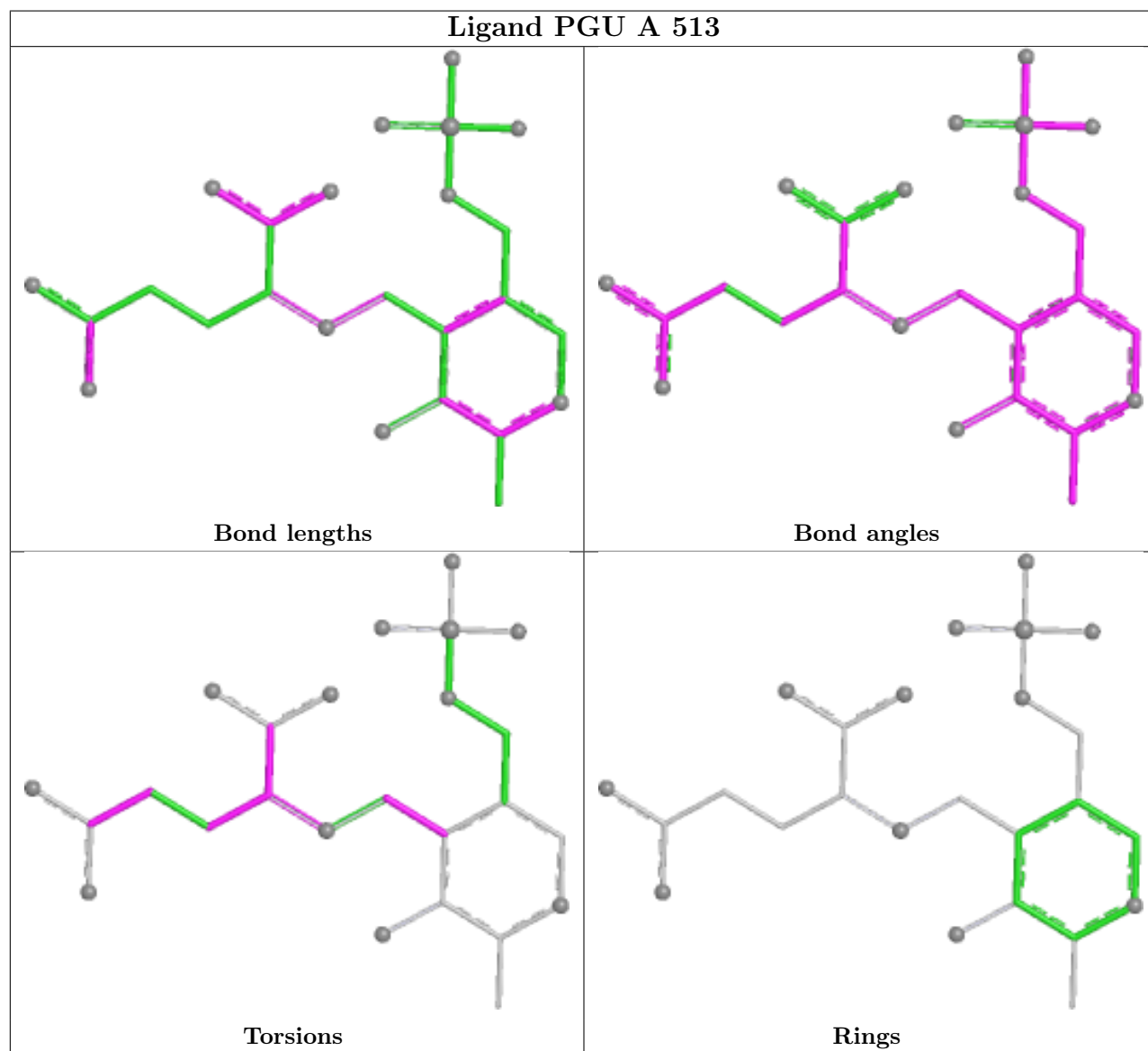
Mol	Chain	Res	Type	Atoms
2	A	513	PGU	C-CA-N-C4A
2	B	913	PGU	C-CA-N-C4A
2	C	1413	PGU	C-CA-N-C4A
2	A	513	PGU	N-CA-CB-CG
2	B	913	PGU	N-CA-CB-CG
2	C	1413	PGU	N-CA-CB-CG
2	A	513	PGU	C5-C4-C4A-N
2	B	913	PGU	C5-C4-C4A-N
2	C	1413	PGU	C5-C4-C4A-N
2	A	513	PGU	C3-C4-C4A-N
2	B	913	PGU	C3-C4-C4A-N
2	B	913	PGU	OXT-C-CA-N
2	A	513	PGU	O-C-CA-N
2	A	513	PGU	OXT-C-CA-N
2	C	1413	PGU	O-C-CA-N
2	C	1413	PGU	C3-C4-C4A-N
2	B	913	PGU	O-C-CA-N
2	C	1413	PGU	OXT-C-CA-N
2	A	513	PGU	OE1-CD-CG-CB
2	C	1413	PGU	OE1-CD-CG-CB
2	A	513	PGU	OE2-CD-CG-CB
2	B	913	PGU	OE1-CD-CG-CB
2	C	1413	PGU	OE2-CD-CG-CB
2	B	913	PGU	OE2-CD-CG-CB
2	B	913	PGU	CA-CB-CG-CD
2	A	513	PGU	C-CA-CB-CG

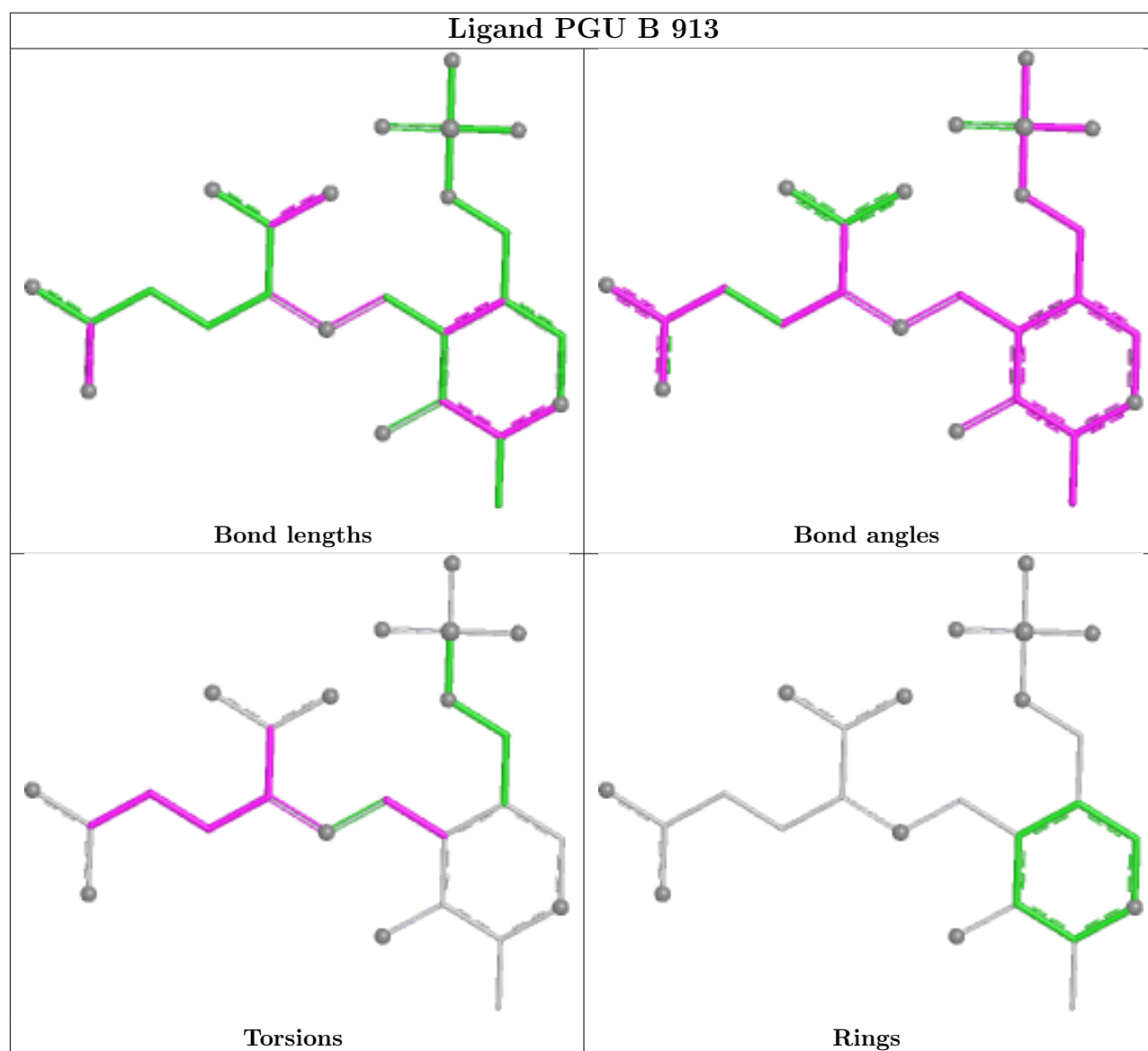
There are no ring outliers.

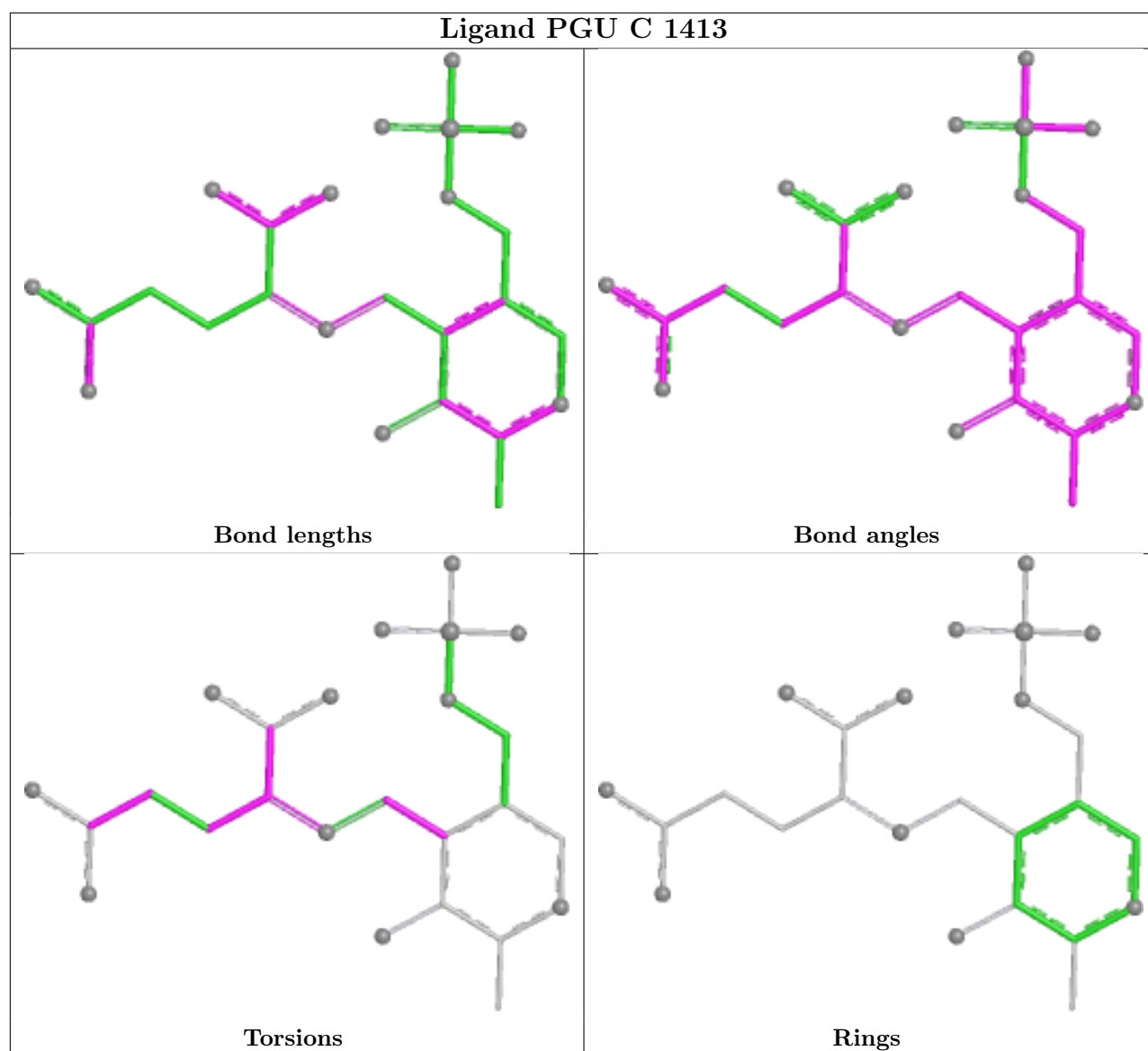
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	513	PGU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.