Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 08:35 AM EST

PDB ID	:	1MAQ
Title	:	CRYSTAL STRUCTURES OF TRUE ENZYMATIC REACTION INTERMEDIATES: ASPARTATE AND GLUTAMATE KETIMINES IN ASPARTATE AMINOTRANSFERASE
Authors	:	Malashkevich, V.N.; Jansonius, J.N.
Deposited on	:	1993-09-10
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

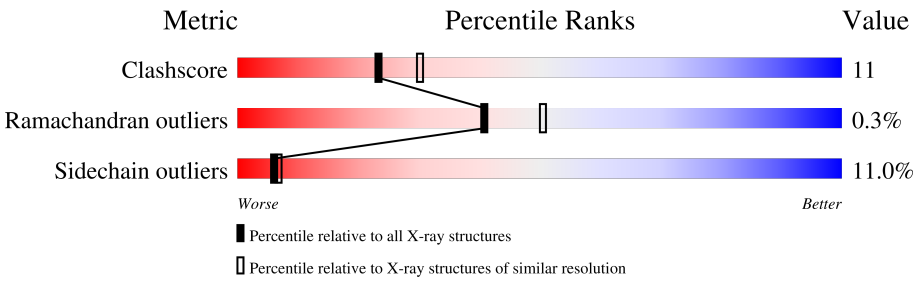
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	67% 26% 7%

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	412	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3489 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.

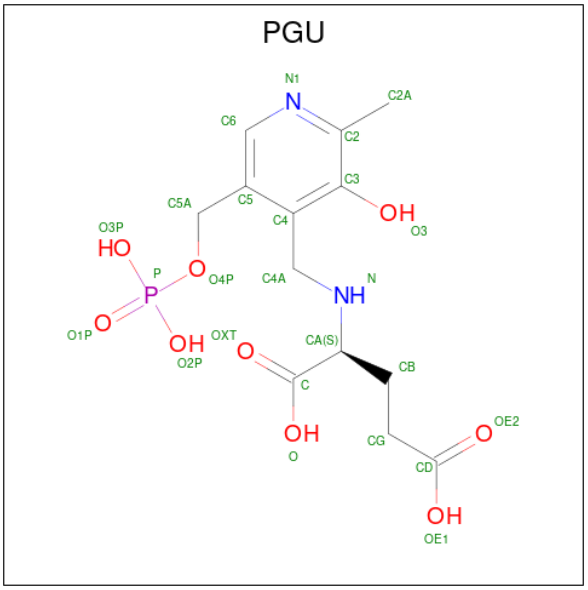
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3161	2004	558	581	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508

- Molecule 2 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-glutamic acid (three-letter code: PGU) (formula: $C_{13}H_{19}N_2O_9P$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	303	303	303	0	0

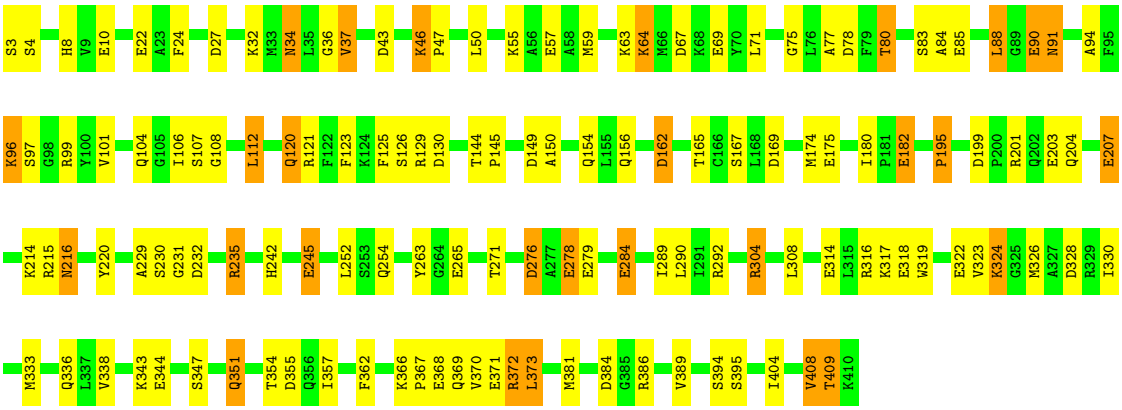
3 Residue-property plots (i)

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: ASPARTATE AMINOTRANSFERASE

Chain A: 67% 26% 7%



4 Data and refinement statistics (i)

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	70.00Å 92.10Å 128.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3489	wwPDB-VP
Average B, all atoms ($Å^2$)	24.0	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: 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	0.81	19/3231 (0.6%)	1.18	26/4360 (0.6%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	GLU	CD-OE2	6.38	1.32	1.25
1	A	278	GLU	CD-OE2	6.27	1.32	1.25
1	A	314	GLU	CD-OE1	6.11	1.32	1.25
1	A	371	GLU	CD-OE1	6.01	1.32	1.25
1	A	175	GLU	CD-OE1	5.92	1.32	1.25
1	A	57	GLU	CD-OE2	5.83	1.32	1.25
1	A	10	GLU	CD-OE1	5.74	1.31	1.25
1	A	368	GLU	CD-OE2	5.72	1.31	1.25
1	A	90	GLU	CD-OE1	5.67	1.31	1.25
1	A	182	GLU	CD-OE1	5.66	1.31	1.25
1	A	279	GLU	CD-OE2	5.66	1.31	1.25
1	A	265	GLU	CD-OE2	5.66	1.31	1.25
1	A	22	GLU	CD-OE1	5.54	1.31	1.25
1	A	69	GLU	CD-OE1	5.54	1.31	1.25
1	A	344	GLU	CD-OE1	5.49	1.31	1.25
1	A	245	GLU	CD-OE1	5.47	1.31	1.25
1	A	203	GLU	CD-OE2	5.37	1.31	1.25
1	A	85	GLU	CD-OE1	5.21	1.31	1.25
1	A	207	GLU	CD-OE1	5.07	1.31	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	A	276	ASP	CB-CG-OD2	-7.64	111.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	276	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	130	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	384	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	27	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	384	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	162	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	A	328	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	169	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	130	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	162	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	67	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	27	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	195	PRO	CB-CA-C	-5.62	97.95	112.00
1	A	199	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	A	232	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	199	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	167	SER	N-CA-CB	5.29	118.43	110.50
1	A	328	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	232	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	355	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	292	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	43	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	149	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3161	0	3154	71	0
2	A	25	0	13	1	0
3	A	303	0	0	14	0
All	All	3489	0	3167	72	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 11.

All (72) 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:A:91:ASN:H	1:A:91:ASN:HD22	0.97	0.94
1:A:91:ASN:H	1:A:91:ASN:ND2	1.65	0.93
1:A:373:LEU:HD23	1:A:381:MET:HE2	1.53	0.88
1:A:373:LEU:HD23	1:A:381:MET:CE	2.04	0.87
1:A:304:ARG:HD3	3:A:463:HOH:O	1.84	0.76
1:A:59:MET:O	1:A:63:LYS:HG3	1.90	0.71
1:A:366:LYS:H	1:A:369:GLN:HE21	1.39	0.70
1:A:404:ILE:O	1:A:409:THR:HB	1.91	0.70
1:A:121:ARG:NE	3:A:656:HOH:O	2.30	0.65
1:A:144:THR:HB	1:A:145:PRO:HD3	1.81	0.63
1:A:97:SER:OG	1:A:99:ARG:HG3	1.98	0.63
1:A:366:LYS:H	1:A:369:GLN:NE2	1.98	0.62
1:A:394:SER:HB3	3:A:538:HOH:O	2.00	0.61
1:A:91:ASN:HD22	1:A:91:ASN:N	1.82	0.60
1:A:162:ASP:OD1	1:A:165:THR:HG22	2.02	0.60
1:A:231:GLY:O	1:A:324:LYS:HD2	2.02	0.60
1:A:372:ARG:HD3	1:A:408:VAL:HG22	1.82	0.60
1:A:91:ASN:ND2	1:A:91:ASN:N	2.39	0.58
1:A:165:THR:HG21	3:A:438:HOH:O	2.02	0.58
1:A:195:PRO:HB3	1:A:386:ARG:HD3	1.84	0.57
1:A:373:LEU:HD23	1:A:381:MET:HE1	1.84	0.57
1:A:80:THR:HG23	3:A:475:HOH:O	2.03	0.57
1:A:75:GLY:HA3	1:A:104:GLN:HB2	1.88	0.56
1:A:338:VAL:HG21	1:A:354:THR:HG23	1.89	0.55
1:A:55:LYS:O	1:A:59:MET:HG3	2.07	0.55
1:A:316:ARG:NH2	3:A:581:HOH:O	2.40	0.55
1:A:37:VAL:HG12	3:A:469:HOH:O	2.08	0.54
1:A:278:GLU:HG3	3:A:598:HOH:O	2.08	0.54
1:A:101:VAL:HG21	1:A:284:GLU:HB2	1.91	0.53
1:A:24:PHE:CE2	1:A:32:LYS:HG3	2.42	0.53
1:A:330:ILE:HG23	1:A:389:VAL:HG12	1.90	0.52
1:A:229:ALA:HB1	1:A:357:ILE:HD12	1.93	0.51
1:A:37:VAL:HG11	3:A:560:HOH:O	2.10	0.51
1:A:319:TRP:O	1:A:323:VAL:HG23	2.11	0.50
1:A:83:SER:HB3	1:A:254:GLN:HE22	1.77	0.50
1:A:370:VAL:HA	1:A:381:MET:HE3	1.93	0.49
1:A:34:ASN:ND2	1:A:36:GLY:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HG22	1:A:106:ILE:O	2.12	0.48
1:A:201:ARG:O	1:A:204:GLN:HB2	2.13	0.48
1:A:180:ILE:O	1:A:215:ARG:NH2	2.43	0.47
1:A:154:GLN:NE2	3:A:676:HOH:O	2.47	0.47
1:A:125:PHE:O	1:A:126:SER:HB2	2.15	0.46
1:A:8:HIS:H	1:A:8:HIS:CD2	2.34	0.46
1:A:242:HIS:HE1	3:A:548:HOH:O	1.98	0.46
1:A:91:ASN:HB3	3:A:566:HOH:O	2.16	0.45
1:A:84:ALA:O	1:A:88:LEU:HB2	2.16	0.45
1:A:90:GLU:O	1:A:96:LYS:NZ	2.30	0.45
1:A:64:LYS:HD2	1:A:64:LYS:HA	1.43	0.45
1:A:333:MET:CE	1:A:336:GLN:NE2	2.80	0.45
1:A:120:GLN:HG3	1:A:150:ALA:O	2.16	0.45
1:A:83:SER:HB3	1:A:254:GLN:NE2	2.32	0.44
1:A:91:ASN:ND2	3:A:685:HOH:O	2.50	0.44
1:A:144:THR:CB	1:A:145:PRO:HD3	2.46	0.44
1:A:182:GLU:HG2	1:A:215:ARG:O	2.17	0.44
1:A:101:VAL:O	1:A:271:THR:HA	2.18	0.43
1:A:366:LYS:HB3	1:A:367:PRO:HD2	2.00	0.43
1:A:50:LEU:N	1:A:50:LEU:HD12	2.33	0.43
2:A:412:PGU:OXT	2:A:412:PGU:HG2	2.18	0.43
1:A:94:ALA:HA	1:A:99:ARG:HD3	2.01	0.42
1:A:156:GLN:NE2	3:A:601:HOH:O	2.51	0.42
1:A:372:ARG:HB3	1:A:408:VAL:CG2	2.50	0.42
1:A:46:LYS:HG3	1:A:47:PRO:HD2	2.01	0.42
1:A:108:GLY:O	1:A:112:LEU:HB2	2.20	0.42
1:A:230:SER:OG	1:A:235:ARG:HG2	2.20	0.42
1:A:123:PHE:O	1:A:129:ARG:NH2	2.53	0.42
1:A:77:ALA:O	1:A:80:THR:HG22	2.20	0.41
1:A:370:VAL:HA	1:A:381:MET:CE	2.50	0.41
1:A:351:GLN:HE21	1:A:351:GLN:HB2	1.32	0.41
1:A:174:MET:CE	1:A:207:GLU:HG3	2.51	0.41
1:A:174:MET:HE1	1:A:207:GLU:HG3	2.02	0.41
1:A:322:GLU:O	1:A:326:MET:HG3	2.21	0.41
1:A:216:ASN:HD22	1:A:216:ASN:HA	1.64	0.41

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	399/401 (100%)	381 (96%)	17 (4%)	1 (0%)	41 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR

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	335/335 (100%)	298 (89%)	37 (11%)	6 7

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	SER
1	A	34	ASN
1	A	37	VAL
1	A	46	LYS
1	A	64	LYS
1	A	71	LEU
1	A	78	ASP
1	A	80	THR
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	96	LYS
1	A	107	SER
1	A	112	LEU
1	A	120	GLN
1	A	214	LYS
1	A	216	ASN
1	A	220	TYR
1	A	235	ARG
1	A	245	GLU
1	A	252	LEU
1	A	276	ASP
1	A	284	GLU
1	A	289	ILE
1	A	290	LEU
1	A	308	LEU
1	A	317	LYS
1	A	324	LYS
1	A	343	LYS
1	A	347	SER
1	A	351	GLN
1	A	362	PHE
1	A	372	ARG
1	A	373	LEU
1	A	395	SER
1	A	408	VAL
1	A	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	34	ASN
1	A	91	ASN
1	A	120	GLN
1	A	156	GLN
1	A	202	GLN
1	A	216	ASN
1	A	234	ASN
1	A	242	HIS
1	A	254	GLN
1	A	286	GLN

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	336	GLN
1	A	340	ASN
1	A	351	GLN
1	A	369	GLN

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)

1 ligand is 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	412	-	25,25,25	2.38	7 (28%)	31,35,35	2.25	11 (35%)

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	412	-	1/1/4/5	12/20/20/20	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	412	PGU	C4A-N	-5.96	1.29	1.46
2	A	412	PGU	CA-N	-5.67	1.33	1.46
2	A	412	PGU	C4A-C4	-5.01	1.45	1.51
2	A	412	PGU	OXT-C	3.24	1.32	1.22
2	A	412	PGU	OE2-CD	3.06	1.32	1.22
2	A	412	PGU	OE1-CD	-2.70	1.21	1.30
2	A	412	PGU	O-C	-2.64	1.21	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	412	PGU	C4A-N-CA	6.08	125.44	113.92
2	A	412	PGU	C6-C5-C4	5.95	122.33	118.12
2	A	412	PGU	C4A-C4-C5	4.11	124.28	119.71
2	A	412	PGU	C5-C6-N1	-3.03	118.78	123.82
2	A	412	PGU	C3-C4-C5	-2.79	116.04	118.72
2	A	412	PGU	OE2-CD-CG	-2.78	114.16	123.08
2	A	412	PGU	O-C-CA	2.36	121.24	113.40
2	A	412	PGU	OE1-CD-CG	2.35	121.57	114.03
2	A	412	PGU	OXT-C-CA	-2.22	114.96	122.26
2	A	412	PGU	C6-N1-C2	2.20	123.25	119.17
2	A	412	PGU	C3-C2-N1	-2.07	118.09	120.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	412	PGU	CA

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	412	PGU	C5A-O4P-P-O1P
2	A	412	PGU	C5A-O4P-P-O2P
2	A	412	PGU	C5A-O4P-P-O3P
2	A	412	PGU	CB-CA-N-C4A
2	A	412	PGU	C5-C4-C4A-N
2	A	412	PGU	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	A	412	PGU	C3-C4-C4A-N
2	A	412	PGU	C-CA-N-C4A
2	A	412	PGU	OE1-CD-CG-CB
2	A	412	PGU	OE2-CD-CG-CB
2	A	412	PGU	O-C-CA-CB
2	A	412	PGU	OXT-C-CA-CB

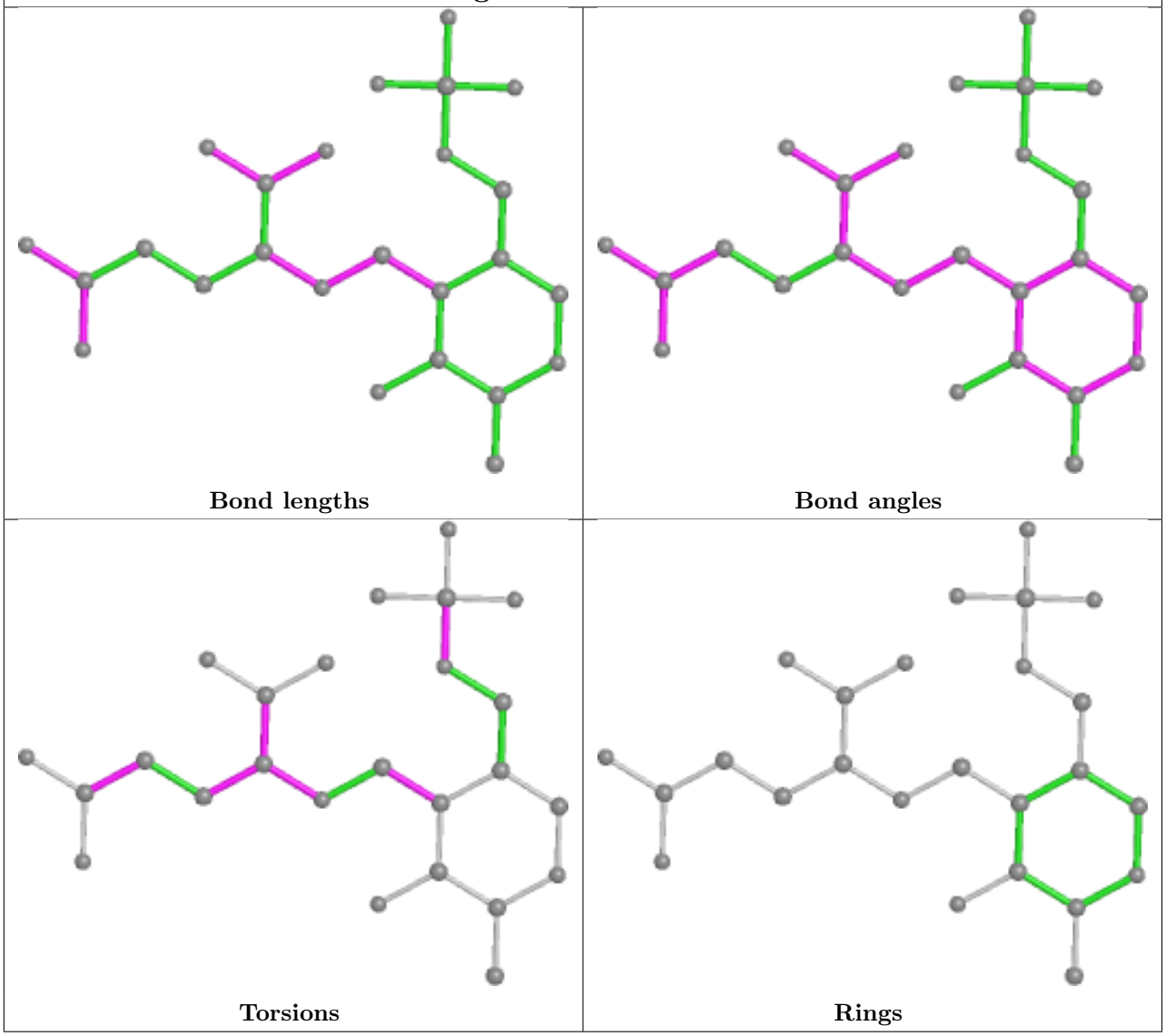
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	412	PGU	1	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 then 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 PGU A 412



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.