Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 12:39 PM EST

PDB ID	:	1AKB
Title	:	STRUCTURAL BASIS FOR THE CATALYTIC ACTIVITY OF ASPARTATE AMINOTRANSFERASE K258H LACKING ITS PYRIDOXAL-5'-PHOSPHATE-BINDING LYSINE RESIDUE
Authors	:	Malashkevich, V.N.; Jansonius, J.N.
Deposited on	:	1994-02-28
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:

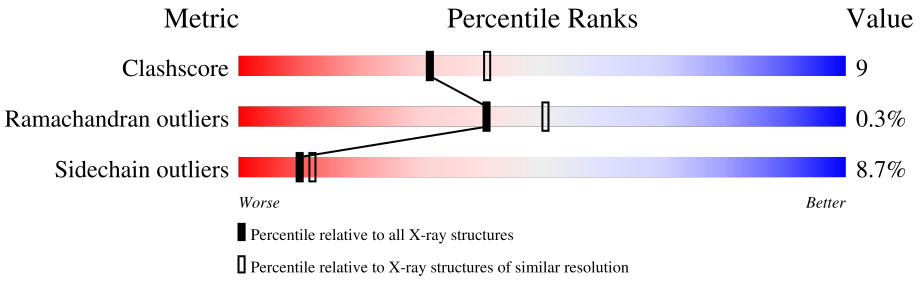
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	75% 19% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3498 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.

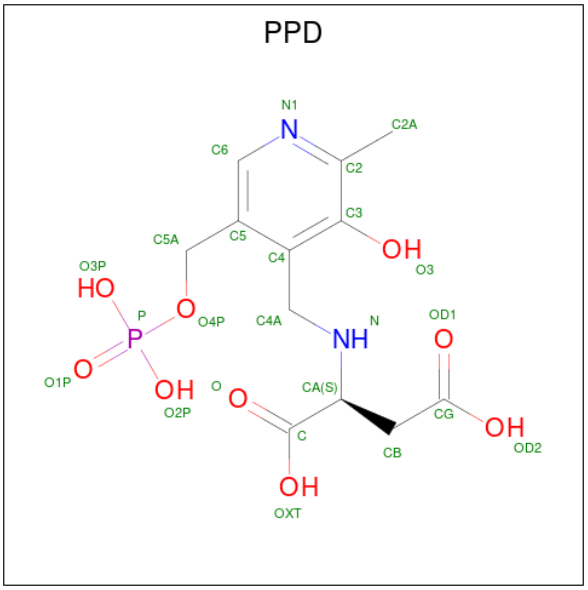
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3162	2004	559	581	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508
A	258	HIS	LYS	engineered mutation	UNP P00508

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYLENE)-AMINO]-SUCCINIC ACID (three-letter code: PPD) (formula: $C_{12}H_{17}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	24	12	2	9	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	312	312	312	0	0

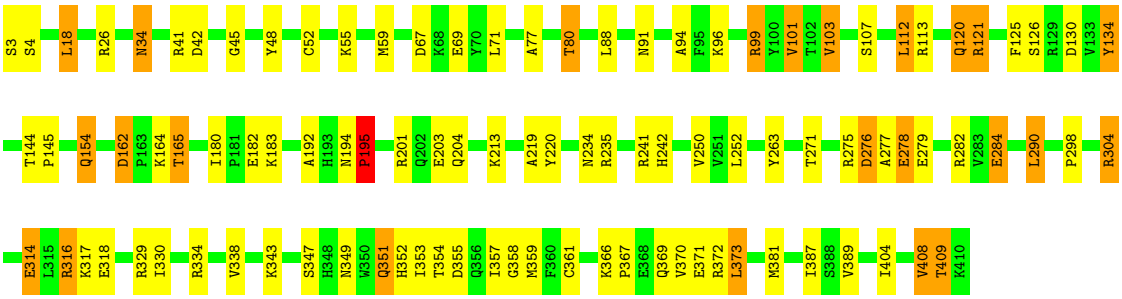
3 Residue-property plots (i)

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: 75% 19% 6%



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	70.10Å 91.80Å 129.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3498	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: PPD

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	0.77	0/3233	1.60	35/4364 (0.8%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ARG	NE-CZ-NH1	23.35	131.98	120.30
1	A	304	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	A	329	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	A	113	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	99	ARG	CD-NE-CZ	9.38	136.73	123.60
1	A	304	ARG	CD-NE-CZ	8.89	136.04	123.60
1	A	162	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	113	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	A	112	LEU	CA-CB-CG	8.05	133.81	115.30
1	A	329	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	41	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	67	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	276	ASP	CB-CA-C	-6.95	96.50	110.40
1	A	316	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	26	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	284	GLU	CA-CB-CG	6.69	128.12	113.40
1	A	41	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	99	ARG	CA-CB-CG	6.17	126.97	113.40
1	A	134	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	A	408	VAL	N-CA-CB	-6.10	98.08	111.50
1	A	235	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	103	VAL	N-CA-CB	-5.84	98.65	111.50
1	A	278	GLU	CB-CG-CD	5.78	129.81	114.20
1	A	359	MET	CA-CB-CG	-5.78	103.47	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	GLU	CG-CD-OE2	-5.71	106.88	118.30
1	A	130	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	101	VAL	N-CA-CB	5.51	123.63	111.50
1	A	26	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	121	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	372	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	69	GLU	CG-CD-OE1	-5.13	108.03	118.30
1	A	134	TYR	CB-CG-CD2	5.13	124.08	121.00
1	A	278	GLU	CG-CD-OE1	5.02	128.34	118.30
1	A	371	GLU	CA-CB-CG	5.02	124.44	113.40
1	A	195	PRO	N-CA-C	5.00	125.10	112.10

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	3162	0	3148	56	0
2	A	24	0	12	1	0
3	A	312	0	0	15	2
All	All	3498	0	3160	57	2

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 (57) 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:366:LYS:H	1:A:369:GLN:HE21	1.22	0.85
1:A:162:ASP:OD2	1:A:165:THR:HB	1.81	0.80
1:A:404:ILE:O	1:A:409:THR:HB	1.84	0.77
1:A:366:LYS:H	1:A:369:GLN:NE2	1.84	0.75
1:A:373:LEU:HD23	1:A:381:MET:HE2	1.69	0.72
1:A:91:ASN:H	1:A:91:ASN:HD22	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD23	1:A:381:MET:CE	2.27	0.64
1:A:91:ASN:H	1:A:91:ASN:ND2	1.97	0.61
1:A:165:THR:HG21	3:A:438:HOH:O	2.00	0.60
1:A:304:ARG:HD3	3:A:464:HOH:O	2.00	0.60
1:A:52:CYS:HB3	1:A:318:GLU:HG2	1.85	0.59
1:A:290:LEU:HD21	3:A:663:HOH:O	2.03	0.58
1:A:45:GLY:HA2	3:A:657:HOH:O	2.04	0.57
1:A:278:GLU:HG3	3:A:601:HOH:O	2.04	0.56
1:A:154:GLN:NE2	3:A:683:HOH:O	2.38	0.56
1:A:366:LYS:HB3	1:A:367:PRO:HD2	1.88	0.55
1:A:373:LEU:HD22	1:A:408:VAL:HG11	1.89	0.54
1:A:338:VAL:HG21	1:A:354:THR:HG23	1.91	0.53
1:A:343:LYS:NZ	3:A:510:HOH:O	2.40	0.53
1:A:370:VAL:HA	1:A:381:MET:HE3	1.90	0.53
1:A:387:ILE:O	1:A:387:ILE:HG13	2.09	0.52
1:A:366:LYS:N	1:A:369:GLN:HE21	2.00	0.52
1:A:234:ASN:HD22	1:A:241:ARG:HH12	1.57	0.52
1:A:120:GLN:NE2	3:A:442:HOH:O	2.42	0.51
1:A:349:ASN:OD1	1:A:351:GLN:HB3	2.11	0.51
1:A:55:LYS:O	1:A:59:MET:HG3	2.10	0.51
1:A:192:ALA:HA	1:A:357:ILE:CD1	2.40	0.51
1:A:314:GLU:HB3	3:A:590:HOH:O	2.10	0.51
1:A:366:LYS:HB3	1:A:367:PRO:CD	2.41	0.51
1:A:381:MET:SD	1:A:387:ILE:HG22	2.52	0.49
1:A:162:ASP:OD1	1:A:164:LYS:HE3	2.12	0.48
1:A:213:LYS:HE2	3:A:637:HOH:O	2.13	0.48
1:A:101:VAL:O	1:A:271:THR:HA	2.15	0.47
1:A:330:ILE:HG23	1:A:389:VAL:HG13	1.97	0.47
1:A:316:ARG:NH2	3:A:584:HOH:O	2.33	0.46
1:A:182:GLU:O	1:A:183:LYS:HB2	2.16	0.46
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.97	0.46
1:A:194:ASN:HA	1:A:195:PRO:HA	1.78	0.45
1:A:353:ILE:HG12	1:A:361:CYS:SG	2.57	0.45
2:A:411:PPD:O3	2:A:411:PPD:N	2.50	0.45
1:A:242:HIS:HE1	3:A:551:HOH:O	2.00	0.44
1:A:34:ASN:C	1:A:34:ASN:HD22	2.21	0.44
1:A:144:THR:N	1:A:145:PRO:HD2	2.34	0.43
1:A:42:ASP:HB3	1:A:48:TYR:HB2	2.01	0.43
1:A:134:TYR:CE2	1:A:180:ILE:HG12	2.54	0.43
1:A:201:ARG:O	1:A:204:GLN:HB2	2.18	0.42
1:A:334:ARG:NH2	1:A:358:GLY:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HA	1:A:381:MET:CE	2.50	0.42
1:A:203:GLU:CD	1:A:203:GLU:H	2.24	0.41
1:A:219:ALA:HB3	1:A:250:VAL:HG12	2.02	0.41
1:A:277:ALA:HB1	3:A:514:HOH:O	2.20	0.41
1:A:80:THR:HG23	3:A:476:HOH:O	2.19	0.41
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.80	0.41
1:A:121:ARG:HB2	3:A:663:HOH:O	2.21	0.41
1:A:77:ALA:O	1:A:80:THR:HG22	2.21	0.40
1:A:125:PHE:O	1:A:126:SER:HB2	2.20	0.40
1:A:352:HIS:HA	1:A:355:ASP:HB2	2.04	0.40

All (2) 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:A:641:HOH:O	3:A:641:HOH:O[3_655]	1.20	1.00
3:A:437:HOH:O	3:A:437:HOH:O[3_655]	1.97	0.23

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%)	382 (96%)	16 (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%)	306 (91%)	29 (9%)	10 12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	SER
1	A	18	LEU
1	A	34	ASN
1	A	71	LEU
1	A	80	THR
1	A	88	LEU
1	A	96	LYS
1	A	103	VAL
1	A	107	SER
1	A	112	LEU
1	A	120	GLN
1	A	154	GLN
1	A	165	THR
1	A	195	PRO
1	A	220	TYR
1	A	252	LEU
1	A	275	ARG
1	A	276	ASP
1	A	282	ARG
1	A	284	GLU
1	A	290	LEU
1	A	298	PRO
1	A	314	GLU
1	A	317	LYS
1	A	347	SER
1	A	351	GLN
1	A	373	LEU
1	A	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	286	GLN
1	A	301	ASN
1	A	336	GLN
1	A	340	ASN
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	PPD	A	411	-	24,24,24	1.24	3 (12%)	30,34,34	2.43	12 (40%)

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	PPD	A	411	-	-	10/19/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PPD	C3-C2	3.16	1.44	1.40
2	A	411	PPD	O-C	2.59	1.30	1.22
2	A	411	PPD	C5-C4	2.10	1.43	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	411	PPD	O4P-C5A-C5	5.69	120.19	109.35
2	A	411	PPD	C2A-C2-C3	5.20	127.32	120.89
2	A	411	PPD	C4A-C4-C5	4.94	125.20	119.71
2	A	411	PPD	C6-C5-C4	3.72	120.75	118.12
2	A	411	PPD	O3-C3-C4	3.08	127.16	118.13
2	A	411	PPD	O3-C3-C2	-3.02	110.92	117.49
2	A	411	PPD	C3-C2-N1	-2.78	117.17	120.77
2	A	411	PPD	OXT-C-O	-2.57	118.26	124.09
2	A	411	PPD	CA-CB-CG	2.48	120.12	112.88
2	A	411	PPD	C4-C4A-N	-2.47	104.98	111.78
2	A	411	PPD	C3-C4-C5	-2.46	116.36	118.72
2	A	411	PPD	O3P-P-O2P	2.20	116.03	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PPD	C4-C5-C5A-O4P
2	A	411	PPD	C6-C5-C5A-O4P
2	A	411	PPD	C5A-O4P-P-O2P
2	A	411	PPD	C5A-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	A	411	PPD	C5-C4-C4A-N
2	A	411	PPD	C-CA-N-C4A
2	A	411	PPD	C3-C4-C4A-N
2	A	411	PPD	O-C-CA-CB
2	A	411	PPD	OXT-C-CA-CB
2	A	411	PPD	C5A-O4P-P-O1P

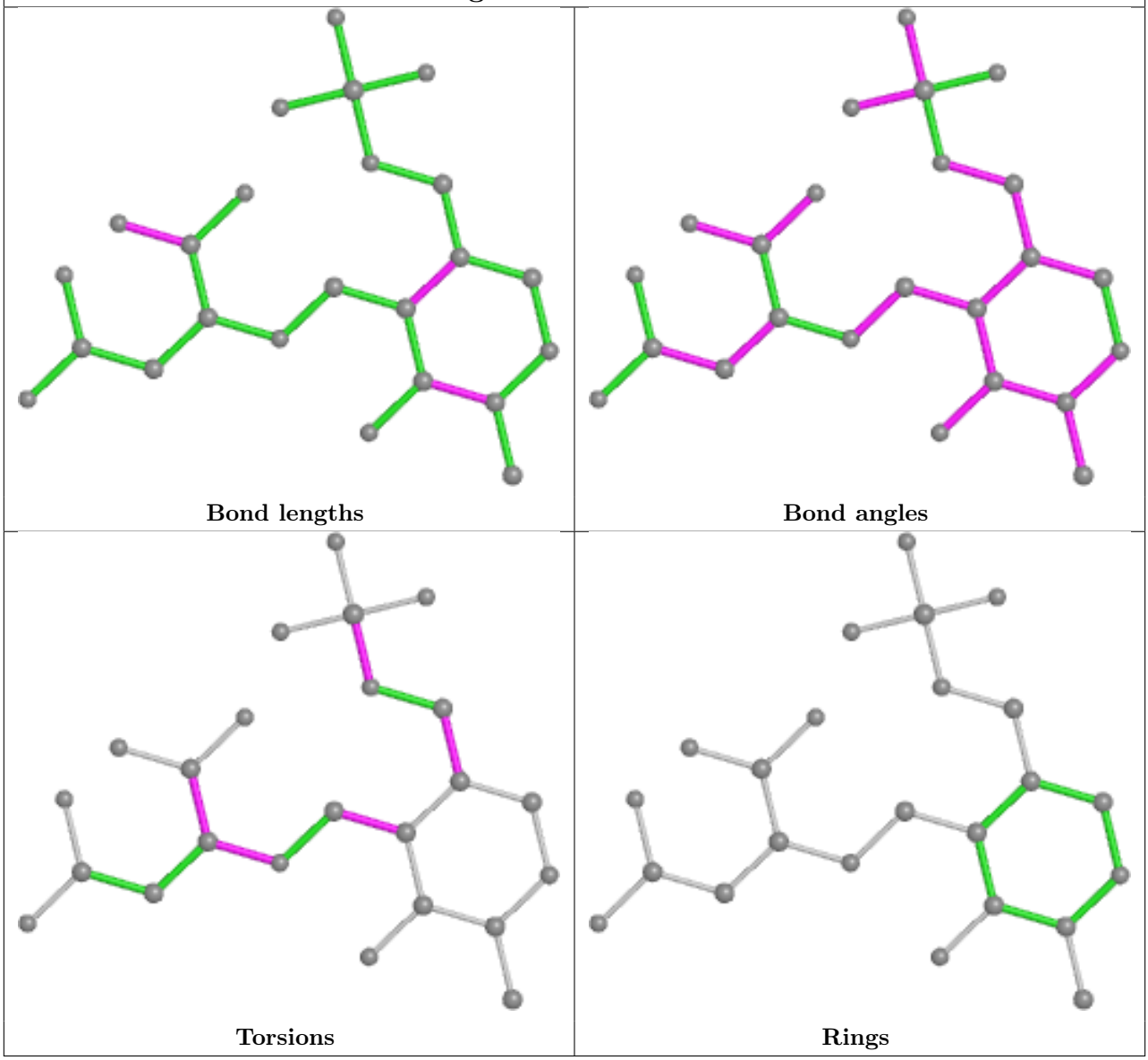
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PPD	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 PPD A 411



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.