



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:38 AM UTC

PDB ID : 1ASD / pdb_00001asd
Title : THE STRUCTURE OF WILD TYPE E. COLI ASPARTATE AMINO-TRANSFERASE RECONSTITUTED WITH N-MEPLP
Authors : Schumacher, C.; Ringe, D.
Deposited on : 1993-08-27
Resolution : 2.20 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

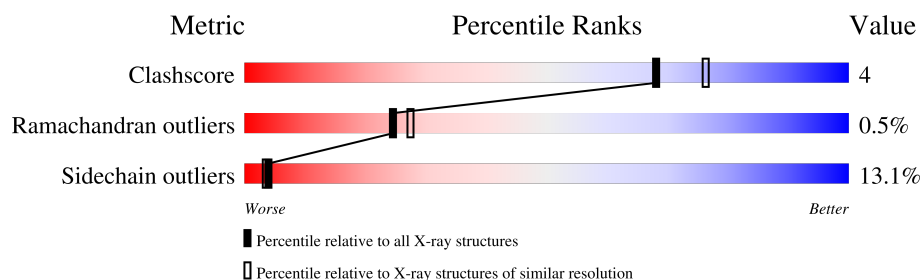
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	396	

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	MAE	A	410	-	X	-	-

2 Entry composition [i](#)

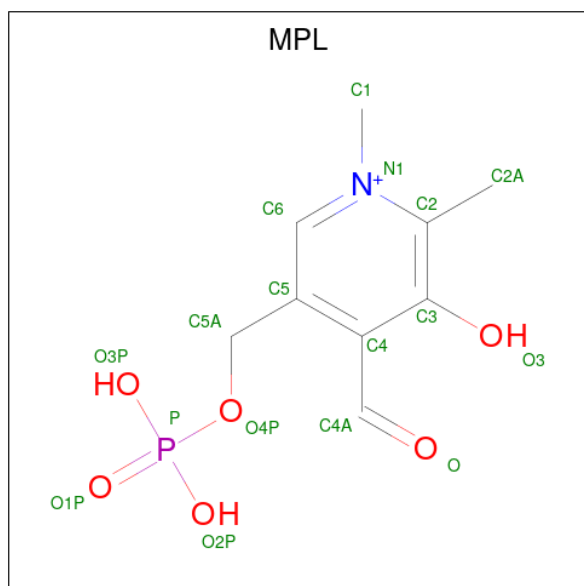
There are 4 unique types of molecules in this entry. The entry contains 3220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

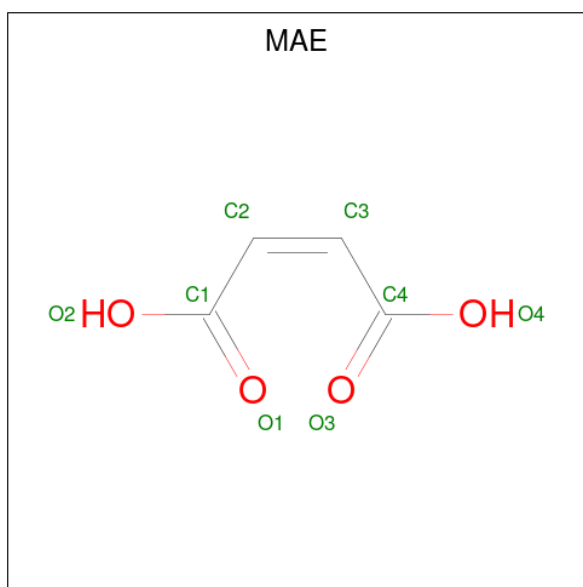
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3069	1936	536	584	13	0	0	0

- Molecule 2 is N-METHYL-PYRIDOXAL-5'-PHOSPHATE (CCD ID: MPL) (formula: $C_9H_{13}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	16	9	1	5	1	0	0

- Molecule 3 is MALEIC ACID (CCD ID: MAE) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is water.

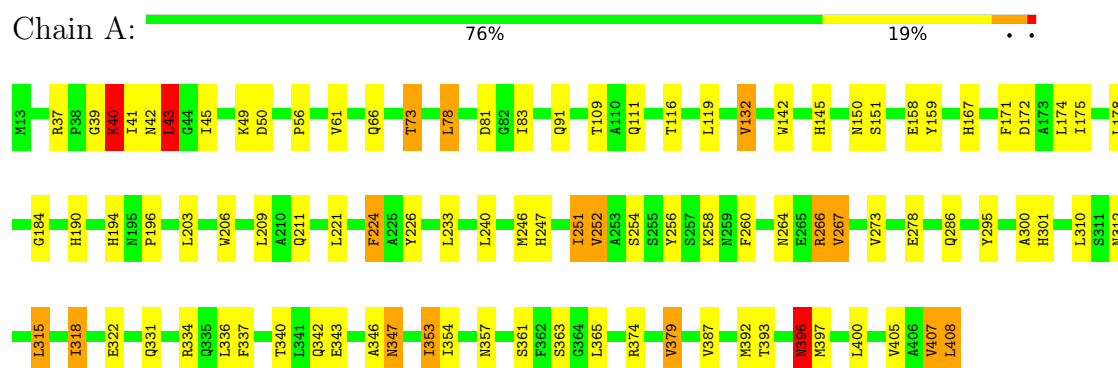
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		

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: ASPARTATE 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	157.96Å 85.41Å 78.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3220	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: MPL, MAE

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	0.97	13/3130 (0.4%)	1.81	46/4240 (1.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	VAL	CA-CB	9.91	1.66	1.54
1	A	251	ILE	CA-CB	7.63	1.65	1.54
1	A	379	VAL	CA-CB	6.78	1.62	1.54
1	A	167	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	301	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	267	VAL	CA-CB	6.46	1.62	1.54
1	A	190	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	247	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	145	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	194	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	190	HIS	CG-ND1	-5.47	1.32	1.38
1	A	318	ILE	CA-CB	5.12	1.61	1.54
1	A	247	HIS	CG-ND1	-5.08	1.32	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ASN	CA-CB-CG	10.24	122.84	112.60
1	A	295	TYR	O-C-N	-10.11	111.12	122.84
1	A	42	ASN	CA-C-O	-9.41	110.91	120.80
1	A	300	ALA	N-CA-C	7.87	119.94	111.36
1	A	295	TYR	N-CA-C	-7.62	99.18	110.46
1	A	50	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	396	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	A	43	LEU	N-CA-C	6.93	125.56	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	A	286	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	142	TRP	CA-C-N	6.77	126.73	119.28
1	A	142	TRP	C-N-CA	6.77	126.73	119.28
1	A	73	THR	CA-CB-OG1	-6.62	99.67	109.60
1	A	150	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	42	ASN	CB-CG-ND2	6.54	126.21	116.40
1	A	190	HIS	CA-C-N	6.43	127.12	119.98
1	A	190	HIS	C-N-CA	6.43	127.12	119.98
1	A	167	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	A	254	SER	N-CA-CB	-6.20	100.89	110.56
1	A	286	GLN	CG-CD-NE2	6.18	125.67	116.40
1	A	337	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	81	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	194	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	A	266	ARG	N-CA-C	5.92	117.83	110.91
1	A	159	TYR	CA-CB-CG	5.88	124.49	113.90
1	A	407	VAL	N-CA-CB	-5.88	101.81	111.98
1	A	374	ARG	CA-CB-CG	5.83	125.75	114.10
1	A	224	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	40	LYS	CA-CB-CG	5.82	125.73	114.10
1	A	42	ASN	N-CA-C	5.67	118.56	111.24
1	A	264	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	396	ASN	CB-CG-ND2	5.62	124.82	116.40
1	A	363	SER	N-CA-C	5.52	119.11	112.38
1	A	206	TRP	CG-CD2-CE3	5.46	139.37	133.90
1	A	91	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	73	THR	CA-CB-CG2	5.45	119.76	110.50
1	A	301	HIS	N-CA-C	5.39	117.60	111.02
1	A	247	HIS	N-CA-C	5.32	118.48	109.76
1	A	150	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	266	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	116	THR	CA-C-N	5.16	125.71	119.98
1	A	116	THR	C-N-CA	5.16	125.71	119.98
1	A	132	VAL	CB-CA-C	-5.13	104.20	111.28
1	A	233	LEU	N-CA-C	5.11	117.24	111.11
1	A	347	ASN	O-C-N	5.05	128.90	122.84
1	A	397	MET	N-CA-C	5.03	116.77	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3069	0	3016	22	0
2	A	16	0	10	3	0
3	A	8	0	2	0	0
4	A	127	0	0	2	0
All	All	3220	0	3028	22	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 4.

All (22) 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:226:TYR:CE1	1:A:258:LYS:HG2	2.11	0.85
1:A:312:ASN:HD22	1:A:315:LEU:H	1.48	0.60
1:A:258:LYS:HB2	4:A:542:HOH:O	2.03	0.58
1:A:405:VAL:HA	1:A:408:LEU:HD22	1.86	0.56
1:A:266:ARG:HH22	2:A:409:MPL:P	2.29	0.56
1:A:226:TYR:HE2	2:A:409:MPL:HO3	1.53	0.55
1:A:37:ARG:O	1:A:40:LYS:HG3	2.09	0.53
1:A:392:MET:HA	1:A:396:ASN:HD21	1.74	0.52
1:A:346:ALA:HB2	1:A:405:VAL:HG12	1.93	0.49
1:A:83:ILE:H	1:A:111:GLN:NE2	2.10	0.49
1:A:43:LEU:HD21	1:A:400:LEU:HD21	1.96	0.48
1:A:340:THR:HA	1:A:343:GLU:HG2	1.96	0.46
1:A:258:LYS:NZ	2:A:409:MPL:H52	2.31	0.45
1:A:361:SER:HB3	1:A:387:VAL:HG23	1.99	0.44
1:A:318:ILE:O	1:A:322:GLU:HG3	2.17	0.43
1:A:334:ARG:HG3	1:A:353:ILE:HD12	2.00	0.43
1:A:132:VAL:HG12	1:A:184:GLY:O	2.19	0.42
1:A:171:PHE:O	1:A:175:ILE:HG12	2.19	0.42
1:A:393:THR:H	1:A:396:ASN:ND2	2.17	0.42
1:A:78:LEU:HB2	4:A:614:HOH:O	2.20	0.41
1:A:41:ILE:HG22	1:A:43:LEU:HD13	2.03	0.41
1:A:256:TYR:O	1:A:260:PHE:HB2	2.20	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	394/396 (100%)	378 (96%)	14 (4%)	2 (0%)	24 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	39	GLY

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	320/320 (100%)	278 (87%)	42 (13%)	4 3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	45	ILE
1	A	49	LYS
1	A	56	PRO
1	A	61	VAL
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	73	THR
1	A	78	LEU
1	A	109	THR
1	A	119	LEU
1	A	151	SER
1	A	158	GLU
1	A	172	ASP
1	A	174	LEU
1	A	178	LEU
1	A	196	PRO
1	A	203	LEU
1	A	209	LEU
1	A	211	GLN
1	A	221	LEU
1	A	224	PHE
1	A	240	LEU
1	A	246	MET
1	A	251	ILE
1	A	252	VAL
1	A	267	VAL
1	A	273	VAL
1	A	278	GLU
1	A	310	LEU
1	A	315	LEU
1	A	331	GLN
1	A	336	LEU
1	A	342	GLN
1	A	347	ASN
1	A	353	ILE
1	A	354	ILE
1	A	357	ASN
1	A	365	LEU
1	A	379	VAL
1	A	396	ASN
1	A	407	VAL
1	A	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	176	ASN
1	A	227	GLN
1	A	312	ASN
1	A	331	GLN
1	A	335	GLN
1	A	357	ASN
1	A	396	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 ⓘ

2 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	$\# Z > 2$
3	MAE	A	410	-	7,7,7	1.58	2 (28%)	8,8,8	1.73	4 (50%)
2	MPL	A	409	1	16,16,17	1.78	2 (12%)	22,24,25	1.69	7 (31%)

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	MAE	A	410	-	-	4/5/5/5	-
2	MPL	A	409	1	-	3/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	MPL	C1-N1	-4.24	1.37	1.47
2	A	409	MPL	C5-C4	-3.02	1.37	1.40
3	A	410	MAE	O4-C4	-2.95	1.22	1.30
3	A	410	MAE	O2-C1	-2.71	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	MPL	O3-C3-C2	3.06	119.95	116.62
3	A	410	MAE	O2-C1-O1	-2.91	116.78	122.70
2	A	409	MPL	C1-N1-C2	2.73	123.45	120.31
2	A	409	MPL	C2-C3-C4	-2.70	119.28	120.53
2	A	409	MPL	O3P-P-O4P	-2.40	100.42	106.67
3	A	410	MAE	O4-C4-O3	-2.26	118.09	122.70
2	A	409	MPL	O3P-P-O2P	2.24	116.19	107.80
3	A	410	MAE	O3-C4-C3	2.19	127.78	121.06
3	A	410	MAE	O2-C1-C2	2.16	124.08	116.16
2	A	409	MPL	C3-C2-N1	2.14	119.48	118.35
2	A	409	MPL	O4P-C5A-C5	-2.10	105.42	109.36

There are no chirality outliers.

All (7) torsion outliers are listed below:

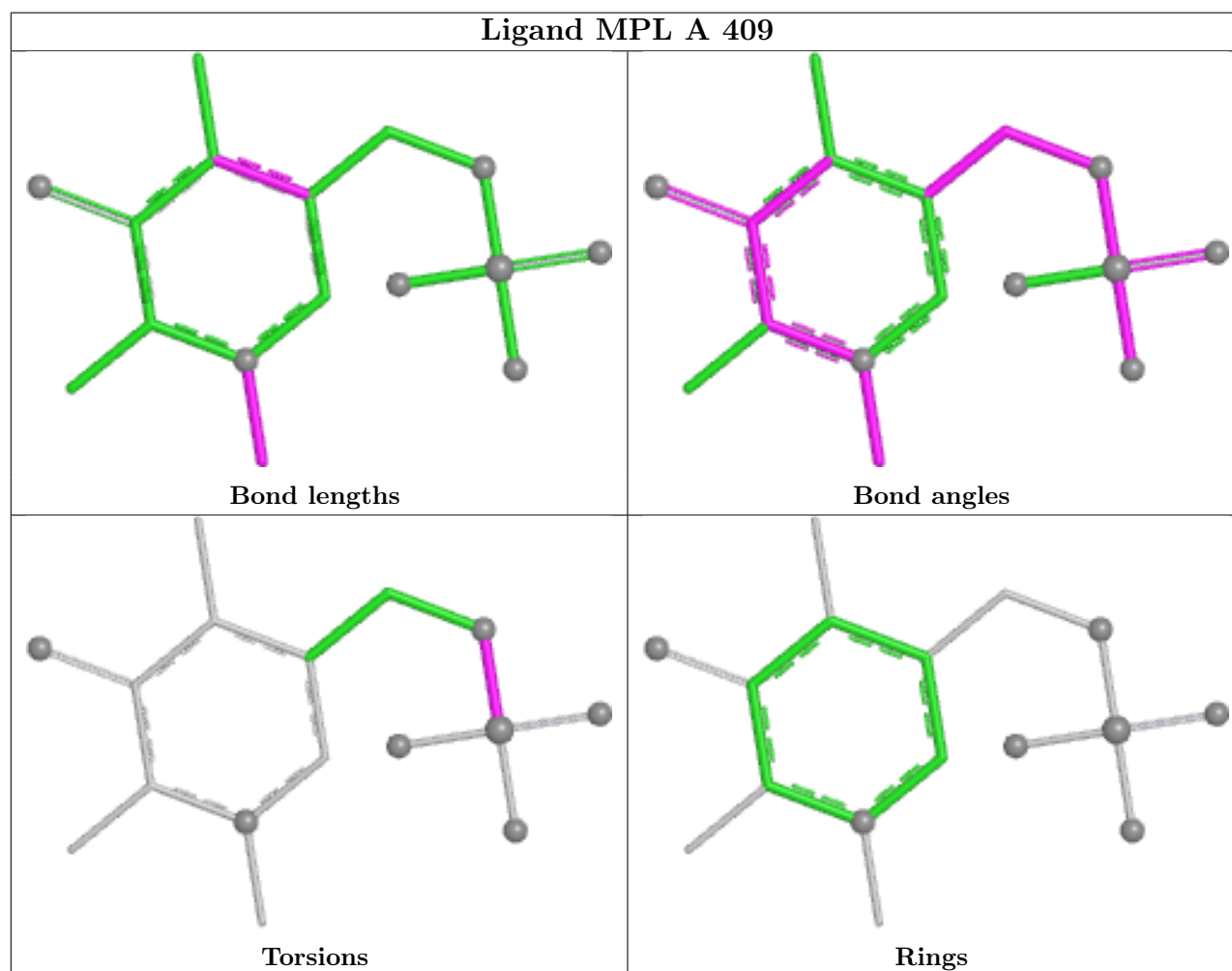
Mol	Chain	Res	Type	Atoms
2	A	409	MPL	C5A-O4P-P-O1P
2	A	409	MPL	C5A-O4P-P-O2P
2	A	409	MPL	C5A-O4P-P-O3P
3	A	410	MAE	O2-C1-C2-C3
3	A	410	MAE	O1-C1-C2-C3
3	A	410	MAE	C2-C3-C4-O4
3	A	410	MAE	C2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	409	MPL	3	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

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.