Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 02:13 pm BST

PDB ID	:	1ASD
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

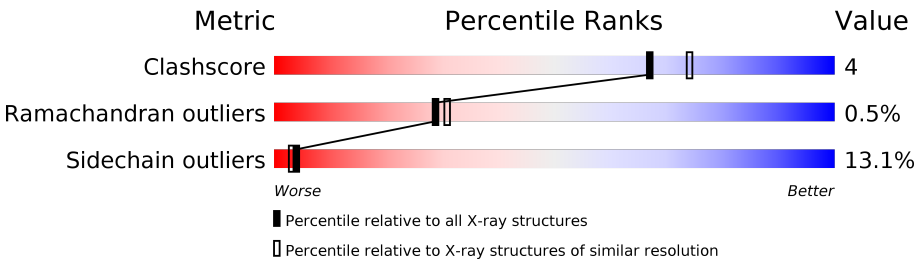
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 on 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	396	75% 20% • •

2 Entry composition (i)

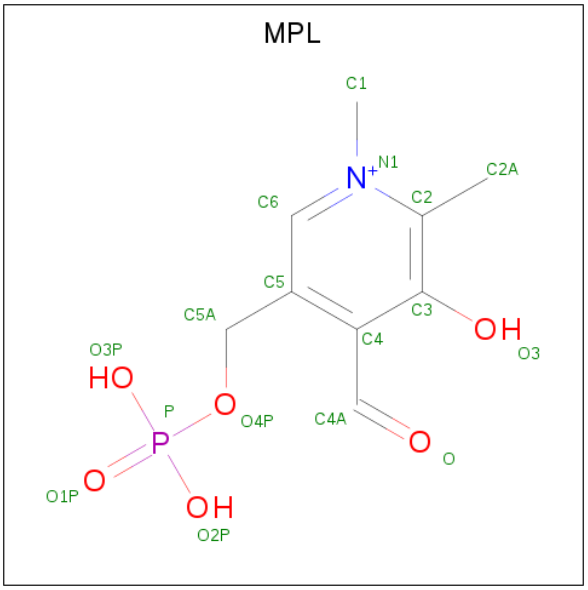
There are 4 unique types of molecules in this entry. The entry contains 3220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

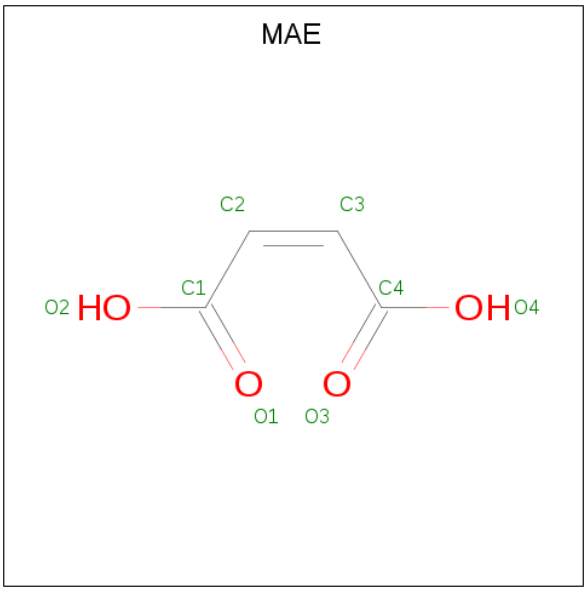
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3069	1936	536	584	13	0	0	0

- Molecule 2 is N-METHYL-PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 (three-letter code: MAE) (formula: $C_4H_4O_4$).



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

- Molecule 4 is water.

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

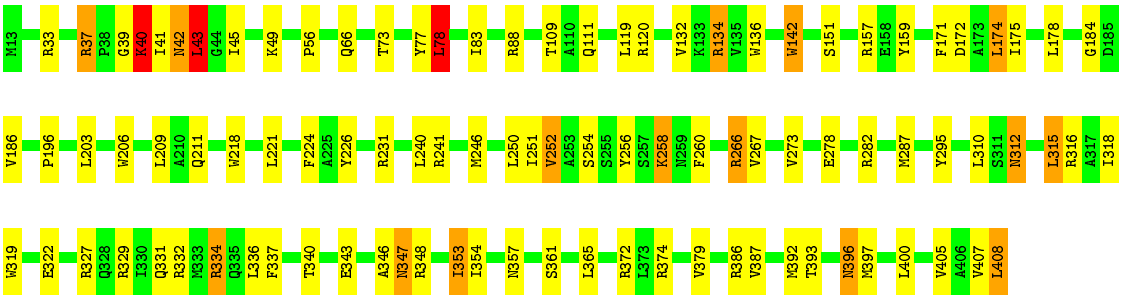
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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:



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	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 (i)

5.1 Standard geometry (i)

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	0.74	1/3130 (0.0%)	1.51	57/4240 (1.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	VAL	CA-CB	5.68	1.66	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	A	266	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	A	218	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	A	231	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	A	136	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	282	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	316	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	327	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	77	TYR	CB-CG-CD2	-7.56	116.47	121.00
1	A	319	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	136	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	A	120	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	334	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	295	TYR	O-C-N	-7.24	111.12	122.70
1	A	250	LEU	CA-CB-CG	6.94	131.27	115.30
1	A	295	TYR	CA-C-N	6.92	132.42	117.20
1	A	329	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	206	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	157	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	319	TRP	CE2-CD2-CG	-6.74	101.91	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	ASN	CA-C-N	6.73	132.01	117.20
1	A	142	TRP	CD1-CG-CD2	6.63	111.61	106.30
1	A	332	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	218	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	134	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	386	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	327	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	254	SER	N-CA-CB	-6.40	100.89	110.50
1	A	348	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	88	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	282	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	206	TRP	CG-CD2-CE3	6.07	139.37	133.90
1	A	33	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	120	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	186	VAL	CG1-CB-CG2	-5.93	101.42	110.90
1	A	142	TRP	CE2-CD2-CG	-5.91	102.57	107.30
1	A	37	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	206	TRP	CD1-CG-CD2	5.88	111.01	106.30
1	A	78	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	159	TYR	CA-CB-CG	5.84	124.49	113.40
1	A	347	ASN	CA-C-N	-5.77	104.51	117.20
1	A	218	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	374	ARG	CA-CB-CG	5.62	125.75	113.40
1	A	40	LYS	CA-CB-CG	5.61	125.73	113.40
1	A	386	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	372	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	174	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	241	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	316	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	43	LEU	N-CA-C	5.39	125.56	111.00
1	A	73	THR	CA-CB-CG2	5.26	119.76	112.40
1	A	157	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	287	MET	CG-SD-CE	-5.24	91.81	100.20
1	A	136	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	A	319	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	A	206	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	A	231	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	3069	0	3016	24	0
2	A	16	0	10	4	0
3	A	8	0	2	0	0
4	A	127	0	0	2	0
All	All	3220	0	3028	24	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 (24) 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	1.55	0.54
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:337:PHE:HD1	1:A:397:MET:HE2	1.84	0.43
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:142:TRP:CZ3	2:A:409:MPL:H13	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	29 31

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

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Mol	Chain	Res	Type
1	A	42	ASN
1	A	45	ILE
1	A	49	LYS
1	A	56	PRO
1	A	66	GLN
1	A	78	LEU
1	A	109	THR
1	A	119	LEU
1	A	134	ARG
1	A	151	SER
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	258	LYS
1	A	267	VAL
1	A	273	VAL
1	A	278	GLU
1	A	310	LEU
1	A	312	ASN
1	A	315	LEU
1	A	331	GLN
1	A	336	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	312	ASN
1	A	396	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	-	1,7,7	0.81	0	2,8,8	1.89	1 (50%)
2	MPL	A	409	1	16,16,17	1.82	2 (12%)	21,24,25	1.75	7 (33%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	MPL	C1-N1	-4.55	1.37	1.47
2	A	409	MPL	C5-C4	-3.04	1.37	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	409	MPL	O3-C3-C2	3.00	119.95	116.58
2	A	409	MPL	C1-N1-C2	2.73	123.45	120.28
2	A	409	MPL	C2-C3-C4	-2.57	119.28	120.56
2	A	409	MPL	O3P-P-O4P	-2.37	100.42	106.73
2	A	409	MPL	O3P-P-O2P	2.24	116.19	107.64
2	A	409	MPL	C3-C2-N1	2.18	119.48	118.32
3	A	410	MAE	C4-C3-C2	2.12	128.21	123.69
2	A	409	MPL	O4P-C5A-C5	-2.06	105.42	109.35

There are no chirality outliers.

All (3) 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

There are no ring outliers.

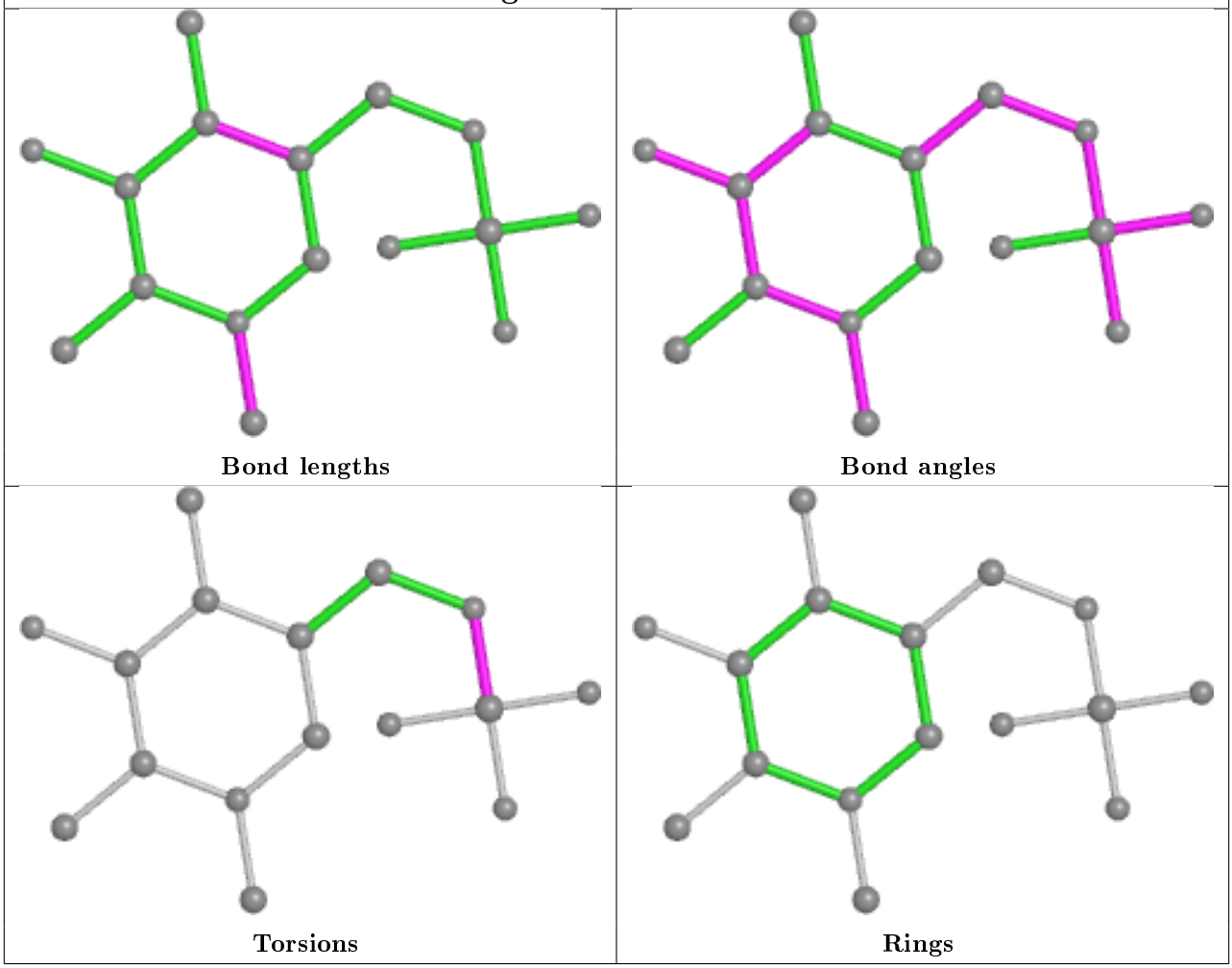
1 monomer is involved in 4 short contacts:

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



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.