



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:03 am GMT

PDB ID : 1ASA
Title : THE STRUCTURAL BASIS FOR THE REDUCED ACTIVITY OF THE
Y226F(Y225F) ACTIVE SITE MUTANT OF E. COLI ASPARTATE
AMINOTRANSFERASE
Authors : Schumacher, C.; Ringe, D.
Deposited on : 1993-08-27
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

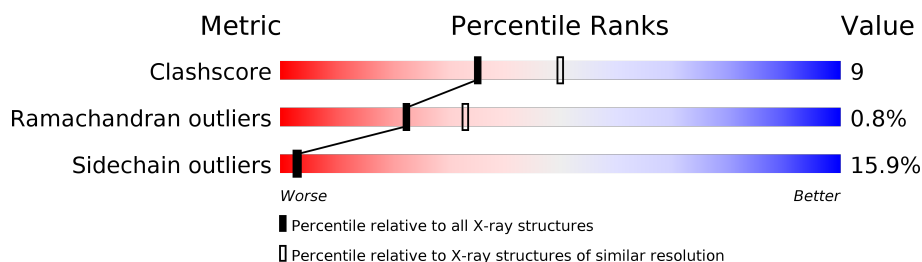
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 65% 28% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3108 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.

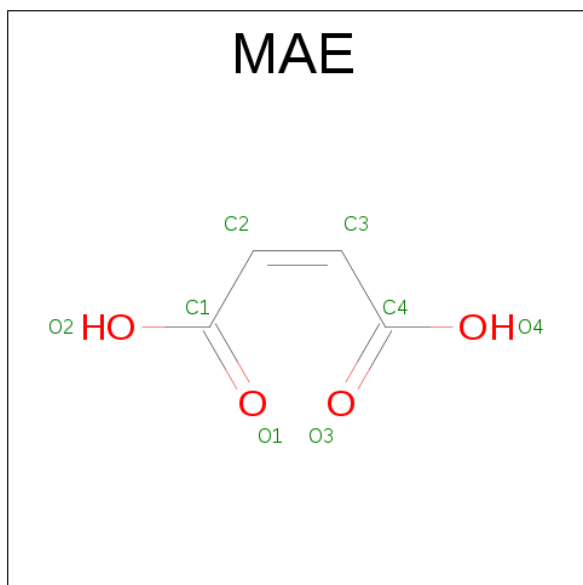
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3069	1936	536	584	13	0	0	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: C₄H₄O₄).



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

- Molecule 4 is water.

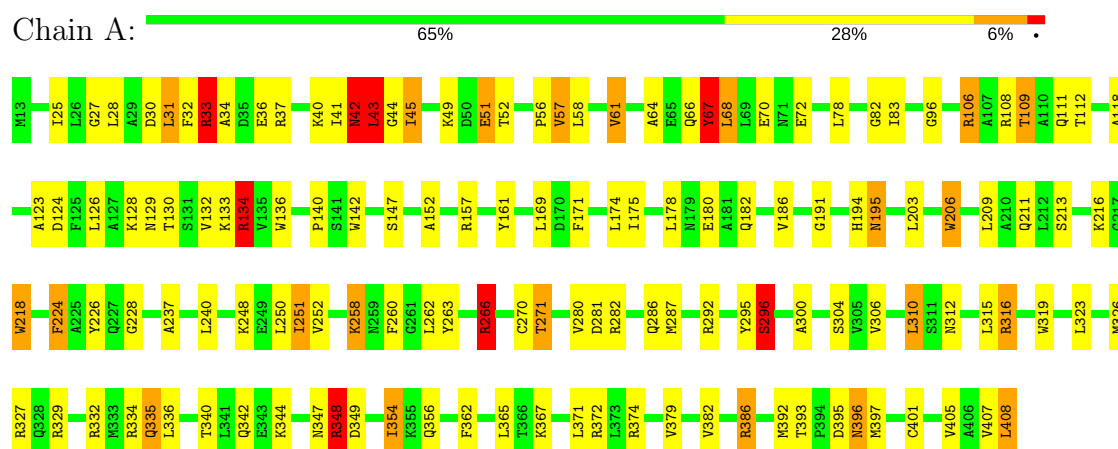
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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	157.50Å 84.80Å 78.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	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	3108	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: MAE, PLP

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	0.87	0/3130	1.61	54/4240 (1.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH2	-14.40	113.10	120.30
1	A	332	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	282	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	A	266	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	A	348	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	319	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	A	42	ASN	CA-C-N	8.43	135.74	117.20
1	A	106	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	295	TYR	CA-C-N	8.14	135.11	117.20
1	A	407	VAL	CG1-CB-CG2	-8.07	97.98	110.90
1	A	136	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	A	319	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	295	TYR	O-C-N	-7.52	110.67	122.70
1	A	218	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	A	287	MET	CG-SD-CE	-7.42	88.32	100.20
1	A	142	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	136	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	142	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	A	33	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	A	281	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	250	LEU	CA-CB-CG	6.61	130.50	115.30
1	A	263	TYR	CB-CG-CD1	-6.51	117.10	121.00
1	A	218	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	108	ARG	NE-CZ-NH2	-6.17	117.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	TRP	CG-CD2-CE3	6.15	139.43	133.90
1	A	147	SER	N-CA-CB	-6.06	101.41	110.50
1	A	37	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	157	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	108	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	42	ASN	CA-C-O	-5.84	107.84	120.10
1	A	96	GLY	CA-C-N	-5.82	104.41	117.20
1	A	206	TRP	CD1-CG-CD2	5.74	110.89	106.30
1	A	329	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	319	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	A	316	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	206	TRP	CE2-CD2-CG	-5.55	102.86	107.30
1	A	296	SER	CA-CB-OG	5.54	126.15	111.20
1	A	134	ARG	CA-CB-CG	5.40	125.28	113.40
1	A	136	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	57	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	A	43	LEU	N-CA-C	5.35	125.44	111.00
1	A	42	ASN	CB-CG-ND2	5.34	129.52	116.70
1	A	334	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	332	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	67	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	371	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	136	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	A	37	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	157	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	386	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	45	ILE	CA-CB-CG1	-5.07	101.36	111.00
1	A	280	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	A	206	TRP	CE2-CD2-CE3	5.06	124.78	118.70
1	A	382	VAL	CG1-CB-CG2	-5.01	102.88	110.90

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	57	0
2	A	15	0	6	1	0
3	A	8	0	2	0	0
4	A	16	0	0	0	0
All	All	3108	0	3024	57	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 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:130:THR:HG22	1:A:132:VAL:H	1.51	0.76
1:A:126:LEU:O	1:A:130:THR:HB	1.88	0.73
1:A:132:VAL:HG21	1:A:186:VAL:HG23	1.72	0.71
1:A:83:ILE:H	1:A:111:GLN:HE21	1.40	0.69
1:A:58:LEU:HB2	1:A:61:VAL:HG13	1.74	0.69
1:A:33:ARG:HA	1:A:33:ARG:HE	1.60	0.67
1:A:195:ASN:HD21	1:A:386:ARG:HH11	1.47	0.62
1:A:266:ARG:HH22	2:A:409:PLP:P	2.23	0.61
1:A:226:TYR:CZ	1:A:258:LYS:HD3	2.35	0.61
1:A:128:LYS:HG3	1:A:129:ASN:ND2	2.16	0.61
1:A:68:LEU:O	1:A:72:GLU:HB2	2.02	0.58
1:A:405:VAL:HA	1:A:408:LEU:HD22	1.87	0.56
1:A:161:TYR:O	1:A:169:LEU:HD12	2.04	0.56
1:A:64:ALA:O	1:A:67:TYR:HB3	2.08	0.53
1:A:133:LYS:HD3	1:A:134:ARG:HH21	1.74	0.53
1:A:312:ASN:HD22	1:A:315:LEU:H	1.55	0.52
1:A:260:PHE:HB3	1:A:262:LEU:HD12	1.92	0.52
1:A:340:THR:O	1:A:344:LYS:HB2	2.09	0.52
1:A:109:THR:HB	1:A:271:THR:HB	1.93	0.51
1:A:347:ASN:ND2	1:A:408:LEU:HG	2.27	0.50
1:A:397:MET:HE2	1:A:401:CYS:SG	2.52	0.49
1:A:128:LYS:NZ	1:A:286:GLN:HE21	2.11	0.48
1:A:171:PHE:O	1:A:175:ILE:HG12	2.13	0.48
1:A:130:THR:CG2	1:A:132:VAL:HG12	2.44	0.48
1:A:356:GLN:HE22	1:A:362:PHE:H	1.61	0.48
1:A:41:ILE:HG22	1:A:43:LEU:HD13	1.94	0.48
1:A:251:ILE:HD13	1:A:270:CYS:SG	2.54	0.47
1:A:292:ARG:HH11	1:A:296:SER:HB2	1.79	0.47
1:A:28:LEU:HA	1:A:31:LEU:HD12	1.95	0.47
1:A:348:ARG:HG2	1:A:349:ASP:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:O	1:A:128:LYS:HG2	2.14	0.47
1:A:213:SER:HA	1:A:218:TRP:CE3	2.50	0.47
1:A:128:LYS:NZ	1:A:129:ASN:HD21	2.13	0.47
1:A:393:THR:H	1:A:396:ASN:ND2	2.13	0.47
1:A:32:PHE:C	1:A:34:ALA:H	2.19	0.46
1:A:392:MET:HA	1:A:396:ASN:HD21	1.79	0.46
1:A:130:THR:HG22	1:A:132:VAL:HG12	1.98	0.46
1:A:224:PHE:HZ	1:A:237:ALA:HA	1.81	0.46
1:A:335:GLN:NE2	1:A:354:ILE:HD11	2.31	0.45
1:A:42:ASN:O	1:A:44:GLY:N	2.49	0.45
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.99	0.45
1:A:78:LEU:HD22	1:A:300:ALA:HB2	1.99	0.44
1:A:109:THR:CG2	1:A:271:THR:HB	2.49	0.43
1:A:140:PRO:O	1:A:194:HIS:HE1	2.01	0.43
1:A:27:GLY:O	1:A:30:ASP:HB2	2.19	0.42
1:A:396:ASN:HD22	1:A:396:ASN:C	2.24	0.41
1:A:82:GLY:HA3	1:A:111:GLN:NE2	2.35	0.41
1:A:191:GLY:HA3	1:A:224:PHE:CD2	2.56	0.41
1:A:25:ILE:HG22	1:A:45:ILE:HG13	2.02	0.41
1:A:25:ILE:CG2	1:A:45:ILE:HG13	2.51	0.41
1:A:396:ASN:HD22	1:A:397:MET:N	2.18	0.41
1:A:112:THR:HG21	1:A:118:ALA:HA	2.03	0.41
1:A:33:ARG:NE	1:A:33:ARG:HA	2.29	0.41
1:A:123:ALA:HB1	1:A:152:ALA:HB2	2.03	0.40
1:A:306:VAL:O	1:A:310:LEU:HB2	2.21	0.40
1:A:228:GLY:O	1:A:327:ARG:HD3	2.22	0.40
1:A:106:ARG:NH2	1:A:248:LYS:HA	2.36	0.40

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%)	374 (95%)	17 (4%)	3 (1%)	22	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	33	ARG
1	A	51	GLU

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%)	269 (84%)	51 (16%)	3	3

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	33	ARG
1	A	36	GLU
1	A	40	LYS
1	A	42	ASN
1	A	49	LYS
1	A	51	GLU
1	A	52	THR
1	A	56	PRO
1	A	57	VAL
1	A	61	VAL
1	A	66	GLN
1	A	67	TYR
1	A	68	LEU
1	A	70	GLU
1	A	109	THR
1	A	134	ARG
1	A	174	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	178	LEU
1	A	180	GLU
1	A	182	GLN
1	A	195	ASN
1	A	203	LEU
1	A	206	TRP
1	A	209	LEU
1	A	211	GLN
1	A	216	LYS
1	A	224	PHE
1	A	240	LEU
1	A	251	ILE
1	A	252	VAL
1	A	258	LYS
1	A	266	ARG
1	A	271	THR
1	A	296	SER
1	A	304	SER
1	A	310	LEU
1	A	316	ARG
1	A	335	GLN
1	A	336	LEU
1	A	342	GLN
1	A	348	ARG
1	A	354	ILE
1	A	365	LEU
1	A	367	LYS
1	A	372	ARG
1	A	374	ARG
1	A	379	VAL
1	A	395	ASP
1	A	396	ASN
1	A	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	111	GLN
1	A	129	ASN
1	A	166	ASN
1	A	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	211	GLN
1	A	286	GLN
1	A	312	ASN
1	A	335	GLN
1	A	356	GLN
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 carbohydrates 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	$\# Z > 2$
2	PLP	A	409	1	15,15,16	1.50	4 (26%)	20,22,23	1.92	4 (20%)
3	MAE	A	410	-	1,7,7	0.55	0	0,8,8	0.00	-

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	PLP	A	409	1	-	0/6/6/8	0/1/1/1
3	MAE	A	410	-	-	0/0/5/5	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	PLP	C3-C2	-2.65	1.38	1.40
2	A	409	PLP	P-O4P	-2.20	1.53	1.60
2	A	409	PLP	P-O3P	-2.09	1.46	1.54
2	A	409	PLP	C5-C4	2.30	1.43	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	PLP	O3P-P-O4P	-3.64	97.04	106.73
2	A	409	PLP	C6-C5-C4	2.30	120.10	118.18
2	A	409	PLP	C4A-C4-C5	2.71	123.59	120.86
2	A	409	PLP	O4P-C5A-C5	5.44	120.27	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	409	PLP	1	0

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.