



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:01 am GMT

PDB ID : 1ASB
Title : THE STRUCTURAL BASIS FOR THE REDUCED ACTIVITY OF THE
D223A(D222A) ACTIVE SITE MUTANT OF E. COLI ASPARTATE
AMINOTRANSFERASE
Authors : Schumacher, C.; Ringe, D.
Deposited on : 1993-08-27
Resolution : 2.60 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

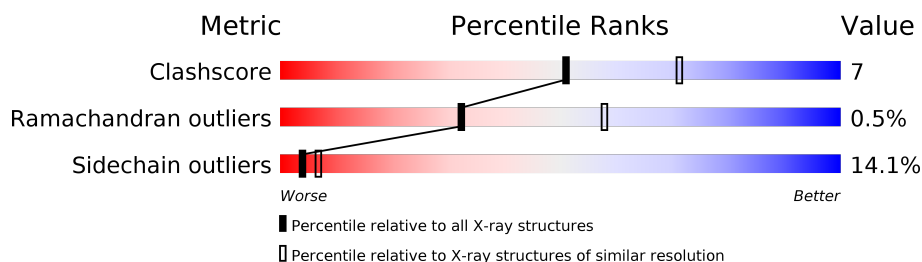
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3109 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.

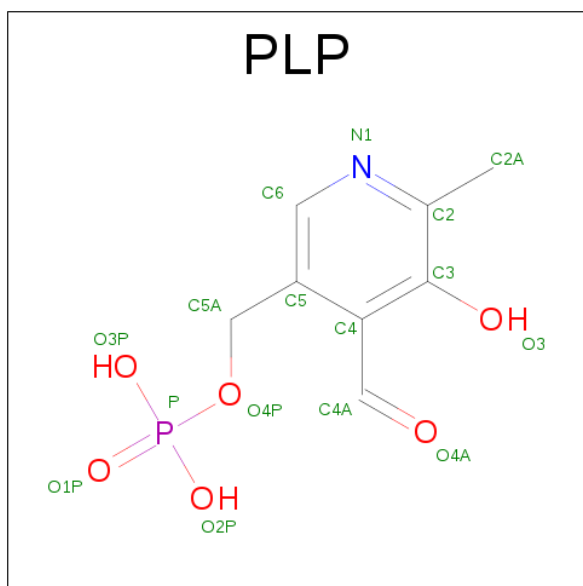
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3066	1935	536	582	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

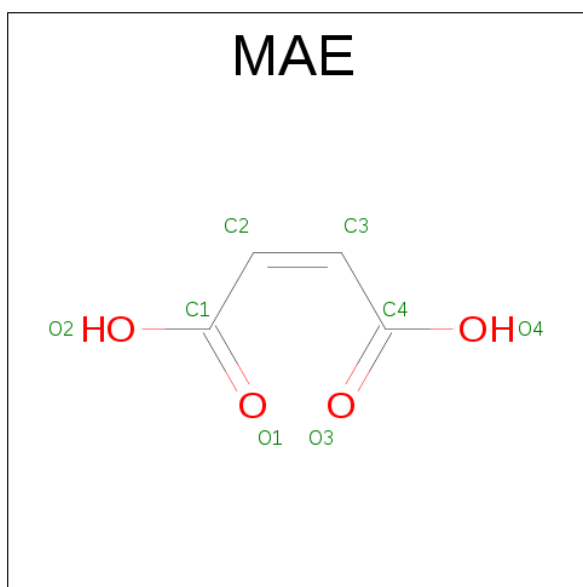
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	ASP	ENGINEERED MUTATION	UNP P00509

- 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.

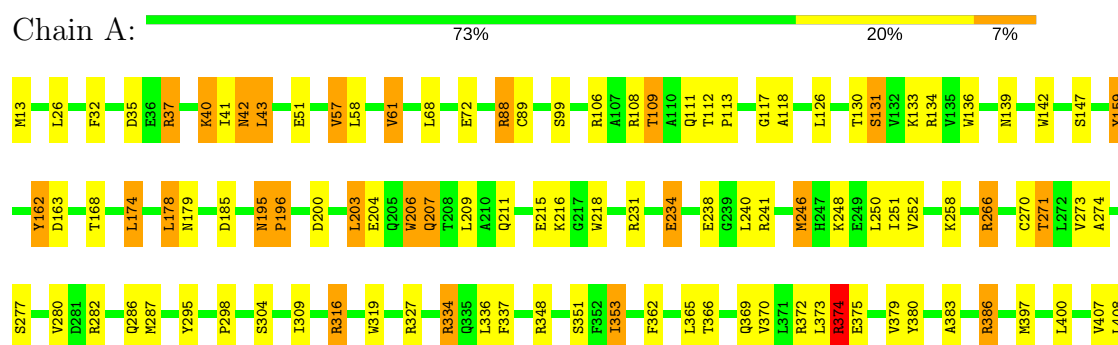
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		

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	159.12Å 86.15Å 79.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3109	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: 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	0.83	1/3127 (0.0%)	1.60	51/4236 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	VAL	CA-CB	5.08	1.65	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH1	13.47	127.04	120.30
1	A	374	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	A	108	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	266	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	316	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	147	SER	N-CA-CB	-8.37	97.95	110.50
1	A	250	LEU	CA-CB-CG	7.79	133.22	115.30
1	A	134	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	185	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	374	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	316	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	295	TYR	O-C-N	-7.37	110.91	122.70
1	A	218	TRP	CD1-CG-CD2	7.22	112.07	106.30
1	A	231	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	136	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	37	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	142	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	206	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	A	142	TRP	CD1-CG-CD2	6.72	111.67	106.30
1	A	380	TYR	CB-CG-CD2	-6.63	117.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	250	LEU	CB-CA-C	-6.61	97.65	110.20
1	A	282	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	295	TYR	CA-C-N	6.45	131.39	117.20
1	A	282	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	42	ASN	CA-C-N	6.36	131.18	117.20
1	A	319	TRP	CD1-CG-CD2	6.18	111.25	106.30
1	A	136	TRP	CD1-CG-CD2	6.13	111.20	106.30
1	A	334	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	287	MET	CG-SD-CE	-5.96	90.66	100.20
1	A	270	CYS	CA-CB-SG	-5.94	103.30	114.00
1	A	327	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	319	TRP	CE2-CD2-CG	-5.84	102.63	107.30
1	A	348	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	246	MET	CG-SD-CE	-5.78	90.94	100.20
1	A	211	GLN	CA-CB-CG	5.75	126.04	113.40
1	A	386	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	163	ASP	CA-C-N	-5.70	104.66	117.20
1	A	159	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	A	206	TRP	CE2-CD2-CG	-5.63	102.80	107.30
1	A	42	ASN	CA-C-O	-5.61	108.33	120.10
1	A	142	TRP	CG-CD2-CE3	5.58	138.93	133.90
1	A	142	TRP	CB-CG-CD1	-5.57	119.76	127.00
1	A	37	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	174	LEU	CA-CB-CG	5.38	127.66	115.30
1	A	147	SER	CB-CA-C	5.31	120.19	110.10
1	A	238	GLU	CA-CB-CG	5.29	125.04	113.40
1	A	334	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	407	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	A	131	SER	N-CA-CB	-5.10	102.86	110.50
1	A	42	ASN	CB-CG-ND2	5.08	128.90	116.70

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	3066	0	3017	39	0
2	A	15	0	6	3	0
3	A	8	0	2	1	0
4	A	20	0	0	0	0
All	All	3109	0	3025	40	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 7.

All (40) 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:58:LEU:HB2	1:A:61:VAL:HG13	1.78	0.65
1:A:159:TYR:HB3	1:A:178:LEU:HD13	1.83	0.61
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.67	0.60
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.67	0.59
1:A:266:ARG:HH22	2:A:409:PLP:P	2.26	0.58
1:A:35:ASP:OD1	1:A:37:ARG:HD3	2.05	0.57
1:A:106:ARG:O	1:A:280:VAL:HG11	2.09	0.53
1:A:126:LEU:O	1:A:130:THR:HB	2.09	0.53
1:A:334:ARG:HG3	1:A:353:ILE:HD12	1.91	0.52
1:A:336:LEU:HG	1:A:397:MET:HG2	1.92	0.52
1:A:41:ILE:HG22	1:A:43:LEU:HD13	1.94	0.50
1:A:111:GLN:OE1	1:A:298:PRO:HB2	2.12	0.49
1:A:195:ASN:HD21	1:A:386:ARG:HH11	1.61	0.49
1:A:162:TYR:HA	1:A:168:THR:O	2.13	0.48
1:A:113:PRO:HD2	1:A:117:GLY:HA3	1.96	0.47
1:A:277:SER:HA	1:A:280:VAL:HG22	1.97	0.47
3:A:410:MAE:C4	3:A:410:MAE:O1	2.62	0.46
1:A:37:ARG:O	1:A:40:LYS:HG3	2.16	0.46
1:A:274:ALA:HB3	1:A:280:VAL:HG12	1.97	0.45
1:A:366:THR:HG23	1:A:369:GLN:OE1	2.17	0.45
1:A:88:ARG:NH2	1:A:89:CYS:SG	2.89	0.45
1:A:112:THR:HG21	1:A:118:ALA:HA	1.99	0.44
1:A:334:ARG:HG3	1:A:353:ILE:CD1	2.48	0.44
1:A:258:LYS:NZ	2:A:409:PLP:O3	2.48	0.44
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.98	0.44
1:A:234:GLU:HG3	1:A:241:ARG:HH12	1.84	0.43
1:A:61:VAL:HA	1:A:309:ILE:HD11	2.00	0.43
1:A:130:THR:HG22	1:A:131:SER:N	2.34	0.42
1:A:109:THR:HG22	1:A:271:THR:HB	2.01	0.42
1:A:195:ASN:HA	1:A:196:PRO:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD22	1:A:379:VAL:HG22	2.01	0.42
1:A:178:LEU:HA	1:A:178:LEU:HD12	1.76	0.41
1:A:373:LEU:HD22	1:A:379:VAL:CG2	2.50	0.41
1:A:68:LEU:O	1:A:72:GLU:HG3	2.21	0.41
1:A:337:PHE:HD1	1:A:397:MET:HE2	1.86	0.41
1:A:266:ARG:NH2	2:A:409:PLP:O2P	2.47	0.41
1:A:207:GLN:HA	1:A:207:GLN:NE2	2.36	0.41
1:A:274:ALA:HB3	1:A:280:VAL:CG1	2.51	0.40
1:A:203:LEU:O	1:A:203:LEU:HD22	2.21	0.40
1:A:32:PHE:CZ	1:A:40:LYS:HD3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	377 (96%)	15 (4%)	2 (0%)	32 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	162	TYR

5.3.2 Protein sidechains ⓘ

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	319/319 (100%)	274 (86%)	45 (14%)	4 7

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	26	LEU
1	A	40	LYS
1	A	42	ASN
1	A	51	GLU
1	A	57	VAL
1	A	61	VAL
1	A	88	ARG
1	A	99	SER
1	A	109	THR
1	A	133	LYS
1	A	139	ASN
1	A	174	LEU
1	A	178	LEU
1	A	179	ASN
1	A	195	ASN
1	A	196	PRO
1	A	200	ASP
1	A	203	LEU
1	A	204	GLU
1	A	206	TRP
1	A	207	GLN
1	A	209	LEU
1	A	215	GLU
1	A	216	LYS
1	A	234	GLU
1	A	240	LEU
1	A	246	MET
1	A	248	LYS
1	A	251	ILE
1	A	252	VAL
1	A	271	THR
1	A	273	VAL
1	A	286	GLN
1	A	304	SER
1	A	316	ARG
1	A	351	SER
1	A	353	ILE

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Mol	Chain	Res	Type
1	A	362	PHE
1	A	365	LEU
1	A	372	ARG
1	A	374	ARG
1	A	375	GLU
1	A	400	LEU
1	A	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	176	ASN
1	A	195	ASN
1	A	207	GLN
1	A	247	HIS
1	A	297	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	$\# Z > 2$
2	PLP	A	409	1	15,15,16	1.52	4 (26%)	20,22,23	1.88	4 (20%)
3	MAE	A	410	-	1,7,7	0.43	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	-2.59	1.38	1.40
2	A	409	PLP	P-O4P	-2.22	1.53	1.60
2	A	409	PLP	P-O3P	-2.09	1.46	1.54
2	A	409	PLP	C5-C4	2.36	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	97.05	106.73
2	A	409	PLP	C6-C5-C4	2.33	120.12	118.18
2	A	409	PLP	C4A-C4-C5	2.69	123.57	120.86
2	A	409	PLP	O4P-C5A-C5	4.61	118.60	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	409	PLP	3	0
3	A	410	MAE	1	0

5.7 Other polymers

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

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.