



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:26 AM UTC

PDB ID : 1ASG / pdb_00001asg
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 : 2.80 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
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

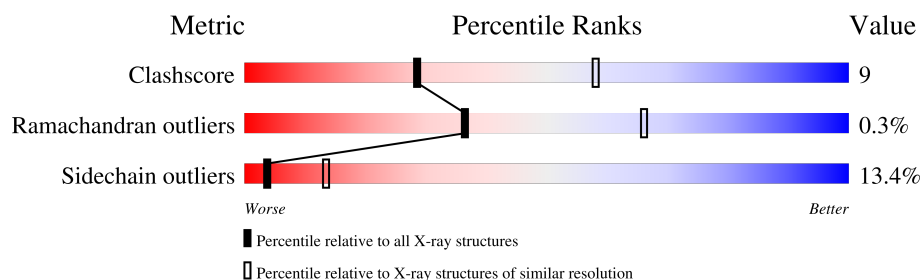
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 3226 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	3068	1936	536	583	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

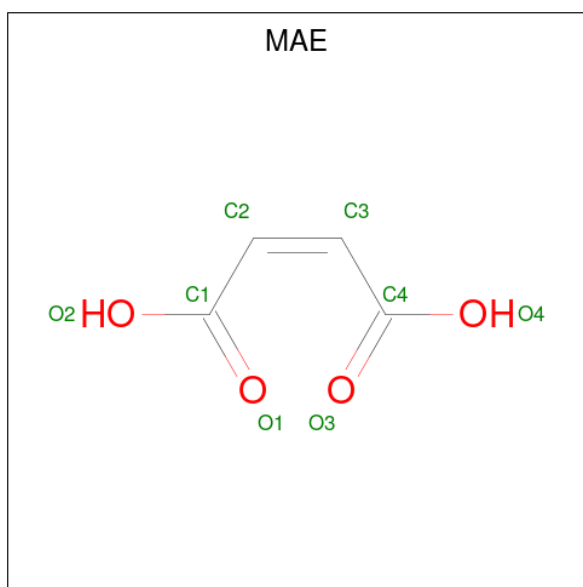
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	PHE	TYR	engineered mutation	UNP P00509

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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 (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.

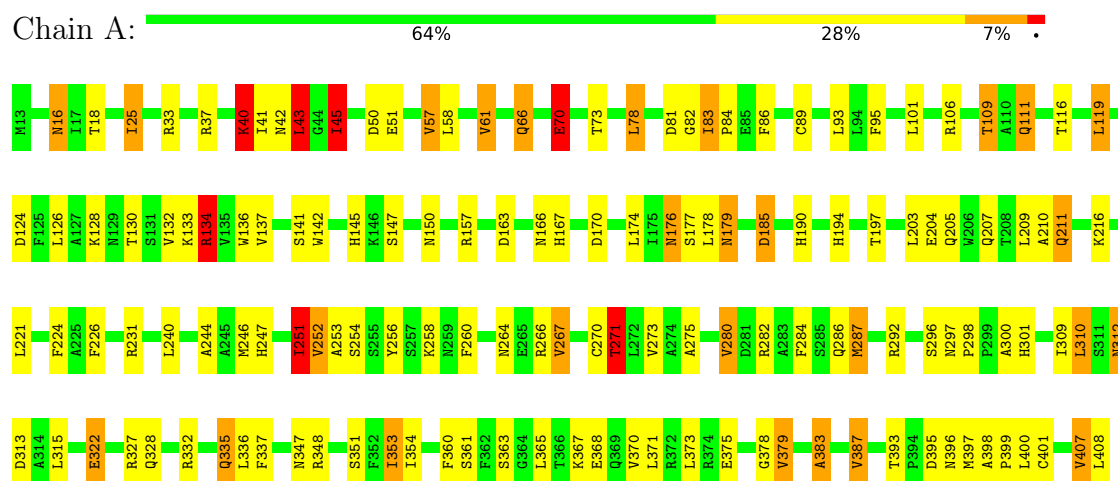
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		

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	157.80Å 85.50Å 78.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3226	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	1.13	16/3129 (0.5%)	1.90	74/4238 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	ILE	CA-CB	9.27	1.66	1.54
1	A	190	HIS	CD2-NE2	-7.93	1.29	1.37
1	A	194	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	247	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	353	ILE	CA-CB	6.83	1.62	1.54
1	A	167	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	271	THR	CA-CB	6.00	1.61	1.53
1	A	145	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	379	VAL	CA-CB	5.67	1.60	1.54
1	A	387	VAL	CA-CB	5.63	1.62	1.54
1	A	252	VAL	CA-CB	5.48	1.61	1.54
1	A	194	HIS	CG-ND1	-5.47	1.32	1.38
1	A	190	HIS	CG-ND1	-5.22	1.32	1.38
1	A	267	VAL	CA-CB	5.20	1.61	1.54
1	A	247	HIS	CG-ND1	-5.12	1.32	1.38
1	A	301	HIS	CD2-NE2	-5.04	1.32	1.37

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASN	CA-C-O	-11.70	108.52	120.80
1	A	42	ASN	OD1-CG-ND2	-10.07	112.53	122.60
1	A	42	ASN	CB-CG-ND2	9.64	130.86	116.40
1	A	81	ASP	CA-CB-CG	7.84	120.44	112.60
1	A	312	ASN	OD1-CG-ND2	-7.73	114.87	122.60
1	A	337	PHE	CA-CB-CG	7.68	121.48	113.80
1	A	150	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	A	266	ARG	NE-CZ-NH2	-7.37	112.57	119.20
1	A	282	ARG	CB-CG-CD	-7.05	95.08	111.30
1	A	50	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	286	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	A	43	LEU	N-CA-C	6.84	125.38	110.80
1	A	298	PRO	N-CA-C	6.83	119.03	110.70
1	A	16	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	207	GLN	CA-CB-CG	6.71	127.52	114.10
1	A	322	GLU	CA-CB-CG	-6.69	100.72	114.10
1	A	163	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	45	ILE	CB-CA-C	-6.62	100.44	111.29
1	A	407	VAL	CG1-CB-CG2	-6.60	96.28	110.80
1	A	176	ASN	CA-CB-CG	6.53	119.13	112.60
1	A	197	THR	N-CA-C	6.42	119.26	111.82
1	A	147	SER	N-CA-CB	-6.37	100.73	110.16
1	A	170	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	312	ASN	CB-CG-ND2	6.23	125.75	116.40
1	A	351	SER	N-CA-C	6.21	120.47	113.01
1	A	396	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	300	ALA	N-CA-C	6.11	117.74	111.14
1	A	73	THR	CA-CB-OG1	-6.08	100.47	109.60
1	A	363	SER	N-CA-C	5.99	119.85	112.54
1	A	360	PHE	N-CA-C	5.98	119.31	110.46
1	A	124	ASP	O-C-N	5.95	128.19	122.07
1	A	25	ILE	N-CA-C	-5.93	107.14	112.12
1	A	264	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	83	ILE	CA-C-N	5.90	125.60	119.05
1	A	83	ILE	C-N-CA	5.90	125.60	119.05
1	A	179	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	216	LYS	CG-CD-CE	-5.83	97.90	111.30
1	A	275	ALA	N-CA-C	5.76	118.34	111.71
1	A	18	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	332	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	A	332	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	A	134	ARG	N-CA-C	5.54	118.13	108.76
1	A	141	SER	CA-C-N	5.53	128.17	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	SER	C-N-CA	5.53	128.17	120.65
1	A	328	GLN	CG-CD-NE2	5.52	124.68	116.40
1	A	194	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	A	282	ARG	N-CA-CB	-5.49	102.02	110.20
1	A	396	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	134	ARG	CB-CG-CD	-5.47	98.73	111.30
1	A	286	GLN	CG-CD-NE2	5.41	124.52	116.40
1	A	301	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	42	ASN	N-CA-C	5.34	118.13	111.24
1	A	353	ILE	N-CA-C	-5.33	105.09	112.50
1	A	111	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	A	185	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	297	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	A	297	ASN	O-C-N	-5.22	116.96	121.71
1	A	383	ALA	N-CA-C	5.19	119.24	113.01
1	A	57	VAL	CB-CA-C	5.19	117.15	111.08
1	A	142	TRP	CA-C-N	5.18	124.80	119.05
1	A	142	TRP	C-N-CA	5.18	124.80	119.05
1	A	70	GLU	CA-CB-CG	5.17	124.45	114.10
1	A	116	THR	N-CA-C	-5.16	105.74	111.36
1	A	95	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	142	TRP	CG-CD2-CE3	5.14	139.04	133.90
1	A	224	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	150	ASN	CB-CG-ND2	5.12	124.08	116.40
1	A	73	THR	CA-CB-CG2	5.11	119.19	110.50
1	A	393	THR	CA-C-N	5.10	124.89	119.28
1	A	393	THR	C-N-CA	5.10	124.89	119.28
1	A	348	ARG	CA-CB-CG	5.06	124.23	114.10
1	A	16	ASN	CB-CA-C	-5.02	105.05	111.22
1	A	335	GLN	CG-CD-NE2	5.00	123.91	116.40
1	A	40	LYS	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	327	ARG	Sidechain

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	3068	0	3016	54	0
2	A	15	0	6	0	0
3	A	8	0	2	0	0
4	A	135	0	0	3	0
All	All	3226	0	3024	54	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 (54) 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:397:MET:HE2	1:A:401:CYS:SG	2.34	0.68
1:A:109:THR:HB	1:A:271:THR:HG22	1.82	0.62
1:A:271:THR:HG23	4:A:592:HOH:O	1.99	0.60
1:A:78:LEU:HB2	4:A:631:HOH:O	2.01	0.60
1:A:109:THR:HG22	1:A:271:THR:HB	1.83	0.60
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.84	0.60
1:A:226:PHE:CE1	1:A:258:LYS:HD3	2.39	0.56
1:A:292:ARG:HA	1:A:296:SER:HA	1.88	0.56
1:A:83:ILE:H	1:A:111:GLN:NE2	2.04	0.55
1:A:133:LYS:CE	1:A:134:ARG:HH12	2.20	0.54
1:A:133:LYS:HD3	1:A:134:ARG:HH12	1.73	0.54
1:A:205:GLN:O	1:A:209:LEU:HB2	2.09	0.53
1:A:361:SER:HB3	1:A:387:VAL:HG23	1.91	0.52
1:A:58:LEU:HD22	1:A:322:GLU:HB3	1.90	0.52
1:A:210:ALA:HB1	1:A:246:MET:HG3	1.92	0.51
1:A:58:LEU:HB2	1:A:61:VAL:HG13	1.93	0.51
1:A:37:ARG:HH21	1:A:378:GLY:CA	2.24	0.51
1:A:361:SER:HB3	1:A:387:VAL:CG2	2.40	0.51
1:A:89:CYS:HB3	1:A:310:LEU:HD23	1.94	0.50
1:A:398:ALA:HB3	1:A:399:PRO:HD3	1.94	0.49
1:A:37:ARG:O	1:A:40:LYS:HG3	2.12	0.49
1:A:130:THR:HG22	1:A:132:VAL:H	1.77	0.49
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:CG2	1:A:132:VAL:HG23	2.44	0.47
1:A:397:MET:HE3	1:A:397:MET:HA	1.96	0.47
1:A:136:TRP:CZ2	1:A:157:ARG:HD3	2.49	0.47
1:A:25:ILE:HG22	1:A:45:ILE:HG23	1.95	0.47
1:A:126:LEU:O	1:A:130:THR:HB	2.14	0.47
1:A:367:LYS:HE3	1:A:368:GLU:OE2	2.16	0.46
1:A:66:GLN:O	1:A:70:GLU:HG2	2.15	0.46
1:A:41:ILE:HG22	1:A:43:LEU:HD13	1.97	0.45
1:A:106:ARG:O	1:A:280:VAL:HG21	2.16	0.45
1:A:347:ASN:HD21	1:A:408:LEU:HB3	1.82	0.45
1:A:61:VAL:HA	1:A:309:ILE:HD11	1.98	0.45
1:A:251:ILE:CD1	1:A:270:CYS:SG	3.05	0.45
1:A:256:TYR:O	1:A:260:PHE:HB2	2.16	0.44
1:A:82:GLY:HA3	1:A:111:GLN:HB3	2.00	0.43
1:A:83:ILE:H	1:A:111:GLN:HE21	1.64	0.43
1:A:373:LEU:HG	1:A:407:VAL:HG21	2.01	0.43
1:A:83:ILE:HG13	1:A:111:GLN:HE22	1.84	0.43
1:A:119:LEU:HD13	1:A:253:ALA:CB	2.49	0.43
1:A:83:ILE:HA	1:A:84:PRO:HD3	1.92	0.42
1:A:284:PHE:CE1	1:A:287:MET:HE2	2.54	0.42
1:A:37:ARG:HH21	1:A:378:GLY:HA2	1.84	0.42
1:A:83:ILE:O	1:A:86:PHE:HB3	2.19	0.42
1:A:246:MET:HE3	1:A:246:MET:HB3	1.81	0.42
1:A:101:LEU:HD11	1:A:244:ALA:HB1	2.02	0.41
1:A:133:LYS:CE	1:A:134:ARG:NH1	2.83	0.41
1:A:134:ARG:NH2	1:A:185:ASP:OD1	2.53	0.41
1:A:231:ARG:HD3	4:A:619:HOH:O	2.21	0.41
1:A:176:ASN:O	1:A:179:ASN:HB2	2.21	0.40
1:A:130:THR:HG22	1:A:132:VAL:HG23	2.02	0.40
1:A:211:GLN:HA	1:A:246:MET:HE2	2.03	0.40
1:A:312:ASN:HD22	1:A:313:ASP:N	2.19	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%)	378 (96%)	15 (4%)	1 (0%)	36 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU

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	320/320 (100%)	277 (87%)	43 (13%)	4 13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	33	ARG
1	A	40	LYS
1	A	45	ILE
1	A	51	GLU
1	A	57	VAL
1	A	61	VAL
1	A	66	GLN
1	A	70	GLU
1	A	78	LEU
1	A	93	LEU
1	A	109	THR
1	A	119	LEU
1	A	128	LYS
1	A	134	ARG
1	A	137	VAL
1	A	166	ASN
1	A	174	LEU

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Mol	Chain	Res	Type
1	A	177	SER
1	A	178	LEU
1	A	203	LEU
1	A	204	GLU
1	A	211	GLN
1	A	221	LEU
1	A	240	LEU
1	A	251	ILE
1	A	252	VAL
1	A	254	SER
1	A	267	VAL
1	A	271	THR
1	A	273	VAL
1	A	280	VAL
1	A	287	MET
1	A	310	LEU
1	A	315	LEU
1	A	336	LEU
1	A	353	ILE
1	A	365	LEU
1	A	371	LEU
1	A	375	GLU
1	A	379	VAL
1	A	395	ASP
1	A	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	71	ASN
1	A	76	ASN
1	A	111	GLN
1	A	129	ASN
1	A	176	ASN
1	A	179	ASN
1	A	211	GLN
1	A	227	GLN
1	A	286	GLN
1	A	297	ASN
1	A	312	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
2	PLP	A	409	1	15,15,16	2.21	5 (33%)	21,22,23	1.88	5 (23%)
3	MAE	A	410	-	7,7,7	1.88	2 (28%)	8,8,8	2.15	2 (25%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	PLP	C3-C2	-4.74	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	PLP	O4P-C5A	-3.84	1.30	1.44
2	A	409	PLP	C2A-C2	-3.60	1.44	1.50
3	A	410	MAE	O4-C4	-3.58	1.21	1.30
3	A	410	MAE	O2-C1	-3.00	1.22	1.30
2	A	409	PLP	O3-C3	-2.22	1.31	1.36
2	A	409	PLP	P-O2P	-2.01	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	MAE	O2-C1-O1	-5.03	112.45	122.70
2	A	409	PLP	C5-C6-N1	-3.96	117.38	123.83
2	A	409	PLP	O4P-C5A-C5	3.48	115.88	109.36
2	A	409	PLP	C6-C5-C4	3.42	120.90	118.10
2	A	409	PLP	C6-N1-C2	2.93	124.52	119.20
3	A	410	MAE	O4-C4-O3	-2.24	118.14	122.70
2	A	409	PLP	O4P-P-O1P	-2.19	100.51	106.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	409	PLP	C4-C5-C5A-O4P
2	A	409	PLP	C6-C5-C5A-O4P
2	A	409	PLP	C5A-O4P-P-O2P
2	A	409	PLP	C5A-O4P-P-O3P
3	A	410	MAE	C2-C3-C4-O3
3	A	410	MAE	C2-C3-C4-O4
3	A	410	MAE	O2-C1-C2-C3
3	A	410	MAE	O1-C1-C2-C3
2	A	409	PLP	C5A-O4P-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

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.