



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 1ASA / pdb_00001asa
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

<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

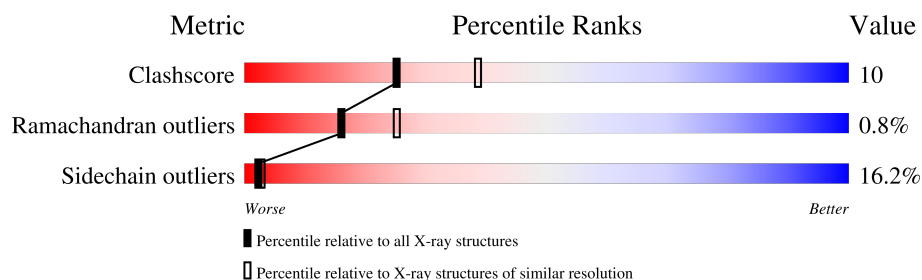
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	

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.

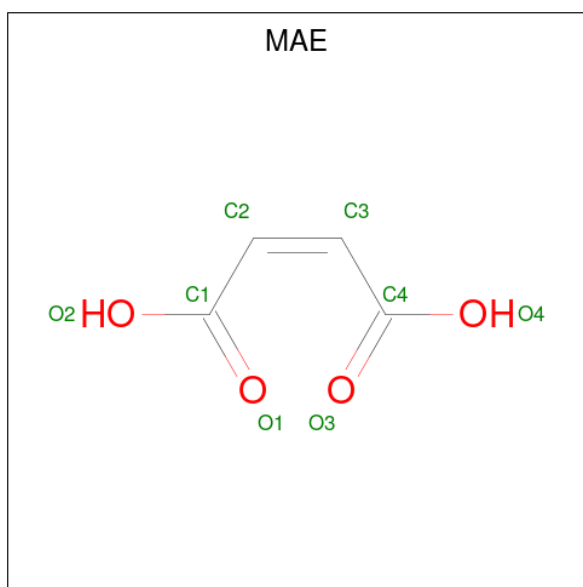
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3069	1936	536	584	13	0	0	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (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.

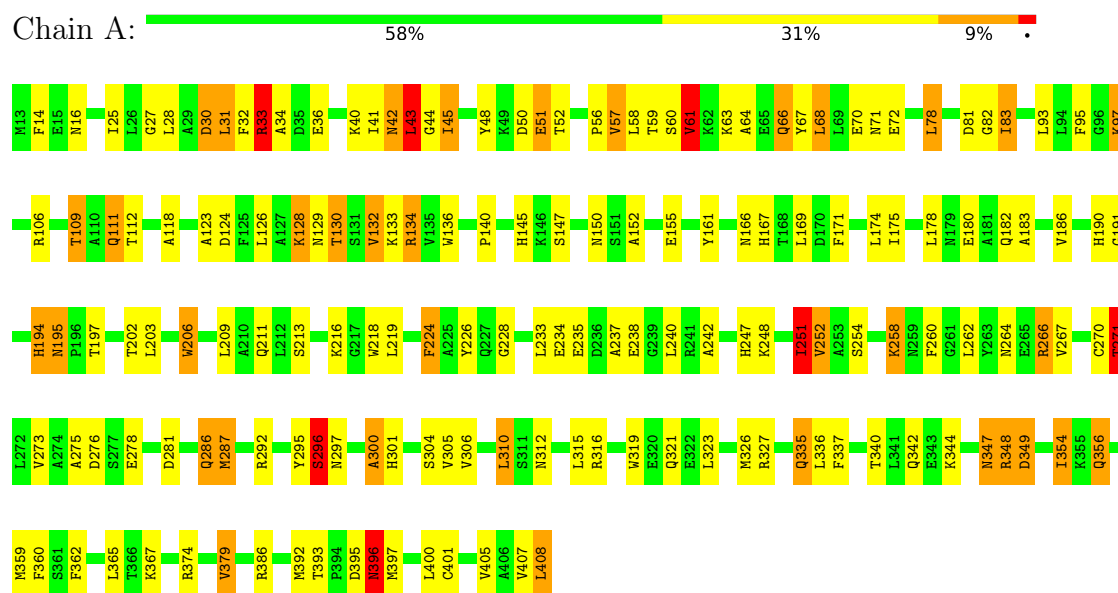
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		

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	157.50Å 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, 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	1.11	15/3130 (0.5%)	1.91	84/4240 (2.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	190	HIS	CD2-NE2	-7.99	1.29	1.37
1	A	145	HIS	CD2-NE2	-7.81	1.29	1.37
1	A	251	ILE	CA-CB	7.05	1.64	1.54
1	A	379	VAL	CA-CB	6.99	1.62	1.54
1	A	61	VAL	CA-CB	6.52	1.63	1.54
1	A	167	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	190	HIS	CG-ND1	-5.90	1.31	1.38
1	A	194	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	305	VAL	CA-CB	5.72	1.61	1.54
1	A	247	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	252	VAL	CA-CB	5.55	1.61	1.54
1	A	271	THR	CA-CB	5.19	1.60	1.53
1	A	247	HIS	CG-ND1	-5.11	1.32	1.38
1	A	167	HIS	CG-ND1	-5.01	1.32	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASN	CA-C-O	-11.88	107.84	120.55
1	A	295	TYR	O-C-N	-9.91	110.67	123.16
1	A	197	THR	N-CA-C	9.12	122.19	111.71
1	A	42	ASN	OD1-CG-ND2	-8.94	113.66	122.60
1	A	111	GLN	OE1-CD-NE2	-8.84	113.76	122.60
1	A	42	ASN	CB-CG-ND2	8.75	129.52	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	HIS	CA-CB-CG	-8.63	105.17	113.80
1	A	30	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	271	THR	CA-C-O	7.66	128.74	120.32
1	A	296	SER	CA-CB-OG	7.52	126.15	111.10
1	A	81	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	347	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	155	GLU	CB-CG-CD	7.03	124.55	112.60
1	A	183	ALA	N-CA-C	-6.93	98.74	109.76
1	A	360	PHE	N-CA-C	6.88	120.72	109.24
1	A	43	LEU	N-CA-C	6.87	125.44	110.80
1	A	347	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	A	396	ASN	CB-CG-ND2	6.84	126.67	116.40
1	A	281	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	266	ARG	NE-CZ-NH2	-6.78	113.10	119.20
1	A	396	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	A	235	GLU	CB-CG-CD	6.59	123.81	112.60
1	A	95	PHE	N-CA-C	6.50	121.38	113.38
1	A	145	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	A	50	ASP	CA-CB-CG	6.41	119.00	112.60
1	A	396	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	264	ASN	CA-CB-CG	6.24	118.84	112.60
1	A	194	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	295	TYR	CA-C-O	-6.15	114.21	121.16
1	A	57	VAL	N-CA-C	-6.00	99.93	108.58
1	A	206	TRP	CE2-CD2-CE3	5.98	124.78	118.80
1	A	147	SER	N-CA-CB	-5.92	101.41	110.16
1	A	295	TYR	N-CA-C	-5.91	100.55	109.95
1	A	150	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	219	LEU	CA-C-N	5.88	125.64	119.76
1	A	219	LEU	C-N-CA	5.88	125.64	119.76
1	A	407	VAL	CG1-CB-CG2	-5.83	97.98	110.80
1	A	321	GLN	N-CA-C	-5.78	104.35	111.40
1	A	301	HIS	N-CA-C	5.73	117.99	111.11
1	A	233	LEU	N-CA-C	5.73	120.83	111.37
1	A	287	MET	CG-SD-CE	-5.72	88.32	100.90
1	A	150	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	128	LYS	CB-CG-CD	5.69	124.39	111.30
1	A	83	ILE	CA-C-N	5.60	125.12	119.19
1	A	83	ILE	C-N-CA	5.60	125.12	119.19
1	A	134	ARG	CA-CB-CG	5.59	125.28	114.10
1	A	130	THR	N-CA-CB	-5.58	101.84	111.55
1	A	166	ASN	OD1-CG-ND2	-5.57	117.03	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ALA	N-CA-C	-5.56	104.85	111.69
1	A	195	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	349	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	136	TRP	CG-CD2-CE3	5.53	139.43	133.90
1	A	337	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	276	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	238	GLU	N-CA-C	5.44	117.21	111.28
1	A	71	ASN	N-CA-C	5.38	119.37	112.26
1	A	97	LYS	N-CA-C	-5.38	98.53	107.99
1	A	132	VAL	O-C-N	5.32	128.41	122.61
1	A	45	ILE	CA-CB-CG1	-5.32	101.36	110.40
1	A	202	THR	N-CA-C	-5.28	103.05	110.50
1	A	275	ALA	N-CA-C	5.27	117.78	111.71
1	A	195	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	195	ASN	CB-CA-C	5.26	116.00	110.17
1	A	305	VAL	N-CA-C	-5.23	105.28	110.62
1	A	97	LYS	CB-CG-CD	5.22	123.31	111.30
1	A	300	ALA	N-CA-C	5.20	118.09	111.69
1	A	111	GLN	CG-CD-NE2	5.20	124.19	116.40
1	A	234	GLU	CA-C-N	5.19	127.23	120.28
1	A	234	GLU	C-N-CA	5.19	127.23	120.28
1	A	14	PHE	N-CA-C	5.18	119.24	113.02
1	A	60	SER	N-CA-C	-5.18	105.81	111.82
1	A	16	ASN	CA-CB-CG	5.17	117.78	112.60
1	A	78	LEU	O-C-N	-5.14	116.99	122.85
1	A	286	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	305	VAL	O-C-N	-5.12	116.90	121.87
1	A	319	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	254	SER	CA-CB-OG	5.11	121.31	111.10
1	A	356	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	254	SER	O-C-N	-5.09	117.24	123.10
1	A	301	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	57	VAL	CB-CA-C	5.04	117.17	110.91
1	A	66	GLN	O-C-N	5.03	127.25	122.07
1	A	33	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A	297	ASN	O-C-N	-5.01	118.00	121.65

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	59	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	59	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 10.

All (59) 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:397:MET:HE2	1:A:401:CYS:SG	2.28	0.74
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:32:PHE:C	1:A:34:ALA:H	2.19	0.51
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:128:LYS:NZ	1:A:286:GLN:HE21	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ILE:HG22	1:A:43:LEU:HD13	1.94	0.48
1:A:356:GLN:HE22	1:A:362:PHE:H	1.61	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
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:397:MET:HE3	1:A:397:MET:HA	1.96	0.47
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:396:ASN:HD22	1:A:396:ASN:C	2.24	0.46
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.98	0.46
1:A:224:PHE:HZ	1:A:237:ALA:HA	1.81	0.46
1:A:42:ASN:O	1:A:44:GLY:N	2.49	0.45
1:A:335:GLN:NE2	1:A:354:ILE:HD11	2.31	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:48:TYR:HB2	1:A:359:MET:HE2	2.03	0.41
1:A:25:ILE:HG22	1:A:45:ILE:HG13	2.02	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:CG2	1:A:45:ILE:HG13	2.51	0.41
1:A:33:ARG:HA	1:A:33:ARG:NE	2.29	0.41
1:A:112:THR:HG21	1:A:118:ALA:HA	2.03	0.41
1:A:396:ASN:HD22	1:A:397:MET:N	2.18	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:106:ARG:NH2	1:A:248:LYS:HA	2.36	0.40
1:A:228:GLY:O	1:A:327:ARG:HD3	2.22	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%)	16 25

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%)	268 (84%)	52 (16%)	2 3

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	36	GLU
1	A	40	LYS
1	A	51	GLU
1	A	52	THR
1	A	56	PRO
1	A	57	VAL
1	A	59	THR

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Mol	Chain	Res	Type
1	A	61	VAL
1	A	63	LYS
1	A	66	GLN
1	A	68	LEU
1	A	70	GLU
1	A	93	LEU
1	A	97	LYS
1	A	109	THR
1	A	174	LEU
1	A	178	LEU
1	A	180	GLU
1	A	182	GLN
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	267	VAL
1	A	271	THR
1	A	273	VAL
1	A	278	GLU
1	A	287	MET
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	374	ARG
1	A	379	VAL
1	A	395	ASP
1	A	396	ASN

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Mol	Chain	Res	Type
1	A	400	LEU
1	A	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	111	GLN
1	A	129	ASN
1	A	195	ASN
1	A	205	GLN
1	A	211	GLN
1	A	227	GLN
1	A	286	GLN
1	A	297	ASN
1	A	312	ASN
1	A	335	GLN
1	A	356	GLN
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 oligosaccharides 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	-	7,7,7	1.64	2 (28%)	8,8,8	1.00	1 (12%)
2	PLP	A	409	1	15,15,16	1.52	4 (26%)	21,22,23	1.95	4 (19%)

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	-	-	2/5/5/5	-
2	PLP	A	409	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	MAE	O4-C4	-3.22	1.22	1.30
3	A	410	MAE	O2-C1	-2.76	1.23	1.30
2	A	409	PLP	C5-C4	2.36	1.43	1.40
2	A	409	PLP	P-O3P	-2.31	1.46	1.54
2	A	409	PLP	P-O4P	-2.28	1.53	1.60
2	A	409	PLP	P-O2P	-2.00	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	PLP	O4P-C5A-C5	5.82	120.27	109.36
2	A	409	PLP	O3P-P-O4P	-3.69	97.04	106.67
2	A	409	PLP	C4A-C4-C5	2.57	123.59	120.94
2	A	409	PLP	C6-C5-C4	2.44	120.10	118.10
3	A	410	MAE	O2-C1-O1	-2.32	117.98	122.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	MAE	C2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	410	MAE	C2-C3-C4-O4

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.