



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:59 am GMT

PDB ID : 1AAW  
Title : THE STRUCTURAL BASIS FOR THE ALTERED SUBSTRATE SPECIFICITY OF THE R292D ACTIVE SITE MUTANT OF ASPARTATE AMINOTRANSFERASE FROM E. COLI  
Authors : Almo, S.C.; Smith, D.L.; Danishefsky, A.T.; Ringe, D.  
Deposited on : 1993-07-13  
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](mailto: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.

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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

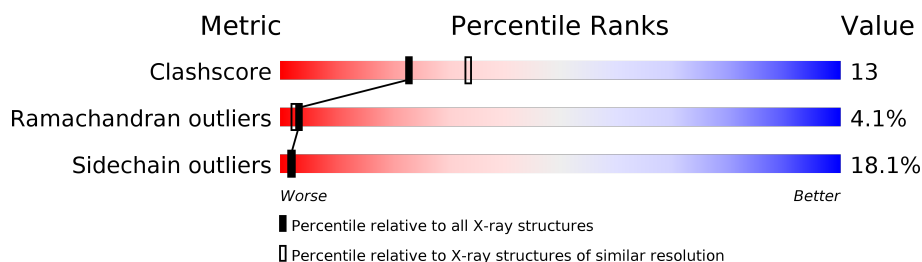
# 1 Overall quality at a glance

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  $\geq 3$ , 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 3 unique types of molecules in this entry. The entry contains 3087 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
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 3 is water.

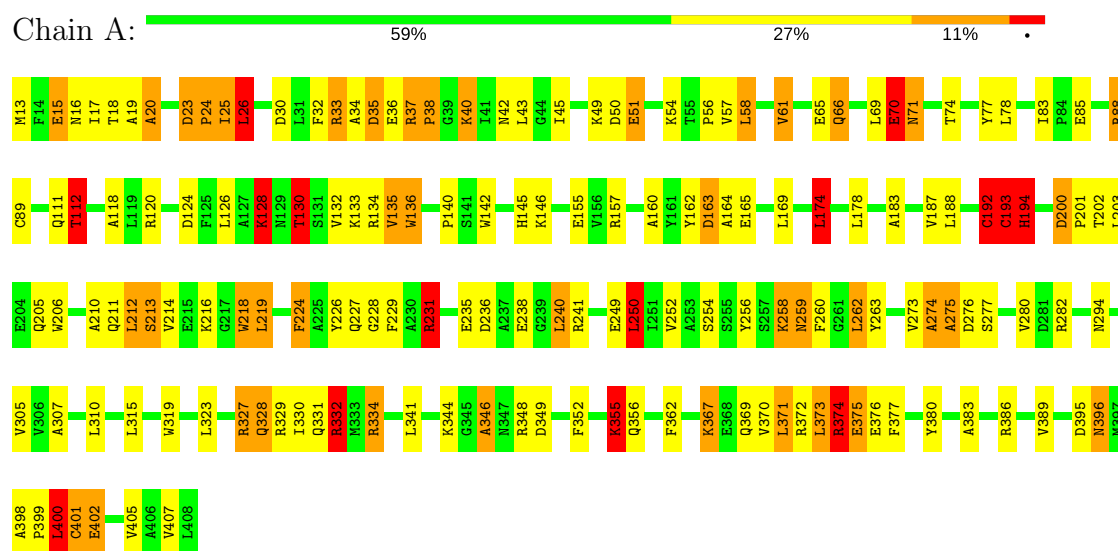
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		

### 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, $\alpha$ , $\beta$ , $\gamma$	156.80Å 86.90Å 80.00Å 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	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: 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	0.89	2/3130 (0.1%)	1.85	87/4240 (2.1%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	TRP	CD1-NE1	-5.86	1.27	1.38
1	A	135	VAL	CA-CB	5.22	1.65	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ARG	NE-CZ-NH1	19.41	130.01	120.30
1	A	334	ARG	NE-CZ-NH2	-15.56	112.52	120.30
1	A	231	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	A	334	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	A	37	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	A	13	MET	CA-CB-CG	-10.59	95.30	113.30
1	A	193	CYS	CA-C-N	-10.33	94.47	117.20
1	A	319	TRP	CD1-CG-CD2	10.03	114.33	106.30
1	A	327	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	A	142	TRP	CD1-CG-CD2	9.50	113.90	106.30
1	A	372	ARG	NE-CZ-NH1	9.33	124.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	372	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	218	TRP	CD1-CG-CD2	8.47	113.07	106.30
1	A	319	TRP	CE2-CD2-CG	-8.36	100.61	107.30
1	A	206	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	A	319	TRP	CG-CD1-NE1	-7.96	102.14	110.10
1	A	355	LYS	CA-C-N	-7.87	99.89	117.20
1	A	142	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	319	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	A	33	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	374	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	346	ALA	CA-C-N	-7.72	100.21	117.20
1	A	371	LEU	CA-CB-CG	7.55	132.67	115.30
1	A	275	ALA	N-CA-CB	7.55	120.67	110.10
1	A	380	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	A	120	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	356	GLN	N-CA-C	-7.32	91.24	111.00
1	A	386	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	400	LEU	CA-CB-CG	7.15	131.75	115.30
1	A	203	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	183	ALA	O-C-N	-7.06	111.20	123.20
1	A	218	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	206	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	A	274	ALA	N-CA-C	6.85	129.49	111.00
1	A	112	THR	N-CA-CB	-6.79	97.40	110.30
1	A	43	LEU	CA-C-N	6.75	129.70	116.20
1	A	15	GLU	CA-C-N	-6.75	102.36	117.20
1	A	241	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	327	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	70	GLU	CA-CB-CG	6.59	127.90	113.40
1	A	332	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	35	ASP	N-CA-C	6.49	128.53	111.00
1	A	136	TRP	CE2-CD2-CG	-6.44	102.15	107.30
1	A	43	LEU	O-C-N	-6.39	112.34	123.20
1	A	282	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	136	TRP	CD1-CG-CD2	6.28	111.32	106.30
1	A	206	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	A	174	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	18	THR	N-CA-C	-6.05	94.65	111.00
1	A	142	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	15	GLU	O-C-N	6.04	132.37	122.70
1	A	275	ALA	CB-CA-C	-6.02	101.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	A	373	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	319	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	A	218	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	A	88	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	319	TRP	CD1-NE1-CE2	5.79	114.21	109.00
1	A	401	CYS	CA-CB-SG	-5.72	103.70	114.00
1	A	250	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	33	ARG	CA-C-N	-5.62	104.85	117.20
1	A	183	ALA	CA-C-N	5.59	127.39	116.20
1	A	130	THR	N-CA-CB	-5.35	100.14	110.30
1	A	142	TRP	CB-CG-CD1	-5.35	120.05	127.00
1	A	219	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	162	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	50	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	163	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	213	SER	N-CA-CB	-5.23	102.65	110.50
1	A	128	LYS	CA-CB-CG	5.21	124.85	113.40
1	A	375	GLU	CA-CB-CG	5.20	124.84	113.40
1	A	15	GLU	CA-CB-CG	5.19	124.81	113.40
1	A	26	LEU	N-CA-C	5.16	124.92	111.00
1	A	183	ALA	N-CA-C	5.12	124.83	111.00
1	A	240	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	332	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	194	HIS	N-CA-C	5.06	124.66	111.00
1	A	120	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	396	ASN	CA-CB-CG	5.05	124.50	113.40
1	A	33	ARG	O-C-N	5.04	130.77	122.70
1	A	407	VAL	C-N-CA	5.04	134.30	121.70
1	A	346	ALA	CA-C-O	5.04	130.67	120.10
1	A	74	THR	OG1-CB-CG2	-5.03	98.42	110.00
1	A	33	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	192	CYS	N-CA-C	-5.01	97.47	111.00
1	A	252	VAL	CA-C-N	-5.01	106.19	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	CYS	Mainchain
1	A	20	ALA	Peptide
1	A	200	ASP	Peptide



## 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	79	1
2	A	15	0	6	0	1
3	A	3	0	0	0	0
All	All	3087	0	3022	79	1

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 13.

All (79) 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:HD3	1.92	1.05
1:A:45:ILE:HD13	1:A:49:LYS:HE2	1.58	0.85
1:A:134:ARG:HH12	1:A:155:GLU:HB3	1.48	0.78
1:A:367:LYS:HE3	1:A:367:LYS:H	1.48	0.77
1:A:229:PHE:HZ	1:A:258:LYS:O	1.68	0.77
1:A:202:THR:H	1:A:205:GLN:HE21	1.34	0.75
1:A:229:PHE:CZ	1:A:258:LYS:O	2.41	0.73
1:A:130:THR:HG22	1:A:132:VAL:H	1.52	0.72
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.72	0.70
1:A:37:ARG:HH22	1:A:376:GLU:HA	1.57	0.69
1:A:193:CYS:SG	1:A:200:ASP:HA	2.33	0.69
1:A:35:ASP:HB2	1:A:40:LYS:HD3	1.76	0.68
1:A:23:ASP:HB3	1:A:26:LEU:HB2	1.73	0.68
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.60	0.67
1:A:134:ARG:NH1	1:A:155:GLU:HB3	2.09	0.67
1:A:371:LEU:HD12	1:A:374:ARG:HH21	1.60	0.65
1:A:259:ASN:HD22	1:A:260:PHE:N	1.98	0.62
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.80	0.62
1:A:328:GLN:HE22	1:A:332:ARG:HG3	1.66	0.60
1:A:348:ARG:NH1	1:A:352:PHE:HE1	1.99	0.60
1:A:212:LEU:HD22	1:A:216:LYS:HD2	1.85	0.59
1:A:160:ALA:O	1:A:174:LEU:HB2	2.03	0.58
1:A:202:THR:H	1:A:205:GLN:NE2	2.01	0.57
1:A:400:LEU:HD23	1:A:401:CYS:SG	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:NZ	1:A:398:ALA:HB1	2.21	0.56
1:A:85:GLU:HG2	1:A:307:ALA:HB1	1.89	0.55
1:A:259:ASN:HD22	1:A:260:PHE:H	1.52	0.55
1:A:61:VAL:HB	1:A:305:VAL:HG11	1.91	0.53
1:A:25:ILE:HG13	1:A:26:LEU:N	2.23	0.52
1:A:61:VAL:O	1:A:65:GLU:HG3	2.09	0.52
1:A:369:GLN:O	1:A:373:LEU:HB2	2.10	0.51
1:A:140:PRO:O	1:A:194:HIS:HE1	1.93	0.51
1:A:371:LEU:HD12	1:A:374:ARG:NH2	2.25	0.51
1:A:231:ARG:NH2	1:A:236:ASP:HA	2.25	0.50
1:A:328:GLN:NE2	1:A:332:ARG:HG3	2.26	0.49
1:A:83:ILE:H	1:A:111:GLN:NE2	2.11	0.49
1:A:57:VAL:HG12	1:A:61:VAL:HG22	1.95	0.49
1:A:192:CYS:HB2	1:A:224:PHE:CE1	2.48	0.49
1:A:35:ASP:HB2	1:A:40:LYS:CD	2.43	0.49
1:A:330:ILE:O	1:A:334:ARG:HG3	2.13	0.49
1:A:35:ASP:O	1:A:37:ARG:N	2.46	0.49
1:A:83:ILE:H	1:A:111:GLN:HE21	1.61	0.48
1:A:32:PHE:O	1:A:40:LYS:HD2	2.14	0.48
1:A:216:LYS:HD3	1:A:218:TRP:CZ2	2.49	0.48
1:A:210:ALA:O	1:A:214:VAL:HG23	2.14	0.48
1:A:226:TYR:CZ	1:A:258:LYS:HD3	2.44	0.47
1:A:193:CYS:SG	1:A:200:ASP:CA	3.03	0.47
1:A:133:LYS:NZ	1:A:133:LYS:HB3	2.30	0.46
1:A:277:SER:HA	1:A:280:VAL:HG12	1.96	0.46
1:A:70:GLU:HB2	1:A:71:ASN:HD22	1.80	0.46
1:A:398:ALA:O	1:A:402:GLU:HB2	2.15	0.46
1:A:192:CYS:SG	1:A:227:GLN:HA	2.55	0.45
1:A:89:CYS:HB3	1:A:310:LEU:HD13	1.97	0.45
1:A:355:LYS:HA	1:A:355:LYS:HD2	1.71	0.45
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.98	0.44
1:A:202:THR:N	1:A:205:GLN:HE21	2.08	0.44
1:A:200:ASP:HB2	1:A:201:PRO:O	2.18	0.44
1:A:250:LEU:HB3	1:A:273:VAL:HG22	1.99	0.44
1:A:136:TRP:HB2	1:A:187:VAL:HG22	2.00	0.43
1:A:145:HIS:NE2	1:A:188:LEU:HD21	2.32	0.43
1:A:344:LYS:HZ1	1:A:398:ALA:HB1	1.84	0.43
1:A:134:ARG:HH21	1:A:157:ARG:HH21	1.65	0.43
1:A:124:ASP:O	1:A:128:LYS:HB3	2.19	0.43
1:A:231:ARG:HH21	1:A:236:ASP:HA	1.84	0.43
1:A:212:LEU:CD2	1:A:216:LYS:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:O	1:A:254:SER:HA	2.19	0.42
1:A:58:LEU:HA	1:A:58:LEU:HD12	1.82	0.42
1:A:15:GLU:O	1:A:16:ASN:HB2	2.19	0.42
1:A:192:CYS:HB2	1:A:224:PHE:CD1	2.54	0.42
1:A:396:ASN:O	1:A:399:PRO:HG2	2.20	0.42
1:A:66:GLN:O	1:A:70:GLU:HG2	2.20	0.41
1:A:401:CYS:O	1:A:405:VAL:HG23	2.21	0.41
1:A:228:GLY:O	1:A:327:ARG:HD3	2.21	0.41
1:A:51:GLU:HA	1:A:329:ARG:NH1	2.35	0.41
1:A:330:ILE:HG23	1:A:389:VAL:CG2	2.51	0.41
1:A:274:ALA:HB3	1:A:280:VAL:HB	2.01	0.41
1:A:249:GLU:HA	1:A:273:VAL:O	2.21	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.86	0.40
1:A:192:CYS:SG	1:A:236:ASP:HB3	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:OH	2:A:409:PLP:O3P[4_566]	2.16	0.04

## 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%)	351 (89%)	27 (7%)	16 (4%)	<b>3</b> <b>2</b>

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	20	ALA

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Mol	Chain	Res	Type
1	A	24	PRO
1	A	34	ALA
1	A	36	GLU
1	A	164	ALA
1	A	165	GLU
1	A	194	HIS
1	A	346	ALA
1	A	19	ALA
1	A	40	LYS
1	A	275	ALA
1	A	163	ASP
1	A	263	TYR
1	A	26	LEU
1	A	38	PRO

### 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%)	262 (82%)	58 (18%)	<b>2</b> <b>2</b>

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	24	PRO
1	A	25	ILE
1	A	30	ASP
1	A	33	ARG
1	A	38	PRO
1	A	42	ASN
1	A	51	GLU
1	A	54	LYS
1	A	56	PRO
1	A	58	LEU
1	A	61	VAL

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Mol	Chain	Res	Type
1	A	66	GLN
1	A	69	LEU
1	A	70	GLU
1	A	71	ASN
1	A	78	LEU
1	A	88	ARG
1	A	112	THR
1	A	126	LEU
1	A	128	LYS
1	A	130	THR
1	A	135	VAL
1	A	146	LYS
1	A	169	LEU
1	A	174	LEU
1	A	192	CYS
1	A	211	GLN
1	A	212	LEU
1	A	213	SER
1	A	219	LEU
1	A	224	PHE
1	A	231	ARG
1	A	235	GLU
1	A	238	GLU
1	A	240	LEU
1	A	250	LEU
1	A	258	LYS
1	A	259	ASN
1	A	262	LEU
1	A	276	ASP
1	A	294	ASN
1	A	315	LEU
1	A	323	LEU
1	A	328	GLN
1	A	331	GLN
1	A	332	ARG
1	A	341	LEU
1	A	349	ASP
1	A	355	LYS
1	A	362	PHE
1	A	367	LYS
1	A	374	ARG
1	A	375	GLU

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Mol	Chain	Res	Type
1	A	377	PHE
1	A	395	ASP
1	A	400	LEU
1	A	402	GLU

Some 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	66	GLN
1	A	71	ASN
1	A	111	GLN
1	A	190	HIS
1	A	205	GLN
1	A	247	HIS
1	A	259	ASN
1	A	294	ASN
1	A	297	ASN
1	A	328	GLN
1	A	339	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](#)

1 ligand is 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	1.53	3 (20%)	20,22,23	2.38	8 (40%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	PLP	C4A-C4	-3.50	1.44	1.51
2	A	409	PLP	C5-C4	-3.01	1.37	1.40
2	A	409	PLP	O3-C3	-2.35	1.31	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	PLP	C3-C2-N1	-3.24	116.49	120.75
2	A	409	PLP	C5A-C5-C6	-3.14	113.93	119.33
2	A	409	PLP	C5-C6-N1	-2.01	120.47	123.87
2	A	409	PLP	C3-C4-C5	2.77	121.78	118.63
2	A	409	PLP	O4P-P-O1P	2.95	114.75	106.47
2	A	409	PLP	C6-N1-C2	3.01	125.05	119.26
2	A	409	PLP	C2A-C2-C3	4.65	126.51	120.96
2	A	409	PLP	O4P-C5A-C5	4.93	119.24	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	0	1

## 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.