



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 AM UTC

PDB ID : 1AAW / pdb_00001aaw
Title : THE STRUCTURAL BASIS FOR THE ALTERED SUBSTRATE SPECIFICITY OF THE R292D ACTIVE SITE MUTANT OF ASPARTATE AMINOTRANSFERASE FROM E. COLI
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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.

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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

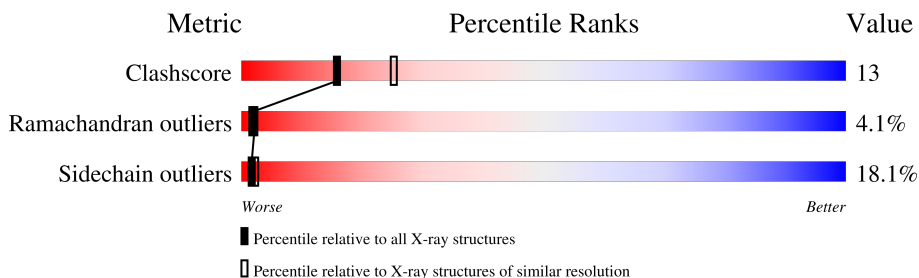
1 Overall quality at a glance

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	

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
2	PLP	A	409	-	X	-	-

2 Entry composition [i](#)

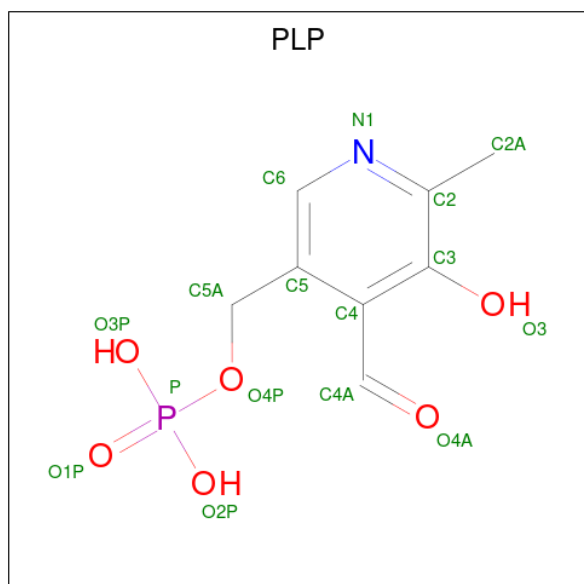
There are 3 unique types of molecules in this entry. The entry contains 3087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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.

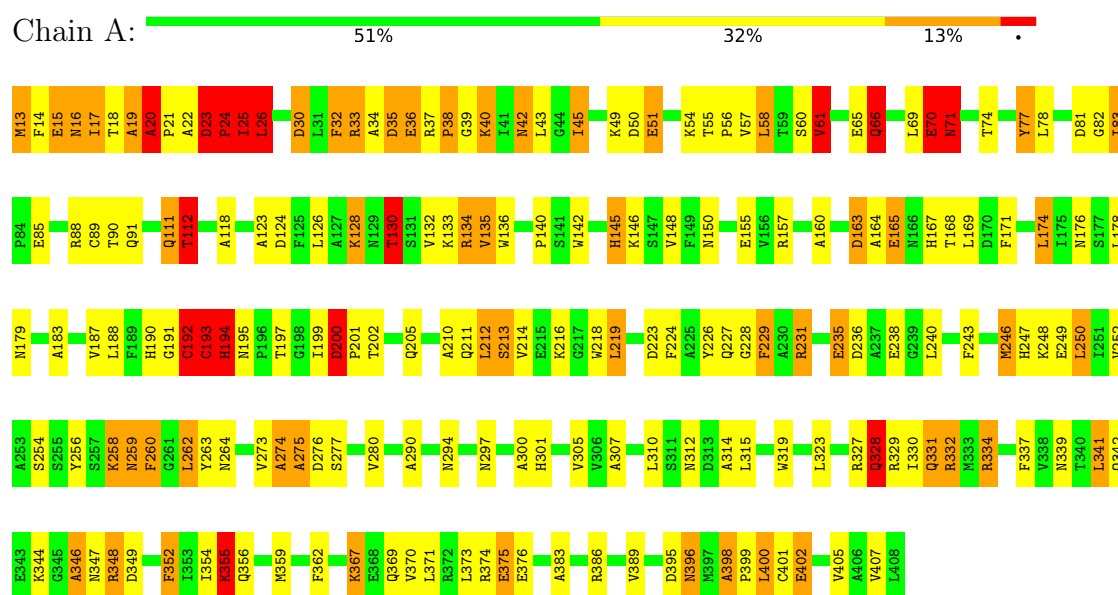
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		

3 Residue-property plots [i](#)

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	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 ²)	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	1.13	12/3130 (0.4%)	2.17	143/4240 (3.4%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	VAL	CA-CB	8.27	1.65	1.54
1	A	301	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	194	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	25	ILE	CA-CB	6.37	1.62	1.54
1	A	194	HIS	CG-ND1	-6.32	1.31	1.38
1	A	247	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	190	HIS	CG-ND1	-5.79	1.31	1.38
1	A	190	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	167	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	61	VAL	CA-CB	5.26	1.60	1.54
1	A	74	THR	CA-CB	5.18	1.63	1.54
1	A	145	HIS	CD2-NE2	-5.08	1.32	1.37

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	N-CA-C	13.87	128.53	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ASN	CA-CB-CG	11.90	124.50	112.60
1	A	274	ALA	N-CA-C	10.41	129.49	114.39
1	A	20	ALA	CA-C-N	10.26	130.02	119.76
1	A	20	ALA	C-N-CA	10.26	130.02	119.76
1	A	356	GLN	N-CA-C	-10.12	91.24	107.93
1	A	183	ALA	N-CA-C	10.08	124.83	112.54
1	A	26	LEU	N-CA-C	9.68	124.92	112.34
1	A	13	MET	CA-CB-CG	-9.40	95.30	114.10
1	A	43	LEU	O-C-N	-8.84	112.34	122.68
1	A	328	GLN	OE1-CD-NE2	-8.76	113.84	122.60
1	A	150	ASN	OD1-CG-ND2	-8.74	113.86	122.60
1	A	32	PHE	N-CA-C	-8.70	99.52	112.04
1	A	21	PRO	N-CA-C	8.69	124.84	111.19
1	A	112	THR	O-C-N	-8.68	115.72	121.88
1	A	231	ARG	NE-CZ-NH1	8.51	130.01	121.50
1	A	183	ALA	O-C-N	-8.38	111.20	122.43
1	A	312	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	A	334	ARG	N-CA-C	-8.19	102.29	111.14
1	A	247	HIS	CA-CB-CG	-8.14	105.66	113.80
1	A	66	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	A	193	CYS	N-CA-C	7.91	121.86	110.24
1	A	15	GLU	O-C-N	7.86	132.37	122.93
1	A	112	THR	N-CA-CB	-7.66	97.40	111.19
1	A	18	THR	N-CA-C	-7.58	94.65	110.80
1	A	301	HIS	CB-CG-CD2	-7.45	121.52	131.20
1	A	248	LYS	N-CA-C	-7.44	104.17	113.55
1	A	171	PHE	N-CA-C	7.44	120.04	111.11
1	A	334	ARG	NE-CZ-NH2	-7.42	112.52	119.20
1	A	301	HIS	N-CA-C	7.38	118.97	111.07
1	A	328	GLN	CG-CD-NE2	7.37	127.45	116.40
1	A	43	LEU	N-CA-C	-7.33	99.96	110.59
1	A	264	ASN	CA-CB-CG	7.26	119.86	112.60
1	A	192	CYS	N-CA-C	-7.21	97.47	109.07
1	A	82	GLY	CA-C-N	7.14	127.73	122.59
1	A	82	GLY	C-N-CA	7.14	127.73	122.59
1	A	346	ALA	CA-C-O	7.11	130.67	120.51
1	A	231	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	A	130	THR	N-CA-CB	-7.10	100.14	111.43
1	A	319	TRP	CG-CD2-CE3	7.02	140.92	133.90
1	A	407	VAL	CA-C-N	7.00	134.30	121.70
1	A	407	VAL	C-N-CA	7.00	134.30	121.70
1	A	39	GLY	N-CA-C	6.95	121.31	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	70	GLU	CA-CB-CG	6.90	127.90	114.10
1	A	111	GLN	N-CA-C	-6.82	99.42	110.20
1	A	328	GLN	CB-CG-CD	6.81	124.18	112.60
1	A	341	LEU	CA-C-O	-6.78	113.31	120.63
1	A	23	ASP	CA-C-N	6.74	128.26	119.84
1	A	23	ASP	C-N-CA	6.74	128.26	119.84
1	A	355	LYS	CA-C-N	6.72	132.47	121.58
1	A	355	LYS	C-N-CA	6.72	132.47	121.58
1	A	150	ASN	CB-CG-ND2	6.70	126.44	116.40
1	A	123	ALA	N-CA-C	6.59	119.06	111.02
1	A	359	MET	N-CA-C	6.56	119.76	111.69
1	A	33	ARG	O-C-N	6.53	130.77	122.93
1	A	194	HIS	N-CA-C	6.50	124.66	110.80
1	A	193	CYS	O-C-N	6.34	130.67	123.06
1	A	197	THR	N-CA-C	6.32	121.06	113.23
1	A	243	PHE	CA-CB-CG	6.27	120.07	113.80
1	A	42	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	112	THR	CB-CA-C	6.26	119.23	108.91
1	A	294	ASN	CB-CG-ND2	6.21	125.72	116.40
1	A	319	TRP	CG-CD1-NE1	-6.20	102.14	110.20
1	A	235	GLU	CB-CG-CD	6.18	123.11	112.60
1	A	337	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	395	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	14	PHE	CA-CB-CG	6.15	119.95	113.80
1	A	342	GLN	CB-CG-CD	6.13	123.02	112.60
1	A	50	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	83	ILE	CA-C-N	6.09	125.57	119.24
1	A	83	ILE	C-N-CA	6.09	125.57	119.24
1	A	66	GLN	CG-CD-NE2	6.08	125.53	116.40
1	A	22	ALA	N-CA-C	6.08	118.81	110.24
1	A	19	ALA	N-CA-C	6.03	123.65	110.80
1	A	275	ALA	N-CA-CB	6.02	120.67	110.49
1	A	55	THR	CA-C-N	6.01	125.98	120.03
1	A	55	THR	C-N-CA	6.01	125.98	120.03
1	A	334	ARG	CA-C-N	6.01	128.65	120.54
1	A	334	ARG	C-N-CA	6.01	128.65	120.54
1	A	294	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	193	CYS	CA-C-O	5.93	127.42	120.96
1	A	30	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	314	ALA	CA-C-N	5.87	128.15	120.28
1	A	314	ALA	C-N-CA	5.87	128.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	A	347	ASN	CA-CB-CG	-5.86	106.74	112.60
1	A	148	VAL	N-CA-C	-5.84	104.63	110.30
1	A	331	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	354	ILE	N-CA-CB	-5.79	102.33	110.26
1	A	165	GLU	N-CA-C	5.79	123.12	110.80
1	A	199	ILE	CB-CA-C	-5.71	103.83	110.91
1	A	213	SER	CA-CB-OG	5.70	122.49	111.10
1	A	16	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	356	GLN	OE1-CD-NE2	-5.64	116.95	122.60
1	A	355	LYS	CA-C-O	5.64	128.57	120.51
1	A	339	ASN	CA-CB-CG	-5.63	106.97	112.60
1	A	14	PHE	N-CA-C	-5.61	106.43	113.72
1	A	176	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	260	PHE	N-CA-C	-5.59	105.81	113.30
1	A	342	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	23	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	194	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	A	195	ASN	N-CA-C	-5.54	98.52	109.10
1	A	199	ILE	CA-C-N	5.52	129.69	120.86
1	A	199	ILE	C-N-CA	5.52	129.69	120.86
1	A	398	ALA	O-C-N	-5.52	115.51	120.92
1	A	90	THR	CA-CB-OG1	-5.51	101.33	109.60
1	A	319	TRP	CE2-CD2-CG	-5.49	100.61	107.20
1	A	74	THR	OG1-CB-CG2	-5.44	98.42	109.30
1	A	168	THR	CA-CB-OG1	-5.41	101.48	109.60
1	A	142	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	A	77	TYR	CA-C-O	5.38	126.88	121.07
1	A	128	LYS	CA-CB-CG	5.38	124.85	114.10
1	A	375	GLU	CA-CB-CG	5.37	124.84	114.10
1	A	15	GLU	CA-CB-CG	5.36	124.81	114.10
1	A	219	LEU	N-CA-C	-5.35	100.21	109.15
1	A	331	GLN	CG-CD-NE2	5.33	124.40	116.40
1	A	200	ASP	N-CA-C	5.32	117.72	110.01
1	A	386	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	300	ALA	N-CA-C	5.27	117.11	111.36
1	A	81	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	60	SER	CA-C-O	-5.22	115.02	120.55
1	A	145	HIS	CA-CB-CG	5.20	119.00	113.80
1	A	352	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	223	ASP	N-CA-C	-5.20	100.26	108.73
1	A	70	GLU	CB-CG-CD	5.19	121.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLY	CA-C-O	5.19	126.71	120.90
1	A	36	GLU	N-CA-C	5.18	121.84	110.80
1	A	252	VAL	CA-C-O	5.17	126.06	120.43
1	A	229	PHE	N-CA-C	5.14	119.65	113.17
1	A	179	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	66	GLN	CB-CG-CD	5.12	121.31	112.60
1	A	142	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	A	71	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	290	ALA	CA-C-N	5.07	126.95	120.56
1	A	290	ALA	C-N-CA	5.07	126.95	120.56
1	A	42	ASN	N-CA-C	5.05	116.88	107.99
1	A	319	TRP	CB-CG-CD1	-5.05	119.33	126.90
1	A	297	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	319	TRP	CD1-CG-CD2	5.02	114.33	106.30
1	A	337	PHE	N-CA-C	-5.02	105.72	111.14
1	A	24	PRO	CA-N-CD	-5.01	104.98	112.00

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 [i](#)

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	81	1
2	A	15	0	6	0	1
3	A	3	0	0	0	0
All	All	3087	0	3022	81	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 (81) 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:344:LYS:HZ2	1:A:398:ALA:HB1	1.69	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
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:214:VAL:HG21	1:A:246:MET:HE3	1.91	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:35:ASP:HB2	1:A:40:LYS:CD	2.43	0.49
1:A:192:CYS:HB2	1:A:224:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:O	1:A:37:ARG:N	2.46	0.49
1:A:330:ILE:O	1:A:334:ARG:HG3	2.13	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:246:MET:HE3	1:A:246:MET:HB3	1.63	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: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
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.82	0.42
1:A:224:PHE:O	1:A:254:SER:HA	2.19	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:51:GLU:HA	1:A:329:ARG:NH1	2.35	0.41
1:A:228:GLY:O	1:A:327:ARG:HD3	2.21	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:HD23	1:A:178:LEU:HA	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 sym-

metry 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%)	2 2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	20	ALA
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 [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%)	262 (82%)	58 (18%)	2 2

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

Mol	Chain	Res	Type
1	A	13	MET
1	A	17	ILE
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	45	ILE
1	A	51	GLU
1	A	54	LYS
1	A	56	PRO
1	A	58	LEU
1	A	61	VAL
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	91	GLN
1	A	112	THR
1	A	126	LEU
1	A	130	THR
1	A	134	ARG
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

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Mol	Chain	Res	Type
1	A	219	LEU
1	A	235	GLU
1	A	238	GLU
1	A	240	LEU
1	A	246	MET
1	A	250	LEU
1	A	258	LYS
1	A	259	ASN
1	A	262	LEU
1	A	276	ASP
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	348	ARG
1	A	349	ASP
1	A	355	LYS
1	A	362	PHE
1	A	367	LYS
1	A	375	GLU
1	A	400	LEU
1	A	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	71	ASN
1	A	76	ASN
1	A	91	GLN
1	A	111	GLN
1	A	129	ASN
1	A	139	ASN
1	A	190	HIS
1	A	205	GLN
1	A	211	GLN
1	A	247	HIS
1	A	259	ASN
1	A	328	GLN
1	A	331	GLN

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Mol	Chain	Res	Type
1	A	335	GLN
1	A	339	ASN
1	A	342	GLN

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](#)

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	1.56	3 (20%)	21,22,23	2.55	10 (47%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	PLP	C4A-C4	-3.54	1.44	1.51
2	A	409	PLP	C5-C4	-3.11	1.37	1.40
2	A	409	PLP	O3-C3	-2.30	1.31	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	PLP	O4P-C5A-C5	5.27	119.24	109.36
2	A	409	PLP	C2A-C2-C3	4.88	126.51	120.80
2	A	409	PLP	C3-C2-N1	-3.54	116.49	120.96
2	A	409	PLP	C5A-C5-C4	3.50	129.55	122.64
2	A	409	PLP	C5A-C5-C6	-3.33	113.93	119.36
2	A	409	PLP	C6-N1-C2	3.23	125.05	119.20
2	A	409	PLP	O4P-P-O1P	3.08	114.75	106.44
2	A	409	PLP	C3-C4-C5	2.66	121.78	118.59
2	A	409	PLP	C5-C6-N1	-2.07	120.47	123.83
2	A	409	PLP	O3P-P-O2P	2.03	115.43	107.80

There are no chirality outliers.

All (5) 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
2	A	409	PLP	C5A-O4P-P-O1P

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

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.