



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:38 PM UTC

PDB ID : 1ASF / pdb_00001asf
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

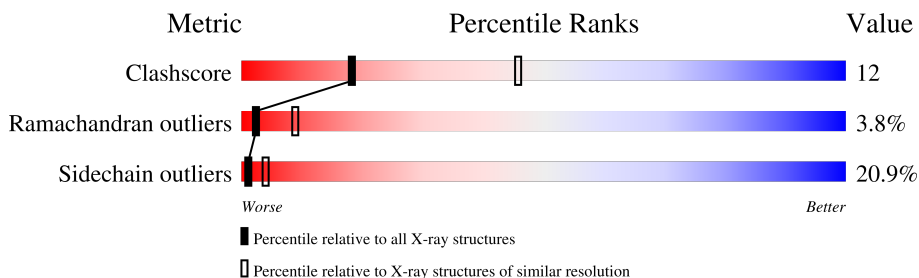
1 Overall quality at a glance

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	47% 37% 12% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3088 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:

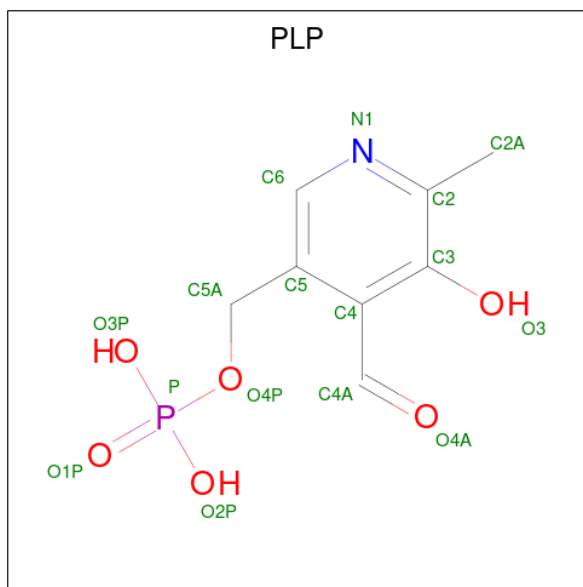
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	PHE	TYR	engineered mutation	UNP P00509

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



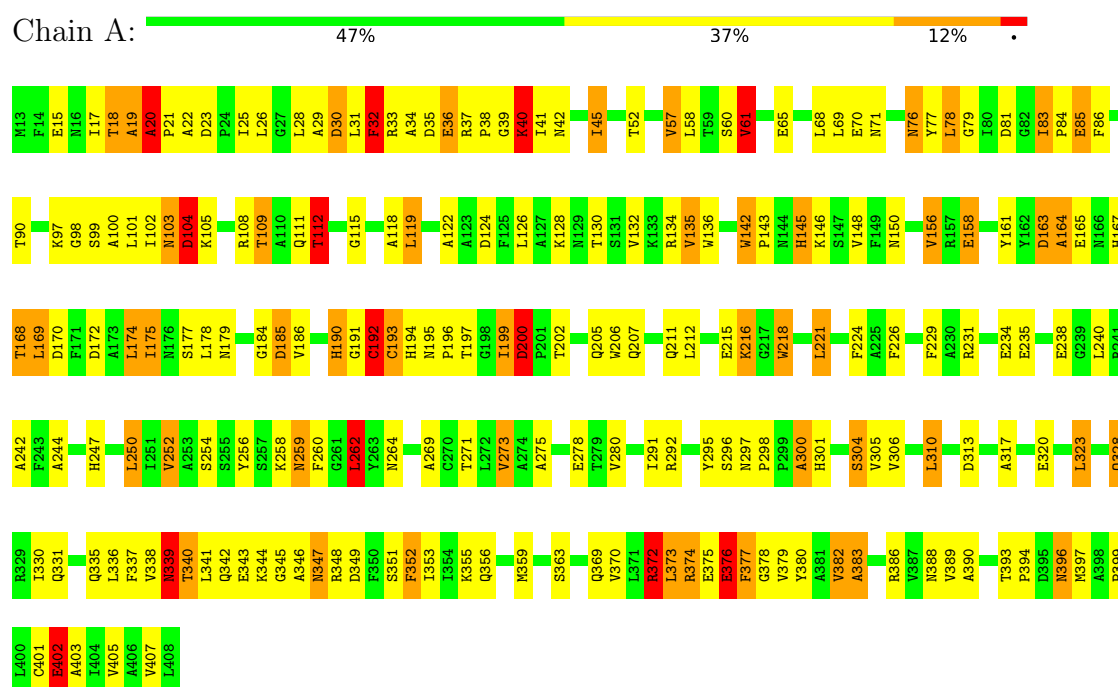
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0

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 87.30Å 80.19Å 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}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3088	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: SO4, 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	1.11	15/3129 (0.5%)	2.08	130/4238 (3.1%)

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	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	HIS	CD2-NE2	-7.48	1.29	1.37
1	A	301	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	145	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	41	ILE	CA-CB	6.38	1.63	1.54
1	A	190	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	61	VAL	CA-CB	6.18	1.63	1.54
1	A	18	THR	CA-CB	6.16	1.63	1.53
1	A	194	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	168	THR	CA-CB	5.80	1.61	1.53
1	A	190	HIS	CG-ND1	-5.67	1.32	1.38
1	A	252	VAL	CA-CB	5.61	1.61	1.54
1	A	145	HIS	CG-ND1	-5.56	1.32	1.38
1	A	194	HIS	CG-ND1	-5.20	1.32	1.38
1	A	247	HIS	CG-ND1	-5.13	1.32	1.38
1	A	135	VAL	CA-CB	5.12	1.61	1.54

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLU	N-CA-C	-10.76	97.39	112.13
1	A	76	ASN	CA-CB-CG	10.55	123.15	112.60
1	A	200	ASP	CA-CB-CG	10.43	123.03	112.60
1	A	150	ASN	CA-CB-CG	9.65	122.25	112.60
1	A	40	LYS	N-CA-C	9.48	122.80	111.33
1	A	103	ASN	CA-C-O	9.35	130.43	120.33
1	A	22	ALA	N-CA-C	9.11	123.19	109.25
1	A	346	ALA	N-CA-C	9.08	123.37	111.75
1	A	20	ALA	CA-C-N	9.03	130.60	120.85
1	A	20	ALA	C-N-CA	9.03	130.60	120.85
1	A	193	CYS	O-C-N	8.68	133.56	123.41
1	A	356	GLN	N-CA-C	-8.47	96.39	109.52
1	A	163	ASP	O-C-N	8.44	132.93	123.48
1	A	81	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	298	PRO	N-CA-C	8.34	120.87	110.70
1	A	163	ASP	CA-C-O	8.20	129.91	120.89
1	A	32	PHE	CA-CB-CG	8.17	121.97	113.80
1	A	348	ARG	N-CA-C	8.10	120.68	109.18
1	A	172	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	199	ILE	N-CA-C	7.99	119.66	107.99
1	A	339	ASN	CA-CB-CG	7.90	120.50	112.60
1	A	71	ASN	N-CA-C	7.89	123.09	113.38
1	A	103	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	103	ASN	CA-C-N	7.85	136.53	121.54
1	A	103	ASN	C-N-CA	7.85	136.53	121.54
1	A	341	LEU	N-CA-C	-7.83	102.34	111.03
1	A	35	ASP	N-CA-C	7.72	122.70	113.28
1	A	301	HIS	N-CA-C	7.63	120.33	111.02
1	A	18	THR	N-CA-CB	-7.58	97.69	110.49
1	A	124	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	194	HIS	N-CA-C	7.41	126.57	110.80
1	A	103	ASN	O-C-N	7.37	132.85	123.12
1	A	349	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	177	SER	N-CA-C	-7.25	105.62	114.75
1	A	197	THR	N-CA-C	7.17	120.92	111.75
1	A	205	GLN	CG-CD-NE2	7.06	126.99	116.40
1	A	396	ASN	CB-CA-C	-6.94	100.27	110.96
1	A	39	GLY	N-CA-C	-6.91	96.79	113.18
1	A	205	GLN	OE1-CD-NE2	-6.89	115.71	122.60
1	A	77	TYR	N-CA-C	6.88	119.98	110.35
1	A	355	LYS	O-C-N	6.81	131.64	122.59
1	A	383	ALA	N-CA-C	6.75	121.12	112.34
1	A	247	HIS	CA-CB-CG	-6.62	107.18	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ILE	CA-CB-CG2	-6.60	99.28	110.50
1	A	42	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	193	CYS	CA-C-N	6.58	134.10	121.54
1	A	193	CYS	C-N-CA	6.58	134.10	121.54
1	A	32	PHE	N-CA-C	6.51	121.59	112.93
1	A	20	ALA	CA-C-O	-6.51	111.24	120.16
1	A	174	LEU	N-CA-C	-6.46	103.28	112.13
1	A	109	THR	N-CA-C	6.40	119.58	108.76
1	A	42	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	355	LYS	CA-C-O	6.35	129.59	120.51
1	A	300	ALA	N-CA-C	6.32	121.74	111.37
1	A	170	ASP	N-CA-C	-6.28	95.40	107.57
1	A	36	GLU	CA-CB-CG	6.25	126.61	114.10
1	A	195	ASN	O-C-N	-6.24	114.44	121.36
1	A	275	ALA	N-CA-C	6.23	124.07	110.80
1	A	175	ILE	CA-CB-CG1	6.18	120.91	110.40
1	A	328	GLN	CB-CG-CD	6.17	123.09	112.60
1	A	229	PHE	N-CA-C	6.17	120.81	113.28
1	A	20	ALA	O-C-N	-6.12	114.28	121.32
1	A	369	GLN	N-CA-C	-6.12	105.95	113.41
1	A	202	THR	CA-C-O	-6.11	114.60	121.81
1	A	231	ARG	CA-CB-CG	6.04	126.19	114.10
1	A	112	THR	N-CA-CB	-6.04	100.30	111.18
1	A	134	ARG	CB-CG-CD	6.02	125.15	111.30
1	A	192	CYS	CA-CB-SG	-6.02	100.56	114.40
1	A	167	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	A	328	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	191	GLY	N-CA-C	5.93	119.38	112.50
1	A	18	THR	CB-CA-C	5.87	122.11	110.42
1	A	363	SER	N-CA-C	5.85	118.44	111.71
1	A	247	HIS	N-CA-C	5.85	119.14	110.48
1	A	103	ASN	CB-CG-ND2	5.85	125.17	116.40
1	A	42	ASN	CB-CG-ND2	5.84	125.16	116.40
1	A	33	ARG	N-CA-C	-5.79	104.97	111.28
1	A	402	GLU	CB-CG-CD	5.78	122.43	112.60
1	A	235	GLU	CB-CG-CD	5.77	122.41	112.60
1	A	158	GLU	N-CA-C	5.73	118.21	108.02
1	A	164	ALA	N-CA-C	5.71	122.97	110.80
1	A	122	ALA	N-CA-C	-5.70	104.70	111.03
1	A	262	LEU	N-CA-CB	-5.70	102.21	110.70
1	A	195	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	264	ASN	CA-CB-CG	5.65	118.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	PRO	CA-C-N	5.65	126.90	119.84
1	A	298	PRO	C-N-CA	5.65	126.90	119.84
1	A	331	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	A	317	ALA	O-C-N	5.62	127.86	122.07
1	A	83	ILE	CA-C-N	5.61	125.07	119.24
1	A	83	ILE	C-N-CA	5.61	125.07	119.24
1	A	190	HIS	N-CA-C	-5.60	99.15	108.34
1	A	242	ALA	N-CA-C	-5.49	105.21	111.14
1	A	269	ALA	N-CA-C	5.46	117.28	108.32
1	A	340	THR	N-CA-C	-5.45	106.13	112.89
1	A	340	THR	CA-CB-OG1	-5.45	101.43	109.60
1	A	195	ASN	N-CA-CB	-5.44	102.06	110.01
1	A	339	ASN	N-CA-C	5.44	119.90	113.16
1	A	115	GLY	N-CA-C	-5.41	105.84	112.77
1	A	41	ILE	O-C-N	-5.41	115.81	122.57
1	A	79	GLY	N-CA-C	-5.40	105.63	112.54
1	A	150	ASN	CB-CA-C	-5.39	102.18	110.81
1	A	374	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	A	33	ARG	O-C-N	5.34	127.78	122.12
1	A	206	TRP	CA-C-N	5.31	127.66	120.38
1	A	206	TRP	C-N-CA	5.31	127.66	120.38
1	A	142	TRP	CA-C-N	5.29	126.46	119.84
1	A	142	TRP	C-N-CA	5.29	126.46	119.84
1	A	235	GLU	N-CA-C	5.28	116.72	111.07
1	A	30	ASP	N-CA-C	5.27	118.50	111.75
1	A	136	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	A	343	GLU	N-CA-CB	-5.24	102.43	110.44
1	A	60	SER	CA-C-O	-5.23	115.00	120.55
1	A	297	ASN	O-C-N	-5.23	118.17	121.88
1	A	15	GLU	O-C-N	5.22	129.53	122.96
1	A	301	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	185	ASP	N-CA-C	5.19	118.56	110.32
1	A	42	ASN	N-CA-C	5.17	117.36	107.75
1	A	313	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	111	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	A	352	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	57	VAL	CB-CA-C	5.14	118.02	110.98
1	A	136	TRP	CG-CD1-NE1	-5.12	103.55	110.20
1	A	31	LEU	N-CA-CB	-5.11	101.45	110.39
1	A	347	ASN	CA-C-O	-5.10	113.22	120.51
1	A	136	TRP	CD1-CG-CD2	5.08	114.42	106.30
1	A	112	THR	CB-CA-C	5.07	117.99	109.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	335	GLN	CA-CB-CG	5.04	124.18	114.10
1	A	19	ALA	N-CA-C	5.01	121.48	110.80
1	A	372	ARG	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ALA	Peptide
1	A	200	ASP	Peptide
1	A	23	ASP	Peptide
1	A	37	ARG	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	3068	0	3016	74	0
2	A	5	0	0	0	0
3	A	15	0	6	0	0
All	All	3088	0	3022	74	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 12.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ($\text{\AA}$)	Clash overlap ($\text{\AA}$)
1:A:196:PRO:HB3	1:A:386:ARG:HG3	1.42	1.01
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.68	0.76
1:A:38:PRO:HD2	1:A:40:LYS:HB3	1.70	0.73
1:A:259:ASN:HB2	1:A:323:LEU:HD21	1.69	0.73
1:A:100:ALA:O	1:A:104:ASP:HB2	1.89	0.73
1:A:193:CYS:SG	1:A:200:ASP:HA	2.30	0.72
1:A:339:ASN:HA	1:A:342:GLN:HB3	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.74	0.67
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.77	0.66
1:A:336:LEU:HG	1:A:397:MET:HG2	1.79	0.64
1:A:25:ILE:HG23	1:A:26:LEU:HG	1.81	0.61
1:A:375:GLU:O	1:A:376:GLU:HB3	1.99	0.60
1:A:99:SER:HB3	1:A:102:ILE:HD12	1.83	0.60
1:A:186:VAL:HG11	1:A:221:LEU:HD12	1.85	0.58
1:A:142:TRP:HB3	1:A:145:HIS:ND1	2.20	0.57
1:A:402:GLU:HG2	1:A:403:ALA:N	2.19	0.56
1:A:375:GLU:O	1:A:375:GLU:HG3	2.04	0.56
1:A:32:PHE:HB2	1:A:380:TYR:CE2	2.41	0.55
1:A:192:CYS:SG	1:A:193:CYS:N	2.80	0.55
1:A:256:TYR:O	1:A:260:PHE:HB2	2.06	0.55
1:A:340:THR:HG22	1:A:401:CYS:SG	2.46	0.55
1:A:132:VAL:HG22	1:A:184:GLY:O	2.07	0.54
1:A:135:VAL:O	1:A:156:VAL:HA	2.08	0.53
1:A:393:THR:HB	1:A:394:PRO:HD2	1.92	0.52
1:A:291:ILE:HG23	1:A:295:TYR:CE1	2.45	0.52
1:A:29:ALA:O	1:A:32:PHE:HB3	2.11	0.51
1:A:83:ILE:HG22	1:A:86:PHE:H	1.76	0.51
1:A:259:ASN:HD22	1:A:259:ASN:H	1.59	0.51
1:A:112:THR:HG21	1:A:118:ALA:N	2.26	0.51
1:A:119:LEU:HD23	1:A:148:VAL:HG11	1.94	0.50
1:A:179:ASN:HA	1:A:216:LYS:HZ1	1.76	0.50
1:A:112:THR:HG21	1:A:118:ALA:CA	2.42	0.49
1:A:108:ARG:HG2	1:A:280:VAL:HG22	1.93	0.49
1:A:119:LEU:HD21	1:A:145:HIS:CD2	2.48	0.48
1:A:38:PRO:HD2	1:A:40:LYS:CB	2.40	0.48
1:A:61:VAL:O	1:A:65:GLU:HG3	2.13	0.48
1:A:161:TYR:O	1:A:169:LEU:HD23	2.13	0.48
1:A:300:ALA:O	1:A:304:SER:HB2	2.14	0.48
1:A:399:PRO:O	1:A:402:GLU:HB3	2.13	0.48
1:A:112:THR:HG21	1:A:118:ALA:CB	2.43	0.47
1:A:338:VAL:CG2	1:A:353:ILE:HB	2.43	0.47
1:A:306:VAL:O	1:A:310:LEU:HB2	2.14	0.47
1:A:340:THR:HG21	1:A:397:MET:HG3	1.96	0.47
1:A:372:ARG:O	1:A:376:GLU:OE1	2.32	0.47
1:A:119:LEU:HD21	1:A:145:HIS:HD2	1.79	0.47
1:A:185:ASP:O	1:A:218:TRP:HA	2.15	0.46
1:A:339:ASN:CA	1:A:342:GLN:HB3	2.46	0.45
1:A:382:VAL:HG12	1:A:386:ARG:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:O	1:A:169:LEU:HA	2.17	0.45
1:A:373:LEU:CD1	1:A:407:VAL:HG11	2.47	0.44
1:A:168:THR:HA	1:A:199:ILE:HD13	1.98	0.44
1:A:85:GLU:H	1:A:85:GLU:CD	2.26	0.44
1:A:323:LEU:HD22	1:A:323:LEU:HA	1.84	0.43
1:A:376:GLU:HG2	1:A:377:PHE:N	2.32	0.43
1:A:337:PHE:HA	1:A:397:MET:SD	2.59	0.43
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.91	0.43
1:A:58:LEU:HB2	1:A:61:VAL:HG13	2.01	0.43
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.67	0.42
1:A:382:VAL:CG1	1:A:386:ARG:HB3	2.49	0.42
1:A:90:THR:CG2	1:A:109:THR:HG21	2.49	0.42
1:A:388:ASN:OD1	1:A:390:ALA:HB3	2.18	0.42
1:A:45:ILE:H	1:A:45:ILE:HG13	1.71	0.42
1:A:90:THR:HG21	1:A:109:THR:HG21	2.00	0.42
1:A:25:ILE:O	1:A:28:LEU:HB2	2.21	0.41
1:A:101:LEU:HD23	1:A:273:VAL:HG21	2.01	0.41
1:A:178:LEU:O	1:A:218:TRP:HZ2	2.02	0.41
1:A:97:LYS:HG3	1:A:98:GLY:N	2.35	0.41
1:A:345:GLY:HA3	1:A:405:VAL:CG2	2.50	0.41
1:A:226:PHE:CE1	1:A:258:LYS:HD3	2.56	0.41
1:A:102:ILE:O	1:A:103:ASN:ND2	2.54	0.41
1:A:244:ALA:HA	1:A:250:LEU:HD11	2.02	0.41
1:A:378:GLY:O	1:A:380:TYR:HD1	2.04	0.40
1:A:61:VAL:HB	1:A:305:VAL:HG11	2.03	0.40
1:A:330:ILE:HD11	1:A:359:MET:HG2	2.04	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%)	334 (85%)	45 (11%)	15 (4%)	2 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	A	34	ALA
1	A	104	ASP
1	A	376	GLU
1	A	36	GLU
1	A	216	LYS
1	A	296	SER
1	A	379	VAL
1	A	19	ALA
1	A	192	CYS
1	A	164	ALA
1	A	218	TRP
1	A	347	ASN
1	A	351	SER
1	A	352	PHE

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%)	253 (79%)	67 (21%)	1 4

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	18	THR
1	A	21	PRO
1	A	30	ASP
1	A	32	PHE
1	A	40	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	45	ILE
1	A	52	THR
1	A	57	VAL
1	A	61	VAL
1	A	68	LEU
1	A	69	LEU
1	A	70	GLU
1	A	76	ASN
1	A	78	LEU
1	A	84	PRO
1	A	85	GLU
1	A	104	ASP
1	A	105	LYS
1	A	112	THR
1	A	119	LEU
1	A	126	LEU
1	A	128	LYS
1	A	130	THR
1	A	143	PRO
1	A	146	LYS
1	A	156	VAL
1	A	158	GLU
1	A	163	ASP
1	A	169	LEU
1	A	174	LEU
1	A	175	ILE
1	A	190	HIS
1	A	207	GLN
1	A	211	GLN
1	A	212	LEU
1	A	215	GLU
1	A	221	LEU
1	A	224	PHE
1	A	234	GLU
1	A	238	GLU
1	A	240	LEU
1	A	250	LEU
1	A	252	VAL
1	A	254	SER
1	A	259	ASN
1	A	262	LEU
1	A	271	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	VAL
1	A	278	GLU
1	A	292	ARG
1	A	304	SER
1	A	310	LEU
1	A	320	GLU
1	A	323	LEU
1	A	328	GLN
1	A	339	ASN
1	A	344	LYS
1	A	372	ARG
1	A	373	LEU
1	A	374	ARG
1	A	376	GLU
1	A	377	PHE
1	A	382	VAL
1	A	389	VAL
1	A	396	ASN
1	A	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	103	ASN
1	A	166	ASN
1	A	176	ASN
1	A	179	ASN
1	A	182	GLN
1	A	227	GLN
1	A	259	ASN
1	A	331	GLN

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 [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	PLP	A	411	1	15,15,16	2.78	4 (26%)	21,22,23	3.26	5 (23%)
2	SO4	A	410	-	4,4,4	0.32	0	6,6,6	0.29	0

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	PLP	A	411	1	-	2/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	411	PLP	O4P-C5A	-7.70	1.16	1.44
3	A	411	PLP	C3-C2	-4.70	1.36	1.41
3	A	411	PLP	C2A-C2	-3.40	1.45	1.50
3	A	411	PLP	O3-C3	-2.25	1.31	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	PLP	O4P-C5A-C5	12.77	133.29	109.36
3	A	411	PLP	C5-C6-N1	-3.96	117.38	123.83
3	A	411	PLP	C6-C5-C4	3.39	120.88	118.10
3	A	411	PLP	C6-N1-C2	2.94	124.54	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	PLP	O4P-P-O1P	-2.19	100.52	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	411	PLP	C4-C5-C5A-O4P
3	A	411	PLP	C6-C5-C5A-O4P

There are no ring outliers.

No monomer is involved in short contacts.

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.