



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:26 PM GMT

PDB ID : 1ASF
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

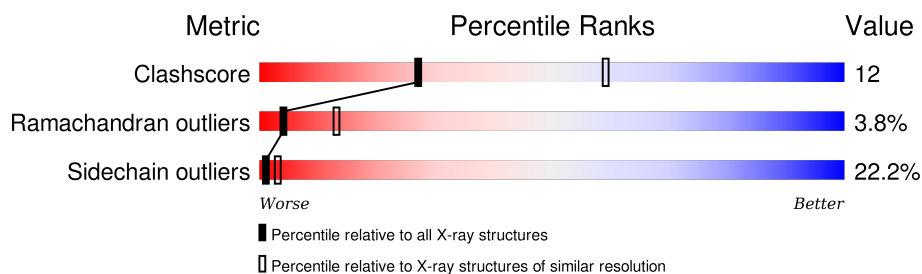
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 54% 35% 9% •

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 (three-letter code: 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 (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



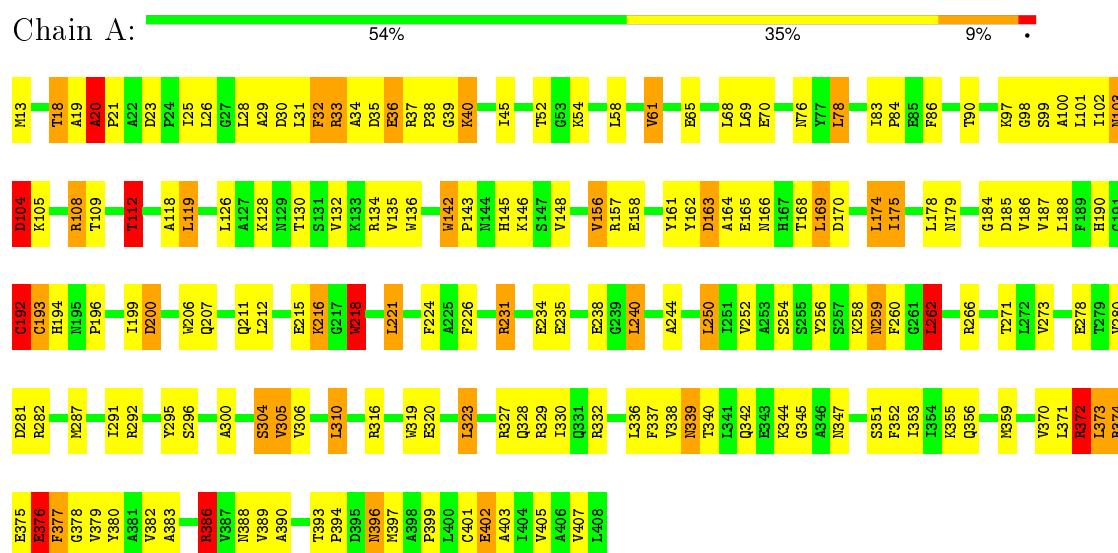
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.80 Å 87.30 Å 80.19 Å 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	0.88	0/3129	1.73	67/4238 (1.6%)

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

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	TRP	CD1-CG-CD2	10.15	114.42	106.30
1	A	163	ASP	CA-C-N	-10.00	95.21	117.20
1	A	108	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	A	355	LYS	CA-C-N	-9.89	95.44	117.20
1	A	103	ASN	CA-C-N	-9.85	95.54	117.20
1	A	108	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	A	134	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	386	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	319	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	A	206	TRP	CD1-CG-CD2	8.74	113.30	106.30
1	A	193	CYS	CA-C-N	-8.74	97.98	117.20
1	A	136	TRP	CE2-CD2-CG	-8.01	100.89	107.30
1	A	142	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	240	LEU	CA-CB-CG	7.66	132.92	115.30
1	A	231	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	192	CYS	CA-CB-SG	-7.47	100.56	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	A	218	TRP	CD1-CG-CD2	7.41	112.22	106.30
1	A	206	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	A	329	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	134	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	319	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	142	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	A	193	CYS	O-C-N	6.79	133.56	122.70
1	A	316	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	386	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	18	THR	N-CA-CB	-6.64	97.69	110.30
1	A	136	TRP	CG-CD1-NE1	-6.55	103.55	110.10
1	A	316	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	39	GLY	N-CA-C	-6.52	96.79	113.10
1	A	218	TRP	CE2-CD2-CG	-6.47	102.12	107.30
1	A	163	ASP	O-C-N	6.39	132.93	122.70
1	A	157	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	103	ASN	O-C-N	6.35	132.85	122.70
1	A	327	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	266	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	20	ALA	CA-C-N	6.21	134.48	117.10
1	A	187	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	A	36	GLU	CA-CB-CG	6.00	126.61	113.40
1	A	174	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	31	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	103	ASN	C-N-CA	5.93	136.53	121.70
1	A	33	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	332	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	231	ARG	CA-CB-CG	5.81	126.19	113.40
1	A	175	ILE	CA-CB-CG2	-5.81	99.28	110.90
1	A	170	ASP	N-CA-C	-5.78	95.40	111.00
1	A	194	HIS	N-CA-C	5.77	126.57	111.00
1	A	319	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	355	LYS	O-C-N	5.59	131.64	122.70
1	A	206	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	A	287	MET	CA-CB-CG	5.56	122.75	113.30
1	A	262	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	18	THR	CA-C-N	5.43	129.14	117.20
1	A	356	GLN	N-CA-C	-5.41	96.39	111.00
1	A	305	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	A	112	THR	N-CA-CB	-5.26	100.30	110.30
1	A	175	ILE	CA-CB-CG1	5.21	120.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	CB-CG-CD	5.21	125.15	111.60
1	A	282	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	142	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	A	371	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	396	ASN	CB-CA-C	-5.07	100.27	110.40
1	A	372	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	13	MET	CA-CB-CG	-5.05	104.72	113.30
1	A	165	GLU	N-CA-C	-5.04	97.39	111.00
1	A	282	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	73	0
2	A	5	0	0	0	0
3	A	15	0	6	0	0
All	All	3088	0	3022	73	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 (73) 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:196:PRO:HB3	1:A:386:ARG:HG3	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:32:PHE:HB2	1:A:380:TYR:CE2	2.41	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	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:323:LEU:HA	1:A:323:LEU:HD22	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:382:VAL:CG1	1:A:386:ARG:HB3	2.49	0.42
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.67	0.42
1:A:388:ASN:OD1	1:A:390:ALA:HB3	2.18	0.42
1:A:90:THR:CG2	1:A:109:THR:HG21	2.49	0.42
1:A:45:ILE:HG13	1:A:45:ILE:H	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%)	4 13

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%)	249 (78%)	71 (22%)	1 3

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	21	PRO
1	A	30	ASP
1	A	32	PHE

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	35	ASP
1	A	40	LYS
1	A	52	THR
1	A	54	LYS
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	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	162	TYR
1	A	163	ASP
1	A	166	ASN
1	A	169	LEU
1	A	174	LEU
1	A	175	ILE
1	A	188	LEU
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	231	ARG
1	A	234	GLU
1	A	235	GLU
1	A	238	GLU
1	A	240	LEU

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	252	VAL
1	A	254	SER
1	A	259	ASN
1	A	262	LEU
1	A	271	THR
1	A	278	GLU
1	A	281	ASP
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	386	ARG
1	A	389	VAL
1	A	396	ASN
1	A	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	166	ASN
1	A	176	ASN
1	A	179	ASN
1	A	205	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 [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](#)

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	SO4	A	410	-	4,4,4	0.70	0	6,6,6	0.17	0
3	PLP	A	411	1	15,15,16	2.81	5 (33%)	21,22,23	3.61	6 (28%)

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	SO4	A	410	-	-	0/0/0/0	0/0/0/0
3	PLP	A	411	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	411	PLP	C3-C2	-6.77	1.36	1.40
3	A	411	PLP	O4P-C5A	-6.74	1.16	1.44
3	A	411	PLP	C2A-C2	-2.67	1.45	1.50
3	A	411	PLP	O3-C3	-2.26	1.31	1.37
3	A	411	PLP	P-O2P	-2.02	1.47	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	PLP	C5-C6-N1	-3.73	117.38	123.86
3	A	411	PLP	O4P-P-O1P	-2.60	100.52	107.14
3	A	411	PLP	O3-C3-C2	2.32	121.69	117.66
3	A	411	PLP	C6-N1-C2	2.58	124.54	119.28
3	A	411	PLP	C6-C5-C4	3.22	120.88	118.15
3	A	411	PLP	O4P-C5A-C5	14.70	133.29	108.99

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.