



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:34 PM UTC

PDB ID : 1AKC / pdb_00001akc
Title : Structural basis for the catalytic activity of aspartate aminotransferase K258H
lacking its pyridoxal-5'-phosphate-binding lysine residue
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1994-02-28
Resolution : 2.30 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**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

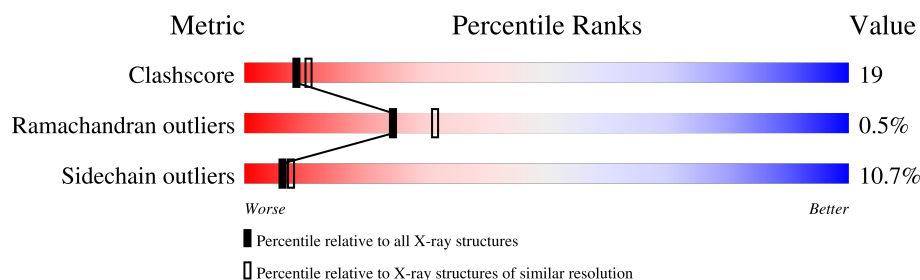
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	401	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3498 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.

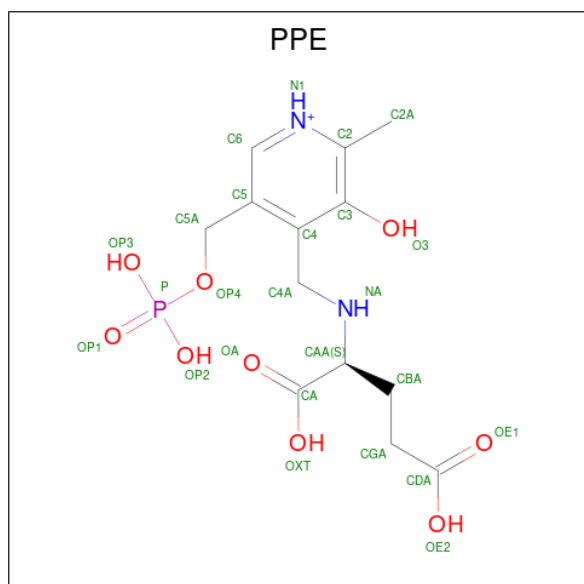
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3162	2004	559	581	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508
A	258	HIS	LYS	conflict	UNP P00508

- Molecule 2 is 4-[(1,3-DICARBOXY-PROPYLAMINO)-METHYL]-3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDINIUM (CCD ID: PPE) (formula: $C_{13}H_{20}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	25	13	2	9	1	0	0

- Molecule 3 is water.

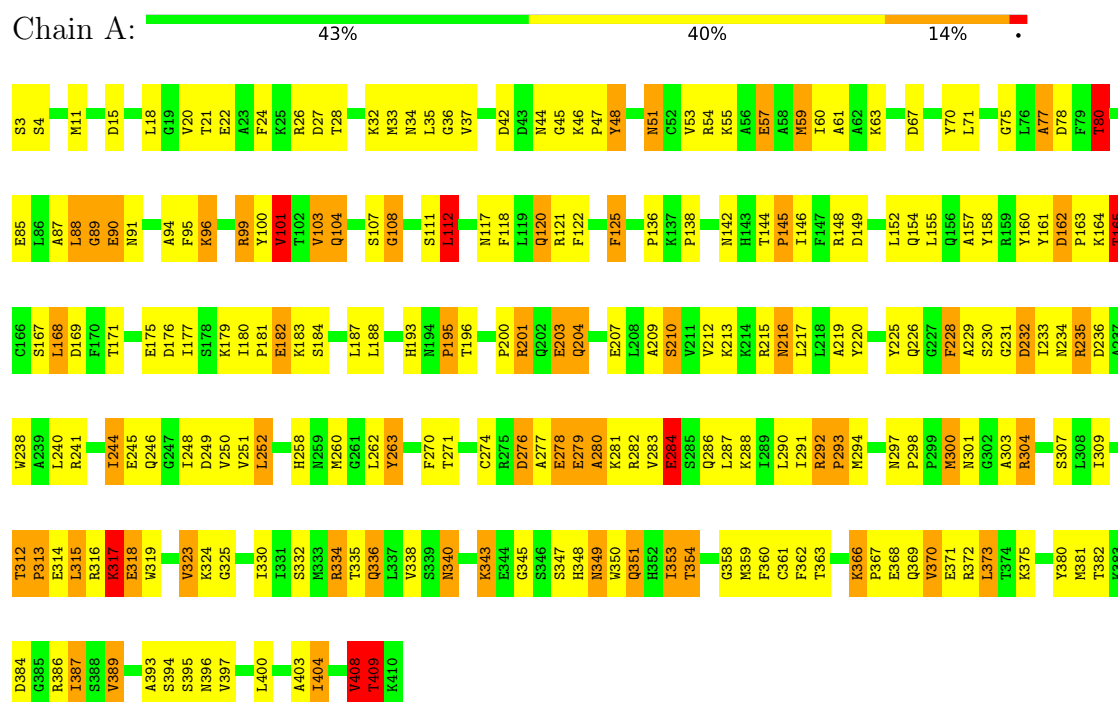
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	311	Total 311	O 311	0	0

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	69.80Å 91.30Å 127.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3498	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: PPE

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	1.04	0/3233	2.30	174/4364 (4.0%)

There are no bond length outliers.

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASP	CA-CB-CG	16.06	128.66	112.60
1	A	99	ARG	CD-NE-CZ	13.96	143.95	124.40
1	A	284	GLU	CA-CB-CG	12.46	139.02	114.10
1	A	278	GLU	CB-CG-CD	10.01	129.62	112.60
1	A	291	ILE	O-C-N	9.99	132.12	121.83
1	A	297	ASN	CB-CA-C	9.85	123.22	110.22
1	A	318	GLU	CA-C-O	9.34	130.45	120.55
1	A	154	GLN	CA-C-O	-8.92	110.76	121.28
1	A	362	PHE	CA-C-N	8.84	132.49	120.38
1	A	362	PHE	C-N-CA	8.84	132.49	120.38
1	A	387	ILE	O-C-N	8.64	132.25	123.00
1	A	363	THR	O-C-N	8.56	131.20	122.12
1	A	304	ARG	NE-CZ-NH2	-8.55	111.50	119.20
1	A	251	VAL	N-CA-C	-8.20	96.22	108.85
1	A	304	ARG	NE-CZ-NH1	8.16	129.66	121.50
1	A	291	ILE	CA-C-O	-7.99	112.39	120.85
1	A	366	LYS	N-CA-CB	7.93	118.93	109.74
1	A	89	GLY	N-CA-C	-7.86	102.97	112.48
1	A	240	LEU	O-C-N	7.80	130.20	122.09
1	A	111	SER	CA-C-N	7.76	130.52	120.44
1	A	111	SER	C-N-CA	7.76	130.52	120.44
1	A	340	ASN	CA-CB-CG	-7.57	105.03	112.60
1	A	334	ARG	CA-C-O	7.51	128.71	120.82
1	A	125	PHE	CA-CB-CG	-7.51	106.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	TYR	CA-CB-CG	7.50	127.39	113.90
1	A	48	TYR	CA-C-O	7.47	128.16	120.24
1	A	270	PHE	O-C-N	7.38	131.94	123.31
1	A	325	GLY	CA-C-N	7.36	130.45	120.44
1	A	325	GLY	C-N-CA	7.36	130.45	120.44
1	A	300	MET	N-CA-C	7.36	121.50	112.23
1	A	297	ASN	N-CA-C	-7.34	101.61	108.22
1	A	54	ARG	CA-C-O	-7.34	113.05	120.90
1	A	136	PRO	CB-CA-C	-7.33	101.38	110.98
1	A	101	VAL	N-CA-CB	7.32	123.44	111.58
1	A	21	THR	CA-CB-OG1	-7.31	98.64	109.60
1	A	363	THR	N-CA-C	7.26	120.11	111.33
1	A	11	MET	CA-C-O	-7.17	112.09	120.62
1	A	117	ASN	CA-CB-CG	7.16	119.76	112.60
1	A	77	ALA	CA-C-N	7.14	129.84	120.28
1	A	77	ALA	C-N-CA	7.14	129.84	120.28
1	A	279	GLU	CA-C-O	7.08	127.93	120.42
1	A	53	VAL	N-CA-C	-6.99	103.96	110.53
1	A	348	HIS	CA-CB-CG	-6.92	106.88	113.80
1	A	298	PRO	N-CA-C	6.92	119.14	110.70
1	A	387	ILE	CA-C-O	-6.84	113.34	121.28
1	A	136	PRO	CA-C-O	-6.79	113.39	121.67
1	A	22	GLU	CA-CB-CG	6.76	127.62	114.10
1	A	47	PRO	CA-C-O	-6.75	113.73	121.36
1	A	396	ASN	CB-CA-C	6.75	121.77	110.44
1	A	359	MET	N-CA-C	6.63	121.21	113.18
1	A	103	VAL	N-CA-CB	-6.55	100.69	111.44
1	A	122	PHE	CA-CB-CG	-6.51	107.29	113.80
1	A	201	ARG	CA-C-O	-6.48	114.17	121.81
1	A	108	GLY	O-C-N	6.46	128.38	122.18
1	A	203	GLU	CA-C-N	6.43	129.22	120.54
1	A	203	GLU	C-N-CA	6.43	129.22	120.54
1	A	258	HIS	CA-CB-CG	-6.41	107.39	113.80
1	A	165	THR	CA-C-N	6.37	131.41	122.36
1	A	165	THR	C-N-CA	6.37	131.41	122.36
1	A	201	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	A	312	THR	CA-C-O	6.27	125.45	119.99
1	A	372	ARG	O-C-N	6.27	128.53	122.07
1	A	26	ARG	N-CA-C	6.26	120.17	112.54
1	A	154	GLN	O-C-N	6.26	130.30	123.10
1	A	158	TYR	CA-CB-CG	6.25	125.16	113.90
1	A	353	ILE	O-C-N	6.24	127.92	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	GLY	O-C-N	6.24	128.06	122.88
1	A	104	GLN	CA-C-O	-6.22	114.34	121.19
1	A	177	ILE	N-CA-C	6.17	116.92	110.62
1	A	409	THR	OG1-CB-CG2	6.17	121.64	109.30
1	A	276	ASP	CA-C-O	-6.14	114.58	121.40
1	A	301	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	A	384	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	397	VAL	N-CA-C	-6.07	104.59	110.72
1	A	244	ILE	CA-C-N	6.06	129.01	120.28
1	A	244	ILE	C-N-CA	6.06	129.01	120.28
1	A	371	GLU	CA-CB-CG	6.01	126.12	114.10
1	A	408	VAL	N-CA-CB	-5.96	97.16	111.23
1	A	188	LEU	O-C-N	5.96	130.54	123.27
1	A	204	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	A	99	ARG	CB-CA-C	-5.91	100.26	110.72
1	A	112	LEU	CA-C-O	5.91	127.02	120.82
1	A	157	ALA	O-C-N	5.91	130.12	123.27
1	A	288	LYS	O-C-N	5.88	128.13	122.07
1	A	87	ALA	CA-C-N	5.88	128.64	120.29
1	A	87	ALA	C-N-CA	5.88	128.64	120.29
1	A	162	ASP	CA-C-O	5.86	125.83	120.09
1	A	363	THR	CA-C-O	-5.85	114.31	120.63
1	A	354	THR	O-C-N	5.84	130.71	122.41
1	A	11	MET	O-C-N	5.84	130.65	122.77
1	A	233	ILE	CA-C-O	-5.83	114.67	120.85
1	A	408	VAL	CA-C-N	5.81	132.71	122.42
1	A	408	VAL	C-N-CA	5.81	132.71	122.42
1	A	209	ALA	CA-C-N	5.80	128.85	120.79
1	A	209	ALA	C-N-CA	5.80	128.85	120.79
1	A	210	SER	O-C-N	5.79	128.27	122.08
1	A	120	GLN	O-C-N	5.78	128.10	122.09
1	A	370	VAL	CA-C-N	5.78	128.34	120.54
1	A	370	VAL	C-N-CA	5.78	128.34	120.54
1	A	232	ASP	CA-C-O	-5.76	114.14	120.30
1	A	59	MET	N-CA-C	-5.75	104.91	111.07
1	A	228	PHE	O-C-N	5.75	129.53	122.34
1	A	284	GLU	N-CA-C	-5.74	104.93	111.07
1	A	164	LYS	O-C-N	5.72	127.96	122.07
1	A	213	LYS	CB-CA-C	5.71	119.75	110.96
1	A	389	VAL	CA-C-O	5.71	126.48	119.58
1	A	312	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	216	ASN	N-CA-CB	-5.61	102.88	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	SER	CA-C-N	5.61	127.73	120.44
1	A	307	SER	C-N-CA	5.61	127.73	120.44
1	A	403	ALA	CA-C-O	5.60	126.47	120.70
1	A	15	ASP	CA-C-O	5.59	124.41	119.71
1	A	400	LEU	CA-C-O	5.58	126.87	120.90
1	A	370	VAL	O-C-N	5.56	127.36	121.91
1	A	404	ILE	N-CA-CB	5.54	116.65	110.51
1	A	323	VAL	O-C-N	5.52	127.52	121.83
1	A	28	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	176	ASP	CA-C-O	-5.51	115.01	121.07
1	A	168	LEU	N-CA-CB	-5.48	101.28	109.71
1	A	345	GLY	O-C-N	5.45	128.65	122.55
1	A	244	ILE	O-C-N	5.43	127.23	121.91
1	A	149	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	252	LEU	CA-C-N	-5.41	115.36	122.99
1	A	252	LEU	C-N-CA	-5.41	115.36	122.99
1	A	353	ILE	CA-C-O	-5.41	115.32	120.95
1	A	61	ALA	CB-CA-C	5.38	119.25	110.96
1	A	293	PRO	CA-C-N	5.38	130.76	122.42
1	A	293	PRO	C-N-CA	5.38	130.76	122.42
1	A	226	GLN	CA-C-N	5.37	131.10	122.40
1	A	226	GLN	C-N-CA	5.37	131.10	122.40
1	A	51	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	A	284	GLU	CB-CA-C	5.36	119.30	110.88
1	A	182	GLU	CA-C-O	5.33	127.06	121.19
1	A	292	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	27	ASP	CB-CA-C	5.33	119.16	109.62
1	A	70	TYR	CA-C-O	-5.29	115.38	121.19
1	A	165	THR	N-CA-CB	-5.25	102.41	110.44
1	A	180	ILE	O-C-N	5.25	126.52	120.69
1	A	349	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	112	LEU	N-CA-CB	-5.21	102.46	110.01
1	A	181	PRO	CA-C-O	5.20	127.24	121.36
1	A	21	THR	CA-C-O	-5.19	114.92	120.42
1	A	77	ALA	CA-C-O	5.19	126.73	120.92
1	A	195	PRO	N-CA-C	5.18	125.58	112.10
1	A	317	LYS	O-C-N	5.18	127.61	122.12
1	A	389	VAL	N-CA-C	-5.18	105.30	112.50
1	A	148	ARG	CA-C-O	-5.18	115.38	120.82
1	A	336	GLN	O-C-N	5.18	127.61	122.12
1	A	366	LYS	CA-CB-CG	5.17	124.44	114.10
1	A	54	ARG	N-CA-CB	5.17	117.64	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	CA-C-O	5.16	126.06	120.43
1	A	307	SER	O-C-N	-5.16	116.76	122.07
1	A	360	PHE	CA-C-O	5.15	127.83	121.60
1	A	286	GLN	OE1-CD-NE2	5.15	127.75	122.60
1	A	359	MET	CA-CB-CG	-5.15	103.81	114.10
1	A	145	PRO	CA-C-N	-5.13	114.09	120.56
1	A	145	PRO	C-N-CA	-5.13	114.09	120.56
1	A	212	VAL	N-CA-CB	-5.13	104.01	110.57
1	A	44	ASN	N-CA-C	-5.11	107.10	113.38
1	A	176	ASP	O-C-N	5.10	127.54	122.08
1	A	88	LEU	N-CA-C	5.09	116.91	111.36
1	A	238	TRP	N-CA-C	5.09	117.23	111.02
1	A	184	SER	N-CA-C	-5.09	103.33	110.35
1	A	280	ALA	O-C-N	5.09	127.51	122.12
1	A	100	TYR	O-C-N	5.07	129.75	123.15
1	A	315	LEU	N-CA-C	-5.07	105.67	111.14
1	A	90	GLU	CA-CB-CG	5.07	124.24	114.10
1	A	245	GLU	CG-CD-OE2	-5.06	106.77	118.40
1	A	99	ARG	CA-CB-CG	5.04	124.18	114.10
1	A	397	VAL	CB-CA-C	5.03	119.17	112.22
1	A	231	GLY	N-CA-C	-5.03	108.30	115.64
1	A	80	THR	CB-CA-C	5.01	118.82	110.90
1	A	22	GLU	CB-CG-CD	5.01	121.11	112.60
1	A	354	THR	CA-CB-OG1	-5.00	102.10	109.60

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	3162	0	3148	119	1
2	A	25	0	15	1	0
3	A	311	0	0	23	1
All	All	3498	0	3163	120	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 19.

All (120) 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:161:TYR:N	3:A:607:HOH:O	2.09	0.85
1:A:142:ASN:O	1:A:146:ILE:HG13	1.77	0.83
1:A:278:GLU:HG3	3:A:601:HOH:O	1.82	0.79
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.64	0.78
1:A:373:LEU:HD23	1:A:381:MET:HE1	1.68	0.76
1:A:366:LYS:H	1:A:369:GLN:HE21	1.37	0.72
1:A:373:LEU:HD22	1:A:408:VAL:HG11	1.71	0.72
1:A:366:LYS:H	1:A:369:GLN:NE2	1.89	0.69
1:A:404:ILE:O	1:A:409:THR:HB	1.92	0.68
1:A:316:ARG:NH2	3:A:584:HOH:O	2.25	0.68
1:A:182:GLU:O	1:A:183:LYS:HB2	1.94	0.67
1:A:234:ASN:HD22	1:A:241:ARG:HH12	1.43	0.66
1:A:165:THR:HG23	1:A:167:SER:OG	1.96	0.65
1:A:370:VAL:HA	1:A:381:MET:HE3	1.80	0.63
1:A:201:ARG:O	1:A:204:GLN:HB2	2.00	0.62
1:A:370:VAL:HG22	1:A:381:MET:HE3	1.83	0.60
1:A:349:ASN:OD1	1:A:351:GLN:HB3	2.03	0.59
1:A:319:TRP:O	1:A:323:VAL:HG23	2.03	0.58
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.85	0.58
1:A:260:MET:HE2	1:A:309:ILE:HG21	1.85	0.57
1:A:101:VAL:HG21	1:A:284:GLU:HB2	1.86	0.56
1:A:45:GLY:HA2	3:A:657:HOH:O	2.06	0.56
1:A:99:ARG:HB3	1:A:274:CYS:O	2.05	0.56
1:A:309:ILE:HA	1:A:315:LEU:HB3	1.88	0.56
1:A:366:LYS:HB3	1:A:367:PRO:CD	2.35	0.56
1:A:42:ASP:HB3	1:A:48:TYR:HB2	1.88	0.55
1:A:338:VAL:HG21	1:A:354:THR:HG23	1.88	0.55
1:A:370:VAL:HA	1:A:381:MET:CE	2.36	0.55
1:A:162:ASP:HB3	1:A:165:THR:HG22	1.89	0.55
1:A:34:ASN:ND2	1:A:36:GLY:H	2.05	0.55
1:A:279:GLU:HG3	1:A:282:ARG:NH2	2.22	0.54
1:A:343:LYS:NZ	3:A:510:HOH:O	2.35	0.53
1:A:55:LYS:O	1:A:59:MET:HG3	2.09	0.53
1:A:277:ALA:HB1	3:A:514:HOH:O	2.08	0.53
1:A:304:ARG:HD3	3:A:464:HOH:O	2.08	0.52
1:A:324:LYS:HD3	3:A:647:HOH:O	2.08	0.52
1:A:330:ILE:HG23	1:A:389:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HG12	1:A:361:CYS:SG	2.50	0.52
1:A:101:VAL:O	1:A:271:THR:HA	2.10	0.52
1:A:244:ILE:HA	1:A:248:ILE:O	2.10	0.51
1:A:121:ARG:NE	3:A:663:HOH:O	2.43	0.51
1:A:334:ARG:O	1:A:338:VAL:HG23	2.11	0.50
1:A:373:LEU:HD23	1:A:381:MET:CE	2.39	0.50
1:A:219:ALA:HB3	1:A:250:VAL:HG12	1.92	0.50
1:A:165:THR:HG21	3:A:438:HOH:O	2.11	0.50
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.94	0.50
1:A:125:PHE:HB3	1:A:183:LYS:HB3	1.93	0.50
1:A:104:GLN:NE2	1:A:303:ALA:HB2	2.27	0.49
1:A:232:ASP:HB3	1:A:235:ARG:HB3	1.93	0.49
1:A:34:ASN:C	1:A:34:ASN:HD22	2.18	0.49
1:A:144:THR:N	1:A:145:PRO:HD2	2.27	0.49
1:A:160:TYR:N	3:A:607:HOH:O	2.30	0.49
1:A:290:LEU:HD21	3:A:663:HOH:O	2.13	0.49
1:A:24:PHE:CE1	1:A:32:LYS:HG3	2.48	0.48
1:A:75:GLY:HA3	1:A:104:GLN:HB2	1.95	0.48
1:A:201:ARG:HD2	1:A:203:GLU:OE1	2.14	0.48
1:A:394:SER:HB3	3:A:541:HOH:O	2.14	0.48
1:A:312:THR:HB	1:A:315:LEU:HB2	1.96	0.48
1:A:144:THR:HB	1:A:145:PRO:HD3	1.95	0.48
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.78	0.47
1:A:300:MET:O	1:A:304:ARG:HG3	2.14	0.47
1:A:366:LYS:HB3	1:A:367:PRO:HD2	1.96	0.47
1:A:89:GLY:HA3	3:A:673:HOH:O	2.13	0.47
1:A:381:MET:SD	1:A:387:ILE:HG22	2.54	0.47
1:A:312:THR:HA	1:A:313:PRO:HD2	1.68	0.47
1:A:314:GLU:HA	1:A:317:LYS:HG2	1.96	0.47
1:A:230:SER:OG	1:A:235:ARG:HG2	2.15	0.46
1:A:229:ALA:HB3	1:A:236:ASP:OD1	2.15	0.46
1:A:317:LYS:HG3	1:A:318:GLU:N	2.30	0.46
1:A:51:ASN:O	1:A:55:LYS:HG3	2.16	0.46
1:A:144:THR:HB	1:A:145:PRO:CD	2.46	0.46
1:A:351:GLN:HE21	1:A:351:GLN:HB2	1.51	0.46
1:A:59:MET:O	1:A:63:LYS:HG3	2.16	0.46
1:A:90:GLU:HG3	3:A:569:HOH:O	2.16	0.46
1:A:57:GLU:HA	1:A:60:ILE:HD12	1.99	0.45
1:A:121:ARG:HB2	3:A:663:HOH:O	2.16	0.45
1:A:225:TYR:HB3	1:A:228:PHE:HB2	1.99	0.45
1:A:332:SER:O	1:A:336:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:O	1:A:263:TYR:C	2.60	0.45
1:A:34:ASN:ND2	1:A:34:ASN:C	2.76	0.44
1:A:171:THR:O	1:A:175:GLU:HG3	2.17	0.44
1:A:193:HIS:CE1	1:A:196:THR:HG23	2.53	0.44
2:A:411:PPE:O3	2:A:411:PPE:NA	2.51	0.44
1:A:91:ASN:ND2	3:A:673:HOH:O	2.51	0.43
1:A:290:LEU:O	1:A:294:MET:HE3	2.17	0.43
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.85	0.43
1:A:77:ALA:O	1:A:80:THR:HG22	2.18	0.43
1:A:340:ASN:HD22	1:A:343:LYS:CE	2.30	0.43
1:A:161:TYR:CE1	1:A:196:THR:HB	2.54	0.43
1:A:279:GLU:O	1:A:280:ALA:C	2.61	0.43
1:A:277:ALA:O	1:A:281:LYS:HG3	2.19	0.42
1:A:33:MET:HE2	1:A:35:LEU:HD21	2.00	0.42
1:A:96:LYS:HD3	3:A:554:HOH:O	2.18	0.42
1:A:168:LEU:CD2	1:A:200:PRO:HA	2.49	0.42
1:A:332:SER:O	1:A:335:THR:HB	2.20	0.42
1:A:353:ILE:HA	1:A:361:CYS:SG	2.59	0.42
1:A:118:PHE:CZ	1:A:283:VAL:HG13	2.54	0.42
1:A:85:GLU:HG3	1:A:95:PHE:CZ	2.54	0.42
1:A:216:ASN:HD22	1:A:216:ASN:HA	1.68	0.42
1:A:260:MET:HE2	1:A:309:ILE:CG2	2.50	0.42
1:A:393:ALA:HB2	3:A:657:HOH:O	2.18	0.42
1:A:112:LEU:HA	1:A:220:TYR:OH	2.19	0.42
1:A:120:GLN:HA	1:A:152:LEU:HD21	2.01	0.42
1:A:207:GLU:HG3	3:A:573:HOH:O	2.19	0.42
1:A:340:ASN:ND2	1:A:343:LYS:NZ	2.68	0.42
1:A:370:VAL:O	1:A:373:LEU:HB2	2.20	0.42
1:A:161:TYR:CD1	1:A:196:THR:HB	2.54	0.41
1:A:162:ASP:OD2	1:A:165:THR:HG22	2.20	0.41
1:A:162:ASP:HA	1:A:163:PRO:HD2	1.94	0.41
1:A:67:ASP:C	1:A:67:ASP:OD1	2.64	0.41
1:A:387:ILE:O	1:A:387:ILE:HG13	2.18	0.41
1:A:282:ARG:NE	3:A:601:HOH:O	2.51	0.41
1:A:340:ASN:HD22	1:A:343:LYS:NZ	2.19	0.41
1:A:215:ARG:HB2	1:A:217:LEU:HG	2.03	0.41
1:A:108:GLY:O	1:A:112:LEU:HB2	2.21	0.40
1:A:350:TRP:O	1:A:353:ILE:HB	2.20	0.40
1:A:20:VAL:CG1	1:A:380:TYR:HB3	2.52	0.40
1:A:246:GLN:NE2	3:A:637:HOH:O	2.53	0.40
1:A:350:TRP:HB2	3:A:545:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:THR:OG1	1:A:386:ARG:HB3	2.20	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:249:ASP:OD2	3:A:704:HOH:O[3_655]	1.98	0.22

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	399/401 (100%)	382 (96%)	15 (4%)	2 (0%)	24 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	A	313	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	335/335 (100%)	299 (89%)	36 (11%)	6 8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	SER
1	A	18	LEU
1	A	37	VAL
1	A	46	LYS
1	A	57	GLU
1	A	71	LEU
1	A	78	ASP
1	A	80	THR
1	A	88	LEU
1	A	96	LYS
1	A	101	VAL
1	A	103	VAL
1	A	107	SER
1	A	112	LEU
1	A	138	PRO
1	A	155	LEU
1	A	165	THR
1	A	179	LYS
1	A	187	LEU
1	A	195	PRO
1	A	210	SER
1	A	235	ARG
1	A	252	LEU
1	A	276	ASP
1	A	284	GLU
1	A	317	LYS
1	A	343	LYS
1	A	347	SER
1	A	351	GLN
1	A	368	GLU
1	A	373	LEU
1	A	375	LYS
1	A	395	SER
1	A	408	VAL
1	A	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN

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Mol	Chain	Res	Type
1	A	120	GLN
1	A	156	GLN
1	A	202	GLN
1	A	216	ASN
1	A	234	ASN
1	A	286	GLN
1	A	340	ASN
1	A	351	GLN
1	A	369	GLN
1	A	405	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	PPE	A	411	-	23,25,25	2.32	6 (26%)	24,35,35	2.64	12 (50%)

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	PPE	A	411	-	-	9/17/20/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PPE	C4A-NA	5.29	1.52	1.46
2	A	411	PPE	OP4-C5A	-5.04	1.38	1.43
2	A	411	PPE	OA-CA	4.95	1.36	1.22
2	A	411	PPE	C3-C4	-3.39	1.39	1.43
2	A	411	PPE	C3-C2	2.72	1.44	1.38
2	A	411	PPE	C5A-C5	2.68	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PPE	O3-C3-C2	-6.95	111.43	118.29
2	A	411	PPE	C2A-C2-C3	4.52	132.63	125.54
2	A	411	PPE	O3-C3-C4	3.64	125.10	116.93
2	A	411	PPE	OA-CA-CAA	-3.63	110.55	122.26
2	A	411	PPE	OXT-CA-CAA	3.28	124.62	113.51
2	A	411	PPE	C3-C2-N1	-3.12	118.45	122.58
2	A	411	PPE	OP2-P-OP1	2.73	121.48	110.83
2	A	411	PPE	OE2-CDA-OE1	2.73	130.35	123.33
2	A	411	PPE	C4-C4A-NA	-2.42	102.62	111.83
2	A	411	PPE	OP4-P-OP1	2.36	112.81	106.44
2	A	411	PPE	C2A-C2-N1	-2.36	108.92	112.46
2	A	411	PPE	OE1-CDA-CGA	-2.32	115.72	123.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PPE	C5A-OP4-P-OP2
2	A	411	PPE	CBA-CAA-NA-C4A
2	A	411	PPE	C4-C5-C5A-OP4
2	A	411	PPE	CA-CAA-NA-C4A
2	A	411	PPE	OA-CA-CAA-CBA
2	A	411	PPE	OXT-CA-CAA-CBA

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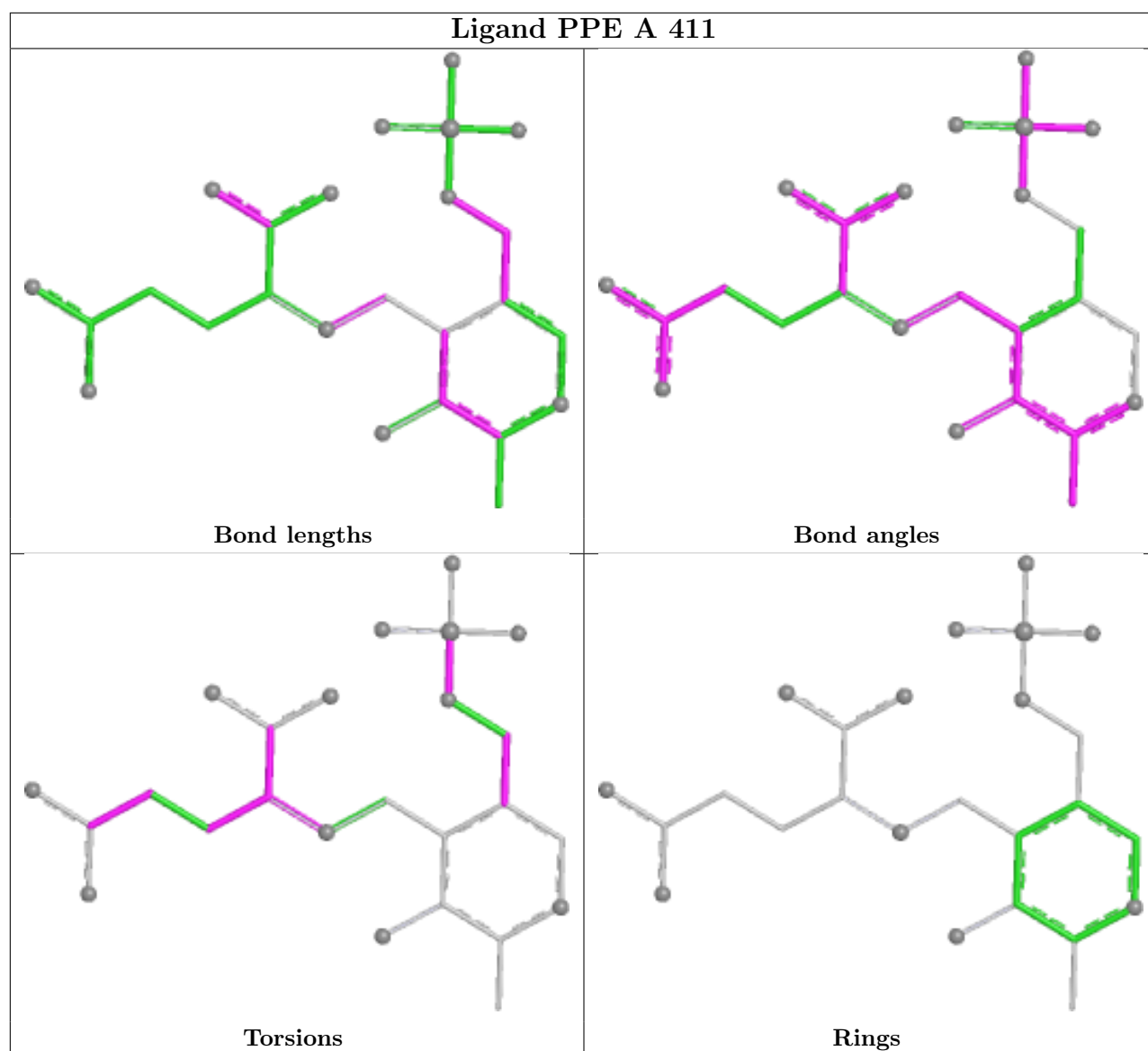
Mol	Chain	Res	Type	Atoms
2	A	411	PPE	CA-CAA-CBA-CGA
2	A	411	PPE	OE1-CDA-CGA-CBA
2	A	411	PPE	OE2-CDA-CGA-CBA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PPE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.