



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 10:24 AM EST

PDB ID : 1AKC  
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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

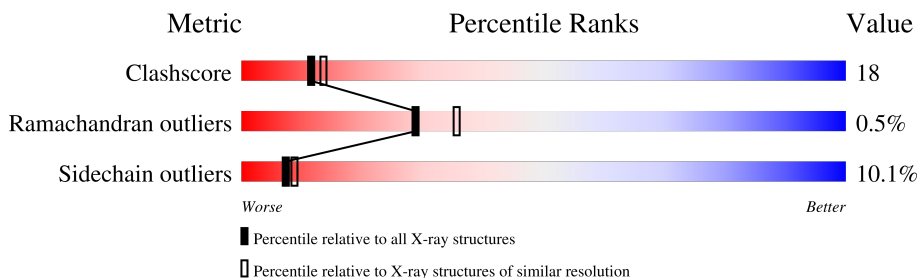
# 1 Overall quality at a glance i

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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  $\geq 3$ , 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.

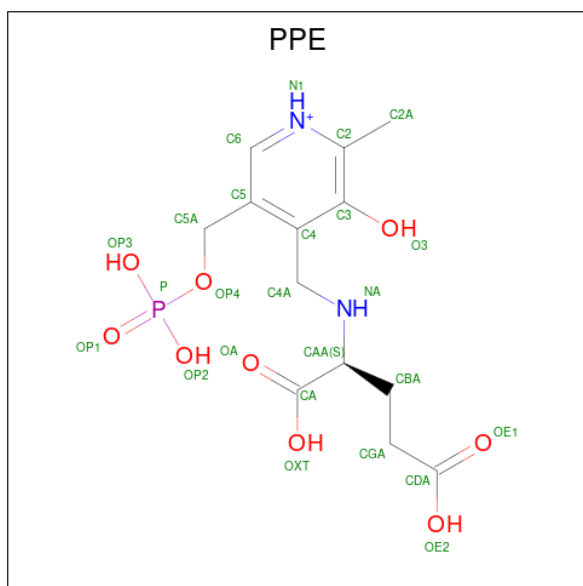
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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 (three-letter code: PPE) (formula: C<sub>13</sub>H<sub>20</sub>N<sub>2</sub>O<sub>9</sub>P).



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

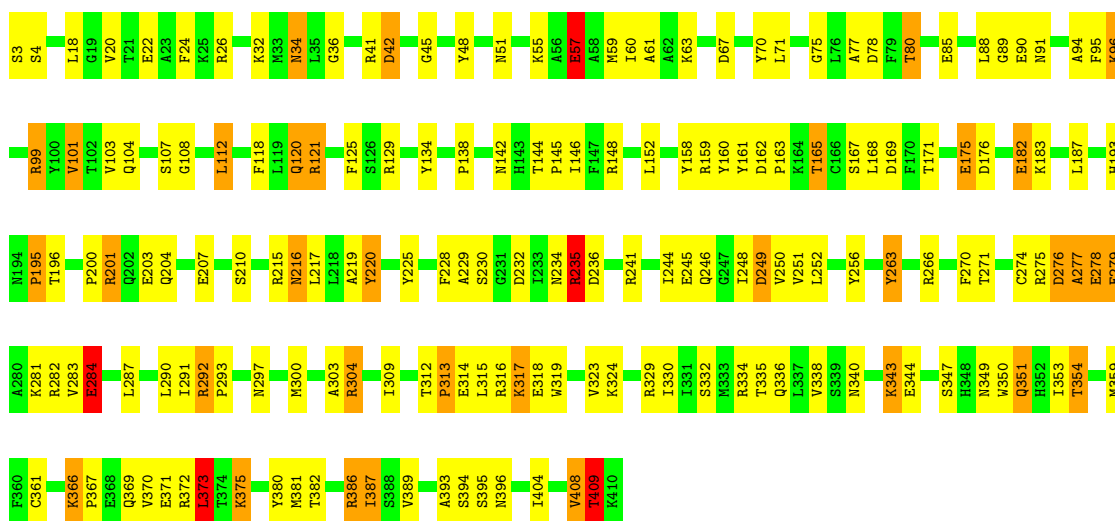
### 3 Residue-property plots

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

Chain A:  56% 34% 8%



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	41.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	0.84	1/3233 (0.0%)	1.80	55/4364 (1.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	LYS	CE-NZ	5.14	1.61	1.49

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ARG	NE-CZ-NH1	18.71	129.66	120.30
1	A	304	ARG	NE-CZ-NH2	-17.59	111.50	120.30
1	A	99	ARG	CD-NE-CZ	14.54	143.95	123.60
1	A	284	GLU	CA-CB-CG	11.64	139.02	113.40
1	A	201	ARG	NE-CZ-NH1	-10.21	115.19	120.30
1	A	148	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	A	175	GLU	OE1-CD-OE2	8.25	133.20	123.30
1	A	292	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	70	TYR	CA-CB-CG	7.36	127.39	113.40
1	A	176	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	41	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	276	ASP	CA-CB-CG	6.94	128.66	113.40
1	A	134	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	A	372	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	386	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	A	266	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	408	VAL	N-CA-CB	-6.52	97.16	111.50
1	A	22	GLU	CA-CB-CG	6.47	127.62	113.40
1	A	182	GLU	OE1-CD-OE2	6.46	131.05	123.30
1	A	297	ASN	CB-CA-C	6.41	123.22	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLU	OE1-CD-OE2	6.30	130.87	123.30
1	A	235	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	158	TYR	CA-CB-CG	6.19	125.16	113.40
1	A	61	ALA	CB-CA-C	6.10	119.25	110.10
1	A	121	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	387	ILE	O-C-N	5.97	132.25	122.70
1	A	291	ILE	O-C-N	5.88	132.12	122.70
1	A	159	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	371	GLU	CA-CB-CG	5.78	126.12	113.40
1	A	270	PHE	O-C-N	5.78	131.94	122.70
1	A	245	GLU	CG-CD-OE2	-5.77	106.77	118.30
1	A	70	TYR	CB-CG-CD1	5.74	124.44	121.00
1	A	278	GLU	CB-CG-CD	5.71	129.62	114.20
1	A	396	ASN	CB-CA-C	5.69	121.77	110.40
1	A	249	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	26	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	359	MET	CA-CB-CG	-5.58	103.81	113.30
1	A	329	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	A	386	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	251	VAL	N-CA-C	-5.47	96.22	111.00
1	A	129	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	277	ALA	N-CA-CB	5.45	117.73	110.10
1	A	344	GLU	CG-CD-OE2	5.44	129.18	118.30
1	A	101	VAL	N-CA-CB	5.42	123.44	111.50
1	A	256	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	373	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	57	GLU	CG-CD-OE1	-5.25	107.80	118.30
1	A	263	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	A	195	PRO	N-CA-C	5.18	125.58	112.10
1	A	67	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	42	ASP	CB-CA-C	5.11	120.63	110.40
1	A	99	ARG	CB-CA-C	-5.07	100.26	110.40
1	A	409	THR	OG1-CB-CG2	5.06	121.64	110.00
1	A	366	LYS	CA-CB-CG	5.02	124.44	113.40
1	A	354	THR	O-C-N	5.00	130.71	122.70

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	111	1
2	A	25	0	15	1	0
3	A	311	0	0	23	1
All	All	3498	0	3163	112	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 18.

All (112) 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: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:201:ARG:O	1:A:204:GLN:HB2	2.00	0.62
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:370:VAL:HA	1:A:381:MET:HE3	1.86	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:373:LEU:HD23	1:A:381:MET:CE	2.39	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
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: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: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:370:VAL:HG13	1:A:381:MET:HE3	1.94	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:317:LYS:HG3	1:A:318:GLU:N	2.30	0.47
1:A:230:SER:OG	1:A:235:ARG:HG2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ALA:HB3	1:A:236:ASP:OD1	2.15	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:373:LEU:HD23	1:A:381:MET:HE2	1.98	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
1:A:34:ASN:C	1:A:34:ASN:HD22	2.18	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: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:277:ALA:O	1:A:281:LYS:HG3	2.19	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: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: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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	29 35

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%)	301 (90%)	34 (10%)	<b>7</b> <b>9</b>

All (34) 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	34	ASN
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	103	VAL
1	A	107	SER
1	A	112	LEU
1	A	120	GLN
1	A	138	PRO
1	A	165	THR
1	A	187	LEU
1	A	195	PRO
1	A	210	SER
1	A	216	ASN
1	A	220	TYR
1	A	235	ARG
1	A	252	LEU
1	A	275	ARG
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	373	LEU
1	A	375	LYS
1	A	395	SER
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
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 [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 monosaccharides 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	PPE	A	411	-	25,25,25	1.64	2 (8%)	31,35,35	3.99	18 (58%)

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	-	-	12/20/20/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PPE	OA-CA	4.79	1.36	1.22
2	A	411	PPE	C3-C2	4.04	1.44	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PPE	C6-C5-C4	11.65	126.36	118.12
2	A	411	PPE	C2A-C2-C3	9.51	132.63	120.89
2	A	411	PPE	C3-C4-C5	-7.25	111.76	118.72
2	A	411	PPE	C4A-C4-C5	6.01	126.39	119.71
2	A	411	PPE	C5A-C5-C6	-5.03	111.10	119.37
2	A	411	PPE	OP4-C5A-C5	4.70	118.31	109.35
2	A	411	PPE	C2A-C2-N1	-4.48	108.92	117.67
2	A	411	PPE	OA-CA-CAA	-3.56	110.55	122.26
2	A	411	PPE	OXT-CA-CAA	3.37	124.62	113.40
2	A	411	PPE	C4-C4A-NA	-3.32	102.62	111.78
2	A	411	PPE	C5-C6-N1	-3.26	118.39	123.82
2	A	411	PPE	OE2-CDA-OE1	2.83	130.35	123.30
2	A	411	PPE	O3-C3-C2	-2.78	111.43	117.49
2	A	411	PPE	OP2-P-OP1	2.76	121.48	110.68
2	A	411	PPE	O3-C3-C4	2.37	125.10	118.13
2	A	411	PPE	OE1-CDA-CGA	-2.29	115.72	123.08
2	A	411	PPE	OP4-P-OP1	2.26	112.81	106.47
2	A	411	PPE	C4-C3-C2	2.21	123.45	120.06

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PPE	C4-C5-C5A-OP4
2	A	411	PPE	C6-C5-C5A-OP4
2	A	411	PPE	C5A-OP4-P-OP2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	411	PPE	C5-C4-C4A-NA
2	A	411	PPE	CA-CAA-NA-C4A
2	A	411	PPE	C3-C4-C4A-NA
2	A	411	PPE	OA-CA-CAA-CBA
2	A	411	PPE	CBA-CAA-NA-C4A
2	A	411	PPE	OXT-CA-CAA-CBA
2	A	411	PPE	CA-CAA-CBA-CGA
2	A	411	PPE	OE1-CDA-CGA-CBA
2	A	411	PPE	OE2-CDA-CGA-CBA

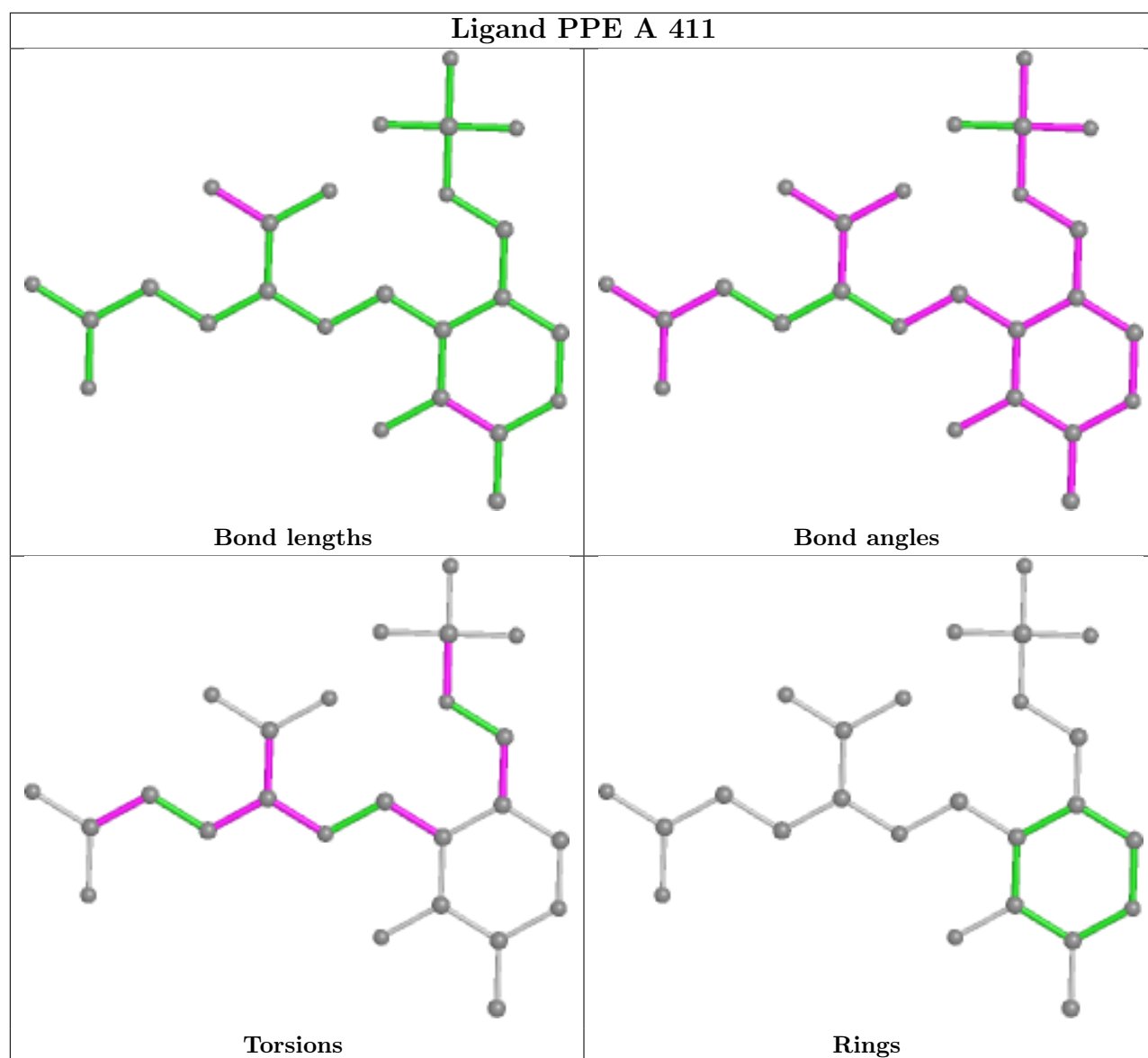
There are no ring outliers.

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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.