



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:42 pm BST

PDB ID : 1OXO
Title : ASPARTATE AMINOTRANSFERASE, H-ASP COMPLEX, OPEN CON-
FORMATION
Authors : Hohenester, E.; Schirmer, T.; Jansonius, J.N.
Deposited on : 1995-12-23
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 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)
Xtriage (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) : 2.11

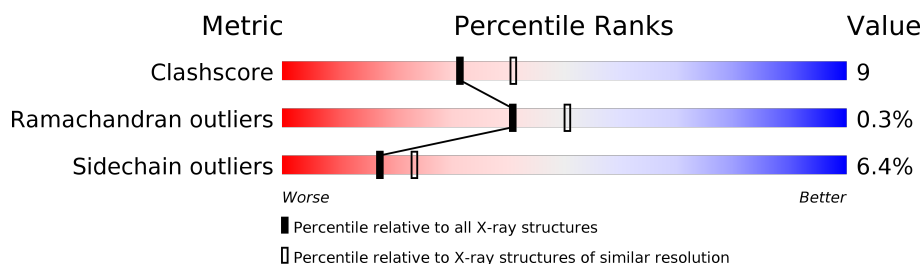
1 Overall quality at a glance

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	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 on 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	
1	B	401	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6905 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.

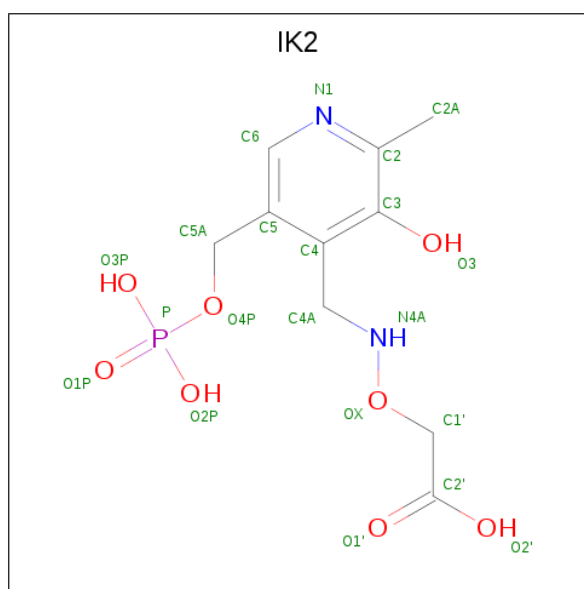
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	16	0	0
			3161	2004	558	581	18			
1	B	401	Total	C	N	O	S	32	0	0
			3161	2004	558	581	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	CONFLICT	UNP P00508
B	47	PRO	SER	CONFLICT	UNP P00508

- Molecule 2 is 4'-DEOXY-4'-ACETYLYAMINO-PYRIDOXAL-5'-PHOSPHATE (three-letter code: IK2) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 3 is water.

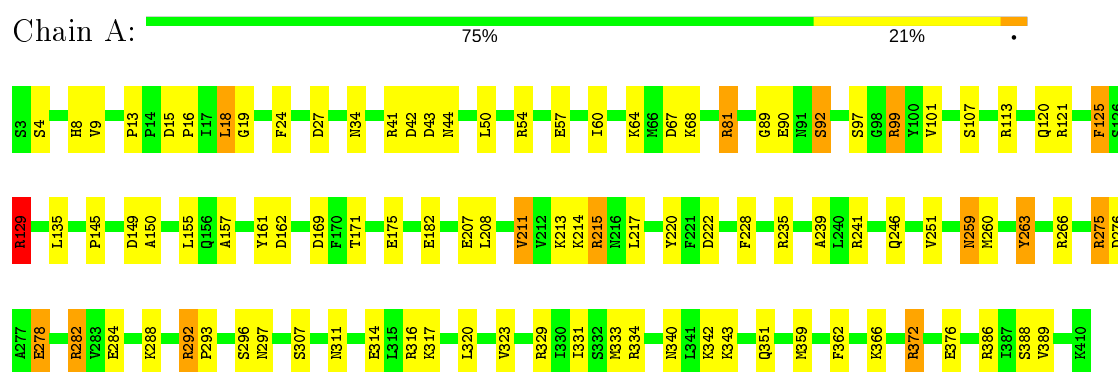
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	275	Total	O	0	0
			275	275		
3	B	266	Total	O	0	0
			266	266		

3 Residue-property plots [i](#)

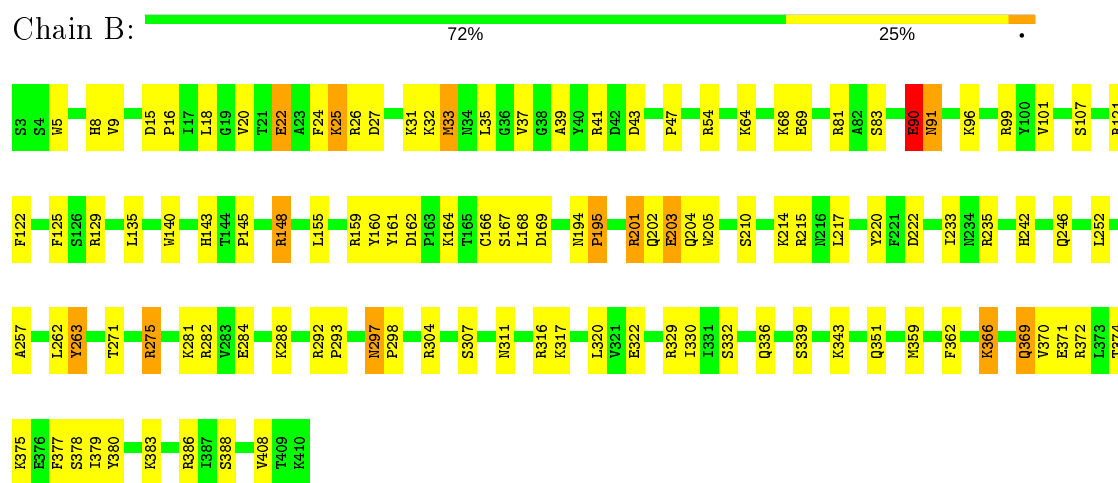
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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



• 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	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.70Å 58.80Å 76.00Å 85.20° 109.20° 115.70°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6905	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: IK2

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	0.85	3/3231 (0.1%)	1.50	36/4360 (0.8%)
1	B	1.10	6/3231 (0.2%)	1.53	39/4360 (0.9%)
All	All	0.98	9/6462 (0.1%)	1.52	75/8720 (0.9%)

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	B	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	ARG	CD-NE	-25.93	1.02	1.46
1	B	203	GLU	CG-CD	-24.75	1.14	1.51
1	A	275	ARG	CD-NE	-21.42	1.10	1.46
1	B	235	ARG	CD-NE	-19.42	1.13	1.46
1	B	22	GLU	CG-CD	-13.78	1.31	1.51
1	B	371	GLU	CG-CD	-13.45	1.31	1.51
1	B	25	LYS	CD-CE	-10.54	1.25	1.51
1	A	317	LYS	CG-CD	-8.79	1.22	1.52
1	A	351	GLN	CG-CD	-5.92	1.37	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ARG	CG-CD-NE	16.27	145.96	111.80
1	B	275	ARG	CD-NE-CZ	-16.10	101.06	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	GLU	CG-CD-OE2	-14.44	89.42	118.30
1	A	282	ARG	NE-CZ-NH1	13.96	127.28	120.30
1	B	22	GLU	CG-CD-OE1	13.26	144.82	118.30
1	B	26	ARG	NE-CZ-NH1	12.86	126.73	120.30
1	B	121	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	B	121	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	275	ARG	CD-NE-CZ	-10.86	108.40	123.60
1	A	41	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	42	ASP	CB-CG-OD2	-10.46	108.88	118.30
1	A	54	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	B	41	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	203	GLU	CB-CG-CD	9.31	139.34	114.20
1	A	113	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	386	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	235	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	A	317	LYS	CB-CG-CD	8.19	132.90	111.60
1	A	316	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	41	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	282	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	B	235	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	A	278	GLU	OE1-CD-OE2	-7.98	113.72	123.30
1	A	278	GLU	CG-CD-OE1	7.70	133.71	118.30
1	A	278	GLU	CB-CG-CD	7.66	134.87	114.20
1	B	41	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	26	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	159	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	235	ARG	CD-NE-CZ	-7.03	113.76	123.60
1	A	275	ARG	CG-CD-NE	7.02	126.53	111.80
1	B	54	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	22	GLU	CB-CG-CD	6.95	132.95	114.20
1	A	251	VAL	CB-CA-C	6.93	124.56	111.40
1	B	372	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	B	292	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	99	ARG	CD-NE-CZ	6.83	133.16	123.60
1	B	159	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	27	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	372	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	143	HIS	N-CA-CB	6.48	122.27	110.60
1	A	149	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	B	33	MET	CA-CB-CG	6.44	124.25	113.30
1	A	266	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	129	ARG	NE-CZ-NH2	-6.13	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	VAL	CB-CA-C	6.05	122.90	111.40
1	B	317	LYS	CD-CE-NZ	-6.04	97.80	111.70
1	B	359	MET	CB-CA-C	5.92	122.24	110.40
1	B	90	GLU	CA-CB-CG	5.83	126.22	113.40
1	A	241	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	33	MET	CB-CA-C	5.77	121.94	110.40
1	B	316	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	43	ASP	CB-CA-C	5.64	121.67	110.40
1	A	182	GLU	CA-CB-CG	5.63	125.80	113.40
1	B	25	LYS	CG-CD-CE	5.59	128.66	111.90
1	B	275	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	210	SER	CB-CA-C	5.58	120.70	110.10
1	B	69	GLU	CG-CD-OE2	5.58	129.46	118.30
1	B	195	PRO	N-CA-C	5.49	126.37	112.10
1	B	148	ARG	CB-CA-C	5.47	121.35	110.40
1	B	252	LEU	N-CA-CB	-5.39	99.62	110.40
1	A	129	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	A	297	ASN	CB-CA-C	5.35	121.10	110.40
1	B	297	ASN	CB-CA-C	5.34	121.08	110.40
1	B	322	GLU	CG-CD-OE2	5.32	128.94	118.30
1	A	239	ALA	CB-CA-C	5.28	118.03	110.10
1	B	205	TRP	CA-CB-CG	5.28	123.73	113.70
1	A	388	SER	N-CA-CB	5.26	118.39	110.50
1	A	161	TYR	CB-CG-CD2	5.24	124.14	121.00
1	A	334	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	388	SER	N-CA-CB	5.22	118.33	110.50
1	A	208	LEU	CB-CG-CD1	-5.16	102.22	111.00
1	A	161	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	A	386	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	67	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	67	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	201	ARG	Sidechain
1	B	304	ARG	Sidechain

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	3161	0	3154	56	0
1	B	3161	0	3154	60	0
2	A	21	0	11	3	0
2	B	21	0	11	4	0
3	A	275	0	0	17	0
3	B	266	0	0	13	0
All	All	6905	0	6330	113	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 9.

All (113) 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:B:90:GLU:O	1:B:96:LYS:HE2	1.48	1.13
1:B:201:ARG:H	1:B:204:GLN:HE21	1.15	0.94
1:B:64:LYS:NZ	3:B:617:HOH:O	2.08	0.81
1:B:135:LEU:HD11	1:B:155:LEU:CD2	2.14	0.76
1:A:333:MET:HE3	3:A:643:HOH:O	1.87	0.74
1:B:101:VAL:HG21	1:B:284:GLU:HB2	1.70	0.73
1:B:203:GLU:HB3	3:B:652:HOH:O	1.88	0.73
1:B:90:GLU:O	1:B:96:LYS:CE	2.33	0.73
1:B:135:LEU:HD11	1:B:155:LEU:HD23	1.72	0.72
1:A:68:LYS:O	1:B:263:TYR:HB2	1.90	0.72
1:A:129:ARG:HA	1:A:129:ARG:HE	1.54	0.71
1:A:60:ILE:O	3:A:535:HOH:O	2.08	0.71
1:A:263:TYR:HB2	1:B:68:LYS:O	1.91	0.71
1:A:57:GLU:OE2	3:A:503:HOH:O	2.10	0.70
1:A:57:GLU:HB3	3:A:592:HOH:O	1.90	0.70
1:A:175:GLU:OE1	3:A:668:HOH:O	2.11	0.68
1:A:372:ARG:HG2	1:A:376:GLU:OE2	1.95	0.66
1:A:18:LEU:HD23	1:A:19:GLY:N	2.10	0.66
1:B:15:ASP:OD2	1:B:18:LEU:HB2	1.95	0.66
1:B:135:LEU:CD1	1:B:155:LEU:HD23	2.29	0.62
1:A:24:PHE:CE2	1:A:34:ASN:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.82	0.62
1:A:282:ARG:CZ	3:A:516:HOH:O	2.48	0.62
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.81	0.62
1:A:307:SER:O	1:A:311:ASN:HB2	2.01	0.61
1:A:9:VAL:O	1:B:282:ARG:HD2	2.00	0.60
1:A:276:ASP:OD1	1:A:278:GLU:HB3	2.03	0.58
1:B:369:GLN:HB3	1:B:408:VAL:HG12	1.86	0.58
1:A:129:ARG:CA	1:A:129:ARG:HE	2.12	0.57
1:A:207:GLU:O	1:A:211:VAL:HG12	2.04	0.57
1:A:81:ARG:HD3	3:A:632:HOH:O	2.05	0.56
1:A:97:SER:OG	1:A:99:ARG:HD3	2.06	0.56
1:B:369:GLN:HB3	1:B:408:VAL:CG1	2.36	0.56
1:A:4:SER:HA	3:B:577:HOH:O	2.06	0.56
1:B:201:ARG:H	1:B:204:GLN:NE2	1.96	0.55
1:A:8:HIS:CD2	1:A:8:HIS:H	2.23	0.55
1:A:282:ARG:HD2	1:B:9:VAL:O	2.07	0.54
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.38	0.53
1:B:160:TYR:O	1:B:168:LEU:HD12	2.08	0.53
1:B:91:ASN:HA	1:B:96:LYS:HE3	1.91	0.52
1:B:215:ARG:HB2	1:B:217:LEU:HG	1.91	0.52
1:B:167:SER:HB2	3:B:491:HOH:O	2.09	0.52
1:B:332:SER:O	1:B:336:GLN:HG3	2.10	0.52
1:A:259:ASN:HD22	1:A:260:MET:N	2.08	0.51
1:A:120:GLN:HG3	1:A:150:ALA:O	2.11	0.51
1:A:329:ARG:O	1:A:333:MET:HG2	2.10	0.51
1:B:257:ALA:HB3	3:B:602:HOH:O	2.09	0.51
1:A:121:ARG:HG3	3:A:466:HOH:O	2.09	0.51
1:A:24:PHE:CD2	1:A:34:ASN:HB2	2.46	0.50
2:A:411:IK2:H4A2	3:A:610:HOH:O	2.10	0.50
1:B:242:HIS:O	1:B:246:GLN:HG2	2.12	0.50
1:B:288:LYS:NZ	3:B:670:HOH:O	2.41	0.50
1:A:125:PHE:HZ	3:A:612:HOH:O	1.95	0.50
1:A:320:LEU:HA	1:A:323:VAL:HG12	1.94	0.49
1:B:329:ARG:O	1:B:332:SER:HB3	2.12	0.49
1:B:33:MET:HG2	1:B:379:ILE:HG12	1.94	0.49
1:A:222:ASP:OD2	2:A:411:IK2:N1	2.45	0.49
1:B:377:PHE:O	1:B:378:SER:HB2	2.14	0.48
1:A:228:PHE:HZ	1:A:359:MET:HE3	1.79	0.47
1:A:135:LEU:O	1:A:157:ALA:HA	2.15	0.47
1:A:342:LYS:NZ	3:A:645:HOH:O	2.48	0.47
1:B:162:ASP:HB2	1:B:169:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HG13	3:B:633:HOH:O	2.16	0.46
1:B:222:ASP:OD2	2:B:411:IK2:N1	2.49	0.46
1:B:214:LYS:HG3	3:B:640:HOH:O	2.15	0.45
1:B:99:ARG:HG3	1:B:99:ARG:O	2.17	0.45
1:A:329:ARG:HG3	3:A:643:HOH:O	2.17	0.45
2:B:411:IK2:H1'1	2:B:411:IK2:H4A1	1.67	0.45
1:A:293:PRO:CG	1:B:145:PRO:HB2	2.47	0.45
1:B:15:ASP:HA	1:B:16:PRO:HD3	1.75	0.45
1:A:284:GLU:HG2	1:A:288:LYS:HD2	1.99	0.45
1:A:44:ASN:HB2	3:A:577:HOH:O	2.17	0.45
1:B:164:LYS:HB2	1:B:164:LYS:HE2	1.73	0.45
1:A:64:LYS:HD2	3:A:658:HOH:O	2.17	0.44
1:B:148:ARG:HD2	3:B:486:HOH:O	2.17	0.44
1:B:374:THR:HG23	1:B:380:TYR:CE1	2.52	0.44
2:B:411:IK2:H4A2	3:B:611:HOH:O	2.17	0.44
1:B:27:ASP:O	1:B:32:LYS:NZ	2.36	0.44
1:B:140:TRP:CH2	2:B:411:IK2:H5A1	2.53	0.44
1:B:24:PHE:CE1	1:B:32:LYS:HG3	2.53	0.43
1:B:31:LYS:NZ	3:B:659:HOH:O	2.46	0.43
1:B:366:LYS:O	1:B:370:VAL:HG23	2.18	0.43
1:A:50:LEU:HD12	1:A:50:LEU:N	2.34	0.43
1:B:33:MET:HE2	1:B:35:LEU:HD21	1.99	0.43
2:A:411:IK2:O4P	2:A:411:IK2:H4A1	2.17	0.43
1:B:24:PHE:HE1	1:B:32:LYS:HG3	1.83	0.43
1:A:215:ARG:HB2	1:A:217:LEU:HG	1.99	0.43
1:B:194:ASN:HA	1:B:195:PRO:HA	1.86	0.43
1:B:161:TYR:OH	1:B:166:CYS:HA	2.19	0.43
1:B:37:VAL:HG12	1:B:39:ALA:O	2.19	0.43
1:A:8:HIS:HE1	1:B:122:PHE:O	2.02	0.42
1:A:89:GLY:O	1:A:92:SER:HB3	2.19	0.42
1:A:331:ILE:HD11	3:A:676:HOH:O	2.19	0.42
1:B:33:MET:HG2	1:B:379:ILE:CG1	2.49	0.42
1:B:101:VAL:O	1:B:271:THR:HA	2.20	0.42
1:B:262:LEU:O	1:B:263:TYR:C	2.59	0.42
1:B:233:ILE:HD13	1:B:320:LEU:HD21	2.02	0.42
1:B:307:SER:O	1:B:311:ASN:HB2	2.19	0.41
1:A:135:LEU:HD11	1:A:155:LEU:CD2	2.50	0.41
1:B:297:ASN:HA	1:B:298:PRO:HD3	1.95	0.41
1:A:101:VAL:HG21	1:A:284:GLU:HB2	2.02	0.41
1:A:145:PRO:HB2	1:B:293:PRO:CG	2.50	0.41
1:A:57:GLU:HG2	3:A:503:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:TRP:O	1:B:8:HIS:HE1	2.03	0.41
1:A:213:LYS:HE3	1:A:246:GLN:O	2.21	0.41
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.67	0.41
1:B:386:ARG:NH1	3:B:459:HOH:O	2.53	0.41
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.85	0.40
1:A:235:ARG:HH11	1:A:235:ARG:HD2	1.69	0.40
1:A:228:PHE:CZ	1:A:359:MET:HE3	2.57	0.40
1:B:101:VAL:CG2	1:B:284:GLU:HB2	2.45	0.40
1:B:47:PRO:HD3	3:B:674:HOH:O	2.22	0.40
1:A:171:THR:HG22	3:A:513:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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%)	385 (96%)	13 (3%)	1 (0%)	41	50
1	B	399/401 (100%)	381 (96%)	17 (4%)	1 (0%)	41	50
All	All	798/802 (100%)	766 (96%)	30 (4%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR

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%)	314 (94%)	21 (6%)	18	24
1	B	335/335 (100%)	313 (93%)	22 (7%)	16	22
All	All	670/670 (100%)	627 (94%)	43 (6%)	17	23

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	18	LEU
1	A	81	ARG
1	A	90	GLU
1	A	92	SER
1	A	107	SER
1	A	125	PHE
1	A	129	ARG
1	A	211	VAL
1	A	214	LYS
1	A	215	ARG
1	A	220	TYR
1	A	259	ASN
1	A	275	ARG
1	A	292	ARG
1	A	296	SER
1	A	314	GLU
1	A	340	ASN
1	A	343	LYS
1	A	362	PHE
1	A	366	LYS
1	B	20	VAL
1	B	22	GLU
1	B	25	LYS
1	B	43	ASP
1	B	81	ARG
1	B	83	SER
1	B	90	GLU
1	B	91	ASN
1	B	107	SER
1	B	125	PHE
1	B	202	GLN
1	B	220	TYR

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Mol	Chain	Res	Type
1	B	275	ARG
1	B	281	LYS
1	B	339	SER
1	B	343	LYS
1	B	351	GLN
1	B	362	PHE
1	B	366	LYS
1	B	369	GLN
1	B	375	LYS
1	B	383	LYS

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	8	HIS
1	A	259	ASN
1	B	204	GLN
1	B	226	GLN
1	B	348	HIS
1	B	351	GLN
1	B	406	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 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	IK2	B	411	-	18,21,21	3.48	6 (33%)	21,29,29	3.56	9 (42%)
2	IK2	A	411	-	18,21,21	3.56	5 (27%)	21,29,29	4.01	11 (52%)

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	IK2	B	411	-	-	7/9/13/13	0/1/1/1
2	IK2	A	411	-	-	5/9/13/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	IK2	C4A-N4A	-13.28	1.24	1.46
2	B	411	IK2	C4A-N4A	-12.70	1.25	1.46
2	B	411	IK2	C5-C4	3.85	1.45	1.40
2	A	411	IK2	C5-C4	3.71	1.45	1.40
2	B	411	IK2	OX-N4A	-3.22	1.41	1.45
2	B	411	IK2	C3-C2	2.89	1.43	1.40
2	A	411	IK2	C3-C2	2.76	1.43	1.40
2	A	411	IK2	C4A-C4	-2.57	1.48	1.51
2	A	411	IK2	P-O3P	-2.51	1.45	1.54
2	B	411	IK2	P-O3P	-2.37	1.45	1.54
2	B	411	IK2	C3-C4	-2.18	1.36	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	IK2	C4-C4A-N4A	13.84	136.88	110.27
2	B	411	IK2	C4-C4A-N4A	7.88	125.42	110.27
2	B	411	IK2	C2A-C2-C3	7.44	130.07	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	IK2	C2A-C2-C3	6.57	129.00	120.89
2	B	411	IK2	O4P-C5A-C5	6.52	121.78	109.35
2	B	411	IK2	C5A-C5-C6	5.02	127.64	119.37
2	A	411	IK2	O4P-C5A-C5	4.80	118.51	109.35
2	A	411	IK2	C4A-C4-C3	4.48	124.84	120.04
2	B	411	IK2	C3-C2-N1	-4.32	115.19	120.77
2	B	411	IK2	C4A-C4-C3	3.88	124.20	120.04
2	B	411	IK2	C4A-C4-C5	-3.87	115.41	119.71
2	A	411	IK2	C3-C2-N1	-3.55	116.18	120.77
2	B	411	IK2	C6-N1-C2	3.48	125.61	119.17
2	A	411	IK2	C6-N1-C2	2.82	124.39	119.17
2	A	411	IK2	O3-C3-C4	2.71	126.07	118.13
2	A	411	IK2	C6-C5-C4	2.63	119.98	118.12
2	A	411	IK2	C5A-C5-C6	2.60	123.66	119.37
2	A	411	IK2	C4A-C4-C5	-2.22	117.24	119.71
2	B	411	IK2	O3-C3-C4	2.19	124.56	118.13
2	A	411	IK2	O3-C3-C2	-2.05	113.03	117.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

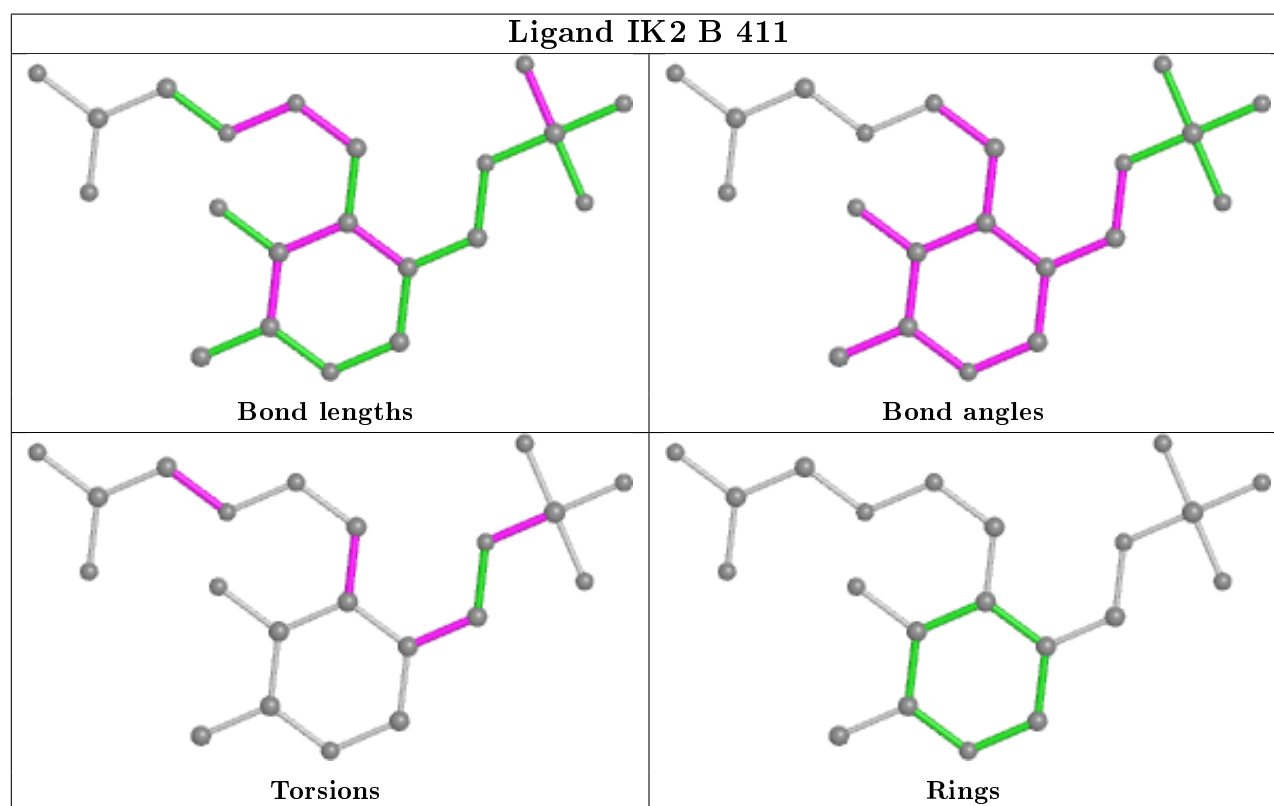
Mol	Chain	Res	Type	Atoms
2	B	411	IK2	C3-C4-C4A-N4A
2	B	411	IK2	C2'-C1'-OX-N4A
2	B	411	IK2	C5A-O4P-P-O3P
2	A	411	IK2	C3-C4-C4A-N4A
2	A	411	IK2	C5A-O4P-P-O1P
2	A	411	IK2	C5A-O4P-P-O2P
2	A	411	IK2	C5A-O4P-P-O3P
2	B	411	IK2	C5-C4-C4A-N4A
2	A	411	IK2	C5-C4-C4A-N4A
2	B	411	IK2	C5A-O4P-P-O1P
2	B	411	IK2	C5A-O4P-P-O2P
2	B	411	IK2	C6-C5-C5A-O4P

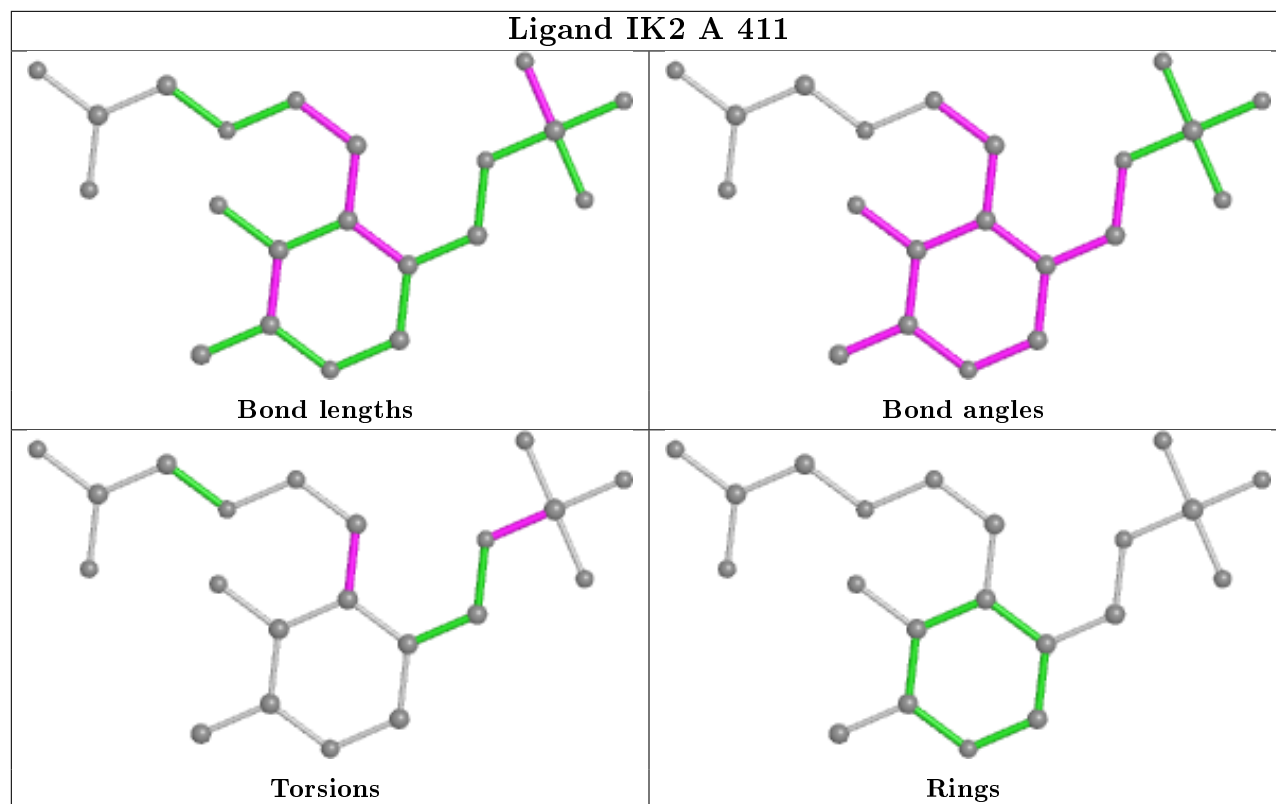
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	411	IK2	4	0
2	A	411	IK2	3	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.