



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:34 AM UTC

PDB ID : 1OXO / pdb_00001oxo
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 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

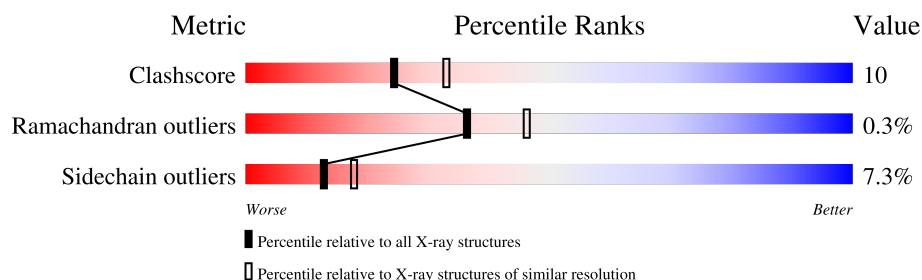
1 Overall quality at a glance

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	 70% 23% 5%
1	B	401	 65% 28% 6%

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.

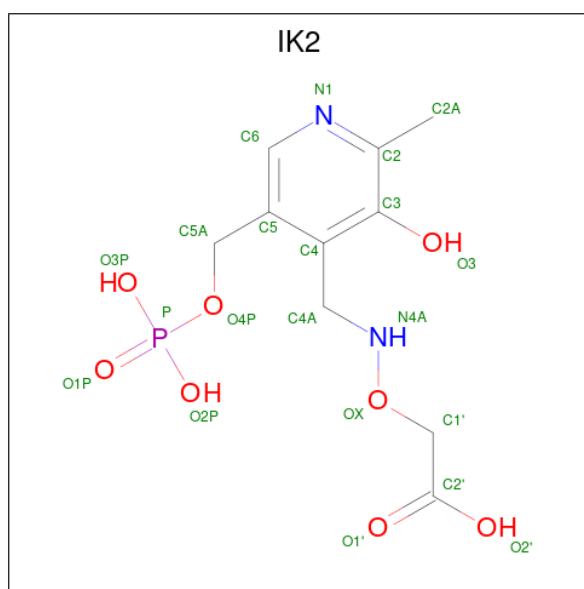
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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'-ACETILYAMINO-PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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		

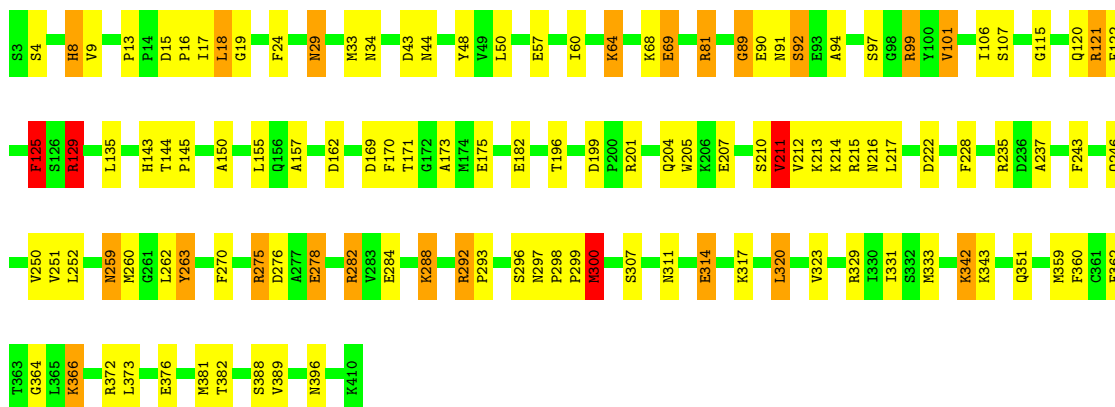
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

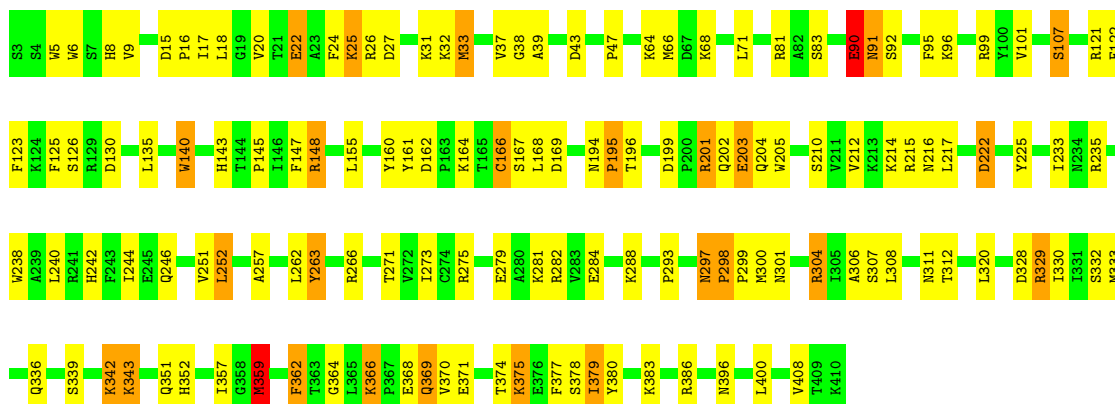
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A: 



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B: 



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	1.02	3/3231 (0.1%)	1.90	64/4360 (1.5%)
1	B	1.19	6/3231 (0.2%)	1.93	75/4360 (1.7%)
All	All	1.11	9/6462 (0.1%)	1.91	139/8720 (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	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	-31.34	1.02	1.46
1	A	275	ARG	CD-NE	-25.87	1.10	1.46
1	B	235	ARG	CD-NE	-23.44	1.13	1.46
1	B	203	GLU	CG-CD	-14.89	1.14	1.52
1	A	317	LYS	CG-CD	-9.96	1.22	1.52
1	B	25	LYS	CD-CE	-9.18	1.25	1.52
1	B	22	GLU	CG-CD	-8.31	1.31	1.52
1	B	371	GLU	CG-CD	-8.11	1.31	1.52
1	A	351	GLN	CG-CD	-5.84	1.37	1.52

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ARG	CD-NE-CZ	-16.67	101.06	124.40
1	B	203	GLU	CB-CG-CD	15.73	139.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ARG	CG-CD-NE	15.44	145.96	112.00
1	A	278	GLU	CB-CG-CD	13.10	134.87	112.60
1	B	22	GLU	CG-CD-OE2	-12.60	89.42	118.40
1	B	22	GLU	CB-CG-CD	11.97	132.95	112.60
1	B	22	GLU	CG-CD-OE1	11.49	144.82	118.40
1	A	275	ARG	CD-NE-CZ	-11.43	108.40	124.40
1	A	317	LYS	CB-CG-CD	9.39	132.90	111.30
1	A	251	VAL	CB-CA-C	9.36	124.56	110.62
1	A	298	PRO	N-CA-C	9.04	121.73	110.70
1	B	297	ASN	CB-CA-C	8.23	121.08	110.22
1	A	297	ASN	CB-CA-C	8.22	121.10	109.92
1	B	143	HIS	N-CA-CB	8.14	122.27	110.06
1	A	199	ASP	CA-CB-CG	7.76	120.36	112.60
1	B	235	ARG	CD-NE-CZ	-7.60	113.76	124.40
1	A	210	SER	O-C-N	7.58	129.97	122.09
1	A	196	THR	N-CA-C	7.55	121.75	112.23
1	B	25	LYS	CG-CD-CE	7.55	128.66	111.30
1	B	121	ARG	N-CA-C	7.50	119.54	111.36
1	B	6	TRP	N-CA-C	7.46	123.30	113.30
1	A	125	PHE	N-CA-C	7.43	121.61	112.54
1	B	196	THR	N-CA-C	7.33	121.46	112.23
1	A	29	ASN	OD1-CG-ND2	7.30	129.91	122.60
1	A	250	VAL	CA-C-N	7.28	133.11	123.06
1	A	250	VAL	C-N-CA	7.28	133.11	123.06
1	B	130	ASP	N-CA-C	7.27	120.51	108.96
1	A	121	ARG	N-CA-C	7.09	118.80	111.14
1	A	89	GLY	N-CA-C	-6.91	102.92	112.18
1	B	71	LEU	N-CA-C	-6.71	101.37	110.36
1	B	148	ARG	CB-CA-C	6.67	121.35	110.88
1	A	278	GLU	CG-CD-OE1	6.65	133.71	118.40
1	A	275	ARG	CG-CD-NE	6.61	126.53	112.00
1	A	17	ILE	N-CA-CB	6.57	118.23	110.55
1	B	92	SER	N-CA-C	-6.50	101.33	110.50
1	B	199	ASP	O-C-N	6.49	127.87	121.57
1	A	314	GLU	CB-CG-CD	6.48	123.61	112.60
1	B	312	THR	O-C-N	6.45	127.25	121.19
1	A	243	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	252	LEU	N-CA-CB	-6.40	99.62	111.52
1	A	122	PHE	N-CA-C	6.36	121.33	113.50
1	A	300	MET	N-CA-C	6.36	120.24	112.23
1	B	216	ASN	N-CA-CB	-6.31	101.68	111.65
1	B	359	MET	CB-CA-C	6.28	122.24	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	CD-NE-CZ	6.26	133.16	124.40
1	A	211	VAL	CB-CA-C	6.26	120.62	112.24
1	B	210	SER	CB-CA-C	6.26	120.70	110.88
1	B	143	HIS	CA-C-O	-6.20	113.94	120.63
1	B	33	MET	CB-CA-C	6.19	121.94	109.38
1	A	91	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	300	MET	N-CA-C	6.10	119.92	112.23
1	B	273	ILE	N-CA-CB	6.09	117.94	111.00
1	B	90	GLU	CA-CB-CG	6.06	126.22	114.10
1	B	222	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	216	ASN	N-CA-CB	-6.04	102.77	111.70
1	B	266	ARG	N-CA-C	6.02	117.96	110.91
1	B	251	VAL	N-CA-C	-6.00	99.09	108.86
1	A	199	ASP	O-C-N	5.99	127.38	121.57
1	B	400	LEU	CA-C-N	5.93	128.50	120.38
1	B	400	LEU	C-N-CA	5.93	128.50	120.38
1	B	357	ILE	N-CA-C	5.88	116.95	108.48
1	A	237	ALA	CA-C-N	5.88	128.48	120.54
1	A	237	ALA	C-N-CA	5.88	128.48	120.54
1	A	182	GLU	CA-CB-CG	5.85	125.80	114.10
1	B	121	ARG	NE-CZ-NH2	-5.83	113.95	119.20
1	A	389	VAL	CB-CA-C	5.82	122.90	111.79
1	A	364	GLY	N-CA-C	-5.80	107.09	115.27
1	A	282	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	B	359	MET	N-CA-C	5.75	118.33	111.71
1	B	299	PRO	CB-CA-C	5.72	118.85	111.64
1	B	235	ARG	O-C-N	5.71	128.17	122.12
1	B	235	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	B	212	VAL	O-C-N	5.67	127.37	121.87
1	B	140	TRP	CB-CA-C	5.66	118.73	109.90
1	A	201	ARG	N-CA-C	-5.65	102.10	110.46
1	A	94	ALA	CA-C-N	5.59	128.04	120.44
1	A	94	ALA	C-N-CA	5.59	128.04	120.44
1	A	270	PHE	CA-C-O	-5.58	114.30	120.38
1	B	352	HIS	CA-CB-CG	5.56	119.36	113.80
1	A	251	VAL	N-CA-CB	5.55	121.05	111.39
1	B	235	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	A	143	HIS	N-CA-CB	5.52	118.73	110.22
1	A	366	LYS	CB-CA-C	5.50	117.40	109.09
1	B	195	PRO	N-CA-C	5.49	126.37	112.10
1	A	342	LYS	CA-C-N	5.47	129.36	120.60
1	A	342	LYS	C-N-CA	5.47	129.36	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	144	THR	O-C-N	5.46	124.69	120.38
1	B	225	TYR	N-CA-C	5.45	119.08	111.56
1	A	170	PHE	N-CA-CB	5.44	118.12	110.12
1	B	301	ASN	N-CA-C	5.44	116.90	110.97
1	A	204	GLN	N-CA-C	-5.44	105.43	111.36
1	B	238	TRP	N-CA-CB	5.41	118.04	109.82
1	A	360	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	43	ASP	CB-CA-C	5.38	121.67	110.32
1	A	210	SER	CA-C-O	-5.36	115.16	120.90
1	B	205	TRP	CA-CB-CG	5.33	123.73	113.60
1	B	362	PHE	N-CA-C	-5.32	99.84	108.41
1	B	17	ILE	O-C-N	5.32	127.25	121.94
1	B	279	GLU	CA-C-N	5.32	127.40	120.28
1	B	279	GLU	C-N-CA	5.32	127.40	120.28
1	B	306	ALA	CA-C-N	5.31	127.40	120.28
1	B	306	ALA	C-N-CA	5.31	127.40	120.28
1	B	235	ARG	CA-C-O	-5.28	114.95	120.55
1	B	244	ILE	O-C-N	5.26	126.97	121.87
1	A	69	GLU	CB-CG-CD	5.26	121.53	112.60
1	A	205	TRP	N-CA-CB	5.25	117.83	110.12
1	A	17	ILE	CB-CA-C	5.24	118.67	111.97
1	B	123	PHE	CA-C-O	-5.24	115.53	121.66
1	B	26	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	A	91	ASN	CB-CA-C	5.22	119.67	110.37
1	B	304	ARG	CA-C-N	5.21	127.13	120.56
1	B	304	ARG	C-N-CA	5.21	127.13	120.56
1	A	8	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	320	LEU	CB-CA-C	5.21	119.44	110.79
1	B	375	LYS	N-CA-C	5.20	116.64	111.07
1	B	298	PRO	N-CA-C	5.19	117.03	110.70
1	B	147	PHE	CB-CA-C	5.18	119.09	110.90
1	A	115	GLY	O-C-N	5.15	127.13	122.19
1	A	388	SER	N-CA-CB	5.14	118.39	110.21
1	B	107	SER	CA-C-N	5.14	125.54	119.94
1	B	107	SER	C-N-CA	5.14	125.54	119.94
1	A	299	PRO	CB-CA-C	5.13	117.67	111.46
1	B	95	PHE	CA-C-N	5.12	127.40	120.38
1	B	95	PHE	C-N-CA	5.12	127.40	120.38
1	A	48	TYR	N-CA-C	5.09	116.61	107.80
1	B	126	SER	N-CA-CB	-5.09	103.09	111.69
1	B	364	GLY	N-CA-C	-5.08	107.53	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	VAL	O-C-N	5.08	126.79	121.87
1	B	33	MET	CA-CB-CG	5.07	124.25	114.10
1	B	166	CYS	N-CA-C	-5.07	104.90	111.74
1	B	329	ARG	CA-C-N	5.07	126.94	120.56
1	B	329	ARG	C-N-CA	5.07	126.94	120.56
1	A	13	PRO	N-CA-CB	5.07	105.85	103.22
1	A	129	ARG	CA-CB-CG	5.05	124.21	114.10
1	A	173	ALA	CA-C-N	5.02	127.01	120.28
1	A	173	ALA	C-N-CA	5.02	127.01	120.28
1	B	342	LYS	N-CA-C	-5.02	105.72	111.14
1	A	216	ASN	OD1-CG-ND2	5.00	127.60	122.60

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	62	0
1	B	3161	0	3154	65	0
2	A	21	0	11	3	0
2	B	21	0	11	5	0
3	A	275	0	0	17	0
3	B	266	0	0	14	0
All	All	6905	0	6330	125	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 10.

All (125) 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:A:228:PHE:CZ	1:A:359:MET:HE3	2.23	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:228:PHE:HZ	1:A:359:MET:HE3	1.57	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
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:HE	1:A:129:ARG:CA	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:H	1:A:8:HIS:CD2	2.23	0.55
1:A:282:ARG:HD2	1:B:9:VAL:O	2.07	0.54
1:B:288:LYS:NZ	3:B:670:HOH:O	2.41	0.54
1:A:373:LEU:HD13	1:A:381:MET:HE3	1.90	0.53
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:411:IK2:H2A2	3:B:440:HOH:O	2.15	0.47
1:B:377:PHE:O	1:B:378:SER:HB2	2.14	0.47
1:A:135:LEU:O	1:A:157:ALA:HA	2.15	0.47
1:B:333:MET:HE2	1:B:333:MET:HA	1.96	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
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:O	1:B:99:ARG:HG3	2.17	0.45
1:B:262:LEU:O	1:B:263:TYR:C	2.59	0.45
1:A:329:ARG:HG3	3:A:643:HOH:O	2.17	0.45
2:B:411:IK2:H4A1	2:B:411:IK2:H1'1	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:A:18:LEU:HD23	1:A:18:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:MET:HE3	1:A:396:ASN:CG	2.43	0.43
1:A:262:LEU:O	1:A:263:TYR:C	2.61	0.43
1:A:50:LEU:N	1:A:50:LEU:HD12	2.34	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:37:VAL:HG12	1:B:39:ALA:O	2.19	0.43
1:B:161:TYR:OH	1:B:166:CYS:HA	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:233:ILE:HD13	1:B:320:LEU:HD21	2.02	0.42
1:A:29:ASN:OD1	1:A:29:ASN:C	2.60	0.42
1:B:240:LEU:C	1:B:240:LEU:HD12	2.44	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:69:GLU:O	1:A:300:MET:HE1	2.19	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
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:B:33:MET:HE1	1:B:396:ASN:OD1	2.21	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:B:342:LYS:O	1:B:343:LYS:C	2.64	0.40
1:B:38:GLY:C	1:B:359:MET:HE1	2.46	0.40
1:B:66:MET:HE2	1:B:66:MET:HB3	1.96	0.40
1:B:47:PRO:HD3	3:B:674:HOH:O	2.22	0.40
1:B:101:VAL:CG2	1:B:284:GLU:HB2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	46
1	B	399/401 (100%)	381 (96%)	17 (4%)	1 (0%)	36	46
All	All	798/802 (100%)	766 (96%)	30 (4%)	2 (0%)	36	46

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%)	311 (93%)	24 (7%)	13	18
1	B	335/335 (100%)	310 (92%)	25 (8%)	12	17
All	All	670/670 (100%)	621 (93%)	49 (7%)	13	18

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	64	LYS
1	A	81	ARG
1	A	90	GLU
1	A	92	SER
1	A	101	VAL
1	A	106	ILE
1	A	107	SER
1	A	125	PHE
1	A	129	ARG
1	A	211	VAL
1	A	214	LYS
1	A	252	LEU
1	A	259	ASN
1	A	275	ARG
1	A	288	LYS
1	A	292	ARG
1	A	296	SER
1	A	300	MET
1	A	314	GLU
1	A	343	LYS
1	A	362	PHE
1	A	366	LYS
1	A	382	THR
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	252	LEU
1	B	281	LYS
1	B	308	LEU
1	B	339	SER
1	B	343	LYS
1	B	351	GLN
1	B	359	MET

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Mol	Chain	Res	Type
1	B	362	PHE
1	B	366	LYS
1	B	368	GLU
1	B	369	GLN
1	B	375	LYS
1	B	379	ILE
1	B	383	LYS

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	8	HIS
1	A	44	ASN
1	A	91	ASN
1	A	189	HIS
1	A	259	ASN
1	B	204	GLN
1	B	226	GLN
1	B	297	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	IK2	A	411	-	19,21,21	1.78	7 (36%)	24,29,29	2.59	11 (45%)
2	IK2	B	411	-	19,21,21	1.70	6 (31%)	24,29,29	3.10	9 (37%)

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	A	411	-	-	5/11/13/13	0/1/1/1
2	IK2	B	411	-	-	8/11/13/13	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	IK2	C5-C4	3.86	1.45	1.40
2	A	411	IK2	C5-C4	3.71	1.45	1.40
2	B	411	IK2	C3-C2	2.72	1.43	1.41
2	A	411	IK2	P-O3P	-2.60	1.45	1.54
2	A	411	IK2	C3-C2	2.60	1.43	1.41
2	A	411	IK2	O1'-C2'	2.52	1.30	1.22
2	B	411	IK2	P-O3P	-2.45	1.45	1.54
2	B	411	IK2	O1'-C2'	2.33	1.29	1.22
2	A	411	IK2	C4A-C4	-2.28	1.48	1.52
2	B	411	IK2	C3-C4	-2.28	1.36	1.40
2	A	411	IK2	C6-C5	-2.13	1.33	1.37
2	B	411	IK2	C6-C5	-2.07	1.33	1.37
2	A	411	IK2	C3-C4	-2.04	1.37	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	IK2	C2A-C2-C3	7.92	130.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	IK2	C2A-C2-C3	7.01	129.00	120.80
2	B	411	IK2	O4P-C5A-C5	6.63	121.78	109.36
2	B	411	IK2	C5A-C5-C6	5.08	127.64	119.36
2	A	411	IK2	O4P-C5A-C5	4.88	118.51	109.36
2	B	411	IK2	C3-C2-N1	-4.58	115.19	120.96
2	B	411	IK2	C4A-C4-C5	-3.98	115.41	119.75
2	B	411	IK2	C5A-C5-C4	-3.80	114.66	122.67
2	A	411	IK2	C3-C2-N1	-3.79	116.18	120.96
2	A	411	IK2	C4A-C4-C3	3.65	124.84	119.98
2	B	411	IK2	C6-N1-C2	3.54	125.61	119.20
2	B	411	IK2	C4A-C4-C3	3.17	124.20	119.98
2	A	411	IK2	C5A-C5-C4	-2.99	116.36	122.67
2	A	411	IK2	C6-N1-C2	2.86	124.39	119.20
2	A	411	IK2	O3-C3-C4	2.72	126.07	118.18
2	A	411	IK2	C5A-C5-C6	2.63	123.66	119.36
2	A	411	IK2	C6-C5-C4	2.54	119.98	118.06
2	A	411	IK2	C4A-C4-C5	-2.30	117.24	119.75
2	B	411	IK2	O3-C3-C4	2.20	124.56	118.18
2	A	411	IK2	O3-C3-C2	-2.20	113.03	117.58

There are no chirality outliers.

All (13) torsion outliers are listed below:

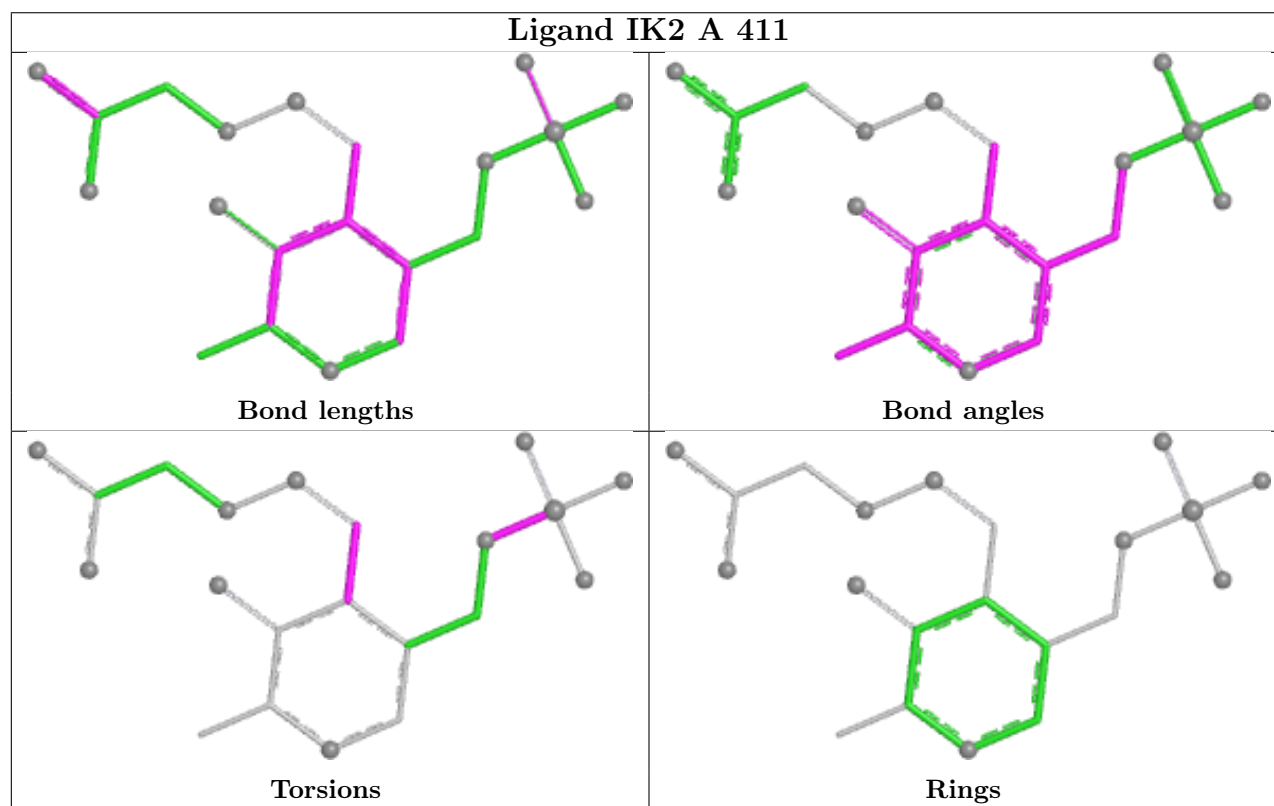
Mol	Chain	Res	Type	Atoms
2	A	411	IK2	C3-C4-C4A-N4A
2	A	411	IK2	C5A-O4P-P-O1P
2	A	411	IK2	C5A-O4P-P-O2P
2	A	411	IK2	C5A-O4P-P-O3P
2	B	411	IK2	C3-C4-C4A-N4A
2	B	411	IK2	C2'-C1'-OX-N4A
2	B	411	IK2	C5A-O4P-P-O3P
2	A	411	IK2	C5-C4-C4A-N4A
2	B	411	IK2	C5-C4-C4A-N4A
2	B	411	IK2	C5A-O4P-P-O1P
2	B	411	IK2	C5A-O4P-P-O2P
2	B	411	IK2	C6-C5-C5A-O4P
2	B	411	IK2	OX-C1'-C2'-O1'

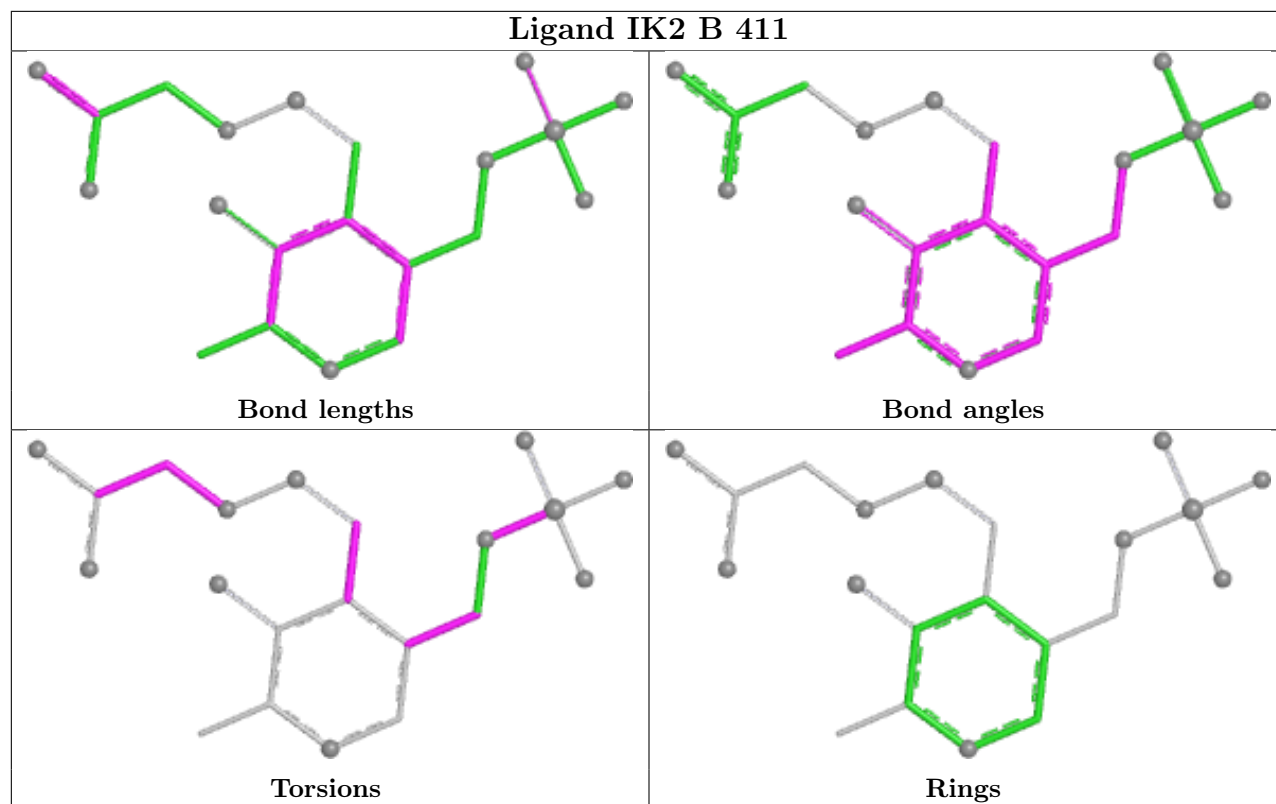
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	IK2	3	0
2	B	411	IK2	5	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.