



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:06 am BST

PDB ID : 1OXP
Title : ASPARTATE AMINOTRANSFERASE, H-ASP COMPLEX, CLOSED CON-
FORMATION
Authors : Hohenester, E.; Schirmer, T.; Jansonius, J.N.
Deposited on : 1995-12-23
Resolution : 2.50 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

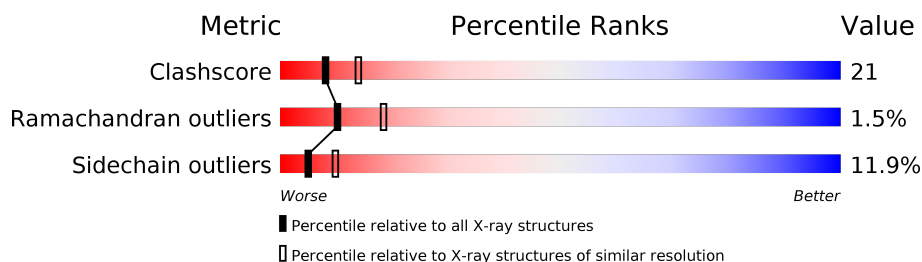
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3397 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.

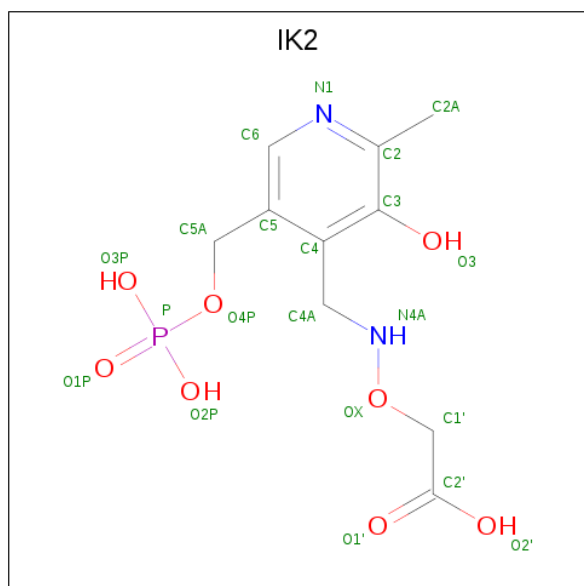
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	5	0	0
			3161	2004	558	581	18			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is 4'-DEOXY-4'-ACETYLYAMINO-PYRIDOXAL-5'-PHOSPHATE (three-letter code: IK2) (formula: $C_{10}H_{15}N_2O_8P$).



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

- Molecule 3 is water.

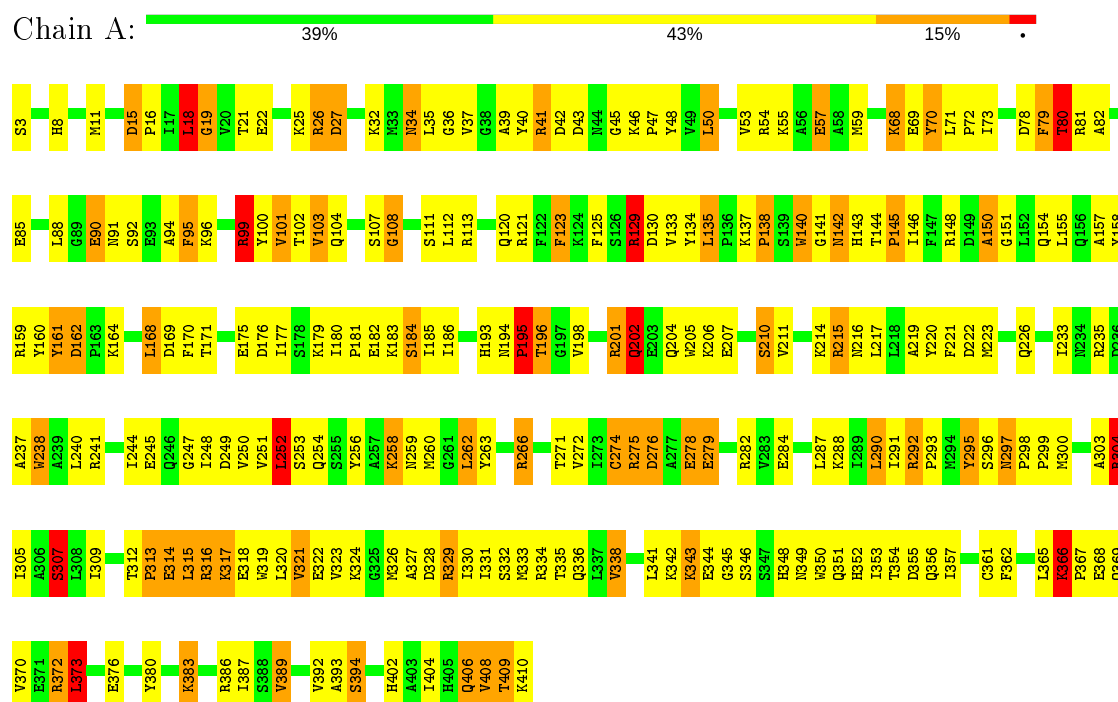
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	215	Total 215	O 215	0	0

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



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	69.50Å 91.55Å 128.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.06	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	3397	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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	0.96	1/3231 (0.0%)	2.47	174/4360 (4.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	LYS	CA-CB	-7.89	1.36	1.53

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH1	21.04	130.82	120.30
1	A	41	ARG	NE-CZ-NH2	-20.30	110.15	120.30
1	A	304	ARG	CD-NE-CZ	18.37	149.32	123.60
1	A	148	ARG	NE-CZ-NH1	18.16	129.38	120.30
1	A	292	ARG	NE-CZ-NH1	-16.72	111.94	120.30
1	A	241	ARG	NE-CZ-NH1	-14.70	112.95	120.30
1	A	99	ARG	NE-CZ-NH1	-13.00	113.80	120.30
1	A	329	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	A	282	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	A	241	ARG	NE-CZ-NH2	12.52	126.56	120.30
1	A	129	ARG	CD-NE-CZ	12.47	141.06	123.60
1	A	317	LYS	CA-CB-CG	12.35	140.57	113.40
1	A	113	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	A	235	ARG	CD-NE-CZ	12.23	140.72	123.60
1	A	148	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	A	304	ARG	NE-CZ-NH2	-11.19	114.70	120.30
1	A	304	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	A	292	ARG	NE-CZ-NH2	10.97	125.78	120.30
1	A	329	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	A	386	ARG	NE-CZ-NH2	10.64	125.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASP	CB-CG-OD2	-10.24	109.08	118.30
1	A	275	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	100	TYR	CB-CG-CD2	10.18	127.11	121.00
1	A	68	LYS	CD-CE-NZ	10.00	134.70	111.70
1	A	27	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	160	TYR	CB-CG-CD1	-9.81	115.11	121.00
1	A	284	GLU	CA-CB-CG	9.56	134.43	113.40
1	A	121	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	148	ARG	CD-NE-CZ	9.28	136.59	123.60
1	A	113	ARG	NH1-CZ-NH2	9.28	129.61	119.40
1	A	100	TYR	CB-CG-CD1	-9.18	115.49	121.00
1	A	304	ARG	CG-CD-NE	9.03	130.76	111.80
1	A	344	GLU	CG-CD-OE2	9.03	136.35	118.30
1	A	15	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	162	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	235	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	27	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	A	113	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	A	195	PRO	N-CA-C	8.08	133.12	112.10
1	A	282	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	295	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	A	362	PHE	CB-CA-C	7.82	126.05	110.40
1	A	81	ARG	CG-CD-NE	7.79	128.15	111.80
1	A	276	ASP	CA-CB-CG	7.68	130.30	113.40
1	A	70	TYR	CB-CG-CD1	7.66	125.60	121.00
1	A	159	ARG	CD-NE-CZ	7.62	134.26	123.60
1	A	372	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	150	ALA	C-N-CA	7.58	138.21	122.30
1	A	222	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	249	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	215	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	297	ASN	CB-CA-C	7.34	125.08	110.40
1	A	159	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	205	TRP	N-CA-CB	7.21	123.57	110.60
1	A	334	ARG	CD-NE-CZ	7.17	133.64	123.60
1	A	275	ARG	NH1-CZ-NH2	7.11	127.22	119.40
1	A	41	ARG	NH1-CZ-NH2	7.03	127.13	119.40
1	A	373	LEU	CA-CB-CG	6.98	131.36	115.30
1	A	71	LEU	CA-CB-CG	6.96	131.31	115.30
1	A	284	GLU	CG-CD-OE2	6.96	132.22	118.30
1	A	276	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	80	THR	CA-CB-CG2	6.81	121.93	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	121	ARG	CD-NE-CZ	6.78	133.09	123.60
1	A	282	ARG	CD-NE-CZ	6.75	133.06	123.60
1	A	256	TYR	O-C-N	6.70	133.42	122.70
1	A	22	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	A	215	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	380	TYR	CA-CB-CG	-6.66	100.75	113.40
1	A	78	ASP	OD1-CG-OD2	6.65	135.94	123.30
1	A	143	HIS	N-CA-CB	6.64	122.56	110.60
1	A	366	LYS	N-CA-CB	6.62	122.51	110.60
1	A	57	GLU	OE1-CD-OE2	6.56	131.18	123.30
1	A	345	GLY	O-C-N	6.52	133.12	122.70
1	A	50	LEU	CA-CB-CG	6.44	130.11	115.30
1	A	215	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	A	26	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	196	THR	N-CA-CB	-6.32	98.30	110.30
1	A	99	ARG	NH1-CZ-NH2	6.29	126.32	119.40
1	A	161	TYR	CA-CB-CG	6.24	125.25	113.40
1	A	201	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	26	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	383	LYS	CA-CB-CG	6.09	126.80	113.40
1	A	238	TRP	N-CA-CB	6.06	121.51	110.60
1	A	237	ALA	N-CA-CB	-6.05	101.63	110.10
1	A	394	SER	C-N-CA	6.01	136.72	121.70
1	A	15	ASP	OD1-CG-OD2	-6.00	111.89	123.30
1	A	22	GLU	CA-CB-CG	6.00	126.60	113.40
1	A	266	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	169	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	408	VAL	C-N-CA	5.95	136.58	121.70
1	A	123	PHE	CB-CG-CD1	-5.95	116.64	120.80
1	A	70	TYR	CA-CB-CG	5.95	124.70	113.40
1	A	202	GLN	C-N-CA	5.94	136.55	121.70
1	A	338	VAL	CG1-CB-CG2	-5.93	101.42	110.90
1	A	102	THR	CA-CB-CG2	5.92	120.69	112.40
1	A	142	ASN	CB-CG-OD1	-5.88	109.83	121.60
1	A	125	PHE	CA-C-O	-5.85	107.81	120.10
1	A	376	GLU	CB-CA-C	-5.85	98.70	110.40
1	A	315	LEU	CB-CA-C	5.84	121.30	110.20
1	A	39	ALA	N-CA-CB	5.83	118.26	110.10
1	A	344	GLU	CG-CD-OE1	-5.80	106.69	118.30
1	A	262	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	102	THR	O-C-N	5.79	131.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ALA	N-CA-CB	5.73	118.12	110.10
1	A	307	SER	CB-CA-C	5.73	120.98	110.10
1	A	50	LEU	CA-C-O	5.72	132.10	120.10
1	A	389	VAL	CB-CA-C	5.71	122.26	111.40
1	A	99	ARG	CA-CB-CG	5.71	125.97	113.40
1	A	345	GLY	CA-C-O	-5.71	110.32	120.60
1	A	19	GLY	CA-C-N	5.70	129.75	117.20
1	A	54	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	278	GLU	CA-CB-CG	5.66	125.85	113.40
1	A	138	PRO	N-CA-CB	-5.65	96.39	102.60
1	A	210	SER	CA-CB-OG	-5.64	95.98	111.20
1	A	389	VAL	CA-CB-CG1	5.64	119.36	110.90
1	A	18	LEU	CB-CG-CD1	5.64	120.58	111.00
1	A	47	PRO	CB-CA-C	5.62	126.05	112.00
1	A	205	TRP	CA-C-O	-5.61	108.32	120.10
1	A	121	ARG	CA-C-O	-5.59	108.36	120.10
1	A	171	THR	CA-CB-OG1	-5.56	97.33	109.00
1	A	316	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	406	GLN	C-N-CA	5.51	135.49	121.70
1	A	35	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	135	LEU	CA-CB-CG	5.51	127.96	115.30
1	A	101	VAL	O-C-N	5.49	131.48	122.70
1	A	42	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	361	CYS	N-CA-C	-5.48	96.21	111.00
1	A	259	ASN	CB-CA-C	5.47	121.34	110.40
1	A	291	ILE	CA-C-O	-5.45	108.65	120.10
1	A	321	VAL	CA-CB-CG1	5.45	119.08	110.90
1	A	150	ALA	N-CA-CB	-5.45	102.47	110.10
1	A	151	GLY	N-CA-C	5.44	126.71	113.10
1	A	275	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	42	ASP	CB-CA-C	5.44	121.28	110.40
1	A	322	GLU	CG-CD-OE1	-5.43	107.44	118.30
1	A	376	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	A	101	VAL	N-CA-CB	5.42	123.42	111.50
1	A	134	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	141	GLY	CA-C-O	5.41	130.34	120.60
1	A	22	GLU	O-C-N	-5.40	114.06	122.70
1	A	158	TYR	CA-CB-CG	5.38	123.63	113.40
1	A	349	ASN	N-CA-CB	-5.38	100.92	110.60
1	A	240	LEU	O-C-N	5.36	131.28	122.70
1	A	103	VAL	CG1-CB-CG2	5.36	119.47	110.90
1	A	288	LYS	CB-CG-CD	-5.35	97.68	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ARG	N-CA-CB	-5.34	100.98	110.60
1	A	108	GLY	O-C-N	5.34	131.24	122.70
1	A	15	ASP	CA-C-O	5.30	131.24	120.10
1	A	121	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	A	344	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	73	ILE	CA-C-O	-5.28	109.01	120.10
1	A	130	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	141	GLY	N-CA-C	5.21	126.11	113.10
1	A	380	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	175	GLU	OE1-CD-OE2	5.16	129.50	123.30
1	A	316	ARG	CG-CD-NE	-5.16	100.96	111.80
1	A	72	PRO	N-CA-CB	5.16	109.49	103.30
1	A	278	GLU	CG-CD-OE1	5.15	128.61	118.30
1	A	176	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	A	95	PHE	O-C-N	-5.06	114.61	122.70
1	A	247	GLY	O-C-N	5.06	130.79	122.70
1	A	140	TRP	CB-CG-CD1	5.05	133.57	127.00
1	A	11	MET	O-C-N	5.05	131.78	123.20
1	A	252	LEU	N-CA-CB	-5.04	100.31	110.40
1	A	134	TYR	O-C-N	5.03	130.75	122.70
1	A	35	LEU	CB-CA-C	5.03	119.76	110.20
1	A	226	GLN	CB-CG-CD	5.03	124.67	111.60
1	A	245	GLU	O-C-N	-5.02	114.67	122.70
1	A	348	HIS	CA-C-O	5.02	130.64	120.10
1	A	279	GLU	CG-CD-OE2	5.02	128.33	118.30
1	A	278	GLU	N-CA-CB	5.02	119.63	110.60
1	A	195	PRO	N-CA-CB	-5.00	97.10	102.60
1	A	103	VAL	N-CA-CB	-5.00	100.50	111.50

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	3161	0	3154	134	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	21	0	10	3	1
3	A	215	0	0	18	1
All	All	3397	0	3164	135	2

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 21.

All (135) 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:177:ILE:HA	1:A:180:ILE:HD12	1.60	0.83
1:A:233:ILE:HD13	1:A:320:LEU:HD21	1.64	0.80
1:A:370:VAL:HG12	1:A:383:LYS:HE2	1.65	0.78
1:A:350:TRP:HB3	1:A:353:ILE:HD12	1.66	0.78
1:A:338:VAL:HG21	1:A:354:THR:HG23	1.67	0.77
1:A:133:VAL:HG13	1:A:185:ILE:HG22	1.68	0.75
1:A:215:ARG:HB2	1:A:217:LEU:HG	1.69	0.74
1:A:129:ARG:HA	1:A:129:ARG:HE	1.52	0.74
1:A:162:ASP:OD1	1:A:164:LYS:HE3	1.88	0.73
1:A:314:GLU:HA	1:A:317:LYS:HD2	1.71	0.72
1:A:41:ARG:HB3	1:A:45:GLY:HA2	1.74	0.69
1:A:370:VAL:HG11	1:A:383:LYS:HA	1.75	0.68
1:A:342:LYS:HG2	3:A:518:HOH:O	1.92	0.68
1:A:312:THR:HB	1:A:315:LEU:HB2	1.75	0.68
1:A:404:ILE:O	1:A:409:THR:HB	1.93	0.68
1:A:244:ILE:HA	1:A:248:ILE:O	1.95	0.67
1:A:34:ASN:HD22	1:A:36:GLY:H	1.42	0.67
1:A:211:VAL:O	1:A:215:ARG:HG2	1.97	0.64
1:A:120:GLN:HG3	1:A:150:ALA:O	1.98	0.64
1:A:196:THR:O	1:A:356:GLN:HG2	1.98	0.64
1:A:373:LEU:HD22	1:A:408:VAL:HG11	1.79	0.63
1:A:193:HIS:ND1	1:A:196:THR:HB	2.12	0.63
1:A:211:VAL:HG22	3:A:528:HOH:O	1.99	0.62
1:A:85:GLU:HG3	1:A:95:PHE:CZ	2.34	0.62
1:A:34:ASN:ND2	1:A:36:GLY:H	1.98	0.61
1:A:366:LYS:HB3	1:A:367:PRO:HD2	1.80	0.61
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.83	0.61
1:A:316:ARG:NH2	3:A:542:HOH:O	2.34	0.60
1:A:179:LYS:NZ	1:A:179:LYS:HB2	2.18	0.59
1:A:111:SER:HB2	1:A:253:SER:OG	2.02	0.59
1:A:194:ASN:ND2	2:A:411:IK2:O3	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:O	1:A:214:LYS:HB3	2.02	0.58
1:A:183:LYS:N	1:A:216:ASN:O	2.36	0.58
1:A:233:ILE:HD13	1:A:320:LEU:CD2	2.32	0.58
1:A:79:PHE:HA	1:A:307:SER:HB2	1.85	0.58
1:A:303:ALA:O	1:A:307:SER:HB3	2.04	0.57
1:A:91:ASN:ND2	1:A:91:ASN:H	2.03	0.57
1:A:137:LYS:HD2	1:A:157:ALA:HB1	1.86	0.57
1:A:182:GLU:O	1:A:183:LYS:HB2	2.05	0.57
1:A:91:ASN:ND2	3:A:610:HOH:O	2.37	0.57
1:A:258:LYS:HD2	1:A:258:LYS:N	2.20	0.56
1:A:332:SER:O	1:A:335:THR:HB	2.06	0.55
1:A:352:HIS:HA	1:A:355:ASP:HB2	1.88	0.55
1:A:144:THR:HB	1:A:145:PRO:HD3	1.89	0.55
1:A:181:PRO:O	1:A:184:SER:OG	2.26	0.54
1:A:170:PHE:CE1	1:A:204:GLN:HB3	2.43	0.54
1:A:40:TYR:OH	1:A:329:ARG:HD3	2.07	0.54
1:A:221:PHE:O	1:A:252:LEU:HA	2.08	0.53
1:A:186:ILE:HG23	1:A:186:ILE:O	2.07	0.53
1:A:333:MET:CE	1:A:336:GLN:HE22	2.22	0.53
1:A:123:PHE:CD2	1:A:185:ILE:HD11	2.44	0.53
1:A:207:GLU:O	1:A:211:VAL:HG23	2.08	0.53
1:A:329:ARG:NH1	1:A:392:VAL:O	2.41	0.53
2:A:411:IK2:C4A	2:A:411:IK2:O4P	2.58	0.52
1:A:366:LYS:HB3	1:A:367:PRO:CD	2.39	0.52
1:A:43:ASP:OD2	1:A:394:SER:OG	2.27	0.52
1:A:251:VAL:HG12	1:A:272:VAL:HG22	1.91	0.52
1:A:183:LYS:HB2	3:A:554:HOH:O	2.09	0.52
1:A:161:TYR:CD1	1:A:196:THR:HG23	2.44	0.52
1:A:356:GLN:HG3	3:A:549:HOH:O	2.11	0.51
1:A:142:ASN:O	1:A:146:ILE:HG13	2.10	0.51
1:A:91:ASN:H	1:A:91:ASN:HD22	1.59	0.51
1:A:80:THR:HG23	3:A:466:HOH:O	2.10	0.51
1:A:104:GLN:NE2	1:A:303:ALA:HB2	2.26	0.51
1:A:15:ASP:OD1	1:A:16:PRO:HD2	2.12	0.50
1:A:298:PRO:HB2	1:A:299:PRO:HD2	1.94	0.50
1:A:314:GLU:H	1:A:314:GLU:CD	2.15	0.50
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.94	0.50
1:A:338:VAL:CG2	1:A:354:THR:HG23	2.40	0.50
1:A:55:LYS:O	1:A:59:MET:HG3	2.10	0.50
1:A:219:ALA:HB3	1:A:250:VAL:HG12	1.95	0.49
1:A:196:THR:HG22	1:A:198:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:VAL:O	1:A:324:LYS:HB2	2.13	0.48
1:A:326:MET:O	1:A:330:ILE:HG13	2.13	0.48
1:A:329:ARG:HH12	1:A:393:ALA:HA	1.78	0.48
1:A:333:MET:HE1	1:A:336:GLN:HE22	1.78	0.48
1:A:108:GLY:O	1:A:112:LEU:HB2	2.14	0.48
1:A:330:ILE:HG23	1:A:389:VAL:HG13	1.94	0.48
1:A:312:THR:O	1:A:313:PRO:C	2.51	0.47
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.76	0.47
1:A:48:TYR:N	3:A:415:HOH:O	2.27	0.47
1:A:327:ALA:HB1	3:A:479:HOH:O	2.14	0.47
1:A:101:VAL:O	1:A:271:THR:HA	2.15	0.47
1:A:258:LYS:NZ	2:A:411:IK2:H4A2	2.30	0.46
1:A:27:ASP:HB3	1:A:32:LYS:HD3	1.98	0.46
1:A:365:LEU:HD23	1:A:369:GLN:NE2	2.31	0.46
1:A:34:ASN:C	1:A:34:ASN:HD22	2.19	0.46
1:A:309:ILE:HA	1:A:315:LEU:HB3	1.98	0.45
1:A:298:PRO:CB	1:A:299:PRO:HD2	2.47	0.45
1:A:69:GLU:HB3	3:A:604:HOH:O	2.16	0.45
1:A:144:THR:CB	1:A:145:PRO:HD3	2.47	0.44
1:A:8:HIS:CD2	1:A:8:HIS:H	2.34	0.44
1:A:223:MET:O	1:A:254:GLN:HA	2.17	0.44
1:A:314:GLU:N	1:A:314:GLU:CD	2.70	0.44
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.93	0.44
1:A:201:ARG:O	1:A:204:GLN:N	2.50	0.44
1:A:15:ASP:O	1:A:16:PRO:C	2.56	0.44
1:A:168:LEU:CD1	1:A:198:VAL:HG12	2.48	0.44
1:A:140:TRP:HA	3:A:560:HOH:O	2.18	0.43
1:A:290:LEU:HD21	3:A:593:HOH:O	2.17	0.43
1:A:137:LYS:HD2	1:A:157:ALA:CB	2.49	0.43
1:A:182:GLU:HA	1:A:215:ARG:O	2.18	0.43
1:A:26:ARG:NH2	3:A:452:HOH:O	2.52	0.43
1:A:357:ILE:HD12	1:A:357:ILE:O	2.18	0.43
1:A:368:GLU:CD	1:A:368:GLU:H	2.23	0.43
1:A:53:VAL:HG13	1:A:305:ILE:HG21	2.01	0.43
1:A:343:LYS:HD3	1:A:343:LYS:C	2.39	0.42
1:A:343:LYS:HE2	3:A:488:HOH:O	2.18	0.42
1:A:387:ILE:HD13	1:A:387:ILE:HG21	1.81	0.42
1:A:338:VAL:O	1:A:341:LEU:HB2	2.19	0.42
1:A:319:TRP:O	1:A:323:VAL:HG23	2.20	0.42
1:A:372:ARG:NH2	3:A:603:HOH:O	2.52	0.42
1:A:318:GLU:HB2	3:A:583:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LYS:HD2	1:A:324:LYS:HA	1.85	0.42
1:A:15:ASP:HB3	1:A:19:GLY:H	1.84	0.42
1:A:179:LYS:HZ2	1:A:179:LYS:HB2	1.85	0.42
1:A:21:THR:O	1:A:25:LYS:HG3	2.20	0.42
1:A:133:VAL:HG13	1:A:185:ILE:CG2	2.43	0.42
1:A:53:VAL:O	1:A:57:GLU:HG3	2.19	0.42
1:A:135:LEU:CD1	1:A:155:LEU:HD22	2.50	0.41
1:A:328:ASP:O	1:A:331:ILE:HB	2.20	0.41
1:A:313:PRO:HB2	1:A:314:GLU:OE2	2.21	0.41
1:A:326:MET:HB2	1:A:326:MET:HE3	1.92	0.41
1:A:402:HIS:O	1:A:406:GLN:HG2	2.19	0.41
1:A:206:LYS:HG3	1:A:238:TRP:HH2	1.85	0.41
1:A:369:GLN:O	1:A:373:LEU:HB2	2.21	0.41
1:A:194:ASN:HA	1:A:195:PRO:HA	1.84	0.41
1:A:260:MET:HB3	1:A:262:LEU:HG	2.03	0.41
1:A:45:GLY:HA2	3:A:588:HOH:O	2.20	0.41
1:A:274:CYS:HB3	1:A:279:GLU:HG2	2.02	0.41
1:A:90:GLU:HG2	3:A:612:HOH:O	2.20	0.41
1:A:300:MET:HB2	1:A:300:MET:HE2	1.90	0.40
1:A:300:MET:O	1:A:304:ARG:HG3	2.22	0.40
1:A:135:LEU:HD11	1:A:155:LEU:HD22	2.02	0.40
1:A:295:TYR:O	1:A:297:ASN:N	2.52	0.40

All (2) 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)
3:A:413:HOH:O	3:A:413:HOH:O[3_655]	2.08	0.12
1:A:70:TYR:OH	2:A:411:IK2:O1P[3_655]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/401 (100%)	366 (92%)	27 (7%)	6 (2%)	10	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	202	GLN
1	A	263	TYR
1	A	296	SER
1	A	266	ARG
1	A	313	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/335 (100%)	295 (88%)	40 (12%)	5	10

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	18	LEU
1	A	34	ASN
1	A	37	VAL
1	A	46	LYS
1	A	50	LEU
1	A	68	LYS
1	A	79	PHE
1	A	80	THR
1	A	88	LEU
1	A	90	GLU
1	A	99	ARG
1	A	103	VAL
1	A	107	SER
1	A	129	ARG

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Mol	Chain	Res	Type
1	A	138	PRO
1	A	145	PRO
1	A	154	GLN
1	A	168	LEU
1	A	184	SER
1	A	195	PRO
1	A	202	GLN
1	A	220	TYR
1	A	252	LEU
1	A	258	LYS
1	A	274	CYS
1	A	275	ARG
1	A	276	ASP
1	A	278	GLU
1	A	290	LEU
1	A	304	ARG
1	A	307	SER
1	A	314	GLU
1	A	343	LYS
1	A	346	SER
1	A	351	GLN
1	A	366	LYS
1	A	373	LEU
1	A	409	THR
1	A	410	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	91	ASN
1	A	154	GLN
1	A	156	GLN
1	A	234	ASN
1	A	242	HIS
1	A	286	GLN
1	A	297	ASN
1	A	336	GLN
1	A	369	GLN

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 carbohydrates 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	IK2	A	411	-	18,21,21	3.82	6 (33%)	21,29,29	4.67	13 (61%)

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	-	-	5/9/13/13	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	IK2	C4A-N4A	-13.82	1.23	1.46
2	A	411	IK2	C3-C2	4.09	1.45	1.40
2	A	411	IK2	C5-C4	4.01	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	IK2	OX-N4A	-3.96	1.40	1.45
2	A	411	IK2	P-O3P	-2.65	1.44	1.54
2	A	411	IK2	C3-C4	-2.35	1.36	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	IK2	C4A-C4-C3	11.82	132.70	120.04
2	A	411	IK2	O3-C3-C2	-7.97	100.14	117.49
2	A	411	IK2	C4A-C4-C5	-7.73	111.11	119.71
2	A	411	IK2	O3-C3-C4	6.54	137.33	118.13
2	A	411	IK2	C4-C4A-N4A	5.62	121.08	110.27
2	A	411	IK2	O4P-C5A-C5	4.95	118.79	109.35
2	A	411	IK2	C3-C2-N1	-4.62	114.80	120.77
2	A	411	IK2	C6-C5-C4	4.19	121.08	118.12
2	A	411	IK2	C6-N1-C2	3.84	126.29	119.17
2	A	411	IK2	C5A-C5-C6	3.33	124.85	119.37
2	A	411	IK2	C5-C6-N1	-2.83	119.10	123.82
2	A	411	IK2	C2A-C2-N1	2.71	122.97	117.67
2	A	411	IK2	C3-C4-C5	-2.64	116.18	118.72

There are no chirality outliers.

All (5) 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-O2P
2	A	411	IK2	C5A-O4P-P-O3P
2	A	411	IK2	C5-C4-C4A-N4A
2	A	411	IK2	C5A-O4P-P-O1P

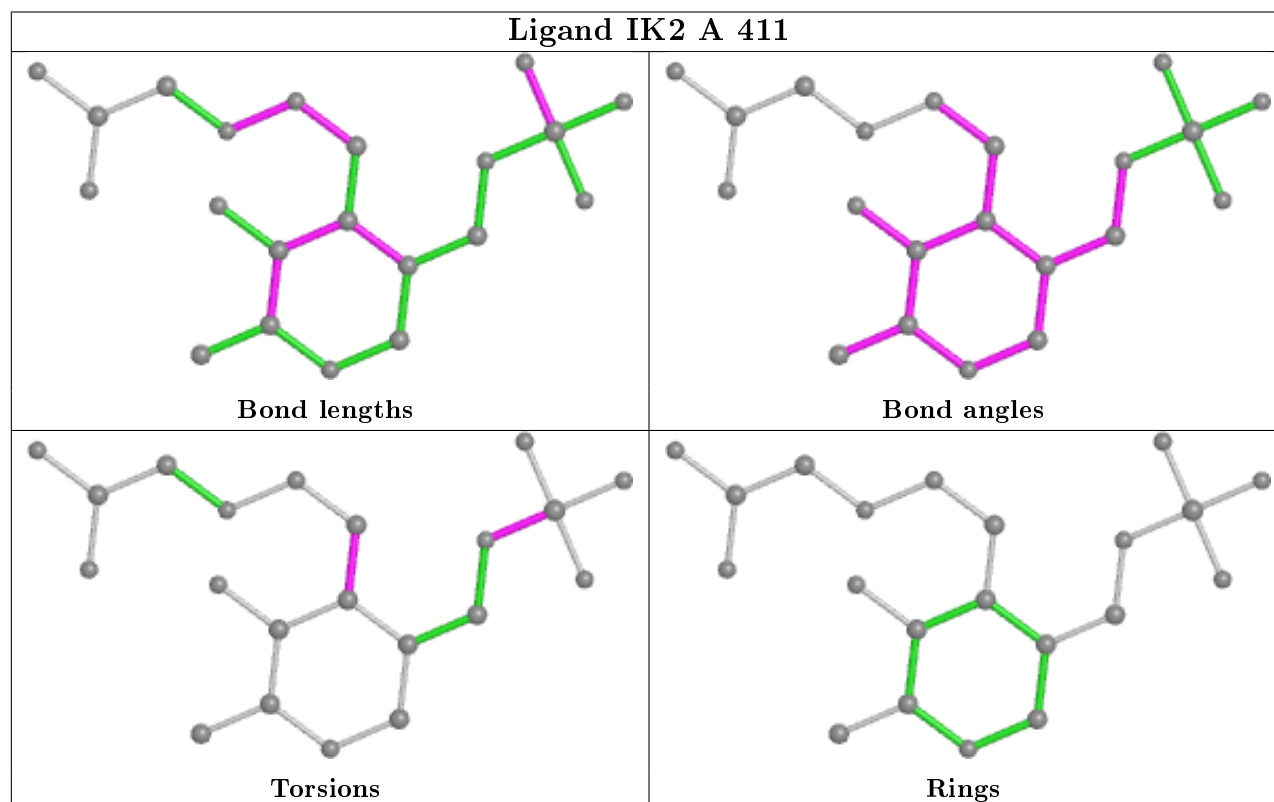
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	IK2	3	1

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.