Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 09:45 AM EST

PDB ID	:	1ADD
Title	:	A PRE-TRANSITION STATE MIMIC OF AN ENZYME: X-RAY STRUCTURE OF ADENOSINE DEAMINASE WITH BOUND 1-DEAZA-ADENOSINE AND ZINC-ACTIVATED WATER
Authors	:	Wilson, D.K.; Quiocho, F.A.
Deposited on	:	1992-12-22
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

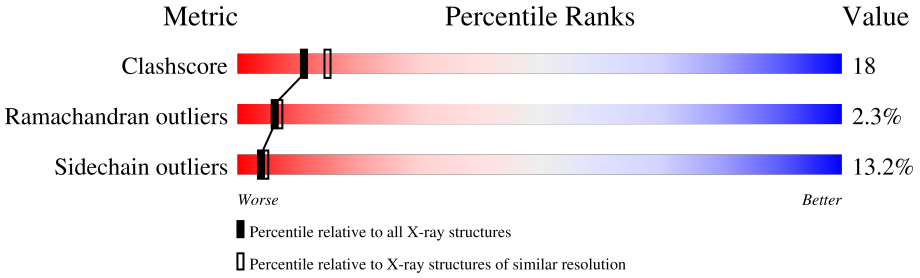
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	349	42% 40% 15% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2922 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.

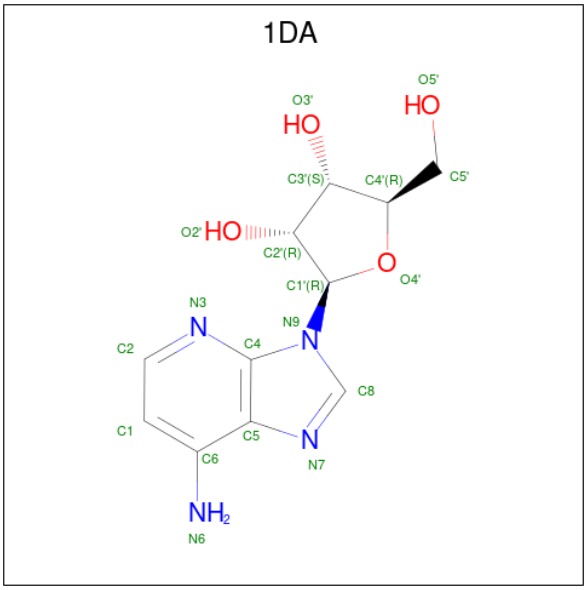
- Molecule 1 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2792	1778	470	530	14	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is 1-DEAZA-ADENOSINE (three-letter code: 1DA) (formula: $C_{11}H_{14}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	19	11	4	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	110	110	110	0	0

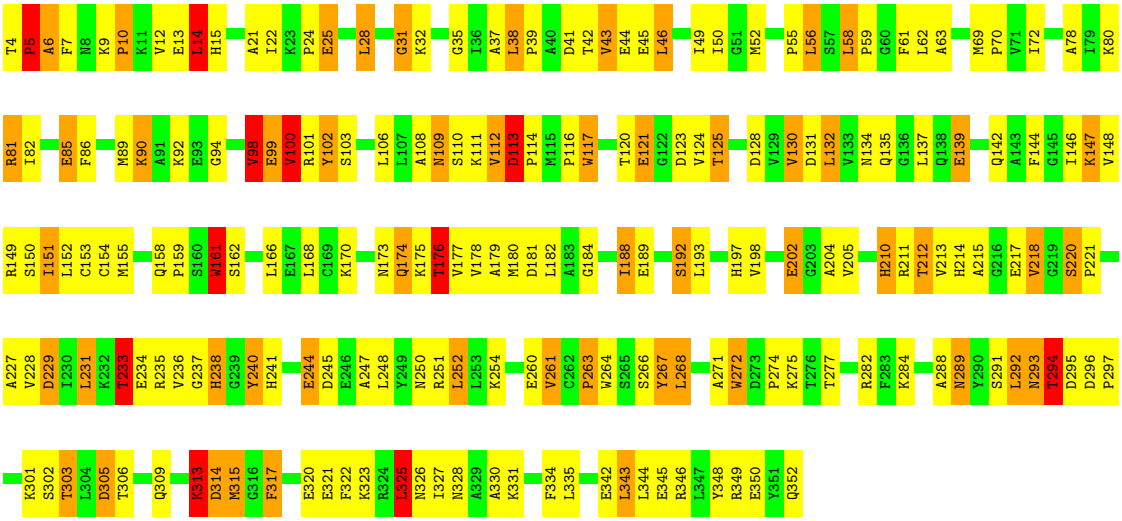
3 Residue-property plots (i)

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: ADENOSINE DEAMINASE

Chain A: 42% 40% 15% •



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.39Å 94.28Å 73.02Å 90.00° 127.05° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2922	wwPDB-VP
Average B, all atoms ($Å^2$)	20.0	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: 1DA, ZN

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	0.66	0/2856	1.04	13/3864 (0.3%)

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	A	0	109

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	TRP	CD1-CG-CD2	9.02	113.52	106.30
1	A	264	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	A	272	TRP	CD1-CG-CD2	8.85	113.38	106.30
1	A	161	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	117	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	A	272	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	264	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	161	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	A	117	TRP	CG-CD1-NE1	-6.26	103.84	110.10
1	A	264	TRP	CG-CD1-NE1	-6.25	103.86	110.10
1	A	161	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	272	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	A	117	TRP	CB-CG-CD1	-5.29	120.13	127.00

There are no chirality outliers.

All (109) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	VAL	Mainchain
1	A	102	TYR	Mainchain
1	A	106	LEU	Mainchain
1	A	112	VAL	Mainchain
1	A	113	ASP	Mainchain
1	A	117	TRP	Mainchain
1	A	12	VAL	Mainchain
1	A	123	ASP	Mainchain
1	A	130	VAL	Mainchain
1	A	131	ASP	Mainchain
1	A	132	LEU	Mainchain
1	A	137	LEU	Mainchain
1	A	139	GLU	Mainchain
1	A	14	LEU	Mainchain
1	A	142	GLN	Mainchain
1	A	144	PHE	Mainchain
1	A	146	ILE	Mainchain
1	A	15	HIS	Mainchain
1	A	150	SER	Mainchain
1	A	151	ILE	Mainchain
1	A	152	LEU	Mainchain
1	A	153	CYS	Mainchain
1	A	154	CYS	Mainchain
1	A	158	GLN	Mainchain
1	A	159	PRO	Mainchain
1	A	161	TRP	Mainchain
1	A	170	LYS	Mainchain
1	A	174	GLN	Mainchain
1	A	176	THR	Mainchain
1	A	177	VAL	Mainchain
1	A	181	ASP	Mainchain
1	A	182	LEU	Mainchain
1	A	184	GLY	Mainchain
1	A	188	ILE	Mainchain
1	A	192	SER	Mainchain
1	A	202	GLU	Mainchain
1	A	204	ALA	Mainchain
1	A	205	VAL	Mainchain
1	A	21	ALA	Mainchain
1	A	210	HIS	Mainchain
1	A	211	ARG	Mainchain
1	A	212	THR	Mainchain
1	A	214	HIS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	215	ALA	Mainchain
1	A	217	GLU	Mainchain
1	A	218	VAL	Mainchain
1	A	22	ILE	Mainchain
1	A	220	SER	Mainchain
1	A	227	ALA	Mainchain
1	A	228	VAL	Mainchain
1	A	229	ASP	Mainchain
1	A	233	THR	Mainchain
1	A	236	VAL	Mainchain
1	A	24	PRO	Mainchain
1	A	240	TYR	Mainchain
1	A	244	GLU	Mainchain
1	A	245	ASP	Mainchain
1	A	247	ALA	Mainchain
1	A	248	LEU	Mainchain
1	A	25	GLU	Mainchain
1	A	250	ASN	Mainchain
1	A	252	LEU	Mainchain
1	A	261	VAL	Mainchain
1	A	267	TYR	Mainchain
1	A	271	ALA	Mainchain
1	A	275	LYS	Mainchain
1	A	28	LEU	Mainchain
1	A	288	ALA	Mainchain
1	A	291	SER	Mainchain
1	A	293	ASN	Mainchain
1	A	294	THR	Mainchain
1	A	296	ASP	Mainchain
1	A	301	LYS	Mainchain
1	A	302	SER	Mainchain
1	A	305	ASP	Mainchain
1	A	306	THR	Mainchain
1	A	31	GLY	Mainchain
1	A	313	LYS	Mainchain
1	A	315	MET	Mainchain
1	A	317	PHE	Mainchain
1	A	320	GLU	Mainchain
1	A	321	GLU	Mainchain
1	A	323	LYS	Mainchain
1	A	325	LEU	Mainchain
1	A	342	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	344	LEU	Mainchain
1	A	345	GLU	Mainchain
1	A	349	ARG	Mainchain
1	A	35	GLY	Mainchain
1	A	37	ALA	Mainchain
1	A	41	ASP	Mainchain
1	A	43	VAL	Mainchain
1	A	46	LEU	Mainchain
1	A	5	PRO	Mainchain
1	A	50	ILE	Mainchain
1	A	55	PRO	Mainchain
1	A	58	LEU	Mainchain
1	A	6	ALA	Mainchain
1	A	62	LEU	Mainchain
1	A	63	ALA	Mainchain
1	A	72	ILE	Mainchain
1	A	80	LYS	Mainchain
1	A	85	GLU	Mainchain
1	A	89	MET	Mainchain
1	A	90	LYS	Mainchain
1	A	92	LYS	Mainchain
1	A	94	GLY	Mainchain
1	A	98	VAL	Mainchain
1	A	99	GLU	Mainchain

5.2 Too-close contacts (i)

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	2792	0	2757	101	0
2	A	1	0	0	0	0
3	A	19	0	14	0	0
4	A	110	0	0	2	0
All	All	2922	0	2771	101	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 18.

All (101) 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:213:VAL:HG23	1:A:233:THR:HG23	1.43	1.01
1:A:103:SER:HB2	1:A:155:MET:CE	2.01	0.91
1:A:155:MET:SD	4:A:482:HOH:O	2.28	0.90
1:A:28:LEU:HD13	1:A:46:LEU:HD22	1.54	0.89
1:A:52:MET:HE1	1:A:56:LEU:HB2	1.59	0.84
1:A:103:SER:HB2	1:A:155:MET:HE3	1.56	0.84
1:A:113:ASP:HB2	1:A:114:PRO:CD	2.12	0.80
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.63	0.80
1:A:237:GLY:O	1:A:238:HIS:HB2	1.82	0.79
1:A:113:ASP:HB2	1:A:114:PRO:HD2	1.65	0.79
1:A:149:ARG:HD3	1:A:178:VAL:HG11	1.65	0.76
1:A:261:VAL:HG12	1:A:263:PRO:HD3	1.68	0.76
1:A:125:THR:HG22	1:A:128:ASP:H	1.53	0.74
1:A:198:VAL:O	1:A:202:GLU:HG3	1.90	0.72
1:A:314:ASP:O	1:A:315:MET:HB2	1.90	0.71
1:A:13:GLU:OE2	1:A:294:THR:HB	1.93	0.68
1:A:113:ASP:CB	1:A:114:PRO:CD	2.71	0.68
1:A:9:LYS:HB3	1:A:10:PRO:HD2	1.75	0.68
1:A:103:SER:HB2	1:A:155:MET:HE2	1.75	0.68
1:A:52:MET:CE	1:A:56:LEU:HB2	2.26	0.66
1:A:109:ASN:C	1:A:109:ASN:HD22	1.99	0.65
1:A:109:ASN:HD21	1:A:124:VAL:H	1.43	0.64
1:A:289:ASN:ND2	1:A:328:ASN:HB3	2.13	0.64
1:A:135:GLN:O	1:A:139:GLU:HG3	1.99	0.63
1:A:149:ARG:HD3	1:A:178:VAL:CG1	2.27	0.63
1:A:162:SER:OG	1:A:197:HIS:HD2	1.82	0.63
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.82	0.62
1:A:235:ARG:NH1	1:A:260:GLU:OE2	2.33	0.61
1:A:325:LEU:C	1:A:325:LEU:HD23	2.21	0.61
1:A:210:HIS:HD2	1:A:234:GLU:OE1	1.84	0.60
1:A:4:THR:O	1:A:4:THR:HG23	2.00	0.60
1:A:99:GLU:OE1	1:A:235:ARG:NH2	2.35	0.60
1:A:86:PHE:CZ	1:A:100:VAL:HG13	2.37	0.59
1:A:213:VAL:CG2	1:A:233:THR:HG23	2.25	0.58
1:A:284:LYS:HD3	1:A:317:PHE:CE1	2.38	0.58
1:A:309:GLN:O	1:A:313:LYS:HE3	2.04	0.57
1:A:166:LEU:HA	1:A:180:MET:CE	2.36	0.56
1:A:330:ALA:HB1	1:A:343:LEU:HD13	1.87	0.56
1:A:81:ARG:O	1:A:85:GLU:HG3	2.06	0.55
1:A:303:THR:HG23	1:A:305:ASP:H	1.71	0.55
1:A:108:ALA:HB3	1:A:112:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:CD1	1:A:46:LEU:HD22	2.34	0.53
1:A:175:LYS:C	1:A:176:THR:HG23	2.29	0.53
1:A:327:ILE:O	1:A:331:LYS:HG3	2.10	0.52
1:A:166:LEU:HA	1:A:180:MET:HE1	1.90	0.52
1:A:28:LEU:HD13	1:A:46:LEU:CD2	2.33	0.52
1:A:325:LEU:C	1:A:325:LEU:CD2	2.79	0.51
1:A:151:ILE:HG12	1:A:179:ALA:HB3	1.93	0.51
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.28	0.51
1:A:162:SER:OG	1:A:197:HIS:CD2	2.63	0.50
1:A:325:LEU:HD23	1:A:326:ASN:N	2.27	0.50
1:A:45:GLU:O	1:A:49:ILE:HG12	2.11	0.50
1:A:322:PHE:O	1:A:325:LEU:HD22	2.12	0.49
1:A:39:PRO:HB2	1:A:49:ILE:HG21	1.94	0.49
1:A:212:THR:HA	1:A:233:THR:HG22	1.93	0.49
1:A:110:SER:O	1:A:112:VAL:HG23	2.12	0.49
1:A:14:LEU:H	1:A:293:ASN:ND2	2.11	0.49
1:A:113:ASP:CB	1:A:114:PRO:HD3	2.42	0.49
1:A:113:ASP:HB2	1:A:161:TRP:HE1	1.78	0.49
1:A:134:ASN:ND2	1:A:176:THR:OG1	2.46	0.48
1:A:210:HIS:CD2	1:A:234:GLU:OE1	2.66	0.48
1:A:13:GLU:HB3	1:A:98:VAL:HG13	1.96	0.48
1:A:81:ARG:HD3	1:A:85:GLU:OE2	2.14	0.48
1:A:325:LEU:CD2	1:A:326:ASN:N	2.77	0.48
1:A:314:ASP:O	1:A:315:MET:CB	2.57	0.47
1:A:4:THR:N	1:A:5:PRO:HD3	2.29	0.47
1:A:125:THR:HG22	1:A:128:ASP:N	2.26	0.47
1:A:237:GLY:O	1:A:238:HIS:CB	2.55	0.47
1:A:109:ASN:C	1:A:109:ASN:ND2	2.67	0.47
1:A:330:ALA:CB	1:A:343:LEU:HD13	2.46	0.46
1:A:220:SER:HB2	1:A:221:PRO:HD2	1.97	0.46
1:A:348:TYR:O	1:A:352:GLN:HG2	2.16	0.46
1:A:229:ASP:OD1	1:A:251:ARG:NH2	2.43	0.46
1:A:267:TYR:CD2	1:A:268:LEU:HD13	2.50	0.46
1:A:240:TYR:CE2	1:A:266:SER:HB3	2.51	0.46
1:A:42:THR:HG22	1:A:44:GLU:H	1.79	0.45
1:A:114:PRO:O	1:A:116:PRO:HD3	2.17	0.45
1:A:147:LYS:HE2	4:A:467:HOH:O	2.16	0.45
1:A:235:ARG:NH2	1:A:334:PHE:CE2	2.85	0.45
1:A:78:ALA:O	1:A:82:ILE:HG23	2.17	0.44
1:A:173:ASN:O	1:A:174:GLN:HB2	2.17	0.44
1:A:213:VAL:N	1:A:233:THR:HG21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:O	1:A:274:PRO:HD3	2.18	0.44
1:A:98:VAL:HG23	1:A:148:VAL:HG22	1.99	0.44
1:A:25:GLU:HG3	1:A:43:VAL:HG11	2.00	0.43
1:A:42:THR:HG22	1:A:44:GLU:HB2	2.01	0.43
1:A:188:ILE:O	1:A:188:ILE:HG22	2.19	0.43
1:A:102:TYR:OH	1:A:130:VAL:HA	2.18	0.43
1:A:241:HIS:HD2	1:A:244:GLU:OE2	2.01	0.43
1:A:90:LYS:HD3	1:A:90:LYS:HA	1.51	0.42
1:A:294:THR:HG21	1:A:297:PRO:HG3	2.00	0.42
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.90	0.42
1:A:166:LEU:CA	1:A:180:MET:CE	2.98	0.42
1:A:9:LYS:O	1:A:10:PRO:C	2.58	0.42
1:A:31:GLY:HA3	1:A:38:LEU:CD2	2.49	0.41
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.92	0.41
1:A:101:ARG:HA	1:A:151:ILE:O	2.21	0.41
1:A:292:LEU:HD22	1:A:325:LEU:HD11	2.02	0.41
1:A:5:PRO:O	1:A:7:PHE:N	2.54	0.40
1:A:69:MET:N	1:A:70:PRO:CD	2.84	0.40
1:A:235:ARG:NH2	1:A:334:PHE:CD2	2.89	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	347/349 (99%)	316 (91%)	23 (7%)	8 (2%)	6 7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	6	ALA

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	10	PRO
1	A	295	ASP
1	A	121	GLU
1	A	5	PRO
1	A	263	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	304/304 (100%)	264 (87%)	40 (13%)	4 4

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

Mol	Chain	Res	Type
1	A	14	LEU
1	A	32	LYS
1	A	38	LEU
1	A	56	LEU
1	A	61	PHE
1	A	81	ARG
1	A	98	VAL
1	A	100	VAL
1	A	109	ASN
1	A	111	LYS
1	A	113	ASP
1	A	120	THR
1	A	121	GLU
1	A	125	THR
1	A	132	LEU
1	A	147	LYS
1	A	168	LEU
1	A	176	THR
1	A	189	GLU
1	A	192	SER

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	218	VAL
1	A	231	LEU
1	A	233	THR
1	A	252	LEU
1	A	254	LYS
1	A	268	LEU
1	A	277	THR
1	A	282	ARG
1	A	289	ASN
1	A	292	LEU
1	A	294	THR
1	A	303	THR
1	A	313	LYS
1	A	314	ASP
1	A	325	LEU
1	A	335	LEU
1	A	343	LEU
1	A	346	ARG
1	A	350	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	119	GLN
1	A	134	ASN
1	A	197	HIS
1	A	210	HIS
1	A	241	HIS
1	A	289	ASN
1	A	293	ASN
1	A	326	ASN

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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	1DA	A	353	-	18,21,21	1.07	1 (5%)	19,31,31	1.39	3 (15%)

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
3	1DA	A	353	-	-	0/2/22/22	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	353	1DA	C6-C5	-3.05	1.37	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	353	1DA	C1-C2-N3	-3.06	119.84	124.58
3	A	353	1DA	C3'-C2'-C1'	2.52	104.77	100.98
3	A	353	1DA	O2'-C2'-C3'	-2.32	104.31	111.82

There are no chirality outliers.

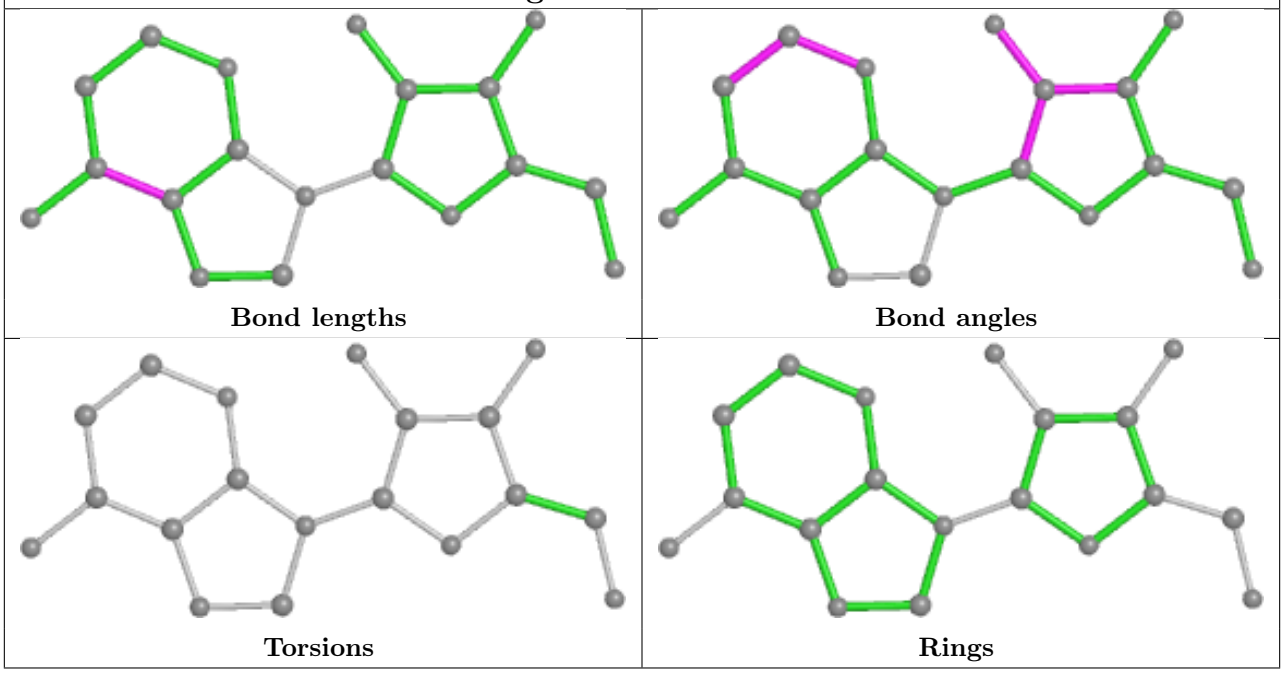
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand 1DA A 353



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.