



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:40 pm BST

PDB ID : 2ADA
Title : ATOMIC STRUCTURE OF ADENOSINE DEAMINASE COMPLEXED
WITH A TRANSITION-STATE ANALOG: UNDERSTANDING CATALY-
SIS AND IMMUNODEFICIENCY MUTATIONS
Authors : Wilson, D.K.; Quioco, F.A.
Deposited on : 1994-12-02
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 ⓘ 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

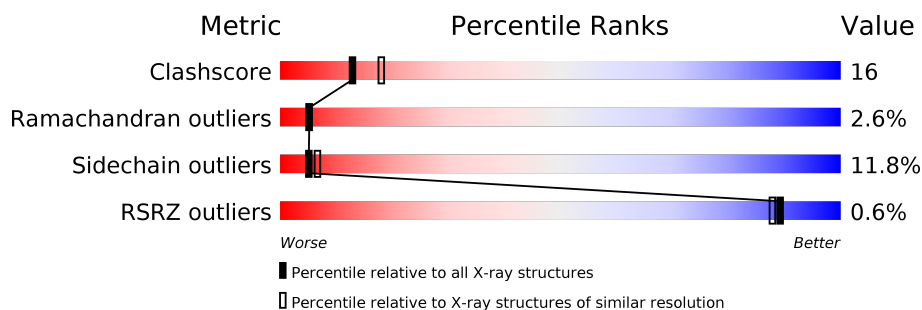
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)
RSRZ outliers	127900	3811 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	<div> <div></div> <div>53%</div> <div>35%</div> <div>10%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2870 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.

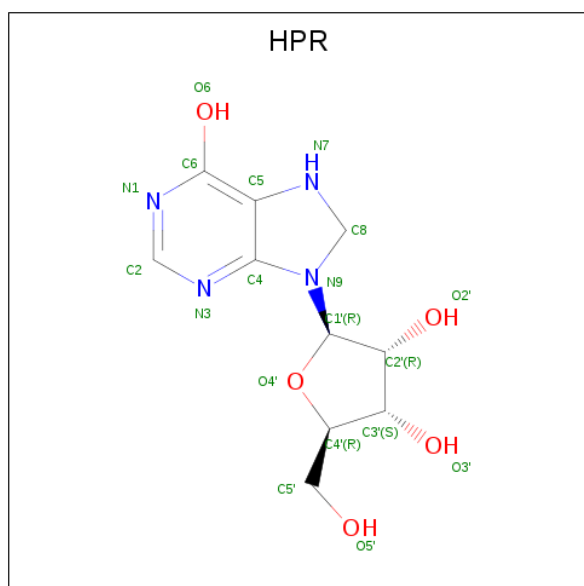
- Molecule 1 is a protein called ADENOSINE DEAMINASE.

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

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

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

- Molecule 3 is 6-HYDROXY-7,8-DIHYDRO PURINE NUCLEOSIDE (three-letter code: HPR) (formula: C₁₀H₁₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	4	5		

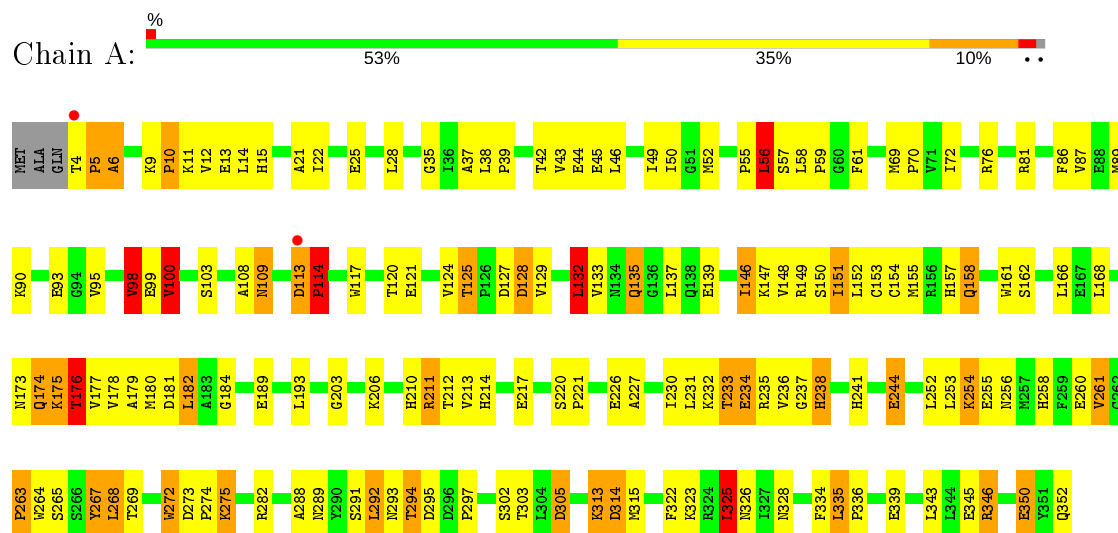
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: ADENOSINE DEAMINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.36 Å 94.11 Å 72.93 Å 90.00° 127.19° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 9.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 96.0 (9.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2870	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HPR, 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	0.62	0/2856	0.91	14/3864 (0.4%)

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	49

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	TRP	CD1-CG-CD2	9.09	113.57	106.30
1	A	117	TRP	CD1-CG-CD2	9.00	113.50	106.30
1	A	161	TRP	CD1-CG-CD2	8.89	113.41	106.30
1	A	272	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	A	117	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	264	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	272	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	161	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	161	TRP	CG-CD1-NE1	-6.22	103.88	110.10
1	A	264	TRP	CG-CD1-NE1	-6.22	103.88	110.10
1	A	117	TRP	CG-CD1-NE1	-6.22	103.88	110.10
1	A	272	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	A	117	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	A	264	TRP	CB-CG-CD1	-5.13	120.33	127.00

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	VAL	Mainchain
1	A	108	ALA	Mainchain
1	A	114	PRO	Mainchain
1	A	12	VAL	Mainchain
1	A	132	LEU	Mainchain
1	A	135	GLN	Mainchain
1	A	137	LEU	Mainchain
1	A	146	ILE	Mainchain
1	A	148	VAL	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	162	SER	Mainchain
1	A	175	LYS	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	21	ALA	Mainchain
1	A	211	ARG	Mainchain
1	A	217	GLU	Mainchain
1	A	22	ILE	Mainchain
1	A	227	ALA	Mainchain
1	A	232	LYS	Mainchain
1	A	234	GLU	Mainchain
1	A	236	VAL	Mainchain
1	A	244	GLU	Mainchain
1	A	261	VAL	Mainchain
1	A	267	TYR	Mainchain
1	A	291	SER	Mainchain
1	A	293	ASN	Mainchain
1	A	302	SER	Mainchain
1	A	305	ASP	Mainchain
1	A	323	LYS	Mainchain
1	A	325	LEU	Mainchain
1	A	345	GLU	Mainchain
1	A	35	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	37	ALA	Mainchain
1	A	55	PRO	Mainchain
1	A	56	LEU	Mainchain
1	A	6	ALA	Mainchain
1	A	72	ILE	Mainchain
1	A	98	VAL	Mainchain
1	A	99	GLU	Mainchain

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	2792	0	2757	92	0
2	A	1	0	0	0	0
3	A	19	0	13	0	0
4	A	58	0	0	0	0
All	All	2870	0	2770	92	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 16.

All (92) 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:113:ASP:HB3	1:A:114:PRO:HD3	1.33	1.05
1:A:292:LEU:HD22	1:A:325:LEU:HD11	1.54	0.90
1:A:113:ASP:HB3	1:A:114:PRO:CD	2.10	0.81
1:A:325:LEU:HD23	1:A:326:ASN:N	1.99	0.78
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.68	0.75
1:A:254:LYS:HE2	1:A:255:GLU:HG3	1.68	0.75
1:A:261:VAL:HG12	1:A:263:PRO:HD3	1.69	0.75
1:A:289:ASN:ND2	1:A:328:ASN:HB3	2.06	0.69
1:A:9:LYS:HB3	1:A:10:PRO:HD2	1.77	0.66
1:A:28:LEU:HD13	1:A:46:LEU:HD22	1.77	0.66
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.77	0.65
1:A:149:ARG:HD3	1:A:178:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:HG23	1:A:305:ASP:H	1.65	0.61
1:A:52:MET:HE3	1:A:56:LEU:HB2	1.81	0.60
1:A:95:VAL:CG1	1:A:98:VAL:HG22	2.31	0.60
1:A:173:ASN:O	1:A:174:GLN:HB2	2.00	0.59
1:A:13:GLU:OE1	1:A:294:THR:HB	2.04	0.57
1:A:314:ASP:O	1:A:315:MET:HB2	2.03	0.57
1:A:175:LYS:C	1:A:176:THR:HG23	2.24	0.57
1:A:166:LEU:HA	1:A:180:MET:HE1	1.87	0.57
1:A:45:GLU:O	1:A:49:ILE:HG12	2.05	0.56
1:A:166:LEU:HA	1:A:180:MET:CE	2.36	0.55
1:A:237:GLY:O	1:A:238:HIS:HB2	2.06	0.55
1:A:39:PRO:HB2	1:A:49:ILE:HG21	1.90	0.54
1:A:149:ARG:HD3	1:A:178:VAL:HG11	1.89	0.53
1:A:89:MET:O	1:A:93:GLU:HG3	2.07	0.53
1:A:282:ARG:O	1:A:282:ARG:HG3	2.09	0.53
1:A:325:LEU:HD23	1:A:325:LEU:C	2.27	0.53
1:A:4:THR:O	1:A:4:THR:HG23	2.09	0.53
1:A:210:HIS:HD2	1:A:234:GLU:OE2	1.92	0.53
1:A:272:TRP:O	1:A:274:PRO:HD3	2.08	0.53
1:A:13:GLU:HB3	1:A:98:VAL:HG13	1.89	0.52
1:A:95:VAL:HG11	1:A:98:VAL:HG22	1.90	0.52
1:A:103:SER:HB2	1:A:155:MET:CE	2.40	0.52
1:A:125:THR:HG23	1:A:127:ASP:H	1.73	0.51
1:A:103:SER:HB2	1:A:155:MET:HE3	1.92	0.51
1:A:213:VAL:N	1:A:233:THR:HG21	2.26	0.50
1:A:289:ASN:HD21	1:A:328:ASN:HB3	1.74	0.50
1:A:76:ARG:HG2	1:A:132:LEU:HD21	1.94	0.50
1:A:42:THR:HG22	1:A:44:GLU:H	1.77	0.50
1:A:253:LEU:HD11	1:A:288:ALA:HB2	1.94	0.50
1:A:109:ASN:HD21	1:A:124:VAL:H	1.60	0.49
1:A:220:SER:HB2	1:A:221:PRO:HD2	1.94	0.49
1:A:25:GLU:HG3	1:A:43:VAL:HG11	1.93	0.49
1:A:294:THR:HG21	1:A:297:PRO:HG3	1.93	0.49
1:A:86:PHE:CZ	1:A:100:VAL:HG13	2.47	0.49
1:A:151:ILE:HG12	1:A:179:ALA:HB3	1.95	0.49
1:A:241:HIS:HD2	1:A:244:GLU:OE2	1.96	0.49
1:A:166:LEU:HB2	1:A:180:MET:HE1	1.95	0.49
1:A:157:HIS:CD2	1:A:158:GLN:HG2	2.48	0.48
1:A:182:LEU:O	1:A:214:HIS:HB2	2.12	0.48
1:A:265:SER:O	1:A:269:THR:HG23	2.14	0.48
1:A:95:VAL:HG12	1:A:98:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLN:O	1:A:139:GLU:HG3	2.14	0.47
1:A:87:VAL:HG13	1:A:146:ILE:HD11	1.95	0.47
1:A:58:LEU:HB3	1:A:59:PRO:CD	2.44	0.46
1:A:113:ASP:CB	1:A:114:PRO:CD	2.86	0.45
1:A:166:LEU:CA	1:A:180:MET:HE1	2.46	0.45
1:A:4:THR:N	1:A:5:PRO:HD3	2.32	0.45
1:A:125:THR:HG22	1:A:128:ASP:OD1	2.17	0.45
1:A:336:PRO:HG2	1:A:339:GLU:OE2	2.16	0.45
1:A:46:LEU:HG	1:A:50:ILE:HD12	1.99	0.45
1:A:125:THR:HG23	1:A:127:ASP:N	2.32	0.44
1:A:322:PHE:HA	1:A:325:LEU:HD22	1.99	0.44
1:A:69:MET:N	1:A:70:PRO:HD2	2.31	0.44
1:A:273:ASP:OD2	1:A:275:LYS:HG3	2.17	0.44
1:A:235:ARG:HD2	1:A:260:GLU:OE2	2.17	0.44
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.85	0.44
1:A:313:LYS:N	1:A:313:LYS:HD3	2.31	0.44
1:A:346:ARG:HD3	1:A:350:GLU:OE2	2.18	0.44
1:A:166:LEU:CB	1:A:180:MET:HE1	2.48	0.44
1:A:125:THR:HG22	1:A:128:ASP:H	1.83	0.43
1:A:56:LEU:HB3	1:A:57:SER:H	1.67	0.43
1:A:176:THR:O	1:A:178:VAL:HG13	2.18	0.43
1:A:109:ASN:C	1:A:109:ASN:HD22	2.22	0.43
1:A:90:LYS:HA	1:A:90:LYS:HD3	1.69	0.43
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.42	0.43
1:A:335:LEU:HA	1:A:335:LEU:HD12	1.88	0.42
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.94	0.42
1:A:203:GLY:HA2	1:A:206:LYS:HG2	2.01	0.42
1:A:235:ARG:HD3	1:A:258:HIS:CD2	2.54	0.42
1:A:292:LEU:HA	1:A:292:LEU:HD12	1.82	0.42
1:A:212:THR:HA	1:A:233:THR:HG22	2.01	0.42
1:A:9:LYS:O	1:A:11:LYS:HG3	2.20	0.41
1:A:294:THR:HG23	1:A:297:PRO:HD3	2.03	0.41
1:A:129:VAL:O	1:A:133:VAL:HG23	2.21	0.41
1:A:179:ALA:HB2	1:A:334:PHE:CD2	2.56	0.41
1:A:303:THR:HG23	1:A:305:ASP:N	2.31	0.41
1:A:267:TYR:CD1	1:A:268:LEU:HD13	2.55	0.41
1:A:213:VAL:H	1:A:233:THR:HG21	1.86	0.40
1:A:226:GLU:HG2	1:A:230:ILE:HD12	2.02	0.40
1:A:322:PHE:O	1:A:325:LEU:HD22	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	347/352 (99%)	318 (92%)	20 (6%)	9 (3%)	5 5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	113	ASP
1	A	6	ALA
1	A	238	HIS
1	A	10	PRO
1	A	176	THR
1	A	295	ASP
1	A	263	PRO
1	A	114	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	304/306 (99%)	268 (88%)	36 (12%)	5 7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	38	LEU

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Mol	Chain	Res	Type
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	120	THR
1	A	121	GLU
1	A	125	THR
1	A	128	ASP
1	A	132	LEU
1	A	147	LYS
1	A	168	LEU
1	A	174	GLN
1	A	189	GLU
1	A	193	LEU
1	A	211	ARG
1	A	231	LEU
1	A	233	THR
1	A	252	LEU
1	A	254	LYS
1	A	256	ASN
1	A	268	LEU
1	A	275	LYS
1	A	292	LEU
1	A	294	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
1	A	352	GLN

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	109	ASN
1	A	119	GLN
1	A	134	ASN
1	A	197	HIS

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Mol	Chain	Res	Type
1	A	210	HIS
1	A	241	HIS
1	A	256	ASN
1	A	289	ASN
1	A	293	ASN
1	A	326	ASN

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 ⓘ

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	HPR	A	353	2	17,21,21	1.34	3 (17%)	20,31,31	1.84	5 (25%)

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	HPR	A	353	2	-	2/6/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	353	HPR	C8-N7	-3.04	1.34	1.43
3	A	353	HPR	C1'-N9	-2.96	1.40	1.46
3	A	353	HPR	O6-C6	2.86	1.42	1.29

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	353	HPR	O6-C6-C5	-5.31	110.92	126.02
3	A	353	HPR	N3-C2-N1	-2.74	124.32	128.60
3	A	353	HPR	C2-N3-C4	2.47	117.59	111.75
3	A	353	HPR	O2'-C2'-C3'	-2.43	103.97	111.82
3	A	353	HPR	N3-C4-N9	2.00	129.40	126.87

There are no chirality outliers.

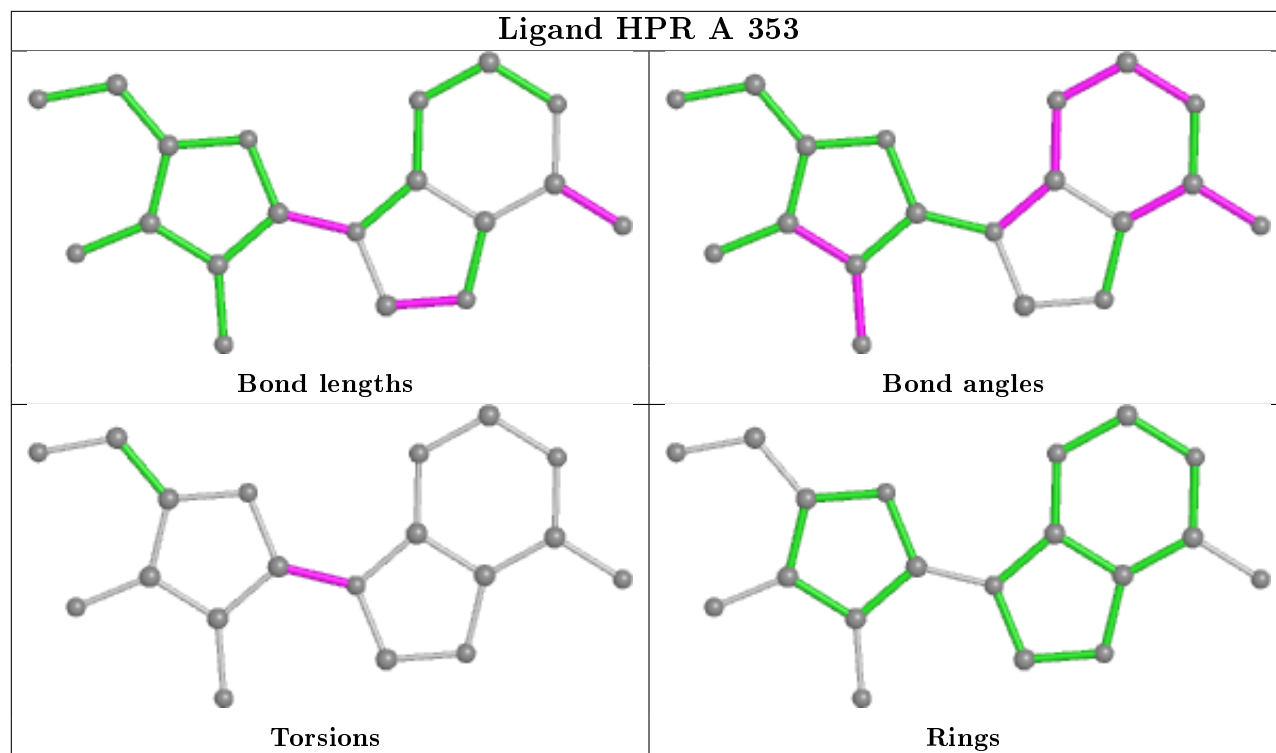
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	353	HPR	C2'-C1'-N9-C8
3	A	353	HPR	O4'-C1'-N9-C8

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/352 (99%)	-0.91	2 (0%) 89 88	5, 17, 41, 69	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	ASP	3.2
1	A	4	THR	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

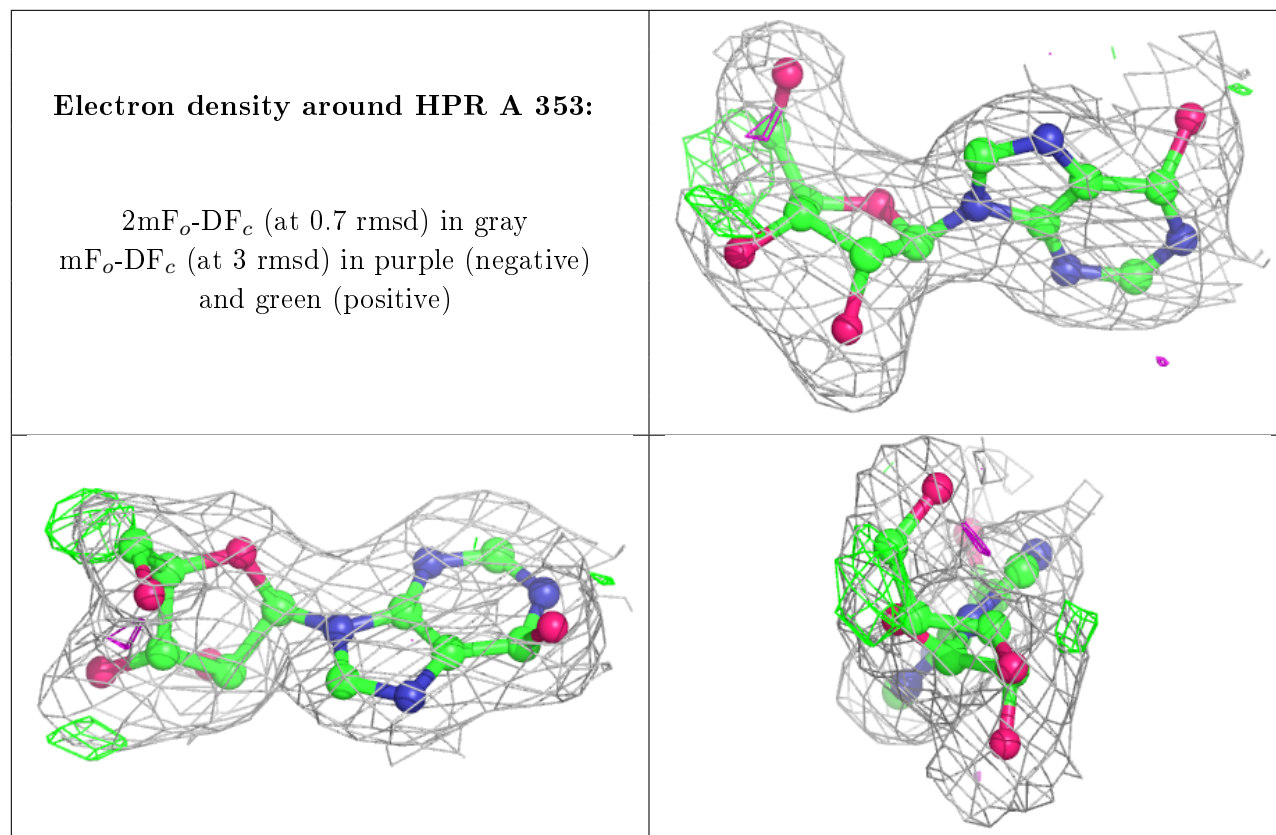
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HPR	A	353	19/19	0.98	0.06	2,6,10,12	0
2	ZN	A	400	1/1	1.00	0.04	12,12,12,12	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.