



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:44 am GMT

PDB ID : 1NDY  
Title : Crystal Structure of Adenosine Deaminase Complexed with FR230513  
Authors : Kinoshita, T.  
Deposited on : 2002-12-09  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

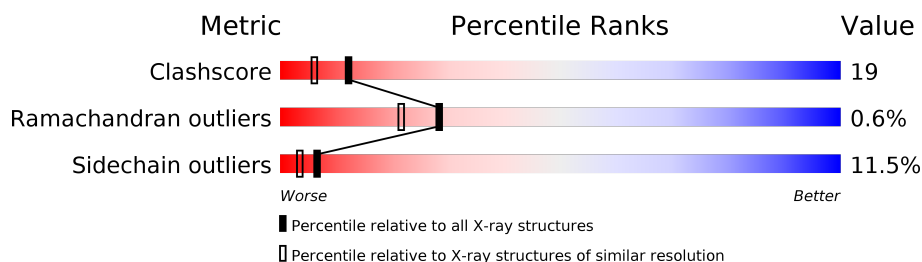
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	356	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3254 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
			2788	1772	471	533	12			

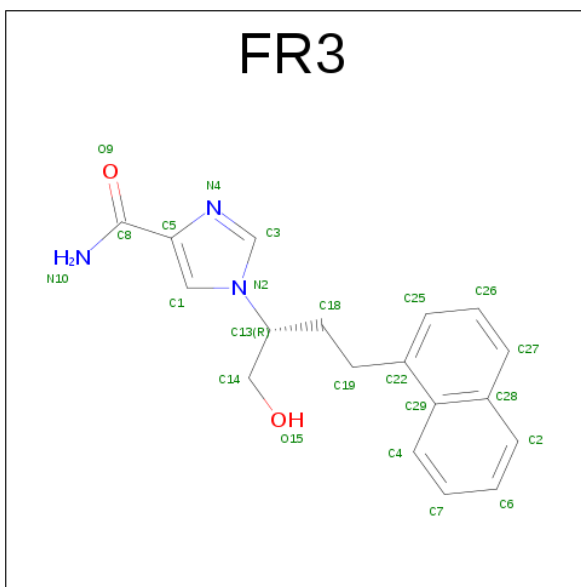
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	ASN	SEE REMARK 999	UNP P56658
A	32	LYS	ARG	SEE REMARK 999	UNP P56658
A	33	ARG	LYS	SEE REMARK 999	UNP P56658
A	57	THR	SER	SEE REMARK 999	UNP P56658
A	60	ASP	GLU	SEE REMARK 999	UNP P56658
A	77	ASP	GLU	SEE REMARK 999	UNP P56658
A	79	ILE	VAL	SEE REMARK 999	UNP P56658
A	199	GLN	LYS	SEE REMARK 999	UNP P56658
A	246	THR	ALA	SEE REMARK 999	UNP P56658
A	261	ILE	VAL	SEE REMARK 999	UNP P56658
A	279	ALA	PRO	SEE REMARK 999	UNP P56658
A	281	ILE	VAL	SEE REMARK 999	UNP P56658
A	313	LYS	ASN	SEE REMARK 999	UNP P56658
A	314	ASP	GLU	SEE REMARK 999	UNP P56658
A	352	ARG	GLY	SEE REMARK 999	UNP P56658

- 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 1-((1R)-1-(HYDROXYMETHYL)-3-(1-NAPHTHYL)PROPYL)-1H-IMIDAZOLE-4-CARBOXAMIDE (three-letter code: FR3) (formula: C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	18	3	2		

- Molecule 4 is water.

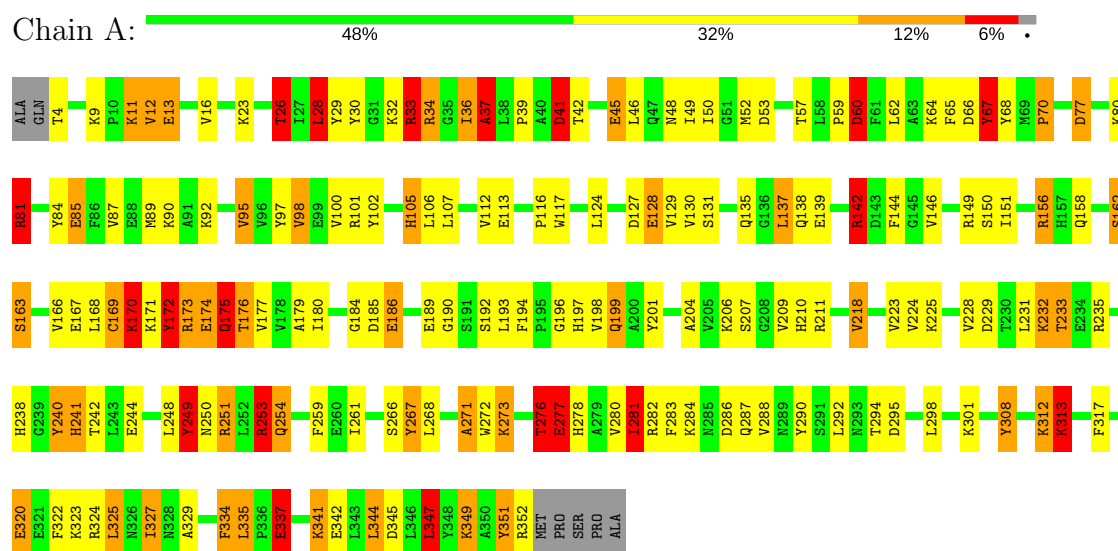
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	442	Total	O	0	0
			442	442		

### 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 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.

Note EDS was not executed.

#### • Molecule 1: Adenosine Deaminase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.92Å 77.92Å 136.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNX	Depositor
R, $R_{free}$	0.203 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: FR3, 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	1.81	41/2852 (1.4%)	2.39	148/3866 (3.8%)

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	1	14

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	GLU	CG-CD	10.86	1.68	1.51
1	A	199	GLN	CG-CD	8.38	1.70	1.51
1	A	85	GLU	CD-OE1	-8.32	1.16	1.25
1	A	198	VAL	CB-CG1	7.52	1.68	1.52
1	A	176	THR	N-CA	7.50	1.61	1.46
1	A	13	GLU	CD-OE1	-7.06	1.17	1.25
1	A	308	TYR	CE2-CZ	6.95	1.47	1.38
1	A	190	GLY	CA-C	6.93	1.62	1.51
1	A	277	GLU	CB-CG	6.90	1.65	1.52
1	A	60	ASP	CB-CG	6.86	1.66	1.51
1	A	101	ARG	CZ-NH2	6.85	1.42	1.33
1	A	322	PHE	CE2-CZ	6.84	1.50	1.37
1	A	142	ARG	NE-CZ	6.72	1.41	1.33
1	A	189	GLU	CG-CD	6.50	1.61	1.51
1	A	249	TYR	CE1-CZ	6.32	1.46	1.38
1	A	194	PHE	CG-CD1	6.31	1.48	1.38
1	A	149	ARG	CZ-NH1	6.22	1.41	1.33
1	A	253	ARG	NE-CZ	6.08	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	TYR	CG-CD2	6.04	1.47	1.39
1	A	196	GLY	CA-C	5.97	1.61	1.51
1	A	342	GLU	CB-CG	5.93	1.63	1.52
1	A	85	GLU	CG-CD	5.91	1.60	1.51
1	A	224	VAL	CB-CG1	5.87	1.65	1.52
1	A	106	LEU	CA-CB	5.61	1.66	1.53
1	A	192	SER	N-CA	5.57	1.57	1.46
1	A	34	ARG	NE-CZ	5.53	1.40	1.33
1	A	60	ASP	CA-CB	5.50	1.66	1.53
1	A	167	GLU	CD-OE1	-5.47	1.19	1.25
1	A	102	TYR	CA-CB	5.46	1.66	1.53
1	A	169	CYS	CB-SG	-5.43	1.73	1.81
1	A	177	VAL	CB-CG1	5.35	1.64	1.52
1	A	240	TYR	CE2-CZ	5.25	1.45	1.38
1	A	342	GLU	CD-OE1	-5.21	1.20	1.25
1	A	320	GLU	CG-CD	5.19	1.59	1.51
1	A	162	SER	CB-OG	5.12	1.49	1.42
1	A	184	GLY	N-CA	5.09	1.53	1.46
1	A	351	TYR	CB-CG	5.08	1.59	1.51
1	A	290	TYR	CG-CD1	5.06	1.45	1.39
1	A	112	VAL	CA-CB	-5.05	1.44	1.54
1	A	131	SER	CA-CB	5.04	1.60	1.52
1	A	186	GLU	CD-OE2	-5.03	1.20	1.25

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ARG	NE-CZ-NH2	19.05	129.82	120.30
1	A	34	ARG	NE-CZ-NH1	16.92	128.76	120.30
1	A	34	ARG	NE-CZ-NH2	-16.53	112.03	120.30
1	A	251	ARG	NE-CZ-NH1	-15.46	112.57	120.30
1	A	267	TYR	CB-CG-CD1	-14.51	112.29	121.00
1	A	101	ARG	NE-CZ-NH2	14.14	127.37	120.30
1	A	251	ARG	NE-CZ-NH2	13.00	126.80	120.30
1	A	60	ASP	CB-CG-OD2	12.84	129.85	118.30
1	A	101	ARG	NE-CZ-NH1	-12.61	113.99	120.30
1	A	253	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	67	TYR	CG-CD1-CE1	-11.46	112.13	121.30
1	A	34	ARG	CD-NE-CZ	10.53	138.34	123.60
1	A	253	ARG	CD-NE-CZ	10.47	138.26	123.60
1	A	170	LYS	CD-CE-NZ	-10.35	87.90	111.70
1	A	218	VAL	CA-CB-CG1	10.33	126.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	10.27	135.99	113.40
1	A	344	LEU	CB-CG-CD1	10.12	128.21	111.00
1	A	30	TYR	CB-CG-CD1	-10.08	114.95	121.00
1	A	81	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	A	325	LEU	CB-CG-CD2	9.70	127.49	111.00
1	A	218	VAL	CA-CB-CG2	9.49	125.14	110.90
1	A	209	VAL	CA-CB-CG1	9.41	125.02	110.90
1	A	277	GLU	CA-CB-CG	9.39	134.07	113.40
1	A	66	ASP	CB-CG-OD2	-9.33	109.91	118.30
1	A	294	THR	CA-CB-OG1	9.25	128.42	109.00
1	A	166	VAL	CA-CB-CG2	9.24	124.76	110.90
1	A	156	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	158	GLN	CG-CD-OE1	9.08	139.76	121.60
1	A	33	ARG	NE-CZ-NH2	9.05	124.83	120.30
1	A	259	PHE	CB-CG-CD1	-8.84	114.61	120.80
1	A	33	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	A	173	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	89	MET	CA-CB-CG	8.57	127.87	113.30
1	A	149	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	201	TYR	CB-CG-CD2	-8.46	115.93	121.00
1	A	95	VAL	CG1-CB-CG2	-8.35	97.54	110.90
1	A	97	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	A	194	PHE	CB-CG-CD2	-8.29	115.00	120.80
1	A	308	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	A	276	THR	N-CA-CB	-8.24	94.65	110.30
1	A	67	TYR	CZ-CE2-CD2	-8.11	112.50	119.80
1	A	233	THR	CA-CB-CG2	8.08	123.71	112.40
1	A	30	TYR	CG-CD1-CE1	-8.04	114.87	121.30
1	A	282	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	267	TYR	CB-CG-CD2	7.95	125.77	121.00
1	A	33	ARG	CD-NE-CZ	-7.92	112.51	123.60
1	A	271	ALA	CB-CA-C	-7.81	98.39	110.10
1	A	223	VAL	CA-CB-CG1	7.77	122.56	110.90
1	A	199	GLN	CA-CB-CG	-7.75	96.34	113.40
1	A	211	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	281	ILE	CB-CG1-CD1	-7.70	92.34	113.90
1	A	281	ILE	CA-CB-CG2	7.62	126.14	110.90
1	A	277	GLU	CB-CG-CD	7.62	134.77	114.20
1	A	129	VAL	CG1-CB-CG2	-7.59	98.76	110.90
1	A	312	LYS	CA-CB-CG	-7.58	96.73	113.40
1	A	254	GLN	CB-CG-CD	-7.52	92.04	111.60
1	A	235	ARG	NE-CZ-NH1	7.42	124.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	VAL	CG1-CB-CG2	7.36	122.67	110.90
1	A	60	ASP	OD1-CG-OD2	-7.31	109.40	123.30
1	A	137	LEU	CB-CG-CD1	7.31	123.43	111.00
1	A	98	VAL	CG1-CB-CG2	-7.25	99.31	110.90
1	A	168	LEU	CB-CG-CD2	7.02	122.93	111.00
1	A	317	PHE	CB-CG-CD2	-7.02	115.89	120.80
1	A	240	TYR	CB-CG-CD1	-7.00	116.80	121.00
1	A	84	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	A	206	LYS	CD-CE-NZ	-6.93	95.75	111.70
1	A	172	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	A	142	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	A	81	ARG	CD-NE-CZ	6.77	133.08	123.60
1	A	334	PHE	CB-CG-CD2	-6.68	116.12	120.80
1	A	347	LEU	CD1-CG-CD2	6.67	130.51	110.50
1	A	29	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	30	TYR	CD1-CG-CD2	6.60	125.16	117.90
1	A	156	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	67	TYR	N-CA-CB	6.58	122.45	110.60
1	A	335	LEU	CB-CG-CD1	6.57	122.17	111.00
1	A	166	VAL	CA-CB-CG1	6.56	120.74	110.90
1	A	327	ILE	CA-CB-CG1	6.56	123.46	111.00
1	A	146	VAL	CA-CB-CG2	6.49	120.63	110.90
1	A	65	PHE	CB-CG-CD2	-6.45	116.28	120.80
1	A	209	VAL	CA-CB-CG2	6.36	120.44	110.90
1	A	67	TYR	CB-CA-C	-6.29	97.83	110.40
1	A	131	SER	CB-CA-C	6.19	121.86	110.10
1	A	158	GLN	CG-CD-NE2	-5.98	102.34	116.70
1	A	66	ASP	CA-CB-CG	-5.94	100.33	113.40
1	A	290	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	335	LEU	CB-CG-CD2	5.91	121.05	111.00
1	A	201	TYR	CD1-CE1-CZ	-5.89	114.50	119.80
1	A	233	THR	CB-CA-C	-5.86	95.77	111.60
1	A	4	THR	CA-CB-CG2	5.86	120.60	112.40
1	A	68	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	A	131	SER	N-CA-CB	-5.85	101.72	110.50
1	A	37	ALA	N-CA-C	5.79	126.64	111.00
1	A	308	TYR	CD1-CG-CD2	5.77	124.24	117.90
1	A	335	LEU	CB-CA-C	-5.74	99.29	110.20
1	A	288	VAL	CA-CB-CG2	-5.72	102.33	110.90
1	A	337	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	87	VAL	CA-CB-CG2	5.70	119.45	110.90
1	A	351	TYR	CB-CG-CD1	-5.69	117.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	TYR	CG-CD2-CE2	-5.69	116.75	121.30
1	A	107	LEU	CB-CG-CD2	5.68	120.65	111.00
1	A	77	ASP	CB-CA-C	5.59	121.59	110.40
1	A	146	VAL	CG1-CB-CG2	-5.59	101.95	110.90
1	A	46	LEU	CD1-CG-CD2	-5.57	93.79	110.50
1	A	149	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	175	GLN	N-CA-C	5.55	125.99	111.00
1	A	267	TYR	CZ-CE2-CD2	-5.55	114.80	119.80
1	A	41	ASP	CB-CA-C	-5.54	99.32	110.40
1	A	12	VAL	CA-CB-CG2	-5.51	102.64	110.90
1	A	67	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	254	GLN	CA-CB-CG	-5.49	101.33	113.40
1	A	105	HIS	CG-ND1-CE1	-5.48	98.57	105.70
1	A	325	LEU	N-CA-CB	-5.38	99.64	110.40
1	A	223	VAL	CG1-CB-CG2	5.32	119.41	110.90
1	A	286	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	62	LEU	CB-CA-C	-5.29	100.15	110.20
1	A	52	MET	CG-SD-CE	5.29	108.66	100.20
1	A	301	LYS	CA-CB-CG	-5.26	101.83	113.40
1	A	313	LYS	C-N-CA	-5.25	108.57	121.70
1	A	26	THR	OG1-CB-CG2	5.25	122.06	110.00
1	A	112	VAL	CA-CB-CG1	5.24	118.76	110.90
1	A	128	GLU	N-CA-CB	-5.24	101.17	110.60
1	A	37	ALA	N-CA-CB	5.22	117.41	110.10
1	A	142	ARG	CD-NE-CZ	-5.21	116.30	123.60
1	A	144	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	A	11	LYS	CA-CB-CG	-5.19	101.98	113.40
1	A	97	TYR	CD1-CG-CD2	5.19	123.61	117.90
1	A	199	GLN	CB-CG-CD	5.18	125.06	111.60
1	A	176	THR	CB-CA-C	-5.16	97.67	111.60
1	A	163	SER	C-N-CA	-5.15	108.83	121.70
1	A	142	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
1	A	127	ASP	CA-C-O	5.13	130.87	120.10
1	A	253	ARG	CG-CD-NE	5.10	122.51	111.80
1	A	282	ARG	CA-C-O	5.09	130.79	120.10
1	A	146	VAL	N-CA-C	-5.08	97.28	111.00
1	A	37	ALA	CA-C-O	5.07	130.74	120.10
1	A	28	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	A	139	GLU	CA-CB-CG	-5.05	102.28	113.40
1	A	68	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
1	A	229	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	232	LYS	CB-CG-CD	5.04	124.70	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	VAL	N-CA-CB	-5.03	100.43	111.50
1	A	12	VAL	CA-CB-CG1	5.03	118.44	110.90
1	A	12	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	A	241	HIS	CB-CA-C	-5.02	100.36	110.40
1	A	102	TYR	CG-CD2-CE2	-5.01	117.29	121.30
1	A	232	LYS	CA-CB-CG	5.00	124.41	113.40
1	A	185	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	THR	CB

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	156	ARG	Sidechain
1	A	172	TYR	Sidechain
1	A	174	GLU	Peptide
1	A	249	TYR	Sidechain
1	A	251	ARG	Sidechain
1	A	267	TYR	Sidechain
1	A	33	ARG	Sidechain
1	A	334	PHE	Sidechain
1	A	34	ARG	Sidechain
1	A	352	ARG	Sidechain
1	A	37	ALA	Peptide
1	A	67	TYR	Sidechain
1	A	81	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	2788	0	2743	106	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	19	0	0
4	A	442	0	0	57	0
All	All	3254	0	2762	106	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 19.

All (106) 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:278:HIS:HD2	1:A:280:VAL:H	1.11	0.95
1:A:327:ILE:HB	4:A:1383:HOH:O	1.74	0.88
1:A:23:LYS:HB2	1:A:26:THR:HG23	1.60	0.83
1:A:324:ARG:HA	4:A:1383:HOH:O	1.80	0.81
1:A:186:GLU:HB3	4:A:1103:HOH:O	1.81	0.80
1:A:344:LEU:HD22	4:A:1099:HOH:O	1.81	0.79
1:A:278:HIS:CD2	1:A:280:VAL:H	2.00	0.79
1:A:26:THR:HG21	1:A:85:GLU:OE2	1.83	0.78
1:A:57:THR:HG22	1:A:60:ASP:HB2	1.65	0.78
1:A:248:LEU:HD13	4:A:1226:HOH:O	1.85	0.76
1:A:249:TYR:HD2	4:A:1047:HOH:O	1.69	0.75
1:A:218:VAL:HG23	4:A:1385:HOH:O	1.89	0.72
1:A:169:CYS:SG	4:A:1177:HOH:O	2.47	0.72
1:A:241:HIS:O	1:A:244:GLU:HG2	1.91	0.71
1:A:308:TYR:HB3	4:A:1201:HOH:O	1.90	0.71
1:A:173:ARG:O	1:A:175:GLN:HB2	1.93	0.69
1:A:67:TYR:HE1	4:A:1431:HOH:O	1.75	0.68
1:A:207:SER:HB2	4:A:1080:HOH:O	1.90	0.68
1:A:105:HIS:CE1	4:A:1257:HOH:O	2.45	0.68
1:A:105:HIS:HE1	4:A:1257:HOH:O	1.77	0.68
1:A:42:THR:HG23	1:A:45:GLU:HB2	1.75	0.68
1:A:172:TYR:CZ	4:A:1386:HOH:O	2.49	0.65
1:A:67:TYR:CE1	4:A:1431:HOH:O	2.49	0.65
1:A:225:LYS:HE2	4:A:1226:HOH:O	1.96	0.64
1:A:39:PRO:HB2	1:A:49:ILE:HD13	1.80	0.64
1:A:151:ILE:HG12	1:A:179:ALA:HB3	1.80	0.64
1:A:9:LYS:HD2	4:A:1295:HOH:O	1.98	0.64
1:A:345:ASP:O	1:A:349:LYS:HD3	2.00	0.62
1:A:128:GLU:HG3	4:A:1262:HOH:O	1.99	0.62
1:A:276:THR:HG21	4:A:1132:HOH:O	1.99	0.62
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:NE1	1:A:276:THR:HG22	2.16	0.60
1:A:241:HIS:HD2	1:A:244:GLU:OE1	1.86	0.59
1:A:228:VAL:HB	4:A:1183:HOH:O	2.02	0.59
1:A:42:THR:CG2	1:A:45:GLU:HB2	2.33	0.59
1:A:323:LYS:HD3	4:A:1203:HOH:O	2.03	0.58
1:A:242:THR:HG21	4:A:1047:HOH:O	2.04	0.58
1:A:42:THR:HG23	1:A:45:GLU:H	1.69	0.57
1:A:92:LYS:HE2	4:A:1096:HOH:O	2.03	0.57
1:A:253:ARG:HG3	1:A:254:GLN:N	2.19	0.56
1:A:49:ILE:HG22	4:A:1431:HOH:O	2.05	0.56
1:A:53:ASP:HA	1:A:268:LEU:HD22	1.87	0.56
1:A:150:SER:HB2	4:A:1138:HOH:O	2.06	0.55
1:A:12:VAL:HG21	1:A:329:ALA:HB3	1.87	0.55
1:A:171:LYS:HD3	1:A:172:TYR:CE2	2.42	0.54
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.42	0.54
1:A:232:LYS:HG2	4:A:1232:HOH:O	2.05	0.54
1:A:284:LYS:HE2	4:A:1168:HOH:O	2.06	0.53
1:A:175:GLN:N	1:A:176:THR:HA	2.22	0.53
1:A:266:SER:OG	1:A:278:HIS:HE1	1.92	0.53
1:A:172:TYR:CE2	4:A:1386:HOH:O	2.60	0.52
1:A:67:TYR:HA	4:A:1380:HOH:O	2.08	0.52
1:A:116:PRO:HB2	1:A:117:TRP:CD1	2.43	0.52
1:A:320:GLU:HA	1:A:323:LYS:HE3	1.92	0.52
1:A:130:VAL:HB	4:A:1386:HOH:O	2.10	0.52
1:A:98:VAL:HG23	4:A:1389:HOH:O	2.10	0.52
1:A:138:GLN:O	1:A:142:ARG:HG2	2.11	0.51
1:A:337:GLU:HG3	1:A:341:LYS:HZ1	1.74	0.51
1:A:26:THR:HB	4:A:1304:HOH:O	2.11	0.51
1:A:250:ASN:O	1:A:253:ARG:HG3	2.11	0.51
1:A:12:VAL:CG2	1:A:329:ALA:HB3	2.41	0.50
1:A:36:ILE:HD13	1:A:70:PRO:HB2	1.93	0.50
1:A:231:LEU:O	1:A:232:LYS:HB2	2.12	0.49
1:A:26:THR:HG22	4:A:1392:HOH:O	2.11	0.49
1:A:57:THR:HG23	1:A:60:ASP:H	1.78	0.49
1:A:64:LYS:HG2	4:A:1227:HOH:O	2.12	0.49
1:A:100:VAL:HG13	4:A:1138:HOH:O	2.13	0.48
1:A:170:LYS:HD3	1:A:207:SER:CB	2.43	0.48
1:A:26:THR:HB	1:A:81:ARG:HH21	1.78	0.48
1:A:28:LEU:HD13	4:A:1186:HOH:O	2.14	0.48
1:A:313:LYS:HD2	1:A:313:LYS:N	2.29	0.48
1:A:180:ILE:HA	4:A:1177:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:HA	4:A:1080:HOH:O	2.14	0.47
1:A:50:ILE:HA	4:A:1431:HOH:O	2.13	0.47
1:A:174:GLU:O	1:A:174:GLU:HG2	2.14	0.47
1:A:11:LYS:HE3	4:A:1308:HOH:O	2.14	0.46
1:A:170:LYS:HD3	1:A:207:SER:HB3	1.98	0.46
1:A:313:LYS:HA	1:A:313:LYS:NZ	2.31	0.46
1:A:57:THR:HG23	1:A:59:PRO:HD2	1.96	0.46
1:A:16:VAL:HG12	4:A:1389:HOH:O	2.15	0.46
1:A:32:LYS:HG3	4:A:1136:HOH:O	2.16	0.45
1:A:67:TYR:HD2	4:A:1380:HOH:O	1.99	0.45
1:A:81:ARG:CZ	4:A:1304:HOH:O	2.65	0.44
1:A:238:HIS:HB3	1:A:240:TYR:CE2	2.52	0.44
1:A:244:GLU:HB3	4:A:1071:HOH:O	2.17	0.44
1:A:351:TYR:HA	4:A:1295:HOH:O	2.18	0.43
1:A:175:GLN:N	1:A:176:THR:CA	2.80	0.43
1:A:298:LEU:HA	4:A:1340:HOH:O	2.19	0.43
1:A:39:PRO:HG3	1:A:67:TYR:CE1	2.54	0.43
1:A:13:GLU:HG2	4:A:1389:HOH:O	2.18	0.43
1:A:95:VAL:HG11	1:A:98:VAL:HB	2.01	0.43
1:A:210:HIS:HE1	4:A:1403:HOH:O	2.01	0.42
1:A:85:GLU:HA	4:A:1211:HOH:O	2.19	0.42
1:A:347:LEU:HG	4:A:1412:HOH:O	2.19	0.42
1:A:41:ASP:HB2	4:A:1199:HOH:O	2.20	0.42
1:A:241:HIS:HE1	4:A:1054:HOH:O	2.03	0.42
1:A:271:ALA:HA	4:A:1385:HOH:O	2.19	0.41
1:A:272:TRP:CD1	1:A:276:THR:HG22	2.55	0.41
1:A:277:GLU:HB2	4:A:1140:HOH:O	2.20	0.41
1:A:281:ILE:HD12	1:A:281:ILE:O	2.21	0.41
1:A:174:GLU:HG3	4:A:1342:HOH:O	2.20	0.41
1:A:273:LYS:HG3	4:A:1132:HOH:O	2.20	0.41
1:A:48:ASN:HD22	1:A:48:ASN:N	2.19	0.41
1:A:90:LYS:HA	1:A:90:LYS:HE2	2.02	0.41
1:A:261:ILE:HD11	1:A:283:PHE:CE2	2.56	0.41
1:A:162:SER:OG	1:A:197:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.



## 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	347/356 (98%)	330 (95%)	15 (4%)	2 (1%)	28	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	295	ASP

### 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	304/309 (98%)	269 (88%)	35 (12%)	6	3

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	28	LEU
1	A	33	ARG
1	A	36	ILE
1	A	41	ASP
1	A	45	GLU
1	A	60	ASP
1	A	67	TYR
1	A	70	PRO

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Mol	Chain	Res	Type
1	A	77	ASP
1	A	113	GLU
1	A	124	LEU
1	A	137	LEU
1	A	142	ARG
1	A	163	SER
1	A	170	LYS
1	A	175	GLN
1	A	193	LEU
1	A	199	GLN
1	A	233	THR
1	A	253	ARG
1	A	273	LYS
1	A	276	THR
1	A	277	GLU
1	A	281	ILE
1	A	287	GLN
1	A	292	LEU
1	A	312	LYS
1	A	313	LYS
1	A	325	LEU
1	A	335	LEU
1	A	337	GLU
1	A	341	LYS
1	A	347	LEU
1	A	349	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	48	ASN
1	A	134	ASN
1	A	138	GLN
1	A	158	GLN
1	A	175	GLN
1	A	197	HIS
1	A	241	HIS
1	A	250	ASN
1	A	278	HIS
1	A	309	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 ⓘ

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	FR3	A	1001	-	22,25,25	1.67	7 (31%)	27,34,34	2.08	6 (22%)

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	FR3	A	1001	-	-	0/7/15/15	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR3	C5-C8	-2.40	1.47	1.50
3	A	1001	FR3	C26-C25	2.11	1.42	1.38
3	A	1001	FR3	C6-C2	2.52	1.42	1.36
3	A	1001	FR3	C7-C6	2.61	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR3	C1-N2	2.63	1.42	1.38
3	A	1001	FR3	C26-C27	2.75	1.43	1.36
3	A	1001	FR3	C14-C13	2.88	1.64	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR3	O9-C8-N10	-3.13	118.13	122.58
3	A	1001	FR3	O9-C8-C5	-2.52	117.51	119.65
3	A	1001	FR3	C19-C18-C13	-2.51	107.26	112.65
3	A	1001	FR3	C4-C29-C28	2.01	120.49	117.89
3	A	1001	FR3	C1-N2-C13	3.92	129.24	125.54
3	A	1001	FR3	C5-C8-N10	7.62	123.83	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.