



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1NDZ  
Title : Crystal Structure of Adenosine Deaminase Complexed with FR235999  
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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

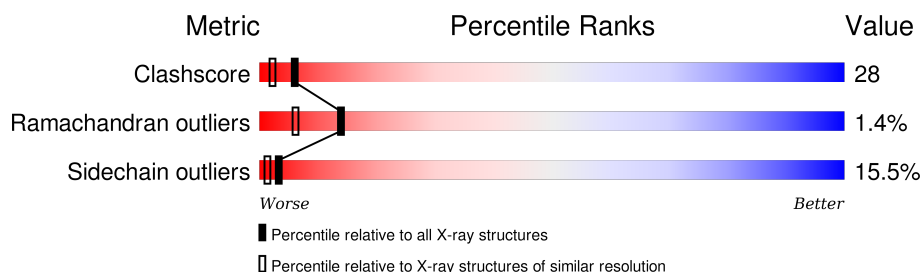
# 1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 3371 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			

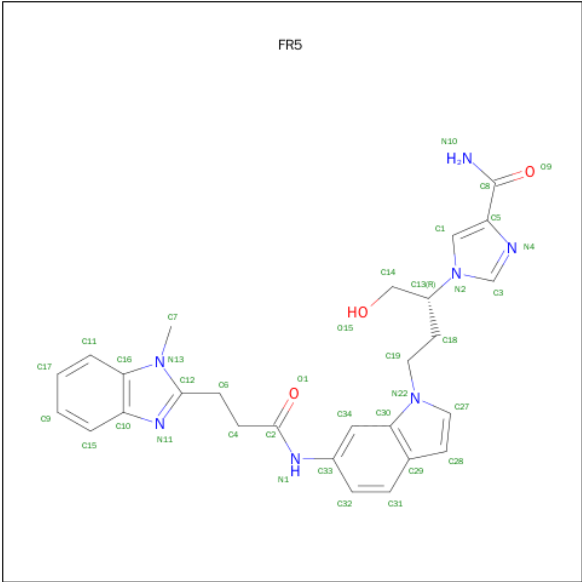
There are 15 discrepancies between the modelled and reference sequences:

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-(6-((3-(1-METHYL-1H-BENZIMIDAZO L-2-YL)PROPANOYL)AMINO)-1H-INDOL-1-YL)PROPYL)-1H-IMIDAZOLE-4-CARBO XAMIDE (three-letter code: FR5) (formula: C<sub>27</sub>H<sub>29</sub>N<sub>7</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	27	7	3		

- Molecule 4 is water.

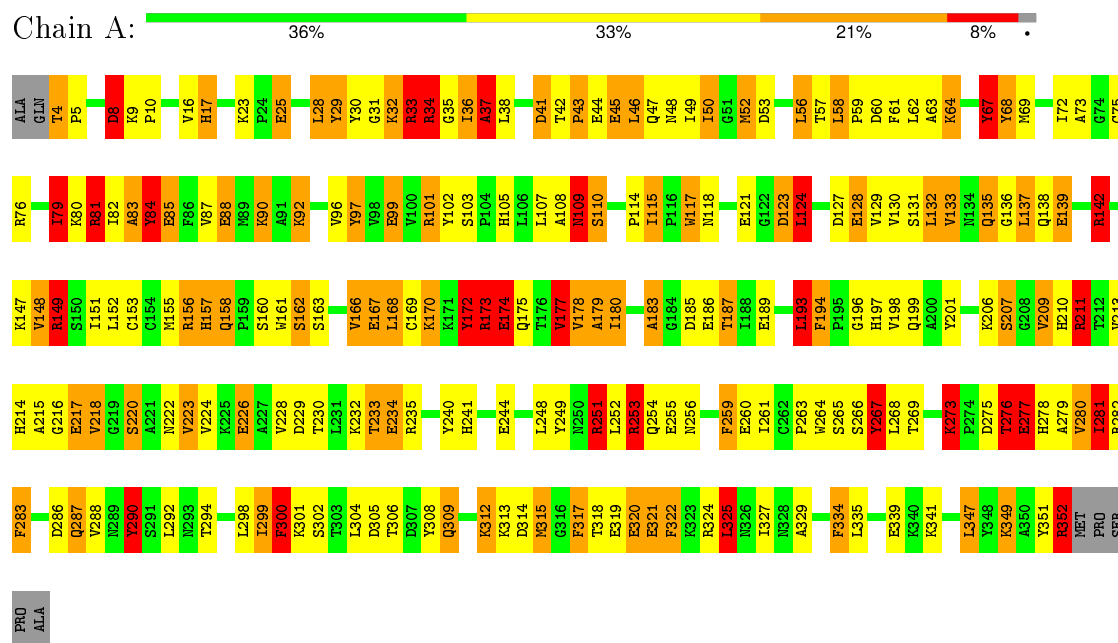
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	545	Total	O	0	0
			545	545		

### 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 errors 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 will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.06 Å 78.06 Å 136.71 Å 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, $R_{free}$	0.210 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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: ZN, FR5

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	1.96	58/2852 (2.0%)	2.46	181/3866 (4.7%)

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	22

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	ARG	CZ-NH2	9.96	1.46	1.33
1	A	160	SER	CA-CB	9.52	1.67	1.52
1	A	110	SER	CB-OG	8.58	1.53	1.42
1	A	199	GLN	CG-CD	8.43	1.70	1.51
1	A	103	SER	CB-OG	7.58	1.52	1.42
1	A	321	GLU	CB-CG	7.55	1.66	1.52
1	A	207	SER	CA-CB	-7.33	1.42	1.52
1	A	339	GLU	CD-OE2	-7.33	1.17	1.25
1	A	213	VAL	N-CA	7.30	1.60	1.46
1	A	213	VAL	CA-CB	7.12	1.69	1.54
1	A	217	GLU	CD-OE1	-6.99	1.18	1.25
1	A	263	PRO	CA-CB	-6.73	1.40	1.53
1	A	156	ARG	CZ-NH1	6.64	1.41	1.33
1	A	213	VAL	CB-CG1	6.36	1.66	1.52
1	A	211	ARG	NE-CZ	-6.29	1.24	1.33
1	A	235	ARG	CZ-NH1	6.29	1.41	1.33
1	A	158	GLN	CD-NE2	-6.24	1.17	1.32
1	A	201	TYR	CD1-CE1	6.22	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ASP	CB-CG	6.16	1.64	1.51
1	A	300	PHE	CG-CD1	6.12	1.48	1.38
1	A	163	SER	CA-CB	6.07	1.62	1.52
1	A	99	GLU	CG-CD	6.05	1.61	1.51
1	A	299	ILE	CA-CB	6.04	1.68	1.54
1	A	277	GLU	CG-CD	6.02	1.60	1.51
1	A	339	GLU	CG-CD	-5.99	1.43	1.51
1	A	131	SER	CB-OG	-5.95	1.34	1.42
1	A	155	MET	N-CA	5.94	1.58	1.46
1	A	226	GLU	CB-CG	5.87	1.63	1.52
1	A	196	GLY	CA-C	5.83	1.61	1.51
1	A	253	ARG	NE-CZ	5.77	1.40	1.33
1	A	96	VAL	CB-CG1	5.71	1.64	1.52
1	A	214	HIS	CG-ND1	-5.71	1.26	1.38
1	A	194	PHE	CG-CD2	5.70	1.47	1.38
1	A	234	GLU	CG-CD	5.66	1.60	1.51
1	A	35	GLY	CA-C	5.66	1.60	1.51
1	A	167	GLU	CD-OE1	-5.63	1.19	1.25
1	A	147	LYS	CD-CE	5.51	1.65	1.51
1	A	162	SER	CB-OG	5.46	1.49	1.42
1	A	198	VAL	CB-CG1	5.44	1.64	1.52
1	A	102	TYR	CG-CD1	5.43	1.46	1.39
1	A	228	VAL	CB-CG2	5.35	1.64	1.52
1	A	210	HIS	CB-CG	5.32	1.59	1.50
1	A	302	SER	CA-CB	-5.32	1.45	1.52
1	A	319	GLU	CG-CD	5.31	1.59	1.51
1	A	133	VAL	CB-CG2	5.29	1.64	1.52
1	A	248	LEU	N-CA	5.28	1.56	1.46
1	A	105	HIS	CE1-NE2	5.25	1.44	1.32
1	A	220	SER	CB-OG	5.24	1.49	1.42
1	A	189	GLU	CD-OE2	-5.23	1.19	1.25
1	A	117	TRP	CD2-CE2	5.23	1.47	1.41
1	A	226	GLU	CG-CD	5.18	1.59	1.51
1	A	339	GLU	CD-OE1	-5.17	1.20	1.25
1	A	157	HIS	CE1-NE2	5.17	1.44	1.32
1	A	324	ARG	CZ-NH2	-5.15	1.26	1.33
1	A	282	ARG	CA-CB	5.14	1.65	1.53
1	A	305	ASP	CA-CB	5.12	1.65	1.53
1	A	214	HIS	CA-CB	5.09	1.65	1.53
1	A	260	GLU	CD-OE1	-5.03	1.20	1.25

All (181) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH2	-18.94	110.83	120.30
1	A	149	ARG	CD-NE-CZ	-14.92	102.72	123.60
1	A	211	ARG	NE-CZ-NH2	-13.77	113.41	120.30
1	A	149	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	A	58	LEU	CB-CA-C	-13.03	85.44	110.20
1	A	240	TYR	CB-CG-CD2	-12.70	113.38	121.00
1	A	308	TYR	CB-CG-CD2	-12.40	113.56	121.00
1	A	155	MET	CG-SD-CE	11.03	117.84	100.20
1	A	8	ASP	CB-CG-OD1	-10.12	109.19	118.30
1	A	166	VAL	CA-CB-CG2	10.05	125.97	110.90
1	A	334	PHE	CB-CG-CD2	-10.00	113.80	120.80
1	A	33	ARG	CD-NE-CZ	-9.79	109.89	123.60
1	A	67	TYR	CB-CG-CD1	-9.78	115.13	121.00
1	A	29	TYR	CB-CG-CD2	-9.66	115.20	121.00
1	A	223	VAL	CA-CB-CG2	9.48	125.13	110.90
1	A	201	TYR	CB-CG-CD2	-9.47	115.32	121.00
1	A	211	ARG	CD-NE-CZ	9.30	136.62	123.60
1	A	156	ARG	NH1-CZ-NH2	9.23	129.55	119.40
1	A	117	TRP	CG-CD1-NE1	9.08	119.18	110.10
1	A	218	VAL	CA-CB-CG1	8.85	124.17	110.90
1	A	175	GLN	C-N-CA	8.77	143.62	121.70
1	A	282	ARG	NE-CZ-NH1	-8.75	115.92	120.30
1	A	81	ARG	CD-NE-CZ	-8.65	111.50	123.60
1	A	187	THR	CA-CB-CG2	-8.64	100.30	112.40
1	A	253	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	A	101	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	A	294	THR	CA-CB-OG1	8.34	126.52	109.00
1	A	251	ARG	CD-NE-CZ	-8.34	111.92	123.60
1	A	193	LEU	CB-CG-CD2	8.26	125.05	111.00
1	A	117	TRP	CD1-CG-CD2	-8.24	99.70	106.30
1	A	37	ALA	CA-C-O	8.22	137.36	120.10
1	A	314	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	194	PHE	CB-CG-CD2	-8.18	115.07	120.80
1	A	185	ASP	CB-CG-OD2	8.14	125.62	118.30
1	A	277	GLU	CA-CB-CG	8.13	131.29	113.40
1	A	170	LYS	CA-CB-CG	-8.03	95.73	113.40
1	A	161	TRP	CH2-CZ2-CE2	7.94	125.34	117.40
1	A	170	LYS	CD-CE-NZ	-7.92	93.49	111.70
1	A	115	ILE	CB-CG1-CD1	-7.88	91.83	113.90
1	A	254	GLN	CB-CA-C	-7.83	94.74	110.40
1	A	158	GLN	CG-CD-OE1	7.81	137.21	121.60
1	A	84	TYR	CB-CG-CD1	-7.75	116.35	121.00
1	A	290	TYR	CB-CA-C	-7.71	94.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	GLU	OE1-CD-OE2	-7.66	114.11	123.30
1	A	73	ALA	CB-CA-C	-7.61	98.69	110.10
1	A	8	ASP	CB-CA-C	-7.54	95.33	110.40
1	A	317	PHE	CB-CG-CD2	-7.50	115.55	120.80
1	A	174	GLU	N-CA-C	7.49	131.23	111.00
1	A	209	VAL	CA-CB-CG1	7.49	122.14	110.90
1	A	37	ALA	N-CA-C	7.45	131.11	111.00
1	A	240	TYR	CD1-CG-CD2	7.44	126.09	117.90
1	A	149	ARG	NH1-CZ-NH2	-7.44	111.22	119.40
1	A	158	GLN	CB-CA-C	-7.43	95.55	110.40
1	A	300	PHE	CB-CG-CD2	7.26	125.88	120.80
1	A	172	TYR	CG-CD2-CE2	-7.20	115.54	121.30
1	A	233	THR	CA-CB-CG2	7.18	122.45	112.40
1	A	199	GLN	CA-CB-CG	-7.11	97.77	113.40
1	A	240	TYR	CG-CD1-CE1	-7.05	115.66	121.30
1	A	335	LEU	CB-CG-CD1	7.04	122.97	111.00
1	A	131	SER	N-CA-CB	-6.99	100.02	110.50
1	A	259	PHE	CB-CG-CD2	-6.95	115.93	120.80
1	A	58	LEU	N-CA-CB	6.92	124.24	110.40
1	A	79	ILE	CA-CB-CG1	6.89	124.09	111.00
1	A	76	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	84	TYR	CD1-CG-CD2	6.86	125.44	117.90
1	A	175	GLN	CA-CB-CG	6.82	128.39	113.40
1	A	101	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	A	79	ILE	CB-CA-C	-6.77	98.05	111.60
1	A	37	ALA	CA-C-N	-6.76	102.32	117.20
1	A	324	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	193	LEU	CB-CG-CD1	6.57	122.17	111.00
1	A	224	VAL	CA-CB-CG2	-6.55	101.07	110.90
1	A	253	ARG	CG-CD-NE	6.53	125.50	111.80
1	A	315	MET	CG-SD-CE	6.48	110.57	100.20
1	A	148	VAL	CG1-CB-CG2	-6.48	100.54	110.90
1	A	35	GLY	C-N-CA	-6.45	105.56	121.70
1	A	67	TYR	CB-CA-C	-6.45	97.49	110.40
1	A	166	VAL	CB-CA-C	-6.44	99.16	111.40
1	A	218	VAL	CG1-CB-CG2	6.42	121.18	110.90
1	A	286	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	180	ILE	CB-CG1-CD1	-6.42	95.94	113.90
1	A	84	TYR	CG-CD1-CE1	-6.38	116.20	121.30
1	A	68	TYR	CD1-CE1-CZ	-6.36	114.08	119.80
1	A	149	ARG	CB-CA-C	-6.29	97.82	110.40
1	A	85	GLU	N-CA-CB	-6.26	99.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	TYR	C-N-CA	-6.25	109.17	122.30
1	A	135	GLN	C-N-CA	-6.25	109.17	122.30
1	A	178	VAL	CG1-CB-CG2	-6.24	100.91	110.90
1	A	349	LYS	CB-CG-CD	6.24	127.81	111.60
1	A	177	VAL	CA-CB-CG2	6.23	120.25	110.90
1	A	174	GLU	C-N-CA	6.19	137.17	121.70
1	A	52	MET	CG-SD-CE	6.17	110.08	100.20
1	A	322	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	A	308	TYR	CB-CG-CD1	6.14	124.69	121.00
1	A	179	ALA	O-C-N	6.14	132.52	122.70
1	A	75	CYS	N-CA-CB	-6.10	99.61	110.60
1	A	105	HIS	CA-CB-CG	-6.08	103.26	113.60
1	A	281	ILE	CA-CB-CG2	6.07	123.03	110.90
1	A	97	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
1	A	253	ARG	CD-NE-CZ	6.05	132.07	123.60
1	A	34	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	58	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	A	67	TYR	N-CA-CB	6.00	121.40	110.60
1	A	187	THR	CB-CA-C	-5.98	95.45	111.60
1	A	314	ASP	CA-CB-CG	5.96	126.51	113.40
1	A	183	ALA	CB-CA-C	-5.92	101.22	110.10
1	A	194	PHE	CZ-CE2-CD2	-5.92	113.00	120.10
1	A	4	THR	N-CA-C	5.88	126.87	111.00
1	A	300	PHE	CB-CG-CD1	-5.87	116.69	120.80
1	A	223	VAL	CA-CB-CG1	5.86	119.70	110.90
1	A	183	ALA	N-CA-CB	-5.84	101.92	110.10
1	A	163	SER	N-CA-CB	5.80	119.20	110.50
1	A	139	GLU	CA-CB-CG	5.75	126.05	113.40
1	A	10	PRO	N-CD-CG	-5.75	94.58	103.20
1	A	273	LYS	CB-CA-C	5.72	121.84	110.40
1	A	85	GLU	CA-CB-CG	5.70	125.93	113.40
1	A	280	VAL	C-N-CA	-5.69	107.48	121.70
1	A	33	ARG	N-CA-CB	-5.65	100.43	110.60
1	A	194	PHE	CG-CD1-CE1	-5.64	114.59	120.80
1	A	233	THR	OG1-CB-CG2	5.63	122.95	110.00
1	A	213	VAL	CA-CB-CG1	-5.62	102.47	110.90
1	A	34	ARG	CD-NE-CZ	5.62	131.47	123.60
1	A	175	GLN	CB-CA-C	-5.62	99.17	110.40
1	A	16	VAL	CG1-CB-CG2	-5.62	101.92	110.90
1	A	215	ALA	N-CA-CB	5.61	117.96	110.10
1	A	325	LEU	CA-CB-CG	5.59	128.17	115.30
1	A	201	TYR	CB-CG-CD1	5.56	124.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	GLN	CB-CG-CD	5.53	125.99	111.60
1	A	352	ARG	N-CA-C	5.52	125.90	111.00
1	A	233	THR	CB-CA-C	-5.51	96.71	111.60
1	A	319	GLU	C-N-CA	-5.51	107.92	121.70
1	A	306	THR	CA-CB-CG2	5.51	120.12	112.40
1	A	132	LEU	CA-CB-CG	-5.50	102.66	115.30
1	A	175	GLN	O-C-N	-5.49	113.91	122.70
1	A	90	LYS	CA-CB-CG	5.49	125.47	113.40
1	A	308	TYR	C-N-CA	-5.48	107.99	121.70
1	A	67	TYR	CD1-CG-CD2	5.48	123.93	117.90
1	A	251	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	36	ILE	CA-CB-CG2	5.44	121.78	110.90
1	A	249	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	267	TYR	CB-CG-CD2	5.44	124.26	121.00
1	A	117	TRP	CB-CG-CD2	5.41	133.64	126.60
1	A	211	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	A	108	ALA	CA-C-N	-5.39	105.33	117.20
1	A	282	ARG	N-CA-CB	-5.38	100.92	110.60
1	A	216	GLY	O-C-N	5.34	131.24	122.70
1	A	240	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	A	117	TRP	CD1-NE1-CE2	-5.32	104.21	109.00
1	A	88	GLU	CA-CB-CG	-5.23	101.89	113.40
1	A	87	VAL	CA-CB-CG1	5.20	118.70	110.90
1	A	139	GLU	CB-CA-C	5.19	120.78	110.40
1	A	166	VAL	CG1-CB-CG2	5.19	119.20	110.90
1	A	324	ARG	C-N-CA	-5.18	108.75	121.70
1	A	287	GLN	CA-CB-CG	5.17	124.77	113.40
1	A	85	GLU	CB-CA-C	5.15	120.70	110.40
1	A	177	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	A	72	ILE	CA-C-O	5.15	130.91	120.10
1	A	67	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	A	43	PRO	O-C-N	5.14	130.92	122.70
1	A	347	LEU	CD1-CG-CD2	5.13	125.89	110.50
1	A	273	LYS	CA-CB-CG	5.11	124.65	113.40
1	A	109	ASN	CB-CA-C	5.11	120.62	110.40
1	A	329	ALA	CA-C-O	5.11	130.82	120.10
1	A	335	LEU	CB-CG-CD2	5.10	119.67	111.00
1	A	229	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	321	GLU	CB-CA-C	5.09	120.59	110.40
1	A	304	LEU	CB-CA-C	5.07	119.84	110.20
1	A	180	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	A	214	HIS	CB-CA-C	-5.06	100.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	PHE	CD1-CE1-CZ	-5.06	114.03	120.10
1	A	17	HIS	CE1-NE2-CD2	-5.05	93.97	106.60
1	A	62	LEU	CD1-CG-CD2	-5.04	95.36	110.50
1	A	123	ASP	N-CA-C	5.04	124.61	111.00
1	A	124	LEU	CB-CG-CD2	5.04	119.57	111.00
1	A	62	LEU	CB-CG-CD1	5.04	119.56	111.00
1	A	63	ALA	C-N-CA	-5.02	109.14	121.70
1	A	335	LEU	N-CA-CB	-5.02	100.37	110.40
1	A	142	ARG	CD-NE-CZ	-5.00	116.60	123.60
1	A	209	VAL	CA-CB-CG2	5.00	118.41	110.90
1	A	85	GLU	N-CA-C	5.00	124.50	111.00
1	A	251	ARG	NE-CZ-NH1	-5.00	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	THR	CB

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	142	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	172	TYR	Sidechain
1	A	173	ARG	Peptide
1	A	194	PHE	Sidechain
1	A	251	ARG	Sidechain
1	A	267	TYR	Sidechain
1	A	276	THR	Peptide
1	A	283	PHE	Sidechain
1	A	29	TYR	Sidechain
1	A	290	TYR	Sidechain
1	A	300	PHE	Sidechain
1	A	322	PHE	Sidechain
1	A	33	ARG	Sidechain
1	A	352	ARG	Sidechain
1	A	37	ALA	Peptide
1	A	41	ASP	Peptide
1	A	67	TYR	Sidechain
1	A	81	ARG	Sidechain
1	A	83	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	84	TYR	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	2742	158	0
2	A	1	0	0	0	0
3	A	37	0	28	4	0
4	A	545	0	0	69	0
All	All	3371	0	2770	159	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 28.

All (159) 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	1.04	0.95
1:A:28:LEU:HD11	1:A:41:ASP:HA	1.51	0.92
1:A:211:ARG:HH22	1:A:234:GLU:HG3	1.32	0.92
1:A:290:TYR:HB3	4:A:1536:HOH:O	1.72	0.89
1:A:268:LEU:HG	4:A:1477:HOH:O	1.73	0.88
1:A:278:HIS:CD2	1:A:280:VAL:H	1.92	0.86
1:A:28:LEU:HD22	1:A:46:LEU:HD13	1.56	0.86
1:A:4:THR:HA	4:A:1520:HOH:O	1.74	0.86
1:A:211:ARG:HH21	1:A:211:ARG:HB2	1.43	0.81
1:A:220:SER:HA	4:A:1139:HOH:O	1.77	0.81
1:A:301:LYS:HA	4:A:1331:HOH:O	1.81	0.81
1:A:139:GLU:HB3	4:A:1285:HOH:O	1.83	0.79
1:A:42:THR:HG23	1:A:45:GLU:H	1.48	0.78
1:A:325:LEU:HB3	4:A:1393:HOH:O	1.84	0.76
1:A:58:LEU:HG	4:A:1200:HOH:O	1.86	0.75
1:A:278:HIS:HD2	1:A:280:VAL:N	1.83	0.73
1:A:153:CYS:SG	4:A:1389:HOH:O	2.45	0.73
1:A:187:THR:HG23	4:A:1373:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE2	4:A:1215:HOH:O	1.91	0.69
1:A:83:ALA:HB3	4:A:1264:HOH:O	1.92	0.68
1:A:80:LYS:HA	4:A:1264:HOH:O	1.93	0.68
1:A:211:ARG:NH2	1:A:211:ARG:HB2	2.09	0.68
1:A:37:ALA:HA	1:A:38:LEU:HG	1.76	0.67
1:A:43:PRO:HG3	4:A:1423:HOH:O	1.94	0.67
1:A:49:ILE:HD12	4:A:1046:HOH:O	1.95	0.67
1:A:69:MET:HA	4:A:1271:HOH:O	1.94	0.67
1:A:82:ILE:HD13	4:A:1495:HOH:O	1.93	0.66
1:A:317:PHE:HE1	4:A:1211:HOH:O	1.80	0.65
1:A:273:LYS:O	1:A:276:THR:HG22	1.96	0.65
1:A:118:ASN:HB3	4:A:1154:HOH:O	1.96	0.65
1:A:151:ILE:HG12	1:A:179:ALA:HB3	1.79	0.64
1:A:251:ARG:O	1:A:255:GLU:HG3	1.98	0.63
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.80	0.63
1:A:57:THR:OG1	1:A:59:PRO:HD2	1.99	0.62
1:A:211:ARG:NH2	1:A:232:LYS:O	2.33	0.62
1:A:28:LEU:HD12	4:A:1537:HOH:O	1.99	0.62
1:A:313:LYS:HB2	4:A:1526:HOH:O	2.02	0.60
1:A:138:GLN:O	1:A:142:ARG:HG2	2.02	0.60
1:A:34:ARG:HH11	1:A:34:ARG:HG2	1.67	0.58
1:A:109:ASN:HB2	4:A:1499:HOH:O	2.03	0.57
1:A:259:PHE:HB2	4:A:1536:HOH:O	2.04	0.57
1:A:17:HIS:CE1	4:A:1389:HOH:O	2.58	0.57
1:A:277:GLU:HA	4:A:1055:HOH:O	2.05	0.57
1:A:61:PHE:HE1	1:A:299:ILE:HG21	1.70	0.57
1:A:256:ASN:HB2	4:A:1194:HOH:O	2.04	0.57
1:A:320:GLU:HG2	4:A:1232:HOH:O	2.05	0.56
1:A:149:ARG:CZ	1:A:174:GLU:HG2	2.36	0.56
1:A:174:GLU:HG3	1:A:178:VAL:HG12	1.87	0.56
1:A:128:GLU:HA	4:A:1432:HOH:O	2.06	0.55
1:A:267:TYR:HD1	4:A:1477:HOH:O	1.89	0.55
1:A:110:SER:HB2	1:A:123:ASP:HA	1.87	0.55
1:A:312:LYS:HB3	1:A:312:LYS:NZ	2.22	0.55
1:A:222:ASN:O	1:A:226:GLU:HG3	2.08	0.55
1:A:130:VAL:HG11	1:A:172:TYR:CD2	2.42	0.54
1:A:193:LEU:HD12	1:A:230:THR:HG21	1.88	0.54
1:A:206:LYS:HE3	4:A:1152:HOH:O	2.08	0.54
1:A:79:ILE:HG12	4:A:1188:HOH:O	2.07	0.53
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.43	0.53
1:A:52:MET:HE2	1:A:56:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:MET:HB3	4:A:1211:HOH:O	2.07	0.53
1:A:114:PRO:HB2	4:A:1067:HOH:O	2.09	0.53
1:A:320:GLU:HB2	4:A:1288:HOH:O	2.09	0.53
1:A:136:GLY:HA3	4:A:1264:HOH:O	2.07	0.52
1:A:312:LYS:HB3	1:A:312:LYS:HZ2	1.73	0.52
1:A:266:SER:OG	1:A:278:HIS:HE1	1.91	0.52
1:A:5:PRO:HG2	1:A:8:ASP:OD1	2.09	0.52
1:A:28:LEU:HD11	1:A:41:ASP:CA	2.34	0.52
1:A:121:GLU:HB3	4:A:1493:HOH:O	2.09	0.52
1:A:186:GLU:HG2	4:A:1426:HOH:O	2.10	0.51
1:A:57:THR:HG23	1:A:60:ASP:H	1.76	0.51
1:A:313:LYS:HE3	1:A:313:LYS:HA	1.92	0.51
1:A:47:GLN:HE22	1:A:298:LEU:HD12	1.75	0.51
1:A:43:PRO:HD2	4:A:1435:HOH:O	2.10	0.50
1:A:46:LEU:HD23	1:A:50:ILE:HD11	1.93	0.50
1:A:137:LEU:HG	1:A:148:VAL:HG11	1.93	0.50
1:A:32:LYS:HG2	4:A:1193:HOH:O	2.11	0.50
1:A:290:TYR:O	1:A:325:LEU:HB2	2.12	0.49
1:A:149:ARG:HG3	1:A:178:VAL:HG11	1.94	0.49
1:A:281:ILE:HB	4:A:1211:HOH:O	2.13	0.49
1:A:312:LYS:HZ3	1:A:313:LYS:HD2	1.76	0.49
1:A:124:LEU:HG	4:A:1156:HOH:O	2.11	0.49
1:A:156:ARG:O	1:A:197:HIS:HE1	1.95	0.49
1:A:167:GLU:HA	1:A:170:LYS:HZ3	1.78	0.49
1:A:36:ILE:HD11	1:A:38:LEU:CD2	2.43	0.48
1:A:61:PHE:CE1	1:A:299:ILE:HG21	2.47	0.48
1:A:138:GLN:O	1:A:142:ARG:NE	2.47	0.48
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.94	0.48
1:A:25:GLU:HA	1:A:43:PRO:HB3	1.94	0.48
1:A:117:TRP:HD1	4:A:1422:HOH:O	1.95	0.48
1:A:90:LYS:HA	1:A:90:LYS:HE2	1.96	0.47
1:A:60:ASP:O	1:A:64:LYS:HD3	2.15	0.47
1:A:277:GLU:HB2	4:A:1213:HOH:O	2.15	0.47
1:A:9:LYS:HD2	4:A:1336:HOH:O	2.14	0.47
1:A:217:GLU:HB3	4:A:1083:HOH:O	2.15	0.47
1:A:180:ILE:HD13	1:A:180:ILE:HG21	1.71	0.47
1:A:183:ALA:HB3	4:A:1117:HOH:O	2.15	0.46
1:A:58:LEU:HB2	1:A:59:PRO:HD3	1.98	0.46
1:A:68:TYR:OH	1:A:299:ILE:HD11	2.15	0.46
1:A:309:GLN:NE2	1:A:312:LYS:HZ1	2.13	0.46
1:A:277:GLU:HB3	4:A:1507:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:OG	1:A:197:HIS:HD2	1.99	0.46
1:A:4:THR:HG21	4:A:1165:HOH:O	2.14	0.46
1:A:61:PHE:CG	3:A:1001:FR5:C15	2.98	0.46
1:A:97:TYR:CE2	1:A:99:GLU:HG3	2.50	0.46
1:A:253:ARG:HB3	4:A:1004:HOH:O	2.15	0.46
1:A:300:PHE:HB2	4:A:1464:HOH:O	2.15	0.45
3:A:1001:FR5:H32	3:A:1001:FR5:O1	2.15	0.45
1:A:23:LYS:HB3	4:A:1196:HOH:O	2.16	0.45
1:A:334:PHE:C	4:A:1503:HOH:O	2.54	0.45
1:A:170:LYS:O	1:A:173:ARG:HG2	2.17	0.45
1:A:169:CYS:HA	1:A:177:VAL:HG21	1.99	0.45
1:A:36:ILE:HD11	1:A:38:LEU:HD21	1.98	0.45
1:A:79:ILE:HD11	1:A:124:LEU:HD11	1.99	0.45
1:A:34:ARG:HG3	4:A:1233:HOH:O	2.16	0.45
1:A:28:LEU:HD13	1:A:38:LEU:HD12	1.99	0.44
1:A:288:VAL:HG12	4:A:1536:HOH:O	2.17	0.44
1:A:261:ILE:N	1:A:261:ILE:HD13	2.33	0.44
1:A:81:ARG:HG2	4:A:1279:HOH:O	2.16	0.44
1:A:133:VAL:HG12	1:A:137:LEU:HD22	2.00	0.44
1:A:80:LYS:CE	1:A:135:GLN:HB3	2.47	0.43
1:A:80:LYS:HE3	4:A:1260:HOH:O	2.17	0.43
1:A:152:LEU:CD1	1:A:168:LEU:HB3	2.48	0.43
1:A:56:LEU:HD13	1:A:60:ASP:HB2	2.00	0.43
1:A:276:THR:HG21	4:A:1096:HOH:O	2.18	0.43
1:A:79:ILE:HD12	1:A:132:LEU:HD12	2.01	0.43
1:A:157:HIS:CD2	1:A:158:GLN:HG2	2.53	0.43
1:A:88:GLU:O	1:A:92:LYS:HG2	2.19	0.43
1:A:58:LEU:HD11	3:A:1001:FR5:H72	2.00	0.43
1:A:115:ILE:HG21	1:A:115:ILE:HD13	1.68	0.43
1:A:318:THR:HG23	4:A:1275:HOH:O	2.18	0.42
1:A:179:ALA:HB2	1:A:334:PHE:CD2	2.54	0.42
1:A:218:VAL:HG13	4:A:1373:HOH:O	2.19	0.42
1:A:313:LYS:CA	1:A:313:LYS:HE3	2.49	0.42
1:A:351:TYR:HD2	4:A:1336:HOH:O	2.01	0.42
1:A:241:HIS:O	1:A:244:GLU:HG3	2.19	0.42
1:A:68:TYR:HD1	4:A:1271:HOH:O	2.00	0.42
1:A:79:ILE:HD13	1:A:129:VAL:HG22	2.00	0.42
1:A:170:LYS:HD3	1:A:207:SER:OG	2.19	0.42
1:A:32:LYS:HB2	4:A:1537:HOH:O	2.19	0.42
1:A:170:LYS:HB2	1:A:170:LYS:HZ3	1.84	0.42
1:A:273:LYS:HE2	4:A:1483:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:HA3	4:A:1265:HOH:O	2.20	0.42
1:A:32:LYS:HG3	4:A:1029:HOH:O	2.19	0.41
1:A:52:MET:HE1	1:A:268:LEU:O	2.20	0.41
1:A:50:ILE:HG21	1:A:50:ILE:HD13	1.62	0.41
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.84	0.41
1:A:46:LEU:CD2	1:A:50:ILE:HD11	2.50	0.41
1:A:58:LEU:CD1	3:A:1001:FR5:H72	2.51	0.41
1:A:327:ILE:HA	1:A:327:ILE:HD13	1.82	0.41
1:A:84:TYR:CD1	4:A:1285:HOH:O	2.74	0.41
1:A:33:ARG:HG3	4:A:1492:HOH:O	2.20	0.41
1:A:47:GLN:HB2	4:A:1247:HOH:O	2.21	0.41
1:A:264:TRP:CD1	1:A:300:PHE:HB3	2.56	0.41
1:A:265:SER:O	1:A:269:THR:HG23	2.20	0.41
1:A:283:PHE:HB3	1:A:288:VAL:HB	2.03	0.40
1:A:309:GLN:NE2	1:A:312:LYS:NZ	2.69	0.40
1:A:23:LYS:HD3	1:A:85:GLU:HG3	2.04	0.40
1:A:149:ARG:CZ	4:A:1399:HOH:O	2.70	0.40
1:A:149:ARG:HD3	1:A:149:ARG:HH11	1.62	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	347/356 (98%)	320 (92%)	22 (6%)	5 (1%)	<b>14</b> <b>6</b>

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLU
1	A	279	ALA
1	A	37	ALA

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Mol	Chain	Res	Type
1	A	44	GLU
1	A	277	GLU

### 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%)	257 (84%)	47 (16%)	<b>3</b> <b>1</b>

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	25	GLU
1	A	28	LEU
1	A	32	LYS
1	A	34	ARG
1	A	45	GLU
1	A	46	LEU
1	A	48	ASN
1	A	50	ILE
1	A	53	ASP
1	A	56	LEU
1	A	64	LYS
1	A	67	TYR
1	A	79	ILE
1	A	92	LYS
1	A	107	LEU
1	A	109	ASN
1	A	124	LEU
1	A	128	GLU
1	A	137	LEU
1	A	142	ARG
1	A	166	VAL
1	A	168	LEU
1	A	173	ARG

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Mol	Chain	Res	Type
1	A	177	VAL
1	A	193	LEU
1	A	209	VAL
1	A	211	ARG
1	A	223	VAL
1	A	233	THR
1	A	253	ARG
1	A	273	LYS
1	A	275	ASP
1	A	276	THR
1	A	277	GLU
1	A	281	ILE
1	A	287	GLN
1	A	292	LEU
1	A	309	GLN
1	A	312	LYS
1	A	320	GLU
1	A	321	GLU
1	A	325	LEU
1	A	341	LYS
1	A	347	LEU
1	A	349	LYS
1	A	352	ARG

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

Mol	Chain	Res	Type
1	A	47	GLN
1	A	134	ASN
1	A	138	GLN
1	A	157	HIS
1	A	197	HIS
1	A	210	HIS
1	A	241	HIS
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	FR5	A	1001	-	35,41,41	2.48	10 (28%)	36,58,58	1.79	7 (19%)

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	FR5	A	1001	-	-	0/16/24/24	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR5	C33-N1	-6.93	1.28	1.41
3	A	1001	FR5	C30-N22	-5.29	1.33	1.39
3	A	1001	FR5	C34-C30	-4.78	1.30	1.40
3	A	1001	FR5	C2-N1	-4.36	1.25	1.35
3	A	1001	FR5	C3-N4	-4.35	1.26	1.35
3	A	1001	FR5	C31-C29	-3.17	1.34	1.41
3	A	1001	FR5	C5-C8	-2.73	1.46	1.51
3	A	1001	FR5	C31-C32	-2.33	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR5	C19-N22	2.74	1.57	1.50
3	A	1001	FR5	C17-C11	3.51	1.44	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR5	C1-N2-C3	-4.78	105.73	108.33
3	A	1001	FR5	C17-C9-C15	-3.71	115.06	120.45
3	A	1001	FR5	C34-C33-N1	-3.25	113.46	122.79
3	A	1001	FR5	C5-C8-N10	-2.81	113.46	116.21
3	A	1001	FR5	C11-C16-C10	-2.56	117.06	121.36
3	A	1001	FR5	C28-C29-C30	2.51	108.34	106.20
3	A	1001	FR5	O9-C8-C5	3.21	122.64	119.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR5	4	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.