



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 AM UTC

PDB ID : 1NDY / pdb_00001ndy
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

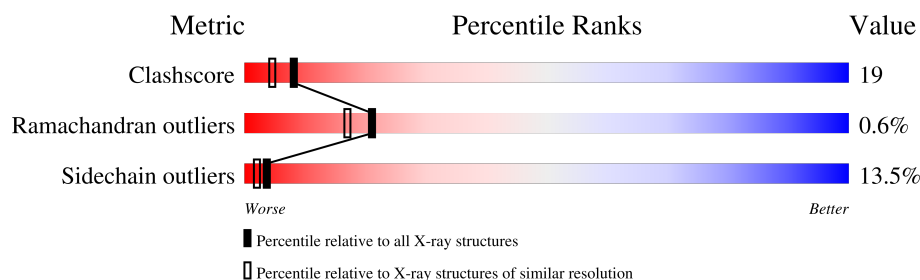
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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 $\leq 5\%$.

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			

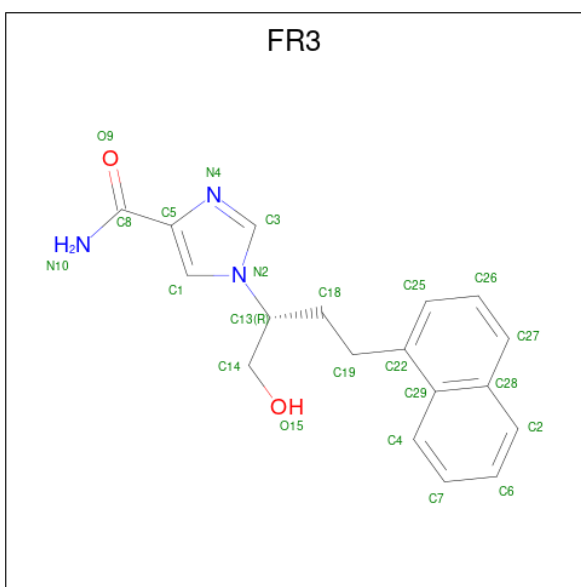
There are 15 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: FR3) (formula: C₁₈H₁₉N₃O₂).



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

- Molecule 4 is water.

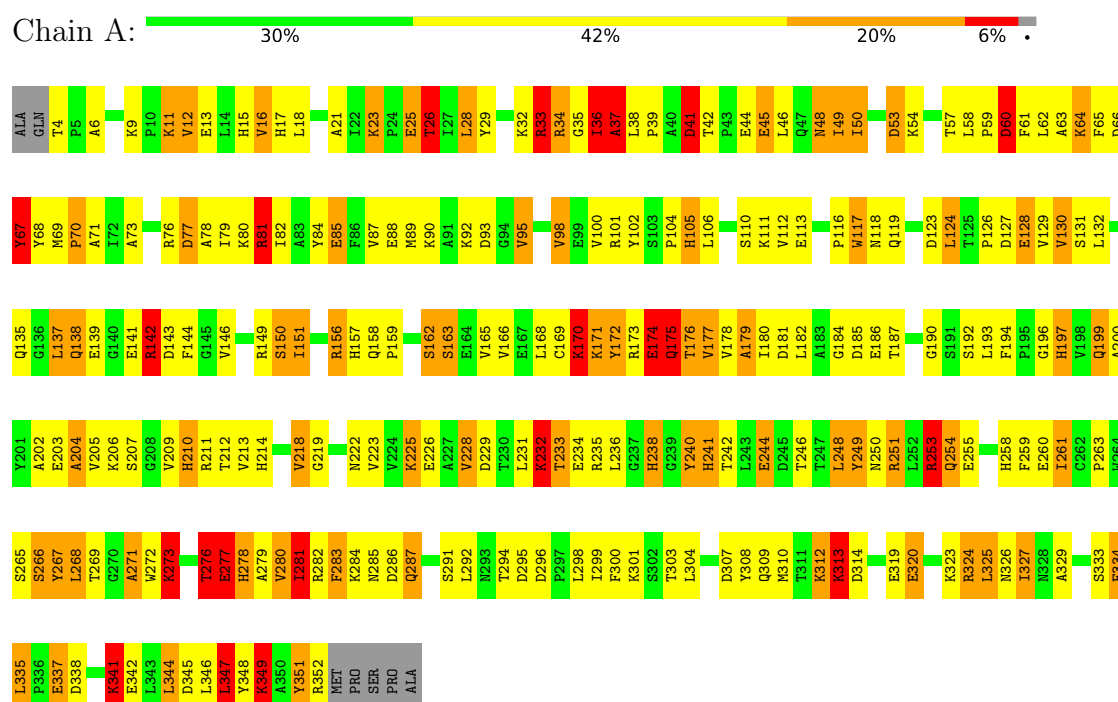
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	442	Total	O	0	0
			442	442		

3 Residue-property plots

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



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, α , β , γ	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 ²)	23.0	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: ZN, FR3

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	2.35	116/2852 (4.1%)	2.80	293/3866 (7.6%)

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 (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	HIS	ND1-CE1	10.12	1.42	1.32
1	A	235	ARG	CA-C	9.66	1.64	1.52
1	A	204	ALA	CA-C	9.19	1.64	1.52
1	A	210	HIS	ND1-CE1	9.01	1.41	1.32
1	A	101	ARG	C-N	8.91	1.44	1.33
1	A	212	THR	CA-C	8.73	1.63	1.52
1	A	192	SER	N-CA	8.67	1.57	1.46
1	A	196	GLY	CA-C	8.31	1.61	1.52
1	A	105	HIS	CD2-NE2	-8.18	1.28	1.37
1	A	15	HIS	CG-ND1	-8.06	1.29	1.38
1	A	181	ASP	CA-C	8.03	1.62	1.52
1	A	176	THR	N-CA	7.95	1.61	1.46
1	A	142	ARG	NE-CZ	7.94	1.41	1.33
1	A	197	HIS	CE1-NE2	7.89	1.40	1.32
1	A	60	ASP	CA-CB	7.77	1.66	1.53
1	A	112	VAL	CA-CB	-7.77	1.44	1.54
1	A	258	HIS	CE1-NE2	7.59	1.40	1.32
1	A	190	GLY	CA-C	7.58	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	N-CA	7.57	1.55	1.46
1	A	17	HIS	ND1-CE1	7.49	1.40	1.32
1	A	65	PHE	CA-C	7.47	1.62	1.52
1	A	106	LEU	CA-CB	7.45	1.66	1.53
1	A	95	VAL	CA-C	7.38	1.60	1.52
1	A	199	GLN	CG-CD	7.31	1.70	1.52
1	A	278	HIS	CE1-NE2	7.28	1.39	1.32
1	A	21	ALA	CA-CB	7.26	1.60	1.53
1	A	58	LEU	C-N	7.25	1.43	1.33
1	A	253	ARG	NE-CZ	7.19	1.41	1.33
1	A	197	HIS	CA-C	7.13	1.61	1.52
1	A	102	TYR	CA-CB	7.12	1.66	1.53
1	A	157	HIS	CE1-NE2	7.05	1.39	1.32
1	A	17	HIS	CG-ND1	-6.99	1.30	1.38
1	A	211	ARG	CA-C	6.92	1.60	1.52
1	A	333	SER	CA-C	-6.92	1.43	1.53
1	A	282	ARG	CA-CB	6.91	1.64	1.53
1	A	334	PHE	CA-C	6.86	1.62	1.52
1	A	263	PRO	CA-C	6.86	1.62	1.52
1	A	105	HIS	ND1-CE1	6.79	1.39	1.32
1	A	151	ILE	CA-C	6.74	1.61	1.52
1	A	15	HIS	CG-CD2	6.59	1.43	1.35
1	A	214	HIS	CA-CB	6.58	1.62	1.53
1	A	296	ASP	CA-C	6.58	1.60	1.52
1	A	101	ARG	CZ-NH2	6.54	1.42	1.33
1	A	34	ARG	NE-CZ	6.53	1.40	1.33
1	A	277	GLU	CG-CD	6.48	1.68	1.52
1	A	248	LEU	N-CA	6.47	1.54	1.46
1	A	213	VAL	C-N	6.46	1.42	1.33
1	A	182	LEU	CA-C	6.40	1.60	1.52
1	A	214	HIS	CG-CD2	6.34	1.42	1.35
1	A	18	LEU	N-CA	6.34	1.53	1.46
1	A	98	VAL	N-CA	6.33	1.53	1.46
1	A	210	HIS	CD2-NE2	6.31	1.44	1.37
1	A	61	PHE	N-CA	6.30	1.53	1.46
1	A	162	SER	N-CA	6.29	1.54	1.46
1	A	93	ASP	CA-C	6.26	1.61	1.52
1	A	159	PRO	C-N	6.18	1.42	1.33
1	A	202	ALA	C-N	6.17	1.42	1.34
1	A	347	LEU	CA-C	6.11	1.60	1.52
1	A	238	HIS	CE1-NE2	6.01	1.38	1.32
1	A	15	HIS	CA-C	6.01	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	ARG	CZ-NH1	5.99	1.41	1.32
1	A	37	ALA	C-N	-5.97	1.26	1.33
1	A	126	PRO	CA-C	5.94	1.60	1.52
1	A	238	HIS	ND1-CE1	5.91	1.38	1.32
1	A	229	ASP	CA-CB	5.88	1.62	1.53
1	A	200	ALA	CA-CB	5.86	1.62	1.53
1	A	141	GLU	CA-C	5.86	1.60	1.52
1	A	158	GLN	CA-CB	-5.80	1.46	1.53
1	A	194	PHE	CA-C	5.79	1.59	1.53
1	A	282	ARG	CA-C	5.78	1.60	1.52
1	A	104	PRO	CA-C	5.78	1.61	1.52
1	A	203	GLU	C-N	5.78	1.41	1.33
1	A	244	GLU	C-N	5.76	1.41	1.33
1	A	36	ILE	CA-CB	5.74	1.62	1.54
1	A	177	VAL	CA-C	5.73	1.59	1.52
1	A	184	GLY	N-CA	5.73	1.53	1.45
1	A	17	HIS	CA-C	5.65	1.59	1.52
1	A	60	ASP	CB-CG	5.64	1.66	1.52
1	A	341	LYS	N-CA	5.64	1.53	1.46
1	A	101	ARG	NE-CZ	5.60	1.39	1.33
1	A	324	ARG	CA-C	5.60	1.60	1.52
1	A	127	ASP	N-CA	5.56	1.52	1.46
1	A	157	HIS	CG-ND1	-5.53	1.32	1.38
1	A	69	MET	C-N	5.50	1.40	1.33
1	A	268	LEU	CA-C	-5.49	1.45	1.52
1	A	175	GLN	CA-CB	-5.49	1.45	1.53
1	A	282	ARG	C-N	5.49	1.40	1.33
1	A	174	GLU	CA-CB	5.47	1.62	1.53
1	A	349	LYS	C-N	5.47	1.41	1.34
1	A	276	THR	C-N	5.44	1.41	1.33
1	A	12	VAL	CA-C	5.40	1.59	1.52
1	A	228	VAL	N-CA	5.38	1.52	1.46
1	A	182	LEU	CB-CG	5.37	1.64	1.53
1	A	73	ALA	CA-C	5.36	1.59	1.52
1	A	98	VAL	C-N	5.34	1.41	1.33
1	A	226	GLU	C-N	5.33	1.41	1.33
1	A	150	SER	C-N	5.33	1.40	1.33
1	A	85	GLU	CA-CB	5.32	1.62	1.53
1	A	260	GLU	CA-CB	5.32	1.59	1.52
1	A	166	VAL	CA-C	5.29	1.59	1.52
1	A	179	ALA	CA-C	5.27	1.59	1.52
1	A	158	GLN	CD-NE2	-5.25	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	N-CA	5.24	1.52	1.46
1	A	241	HIS	ND1-CE1	5.24	1.37	1.32
1	A	89	MET	CG-SD	5.24	1.93	1.80
1	A	259	PHE	N-CA	5.23	1.52	1.46
1	A	291	SER	CA-C	5.13	1.58	1.52
1	A	269	THR	C-N	-5.11	1.26	1.33
1	A	266	SER	N-CA	5.08	1.52	1.46
1	A	310	MET	C-N	5.08	1.40	1.33
1	A	15	HIS	CB-CG	5.04	1.57	1.50
1	A	163	SER	CA-C	5.04	1.59	1.52
1	A	205	VAL	CA-C	5.04	1.58	1.52
1	A	303	THR	CA-C	5.02	1.59	1.52
1	A	170	LYS	CA-C	5.01	1.59	1.52
1	A	185	ASP	CA-CB	5.01	1.59	1.52

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	23.39	135.99	112.60
1	A	277	GLU	CB-CG-CD	13.04	134.77	112.60
1	A	294	THR	CA-CB-OG1	12.55	128.42	109.60
1	A	175	GLN	N-CA-C	12.30	125.99	110.61
1	A	66	ASP	CA-CB-CG	-12.27	100.33	112.60
1	A	254	GLN	CB-CG-CD	-12.10	92.04	112.60
1	A	81	ARG	NE-CZ-NH2	11.81	129.82	119.20
1	A	26	THR	N-CA-C	10.66	124.19	111.82
1	A	35	GLY	CA-C-N	-10.55	109.92	121.84
1	A	35	GLY	C-N-CA	-10.55	109.92	121.84
1	A	276	THR	N-CA-CB	-10.22	94.65	111.20
1	A	281	ILE	CB-CG1-CD1	-10.22	92.34	113.80
1	A	277	GLU	CA-CB-CG	9.98	134.07	114.10
1	A	34	ARG	CD-NE-CZ	9.96	138.34	124.40
1	A	49	ILE	N-CA-C	9.93	119.86	110.53
1	A	253	ARG	CD-NE-CZ	9.90	138.26	124.40
1	A	33	ARG	N-CA-C	9.78	122.96	111.71
1	A	282	ARG	CA-C-O	9.66	130.79	120.55
1	A	127	ASP	CA-C-O	9.57	130.87	120.82
1	A	158	GLN	CG-CD-OE1	9.48	139.76	120.80
1	A	218	VAL	CA-CB-CG1	9.41	126.39	110.40
1	A	158	GLN	CG-CD-NE2	-9.37	102.34	116.40
1	A	281	ILE	CA-CB-CG2	9.20	126.14	110.50
1	A	101	ARG	NE-CZ-NH2	9.08	127.37	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ASP	N-CA-C	9.02	124.06	112.34
1	A	347	LEU	CD1-CG-CD2	8.96	130.51	110.80
1	A	251	ARG	NE-CZ-NH1	-8.93	112.57	121.50
1	A	324	ARG	CA-C-O	8.90	130.42	120.90
1	A	199	GLN	CA-CB-CG	-8.88	96.34	114.10
1	A	36	ILE	CA-C-O	8.75	126.64	119.29
1	A	105	HIS	CB-CG-CD2	-8.75	119.83	131.20
1	A	312	LYS	CA-CB-CG	-8.68	96.73	114.10
1	A	218	VAL	CA-CB-CG2	8.67	125.14	110.40
1	A	138	GLN	OE1-CD-NE2	-8.63	113.97	122.60
1	A	349	LYS	N-CA-C	8.63	120.31	111.07
1	A	313	LYS	CA-C-N	-8.61	108.57	122.26
1	A	313	LYS	C-N-CA	-8.61	108.57	122.26
1	A	209	VAL	CA-CB-CG1	8.60	125.02	110.40
1	A	33	ARG	CD-NE-CZ	-8.50	112.51	124.40
1	A	258	HIS	CA-CB-CG	-8.48	105.31	113.80
1	A	166	VAL	CA-CB-CG2	8.45	124.76	110.40
1	A	251	ARG	NE-CZ-NH2	8.45	126.80	119.20
1	A	87	VAL	CA-C-O	8.39	129.67	120.95
1	A	267	TYR	N-CA-C	8.33	119.98	111.07
1	A	67	TYR	N-CA-CB	8.22	122.45	110.20
1	A	89	MET	N-CA-C	8.18	120.20	111.28
1	A	34	ARG	NE-CZ-NH2	-7.96	112.03	119.20
1	A	105	HIS	CA-CB-CG	-7.92	105.88	113.80
1	A	88	GLU	N-CA-C	7.88	120.56	111.11
1	A	307	ASP	CA-CB-CG	-7.81	104.79	112.60
1	A	146	VAL	N-CA-C	-7.77	97.28	108.48
1	A	233	THR	CA-CB-CG2	7.77	123.71	110.50
1	A	271	ALA	CB-CA-C	-7.76	98.39	110.81
1	A	46	LEU	CD1-CG-CD2	-7.73	93.79	110.80
1	A	223	VAL	N-CA-C	7.68	118.48	110.72
1	A	327	ILE	CA-CB-CG1	7.68	123.46	110.40
1	A	101	ARG	NE-CZ-NH1	-7.51	113.99	121.50
1	A	170	LYS	CD-CE-NZ	-7.50	87.90	111.90
1	A	271	ALA	N-CA-C	7.50	120.11	111.11
1	A	34	ARG	CA-C-O	7.50	127.30	119.05
1	A	37	ALA	N-CA-C	7.43	126.64	110.80
1	A	44	GLU	N-CA-C	7.43	120.32	111.33
1	A	232	LYS	CB-CA-C	-7.35	101.29	111.73
1	A	234	GLU	CA-C-O	7.33	126.81	118.97
1	A	199	GLN	CB-CG-CD	7.33	125.06	112.60
1	A	268	LEU	N-CA-C	7.28	120.26	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH1	7.26	128.76	121.50
1	A	206	LYS	N-CA-C	7.25	119.18	111.28
1	A	64	LYS	O-C-N	7.22	129.78	122.12
1	A	6	ALA	N-CA-C	7.19	121.15	112.38
1	A	37	ALA	CA-C-O	7.15	130.74	120.51
1	A	166	VAL	CB-CA-C	-7.15	102.35	112.22
1	A	223	VAL	CA-CB-CG1	7.15	122.56	110.40
1	A	279	ALA	N-CA-C	7.11	120.85	111.75
1	A	283	PHE	CA-CB-CG	7.10	120.90	113.80
1	A	181	ASP	CA-CB-CG	7.05	119.65	112.60
1	A	67	TYR	CB-CA-C	-7.04	97.83	110.70
1	A	324	ARG	N-CA-C	7.03	119.55	111.11
1	A	286	ASP	CA-C-N	-7.00	111.79	122.08
1	A	286	ASP	C-N-CA	-7.00	111.79	122.08
1	A	76	ARG	CA-C-N	-6.98	109.71	120.31
1	A	76	ARG	C-N-CA	-6.98	109.71	120.31
1	A	89	MET	CA-C-O	6.97	127.94	120.55
1	A	163	SER	CA-C-N	-6.97	108.83	120.68
1	A	163	SER	C-N-CA	-6.97	108.83	120.68
1	A	255	GLU	CA-C-O	6.96	127.85	119.43
1	A	312	LYS	N-CA-C	6.89	118.48	110.97
1	A	89	MET	CA-CB-CG	6.88	127.87	114.10
1	A	351	TYR	CA-C-N	-6.88	109.32	121.70
1	A	351	TYR	C-N-CA	-6.88	109.32	121.70
1	A	157	HIS	CA-CB-CG	-6.83	106.97	113.80
1	A	232	LYS	N-CA-C	6.82	120.95	111.74
1	A	233	THR	CB-CA-C	-6.78	95.77	109.68
1	A	238	HIS	CA-CB-CG	-6.67	107.13	113.80
1	A	131	SER	CB-CA-C	6.67	121.86	110.79
1	A	179	ALA	O-C-N	6.66	129.95	123.29
1	A	41	ASP	CB-CA-C	-6.62	99.32	110.44
1	A	325	LEU	N-CA-CB	-6.60	99.64	110.40
1	A	326	ASN	CA-C-N	-6.59	111.06	120.42
1	A	326	ASN	C-N-CA	-6.59	111.06	120.42
1	A	143	ASP	N-CA-C	6.58	119.79	111.69
1	A	218	VAL	N-CA-CB	-6.54	100.43	111.23
1	A	246	THR	N-CA-C	6.53	118.39	111.28
1	A	344	LEU	CD1-CG-CD2	-6.51	96.47	110.80
1	A	162	SER	CA-C-N	-6.49	109.88	120.72
1	A	162	SER	C-N-CA	-6.49	109.88	120.72
1	A	346	LEU	N-CA-C	6.49	118.04	110.97
1	A	63	ALA	N-CA-C	6.46	119.14	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LYS	N-CA-C	6.45	118.31	111.28
1	A	273	LYS	CA-C-O	6.44	124.42	119.46
1	A	82	ILE	N-CA-C	6.43	117.18	110.62
1	A	241	HIS	CA-CB-CG	-6.42	107.38	113.80
1	A	177	VAL	N-CA-C	6.42	118.04	108.54
1	A	64	LYS	N-CA-CB	6.42	119.55	110.12
1	A	84	TYR	N-CA-C	6.41	118.80	111.11
1	A	62	LEU	N-CA-C	6.41	119.08	111.71
1	A	175	GLN	CB-CG-CD	-6.39	101.73	112.60
1	A	105	HIS	ND1-CG-CD2	6.39	112.49	106.10
1	A	105	HIS	ND1-CE1-NE2	6.38	114.78	108.40
1	A	254	GLN	CA-CB-CG	-6.38	101.33	114.10
1	A	26	THR	OG1-CB-CG2	6.38	122.06	109.30
1	A	118	ASN	OD1-CG-ND2	-6.34	116.25	122.60
1	A	26	THR	CA-CB-OG1	6.32	119.08	109.60
1	A	105	HIS	CG-ND1-CE1	-6.31	98.57	109.30
1	A	287	GLN	N-CA-C	6.30	120.22	111.90
1	A	175	GLN	N-CA-CB	-6.28	102.86	111.65
1	A	50	ILE	CA-C-N	-6.27	112.75	120.64
1	A	50	ILE	C-N-CA	-6.27	112.75	120.64
1	A	280	VAL	CA-C-N	-6.27	111.88	120.46
1	A	280	VAL	C-N-CA	-6.27	111.88	120.46
1	A	111	LYS	N-CA-C	6.26	120.06	111.54
1	A	338	ASP	N-CA-C	6.26	118.10	111.28
1	A	33	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	A	174	GLU	CB-CG-CD	6.25	123.23	112.60
1	A	117	TRP	CA-C-N	-6.25	113.88	124.31
1	A	117	TRP	C-N-CA	-6.25	113.88	124.31
1	A	41	ASP	CA-CB-CG	-6.22	106.38	112.60
1	A	313	LYS	N-CA-C	6.20	119.02	111.82
1	A	81	ARG	CD-NE-CZ	6.20	133.08	124.40
1	A	166	VAL	N-CA-CB	6.20	119.88	110.58
1	A	286	ASP	N-CA-C	6.19	120.69	113.20
1	A	81	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	A	11	LYS	CA-C-N	-6.17	114.54	123.06
1	A	11	LYS	C-N-CA	-6.17	114.54	123.06
1	A	210	HIS	CA-CB-CG	-6.16	107.64	113.80
1	A	301	LYS	CA-CB-CG	-6.13	101.83	114.10
1	A	240	TYR	N-CA-C	6.12	117.95	111.28
1	A	93	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	139	GLU	N-CA-C	6.10	118.43	111.11
1	A	66	ASP	CA-C-N	-6.10	110.16	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ASP	C-N-CA	-6.10	110.16	120.58
1	A	128	GLU	N-CA-CB	-6.09	101.17	110.12
1	A	77	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	166	VAL	CA-CB-CG1	6.08	120.74	110.40
1	A	276	THR	CA-CB-OG1	6.07	118.70	109.60
1	A	11	LYS	CA-CB-CG	-6.06	101.98	114.10
1	A	197	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	236	LEU	CD1-CG-CD2	6.05	124.11	110.80
1	A	67	TYR	CG-CD1-CE1	-6.04	112.13	121.20
1	A	82	ILE	O-C-N	6.04	127.73	121.87
1	A	95	VAL	CG1-CB-CG2	-6.03	97.54	110.80
1	A	146	VAL	CA-CB-CG2	6.02	120.63	110.40
1	A	325	LEU	CD1-CG-CD2	6.01	124.03	110.80
1	A	199	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	A	123	ASP	N-CA-C	5.98	119.73	111.71
1	A	4	THR	CA-CB-CG2	5.94	120.60	110.50
1	A	342	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	187	THR	CA-C-O	5.92	126.22	119.18
1	A	139	GLU	CA-CB-CG	-5.91	102.28	114.10
1	A	209	VAL	CA-CB-CG2	5.91	120.44	110.40
1	A	225	LYS	CA-C-O	5.90	126.68	120.42
1	A	124	LEU	CD1-CG-CD2	5.86	123.69	110.80
1	A	253	ARG	CA-C-N	-5.86	111.84	120.28
1	A	253	ARG	C-N-CA	-5.86	111.84	120.28
1	A	101	ARG	O-C-N	5.85	130.44	123.24
1	A	342	GLU	N-CA-C	5.84	117.65	111.28
1	A	314	ASP	CA-C-O	5.84	125.47	119.05
1	A	344	LEU	CB-CG-CD1	5.84	128.21	110.70
1	A	232	LYS	CB-CG-CD	5.83	124.70	111.30
1	A	319	GLU	N-CA-C	5.81	117.28	111.07
1	A	64	LYS	CA-C-O	-5.80	114.40	120.55
1	A	53	ASP	N-CA-C	5.79	121.64	113.02
1	A	142	ARG	CD-NE-CZ	-5.79	116.30	124.40
1	A	178	VAL	N-CA-C	5.78	118.45	112.90
1	A	326	ASN	CA-CB-CG	-5.78	106.83	112.60
1	A	68	TYR	CB-CA-C	5.76	119.06	109.56
1	A	281	ILE	N-CA-C	5.72	116.45	110.62
1	A	131	SER	N-CA-CB	-5.71	101.72	110.12
1	A	205	VAL	CA-C-N	-5.71	112.63	120.28
1	A	205	VAL	C-N-CA	-5.71	112.63	120.28
1	A	175	GLN	CG-CD-NE2	-5.71	107.84	116.40
1	A	156	ARG	CB-CA-C	-5.70	101.28	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CA-C	5.69	121.59	110.67
1	A	267	TYR	CB-CG-CD1	-5.67	112.29	120.80
1	A	62	LEU	CB-CA-C	-5.66	100.15	110.63
1	A	190	GLY	CA-C-N	-5.66	111.27	120.72
1	A	190	GLY	C-N-CA	-5.66	111.27	120.72
1	A	266	SER	N-CA-C	5.64	117.43	111.28
1	A	342	GLU	CA-C-O	5.64	126.53	120.55
1	A	78	ALA	N-CA-C	5.63	117.42	111.28
1	A	137	LEU	N-CA-C	-5.63	105.22	111.36
1	A	60	ASP	OD1-CG-OD2	-5.62	109.40	122.90
1	A	335	LEU	CB-CA-C	-5.61	99.29	109.45
1	A	119	GLN	N-CA-CB	5.59	118.19	109.97
1	A	325	LEU	CB-CG-CD2	5.59	127.49	110.70
1	A	130	VAL	CA-C-O	5.59	126.77	120.95
1	A	277	GLU	CA-C-N	-5.59	112.93	120.87
1	A	277	GLU	C-N-CA	-5.59	112.93	120.87
1	A	158	GLN	CB-CA-C	-5.59	102.42	111.14
1	A	163	SER	CA-C-O	5.58	126.24	119.38
1	A	327	ILE	N-CA-C	5.58	116.36	110.72
1	A	33	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	A	132	LEU	CA-C-O	5.54	126.43	120.55
1	A	261	ILE	CA-CB-CG2	5.53	119.90	110.50
1	A	25	GLU	N-CA-C	5.49	117.98	111.33
1	A	129	VAL	CG1-CB-CG2	-5.47	98.76	110.80
1	A	98	VAL	CA-C-N	-5.47	115.39	123.05
1	A	98	VAL	C-N-CA	-5.47	115.39	123.05
1	A	197	HIS	N-CA-C	5.47	117.04	111.14
1	A	254	GLN	CA-C-N	-5.46	113.16	122.56
1	A	254	GLN	C-N-CA	-5.46	113.16	122.56
1	A	196	GLY	CA-C-N	-5.44	113.04	120.44
1	A	196	GLY	C-N-CA	-5.44	113.04	120.44
1	A	76	ARG	CA-C-O	5.44	127.01	120.92
1	A	106	LEU	CA-C-O	5.43	126.11	119.05
1	A	255	GLU	N-CA-C	5.41	119.52	113.02
1	A	67	TYR	N-CA-C	5.41	118.34	111.69
1	A	307	ASP	CA-C-N	-5.41	112.09	120.31
1	A	307	ASP	C-N-CA	-5.41	112.09	120.31
1	A	241	HIS	CB-CA-C	-5.41	100.36	110.36
1	A	205	VAL	N-CA-C	5.40	115.60	110.42
1	A	177	VAL	CG1-CB-CG2	5.39	122.67	110.80
1	A	118	ASN	CB-CG-OD1	5.38	131.57	120.80
1	A	304	LEU	CA-C-O	5.38	126.16	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	TYR	CA-C-O	5.36	126.63	120.90
1	A	165	VAL	CA-C-N	-5.35	112.83	120.42
1	A	165	VAL	C-N-CA	-5.35	112.83	120.42
1	A	285	ASN	CA-C-O	5.35	126.12	119.97
1	A	348	TYR	CB-CA-C	-5.33	101.94	110.79
1	A	87	VAL	CA-CB-CG2	5.33	119.45	110.40
1	A	273	LYS	N-CA-C	5.33	117.30	109.42
1	A	277	GLU	CB-CA-C	-5.32	102.66	110.06
1	A	320	GLU	CA-C-N	-5.32	112.73	120.29
1	A	320	GLU	C-N-CA	-5.32	112.73	120.29
1	A	234	GLU	CB-CG-CD	-5.32	103.56	112.60
1	A	240	TYR	CA-C-N	-5.30	111.71	122.31
1	A	240	TYR	C-N-CA	-5.30	111.71	122.31
1	A	48	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	194	PHE	N-CA-CB	-5.23	102.06	109.75
1	A	98	VAL	CG1-CB-CG2	-5.22	99.31	110.80
1	A	346	LEU	CA-C-O	5.22	126.48	121.00
1	A	254	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	A	233	THR	OG1-CB-CG2	5.21	119.71	109.30
1	A	158	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	176	THR	CB-CA-C	-5.20	97.67	109.10
1	A	79	ILE	N-CA-CB	-5.18	104.48	110.55
1	A	232	LYS	CA-CB-CG	5.16	124.41	114.10
1	A	60	ASP	N-CA-C	-5.15	105.74	112.23
1	A	119	GLN	CA-C-N	-5.15	110.51	121.32
1	A	119	GLN	C-N-CA	-5.15	110.51	121.32
1	A	110	SER	CB-CA-C	-5.15	101.05	110.62
1	A	38	LEU	N-CA-C	-5.14	100.53	108.55
1	A	48	ASN	N-CA-C	5.14	116.96	111.36
1	A	294	THR	N-CA-C	5.14	118.70	112.23
1	A	300	PHE	CA-C-O	5.13	125.36	119.35
1	A	326	ASN	O-C-N	5.13	128.00	122.15
1	A	168	LEU	N-CA-C	5.13	116.95	111.36
1	A	41	ASP	N-CA-C	5.12	120.65	113.02
1	A	299	ILE	CA-CB-CG1	-5.12	101.70	110.40
1	A	4	THR	CA-C-O	-5.12	112.10	120.80
1	A	38	LEU	CD1-CG-CD2	-5.11	99.56	110.80
1	A	192	SER	CA-C-N	-5.10	114.64	122.60
1	A	192	SER	C-N-CA	-5.10	114.64	122.60
1	A	128	GLU	N-CA-C	5.09	116.83	111.28
1	A	71	ALA	CA-C-N	-5.08	117.95	123.08
1	A	71	ALA	C-N-CA	-5.08	117.95	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	TYR	N-CA-C	5.08	119.74	111.37
1	A	144	PHE	CA-C-N	-5.07	112.70	120.91
1	A	144	PHE	C-N-CA	-5.07	112.70	120.91
1	A	211	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	142	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A	265	SER	CB-CA-C	-5.05	102.72	110.81
1	A	170	LYS	CG-CD-CE	5.05	122.92	111.30
1	A	301	LYS	N-CA-C	5.05	118.56	111.74
1	A	206	LYS	CD-CE-NZ	-5.05	95.75	111.90
1	A	309	GLN	CA-C-O	5.05	125.77	120.42
1	A	171	LYS	O-C-N	5.04	127.54	122.09
1	A	222	ASN	CA-C-N	-5.03	113.28	120.42
1	A	222	ASN	C-N-CA	-5.03	113.28	120.42
1	A	53	ASP	CA-C-O	5.02	124.81	119.34
1	A	273	LYS	CB-CG-CD	-5.02	99.75	111.30
1	A	219	GLY	N-CA-C	-5.01	102.99	112.51
1	A	296	ASP	CB-CA-C	-5.01	102.89	111.15

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	108	0
2	A	1	0	0	0	0
3	A	23	0	19	0	0
4	A	442	0	0	58	0
All	All	3254	0	2762	108	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 (108) 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:42:THR:HG23	1:A:45:GLU:HB2	1.75	0.68
1:A:105:HIS:HE1	4:A:1257:HOH:O	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HB2	1:A:49:ILE:HD13	1.80	0.64
1:A:225:LYS:HE2	4:A:1226:HOH:O	1.96	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
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:67:TYR:HA	4:A:1380:HOH:O	2.08	0.52
1:A:172:TYR:CE2	4:A:1386:HOH:O	2.60	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: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:26:THR:HG22	4:A:1392:HOH:O	2.11	0.49
1:A:231:LEU:O	1:A:232:LYS:HB2	2.12	0.49
1:A:57:THR:HG23	1:A:60:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:GLU:HG3	1:A:341:LYS:HZ1	1.77	0.48
1:A:28:LEU:HD13	4:A:1186:HOH:O	2.14	0.48
1:A:313:LYS:N	1:A:313:LYS:HD2	2.29	0.48
1:A:180:ILE:HA	4:A:1177:HOH:O	2.13	0.47
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:NZ	1:A:313:LYS:HA	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:281:ILE:C	1:A:281:ILE:HD12	2.43	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:41:ASP:HB2	4:A:1199:HOH:O	2.20	0.42
1:A:347:LEU:HG	4:A:1412:HOH:O	2.19	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:N	1:A:48:ASN:HD22	2.19	0.41
1:A:90:LYS:HE2	1:A:90:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HD11	1:A:283:PHE:CE2	2.56	0.41
1:A:13:GLU:C	4:A:1389:HOH:O	2.64	0.40
1:A:162:SER:OG	1:A:197:HIS:HD2	2.04	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%)	330 (95%)	15 (4%)	2 (1%)	21 17

All (2) Ramachandran outliers are listed below:

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

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	304/309 (98%)	263 (86%)	41 (14%)	4 2

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	23	LYS
1	A	25	GLU
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	54	LYS
1	A	60	ASP
1	A	67	TYR
1	A	70	PRO
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	177	VAL
1	A	193	LEU
1	A	199	GLN
1	A	232	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	134	ASN
1	A	138	GLN
1	A	175	GLN
1	A	197	HIS
1	A	241	HIS
1	A	250	ASN
1	A	278	HIS

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 oligosaccharides 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	-	25,25,25	1.93	7 (28%)	29,34,34	1.92	4 (13%)

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	-	-	3/15/15/15	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	C13-N2	4.31	1.53	1.48
3	A	1001	FR3	C1-C5	-3.89	1.32	1.37
3	A	1001	FR3	C26-C27	3.05	1.43	1.36
3	A	1001	FR3	C14-C13	3.02	1.64	1.52
3	A	1001	FR3	C7-C6	2.79	1.44	1.38
3	A	1001	FR3	C6-C2	2.78	1.42	1.36
3	A	1001	FR3	C26-C25	2.34	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR3	C5-C8-N10	7.44	123.83	116.28
3	A	1001	FR3	C1-N2-C3	-3.71	103.91	106.37
3	A	1001	FR3	O9-C8-C5	-2.85	117.51	120.25
3	A	1001	FR3	O9-C8-N10	-2.12	118.13	122.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

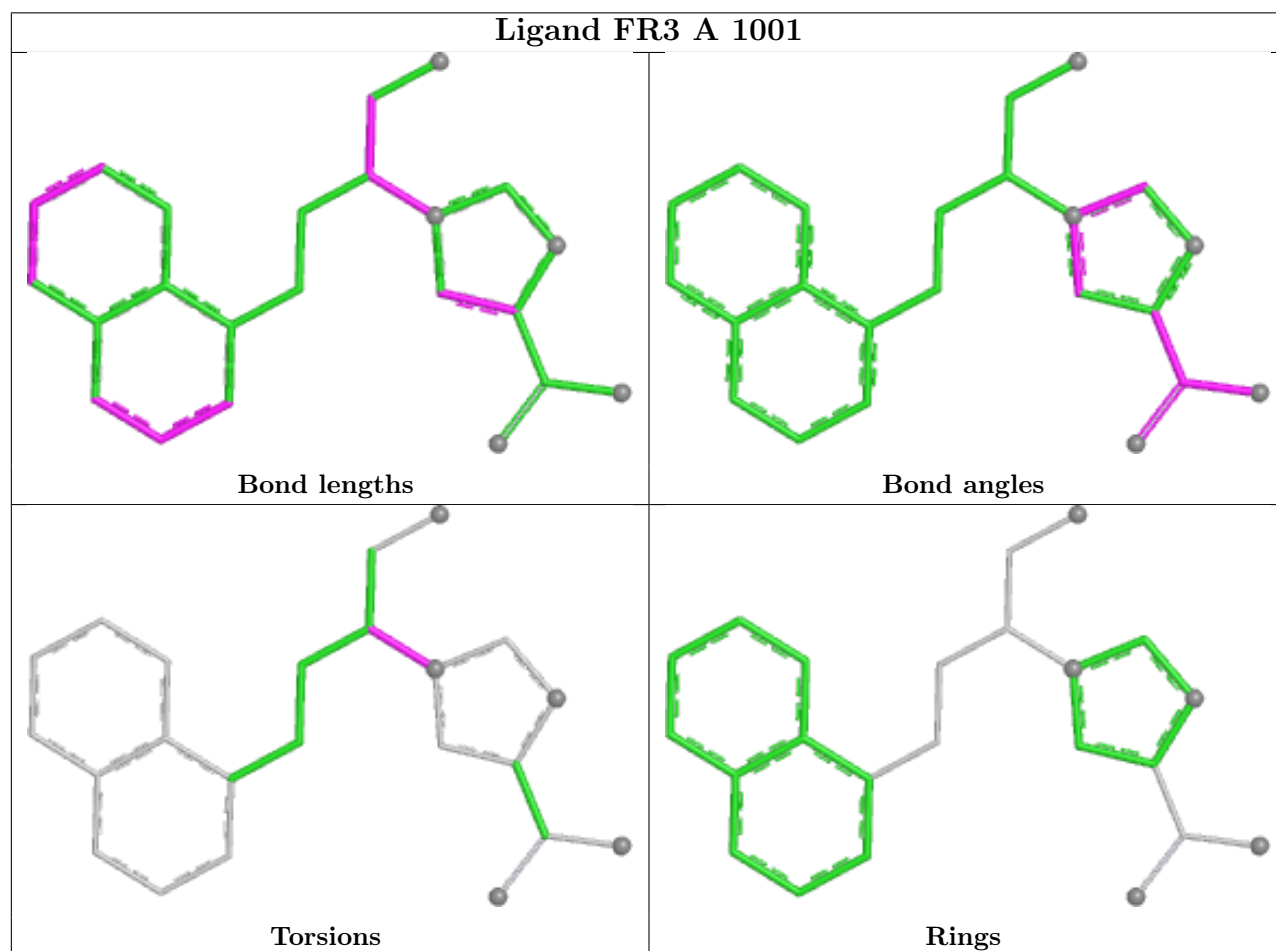
Mol	Chain	Res	Type	Atoms
3	A	1001	FR3	C18-C13-N2-C1
3	A	1001	FR3	C14-C13-N2-C1
3	A	1001	FR3	C18-C13-N2-C3

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

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.