



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:56 PM UTC

PDB ID : 1NDW / pdb_00001ndw
Title : Crystal Structure of Adenosine Deaminase Complexed with FR221647
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

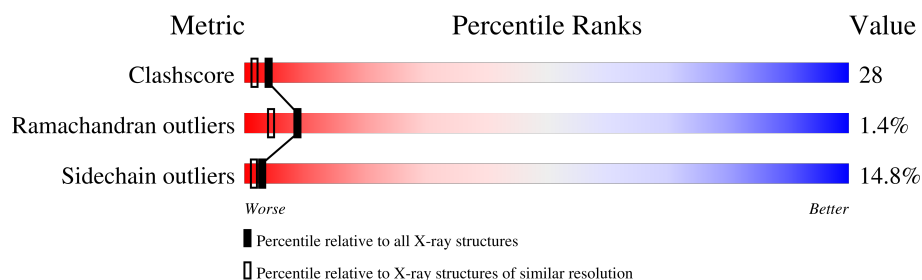
1 Overall quality at a glance

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	22% 42% 27% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3288 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			

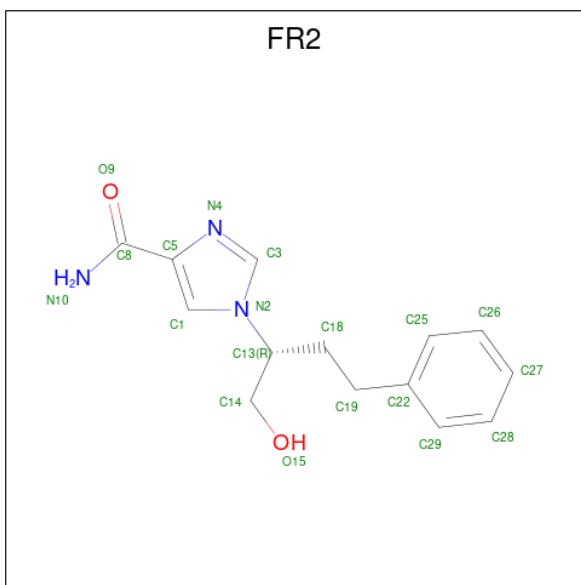
There are 15 discrepancies between the modelled and reference sequences:

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-PHENYLPROPYL)-1H-IMIDAZOLE-4-CARBOXAMIDE (CCD ID: FR2) (formula: C₁₄H₁₇N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 4 is water.

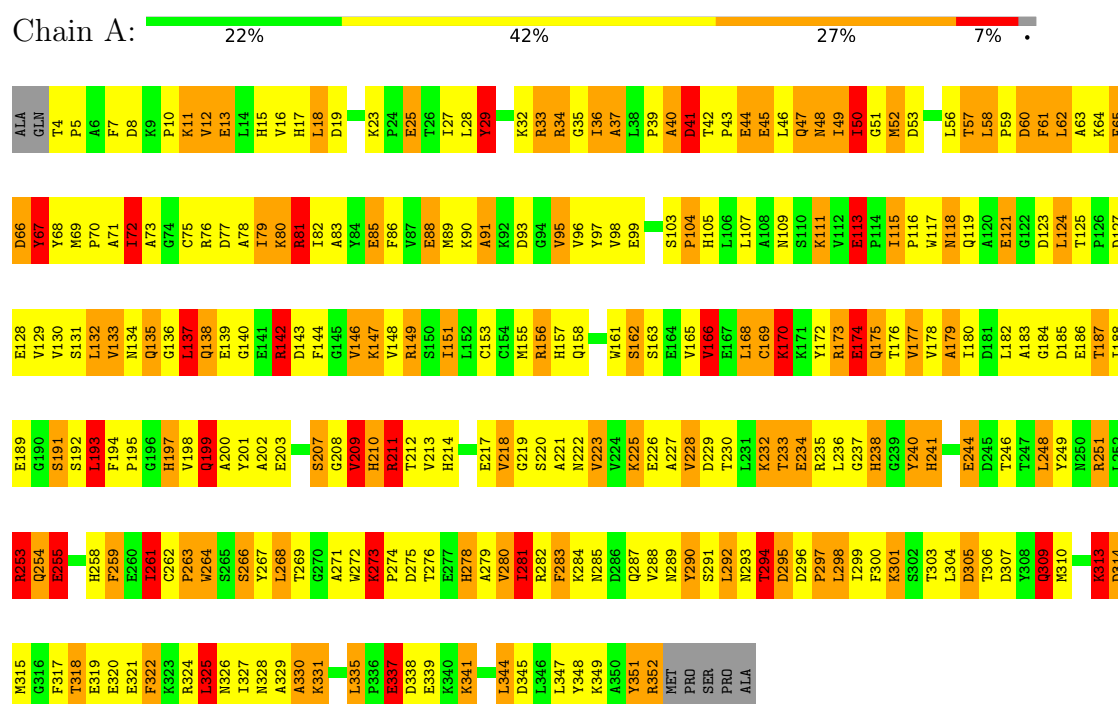
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	480	Total	O	0	0
			480	480		

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	77.63Å 77.63Å 135.66Å 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}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.206 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3288	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: FR2, 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	2.32	113/2852 (4.0%)	2.87	320/3866 (8.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	13

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	VAL	CA-CB	10.69	1.69	1.54
1	A	211	ARG	CD-NE	-9.73	1.32	1.46
1	A	288	VAL	CA-C	9.34	1.64	1.52
1	A	210	HIS	CG-CD2	9.33	1.46	1.35
1	A	197	HIS	CE1-NE2	9.11	1.41	1.32
1	A	211	ARG	CZ-NH2	-8.82	1.22	1.33
1	A	210	HIS	CE1-NE2	8.80	1.41	1.32
1	A	324	ARG	NE-CZ	8.80	1.42	1.33
1	A	330	ALA	CA-CB	8.74	1.67	1.53
1	A	17	HIS	CA-CB	8.69	1.65	1.53
1	A	201	TYR	CA-C	8.65	1.64	1.52
1	A	232	LYS	CA-C	8.60	1.64	1.53
1	A	258	HIS	ND1-CE1	8.37	1.41	1.32
1	A	86	PHE	N-CA	8.09	1.56	1.46
1	A	183	ALA	CA-CB	8.03	1.67	1.54
1	A	173	ARG	NE-CZ	8.02	1.41	1.33
1	A	258	HIS	CA-CB	7.80	1.64	1.53
1	A	103	SER	CA-CB	7.57	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	ALA	CA-CB	7.54	1.65	1.53
1	A	10	PRO	CA-C	7.49	1.62	1.52
1	A	197	HIS	ND1-CE1	7.49	1.40	1.32
1	A	91	ALA	N-CA	7.43	1.55	1.46
1	A	146	VAL	CA-C	-7.29	1.44	1.52
1	A	79	ILE	C-N	7.28	1.44	1.34
1	A	127	ASP	CA-C	7.27	1.62	1.52
1	A	327	ILE	CA-C	7.25	1.63	1.52
1	A	226	GLU	C-N	7.21	1.43	1.33
1	A	81	ARG	NE-CZ	7.21	1.41	1.33
1	A	185	ASP	CA-CB	7.18	1.61	1.52
1	A	15	HIS	ND1-CE1	7.02	1.39	1.32
1	A	77	ASP	CA-CB	7.02	1.64	1.53
1	A	295	ASP	C-N	6.96	1.43	1.33
1	A	326	ASN	CA-C	-6.93	1.43	1.52
1	A	104	PRO	N-CA	-6.92	1.38	1.47
1	A	155	MET	N-CA	6.84	1.54	1.46
1	A	136	GLY	CA-C	6.82	1.59	1.52
1	A	49	ILE	CA-C	6.78	1.60	1.52
1	A	248	LEU	CA-C	6.70	1.61	1.52
1	A	284	LYS	N-CA	6.63	1.54	1.46
1	A	130	VAL	CA-C	6.61	1.61	1.52
1	A	137	LEU	CA-C	6.56	1.61	1.52
1	A	339	GLU	CA-C	-6.55	1.44	1.52
1	A	296	ASP	CA-C	6.54	1.60	1.52
1	A	200	ALA	CA-C	-6.50	1.44	1.52
1	A	326	ASN	CA-CB	6.49	1.64	1.53
1	A	15	HIS	CG-ND1	-6.45	1.31	1.38
1	A	248	LEU	N-CA	6.42	1.54	1.46
1	A	17	HIS	CD2-NE2	6.37	1.44	1.37
1	A	278	HIS	ND1-CE1	6.28	1.38	1.32
1	A	210	HIS	ND1-CE1	6.28	1.38	1.32
1	A	147	LYS	CA-C	6.28	1.61	1.52
1	A	191	SER	CA-CB	6.18	1.63	1.53
1	A	169	CYS	C-N	6.18	1.42	1.33
1	A	65	PHE	CA-CB	6.17	1.64	1.53
1	A	134	ASN	CA-C	6.12	1.60	1.52
1	A	18	LEU	CA-C	6.05	1.60	1.52
1	A	271	ALA	CA-CB	6.04	1.63	1.53
1	A	234	GLU	N-CA	6.02	1.53	1.46
1	A	288	VAL	N-CA	5.90	1.53	1.46
1	A	328	ASN	N-CA	5.87	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	HIS	CE1-NE2	5.87	1.38	1.32
1	A	138	GLN	CA-C	5.86	1.60	1.52
1	A	214	HIS	CG-CD2	5.75	1.42	1.35
1	A	229	ASP	N-CA	5.75	1.53	1.46
1	A	283	PHE	C-N	5.71	1.41	1.33
1	A	60	ASP	CA-C	5.71	1.60	1.52
1	A	214	HIS	CA-CB	5.64	1.61	1.53
1	A	237	GLY	CA-C	5.63	1.59	1.51
1	A	15	HIS	CA-C	5.60	1.59	1.53
1	A	129	VAL	CA-C	5.59	1.59	1.52
1	A	282	ARG	C-N	5.53	1.40	1.33
1	A	305	ASP	CA-CB	5.51	1.62	1.53
1	A	139	GLU	C-N	5.51	1.40	1.33
1	A	289	ASN	CA-CB	5.50	1.59	1.52
1	A	195	PRO	N-CD	-5.49	1.40	1.47
1	A	177	VAL	N-CA	5.47	1.52	1.46
1	A	90	LYS	N-CA	5.46	1.53	1.46
1	A	249	TYR	CA-C	-5.43	1.46	1.52
1	A	222	ASN	CA-C	5.43	1.60	1.52
1	A	220	SER	CA-C	-5.42	1.45	1.53
1	A	241	HIS	CE1-NE2	5.38	1.38	1.32
1	A	58	LEU	C-N	5.38	1.41	1.33
1	A	96	VAL	C-N	5.36	1.40	1.33
1	A	211	ARG	NE-CZ	-5.36	1.27	1.33
1	A	345	ASP	N-CA	5.32	1.52	1.46
1	A	241	HIS	CG-ND1	-5.31	1.32	1.38
1	A	210	HIS	N-CA	5.31	1.52	1.45
1	A	58	LEU	CA-C	5.29	1.58	1.52
1	A	170	LYS	CA-C	5.26	1.59	1.52
1	A	264	TRP	CA-CB	5.25	1.61	1.53
1	A	199	GLN	C-O	-5.24	1.17	1.24
1	A	210	HIS	CD2-NE2	5.24	1.43	1.37
1	A	105	HIS	ND1-CE1	5.22	1.37	1.32
1	A	179	ALA	CA-CB	5.21	1.62	1.53
1	A	293	ASN	N-CA	-5.21	1.39	1.46
1	A	158	GLN	C-N	5.20	1.40	1.33
1	A	341	LYS	N-CA	5.17	1.52	1.46
1	A	155	MET	C-N	5.17	1.40	1.33
1	A	262	CYS	CA-C	5.15	1.58	1.52
1	A	16	VAL	CA-CB	5.15	1.61	1.54
1	A	65	PHE	CA-C	5.14	1.59	1.52
1	A	17	HIS	ND1-CE1	5.12	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	SER	CA-C	-5.11	1.45	1.52
1	A	278	HIS	CE1-NE2	5.11	1.37	1.32
1	A	133	VAL	C-O	-5.11	1.18	1.24
1	A	268	LEU	CA-C	-5.10	1.45	1.52
1	A	264	TRP	CA-C	5.09	1.59	1.52
1	A	178	VAL	CA-C	5.08	1.58	1.52
1	A	161	TRP	NE1-CE2	5.07	1.43	1.37
1	A	197	HIS	C-N	5.07	1.40	1.33
1	A	25	GLU	CA-CB	5.07	1.61	1.53
1	A	344	LEU	CB-CG	5.05	1.63	1.53
1	A	98	VAL	C-N	5.05	1.40	1.33

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	VAL	CA-CB-CG2	-20.97	74.76	110.40
1	A	149	ARG	NE-CZ-NH1	17.32	138.81	121.50
1	A	149	ARG	CD-NE-CZ	15.67	146.34	124.40
1	A	209	VAL	CA-CB-CG2	13.19	132.81	110.40
1	A	60	ASP	CA-CB-CG	12.19	124.79	112.60
1	A	77	ASP	CA-CB-CG	11.94	124.54	112.60
1	A	304	LEU	N-CA-C	11.70	126.73	111.75
1	A	254	GLN	CA-CB-CG	-11.64	90.81	114.10
1	A	41	ASP	N-CA-C	10.65	126.26	112.41
1	A	36	ILE	N-CA-C	10.63	121.13	110.82
1	A	66	ASP	N-CA-C	10.61	122.60	111.14
1	A	149	ARG	NH1-CZ-NH2	-10.18	106.06	119.30
1	A	233	THR	CA-CB-OG1	9.88	124.41	109.60
1	A	345	ASP	CA-CB-CG	9.79	122.39	112.60
1	A	254	GLN	N-CA-C	9.74	123.11	111.33
1	A	339	GLU	N-CA-C	9.54	121.67	111.28
1	A	254	GLN	CB-CG-CD	-9.49	96.47	112.60
1	A	326	ASN	CA-CB-CG	-9.42	103.18	112.60
1	A	211	ARG	CB-CG-CD	-9.34	89.82	111.30
1	A	157	HIS	CA-CB-CG	-9.27	104.53	113.80
1	A	299	ILE	N-CA-C	9.26	120.06	110.62
1	A	269	THR	CA-C-N	-9.03	109.13	123.31
1	A	269	THR	C-N-CA	-9.03	109.13	123.31
1	A	58	LEU	CD1-CG-CD2	-8.94	91.13	110.80
1	A	49	ILE	N-CA-C	8.93	118.96	110.30
1	A	309	GLN	CB-CG-CD	8.88	127.69	112.60
1	A	35	GLY	CA-C-N	-8.88	108.05	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLY	C-N-CA	-8.88	108.05	120.74
1	A	146	VAL	CG1-CB-CG2	-8.76	91.53	110.80
1	A	304	LEU	CA-C-O	8.74	129.99	120.20
1	A	49	ILE	N-CA-CB	-8.67	101.17	110.62
1	A	233	THR	N-CA-CB	8.60	122.68	110.04
1	A	233	THR	CB-CA-C	-8.59	94.24	109.62
1	A	15	HIS	CE1-NE2-CD2	-8.55	100.45	109.00
1	A	56	LEU	CA-C-N	-8.50	107.91	120.75
1	A	56	LEU	C-N-CA	-8.50	107.91	120.75
1	A	158	GLN	CB-CA-C	-8.40	98.04	111.14
1	A	89	MET	CA-CB-CG	8.39	130.89	114.10
1	A	221	ALA	N-CA-C	8.37	122.59	112.38
1	A	72	ILE	N-CA-C	8.29	118.94	111.81
1	A	192	SER	N-CA-C	8.27	122.47	112.38
1	A	139	GLU	CB-CA-C	8.24	124.86	110.85
1	A	40	ALA	CA-C-N	-8.19	109.64	122.49
1	A	40	ALA	C-N-CA	-8.19	109.64	122.49
1	A	50	ILE	N-CA-C	8.15	118.94	110.62
1	A	175	GLN	CA-C-N	8.10	136.28	121.70
1	A	175	GLN	C-N-CA	8.10	136.28	121.70
1	A	37	ALA	N-CA-CB	8.05	124.10	110.49
1	A	176	THR	CA-C-N	-8.05	110.55	121.66
1	A	176	THR	C-N-CA	-8.05	110.55	121.66
1	A	254	GLN	CA-C-N	-8.04	109.78	122.73
1	A	254	GLN	C-N-CA	-8.04	109.78	122.73
1	A	135	GLN	N-CA-C	8.03	120.82	111.02
1	A	146	VAL	CA-C-O	-7.96	112.04	120.48
1	A	111	LYS	CA-CB-CG	7.80	129.71	114.10
1	A	213	VAL	CA-C-N	-7.64	110.23	121.24
1	A	213	VAL	C-N-CA	-7.64	110.23	121.24
1	A	251	ARG	CD-NE-CZ	-7.62	113.74	124.40
1	A	337	GLU	CB-CG-CD	7.58	125.48	112.60
1	A	81	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	A	223	VAL	N-CA-C	7.49	118.29	110.72
1	A	328	ASN	CA-CB-CG	-7.49	105.11	112.60
1	A	53	ASP	CA-C-O	7.47	127.48	119.34
1	A	225	LYS	CB-CA-C	-7.46	98.41	110.79
1	A	254	GLN	OE1-CD-NE2	7.45	130.05	122.60
1	A	44	GLU	N-CA-C	7.40	119.34	111.28
1	A	162	SER	N-CA-C	7.36	120.35	111.82
1	A	60	ASP	CA-C-O	7.32	128.31	120.55
1	A	91	ALA	N-CA-C	7.32	119.89	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	N-CA-C	7.32	119.26	111.28
1	A	309	GLN	CA-CB-CG	7.31	128.73	114.10
1	A	269	THR	CA-CB-CG2	7.25	122.83	110.50
1	A	48	ASN	CA-CB-CG	7.25	119.85	112.60
1	A	351	TYR	CA-C-N	-7.25	108.65	121.70
1	A	351	TYR	C-N-CA	-7.25	108.65	121.70
1	A	222	ASN	CA-C-N	-7.22	110.17	120.42
1	A	222	ASN	C-N-CA	-7.22	110.17	120.42
1	A	298	LEU	CD1-CG-CD2	-7.20	94.97	110.80
1	A	142	ARG	CB-CG-CD	7.13	127.69	111.30
1	A	222	ASN	CA-C-O	7.12	128.15	119.97
1	A	268	LEU	N-CA-C	7.09	120.83	111.75
1	A	69	MET	N-CA-C	7.09	123.30	113.45
1	A	268	LEU	N-CA-CB	7.05	121.28	110.14
1	A	81	ARG	N-CA-C	7.04	119.03	111.36
1	A	132	LEU	CA-C-N	-7.03	110.44	120.42
1	A	132	LEU	C-N-CA	-7.03	110.44	120.42
1	A	325	LEU	CB-CG-CD2	7.01	131.74	110.70
1	A	222	ASN	CA-CB-CG	-6.94	105.66	112.60
1	A	173	ARG	CA-C-N	6.91	134.74	121.54
1	A	173	ARG	C-N-CA	6.91	134.74	121.54
1	A	197	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	281	ILE	CA-CB-CG1	6.88	122.10	110.40
1	A	170	LYS	CD-CE-NZ	-6.87	89.93	111.90
1	A	266	SER	N-CA-C	6.82	118.71	111.28
1	A	8	ASP	CA-CB-CG	-6.81	105.79	112.60
1	A	197	HIS	ND1-CE1-NE2	-6.79	101.61	108.40
1	A	66	ASP	CA-C-O	6.79	127.69	120.70
1	A	335	LEU	CB-CA-C	-6.79	98.58	109.37
1	A	262	CYS	CA-C-N	6.75	126.21	118.85
1	A	262	CYS	C-N-CA	6.75	126.21	118.85
1	A	221	ALA	CB-CA-C	-6.75	96.09	110.32
1	A	307	ASP	CA-C-N	-6.72	110.10	120.31
1	A	307	ASP	C-N-CA	-6.72	110.10	120.31
1	A	62	LEU	N-CA-C	6.70	118.58	111.28
1	A	176	THR	N-CA-CB	-6.70	100.12	111.50
1	A	158	GLN	CA-CB-CG	6.69	127.48	114.10
1	A	15	HIS	CG-CD2-NE2	6.67	113.87	107.20
1	A	17	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
1	A	139	GLU	CB-CG-CD	6.60	123.81	112.60
1	A	199	GLN	CB-CG-CD	6.58	123.79	112.60
1	A	96	VAL	CA-C-O	6.57	126.17	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	THR	N-CA-C	6.57	118.44	111.28
1	A	125	THR	N-CA-C	6.55	119.13	110.36
1	A	7	PHE	CA-C-O	6.55	129.21	120.89
1	A	258	HIS	CA-CB-CG	-6.54	107.26	113.80
1	A	151	ILE	N-CA-CB	-6.53	102.33	111.99
1	A	13	GLU	CA-C-N	-6.52	112.39	122.49
1	A	13	GLU	C-N-CA	-6.52	112.39	122.49
1	A	76	ARG	N-CA-C	6.52	124.68	110.80
1	A	214	HIS	ND1-CE1-NE2	6.51	114.91	108.40
1	A	143	ASP	N-CA-C	6.46	121.37	112.90
1	A	34	ARG	CA-C-O	6.46	126.01	118.90
1	A	273	LYS	O-C-N	6.43	127.27	121.35
1	A	294	THR	OG1-CB-CG2	6.41	122.12	109.30
1	A	241	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	45	GLU	N-CA-C	6.39	118.04	111.14
1	A	251	ARG	NE-CZ-NH1	-6.39	115.11	121.50
1	A	51	GLY	CA-C-N	-6.35	111.81	122.29
1	A	51	GLY	C-N-CA	-6.35	111.81	122.29
1	A	281	ILE	CA-CB-CG2	6.35	121.30	110.50
1	A	226	GLU	CA-C-N	-6.32	111.81	120.28
1	A	226	GLU	C-N-CA	-6.32	111.81	120.28
1	A	45	GLU	CB-CA-C	-6.32	100.92	110.90
1	A	169	CYS	N-CA-C	6.32	118.97	111.33
1	A	281	ILE	N-CA-C	6.29	118.95	111.09
1	A	109	ASN	CA-C-O	6.27	126.17	119.34
1	A	89	MET	CB-CA-C	6.25	121.47	110.85
1	A	187	THR	OG1-CB-CG2	-6.24	96.83	109.30
1	A	118	ASN	CA-CB-CG	6.24	118.84	112.60
1	A	131	SER	N-CA-CB	6.24	119.94	110.28
1	A	301	LYS	CB-CA-C	-6.24	102.60	111.95
1	A	166	VAL	CB-CA-C	-6.22	102.51	112.16
1	A	157	HIS	CA-C-N	-6.20	115.64	123.15
1	A	157	HIS	C-N-CA	-6.20	115.64	123.15
1	A	128	GLU	N-CA-C	6.18	118.02	111.28
1	A	218	VAL	CA-CB-CG1	6.18	120.90	110.40
1	A	223	VAL	CA-CB-CG1	6.16	120.88	110.40
1	A	115	ILE	CA-C-N	-6.15	113.94	120.03
1	A	115	ILE	C-N-CA	-6.15	113.94	120.03
1	A	47	GLN	CA-C-N	-6.15	110.38	121.14
1	A	47	GLN	C-N-CA	-6.15	110.38	121.14
1	A	49	ILE	CA-CB-CG2	6.12	120.91	110.50
1	A	288	VAL	N-CA-CB	-6.12	101.13	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	THR	CA-CB-CG2	6.09	120.85	110.50
1	A	184	GLY	CA-C-N	-6.09	113.46	122.41
1	A	184	GLY	C-N-CA	-6.09	113.46	122.41
1	A	113	GLU	CA-CB-CG	6.08	126.25	114.10
1	A	325	LEU	CB-CA-C	6.07	121.17	110.85
1	A	67	TYR	CA-C-N	-6.06	110.89	122.53
1	A	67	TYR	C-N-CA	-6.06	110.89	122.53
1	A	193	LEU	CA-C-N	-6.05	111.97	120.39
1	A	193	LEU	C-N-CA	-6.05	111.97	120.39
1	A	166	VAL	CG1-CB-CG2	6.03	124.07	110.80
1	A	325	LEU	CA-CB-CG	6.02	137.36	116.30
1	A	156	ARG	CA-CB-CG	-6.00	102.09	114.10
1	A	289	ASN	CA-C-O	5.99	127.14	120.92
1	A	89	MET	N-CA-CB	-5.97	101.33	110.16
1	A	235	ARG	CA-C-O	-5.92	114.71	121.40
1	A	211	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	63	ALA	N-CA-C	5.91	118.50	111.71
1	A	317	PHE	CA-C-N	-5.91	112.45	122.67
1	A	317	PHE	C-N-CA	-5.91	112.45	122.67
1	A	53	ASP	CB-CA-C	5.89	120.34	110.44
1	A	180	ILE	CB-CG1-CD1	-5.89	101.44	113.80
1	A	198	VAL	N-CA-C	5.88	116.53	110.36
1	A	280	VAL	CA-C-N	-5.87	110.67	120.30
1	A	280	VAL	C-N-CA	-5.87	110.67	120.30
1	A	48	ASN	N-CA-CB	5.87	119.97	110.40
1	A	228	VAL	CA-CB-CG2	-5.86	100.43	110.40
1	A	236	LEU	CA-C-O	-5.86	114.49	120.71
1	A	123	ASP	CA-C-N	-5.86	114.85	123.05
1	A	123	ASP	C-N-CA	-5.86	114.85	123.05
1	A	88	GLU	CA-C-O	5.83	126.93	120.63
1	A	253	ARG	CB-CG-CD	5.81	124.66	111.30
1	A	168	LEU	N-CA-C	5.80	118.07	111.11
1	A	246	THR	N-CA-C	5.76	117.23	111.07
1	A	226	GLU	CA-CB-CG	-5.75	102.59	114.10
1	A	223	VAL	CA-C-N	-5.75	112.59	120.46
1	A	223	VAL	C-N-CA	-5.75	112.59	120.46
1	A	318	THR	N-CA-CB	-5.71	101.61	110.46
1	A	289	ASN	N-CA-CB	-5.68	101.89	110.35
1	A	129	VAL	CA-C-N	-5.67	112.70	120.46
1	A	129	VAL	C-N-CA	-5.67	112.70	120.46
1	A	249	TYR	CB-CA-C	5.67	119.77	110.88
1	A	314	ASP	N-CA-C	5.65	119.25	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	209	VAL	CA-CB-CG1	5.64	119.99	110.40
1	A	162	SER	CA-C-N	-5.64	111.74	120.31
1	A	162	SER	C-N-CA	-5.64	111.74	120.31
1	A	307	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	249	TYR	CA-C-O	5.61	126.71	120.82
1	A	349	LYS	N-CA-C	5.61	117.08	111.07
1	A	261	ILE	CA-CB-CG1	5.61	119.93	110.40
1	A	313	LYS	CA-C-N	-5.60	113.35	122.65
1	A	313	LYS	C-N-CA	-5.60	113.35	122.65
1	A	331	LYS	CB-CG-CD	-5.58	98.46	111.30
1	A	214	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	229	ASP	CA-C-N	-5.57	112.87	122.79
1	A	229	ASP	C-N-CA	-5.57	112.87	122.79
1	A	172	TYR	N-CA-CB	-5.56	102.75	110.65
1	A	303	THR	N-CA-C	-5.55	100.86	109.14
1	A	131	SER	CA-C-O	-5.53	113.61	119.97
1	A	253	ARG	CG-CD-NE	5.53	124.16	112.00
1	A	254	GLN	CG-CD-NE2	-5.52	108.11	116.40
1	A	212	THR	N-CA-C	-5.52	100.97	109.52
1	A	279	ALA	N-CA-C	5.52	119.51	112.34
1	A	300	PHE	O-C-N	5.51	129.98	122.37
1	A	324	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	A	217	GLU	CA-C-N	-5.51	115.97	122.36
1	A	217	GLU	C-N-CA	-5.51	115.97	122.36
1	A	99	GLU	CA-C-O	-5.51	114.26	120.32
1	A	121	GLU	CA-C-N	-5.51	111.22	123.12
1	A	121	GLU	C-N-CA	-5.51	111.22	123.12
1	A	175	GLN	O-C-N	-5.50	115.27	122.59
1	A	33	ARG	N-CA-C	5.50	119.09	112.38
1	A	15	HIS	ND1-CE1-NE2	5.49	113.89	108.40
1	A	283	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	161	TRP	CH2-CZ2-CE2	5.47	124.62	117.50
1	A	177	VAL	CG1-CB-CG2	5.46	122.80	110.80
1	A	90	LYS	CA-C-O	5.45	126.24	119.97
1	A	207	SER	N-CA-C	5.45	120.04	113.17
1	A	146	VAL	O-C-N	5.43	128.88	123.18
1	A	174	GLU	N-CA-C	5.41	122.33	110.80
1	A	263	PRO	CB-CA-C	-5.41	104.44	112.55
1	A	79	ILE	CA-CB-CG1	-5.41	101.21	110.40
1	A	148	VAL	CA-C-N	-5.40	114.11	122.59
1	A	148	VAL	C-N-CA	-5.40	114.11	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	VAL	CA-C-N	-5.38	111.96	120.47
1	A	165	VAL	C-N-CA	-5.38	111.96	120.47
1	A	203	GLU	CA-C-O	5.38	126.26	120.55
1	A	158	GLN	CG-CD-NE2	-5.38	108.33	116.40
1	A	51	GLY	N-CA-C	5.37	125.91	113.18
1	A	285	ASN	CB-CA-C	-5.37	100.37	110.67
1	A	161	TRP	CA-C-N	-5.36	112.16	120.31
1	A	161	TRP	C-N-CA	-5.36	112.16	120.31
1	A	273	LYS	CG-CD-CE	5.35	123.61	111.30
1	A	326	ASN	CA-C-N	-5.35	111.52	120.30
1	A	326	ASN	C-N-CA	-5.35	111.52	120.30
1	A	44	GLU	CB-CA-C	-5.33	101.94	110.79
1	A	210	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	71	ALA	CA-C-N	-5.32	116.07	122.35
1	A	71	ALA	C-N-CA	-5.32	116.07	122.35
1	A	225	LYS	CG-CD-CE	-5.32	99.07	111.30
1	A	255	GLU	CB-CG-CD	-5.32	103.56	112.60
1	A	338	ASP	CA-C-O	5.31	126.39	120.82
1	A	158	GLN	N-CA-CB	5.31	119.38	110.99
1	A	37	ALA	CB-CA-C	-5.30	99.87	110.42
1	A	227	ALA	N-CA-C	5.29	117.05	111.28
1	A	148	VAL	CB-CA-C	-5.29	103.28	110.42
1	A	137	LEU	N-CA-CB	-5.28	102.36	110.12
1	A	29	TYR	N-CA-C	5.28	117.46	111.02
1	A	140	GLY	N-CA-C	5.27	119.02	112.64
1	A	119	GLN	CA-C-N	-5.26	110.19	121.45
1	A	119	GLN	C-N-CA	-5.26	110.19	121.45
1	A	80	LYS	CA-C-O	5.26	126.02	119.97
1	A	12	VAL	CA-CB-CG1	5.25	119.33	110.40
1	A	45	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	149	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	A	99	GLU	O-C-N	5.24	129.45	123.27
1	A	309	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	A	218	VAL	N-CA-C	5.22	118.22	113.20
1	A	209	VAL	N-CA-C	5.22	115.82	108.36
1	A	259	PHE	N-CA-C	5.22	117.23	108.73
1	A	191	SER	CA-C-N	-5.21	112.27	120.60
1	A	191	SER	C-N-CA	-5.21	112.27	120.60
1	A	320	GLU	O-C-N	5.21	127.64	122.12
1	A	298	LEU	CA-C-O	-5.21	115.34	121.07
1	A	208	GLY	CA-C-N	-5.20	116.38	122.93
1	A	208	GLY	C-N-CA	-5.20	116.38	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ILE	CB-CG1-CD1	-5.20	102.89	113.80
1	A	146	VAL	CA-C-N	-5.20	114.07	121.50
1	A	146	VAL	C-N-CA	-5.20	114.07	121.50
1	A	275	ASP	CA-C-N	-5.19	113.72	122.29
1	A	275	ASP	C-N-CA	-5.19	113.72	122.29
1	A	65	PHE	CA-C-O	5.19	125.76	119.38
1	A	105	HIS	CA-C-O	5.18	126.22	120.63
1	A	72	ILE	CB-CA-C	-5.17	105.60	111.55
1	A	134	ASN	N-CA-C	5.16	117.30	111.11
1	A	255	GLU	CB-CA-C	-5.14	102.45	110.94
1	A	170	LYS	CG-CD-CE	5.14	123.12	111.30
1	A	80	LYS	CA-C-N	-5.14	113.00	120.29
1	A	80	LYS	C-N-CA	-5.14	113.00	120.29
1	A	290	TYR	O-C-N	5.13	129.10	123.25
1	A	327	ILE	CB-CG1-CD1	-5.13	103.03	113.80
1	A	244	GLU	N-CA-C	5.12	119.40	113.20
1	A	142	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	A	95	VAL	CA-CB-CG1	5.11	119.09	110.40
1	A	172	TYR	N-CA-C	5.11	118.39	112.97
1	A	297	PRO	CB-CA-C	5.11	121.05	112.62
1	A	162	SER	CA-C-O	5.10	125.84	119.97
1	A	36	ILE	N-CA-CB	5.10	117.86	110.52
1	A	217	GLU	CA-C-O	5.09	126.00	120.55
1	A	103	SER	CA-C-O	5.09	125.02	119.32
1	A	158	GLN	CB-CG-CD	5.08	121.23	112.60
1	A	226	GLU	CB-CG-CD	5.08	121.23	112.60
1	A	318	THR	N-CA-C	5.08	117.97	110.46
1	A	37	ALA	CA-C-O	5.07	127.76	120.51
1	A	99	GLU	CA-CB-CG	-5.04	104.01	114.10
1	A	189	GLU	CB-CG-CD	-5.04	104.03	112.60
1	A	240	TYR	CB-CA-C	-5.04	102.42	110.79
1	A	182	LEU	O-C-N	5.03	129.16	123.27
1	A	57	THR	N-CA-CB	5.02	117.42	110.04
1	A	281	ILE	CA-C-N	-5.02	113.91	120.44
1	A	281	ILE	C-N-CA	-5.02	113.91	120.44
1	A	128	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	52	MET	CA-C-N	-5.02	114.11	122.08
1	A	52	MET	C-N-CA	-5.02	114.11	122.08
1	A	293	ASN	OD1-CG-ND2	5.00	127.61	122.60
1	A	61	PHE	N-CA-C	5.00	116.42	111.07
1	A	326	ASN	OD1-CG-ND2	-5.00	117.60	122.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	THR	CB
1	A	294	THR	CB

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	153	CYS	Peptide
1	A	173	ARG	Sidechain,Peptide
1	A	194	PHE	Sidechain
1	A	211	ARG	Sidechain
1	A	251	ARG	Sidechain
1	A	29	TYR	Sidechain
1	A	351	TYR	Sidechain
1	A	352	ARG	Sidechain
1	A	61	PHE	Sidechain
1	A	67	TYR	Sidechain
1	A	81	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2788	0	2743	156	0
2	A	1	0	0	0	0
3	A	19	0	17	2	0
4	A	480	0	0	63	0
All	All	3288	0	2760	156	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 (156) 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:12:VAL:HB	4:A:1133:HOH:O	1.64	0.97
1:A:57:THR:HB	1:A:59:PRO:HD2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:HIS:HD2	1:A:280:VAL:H	1.18	0.91
1:A:187:THR:HG22	4:A:1355:HOH:O	1.77	0.83
1:A:325:LEU:HG	4:A:1356:HOH:O	1.81	0.78
1:A:115:ILE:HB	4:A:1293:HOH:O	1.83	0.78
1:A:263:PRO:HD3	4:A:1371:HOH:O	1.82	0.77
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.66	0.77
1:A:322:PHE:HA	1:A:325:LEU:HD22	1.65	0.77
1:A:218:VAL:HB	4:A:1329:HOH:O	1.84	0.76
1:A:68:TYR:HD1	4:A:1340:HOH:O	1.68	0.76
1:A:72:ILE:HG22	1:A:78:ALA:HB1	1.69	0.73
1:A:264:TRP:HA	4:A:1394:HOH:O	1.88	0.73
1:A:264:TRP:HE3	4:A:1394:HOH:O	1.72	0.73
1:A:337:GLU:HG3	1:A:341:LYS:HE3	1.70	0.72
1:A:292:LEU:HA	4:A:1371:HOH:O	1.89	0.71
1:A:27:ILE:HD13	1:A:68:TYR:HB2	1.71	0.71
1:A:11:LYS:HE3	4:A:1441:HOH:O	1.91	0.71
1:A:267:TYR:HB2	1:A:272:TRP:HE3	1.55	0.70
1:A:310:MET:SD	4:A:1394:HOH:O	2.48	0.70
1:A:50:ILE:HG21	1:A:68:TYR:HD2	1.57	0.69
1:A:298:LEU:HD12	4:A:1085:HOH:O	1.93	0.69
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.27	0.68
1:A:278:HIS:CD2	1:A:280:VAL:H	2.08	0.68
1:A:267:TYR:HB2	1:A:272:TRP:CE3	2.29	0.67
1:A:58:LEU:C	1:A:58:LEU:HD23	2.21	0.66
1:A:138:GLN:O	1:A:142:ARG:HG2	1.95	0.66
1:A:72:ILE:HD13	4:A:1326:HOH:O	1.95	0.65
1:A:266:SER:OG	1:A:278:HIS:HE1	1.78	0.65
1:A:115:ILE:HG21	4:A:1260:HOH:O	1.96	0.65
1:A:325:LEU:HD23	4:A:1356:HOH:O	1.98	0.63
1:A:73:ALA:HB2	4:A:1393:HOH:O	1.98	0.63
1:A:169:CYS:SG	4:A:1342:HOH:O	2.56	0.62
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.82	0.61
1:A:23:LYS:HD2	1:A:85:GLU:CG	2.30	0.61
1:A:23:LYS:HG3	4:A:1363:HOH:O	2.01	0.60
1:A:66:ASP:HA	4:A:1183:HOH:O	2.01	0.60
1:A:116:PRO:HB2	1:A:117:TRP:CD1	2.36	0.60
1:A:107:LEU:HD13	4:A:1393:HOH:O	2.01	0.60
1:A:264:TRP:CE3	4:A:1394:HOH:O	2.52	0.60
1:A:241:HIS:HD2	1:A:244:GLU:OE2	1.83	0.60
1:A:121:GLU:HA	4:A:1260:HOH:O	2.02	0.59
1:A:337:GLU:HG3	1:A:341:LYS:CE	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD22	4:A:1325:HOH:O	2.02	0.59
1:A:309:GLN:HE21	1:A:313:LYS:HD3	1.67	0.59
1:A:287:GLN:HG2	4:A:1330:HOH:O	2.02	0.58
1:A:79:ILE:HD12	1:A:124:LEU:HD11	1.85	0.58
1:A:337:GLU:O	1:A:341:LYS:HG2	2.04	0.58
1:A:322:PHE:HA	1:A:325:LEU:CD2	2.34	0.57
1:A:179:ALA:C	4:A:1342:HOH:O	2.47	0.57
1:A:47:GLN:OE1	1:A:301:LYS:HG2	2.05	0.57
1:A:276:THR:HB	4:A:1234:HOH:O	2.02	0.57
1:A:211:ARG:NH2	1:A:232:LYS:O	2.37	0.57
1:A:118:ASN:HB3	4:A:1190:HOH:O	2.05	0.56
1:A:273:LYS:HG2	4:A:1156:HOH:O	2.04	0.56
1:A:50:ILE:HG21	1:A:68:TYR:CD2	2.40	0.56
1:A:347:LEU:HG	4:A:1018:HOH:O	2.05	0.56
1:A:331:LYS:HG3	1:A:344:LEU:HD21	1.87	0.56
1:A:72:ILE:HG22	1:A:78:ALA:CB	2.36	0.56
1:A:13:GLU:OE1	1:A:294:THR:HB	2.05	0.55
1:A:248:LEU:HD12	4:A:1207:HOH:O	2.06	0.55
1:A:281:ILE:C	1:A:281:ILE:HD12	2.32	0.55
1:A:166:VAL:O	1:A:170:LYS:HG3	2.06	0.55
1:A:264:TRP:HZ2	4:A:1092:HOH:O	1.88	0.55
1:A:318:THR:HB	4:A:1449:HOH:O	2.08	0.54
1:A:209:VAL:HG13	4:A:1342:HOH:O	2.07	0.54
1:A:11:LYS:HD3	4:A:1178:HOH:O	2.06	0.54
1:A:72:ILE:HG23	4:A:1326:HOH:O	2.07	0.54
1:A:107:LEU:HG	4:A:1341:HOH:O	2.08	0.54
1:A:162:SER:OG	1:A:197:HIS:HD2	1.90	0.54
1:A:72:ILE:CG2	1:A:78:ALA:HB1	2.38	0.53
1:A:62:LEU:HD13	4:A:1401:HOH:O	2.08	0.53
1:A:188:ILE:HB	1:A:191:SER:HB3	1.90	0.53
1:A:147:LYS:HE3	4:A:1217:HOH:O	2.09	0.53
1:A:142:ARG:HB3	4:A:1016:HOH:O	2.07	0.53
1:A:261:ILE:HD11	1:A:283:PHE:CE2	2.44	0.52
1:A:18:LEU:HG	4:A:1203:HOH:O	2.09	0.52
1:A:52:MET:HE2	1:A:268:LEU:HB3	1.91	0.51
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.92	0.51
1:A:80:LYS:HE3	1:A:135:GLN:CB	2.39	0.51
1:A:5:PRO:HD3	4:A:1479:HOH:O	2.10	0.51
1:A:70:PRO:HD3	4:A:1183:HOH:O	2.10	0.51
1:A:34:ARG:NH1	1:A:75:CYS:HB2	2.26	0.50
1:A:104:PRO:HD2	4:A:1164:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLN:HB2	4:A:1024:HOH:O	2.10	0.50
1:A:322:PHE:O	1:A:325:LEU:HD22	2.12	0.50
1:A:78:ALA:O	1:A:82:ILE:HG23	2.11	0.49
1:A:42:THR:O	1:A:43:PRO:C	2.55	0.49
1:A:29:TYR:OH	1:A:33:ARG:NH1	2.47	0.48
1:A:199:GLN:HG2	4:A:1230:HOH:O	2.11	0.48
1:A:348:TYR:HB3	1:A:352:ARG:NH2	2.28	0.48
1:A:33:ARG:HG3	4:A:1424:HOH:O	2.13	0.48
1:A:210:HIS:HD2	1:A:234:GLU:OE2	1.96	0.48
1:A:81:ARG:O	1:A:85:GLU:HB2	2.13	0.48
1:A:273:LYS:HD3	1:A:273:LYS:H	1.78	0.48
1:A:11:LYS:HE2	1:A:93:ASP:O	2.14	0.47
1:A:156:ARG:HD2	1:A:186:GLU:HA	1.96	0.47
1:A:261:ILE:HD11	1:A:283:PHE:HE2	1.79	0.47
1:A:290:TYR:CE2	1:A:325:LEU:HD12	2.49	0.47
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.96	0.47
1:A:46:LEU:O	1:A:47:GLN:C	2.56	0.47
1:A:321:GLU:HG3	1:A:325:LEU:HD13	1.97	0.47
1:A:65:PHE:CD1	3:A:1001:FR2:H25	2.50	0.46
1:A:193:LEU:HD12	1:A:230:THR:HG21	1.97	0.46
1:A:156:ARG:O	1:A:197:HIS:HE1	1.98	0.46
1:A:12:VAL:CG2	1:A:329:ALA:HB3	2.46	0.45
1:A:91:ALA:HB2	4:A:1122:HOH:O	2.15	0.45
1:A:133:VAL:HG12	1:A:137:LEU:HD22	1.97	0.45
1:A:322:PHE:CA	1:A:325:LEU:HD22	2.43	0.45
1:A:255:GLU:H	1:A:255:GLU:HG2	1.59	0.45
1:A:19:ASP:HA	4:A:1203:HOH:O	2.17	0.45
1:A:52:MET:HE1	4:A:1188:HOH:O	2.17	0.45
1:A:170:LYS:HD2	1:A:207:SER:CB	2.47	0.45
1:A:82:ILE:HG21	1:A:82:ILE:HD13	1.75	0.45
1:A:113:GLU:HG2	4:A:1104:HOH:O	2.16	0.45
1:A:34:ARG:CZ	1:A:75:CYS:HB2	2.48	0.44
1:A:313:LYS:NZ	1:A:313:LYS:HA	2.32	0.44
1:A:259:PHE:HB3	1:A:261:ILE:CD1	2.48	0.44
1:A:4:THR:HB	4:A:1480:HOH:O	2.17	0.44
1:A:49:ILE:HD13	1:A:49:ILE:HG21	1.71	0.44
1:A:97:TYR:HA	1:A:147:LYS:O	2.18	0.43
1:A:57:THR:HG23	4:A:1298:HOH:O	2.18	0.43
1:A:267:TYR:CD2	1:A:274:PRO:HG3	2.53	0.43
1:A:305:ASP:O	1:A:309:GLN:HB2	2.17	0.43
1:A:88:GLU:HG3	1:A:144:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HG2	4:A:1213:HOH:O	2.18	0.43
1:A:23:LYS:HD2	1:A:85:GLU:HG2	1.99	0.43
1:A:40:ALA:HB2	1:A:49:ILE:HD12	2.01	0.43
1:A:23:LYS:HD2	1:A:85:GLU:HG3	2.01	0.43
1:A:72:ILE:HD13	1:A:72:ILE:HG23	1.70	0.42
1:A:151:ILE:HG13	4:A:1400:HOH:O	2.19	0.42
1:A:45:GLU:HG3	4:A:1432:HOH:O	2.19	0.42
1:A:218:VAL:CB	4:A:1329:HOH:O	2.56	0.42
1:A:50:ILE:HG22	1:A:64:LYS:HG2	2.01	0.42
1:A:281:ILE:HD12	1:A:281:ILE:O	2.19	0.42
1:A:211:ARG:NH2	1:A:211:ARG:HB2	2.34	0.42
1:A:162:SER:OG	1:A:197:HIS:CD2	2.72	0.42
1:A:318:THR:O	1:A:319:GLU:C	2.62	0.42
1:A:40:ALA:O	1:A:41:ASP:OD1	2.38	0.42
1:A:62:LEU:HD22	3:A:1001:FR2:C26	2.50	0.42
1:A:330:ALA:HB2	4:A:1018:HOH:O	2.20	0.42
1:A:209:VAL:CG1	4:A:1342:HOH:O	2.66	0.42
1:A:261:ILE:HB	1:A:291:SER:O	2.20	0.42
1:A:253:ARG:HH11	1:A:253:ARG:CG	2.33	0.41
1:A:39:PRO:HA	4:A:1051:HOH:O	2.19	0.41
1:A:238:HIS:HB3	1:A:240:TYR:CE2	2.55	0.41
1:A:228:VAL:HG22	4:A:1151:HOH:O	2.19	0.41
1:A:309:GLN:NE2	1:A:313:LYS:HD3	2.35	0.41
1:A:40:ALA:HB1	1:A:45:GLU:HB3	2.01	0.41
1:A:12:VAL:HG21	1:A:329:ALA:HB3	2.02	0.41
1:A:67:TYR:HD2	4:A:1292:HOH:O	2.02	0.41
1:A:267:TYR:HD2	1:A:274:PRO:HG3	1.85	0.41
1:A:95:VAL:O	1:A:146:VAL:HG21	2.20	0.41
1:A:186:GLU:CD	1:A:219:GLY:H	2.29	0.40
1:A:322:PHE:HD2	1:A:325:LEU:HD21	1.86	0.40
1:A:276:THR:HG23	4:A:1232:HOH:O	2.21	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%)	323 (93%)	19 (6%)	5 (1%)	9 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	174	GLU
1	A	315	MET
1	A	238	HIS
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%)	259 (85%)	45 (15%)	3 1

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	25	GLU
1	A	28	LEU
1	A	32	LYS
1	A	36	ILE
1	A	41	ASP
1	A	44	GLU
1	A	48	ASN
1	A	50	ILE
1	A	60	ASP
1	A	72	ILE
1	A	85	GLU
1	A	111	LYS
1	A	113	GLU

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	137	LEU
1	A	142	ARG
1	A	149	ARG
1	A	163	SER
1	A	166	VAL
1	A	168	LEU
1	A	170	LYS
1	A	174	GLU
1	A	177	VAL
1	A	193	LEU
1	A	199	GLN
1	A	209	VAL
1	A	211	ARG
1	A	223	VAL
1	A	225	LYS
1	A	233	THR
1	A	253	ARG
1	A	254	GLN
1	A	255	GLU
1	A	261	ILE
1	A	273	LYS
1	A	281	ILE
1	A	292	LEU
1	A	294	THR
1	A	309	GLN
1	A	313	LYS
1	A	314	ASP
1	A	325	LEU
1	A	335	LEU
1	A	337	GLU

Sometimes 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	197	HIS
1	A	210	HIS
1	A	241	HIS
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	278	HIS
1	A	287	GLN
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 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	FR2	A	1001	-	20,20,20	1.44	3 (15%)	21,26,26	1.79	7 (33%)

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	FR2	A	1001	-	-	3/15/15/15	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR2	C1-C5	-3.19	1.33	1.37
3	A	1001	FR2	C1-N2	3.09	1.44	1.37
3	A	1001	FR2	C3-N2	-2.41	1.32	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR2	C18-C13-N2	3.57	116.26	110.44
3	A	1001	FR2	O15-C14-C13	-3.28	98.82	111.51
3	A	1001	FR2	C27-C28-C29	-2.63	116.99	120.24
3	A	1001	FR2	C5-C8-N10	2.55	118.87	116.28
3	A	1001	FR2	C1-N2-C3	2.48	108.01	106.37
3	A	1001	FR2	C8-C5-N4	2.38	126.66	121.52
3	A	1001	FR2	C3-N4-C5	2.12	107.11	104.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

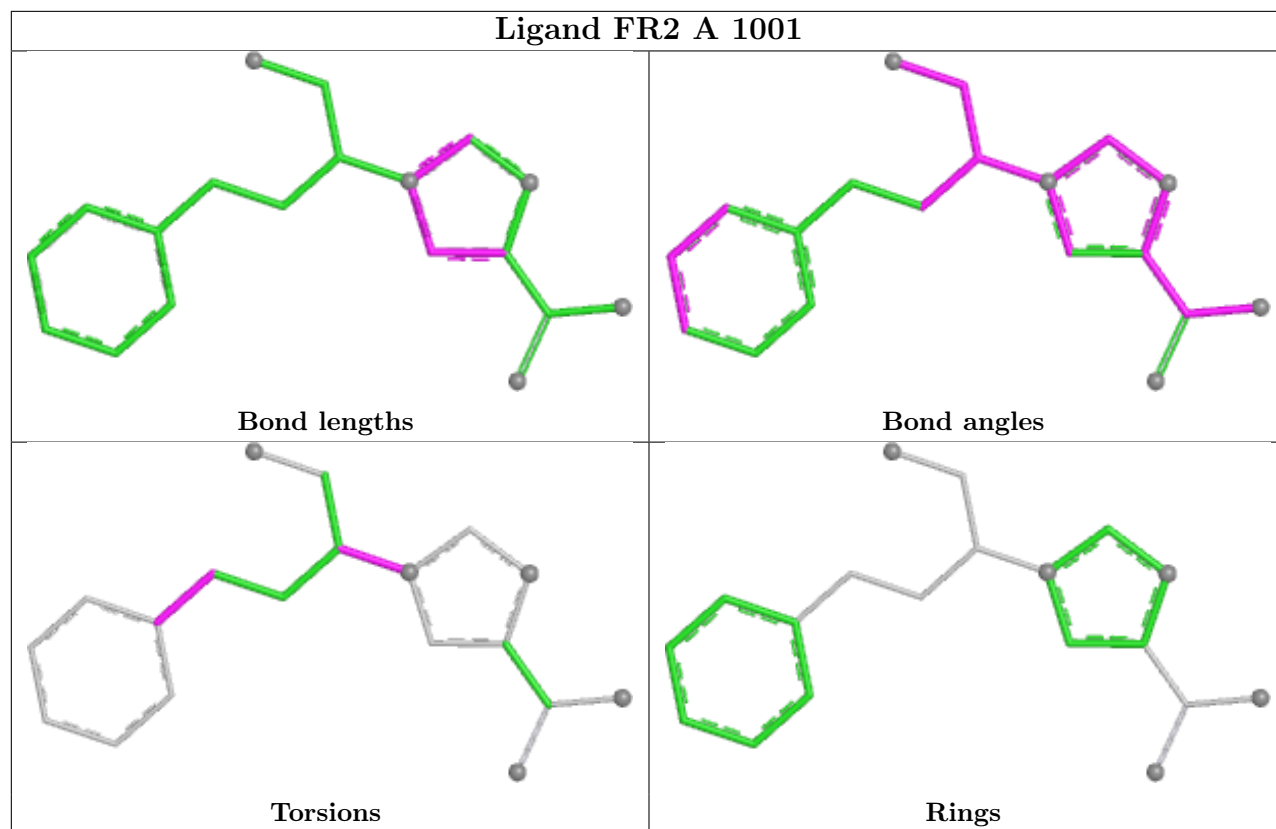
Mol	Chain	Res	Type	Atoms
3	A	1001	FR2	C18-C19-C22-C29
3	A	1001	FR2	C18-C19-C22-C25
3	A	1001	FR2	C18-C13-N2-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR2	2	0

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.