



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:51 PM UTC

PDB ID : 1NDZ / pdb_00001ndz
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

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

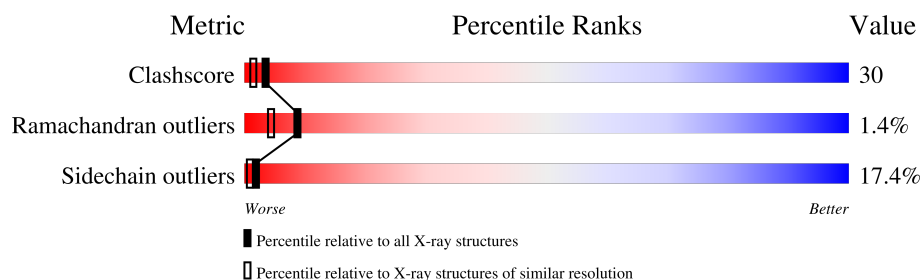
1 Overall quality at a glance

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	17% 42% 28% 12% .

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			

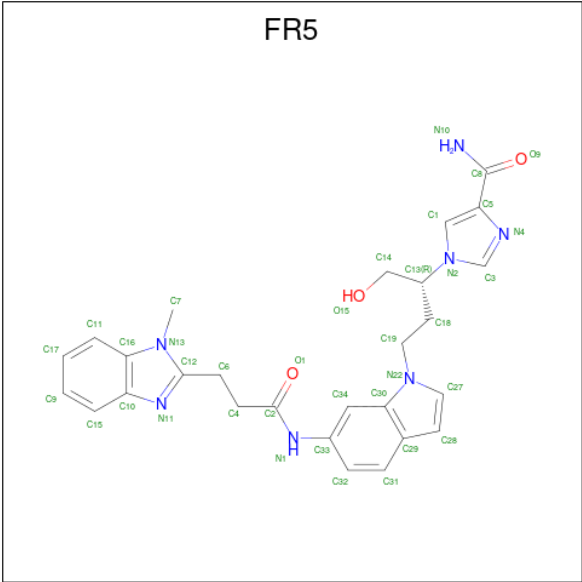
There are 15 discrepancies between the modelled and reference sequences:

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 (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-(6-((3-(1-METHYL-1H-BENZIMIDAZO L-2-YL)PROPANOYL)AMINO)-1H-INDOL-1-YL)PROPYL)-1H-IMIDAZOLE-4-CARBO XAMIDE (CCD ID: FR5) (formula: C₂₇H₂₉N₇O₃).



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

- Molecule 4 is water.

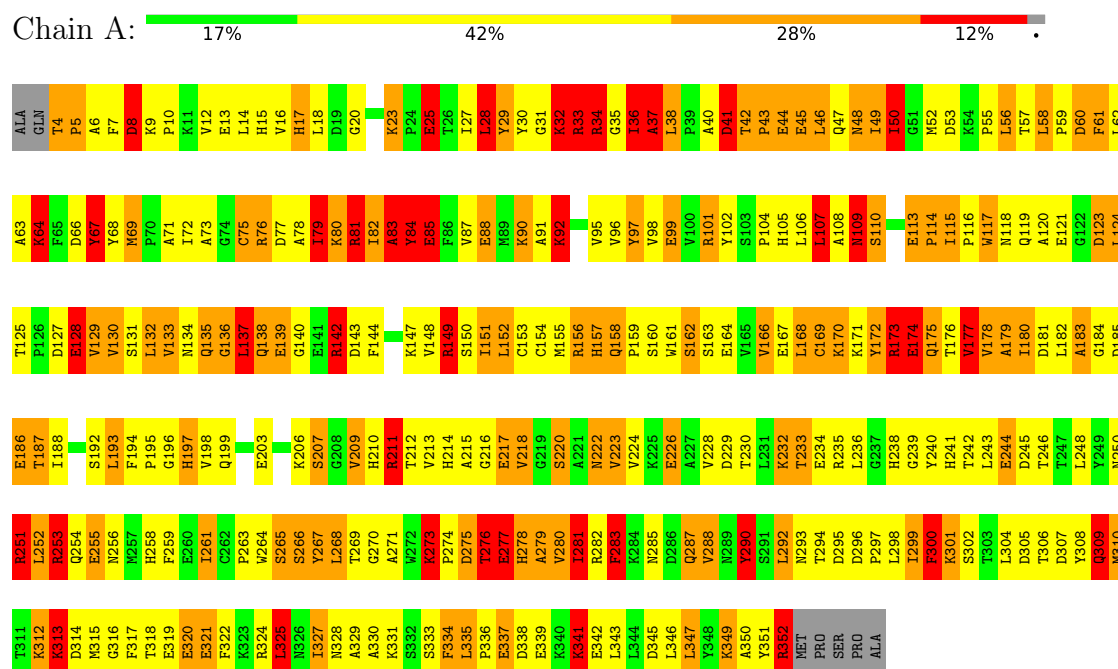
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	545	Total	O	0	0
			545	545		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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	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 ²)	31.0	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: FR5, 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	2.61	181/2852 (6.3%)	3.06	404/3866 (10.5%)

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 (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	HIS	CE1-NE2	12.17	1.44	1.32
1	A	157	HIS	CE1-NE2	11.99	1.44	1.32
1	A	213	VAL	N-CA	11.68	1.60	1.46
1	A	213	VAL	CA-CB	11.21	1.69	1.54
1	A	15	HIS	CD2-NE2	11.21	1.50	1.37
1	A	299	ILE	CA-CB	11.10	1.68	1.54
1	A	214	HIS	CG-ND1	-10.96	1.26	1.38
1	A	210	HIS	CD2-NE2	10.77	1.49	1.37
1	A	17	HIS	CE1-NE2	10.22	1.42	1.32
1	A	155	MET	N-CA	10.08	1.58	1.46
1	A	12	VAL	CA-C	9.90	1.64	1.52
1	A	282	ARG	CZ-NH2	9.65	1.46	1.33
1	A	258	HIS	ND1-CE1	9.48	1.42	1.32
1	A	17	HIS	ND1-CE1	9.46	1.42	1.32
1	A	27	ILE	CA-C	9.21	1.63	1.52
1	A	278	HIS	CE1-NE2	9.18	1.41	1.32
1	A	248	LEU	N-CA	8.85	1.56	1.46
1	A	263	PRO	CA-CB	-8.47	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	HIS	ND1-CE1	8.45	1.41	1.32
1	A	214	HIS	CA-CB	8.37	1.65	1.53
1	A	310	MET	CA-C	8.35	1.63	1.52
1	A	210	HIS	CE1-NE2	8.21	1.40	1.32
1	A	17	HIS	CD2-NE2	8.19	1.46	1.37
1	A	207	SER	CA-CB	-8.13	1.42	1.53
1	A	209	VAL	CA-C	8.09	1.62	1.52
1	A	211	ARG	N-CA	8.06	1.56	1.46
1	A	196	GLY	CA-C	8.05	1.61	1.51
1	A	295	ASP	C-N	7.97	1.43	1.33
1	A	238	HIS	CE1-NE2	7.90	1.40	1.32
1	A	325	LEU	CA-C	-7.83	1.42	1.52
1	A	197	HIS	CA-C	7.82	1.62	1.52
1	A	99	GLU	CA-C	7.81	1.62	1.52
1	A	160	SER	CA-CB	7.78	1.67	1.53
1	A	278	HIS	ND1-CE1	7.76	1.40	1.32
1	A	91	ALA	N-CA	7.75	1.55	1.46
1	A	17	HIS	CA-C	7.72	1.62	1.52
1	A	282	ARG	CA-CB	7.67	1.65	1.53
1	A	151	ILE	CA-C	7.64	1.62	1.52
1	A	155	MET	CA-CB	7.63	1.65	1.53
1	A	158	GLN	CD-NE2	-7.62	1.17	1.33
1	A	96	VAL	C-N	7.54	1.43	1.33
1	A	181	ASP	CA-C	7.50	1.62	1.52
1	A	211	ARG	NE-CZ	-7.43	1.24	1.33
1	A	150	SER	CA-C	7.41	1.61	1.52
1	A	17	HIS	CA-CB	7.39	1.64	1.53
1	A	182	LEU	C-O	-7.37	1.15	1.24
1	A	199	GLN	CG-CD	7.35	1.70	1.52
1	A	106	LEU	CA-C	7.32	1.63	1.52
1	A	296	ASP	CA-C	7.28	1.61	1.52
1	A	220	SER	CA-C	-7.21	1.43	1.53
1	A	183	ALA	CA-C	7.19	1.62	1.52
1	A	248	LEU	CA-C	7.14	1.61	1.52
1	A	228	VAL	CA-C	7.04	1.61	1.52
1	A	97	TYR	CA-C	7.03	1.60	1.52
1	A	305	ASP	CA-CB	6.98	1.65	1.53
1	A	58	LEU	N-CA	6.95	1.53	1.46
1	A	184	GLY	CA-C	-6.91	1.44	1.52
1	A	197	HIS	ND1-CE1	6.86	1.39	1.32
1	A	98	VAL	N-CA	6.82	1.54	1.46
1	A	253	ARG	NE-CZ	6.82	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	HIS	CA-C	6.81	1.64	1.53
1	A	261	ILE	CA-CB	-6.80	1.45	1.54
1	A	304	LEU	C-N	6.79	1.43	1.34
1	A	246	THR	CA-C	-6.79	1.43	1.52
1	A	210	HIS	CB-CG	6.77	1.59	1.50
1	A	197	HIS	CE1-NE2	6.74	1.39	1.32
1	A	258	HIS	N-CA	6.73	1.54	1.46
1	A	161	TRP	CA-C	6.68	1.61	1.52
1	A	297	PRO	CA-C	6.60	1.62	1.52
1	A	134	ASN	CA-C	6.58	1.61	1.52
1	A	157	HIS	CG-CD2	6.55	1.43	1.35
1	A	182	LEU	N-CA	6.55	1.54	1.46
1	A	278	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	341	LYS	N-CA	6.50	1.54	1.46
1	A	35	GLY	CA-C	6.48	1.60	1.51
1	A	102	TYR	CA-CB	6.43	1.64	1.53
1	A	159	PRO	C-N	6.40	1.42	1.33
1	A	156	ARG	CZ-NH1	6.38	1.41	1.32
1	A	211	ARG	C-O	6.36	1.30	1.23
1	A	115	ILE	CB-CG1	-6.34	1.40	1.53
1	A	324	ARG	N-CA	6.32	1.53	1.46
1	A	232	LYS	CA-C	6.29	1.61	1.53
1	A	144	PHE	CA-C	6.28	1.60	1.52
1	A	125	THR	CA-C	6.26	1.60	1.53
1	A	17	HIS	C-N	-6.23	1.25	1.33
1	A	188	ILE	CA-C	6.22	1.60	1.52
1	A	258	HIS	CE1-NE2	6.22	1.38	1.32
1	A	102	TYR	CA-C	-6.18	1.45	1.52
1	A	105	HIS	CG-CD2	6.16	1.42	1.35
1	A	261	ILE	CA-C	6.15	1.59	1.52
1	A	129	VAL	CA-C	6.12	1.60	1.52
1	A	15	HIS	CG-CD2	6.11	1.42	1.35
1	A	157	HIS	C-N	6.10	1.42	1.33
1	A	166	VAL	C-O	-6.09	1.17	1.24
1	A	258	HIS	C-O	6.07	1.31	1.24
1	A	235	ARG	CZ-NH1	6.06	1.41	1.32
1	A	255	GLU	CA-C	6.01	1.61	1.52
1	A	293	ASN	CA-C	5.97	1.59	1.52
1	A	157	HIS	ND1-CE1	5.94	1.38	1.32
1	A	38	LEU	N-CA	-5.92	1.40	1.45
1	A	280	VAL	CA-CB	5.91	1.63	1.54
1	A	192	SER	N-CA	5.90	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	HIS	ND1-CE1	5.89	1.38	1.32
1	A	149	ARG	NE-CZ	5.89	1.39	1.33
1	A	251	ARG	NE-CZ	5.88	1.39	1.33
1	A	294	THR	C-N	5.83	1.41	1.33
1	A	17	HIS	CG-CD2	5.83	1.42	1.35
1	A	242	THR	CA-CB	5.83	1.62	1.53
1	A	226	GLU	C-N	5.81	1.41	1.33
1	A	13	GLU	CA-CB	5.80	1.63	1.53
1	A	243	LEU	CA-C	5.79	1.60	1.52
1	A	152	LEU	CA-C	5.74	1.59	1.52
1	A	169	CYS	CA-CB	5.74	1.63	1.53
1	A	29	TYR	CA-C	-5.73	1.45	1.52
1	A	214	HIS	CG-CD2	5.71	1.42	1.35
1	A	43	PRO	CA-C	-5.71	1.44	1.52
1	A	28	LEU	N-CA	5.68	1.53	1.46
1	A	158	GLN	CA-CB	5.68	1.61	1.53
1	A	162	SER	N-CA	5.67	1.53	1.46
1	A	76	ARG	NE-CZ	5.65	1.39	1.33
1	A	302	SER	CA-CB	-5.63	1.45	1.53
1	A	110	SER	CB-OG	5.62	1.53	1.42
1	A	182	LEU	CB-CG	5.62	1.64	1.53
1	A	67	TYR	C-N	5.62	1.41	1.33
1	A	263	PRO	N-CA	-5.62	1.40	1.47
1	A	328	ASN	CA-CB	5.61	1.62	1.53
1	A	245	ASP	CA-C	-5.61	1.46	1.52
1	A	95	VAL	CA-C	5.60	1.59	1.52
1	A	156	ARG	C-N	5.60	1.42	1.33
1	A	336	PRO	CA-CB	5.59	1.60	1.53
1	A	252	LEU	CA-C	5.58	1.59	1.52
1	A	288	VAL	CA-CB	5.54	1.59	1.54
1	A	223	VAL	CA-CB	5.49	1.61	1.54
1	A	324	ARG	CZ-NH2	-5.46	1.26	1.33
1	A	345	ASP	N-CA	5.46	1.52	1.46
1	A	333	SER	N-CA	-5.45	1.38	1.45
1	A	151	ILE	CA-CB	5.43	1.61	1.54
1	A	58	LEU	CB-CG	-5.43	1.42	1.53
1	A	330	ALA	C-O	-5.43	1.17	1.24
1	A	295	ASP	CA-CB	5.42	1.62	1.53
1	A	265	SER	C-N	-5.42	1.26	1.34
1	A	129	VAL	N-CA	-5.40	1.40	1.46
1	A	290	TYR	CA-C	5.40	1.59	1.52
1	A	66	ASP	N-CA	5.40	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	ARG	C-N	-5.38	1.25	1.33
1	A	228	VAL	N-CA	5.38	1.52	1.46
1	A	20	GLY	CA-C	5.36	1.59	1.51
1	A	62	LEU	C-N	5.36	1.41	1.33
1	A	58	LEU	CA-C	-5.30	1.46	1.52
1	A	222	ASN	CA-CB	5.30	1.61	1.53
1	A	163	SER	CA-CB	5.28	1.62	1.53
1	A	218	VAL	CA-CB	-5.27	1.48	1.54
1	A	266	SER	CA-C	5.27	1.59	1.52
1	A	164	GLU	CA-C	5.26	1.59	1.52
1	A	63	ALA	CA-C	-5.26	1.45	1.52
1	A	321	GLU	CA-C	5.25	1.59	1.52
1	A	123	ASP	CA-CB	-5.24	1.46	1.53
1	A	203	GLU	CA-CB	-5.23	1.44	1.53
1	A	195	PRO	C-N	5.22	1.40	1.33
1	A	61	PHE	C-N	5.22	1.41	1.33
1	A	327	ILE	CA-CB	5.21	1.60	1.54
1	A	343	LEU	CA-CB	5.18	1.61	1.53
1	A	342	GLU	C-N	5.17	1.40	1.33
1	A	107	LEU	CB-CG	-5.16	1.43	1.53
1	A	131	SER	C-N	5.16	1.40	1.33
1	A	199	GLN	CD-NE2	5.16	1.44	1.33
1	A	155	MET	SD-CE	-5.15	1.66	1.79
1	A	60	ASP	C-N	5.14	1.40	1.33
1	A	7	PHE	C-N	5.12	1.40	1.33
1	A	226	GLU	CA-C	5.12	1.59	1.52
1	A	17	HIS	CG-ND1	-5.12	1.32	1.38
1	A	307	ASP	C-N	5.10	1.41	1.34
1	A	235	ARG	NE-CZ	5.06	1.38	1.33
1	A	296	ASP	N-CA	5.06	1.51	1.46
1	A	127	ASP	CB-CG	5.05	1.64	1.52
1	A	155	MET	CA-C	5.05	1.58	1.52
1	A	282	ARG	C-O	5.05	1.30	1.24
1	A	278	HIS	N-CA	5.04	1.52	1.46
1	A	69	MET	C-N	5.03	1.40	1.34
1	A	211	ARG	CA-CB	5.02	1.62	1.53
1	A	132	LEU	C-N	5.00	1.40	1.33

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	CD-NE-CZ	-15.49	102.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	HIS	CE1-NE2-CD2	-15.04	93.97	109.00
1	A	314	ASP	CA-CB-CG	13.91	126.51	112.60
1	A	58	LEU	CB-CA-C	-12.41	85.44	112.38
1	A	175	GLN	CA-C-N	12.18	143.62	121.70
1	A	175	GLN	C-N-CA	12.18	143.62	121.70
1	A	37	ALA	CA-C-O	11.78	137.36	120.51
1	A	17	HIS	ND1-CE1-NE2	11.44	119.84	108.40
1	A	294	THR	CA-CB-OG1	11.28	126.52	109.60
1	A	79	ILE	CB-CA-C	-10.66	98.05	112.02
1	A	35	GLY	CA-C-N	-10.61	105.56	120.74
1	A	35	GLY	C-N-CA	-10.61	105.56	120.74
1	A	105	HIS	CA-CB-CG	-10.54	103.26	113.80
1	A	273	LYS	CB-CA-C	10.52	121.84	109.85
1	A	115	ILE	CB-CG1-CD1	-10.46	91.83	113.80
1	A	33	ARG	CD-NE-CZ	-10.37	109.89	124.40
1	A	349	LYS	N-CA-C	10.09	121.86	111.07
1	A	158	GLN	OE1-CD-NE2	-9.90	112.70	122.60
1	A	166	VAL	CB-CA-C	-9.83	99.16	112.04
1	A	223	VAL	N-CA-C	9.81	120.62	110.62
1	A	135	GLN	CA-C-N	-9.73	109.17	119.98
1	A	135	GLN	C-N-CA	-9.73	109.17	119.98
1	A	329	ALA	CA-C-O	9.69	130.82	120.55
1	A	72	ILE	CA-C-O	9.62	130.91	120.32
1	A	166	VAL	N-CA-CB	9.61	122.48	110.47
1	A	174	GLU	N-CA-C	9.59	131.23	110.80
1	A	37	ALA	N-CA-C	9.54	131.11	110.80
1	A	64	LYS	N-CA-C	9.50	122.84	111.82
1	A	254	GLN	CB-CA-C	-9.48	94.74	110.85
1	A	280	VAL	CA-C-N	-9.47	107.48	120.46
1	A	280	VAL	C-N-CA	-9.47	107.48	120.46
1	A	123	ASP	N-CA-C	9.46	124.61	111.56
1	A	158	GLN	CB-CA-C	-9.46	95.55	111.15
1	A	313	LYS	N-CA-C	9.38	121.58	111.36
1	A	85	GLU	N-CA-C	9.36	124.50	113.18
1	A	156	ARG	NE-CZ-NH2	-9.30	110.83	119.20
1	A	81	ARG	CD-NE-CZ	-9.22	111.50	124.40
1	A	170	LYS	CA-CB-CG	-9.19	95.73	114.10
1	A	281	ILE	N-CA-C	9.18	119.98	110.62
1	A	166	VAL	CA-CB-CG2	9.16	125.97	110.40
1	A	282	ARG	CA-C-O	9.05	130.14	120.55
1	A	254	GLN	OE1-CD-NE2	9.01	131.61	122.60
1	A	338	ASP	CA-CB-CG	9.00	121.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	CD-NE-CZ	-8.91	111.92	124.40
1	A	218	VAL	CB-CA-C	8.90	119.37	110.65
1	A	66	ASP	CA-CB-CG	-8.89	103.71	112.60
1	A	30	TYR	CA-C-N	-8.87	109.17	120.34
1	A	30	TYR	C-N-CA	-8.87	109.17	120.34
1	A	350	ALA	N-CA-C	8.77	122.98	111.75
1	A	211	ARG	CD-NE-CZ	8.73	136.62	124.40
1	A	128	GLU	N-CA-C	8.70	120.76	111.28
1	A	223	VAL	CA-CB-CG2	8.66	125.13	110.40
1	A	127	ASP	CA-C-O	8.66	129.73	120.55
1	A	175	GLN	CB-CA-C	-8.61	99.17	111.14
1	A	277	GLU	CA-CB-CG	8.59	131.29	114.10
1	A	174	GLU	CA-C-N	8.56	137.17	122.95
1	A	174	GLU	C-N-CA	8.56	137.17	122.95
1	A	67	TYR	CB-CA-C	-8.53	97.49	110.88
1	A	179	ALA	O-C-N	8.51	132.52	123.42
1	A	180	ILE	CB-CG1-CD1	-8.51	95.94	113.80
1	A	115	ILE	CA-C-O	8.49	127.60	119.71
1	A	66	ASP	CA-C-N	-8.42	109.50	120.44
1	A	66	ASP	C-N-CA	-8.42	109.50	120.44
1	A	136	GLY	N-CA-C	8.36	122.75	112.73
1	A	341	LYS	CA-C-O	8.21	129.38	120.10
1	A	158	GLN	CG-CD-OE1	8.21	137.21	120.80
1	A	199	GLN	CA-CB-CG	-8.17	97.77	114.10
1	A	69	MET	CA-C-N	-8.13	111.35	119.56
1	A	69	MET	C-N-CA	-8.13	111.35	119.56
1	A	308	TYR	CA-C-N	-8.10	107.99	120.31
1	A	308	TYR	C-N-CA	-8.10	107.99	120.31
1	A	218	VAL	CA-CB-CG1	8.10	124.17	110.40
1	A	5	PRO	CB-CA-C	8.08	121.24	111.46
1	A	335	LEU	N-CA-CB	-8.08	100.37	109.74
1	A	79	ILE	CA-CB-CG1	8.05	124.09	110.40
1	A	177	VAL	N-CA-C	8.03	119.44	108.84
1	A	301	LYS	N-CA-C	7.96	122.44	112.24
1	A	48	ASN	N-CA-C	7.94	120.94	111.33
1	A	16	VAL	CA-C-O	7.93	129.39	120.90
1	A	255	GLU	N-CA-C	7.93	122.79	113.20
1	A	83	ALA	N-CA-C	7.90	121.04	111.40
1	A	81	ARG	N-CA-C	7.90	120.89	111.33
1	A	158	GLN	CB-CG-CD	-7.89	99.19	112.60
1	A	156	ARG	NH1-CZ-NH2	7.88	129.55	119.30
1	A	199	GLN	CB-CG-CD	7.87	125.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TYR	N-CA-CB	7.86	121.40	110.01
1	A	277	GLU	CA-C-N	-7.79	110.36	121.50
1	A	277	GLU	C-N-CA	-7.79	110.36	121.50
1	A	120	ALA	N-CA-C	7.76	121.02	110.55
1	A	8	ASP	CA-CB-CG	-7.72	104.88	112.60
1	A	155	MET	CG-SD-CE	7.70	117.84	100.90
1	A	343	LEU	N-CA-C	7.68	124.04	111.37
1	A	324	ARG	CA-C-N	-7.60	108.75	120.31
1	A	324	ARG	C-N-CA	-7.60	108.75	120.31
1	A	8	ASP	CB-CA-C	-7.58	95.33	110.42
1	A	67	TYR	N-CA-C	7.58	119.19	111.07
1	A	319	GLU	CA-C-N	-7.56	107.92	121.14
1	A	319	GLU	C-N-CA	-7.56	107.92	121.14
1	A	58	LEU	N-CA-CB	7.49	124.24	110.08
1	A	187	THR	CB-CA-C	-7.43	95.45	109.72
1	A	294	THR	CA-C-O	-7.38	111.07	119.41
1	A	281	ILE	CA-CB-CG2	7.37	123.03	110.50
1	A	63	ALA	CA-C-N	-7.35	109.14	120.31
1	A	63	ALA	C-N-CA	-7.35	109.14	120.31
1	A	76	ARG	CA-C-O	7.33	129.13	120.92
1	A	268	LEU	CA-C-N	-7.29	110.98	122.65
1	A	268	LEU	C-N-CA	-7.29	110.98	122.65
1	A	91	ALA	CA-C-O	7.25	128.46	120.63
1	A	60	ASP	CA-C-N	-7.24	110.73	120.79
1	A	60	ASP	C-N-CA	-7.24	110.73	120.79
1	A	216	GLY	O-C-N	7.19	131.24	122.32
1	A	217	GLU	O-C-N	7.18	130.44	122.11
1	A	197	HIS	ND1-CE1-NE2	-7.18	101.22	108.40
1	A	349	LYS	CB-CG-CD	7.18	127.81	111.30
1	A	88	GLU	N-CA-C	7.16	123.19	111.37
1	A	66	ASP	N-CA-C	7.16	119.16	111.36
1	A	175	GLN	CA-CB-CG	7.15	128.39	114.10
1	A	178	VAL	CB-CA-C	-7.15	103.07	110.93
1	A	107	LEU	N-CA-C	-7.11	102.91	112.94
1	A	71	ALA	N-CA-C	7.09	119.01	111.28
1	A	343	LEU	CA-C-O	7.06	128.83	120.92
1	A	233	THR	CA-CB-CG2	7.03	122.45	110.50
1	A	290	TYR	CB-CA-C	-7.03	94.99	110.67
1	A	282	ARG	CA-C-N	-7.02	109.64	120.31
1	A	282	ARG	C-N-CA	-7.02	109.64	120.31
1	A	62	LEU	CD1-CG-CD2	-7.02	95.36	110.80
1	A	224	VAL	CA-C-N	-7.00	110.89	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	VAL	C-N-CA	-7.00	110.89	120.28
1	A	64	LYS	CA-C-N	-6.99	110.18	120.38
1	A	64	LYS	C-N-CA	-6.99	110.18	120.38
1	A	61	PHE	N-CA-C	6.98	119.54	111.02
1	A	179	ALA	N-CA-C	-6.97	98.13	108.79
1	A	254	GLN	CB-CG-CD	-6.96	100.76	112.60
1	A	50	ILE	N-CA-C	6.91	117.70	110.72
1	A	117	TRP	CG-CD1-NE1	6.91	119.18	110.20
1	A	209	VAL	CA-CB-CG1	6.90	122.14	110.40
1	A	40	ALA	N-CA-C	6.90	117.69	108.38
1	A	325	LEU	N-CA-C	6.89	119.81	111.82
1	A	116	PRO	N-CA-C	6.87	121.85	111.14
1	A	347	LEU	CD1-CG-CD2	6.86	125.89	110.80
1	A	244	GLU	N-CA-C	6.86	121.35	113.19
1	A	87	VAL	CA-C-O	6.83	128.05	120.95
1	A	233	THR	OG1-CB-CG2	6.83	122.95	109.30
1	A	300	PHE	CA-C-N	-6.80	112.53	122.40
1	A	300	PHE	C-N-CA	-6.80	112.53	122.40
1	A	210	HIS	CA-C-N	-6.79	110.92	122.33
1	A	210	HIS	C-N-CA	-6.79	110.92	122.33
1	A	109	ASN	CB-CA-C	6.72	120.62	109.80
1	A	4	THR	CA-C-N	-6.71	112.85	119.90
1	A	4	THR	C-N-CA	-6.71	112.85	119.90
1	A	282	ARG	N-CA-C	6.70	118.58	111.28
1	A	60	ASP	CA-C-O	6.65	127.47	120.42
1	A	199	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	A	214	HIS	CB-CA-C	-6.65	100.29	110.26
1	A	108	ALA	CA-C-N	-6.65	110.87	121.44
1	A	108	ALA	C-N-CA	-6.65	110.87	121.44
1	A	73	ALA	CB-CA-C	-6.64	98.69	109.72
1	A	113	GLU	CB-CG-CD	6.64	123.89	112.60
1	A	36	ILE	CA-CB-CG2	6.63	121.78	110.50
1	A	306	THR	CA-C-N	-6.63	110.23	120.31
1	A	306	THR	C-N-CA	-6.63	110.23	120.31
1	A	149	ARG	CB-CA-C	-6.61	97.82	110.24
1	A	60	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	77	ASP	O-C-N	6.60	128.87	122.07
1	A	296	ASP	CA-C-N	6.59	126.83	119.32
1	A	296	ASP	C-N-CA	6.59	126.83	119.32
1	A	85	GLU	N-CA-CB	-6.59	99.34	110.41
1	A	274	PRO	N-CA-C	6.56	122.37	113.84
1	A	278	HIS	CA-CB-CG	-6.55	107.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	CYS	N-CA-CB	-6.54	99.61	110.47
1	A	58	LEU	N-CA-C	6.53	121.73	113.25
1	A	115	ILE	N-CA-CB	6.50	116.13	110.08
1	A	197	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	A	129	VAL	N-CA-C	6.49	117.17	110.36
1	A	197	HIS	CE1-NE2-CD2	6.48	115.48	109.00
1	A	210	HIS	CE1-NE2-CD2	-6.48	102.52	109.00
1	A	80	LYS	CA-C-O	6.48	127.62	120.82
1	A	13	GLU	CA-C-O	6.47	128.24	120.28
1	A	131	SER	N-CA-CB	-6.45	100.02	109.82
1	A	44	GLU	CB-CG-CD	-6.45	101.64	112.60
1	A	17	HIS	CG-CD2-NE2	6.44	113.64	107.20
1	A	211	ARG	NE-CZ-NH2	-6.43	113.41	119.20
1	A	25	GLU	N-CA-C	6.43	120.22	112.38
1	A	295	ASP	CA-C-N	-6.38	116.66	122.28
1	A	295	ASP	C-N-CA	-6.38	116.66	122.28
1	A	49	ILE	N-CA-C	6.36	117.15	110.72
1	A	210	HIS	CA-CB-CG	-6.36	107.44	113.80
1	A	177	VAL	N-CA-CB	6.35	117.87	110.82
1	A	186	GLU	CB-CG-CD	6.35	123.39	112.60
1	A	187	THR	CA-CB-OG1	6.34	119.11	109.60
1	A	233	THR	CB-CA-C	-6.33	96.71	109.68
1	A	91	ALA	CA-C-N	-6.31	110.09	121.14
1	A	91	ALA	C-N-CA	-6.31	110.09	121.14
1	A	36	ILE	CB-CG1-CD1	-6.30	100.57	113.80
1	A	66	ASP	N-CA-CB	6.27	119.45	110.16
1	A	236	LEU	N-CA-C	6.27	119.17	109.07
1	A	14	LEU	N-CA-CB	-6.27	101.19	110.53
1	A	282	ARG	N-CA-CB	-6.26	100.92	110.12
1	A	304	LEU	CA-C-O	6.26	127.17	120.10
1	A	82	ILE	O-C-N	6.25	128.86	121.80
1	A	266	SER	CA-C-O	-6.23	112.80	119.97
1	A	149	ARG	NH1-CZ-NH2	-6.22	111.22	119.30
1	A	138	GLN	CA-C-O	6.21	127.10	120.70
1	A	158	GLN	N-CA-CB	6.21	118.79	111.09
1	A	347	LEU	N-CA-C	6.21	117.71	111.07
1	A	349	LYS	CA-C-O	6.17	127.30	120.82
1	A	281	ILE	CA-C-N	-6.17	112.02	120.28
1	A	281	ILE	C-N-CA	-6.17	112.02	120.28
1	A	187	THR	N-CA-C	6.16	120.80	113.28
1	A	173	ARG	N-CA-CB	6.14	119.07	110.04
1	A	253	ARG	CG-CD-NE	6.14	125.50	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	VAL	CA-C-N	-6.14	110.39	121.62
1	A	178	VAL	C-N-CA	-6.14	110.39	121.62
1	A	43	PRO	O-C-N	6.13	130.92	122.64
1	A	104	PRO	CA-C-N	-6.12	111.44	120.38
1	A	104	PRO	C-N-CA	-6.12	111.44	120.38
1	A	157	HIS	CA-C-N	-6.11	116.26	122.74
1	A	157	HIS	C-N-CA	-6.11	116.26	122.74
1	A	88	GLU	CA-CB-CG	-6.10	101.89	114.10
1	A	32	LYS	CG-CD-CE	6.09	125.31	111.30
1	A	38	LEU	O-C-N	6.07	125.59	121.71
1	A	130	VAL	O-C-N	6.04	127.73	121.87
1	A	278	HIS	ND1-CE1-NE2	-6.04	102.36	108.40
1	A	325	LEU	CA-C-N	-6.04	111.13	120.31
1	A	325	LEU	C-N-CA	-6.04	111.13	120.31
1	A	161	TRP	CH2-CZ2-CE2	6.03	125.34	117.50
1	A	33	ARG	N-CA-CB	-6.00	100.43	110.39
1	A	187	THR	CA-CB-CG2	-6.00	100.30	110.50
1	A	329	ALA	N-CA-C	5.98	117.80	111.28
1	A	101	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	A	139	GLU	CA-CB-CG	5.97	126.05	114.10
1	A	81	ARG	CA-C-N	-5.97	110.51	120.30
1	A	81	ARG	C-N-CA	-5.97	110.51	120.30
1	A	266	SER	N-CA-C	5.96	118.73	111.82
1	A	115	ILE	N-CA-C	5.93	114.77	108.95
1	A	48	ASN	CB-CA-C	-5.93	100.60	110.68
1	A	85	GLU	CA-CB-CG	5.92	125.93	114.10
1	A	109	ASN	CA-C-O	5.92	125.47	118.79
1	A	349	LYS	CG-CD-CE	5.91	124.89	111.30
1	A	321	GLU	CB-CA-C	5.90	120.59	110.79
1	A	87	VAL	N-CA-C	5.90	116.64	110.62
1	A	183	ALA	N-CA-CB	-5.89	101.92	111.22
1	A	92	LYS	N-CA-C	5.88	120.18	112.89
1	A	212	THR	CA-CB-OG1	5.88	118.42	109.60
1	A	139	GLU	CA-C-O	5.86	126.73	120.10
1	A	18	LEU	CD1-CG-CD2	5.85	123.67	110.80
1	A	144	PHE	CA-C-O	5.84	126.08	119.18
1	A	4	THR	OG1-CB-CG2	5.84	120.97	109.30
1	A	250	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	246	THR	N-CA-C	5.81	119.55	112.23
1	A	127	ASP	CA-C-N	-5.80	112.50	120.28
1	A	127	ASP	C-N-CA	-5.80	112.50	120.28
1	A	177	VAL	CA-CB-CG2	5.79	120.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASN	CA-C-N	-5.77	112.09	120.29
1	A	250	ASN	C-N-CA	-5.77	112.09	120.29
1	A	325	LEU	CD1-CG-CD2	5.77	123.49	110.80
1	A	163	SER	N-CA-CB	5.76	119.20	110.28
1	A	170	LYS	CD-CE-NZ	-5.75	93.49	111.90
1	A	177	VAL	CA-C-N	-5.75	114.73	122.72
1	A	177	VAL	C-N-CA	-5.75	114.73	122.72
1	A	10	PRO	N-CD-CG	-5.75	94.58	103.20
1	A	331	LYS	O-C-N	5.72	128.19	122.12
1	A	321	GLU	N-CA-C	5.71	117.51	111.28
1	A	79	ILE	N-CA-CB	5.71	117.87	110.57
1	A	158	GLN	CG-CD-NE2	-5.70	107.86	116.40
1	A	258	HIS	ND1-CG-CD2	5.69	111.79	106.10
1	A	213	VAL	CA-C-N	-5.69	113.04	121.24
1	A	213	VAL	C-N-CA	-5.69	113.04	121.24
1	A	90	LYS	CA-CB-CG	5.69	125.47	114.10
1	A	281	ILE	CA-C-O	5.68	126.86	120.95
1	A	109	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	A	4	THR	N-CA-C	5.67	126.87	111.00
1	A	271	ALA	N-CA-C	5.67	118.19	111.33
1	A	279	ALA	N-CA-C	5.67	122.87	110.80
1	A	306	THR	CA-CB-CG2	5.66	120.12	110.50
1	A	41	ASP	N-CA-C	5.65	121.08	112.54
1	A	160	SER	CA-C-N	-5.65	111.55	122.06
1	A	160	SER	C-N-CA	-5.65	111.55	122.06
1	A	228	VAL	CA-C-O	5.62	127.65	120.96
1	A	23	LYS	CG-CD-CE	5.62	124.22	111.30
1	A	69	MET	CA-C-O	5.62	123.50	118.33
1	A	254	GLN	O-C-N	5.60	128.54	122.15
1	A	58	LEU	CA-C-O	5.60	123.78	118.63
1	A	275	ASP	CA-C-N	-5.58	113.44	122.82
1	A	275	ASP	C-N-CA	-5.58	113.44	122.82
1	A	151	ILE	N-CA-CB	-5.58	103.37	111.52
1	A	282	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	A	42	THR	N-CA-C	5.57	118.00	110.31
1	A	142	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	A	84	TYR	N-CA-C	5.57	122.67	110.80
1	A	119	GLN	CB-CG-CD	-5.56	103.15	112.60
1	A	292	LEU	CD1-CG-CD2	5.56	123.02	110.80
1	A	147	LYS	CA-C-O	-5.55	114.36	120.69
1	A	349	LYS	N-CA-CB	-5.55	101.96	110.01
1	A	299	ILE	CA-C-N	-5.55	113.77	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ILE	C-N-CA	-5.55	113.77	122.65
1	A	158	GLN	CA-C-O	5.55	127.65	121.22
1	A	197	HIS	CA-CB-CG	-5.54	108.25	113.80
1	A	135	GLN	CG-CD-NE2	-5.54	108.09	116.40
1	A	34	ARG	N-CA-C	5.54	120.15	113.17
1	A	6	ALA	N-CA-C	5.54	122.59	110.80
1	A	49	ILE	CA-C-N	-5.52	112.59	120.42
1	A	49	ILE	C-N-CA	-5.52	112.59	120.42
1	A	16	VAL	CA-C-N	-5.51	115.11	122.72
1	A	16	VAL	C-N-CA	-5.51	115.11	122.72
1	A	139	GLU	CB-CA-C	5.49	120.78	110.63
1	A	224	VAL	CA-CB-CG2	-5.49	101.07	110.40
1	A	218	VAL	N-CA-CB	-5.48	104.72	112.12
1	A	119	GLN	CA-C-N	-5.48	109.82	121.32
1	A	119	GLN	C-N-CA	-5.48	109.82	121.32
1	A	149	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	A	253	ARG	CD-NE-CZ	5.48	132.07	124.40
1	A	223	VAL	CA-CB-CG1	5.47	119.70	110.40
1	A	299	ILE	N-CA-C	5.47	116.24	110.72
1	A	49	ILE	CB-CG1-CD1	-5.46	102.33	113.80
1	A	48	ASN	CA-C-N	-5.46	112.66	120.42
1	A	48	ASN	C-N-CA	-5.46	112.66	120.42
1	A	85	GLU	CB-CG-CD	-5.46	103.32	112.60
1	A	157	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	316	GLY	CA-C-N	-5.44	113.14	120.87
1	A	316	GLY	C-N-CA	-5.44	113.14	120.87
1	A	339	GLU	N-CA-C	5.44	118.13	111.82
1	A	101	ARG	O-C-N	5.44	129.75	123.17
1	A	116	PRO	N-CA-CB	-5.44	98.47	103.31
1	A	99	GLU	O-C-N	5.43	129.68	123.27
1	A	338	ASP	N-CA-C	5.43	116.88	111.07
1	A	72	ILE	CA-C-N	-5.42	113.02	120.71
1	A	72	ILE	C-N-CA	-5.42	113.02	120.71
1	A	270	GLY	N-CA-C	5.42	122.74	115.59
1	A	185	ASP	N-CA-C	5.41	117.54	108.23
1	A	55	PRO	CA-C-N	-5.41	113.82	122.53
1	A	55	PRO	C-N-CA	-5.41	113.82	122.53
1	A	346	LEU	CA-C-N	-5.40	113.42	120.44
1	A	346	LEU	C-N-CA	-5.40	113.42	120.44
1	A	85	GLU	CB-CA-C	5.40	120.70	109.95
1	A	307	ASP	CA-C-O	5.40	126.18	119.97
1	A	282	ARG	CA-CB-CG	-5.39	103.31	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LYS	CB-CA-C	5.39	119.34	110.88
1	A	178	VAL	N-CA-C	5.39	118.32	113.10
1	A	135	GLN	CG-CD-OE1	5.36	131.53	120.80
1	A	176	THR	CA-CB-OG1	5.36	117.64	109.60
1	A	12	VAL	O-C-N	5.36	128.66	123.03
1	A	278	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	214	HIS	N-CA-CB	5.35	117.95	109.71
1	A	163	SER	N-CA-C	5.34	118.01	111.82
1	A	287	GLN	CA-CB-CG	5.33	124.77	114.10
1	A	78	ALA	CA-C-O	-5.33	114.07	120.10
1	A	309	GLN	N-CA-C	5.33	118.00	111.82
1	A	240	TYR	CD1-CG-CD2	5.33	126.09	118.10
1	A	246	THR	CA-C-O	5.32	126.07	119.79
1	A	352	ARG	N-CA-C	5.32	125.90	111.00
1	A	285	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	197	HIS	ND1-CG-CD2	5.30	111.40	106.10
1	A	132	LEU	N-CA-C	5.29	117.04	111.28
1	A	58	LEU	CD1-CG-CD2	5.28	122.42	110.80
1	A	239	GLY	N-CA-C	5.28	122.91	115.30
1	A	273	LYS	CA-CB-CG	5.27	124.65	114.10
1	A	336	PRO	CA-C-O	5.26	127.33	121.43
1	A	215	ALA	CA-C-O	5.26	126.64	120.43
1	A	261	ILE	CA-C-N	-5.26	115.78	122.98
1	A	261	ILE	C-N-CA	-5.26	115.78	122.98
1	A	334	PHE	N-CA-C	5.25	118.50	112.57
1	A	147	LYS	CB-CG-CD	5.24	123.36	111.30
1	A	171	LYS	N-CA-C	5.23	117.06	111.36
1	A	143	ASP	CA-C-N	-5.23	114.13	122.29
1	A	143	ASP	C-N-CA	-5.23	114.13	122.29
1	A	197	HIS	CG-CD2-NE2	-5.22	101.98	107.20
1	A	258	HIS	CG-CD2-NE2	-5.22	101.98	107.20
1	A	276	THR	N-CA-CB	-5.21	103.15	111.43
1	A	296	ASP	CB-CA-C	-5.20	103.65	110.87
1	A	48	ASN	N-CA-CB	5.18	117.83	110.06
1	A	149	ARG	N-CA-CB	5.18	118.83	111.05
1	A	157	HIS	ND1-CG-CD2	5.18	111.28	106.10
1	A	253	ARG	CB-CG-CD	5.18	123.21	111.30
1	A	283	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	335	LEU	CB-CA-C	-5.17	101.14	109.37
1	A	114	PRO	CA-CB-CG	5.17	113.82	104.00
1	A	34	ARG	CB-CG-CD	5.16	123.17	111.30
1	A	334	PHE	CA-C-O	5.16	126.81	120.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	CA-C-O	5.15	125.60	120.09
1	A	133	VAL	CA-C-N	-5.15	113.86	120.65
1	A	133	VAL	C-N-CA	-5.15	113.86	120.65
1	A	294	THR	O-C-N	5.13	129.65	122.36
1	A	226	GLU	CA-C-N	-5.12	113.42	120.28
1	A	226	GLU	C-N-CA	-5.12	113.42	120.28
1	A	352	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	A	108	ALA	CA-C-O	5.09	128.35	121.89
1	A	135	GLN	N-CA-C	5.08	119.70	111.37
1	A	175	GLN	O-C-N	-5.08	113.91	121.63
1	A	276	THR	N-CA-C	5.08	117.13	109.41
1	A	229	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	157	HIS	CA-C-O	5.07	125.61	119.11
1	A	43	PRO	N-CA-C	-5.07	102.03	112.47
1	A	137	LEU	CD1-CG-CD2	5.07	121.95	110.80
1	A	154	CYS	CA-C-N	-5.06	115.86	123.00
1	A	154	CYS	C-N-CA	-5.06	115.86	123.00
1	A	72	ILE	N-CA-CB	-5.05	102.02	110.86
1	A	32	LYS	CB-CG-CD	5.05	122.91	111.30
1	A	34	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	76	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	198	VAL	CA-C-N	-5.03	112.67	120.31
1	A	198	VAL	C-N-CA	-5.03	112.67	120.31
1	A	27	ILE	N-CA-C	-5.03	105.42	110.30
1	A	17	HIS	CB-CA-C	-5.01	101.48	109.75

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

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Mol	Chain	Res	Type	Group
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
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	2743	166	0
2	A	1	0	0	0	0
3	A	37	0	28	2	0
4	A	545	0	0	71	0
All	All	3371	0	2771	167	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 30.

All (167) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:211:ARG:HH21	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:52:MET:HE3	1:A:56:LEU:HG	1.60	0.80
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
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:HB2	1:A:211:ARG:NH2	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:312:LYS:HZ2	1:A:312:LYS:HB3	1.68	0.57
1:A:61:PHE:HE1	1:A:299:ILE:HG21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASN:HB2	4:A:1194:HOH:O	2.04	0.57
1:A:310:MET:HE2	1:A:315:MET:CE	2.35	0.56
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:222:ASN:O	1:A:226:GLU:HG3	2.08	0.55
1:A:312:LYS:HB3	1:A:312:LYS:NZ	2.22	0.55
1:A:117:TRP:CD1	4:A:1422:HOH:O	2.59	0.54
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:52:MET:HE3	1:A:56:LEU:CG	2.34	0.53
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.43	0.53
1:A:114:PRO:HB2	4:A:1067:HOH:O	2.09	0.53
1:A:315:MET:HB3	4:A:1211:HOH:O	2.07	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:5:PRO:HG2	1:A:8:ASP:OD1	2.09	0.52
1:A:266:SER:OG	1:A:278:HIS:HE1	1.91	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:47:GLN:HE22	1:A:298:LEU:HD12	1.75	0.51
1:A:57:THR:HG23	1:A:60:ASP:H	1.76	0.51
1:A:313:LYS:HA	1:A:313:LYS:HE3	1.92	0.51
1:A:334:PHE:C	4:A:1503:HOH:O	2.54	0.51
1:A:43:PRO:HD2	4:A:1435:HOH:O	2.10	0.50
1:A:315:MET:HE2	4:A:1335:HOH:O	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HE2	1:A:315:MET:HE2	1.94	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:25:GLU:HA	1:A:43:PRO:HB3	1.94	0.48
1:A:80:LYS:HE3	1:A:135:GLN:HB3	1.94	0.48
1:A:117:TRP:HD1	4:A:1422:HOH:O	1.95	0.48
1:A:90:LYS:HE2	1:A:90:LYS:HA	1.96	0.47
1:A:309:GLN:NE2	1:A:312:LYS:HZ1	2.13	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:312:LYS:HZ3	1:A:313:LYS:HD2	1.79	0.47
1:A:9:LYS:HD2	4:A:1336:HOH:O	2.14	0.47
1:A:180:ILE:HG21	1:A:180:ILE:HD13	1.71	0.47
1:A:217:GLU:HB3	4:A:1083:HOH:O	2.15	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:162:SER:OG	1:A:197:HIS:HD2	1.99	0.46
1:A:277:GLU:HB3	4:A:1507:HOH:O	2.14	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:O1	3:A:1001:FR5:H32	2.15	0.45
1:A:23:LYS:HB3	4:A:1196:HOH:O	2.16	0.45
1:A:169:CYS:HA	1:A:177:VAL:HG21	1.99	0.45
1:A:170:LYS:O	1:A:173:ARG:HG2	2.17	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:69:MET:HE1	1:A:107:LEU:CD1	2.48	0.44
1:A:28:LEU:HD13	1:A:38:LEU:HD12	1.99	0.44
1:A:75:CYS:O	1:A:76:ARG:C	2.60	0.44
1:A:337:GLU:CD	1:A:341:LYS:HZ2	2.25	0.44
1:A:261:ILE:N	1:A:261:ILE:HD13	2.33	0.44
1:A:288:VAL:HG12	4:A:1536:HOH:O	2.17	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:25:GLU:H	1:A:25:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:241:HIS:HD2	1:A:244:GLU:CD	2.26	0.43
1:A:88:GLU:O	1:A:92:LYS:HG2	2.19	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:113:GLU:CD	1:A:114:PRO:HA	2.43	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:241:HIS:O	1:A:244:GLU:HG3	2.19	0.42
1:A:313:LYS:HE3	1:A:313:LYS:CA	2.49	0.42
1:A:351:TYR:HD2	4:A:1336:HOH:O	2.01	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:HZ3	1:A:170:LYS:HB2	1.84	0.42
1:A:31:GLY:HA3	4:A:1265:HOH:O	2.20	0.42
1:A:273:LYS:HE2	4:A:1483:HOH:O	2.20	0.42
1:A:32:LYS:HG3	4:A:1029:HOH:O	2.19	0.41
1:A:50:ILE:HG21	1:A:50:ILE:HD13	1.62	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.84	0.41
1:A:46:LEU:CD2	1:A:50:ILE:HD11	2.50	0.41
1:A:327:ILE:HA	1:A:327:ILE:HD13	1.82	0.41
1:A:33:ARG:HG3	4:A:1492:HOH:O	2.20	0.41
1:A:84:TYR:CD1	4:A:1285:HOH:O	2.74	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:HH11	1:A:149:ARG:HD3	1.62	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%)	320 (92%)	22 (6%)	5 (1%)	9 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLU
1	A	279	ALA
1	A	37	ALA
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%)	251 (83%)	53 (17%)	2 1

All (53) 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	36	ILE

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Mol	Chain	Res	Type
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	85	GLU
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
1	A	175	GLN
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	313	LYS
1	A	320	GLU
1	A	321	GLU
1	A	325	LEU
1	A	335	LEU

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Mol	Chain	Res	Type
1	A	337	GLU
1	A	341	LYS
1	A	347	LEU
1	A	349	LYS
1	A	352	ARG

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	47	GLN
1	A	134	ASN
1	A	138	GLN
1	A	157	HIS
1	A	158	GLN
1	A	197	HIS
1	A	210	HIS
1	A	241	HIS
1	A	278	HIS
1	A	309	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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	-	41,41,41	2.58	15 (36%)	52,58,58	1.89	16 (30%)

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	-	-	3/24/24/24	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR5	C33-N1	-6.55	1.28	1.41
3	A	1001	FR5	C34-C30	-5.72	1.30	1.39
3	A	1001	FR5	C2-N1	-4.93	1.25	1.35
3	A	1001	FR5	C1-C5	-4.87	1.31	1.37
3	A	1001	FR5	C19-N22	4.86	1.57	1.47
3	A	1001	FR5	C32-C31	-4.53	1.31	1.38
3	A	1001	FR5	C31-C29	-3.88	1.34	1.41
3	A	1001	FR5	C6-C12	3.56	1.54	1.49
3	A	1001	FR5	C17-C11	3.39	1.44	1.38
3	A	1001	FR5	C30-N22	-3.34	1.33	1.39
3	A	1001	FR5	C34-C33	-3.14	1.34	1.39
3	A	1001	FR5	C12-N13	-2.26	1.33	1.36
3	A	1001	FR5	C18-C19	2.18	1.59	1.52
3	A	1001	FR5	C29-C30	-2.05	1.38	1.41
3	A	1001	FR5	C3-N4	-2.01	1.26	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR5	C4-C6-C12	-4.92	106.97	111.62
3	A	1001	FR5	C11-C16-C10	-4.48	117.06	122.23
3	A	1001	FR5	C17-C9-C15	-4.20	115.06	120.24
3	A	1001	FR5	C29-C30-N22	-3.27	104.39	107.62
3	A	1001	FR5	C16-C10-N11	-3.05	106.32	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR5	C5-C8-N10	-2.77	113.46	116.28
3	A	1001	FR5	C14-C13-N2	2.65	116.67	110.52
3	A	1001	FR5	C10-C16-N13	2.55	107.48	105.68
3	A	1001	FR5	O9-C8-C5	2.49	122.64	120.25
3	A	1001	FR5	O15-C14-C13	2.44	120.97	111.51
3	A	1001	FR5	C19-N22-C30	-2.35	122.38	126.55
3	A	1001	FR5	C30-N22-C27	2.33	113.14	108.32
3	A	1001	FR5	C11-C16-N13	2.26	134.54	129.88
3	A	1001	FR5	C6-C4-C2	2.18	117.16	112.67
3	A	1001	FR5	C34-C33-N1	-2.05	113.46	120.13
3	A	1001	FR5	C9-C15-C10	2.05	122.74	118.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

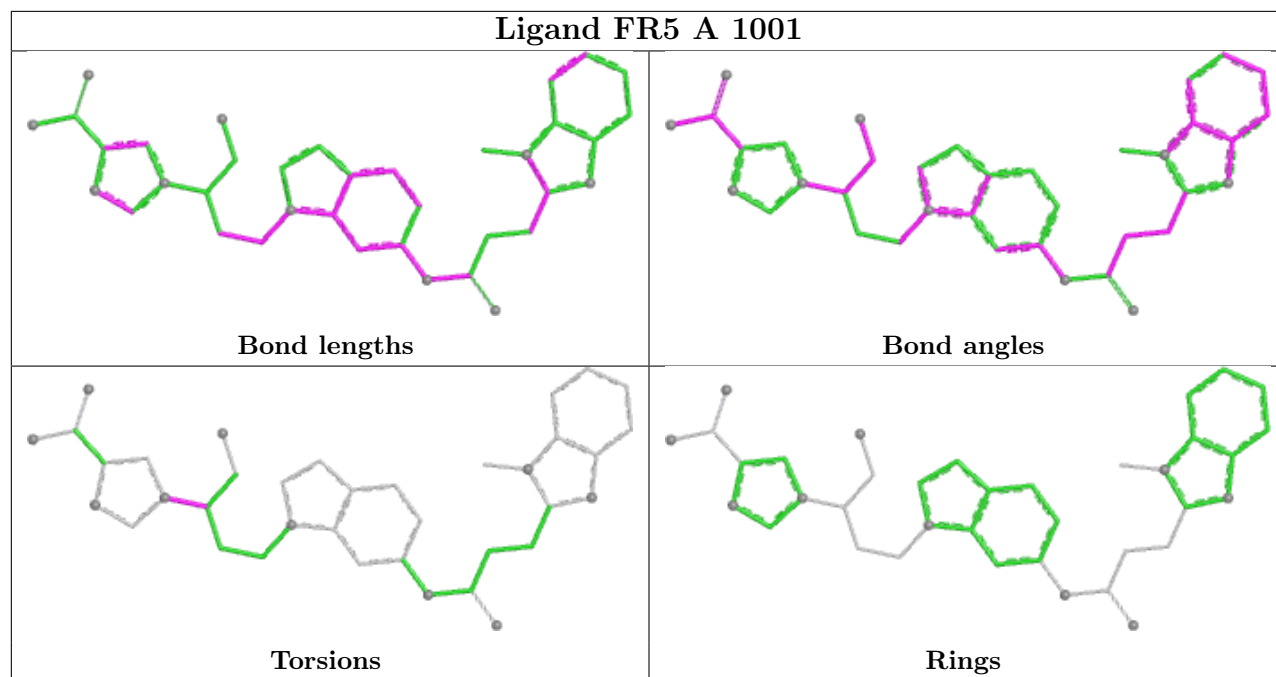
Mol	Chain	Res	Type	Atoms
3	A	1001	FR5	C18-C13-N2-C3
3	A	1001	FR5	C14-C13-N2-C1
3	A	1001	FR5	C18-C13-N2-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR5	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.