



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:29 AM UTC

PDB ID : 1NDV / pdb_00001ndv
Title : Crystal Structure of Adenosine Deaminase complexed with FR117016
Authors : Kinoshita, T.
Deposited on : 2002-12-09
Resolution : 2.30 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

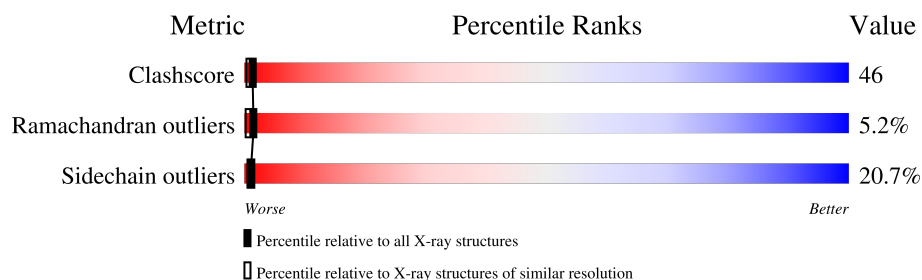
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	9% 33% 40% 16% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3272 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			

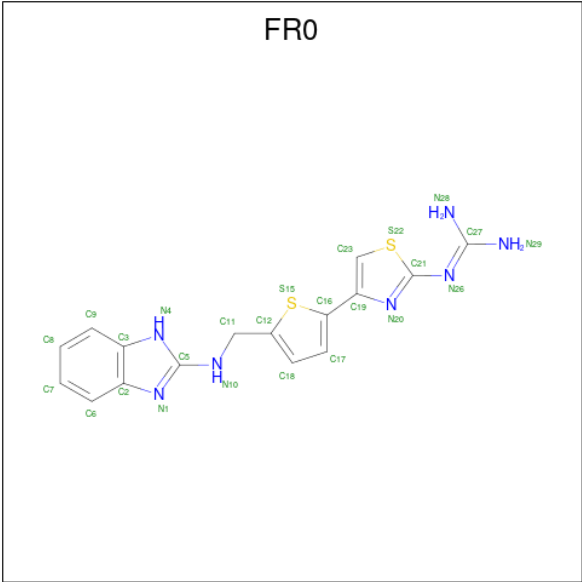
There are 15 discrepancies between the modelled and reference sequences:

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 N''-(4-(5-((1H-BENZIMIDAZOL-2-YLAMINO)METHYL)-2-THIENYL)-1,3-THIAZOL-2-YL)GUANIDINE (CCD ID: FR0) (formula: C₁₆H₁₅N₇S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			25	16	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	458	Total	O	0	0
			458	458		

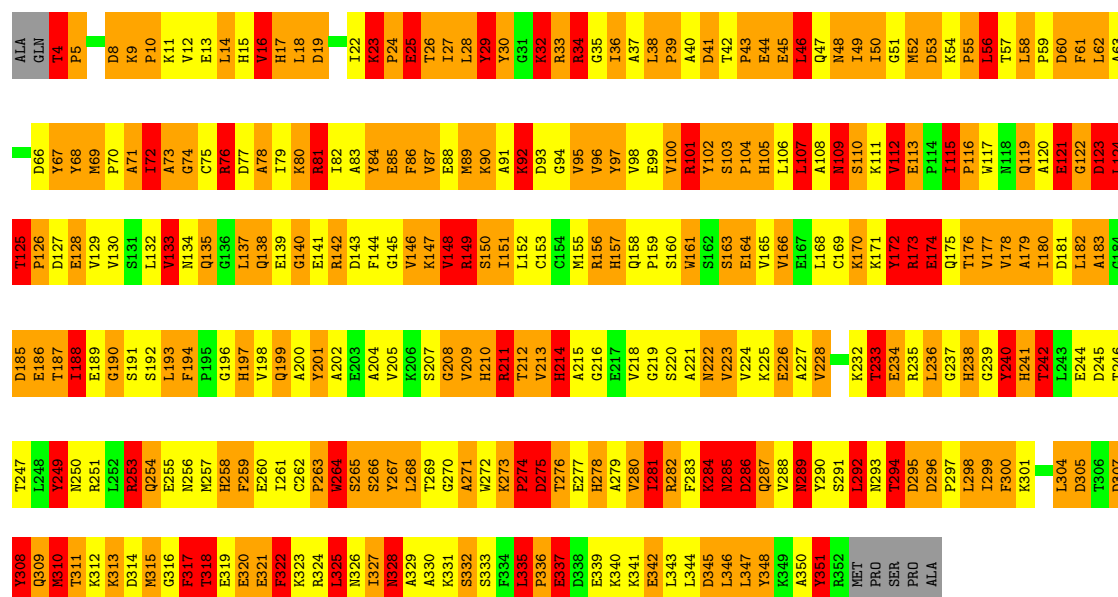
3 Residue-property plots

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

Chain A: 



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	78.03Å 78.03Å 136.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.225 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3272	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: FR0, 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	2.33	134/2852 (4.7%)	3.21	476/3866 (12.3%)

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	0	23

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ARG	NE-CZ	11.35	1.45	1.33
1	A	213	VAL	CA-CB	10.63	1.68	1.54
1	A	150	SER	CA-C	9.67	1.64	1.52
1	A	247	THR	CA-CB	9.13	1.68	1.53
1	A	188	ILE	CA-CB	-9.08	1.42	1.54
1	A	299	ILE	CA-CB	8.85	1.65	1.54
1	A	83	ALA	CA-C	8.80	1.64	1.52
1	A	238	HIS	C-N	8.62	1.44	1.33
1	A	228	VAL	CA-C	8.51	1.62	1.52
1	A	157	HIS	CE1-NE2	8.47	1.41	1.32
1	A	236	LEU	CA-C	8.27	1.62	1.52
1	A	238	HIS	CA-C	8.18	1.63	1.52
1	A	15	HIS	CA-C	8.11	1.63	1.53
1	A	157	HIS	CG-CD2	8.04	1.44	1.35
1	A	97	TYR	C-N	-8.02	1.22	1.33
1	A	17	HIS	CA-CB	7.98	1.64	1.53
1	A	218	VAL	CA-C	7.77	1.62	1.53
1	A	157	HIS	ND1-CE1	7.75	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ARG	CD-NE	7.66	1.56	1.46
1	A	241	HIS	ND1-CE1	7.59	1.40	1.32
1	A	232	LYS	CA-C	7.58	1.62	1.53
1	A	259	PHE	CA-C	7.58	1.62	1.52
1	A	11	LYS	C-N	7.51	1.44	1.33
1	A	279	ALA	C-N	7.48	1.42	1.34
1	A	158	GLN	C-N	7.42	1.42	1.34
1	A	222	ASN	CA-CB	7.40	1.65	1.53
1	A	328	ASN	N-CA	7.34	1.55	1.46
1	A	261	ILE	CA-CB	-7.34	1.45	1.54
1	A	209	VAL	CA-C	-7.31	1.44	1.52
1	A	227	ALA	N-CA	7.27	1.55	1.46
1	A	327	ILE	CA-C	7.22	1.61	1.52
1	A	19	ASP	CA-C	-7.13	1.41	1.52
1	A	104	PRO	CA-C	7.11	1.62	1.52
1	A	264	TRP	CA-C	-7.08	1.43	1.52
1	A	196	GLY	C-N	7.05	1.42	1.33
1	A	36	ILE	CA-C	7.02	1.62	1.52
1	A	91	ALA	N-CA	6.90	1.54	1.46
1	A	155	MET	CA-C	6.90	1.61	1.52
1	A	174	GLU	CA-C	6.86	1.61	1.52
1	A	350	ALA	CA-C	-6.79	1.43	1.52
1	A	86	PHE	N-CA	6.76	1.54	1.46
1	A	282	ARG	NE-CZ	6.74	1.40	1.33
1	A	214	HIS	CA-CB	-6.69	1.43	1.53
1	A	190	GLY	CA-C	6.58	1.61	1.51
1	A	89	MET	N-CA	6.55	1.54	1.46
1	A	214	HIS	CG-CD2	6.52	1.43	1.35
1	A	264	TRP	CA-CB	6.51	1.63	1.53
1	A	278	HIS	CG-CD2	6.46	1.43	1.35
1	A	53	ASP	C-N	6.46	1.41	1.33
1	A	197	HIS	CG-ND1	-6.46	1.31	1.38
1	A	339	GLU	CA-C	-6.46	1.43	1.52
1	A	25	GLU	CA-C	6.44	1.61	1.52
1	A	177	VAL	CA-C	-6.44	1.45	1.52
1	A	247	THR	CA-C	6.43	1.61	1.52
1	A	12	VAL	CA-CB	-6.42	1.46	1.54
1	A	335	LEU	CA-C	6.42	1.60	1.53
1	A	17	HIS	CE1-NE2	6.40	1.39	1.32
1	A	329	ALA	CA-CB	-6.32	1.43	1.53
1	A	241	HIS	CG-ND1	-6.27	1.31	1.38
1	A	312	LYS	CA-C	6.25	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	PHE	C-N	6.23	1.42	1.34
1	A	105	HIS	CA-C	-6.16	1.44	1.52
1	A	208	GLY	CA-C	6.16	1.60	1.51
1	A	68	TYR	CA-C	-6.10	1.44	1.52
1	A	247	THR	N-CA	6.08	1.54	1.46
1	A	105	HIS	CG-ND1	-6.07	1.31	1.38
1	A	17	HIS	CA-C	6.00	1.60	1.52
1	A	325	LEU	CA-C	-5.94	1.44	1.52
1	A	105	HIS	C-O	-5.94	1.17	1.24
1	A	138	GLN	CA-C	5.93	1.60	1.52
1	A	103	SER	CA-CB	5.93	1.62	1.52
1	A	224	VAL	CA-C	-5.88	1.44	1.52
1	A	86	PHE	CA-CB	5.85	1.62	1.53
1	A	290	TYR	CA-C	5.80	1.60	1.52
1	A	215	ALA	CA-C	-5.79	1.45	1.52
1	A	189	GLU	CG-CD	5.79	1.66	1.52
1	A	147	LYS	N-CA	5.76	1.53	1.46
1	A	253	ARG	CA-CB	5.75	1.62	1.53
1	A	161	TRP	CA-C	5.74	1.60	1.52
1	A	212	THR	CA-CB	5.72	1.66	1.54
1	A	97	TYR	N-CA	5.72	1.53	1.46
1	A	44	GLU	CA-C	-5.70	1.45	1.52
1	A	304	LEU	C-N	5.69	1.41	1.33
1	A	222	ASN	C-N	5.69	1.40	1.34
1	A	156	ARG	CA-C	5.64	1.60	1.52
1	A	26	THR	CA-C	-5.62	1.44	1.52
1	A	329	ALA	CA-C	-5.60	1.45	1.52
1	A	94	GLY	CA-C	5.58	1.59	1.51
1	A	142	ARG	NE-CZ	5.56	1.39	1.33
1	A	19	ASP	C-O	-5.55	1.16	1.24
1	A	223	VAL	CA-CB	5.54	1.62	1.54
1	A	226	GLU	CA-C	5.53	1.59	1.52
1	A	289	ASN	C-N	5.53	1.41	1.33
1	A	153	CYS	C-N	5.53	1.41	1.33
1	A	69	MET	CA-CB	5.51	1.60	1.53
1	A	99	GLU	CA-C	-5.47	1.46	1.52
1	A	35	GLY	C-N	-5.45	1.27	1.34
1	A	265	SER	CA-CB	-5.45	1.44	1.53
1	A	255	GLU	CA-C	5.43	1.60	1.52
1	A	278	HIS	CB-CG	5.43	1.57	1.50
1	A	193	LEU	CA-C	-5.42	1.45	1.52
1	A	194	PHE	N-CA	5.40	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	GLN	C-N	5.39	1.40	1.33
1	A	151	ILE	CA-CB	5.38	1.61	1.54
1	A	348	TYR	CA-C	5.36	1.59	1.52
1	A	345	ASP	C-N	5.36	1.40	1.33
1	A	181	ASP	N-CA	-5.35	1.39	1.45
1	A	286	ASP	CA-CB	5.35	1.61	1.53
1	A	227	ALA	CA-CB	5.35	1.61	1.53
1	A	17	HIS	ND1-CE1	5.35	1.37	1.32
1	A	238	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	51	GLY	N-CA	-5.31	1.40	1.45
1	A	333	SER	CA-C	-5.31	1.45	1.53
1	A	342	GLU	C-N	5.27	1.40	1.33
1	A	197	HIS	CB-CG	-5.24	1.42	1.50
1	A	326	ASN	CA-C	-5.23	1.45	1.52
1	A	263	PRO	C-N	-5.22	1.26	1.33
1	A	238	HIS	CE1-NE2	5.19	1.37	1.32
1	A	245	ASP	CA-CB	-5.19	1.47	1.53
1	A	102	TYR	CA-CB	5.17	1.62	1.53
1	A	197	HIS	ND1-CE1	5.15	1.37	1.32
1	A	197	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	123	ASP	CA-C	5.11	1.59	1.52
1	A	102	TYR	C-O	-5.11	1.17	1.23
1	A	111	LYS	CA-C	5.09	1.59	1.53
1	A	285	ASN	CA-C	5.09	1.59	1.52
1	A	313	LYS	CA-C	-5.09	1.46	1.52
1	A	268	LEU	CB-CG	5.08	1.63	1.53
1	A	201	TYR	CA-C	5.06	1.59	1.52
1	A	220	SER	CA-C	-5.05	1.46	1.53
1	A	326	ASN	N-CA	5.05	1.52	1.46
1	A	17	HIS	CB-CG	5.03	1.57	1.50
1	A	17	HIS	CD2-NE2	5.02	1.43	1.37
1	A	50	ILE	CA-C	-5.01	1.46	1.52

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ALA	N-CA-C	15.79	128.49	111.28
1	A	36	ILE	N-CA-C	13.34	129.59	111.17
1	A	209	VAL	N-CA-C	13.33	125.96	109.30
1	A	164	GLU	CA-CB-CG	12.49	139.08	114.10
1	A	223	VAL	CA-CB-CG2	12.00	130.80	110.40
1	A	211	ARG	NE-CZ-NH1	-11.35	110.15	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	CB-CA-C	11.34	128.95	110.81
1	A	273	LYS	CA-C-O	11.17	128.06	119.46
1	A	28	LEU	N-CA-C	11.02	123.29	111.28
1	A	89	MET	N-CA-C	10.50	124.03	111.33
1	A	211	ARG	NE-CZ-NH2	10.47	128.62	119.20
1	A	197	HIS	CA-CB-CG	-10.42	103.38	113.80
1	A	111	LYS	N-CA-C	10.34	125.60	111.54
1	A	228	VAL	N-CA-C	10.19	119.99	110.42
1	A	146	VAL	CA-C-N	-10.17	106.87	121.42
1	A	146	VAL	C-N-CA	-10.17	106.87	121.42
1	A	157	HIS	CA-CB-CG	-10.00	103.80	113.80
1	A	149	ARG	CD-NE-CZ	-9.99	110.41	124.40
1	A	32	LYS	CB-CA-C	9.99	127.66	110.68
1	A	181	ASP	CA-CB-CG	9.93	122.53	112.60
1	A	333	SER	CA-C-N	-9.92	106.50	122.66
1	A	333	SER	C-N-CA	-9.92	106.50	122.66
1	A	294	THR	CA-CB-CG2	9.88	127.30	110.50
1	A	183	ALA	N-CA-C	9.87	122.78	108.86
1	A	177	VAL	O-C-N	9.77	133.44	123.18
1	A	77	ASP	CA-CB-CG	9.73	122.33	112.60
1	A	282	ARG	NH1-CZ-NH2	-9.69	106.70	119.30
1	A	251	ARG	NE-CZ-NH1	-9.62	111.88	121.50
1	A	283	PHE	CA-CB-CG	9.37	123.17	113.80
1	A	311	THR	N-CA-C	9.34	121.06	111.07
1	A	328	ASN	CA-CB-CG	9.32	121.92	112.60
1	A	242	THR	CA-CB-CG2	9.13	126.02	110.50
1	A	261	ILE	N-CA-C	9.10	120.90	108.89
1	A	226	GLU	N-CA-C	9.09	121.19	111.28
1	A	142	ARG	N-CA-C	9.08	122.36	111.82
1	A	295	ASP	N-CA-C	9.07	130.12	110.80
1	A	346	LEU	CB-CA-C	-9.06	95.70	110.74
1	A	87	VAL	CA-C-O	9.03	130.95	121.29
1	A	41	ASP	CA-CB-CG	-8.98	103.62	112.60
1	A	259	PHE	O-C-N	-8.90	112.77	123.27
1	A	103	SER	O-C-N	-8.89	113.17	121.35
1	A	32	LYS	N-CA-CB	-8.86	96.77	110.06
1	A	15	HIS	CE1-NE2-CD2	-8.72	100.28	109.00
1	A	340	LYS	CA-CB-CG	8.65	131.41	114.10
1	A	15	HIS	CA-CB-CG	-8.64	105.16	113.80
1	A	279	ALA	N-CA-CB	-8.61	95.74	109.78
1	A	284	LYS	CA-C-N	-8.59	107.92	120.28
1	A	284	LYS	C-N-CA	-8.59	107.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	SER	CA-C-O	8.54	129.83	119.49
1	A	291	SER	CA-C-O	-8.50	111.99	121.51
1	A	36	ILE	CA-C-N	8.47	136.95	121.70
1	A	36	ILE	C-N-CA	8.47	136.95	121.70
1	A	34	ARG	CD-NE-CZ	-8.46	112.56	124.40
1	A	105	HIS	CA-CB-CG	-8.45	105.35	113.80
1	A	10	PRO	O-C-N	8.44	133.29	123.00
1	A	27	ILE	CA-C-N	-8.44	108.98	120.28
1	A	27	ILE	C-N-CA	-8.44	108.98	120.28
1	A	156	ARG	CD-NE-CZ	8.42	136.19	124.40
1	A	166	VAL	CB-CA-C	-8.39	99.15	112.16
1	A	298	LEU	CA-C-O	8.36	130.27	121.07
1	A	337	GLU	N-CA-C	8.36	121.32	111.71
1	A	4	THR	CA-C-N	-8.35	111.16	119.76
1	A	4	THR	C-N-CA	-8.35	111.16	119.76
1	A	266	SER	N-CA-C	8.30	122.38	111.75
1	A	285	ASN	OD1-CG-ND2	-8.27	114.33	122.60
1	A	335	LEU	CD1-CG-CD2	8.23	128.91	110.80
1	A	174	GLU	CA-CB-CG	8.23	130.55	114.10
1	A	84	TYR	CA-C-O	8.21	129.69	120.90
1	A	253	ARG	CA-CB-CG	8.20	130.51	114.10
1	A	25	GLU	CA-C-N	-8.12	109.14	122.54
1	A	25	GLU	C-N-CA	-8.12	109.14	122.54
1	A	119	GLN	N-CA-C	8.12	121.06	110.43
1	A	182	LEU	CA-C-N	-8.03	109.61	122.53
1	A	182	LEU	C-N-CA	-8.03	109.61	122.53
1	A	32	LYS	CA-CB-CG	8.01	130.12	114.10
1	A	80	LYS	CA-C-N	-8.01	109.66	120.79
1	A	80	LYS	C-N-CA	-8.01	109.66	120.79
1	A	101	ARG	CD-NE-CZ	-7.99	113.21	124.40
1	A	299	ILE	CA-CB-CG2	7.98	124.06	110.50
1	A	278	HIS	N-CA-CB	7.97	123.41	110.42
1	A	107	LEU	CA-C-N	-7.96	104.60	121.32
1	A	107	LEU	C-N-CA	-7.96	104.60	121.32
1	A	110	SER	CA-C-O	-7.96	111.97	121.60
1	A	308	TYR	CB-CG-CD2	-7.95	108.87	120.80
1	A	27	ILE	N-CA-C	7.92	117.98	110.30
1	A	122	GLY	CA-C-O	7.91	129.94	121.87
1	A	68	TYR	N-CA-C	7.90	122.19	112.23
1	A	275	ASP	CA-C-N	-7.89	108.63	122.20
1	A	275	ASP	C-N-CA	-7.89	108.63	122.20
1	A	109	ASN	CB-CA-C	7.87	122.18	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASP	CA-C-N	-7.86	109.75	120.44
1	A	127	ASP	C-N-CA	-7.86	109.75	120.44
1	A	282	ARG	NE-CZ-NH2	7.86	126.27	119.20
1	A	78	ALA	CA-C-N	-7.82	110.71	120.56
1	A	78	ALA	C-N-CA	-7.82	110.71	120.56
1	A	340	LYS	CA-C-N	-7.78	109.86	120.28
1	A	340	LYS	C-N-CA	-7.78	109.86	120.28
1	A	180	ILE	CB-CG1-CD1	-7.75	97.52	113.80
1	A	119	GLN	CA-C-N	-7.74	108.49	122.12
1	A	119	GLN	C-N-CA	-7.74	108.49	122.12
1	A	271	ALA	N-CA-C	7.72	119.70	111.28
1	A	186	GLU	CB-CA-C	-7.68	95.13	110.42
1	A	176	THR	CA-C-N	-7.68	113.67	123.19
1	A	176	THR	C-N-CA	-7.68	113.67	123.19
1	A	49	ILE	N-CA-C	7.65	118.24	110.82
1	A	81	ARG	N-CA-C	7.61	120.31	111.02
1	A	50	ILE	CA-C-N	-7.59	116.49	121.65
1	A	50	ILE	C-N-CA	-7.59	116.49	121.65
1	A	259	PHE	CA-C-O	7.58	128.66	120.32
1	A	60	ASP	CA-C-O	7.58	129.01	120.90
1	A	265	SER	N-CA-C	7.57	123.86	111.37
1	A	100	VAL	CG1-CB-CG2	-7.56	94.17	110.80
1	A	337	GLU	N-CA-CB	7.55	121.85	110.22
1	A	233	THR	N-CA-C	7.53	120.59	110.35
1	A	91	ALA	CA-C-N	-7.53	108.55	120.60
1	A	91	ALA	C-N-CA	-7.53	108.55	120.60
1	A	9	LYS	CA-C-N	-7.53	112.58	120.03
1	A	9	LYS	C-N-CA	-7.53	112.58	120.03
1	A	249	TYR	N-CA-C	7.50	123.68	111.37
1	A	339	GLU	CA-CB-CG	-7.47	99.15	114.10
1	A	326	ASN	CA-CB-CG	-7.46	105.14	112.60
1	A	89	MET	CB-CA-C	-7.39	98.11	110.68
1	A	192	SER	N-CA-C	7.38	121.39	112.38
1	A	247	THR	CA-CB-OG1	7.34	120.60	109.60
1	A	81	ARG	NE-CZ-NH2	7.31	125.78	119.20
1	A	210	HIS	N-CA-C	7.31	119.76	110.33
1	A	45	GLU	CA-C-N	-7.28	109.61	121.19
1	A	45	GLU	C-N-CA	-7.28	109.61	121.19
1	A	23	LYS	CA-CB-CG	-7.27	99.56	114.10
1	A	251	ARG	NE-CZ-NH2	7.25	125.72	119.20
1	A	72	ILE	CA-C-N	-7.23	109.39	121.39
1	A	72	ILE	C-N-CA	-7.23	109.39	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	HIS	N-CA-CB	7.22	120.49	110.01
1	A	169	CYS	CA-C-N	-7.21	109.45	121.92
1	A	169	CYS	C-N-CA	-7.21	109.45	121.92
1	A	218	VAL	CA-C-O	7.20	128.18	120.26
1	A	173	ARG	N-CA-C	7.17	120.79	110.10
1	A	194	PHE	CB-CA-C	-7.17	98.53	109.50
1	A	188	ILE	N-CA-CB	-7.17	99.40	111.23
1	A	350	ALA	N-CA-C	7.15	121.26	112.54
1	A	332	SER	CA-CB-OG	-7.14	96.82	111.10
1	A	273	LYS	N-CA-C	7.13	119.98	109.42
1	A	93	ASP	CA-C-N	-7.13	109.36	120.91
1	A	93	ASP	C-N-CA	-7.13	109.36	120.91
1	A	201	TYR	N-CA-C	7.12	120.08	111.82
1	A	71	ALA	N-CA-C	7.11	119.11	111.36
1	A	270	GLY	N-CA-C	7.10	124.80	115.36
1	A	116	PRO	N-CA-C	7.09	122.34	111.34
1	A	187	THR	CA-C-N	-7.07	109.24	121.97
1	A	187	THR	C-N-CA	-7.07	109.24	121.97
1	A	288	VAL	N-CA-C	7.03	118.65	109.58
1	A	140	GLY	CA-C-N	-7.01	110.89	120.28
1	A	140	GLY	C-N-CA	-7.01	110.89	120.28
1	A	142	ARG	CB-CG-CD	7.00	127.39	111.30
1	A	84	TYR	O-C-N	-6.95	114.87	122.09
1	A	158	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	A	152	LEU	O-C-N	-6.93	115.29	123.06
1	A	267	TYR	CA-C-N	-6.93	109.02	121.14
1	A	267	TYR	C-N-CA	-6.93	109.02	121.14
1	A	194	PHE	N-CA-C	6.90	118.06	109.57
1	A	124	LEU	N-CA-CB	6.89	120.51	110.58
1	A	188	ILE	N-CA-C	6.89	123.66	109.34
1	A	86	PHE	CA-CB-CG	-6.87	106.93	113.80
1	A	74	GLY	CA-C-N	-6.85	113.33	122.85
1	A	74	GLY	C-N-CA	-6.85	113.33	122.85
1	A	286	ASP	N-CA-C	6.79	120.54	112.93
1	A	295	ASP	CA-C-N	-6.79	114.93	123.15
1	A	295	ASP	C-N-CA	-6.79	114.93	123.15
1	A	279	ALA	CB-CA-C	6.78	122.00	110.74
1	A	314	ASP	CA-C-N	-6.78	111.36	122.54
1	A	314	ASP	C-N-CA	-6.78	111.36	122.54
1	A	61	PHE	CA-C-O	-6.77	113.89	121.00
1	A	300	PHE	N-CA-C	6.75	121.22	112.92
1	A	304	LEU	CD1-CG-CD2	-6.75	95.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLU	CA-C-O	-6.74	113.14	121.02
1	A	38	LEU	N-CA-C	6.72	119.70	109.41
1	A	104	PRO	CA-C-O	6.72	130.67	120.05
1	A	283	PHE	CA-C-O	6.72	127.69	120.10
1	A	262	CYS	N-CA-C	6.71	124.63	109.81
1	A	281	ILE	CA-CB-CG1	6.71	121.80	110.40
1	A	51	GLY	CA-C-O	6.70	126.17	120.94
1	A	310	MET	CA-C-O	6.69	128.85	121.02
1	A	88	GLU	CA-C-N	-6.64	111.28	120.38
1	A	88	GLU	C-N-CA	-6.64	111.28	120.38
1	A	182	LEU	CD1-CG-CD2	-6.63	96.22	110.80
1	A	158	GLN	N-CA-C	6.62	120.39	109.79
1	A	275	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	210	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	126	PRO	CA-C-O	6.60	130.15	119.86
1	A	143	ASP	N-CA-C	6.58	119.78	111.69
1	A	120	ALA	N-CA-C	6.58	120.05	109.86
1	A	109	ASN	N-CA-CB	-6.57	102.31	110.98
1	A	34	ARG	NE-CZ-NH2	-6.56	113.29	119.20
1	A	317	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	292	LEU	CD1-CG-CD2	-6.53	96.43	110.80
1	A	185	ASP	N-CA-CB	-6.53	99.62	110.39
1	A	91	ALA	CA-C-O	6.52	127.33	120.42
1	A	125	THR	CA-C-N	6.51	126.28	119.05
1	A	125	THR	C-N-CA	6.51	126.28	119.05
1	A	80	LYS	N-CA-C	6.50	118.45	111.36
1	A	165	VAL	N-CA-C	6.49	122.84	109.34
1	A	246	THR	N-CA-C	6.49	120.30	112.38
1	A	156	ARG	N-CA-C	6.48	119.17	111.33
1	A	28	LEU	CA-C-N	-6.48	111.59	120.28
1	A	28	LEU	C-N-CA	-6.48	111.59	120.28
1	A	345	ASP	O-C-N	6.46	131.19	122.59
1	A	285	ASN	N-CA-C	6.46	119.14	111.71
1	A	95	VAL	CA-CB-CG2	6.45	121.37	110.40
1	A	238	HIS	ND1-CE1-NE2	-6.45	101.95	108.40
1	A	351	TYR	CA-C-N	-6.44	110.11	121.70
1	A	351	TYR	C-N-CA	-6.44	110.11	121.70
1	A	108	ALA	N-CA-C	6.42	119.21	110.55
1	A	241	HIS	CA-CB-CG	-6.41	107.39	113.80
1	A	179	ALA	O-C-N	6.41	130.55	123.25
1	A	198	VAL	N-CA-C	6.40	117.15	110.62
1	A	15	HIS	CG-CD2-NE2	6.39	113.59	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	VAL	N-CA-C	6.39	120.99	112.04
1	A	199	GLN	CB-CG-CD	6.36	123.42	112.60
1	A	172	TYR	N-CA-C	6.35	119.71	112.97
1	A	281	ILE	N-CA-C	6.35	117.10	110.62
1	A	148	VAL	CA-C-N	-6.35	111.66	123.03
1	A	148	VAL	C-N-CA	-6.35	111.66	123.03
1	A	63	ALA	CA-C-N	-6.35	111.69	120.38
1	A	63	ALA	C-N-CA	-6.35	111.69	120.38
1	A	261	ILE	CB-CA-C	-6.34	102.90	111.15
1	A	325	LEU	N-CA-C	6.33	118.98	111.71
1	A	5	PRO	N-CA-CB	-6.32	97.68	103.31
1	A	268	LEU	CD1-CG-CD2	-6.32	96.89	110.80
1	A	146	VAL	O-C-N	-6.32	116.02	123.03
1	A	233	THR	CB-CA-C	-6.31	98.32	109.62
1	A	221	ALA	CA-C-N	-6.30	110.73	120.31
1	A	221	ALA	C-N-CA	-6.30	110.73	120.31
1	A	271	ALA	CA-C-O	6.30	127.23	120.55
1	A	90	LYS	N-CA-CB	6.29	119.37	110.12
1	A	101	ARG	N-CA-C	6.29	119.44	109.50
1	A	62	LEU	CA-C-O	6.28	127.19	119.97
1	A	170	LYS	CA-C-O	6.26	126.03	119.14
1	A	246	THR	CA-C-O	6.23	127.03	119.49
1	A	32	LYS	N-CA-C	6.23	118.87	111.33
1	A	155	MET	O-C-N	-6.23	115.97	123.13
1	A	56	LEU	N-CA-C	6.23	124.06	110.80
1	A	240	TYR	CA-C-O	6.22	127.01	120.42
1	A	174	GLU	CB-CG-CD	6.21	123.15	112.60
1	A	157	HIS	CB-CA-C	6.20	122.29	109.95
1	A	274	PRO	N-CA-CB	-6.19	96.75	103.25
1	A	213	VAL	CA-C-N	-6.19	112.65	121.50
1	A	213	VAL	C-N-CA	-6.19	112.65	121.50
1	A	299	ILE	CB-CA-C	6.18	127.90	111.34
1	A	287	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	A	255	GLU	CA-C-O	6.17	127.00	119.11
1	A	232	LYS	N-CA-C	6.15	119.90	111.54
1	A	25	GLU	O-C-N	-6.15	114.42	122.59
1	A	133	VAL	CB-CA-C	-6.12	103.89	112.14
1	A	115	ILE	CA-C-N	6.11	126.46	119.92
1	A	115	ILE	C-N-CA	6.11	126.46	119.92
1	A	322	PHE	CA-C-N	-6.11	110.45	121.14
1	A	322	PHE	C-N-CA	-6.11	110.45	121.14
1	A	245	ASP	N-CA-CB	-6.10	101.47	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	SER	O-C-N	6.10	130.64	122.96
1	A	76	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	238	HIS	CE1-NE2-CD2	6.09	115.09	109.00
1	A	33	ARG	CA-C-O	6.08	127.00	120.55
1	A	151	ILE	CA-C-N	-6.08	111.67	122.07
1	A	151	ILE	C-N-CA	-6.08	111.67	122.07
1	A	324	ARG	CA-C-O	6.07	127.04	120.55
1	A	11	LYS	CA-C-N	6.06	130.92	123.10
1	A	11	LYS	C-N-CA	6.06	130.92	123.10
1	A	299	ILE	N-CA-CB	-6.06	98.04	111.50
1	A	325	LEU	CB-CG-CD2	6.05	128.86	110.70
1	A	23	LYS	N-CA-C	6.05	119.08	110.24
1	A	241	HIS	N-CA-C	6.05	119.76	112.38
1	A	194	PHE	N-CA-CB	6.04	119.96	109.57
1	A	19	ASP	N-CA-CB	6.03	119.21	110.47
1	A	179	ALA	N-CA-CB	6.02	121.72	111.66
1	A	282	ARG	CA-C-N	-6.02	111.61	120.28
1	A	282	ARG	C-N-CA	-6.02	111.61	120.28
1	A	316	GLY	CA-C-O	6.01	126.52	119.19
1	A	44	GLU	CB-CA-C	-6.00	99.66	110.35
1	A	317	PHE	N-CA-C	6.00	117.80	109.15
1	A	204	ALA	N-CA-C	5.98	118.29	111.11
1	A	253	ARG	CA-C-N	-5.98	111.67	120.28
1	A	253	ARG	C-N-CA	-5.98	111.67	120.28
1	A	276	THR	N-CA-C	5.97	115.98	108.45
1	A	175	GLN	CA-C-N	5.96	132.43	121.70
1	A	175	GLN	C-N-CA	5.96	132.43	121.70
1	A	213	VAL	N-CA-C	5.95	116.86	108.17
1	A	152	LEU	CA-C-N	-5.95	114.39	123.07
1	A	152	LEU	C-N-CA	-5.95	114.39	123.07
1	A	81	ARG	CB-CG-CD	5.93	124.94	111.30
1	A	11	LYS	O-C-N	5.92	130.14	123.27
1	A	62	LEU	N-CA-C	5.91	118.67	111.82
1	A	215	ALA	N-CA-C	5.91	117.38	108.46
1	A	251	ARG	CB-CG-CD	-5.90	97.74	111.30
1	A	66	ASP	N-CA-C	5.89	117.70	111.28
1	A	170	LYS	CB-CG-CD	-5.89	97.75	111.30
1	A	275	ASP	N-CA-C	5.89	120.07	113.01
1	A	73	ALA	N-CA-C	5.87	119.17	110.48
1	A	299	ILE	N-CA-C	-5.87	104.35	112.50
1	A	258	HIS	ND1-CE1-NE2	-5.86	102.54	108.40
1	A	285	ASN	CA-C-N	-5.84	112.95	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASN	C-N-CA	-5.84	112.95	122.65
1	A	314	ASP	CA-CB-CG	-5.83	106.77	112.60
1	A	238	HIS	N-CA-C	5.81	123.18	110.80
1	A	202	ALA	CA-C-O	5.80	126.57	120.42
1	A	84	TYR	CA-C-N	-5.80	112.51	120.28
1	A	84	TYR	C-N-CA	-5.80	112.51	120.28
1	A	318	THR	CA-C-N	-5.80	112.97	122.54
1	A	318	THR	C-N-CA	-5.80	112.97	122.54
1	A	138	GLN	CA-C-O	5.79	126.56	120.42
1	A	207	SER	CA-C-O	5.78	126.77	119.95
1	A	260	GLU	CA-C-N	-5.78	113.69	121.66
1	A	260	GLU	C-N-CA	-5.78	113.69	121.66
1	A	36	ILE	O-C-N	-5.76	116.09	121.90
1	A	8	ASP	N-CA-C	5.74	119.39	112.38
1	A	308	TYR	N-CA-C	5.74	119.54	112.54
1	A	307	ASP	N-CA-C	5.74	117.99	111.11
1	A	132	LEU	CB-CA-C	-5.73	101.89	110.88
1	A	186	GLU	CB-CG-CD	-5.72	102.87	112.60
1	A	305	ASP	N-CA-C	5.72	117.51	111.28
1	A	119	GLN	CB-CA-C	-5.72	97.82	109.65
1	A	143	ASP	CA-C-N	-5.72	113.11	122.54
1	A	143	ASP	C-N-CA	-5.72	113.11	122.54
1	A	237	GLY	N-CA-C	5.71	126.71	113.18
1	A	135	GLN	N-CA-C	5.71	122.96	110.80
1	A	239	GLY	O-C-N	5.70	128.57	122.41
1	A	53	ASP	CA-C-N	5.69	132.50	122.08
1	A	53	ASP	C-N-CA	5.69	132.50	122.08
1	A	138	GLN	N-CA-C	5.69	117.57	111.36
1	A	234	GLU	CA-C-O	5.69	125.64	119.15
1	A	201	TYR	CA-C-O	5.69	126.51	119.97
1	A	251	ARG	N-CA-C	5.69	118.68	111.69
1	A	329	ALA	CA-C-N	-5.69	111.06	121.52
1	A	329	ALA	C-N-CA	-5.69	111.06	121.52
1	A	218	VAL	CA-CB-CG2	5.67	120.04	110.40
1	A	200	ALA	O-C-N	5.67	127.99	122.09
1	A	218	VAL	N-CA-C	5.67	117.66	111.77
1	A	166	VAL	CA-CB-CG1	5.66	120.03	110.40
1	A	72	ILE	CB-CG1-CD1	-5.66	101.92	113.80
1	A	26	THR	O-C-N	5.66	129.41	122.34
1	A	73	ALA	CA-C-N	-5.64	110.36	121.41
1	A	73	ALA	C-N-CA	-5.64	110.36	121.41
1	A	218	VAL	N-CA-CB	-5.64	104.83	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLU	CA-CB-CG	5.64	125.37	114.10
1	A	238	HIS	CA-CB-CG	5.63	119.43	113.80
1	A	246	THR	CA-CB-CG2	5.61	120.04	110.50
1	A	145	GLY	N-CA-C	5.61	122.56	114.10
1	A	89	MET	CA-C-N	-5.60	112.78	120.28
1	A	89	MET	C-N-CA	-5.60	112.78	120.28
1	A	18	LEU	CA-C-O	5.59	127.19	120.92
1	A	170	LYS	CA-CB-CG	-5.58	102.94	114.10
1	A	85	GLU	N-CA-C	5.57	117.35	111.28
1	A	214	HIS	ND1-CE1-NE2	5.55	113.95	108.40
1	A	336	PRO	O-C-N	5.55	129.89	123.01
1	A	179	ALA	CA-C-O	-5.54	115.34	121.33
1	A	68	TYR	CB-CA-C	-5.53	99.09	110.38
1	A	282	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	A	315	MET	CB-CA-C	5.52	119.31	110.09
1	A	176	THR	CB-CA-C	-5.51	96.98	109.10
1	A	247	THR	CA-CB-CG2	5.51	119.86	110.50
1	A	222	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	221	ALA	N-CA-C	5.50	119.49	112.34
1	A	121	GLU	N-CA-C	5.49	122.48	110.80
1	A	121	GLU	CA-C-N	-5.48	112.43	121.04
1	A	121	GLU	C-N-CA	-5.48	112.43	121.04
1	A	225	LYS	CA-C-N	-5.48	112.93	120.28
1	A	225	LYS	C-N-CA	-5.48	112.93	120.28
1	A	41	ASP	CA-C-N	-5.47	110.55	120.94
1	A	41	ASP	C-N-CA	-5.47	110.55	120.94
1	A	96	VAL	CA-C-O	5.46	126.18	119.58
1	A	133	VAL	N-CA-CB	5.46	117.96	110.54
1	A	244	GLU	CA-CB-CG	-5.45	103.20	114.10
1	A	312	LYS	CA-C-O	5.45	126.73	120.90
1	A	89	MET	CA-C-O	5.45	126.52	120.63
1	A	164	GLU	CB-CG-CD	-5.45	103.34	112.60
1	A	26	THR	N-CA-C	5.44	120.02	113.17
1	A	32	LYS	O-C-N	-5.44	116.36	122.12
1	A	125	THR	N-CA-C	5.44	121.82	109.81
1	A	253	ARG	O-C-N	-5.42	116.45	122.09
1	A	166	VAL	CG1-CB-CG2	5.42	122.73	110.80
1	A	128	GLU	N-CA-CB	5.42	117.93	110.07
1	A	169	CYS	CA-C-O	5.42	126.05	119.38
1	A	348	TYR	O-C-N	-5.42	116.49	122.07
1	A	254	GLN	N-CA-CB	5.42	118.56	110.22
1	A	293	ASN	OD1-CG-ND2	-5.40	117.20	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	N-CA-CB	-5.40	103.64	111.52
1	A	304	LEU	O-C-N	5.39	127.84	122.12
1	A	101	ARG	CA-C-N	-5.38	110.98	121.91
1	A	101	ARG	C-N-CA	-5.38	110.98	121.91
1	A	337	GLU	CA-C-N	-5.38	113.13	120.44
1	A	337	GLU	C-N-CA	-5.38	113.13	120.44
1	A	59	PRO	N-CA-C	5.37	121.00	113.53
1	A	258	HIS	CE1-NE2-CD2	5.37	114.37	109.00
1	A	66	ASP	O-C-N	-5.36	116.43	122.12
1	A	95	VAL	N-CA-C	5.36	115.82	107.99
1	A	282	ARG	CB-CG-CD	5.35	123.60	111.30
1	A	163	SER	CA-C-N	-5.34	112.19	120.31
1	A	163	SER	C-N-CA	-5.34	112.19	120.31
1	A	58	LEU	N-CA-C	5.33	121.59	109.81
1	A	153	CYS	CA-C-O	-5.33	114.81	120.40
1	A	343	LEU	CD1-CG-CD2	-5.33	99.08	110.80
1	A	46	LEU	N-CA-CB	5.32	118.77	109.72
1	A	96	VAL	CG1-CB-CG2	-5.32	99.10	110.80
1	A	30	TYR	CA-CB-CG	-5.31	104.34	113.90
1	A	14	LEU	CD1-CG-CD2	-5.30	99.13	110.80
1	A	179	ALA	CB-CA-C	-5.30	99.05	110.45
1	A	156	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	204	ALA	O-C-N	5.27	127.58	122.09
1	A	309	GLN	O-C-N	5.27	127.51	122.03
1	A	205	VAL	CA-CB-CG2	5.27	119.35	110.40
1	A	183	ALA	CB-CA-C	-5.26	99.02	111.65
1	A	87	VAL	CA-CB-CG2	5.25	119.32	110.40
1	A	211	ARG	N-CA-C	5.25	117.92	108.48
1	A	300	PHE	O-C-N	5.24	128.63	122.34
1	A	209	VAL	CA-CB-CG2	5.24	119.30	110.40
1	A	16	VAL	CG1-CB-CG2	5.23	122.31	110.80
1	A	282	ARG	CB-CA-C	5.23	119.75	110.85
1	A	103	SER	CA-C-O	5.23	123.19	119.32
1	A	11	LYS	CA-CB-CG	5.23	124.55	114.10
1	A	236	LEU	CD1-CG-CD2	-5.23	99.30	110.80
1	A	87	VAL	N-CA-C	5.22	115.37	110.30
1	A	310	MET	N-CA-CB	-5.21	100.86	109.72
1	A	335	LEU	N-CA-C	5.21	116.98	109.48
1	A	157	HIS	CA-C-O	5.20	125.77	119.11
1	A	12	VAL	CG1-CB-CG2	-5.20	99.37	110.80
1	A	296	ASP	CB-CA-C	-5.20	103.04	111.14
1	A	341	LYS	O-C-N	5.20	127.63	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASP	CB-CA-C	5.19	118.94	110.17
1	A	27	ILE	CA-CB-CG2	-5.18	101.69	110.50
1	A	332	SER	N-CA-C	5.17	119.30	113.15
1	A	290	TYR	N-CA-C	5.17	116.52	109.18
1	A	113	GLU	N-CA-C	5.17	117.11	109.62
1	A	141	GLU	CB-CA-C	5.16	119.36	110.79
1	A	317	PHE	CB-CA-C	-5.16	102.83	110.67
1	A	9	LYS	N-CA-C	5.16	121.21	109.81
1	A	220	SER	CB-CA-C	-5.16	99.73	110.40
1	A	214	HIS	CA-CB-CG	5.15	118.95	113.80
1	A	137	LEU	N-CA-C	5.15	116.89	111.28
1	A	28	LEU	CB-CA-C	-5.15	102.25	110.79
1	A	32	LYS	CA-C-N	-5.14	113.39	120.28
1	A	32	LYS	C-N-CA	-5.14	113.39	120.28
1	A	132	LEU	CA-C-N	-5.14	113.41	120.46
1	A	132	LEU	C-N-CA	-5.14	113.41	120.46
1	A	157	HIS	CA-C-N	-5.14	117.13	122.89
1	A	157	HIS	C-N-CA	-5.14	117.13	122.89
1	A	223	VAL	CA-CB-CG1	5.14	119.14	110.40
1	A	105	HIS	CA-C-O	-5.14	115.08	120.63
1	A	72	ILE	N-CA-C	5.13	119.58	112.35
1	A	258	HIS	CG-CD2-NE2	-5.12	102.08	107.20
1	A	148	VAL	N-CA-C	5.12	115.40	107.78
1	A	173	ARG	N-CA-CB	5.12	117.52	109.69
1	A	29	TYR	N-CA-CB	5.11	117.64	110.12
1	A	256	ASN	CA-C-N	-5.11	113.03	120.75
1	A	256	ASN	C-N-CA	-5.11	113.03	120.75
1	A	66	ASP	CA-C-O	5.11	125.97	120.55
1	A	109	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	166	VAL	N-CA-CB	5.09	119.36	110.65
1	A	212	THR	CA-C-N	-5.07	115.39	122.75
1	A	212	THR	C-N-CA	-5.07	115.39	122.75
1	A	307	ASP	CA-C-N	-5.06	112.27	120.72
1	A	307	ASP	C-N-CA	-5.06	112.27	120.72
1	A	92	LYS	CB-CA-C	-5.04	99.69	110.32
1	A	45	GLU	CA-CB-CG	5.03	124.16	114.10
1	A	139	GLU	CA-CB-CG	-5.03	104.04	114.10
1	A	204	ALA	N-CA-CB	5.03	117.44	109.94
1	A	92	LYS	CA-C-N	-5.02	113.29	122.38
1	A	92	LYS	C-N-CA	-5.02	113.29	122.38
1	A	119	GLN	CG-CD-OE1	5.02	130.85	120.80
1	A	222	ASN	CA-C-N	-5.02	112.30	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ASN	C-N-CA	-5.02	112.30	120.64
1	A	241	HIS	N-CA-CB	5.02	118.85	110.32
1	A	51	GLY	CA-C-N	-5.02	113.61	122.74
1	A	51	GLY	C-N-CA	-5.02	113.61	122.74
1	A	104	PRO	CA-C-N	-5.01	113.52	120.38
1	A	104	PRO	C-N-CA	-5.01	113.52	120.38
1	A	212	THR	N-CA-CB	5.01	120.84	111.53
1	A	194	PHE	CA-C-O	5.00	123.91	119.71

There are no chirality outliers.

All (23) 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	19	ASP	Peptide
1	A	201	TYR	Sidechain
1	A	208	GLY	Peptide
1	A	211	ARG	Sidechain
1	A	214	HIS	Sidechain
1	A	240	TYR	Sidechain
1	A	249	TYR	Sidechain
1	A	259	PHE	Sidechain
1	A	264	TRP	Peptide
1	A	275	ASP	Peptide
1	A	29	TYR	Sidechain
1	A	317	PHE	Sidechain
1	A	328	ASN	Mainchain
1	A	34	ARG	Sidechain
1	A	348	TYR	Sidechain
1	A	351	TYR	Sidechain
1	A	45	GLU	Peptide
1	A	55	PRO	Peptide
1	A	67	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	253	0
2	A	1	0	0	0	0
3	A	25	0	15	6	0
4	A	458	0	0	88	0
All	All	3272	0	2758	254	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 46.

All (254) 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:36:ILE:HD12	1:A:37:ALA:HA	1.38	1.02
1:A:278:HIS:HD2	1:A:280:VAL:H	1.15	0.94
1:A:337:GLU:HA	4:A:1395:HOH:O	1.67	0.94
1:A:310:MET:HE2	1:A:315:MET:HE3	1.52	0.90
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.59	0.85
1:A:330:ALA:HB3	4:A:1072:HOH:O	1.77	0.84
1:A:105:HIS:HA	4:A:1301:HOH:O	1.76	0.83
1:A:68:TYR:OH	1:A:299:ILE:HD11	1.78	0.82
1:A:151:ILE:HG12	1:A:179:ALA:HB3	1.63	0.81
1:A:182:LEU:HD23	4:A:1421:HOH:O	1.79	0.81
1:A:52:MET:HE2	1:A:268:LEU:HB3	1.62	0.80
1:A:164:GLU:HB3	4:A:1432:HOH:O	1.82	0.79
1:A:269:THR:HG22	3:A:1001:FR0:C9	2.13	0.78
1:A:76:ARG:HH11	1:A:76:ARG:HB2	1.47	0.78
1:A:331:LYS:HG3	1:A:344:LEU:HD21	1.66	0.78
1:A:258:HIS:HA	1:A:289:ASN:O	1.84	0.77
1:A:298:LEU:HD22	4:A:1414:HOH:O	1.83	0.77
1:A:236:LEU:HD23	4:A:1367:HOH:O	1.86	0.76
1:A:125:THR:HG23	1:A:128:GLU:HB2	1.68	0.75
1:A:110:SER:O	1:A:112:VAL:HG12	1.87	0.74
1:A:174:GLU:O	1:A:176:THR:HA	1.87	0.74
1:A:27:ILE:HG21	4:A:1062:HOH:O	1.87	0.73
1:A:106:LEU:HB3	1:A:117:TRP:HZ2	1.52	0.73
1:A:301:LYS:HE3	4:A:1194:HOH:O	1.88	0.73
1:A:102:TYR:CZ	1:A:133:VAL:HG21	2.23	0.72
1:A:347:LEU:HD13	4:A:1307:HOH:O	1.90	0.72
1:A:116:PRO:HD2	4:A:1359:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:O	1:A:345:ASP:HB3	1.90	0.71
1:A:278:HIS:CD2	1:A:280:VAL:H	2.04	0.71
1:A:266:SER:OG	1:A:278:HIS:HE1	1.75	0.70
1:A:14:LEU:HD12	4:A:1416:HOH:O	1.91	0.69
1:A:174:GLU:HA	4:A:1327:HOH:O	1.92	0.69
1:A:87:VAL:HG21	1:A:140:GLY:HA3	1.73	0.69
1:A:89:MET:SD	4:A:1289:HOH:O	2.50	0.69
1:A:97:TYR:CE1	4:A:1408:HOH:O	2.47	0.68
1:A:100:VAL:HG23	4:A:1211:HOH:O	1.94	0.67
1:A:308:TYR:CD2	1:A:322:PHE:CD2	2.82	0.67
1:A:183:ALA:HB3	4:A:1335:HOH:O	1.93	0.66
1:A:171:LYS:HD3	1:A:172:TYR:CZ	2.29	0.66
1:A:188:ILE:HB	4:A:1396:HOH:O	1.95	0.66
1:A:30:TYR:O	1:A:34:ARG:HB2	1.96	0.66
1:A:16:VAL:HG13	4:A:1211:HOH:O	1.95	0.66
1:A:58:LEU:HG	4:A:1036:HOH:O	1.96	0.65
1:A:22:ILE:HB	4:A:1414:HOH:O	1.97	0.65
1:A:212:THR:HA	1:A:233:THR:HG22	1.79	0.64
1:A:277:GLU:HA	4:A:1118:HOH:O	1.97	0.64
1:A:129:VAL:O	1:A:133:VAL:HG23	1.97	0.64
1:A:125:THR:O	1:A:129:VAL:HG23	1.97	0.64
1:A:133:VAL:HG22	4:A:1013:HOH:O	1.98	0.64
1:A:275:ASP:OD1	1:A:276:THR:HB	1.97	0.64
1:A:178:VAL:HG21	4:A:1244:HOH:O	1.97	0.63
1:A:323:LYS:HB3	1:A:351:TYR:CD1	2.33	0.63
1:A:67:TYR:HB2	4:A:1278:HOH:O	1.97	0.63
1:A:308:TYR:CD2	1:A:322:PHE:CE2	2.86	0.63
1:A:34:ARG:HB3	1:A:36:ILE:HG23	1.79	0.63
1:A:298:LEU:HB3	1:A:299:ILE:HG13	1.80	0.62
1:A:346:LEU:HB2	4:A:1179:HOH:O	1.99	0.62
1:A:238:HIS:HB3	1:A:240:TYR:CZ	2.33	0.62
1:A:50:ILE:HD12	1:A:298:LEU:HD21	1.83	0.61
1:A:134:ASN:O	1:A:138:GLN:HG3	2.02	0.59
1:A:327:ILE:HD13	1:A:347:LEU:HD23	1.85	0.59
1:A:161:TRP:HH2	4:A:1089:HOH:O	1.84	0.59
1:A:147:LYS:HE3	4:A:1333:HOH:O	2.03	0.59
1:A:228:VAL:HG22	4:A:1231:HOH:O	2.03	0.59
1:A:210:HIS:HB2	4:A:1441:HOH:O	2.01	0.58
1:A:174:GLU:C	1:A:176:THR:HA	2.29	0.57
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.40	0.57
1:A:115:ILE:HA	4:A:1359:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD13	1:A:124:LEU:HD11	1.87	0.56
1:A:235:ARG:HD3	1:A:332:SER:O	2.05	0.56
1:A:61:PHE:CE1	3:A:1001:FR0:H9	2.40	0.56
1:A:86:PHE:CE2	1:A:90:LYS:HE3	2.40	0.56
1:A:87:VAL:HB	4:A:1249:HOH:O	2.04	0.56
1:A:188:ILE:HD12	4:A:1396:HOH:O	2.06	0.56
1:A:76:ARG:HB2	1:A:76:ARG:NH1	2.17	0.56
1:A:106:LEU:HB3	1:A:117:TRP:CZ2	2.37	0.56
1:A:109:ASN:HB2	4:A:1106:HOH:O	2.04	0.56
1:A:156:ARG:HD3	1:A:191:SER:OG	2.05	0.56
1:A:137:LEU:HG	1:A:148:VAL:HG11	1.88	0.56
1:A:254:GLN:HB3	4:A:1066:HOH:O	2.06	0.55
1:A:271:ALA:HA	4:A:1027:HOH:O	2.06	0.55
1:A:310:MET:HE2	1:A:315:MET:CE	2.30	0.55
1:A:39:PRO:HA	4:A:1439:HOH:O	2.07	0.55
1:A:124:LEU:HA	4:A:1222:HOH:O	2.06	0.55
1:A:292:LEU:HD22	4:A:1266:HOH:O	2.06	0.55
1:A:30:TYR:CD1	1:A:78:ALA:HB2	2.42	0.55
1:A:171:LYS:HD3	1:A:172:TYR:CE2	2.42	0.54
1:A:289:ASN:OD1	1:A:328:ASN:HB3	2.08	0.54
1:A:308:TYR:HD2	1:A:322:PHE:CE2	2.25	0.54
1:A:36:ILE:HG12	1:A:71:ALA:HB2	1.90	0.54
1:A:46:LEU:HA	4:A:1283:HOH:O	2.08	0.54
1:A:210:HIS:HE1	4:A:1343:HOH:O	1.90	0.54
1:A:28:LEU:O	1:A:29:TYR:C	2.45	0.53
1:A:79:ILE:HG13	1:A:107:LEU:HG	1.90	0.53
1:A:117:TRP:HD1	1:A:119:GLN:NE2	2.06	0.53
1:A:272:TRP:CD1	1:A:277:GLU:O	2.61	0.53
1:A:29:TYR:C	1:A:29:TYR:CD1	2.87	0.53
1:A:86:PHE:HD1	4:A:1025:HOH:O	1.92	0.53
1:A:48:ASN:OD1	1:A:48:ASN:N	2.41	0.53
1:A:23:LYS:O	1:A:27:ILE:HG13	2.10	0.52
1:A:98:VAL:CG1	1:A:148:VAL:HG22	2.39	0.52
1:A:49:ILE:HB	4:A:1283:HOH:O	2.08	0.52
1:A:26:THR:HG21	1:A:81:ARG:NH2	2.25	0.52
1:A:79:ILE:HG23	4:A:1013:HOH:O	2.10	0.52
1:A:272:TRP:CD1	1:A:278:HIS:HA	2.45	0.52
1:A:328:ASN:O	1:A:331:LYS:HB2	2.10	0.52
1:A:281:ILE:HD13	4:A:1041:HOH:O	2.09	0.52
1:A:222:ASN:O	1:A:226:GLU:HG3	2.10	0.52
1:A:105:HIS:CE1	4:A:1432:HOH:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:OG	1:A:278:HIS:CE1	2.60	0.52
1:A:33:ARG:HB3	4:A:1086:HOH:O	2.09	0.51
1:A:179:ALA:HB2	4:A:1441:HOH:O	2.09	0.51
1:A:107:LEU:HB2	1:A:129:VAL:HG11	1.91	0.51
1:A:284:LYS:HD2	1:A:317:PHE:HZ	1.75	0.51
1:A:156:ARG:HB3	4:A:1396:HOH:O	2.10	0.51
1:A:50:ILE:HG21	4:A:1278:HOH:O	2.10	0.50
1:A:69:MET:N	1:A:70:PRO:HD2	2.26	0.50
1:A:170:LYS:O	1:A:173:ARG:HG2	2.12	0.50
1:A:173:ARG:HD3	4:A:1068:HOH:O	2.12	0.50
1:A:14:LEU:HB2	4:A:1416:HOH:O	2.12	0.50
1:A:47:GLN:NE2	1:A:301:LYS:HG2	2.26	0.49
1:A:23:LYS:HB2	1:A:85:GLU:OE2	2.13	0.49
1:A:305:ASP:O	1:A:309:GLN:HB2	2.12	0.49
1:A:117:TRP:HD1	1:A:119:GLN:HE21	1.61	0.49
1:A:346:LEU:HD22	4:A:1153:HOH:O	2.12	0.49
1:A:311:THR:O	1:A:317:PHE:HD1	1.95	0.49
1:A:4:THR:HB	1:A:5:PRO:CD	2.43	0.49
1:A:249:TYR:HE2	4:A:1295:HOH:O	1.94	0.49
1:A:250:ASN:O	1:A:254:GLN:HG3	2.13	0.48
1:A:22:ILE:HG23	1:A:82:ILE:CG2	2.43	0.48
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.94	0.48
1:A:13:GLU:OE1	1:A:294:THR:HB	2.13	0.48
1:A:61:PHE:CZ	3:A:1001:FR0:H9	2.49	0.48
1:A:84:TYR:CZ	1:A:144:PHE:CE1	3.01	0.48
1:A:292:LEU:HD13	4:A:1418:HOH:O	2.13	0.48
1:A:282:ARG:NH1	1:A:282:ARG:HG2	2.29	0.48
1:A:117:TRP:CE3	4:A:1363:HOH:O	2.56	0.48
1:A:287:GLN:HA	4:A:1186:HOH:O	2.14	0.48
1:A:72:ILE:HD13	1:A:72:ILE:H	1.77	0.48
1:A:149:ARG:HD3	1:A:178:VAL:CG1	2.43	0.48
1:A:149:ARG:HD3	1:A:178:VAL:HG11	1.96	0.48
1:A:147:LYS:HB3	4:A:1254:HOH:O	2.13	0.48
1:A:68:TYR:HD2	4:A:1278:HOH:O	1.96	0.47
1:A:84:TYR:CZ	1:A:144:PHE:CZ	3.02	0.47
1:A:241:HIS:O	1:A:242:THR:C	2.56	0.47
1:A:250:ASN:HA	1:A:253:ARG:HD3	1.96	0.47
1:A:34:ARG:NH2	1:A:73:ALA:O	2.48	0.47
1:A:104:PRO:O	1:A:105:HIS:C	2.54	0.47
1:A:18:LEU:HD22	4:A:1082:HOH:O	2.14	0.47
1:A:101:ARG:HA	4:A:1310:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:OE1	1:A:216:GLY:N	2.41	0.47
1:A:72:ILE:HG23	1:A:72:ILE:HD12	1.62	0.47
1:A:273:LYS:HE3	4:A:1334:HOH:O	2.15	0.46
1:A:156:ARG:HA	1:A:197:HIS:CE1	2.50	0.46
1:A:185:ASP:OD2	1:A:187:THR:OG1	2.28	0.46
1:A:267:TYR:CE1	1:A:268:LEU:HD23	2.51	0.46
1:A:10:PRO:HB3	1:A:96:VAL:HG13	1.98	0.46
1:A:47:GLN:O	1:A:301:LYS:HD3	2.15	0.46
1:A:134:ASN:C	1:A:138:GLN:HG3	2.40	0.46
1:A:36:ILE:HD11	1:A:38:LEU:HD11	1.97	0.46
1:A:130:VAL:HG11	1:A:172:TYR:CD2	2.51	0.46
1:A:257:MET:HE2	4:A:1380:HOH:O	2.15	0.46
1:A:319:GLU:O	1:A:323:LYS:HG3	2.16	0.46
1:A:97:TYR:HB2	4:A:1254:HOH:O	2.16	0.45
1:A:40:ALA:HB3	1:A:46:LEU:HD13	1.98	0.45
1:A:56:LEU:HD22	1:A:60:ASP:OD1	2.16	0.45
1:A:235:ARG:HD2	1:A:258:HIS:CD2	2.52	0.45
1:A:74:GLY:C	1:A:124:LEU:HD12	2.41	0.45
1:A:159:PRO:HG3	1:A:194:PHE:CD2	2.52	0.45
1:A:263:PRO:HD2	1:A:307:ASP:OD2	2.16	0.45
1:A:24:PRO:O	1:A:25:GLU:C	2.57	0.45
1:A:163:SER:HB3	4:A:1209:HOH:O	2.16	0.45
1:A:309:GLN:HB3	4:A:1122:HOH:O	2.17	0.45
1:A:9:LYS:H	1:A:9:LYS:HG2	1.44	0.45
1:A:68:TYR:OH	1:A:299:ILE:CD1	2.59	0.45
1:A:280:VAL:HG22	4:A:1370:HOH:O	2.17	0.45
1:A:30:TYR:CE1	1:A:78:ALA:HB2	2.52	0.44
1:A:39:PRO:O	1:A:40:ALA:HB2	2.17	0.44
1:A:156:ARG:CB	4:A:1396:HOH:O	2.65	0.44
1:A:282:ARG:HD2	1:A:286:ASP:OD1	2.17	0.44
1:A:68:TYR:CE1	1:A:69:MET:SD	3.10	0.44
1:A:116:PRO:HB2	1:A:117:TRP:CE2	2.53	0.44
1:A:308:TYR:HD2	1:A:322:PHE:CD2	2.30	0.44
1:A:27:ILE:HA	4:A:1133:HOH:O	2.17	0.44
1:A:183:ALA:HB2	1:A:214:HIS:CE1	2.52	0.44
1:A:281:ILE:O	1:A:281:ILE:HD12	2.18	0.44
1:A:32:LYS:HE3	4:A:1356:HOH:O	2.18	0.44
1:A:28:LEU:HD22	1:A:46:LEU:HD21	1.99	0.43
1:A:188:ILE:HA	4:A:1393:HOH:O	2.17	0.43
1:A:84:TYR:OH	1:A:144:PHE:CZ	2.68	0.43
1:A:157:HIS:C	1:A:157:HIS:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:NE1	1:A:277:GLU:O	2.51	0.43
1:A:61:PHE:CD1	3:A:1001:FR0:C9	3.01	0.43
1:A:137:LEU:HG	1:A:148:VAL:CG1	2.47	0.43
1:A:320:GLU:H	1:A:320:GLU:HG3	1.48	0.43
1:A:4:THR:HB	1:A:5:PRO:HD3	2.00	0.43
1:A:62:LEU:HB3	4:A:1375:HOH:O	2.19	0.43
1:A:75:CYS:O	1:A:76:ARG:C	2.61	0.43
1:A:121:GLU:HB3	1:A:122:GLY:H	1.61	0.43
1:A:150:SER:HB2	4:A:1310:HOH:O	2.18	0.43
1:A:187:THR:O	1:A:188:ILE:C	2.57	0.43
1:A:273:LYS:HA	1:A:274:PRO:HD2	1.76	0.43
1:A:317:PHE:N	1:A:317:PHE:CD1	2.86	0.43
1:A:325:LEU:C	1:A:325:LEU:CD2	2.92	0.43
1:A:17:HIS:O	1:A:18:LEU:C	2.61	0.43
1:A:112:VAL:HG13	4:A:1359:HOH:O	2.18	0.43
1:A:264:TRP:HA	4:A:1145:HOH:O	2.18	0.43
1:A:16:VAL:CG1	4:A:1211:HOH:O	2.60	0.43
1:A:27:ILE:HG12	4:A:1133:HOH:O	2.19	0.43
1:A:69:MET:HB3	4:A:1455:HOH:O	2.18	0.43
1:A:219:GLY:O	1:A:241:HIS:ND1	2.51	0.43
1:A:272:TRP:NE1	1:A:278:HIS:HA	2.33	0.43
1:A:212:THR:HA	1:A:233:THR:CG2	2.48	0.43
1:A:284:LYS:HD2	1:A:317:PHE:CZ	2.54	0.43
1:A:285:ASN:HB2	4:A:1059:HOH:O	2.19	0.43
1:A:296:ASP:HB2	1:A:300:PHE:CE2	2.54	0.43
1:A:106:LEU:HD21	4:A:1089:HOH:O	2.18	0.42
1:A:74:GLY:HA2	1:A:109:ASN:HB3	2.01	0.42
1:A:103:SER:O	1:A:104:PRO:C	2.61	0.42
1:A:210:HIS:CE1	4:A:1343:HOH:O	2.68	0.42
1:A:32:LYS:HE2	1:A:32:LYS:O	2.19	0.42
1:A:61:PHE:CG	3:A:1001:FR0:C9	3.03	0.42
1:A:84:TYR:O	1:A:85:GLU:C	2.60	0.42
1:A:97:TYR:HE1	4:A:1408:HOH:O	1.96	0.42
1:A:178:VAL:C	4:A:1441:HOH:O	2.62	0.42
1:A:115:ILE:HA	1:A:116:PRO:HD2	1.87	0.42
1:A:125:THR:HA	1:A:126:PRO:HD3	1.86	0.42
1:A:325:LEU:HB2	4:A:1329:HOH:O	2.19	0.42
1:A:42:THR:HA	1:A:43:PRO:HD2	1.75	0.42
1:A:23:LYS:HB3	1:A:25:GLU:HG2	2.01	0.41
1:A:92:LYS:HZ3	1:A:92:LYS:HG3	1.72	0.41
1:A:116:PRO:HB2	1:A:117:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:O	1:A:137:LEU:HB2	2.21	0.41
1:A:313:LYS:C	4:A:1200:HOH:O	2.63	0.41
1:A:42:THR:C	1:A:44:GLU:H	2.27	0.41
1:A:95:VAL:O	1:A:146:VAL:HG13	2.20	0.41
1:A:188:ILE:H	1:A:188:ILE:HG13	1.58	0.41
1:A:23:LYS:HD3	1:A:85:GLU:OE2	2.20	0.41
1:A:80:LYS:O	1:A:81:ARG:C	2.62	0.41
1:A:298:LEU:CB	1:A:299:ILE:HG13	2.49	0.41
3:A:1001:FR0:S22	4:A:1386:HOH:O	2.62	0.41
1:A:36:ILE:H	1:A:36:ILE:HG13	1.39	0.41
1:A:116:PRO:HB2	1:A:117:TRP:CD2	2.56	0.41
1:A:335:LEU:HA	1:A:336:PRO:HD2	1.83	0.41
1:A:72:ILE:HB	1:A:78:ALA:HB1	2.03	0.41
1:A:123:ASP:O	1:A:125:THR:HG22	2.20	0.41
1:A:148:VAL:CA	4:A:1408:HOH:O	2.68	0.41
1:A:264:TRP:HE1	1:A:300:PHE:HB3	1.86	0.41
1:A:327:ILE:HA	4:A:1072:HOH:O	2.21	0.40
1:A:36:ILE:HD11	1:A:38:LEU:CD1	2.51	0.40
1:A:323:LYS:HB3	1:A:351:TYR:CE1	2.56	0.40
1:A:36:ILE:HG12	1:A:71:ALA:CB	2.52	0.40
1:A:130:VAL:CG1	1:A:172:TYR:CD2	3.05	0.40
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.77	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%)	289 (83%)	40 (12%)	18 (5%)	1 1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	56	LEU
1	A	121	GLU
1	A	135	GLN
1	A	289	ASN
1	A	322	PHE
1	A	24	PRO
1	A	242	THR
1	A	274	PRO
1	A	43	PRO
1	A	55	PRO
1	A	190	GLY
1	A	295	ASP
1	A	39	PRO
1	A	318	THR
1	A	321	GLU
1	A	112	VAL
1	A	188	ILE

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%)	241 (79%)	63 (21%)	1 1

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASP
1	A	16	VAL
1	A	23	LYS
1	A	25	GLU
1	A	32	LYS
1	A	34	ARG
1	A	41	ASP
1	A	46	LEU

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Mol	Chain	Res	Type
1	A	48	ASN
1	A	52	MET
1	A	53	ASP
1	A	54	LYS
1	A	57	THR
1	A	72	ILE
1	A	76	ARG
1	A	81	ARG
1	A	92	LYS
1	A	107	LEU
1	A	109	ASN
1	A	112	VAL
1	A	113	GLU
1	A	115	ILE
1	A	123	ASP
1	A	124	LEU
1	A	125	THR
1	A	133	VAL
1	A	148	VAL
1	A	149	ARG
1	A	160	SER
1	A	166	VAL
1	A	168	LEU
1	A	173	ARG
1	A	174	GLU
1	A	177	VAL
1	A	178	VAL
1	A	180	ILE
1	A	193	LEU
1	A	199	GLN
1	A	209	VAL
1	A	211	ARG
1	A	223	VAL
1	A	233	THR
1	A	234	GLU
1	A	253	ARG
1	A	265	SER
1	A	274	PRO
1	A	281	ILE
1	A	284	LYS
1	A	285	ASN
1	A	286	ASP

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Mol	Chain	Res	Type
1	A	292	LEU
1	A	294	THR
1	A	304	LEU
1	A	308	TYR
1	A	310	MET
1	A	318	THR
1	A	320	GLU
1	A	321	GLU
1	A	325	LEU
1	A	335	LEU
1	A	337	GLU
1	A	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	134	ASN
1	A	138	GLN
1	A	157	HIS
1	A	197	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	FR0	A	1001	-	28,28,28	2.62	9 (32%)	37,39,39	4.98	15 (40%)

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	FR0	A	1001	-	-	7/13/13/13	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR0	C19-C16	-6.98	1.36	1.45
3	A	1001	FR0	C5-N10	6.74	1.48	1.34
3	A	1001	FR0	C19-N20	5.32	1.50	1.38
3	A	1001	FR0	C21-N20	4.05	1.36	1.31
3	A	1001	FR0	C16-S15	3.52	1.81	1.73
3	A	1001	FR0	C5-N4	-2.59	1.31	1.35
3	A	1001	FR0	C3-C2	2.14	1.43	1.40
3	A	1001	FR0	C8-C7	2.11	1.42	1.38
3	A	1001	FR0	C27-N26	2.08	1.36	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR0	C21-N20-C19	19.70	121.07	110.56
3	A	1001	FR0	C23-C19-C16	10.64	154.03	126.71
3	A	1001	FR0	C23-C19-N20	-10.11	101.52	115.43
3	A	1001	FR0	S22-C21-N20	-9.63	104.76	114.49
3	A	1001	FR0	C19-C23-S22	8.25	119.78	110.24
3	A	1001	FR0	C17-C16-C19	-5.91	117.36	128.41
3	A	1001	FR0	C19-C16-S15	5.69	132.40	119.42
3	A	1001	FR0	C23-S22-C21	5.09	92.17	89.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR0	C2-N1-C5	3.17	107.93	104.21
3	A	1001	FR0	C3-C2-N1	-2.62	105.83	109.42
3	A	1001	FR0	C12-C11-N10	-2.58	106.97	112.30
3	A	1001	FR0	S22-C21-N26	2.51	123.14	117.76
3	A	1001	FR0	C11-C12-S15	2.50	126.31	120.70
3	A	1001	FR0	C11-C12-C18	-2.46	120.27	127.56
3	A	1001	FR0	C6-C2-N1	2.01	133.91	128.21

There are no chirality outliers.

All (7) torsion outliers are listed below:

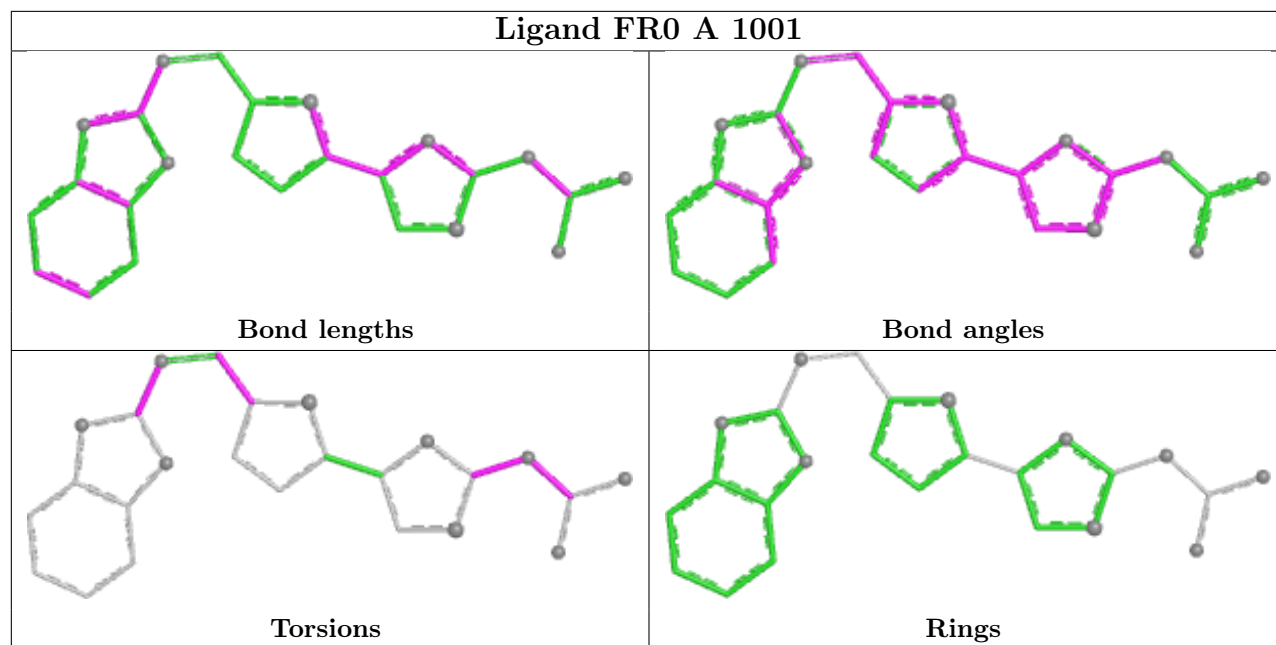
Mol	Chain	Res	Type	Atoms
3	A	1001	FR0	N28-C27-N26-C21
3	A	1001	FR0	N29-C27-N26-C21
3	A	1001	FR0	N10-C11-C12-S15
3	A	1001	FR0	N10-C11-C12-C18
3	A	1001	FR0	S22-C21-N26-C27
3	A	1001	FR0	N1-C5-N10-C11
3	A	1001	FR0	N20-C21-N26-C27

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR0	6	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.