



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:03 AM UTC

PDB ID : 1O5R / pdb_00001o5r
Title : Crystal structure of adenosine deaminase complexed with a potent inhibitor
Authors : Kinoshita, T.
Deposited on : 2003-10-05
Resolution : 2.35 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

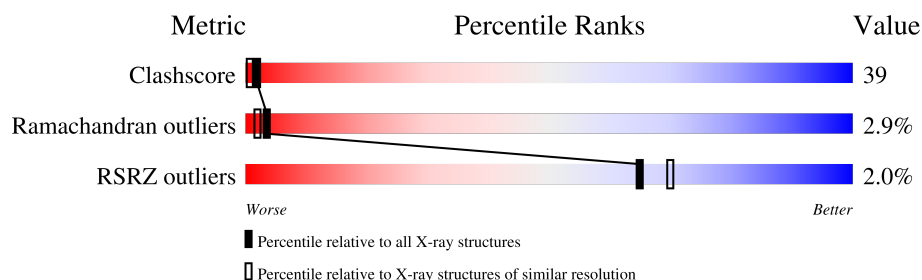
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

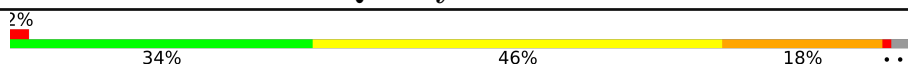
The reported resolution of this entry is 2.35 Å.

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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3049 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
			2789	1772	471	534	12			

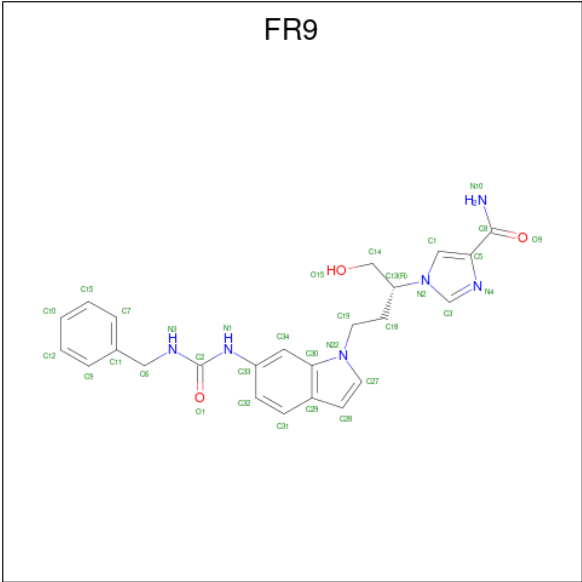
There are 15 discrepancies between the modelled and reference sequences:

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)-3-(6-[(BENZYLAMINO)CARBONYLAMINO]-1H-INDOL-1-YL)-1-(HYDROXYMETHYL)PROPYL]-1H-IMIDAZOLE-4-CARBOXAMIDE (CCD ID: FR9) (formula: C₂₄H₂₆N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	24	6	3		

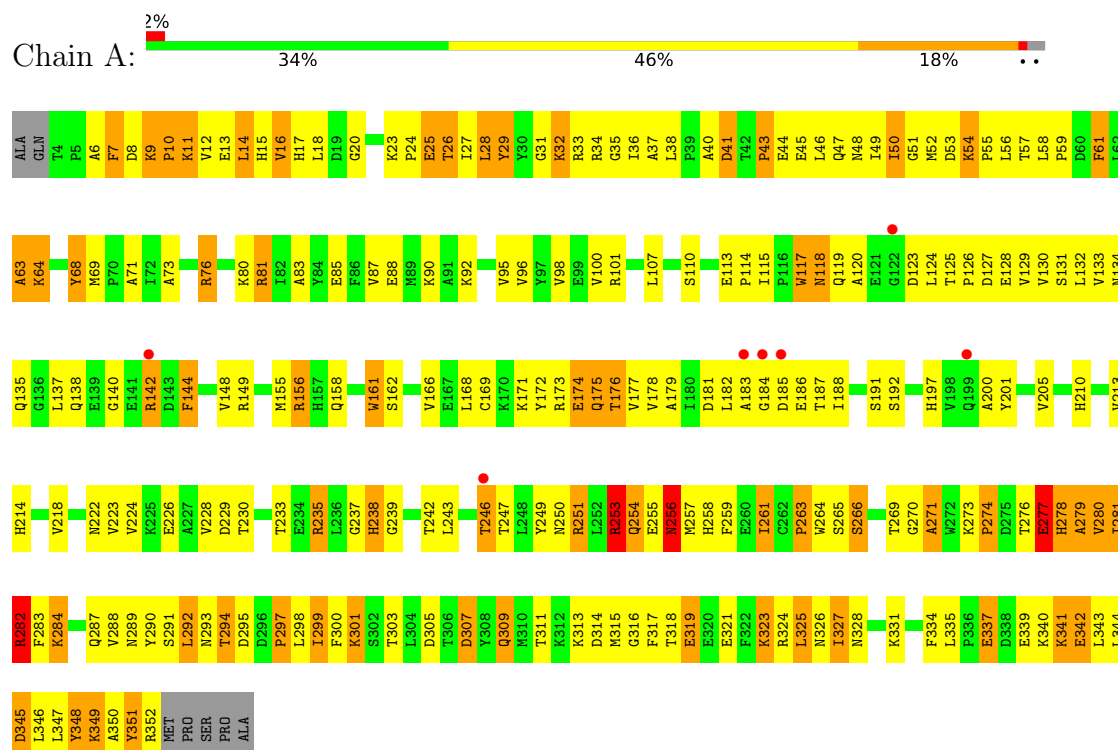
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	226	Total	O	0	0
			226	226		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Adenosine deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.44Å 78.44Å 137.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.35 12.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.35) 98.4 (12.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.05Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.228 , 0.242 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 101.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3049	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FR9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.68	51/2853 (1.8%)	2.20	145/3867 (3.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	GLU	C-N	-17.29	1.09	1.33
1	A	161	TRP	NE1-CE2	10.46	1.49	1.37
1	A	292	LEU	C-O	-10.35	1.11	1.24
1	A	117	TRP	NE1-CE2	10.21	1.48	1.37
1	A	287	GLN	C-N	-10.01	1.22	1.33
1	A	12	VAL	C-O	-8.68	1.14	1.24
1	A	287	GLN	CA-C	-8.43	1.41	1.53
1	A	327	ILE	C-N	-8.36	1.23	1.33
1	A	14	LEU	C-N	-8.24	1.23	1.33
1	A	278	HIS	CE1-NE2	7.98	1.40	1.32
1	A	8	ASP	CA-C	-7.91	1.44	1.53
1	A	11	LYS	CA-C	-7.88	1.43	1.52
1	A	299	ILE	CB-CG1	-7.82	1.37	1.53
1	A	297	PRO	CA-C	7.47	1.63	1.52
1	A	287	GLN	C-O	-7.02	1.13	1.23
1	A	253	ARG	NE-CZ	6.76	1.40	1.33
1	A	279	ALA	C-N	6.72	1.42	1.34
1	A	287	GLN	CA-CB	-6.60	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ALA	CA-C	6.47	1.61	1.52
1	A	17	HIS	ND1-CE1	6.30	1.38	1.32
1	A	9	LYS	C-O	-6.29	1.18	1.24
1	A	7	PHE	CA-C	-6.27	1.45	1.52
1	A	297	PRO	C-N	6.19	1.41	1.33
1	A	292	LEU	CA-CB	-6.07	1.44	1.53
1	A	351	TYR	C-O	-6.06	1.16	1.24
1	A	50	ILE	C-O	-6.04	1.17	1.24
1	A	265	SER	N-CA	-6.00	1.39	1.46
1	A	15	HIS	CA-C	5.89	1.61	1.53
1	A	26	THR	CB-OG1	-5.89	1.34	1.43
1	A	327	ILE	CA-C	5.85	1.61	1.52
1	A	20	GLY	N-CA	5.84	1.53	1.45
1	A	299	ILE	C-N	-5.79	1.26	1.33
1	A	259	PHE	CA-C	5.76	1.59	1.52
1	A	249	TYR	N-CA	-5.70	1.39	1.46
1	A	247	THR	CA-CB	5.63	1.62	1.53
1	A	277	GLU	CA-CB	5.56	1.62	1.53
1	A	247	THR	CB-OG1	-5.51	1.34	1.43
1	A	300	PHE	N-CA	5.47	1.52	1.46
1	A	12	VAL	CA-C	-5.40	1.46	1.52
1	A	28	LEU	CA-CB	-5.35	1.45	1.53
1	A	277	GLU	CA-C	-5.30	1.45	1.52
1	A	289	ASN	CA-CB	-5.27	1.46	1.53
1	A	303	THR	CA-CB	5.21	1.63	1.53
1	A	29	TYR	C-N	5.20	1.41	1.33
1	A	257	MET	CG-SD	-5.17	1.67	1.80
1	A	300	PHE	CA-C	5.16	1.60	1.52
1	A	350	ALA	CA-CB	-5.14	1.44	1.53
1	A	6	ALA	C-O	-5.11	1.17	1.24
1	A	263	PRO	CA-CB	-5.07	1.45	1.53
1	A	263	PRO	CA-C	-5.04	1.45	1.52
1	A	12	VAL	CA-CB	-5.01	1.48	1.54

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	HIS	CA-CB-CG	13.23	127.03	113.80
1	A	277	GLU	CB-CG-CD	11.50	132.16	112.60
1	A	307	ASP	CA-CB-CG	11.21	123.81	112.60
1	A	282	ARG	CD-NE-CZ	-11.20	108.72	124.40
1	A	295	ASP	CA-CB-CG	11.18	123.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ASP	N-CA-C	10.43	126.21	113.38
1	A	29	TYR	N-CA-C	10.11	123.25	111.11
1	A	253	ARG	CA-C-O	10.06	131.66	120.90
1	A	53	ASP	CA-CB-CG	9.66	122.26	112.60
1	A	246	THR	O-C-N	-9.30	110.30	122.39
1	A	282	ARG	CA-CB-CG	-9.14	95.83	114.10
1	A	253	ARG	CB-CG-CD	9.07	132.15	111.30
1	A	251	ARG	CD-NE-CZ	-9.02	111.78	124.40
1	A	73	ALA	CA-C-N	-9.00	103.77	121.41
1	A	73	ALA	C-N-CA	-9.00	103.77	121.41
1	A	261	ILE	CA-C-N	-8.58	111.23	122.98
1	A	261	ILE	C-N-CA	-8.58	111.23	122.98
1	A	349	LYS	CG-CD-CE	8.48	130.80	111.30
1	A	339	GLU	CA-C-O	8.37	129.59	119.97
1	A	41	ASP	CA-C-O	8.08	127.79	118.90
1	A	44	GLU	CA-C-N	-8.04	108.00	121.92
1	A	44	GLU	C-N-CA	-8.04	108.00	121.92
1	A	254	GLN	CB-CG-CD	-7.99	99.02	112.60
1	A	277	GLU	CA-C-N	-7.96	108.47	122.07
1	A	277	GLU	C-N-CA	-7.96	108.47	122.07
1	A	280	VAL	N-CA-C	7.88	120.91	111.05
1	A	345	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	271	ALA	N-CA-C	7.75	120.71	111.33
1	A	8	ASP	CB-CA-C	-7.71	101.01	111.88
1	A	337	GLU	O-C-N	-7.66	113.47	122.20
1	A	281	ILE	CA-C-O	7.65	128.91	120.95
1	A	253	ARG	O-C-N	-7.57	114.22	122.09
1	A	49	ILE	CA-C-O	7.55	125.54	118.90
1	A	324	ARG	CD-NE-CZ	-7.53	113.86	124.40
1	A	327	ILE	N-CA-C	7.52	120.49	111.09
1	A	28	LEU	N-CA-C	7.51	120.12	111.11
1	A	271	ALA	CA-C-O	7.51	128.74	120.63
1	A	294	THR	CA-C-O	7.44	127.65	119.24
1	A	298	LEU	N-CA-C	7.42	119.06	110.97
1	A	294	THR	N-CA-CB	-7.33	100.84	110.59
1	A	276	THR	CA-C-O	-7.32	112.79	120.99
1	A	68	TYR	CG-CD2-CE2	-7.21	110.38	121.20
1	A	15	HIS	CB-CA-C	-7.21	100.81	111.77
1	A	32	LYS	CA-C-N	-7.01	108.15	121.54
1	A	32	LYS	C-N-CA	-7.01	108.15	121.54
1	A	282	ARG	CA-C-N	-7.00	110.21	120.28
1	A	282	ARG	C-N-CA	-7.00	110.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ASN	N-CA-C	6.95	125.60	110.80
1	A	284	LYS	N-CA-C	6.86	118.41	111.07
1	A	318	THR	CA-C-N	-6.86	108.60	122.31
1	A	318	THR	C-N-CA	-6.86	108.60	122.31
1	A	284	LYS	CA-C-O	6.85	128.01	120.82
1	A	311	THR	N-CA-C	6.84	118.82	111.36
1	A	351	TYR	CA-C-N	-6.78	109.51	121.70
1	A	351	TYR	C-N-CA	-6.78	109.51	121.70
1	A	299	ILE	CA-C-N	-6.77	111.83	122.73
1	A	299	ILE	C-N-CA	-6.77	111.83	122.73
1	A	36	ILE	N-CA-C	6.77	121.91	112.50
1	A	11	LYS	CB-CG-CD	6.74	126.81	111.30
1	A	269	THR	CA-C-N	-6.69	112.31	122.28
1	A	269	THR	C-N-CA	-6.69	112.31	122.28
1	A	326	ASN	CA-CB-CG	-6.68	105.92	112.60
1	A	254	GLN	N-CA-C	6.67	121.64	112.90
1	A	279	ALA	N-CA-CB	-6.67	99.21	110.49
1	A	61	PHE	N-CA-C	6.60	118.56	111.36
1	A	63	ALA	CA-C-O	6.57	127.53	119.97
1	A	341	LYS	N-CA-C	6.51	119.69	111.69
1	A	249	TYR	N-CA-C	6.47	118.92	111.02
1	A	350	ALA	N-CA-C	6.46	119.14	111.71
1	A	274	PRO	CA-C-N	-6.40	112.32	122.95
1	A	274	PRO	C-N-CA	-6.40	112.32	122.95
1	A	300	PHE	N-CA-C	6.40	120.01	112.72
1	A	9	LYS	CA-C-N	-6.39	113.70	120.03
1	A	9	LYS	C-N-CA	-6.39	113.70	120.03
1	A	28	LEU	CA-C-O	6.29	127.64	120.90
1	A	282	ARG	N-CA-C	6.24	118.09	111.28
1	A	251	ARG	CB-CG-CD	6.24	125.65	111.30
1	A	68	TYR	N-CA-C	6.21	120.99	113.41
1	A	34	ARG	CA-C-N	-6.17	112.82	122.51
1	A	34	ARG	C-N-CA	-6.17	112.82	122.51
1	A	342	GLU	O-C-N	-6.12	115.06	122.22
1	A	15	HIS	N-CA-CB	6.11	122.13	110.82
1	A	346	LEU	CA-C-O	6.03	127.67	120.92
1	A	6	ALA	O-C-N	6.01	129.25	122.22
1	A	316	GLY	CA-C-N	-6.00	112.55	120.95
1	A	316	GLY	C-N-CA	-6.00	112.55	120.95
1	A	31	GLY	O-C-N	6.00	127.94	122.18
1	A	345	ASP	N-CA-C	5.99	118.32	111.02
1	A	342	GLU	CB-CG-CD	5.99	122.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASP	N-CA-C	5.98	120.57	113.16
1	A	18	LEU	N-CA-C	5.96	118.27	111.11
1	A	7	PHE	N-CA-CB	-5.96	101.78	110.84
1	A	25	GLU	N-CA-C	5.95	123.47	110.80
1	A	264	TRP	N-CA-C	5.95	117.76	111.28
1	A	348	TYR	CA-C-N	-5.89	111.35	120.31
1	A	348	TYR	C-N-CA	-5.89	111.35	120.31
1	A	250	ASN	CA-C-O	5.86	126.58	119.49
1	A	293	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	49	ILE	CB-CA-C	-5.78	104.58	110.88
1	A	294	THR	CA-CB-CG2	5.75	120.28	110.50
1	A	291	SER	N-CA-C	5.72	118.11	109.41
1	A	313	LYS	CA-C-N	-5.69	112.08	122.38
1	A	313	LYS	C-N-CA	-5.69	112.08	122.38
1	A	40	ALA	CA-C-O	-5.69	114.84	121.10
1	A	235	ARG	CD-NE-CZ	-5.69	116.44	124.40
1	A	297	PRO	N-CA-C	5.68	121.42	113.53
1	A	257	MET	CA-CB-CG	-5.62	102.85	114.10
1	A	261	ILE	CB-CA-C	-5.62	102.96	111.33
1	A	73	ALA	N-CA-C	5.57	118.35	110.50
1	A	26	THR	CA-CB-CG2	5.55	119.94	110.50
1	A	325	LEU	CB-CA-C	5.52	121.53	109.99
1	A	16	VAL	CA-C-N	-5.49	115.47	122.77
1	A	16	VAL	C-N-CA	-5.49	115.47	122.77
1	A	266	SER	N-CA-C	5.48	119.23	112.54
1	A	309	GLN	N-CA-C	5.48	116.93	111.07
1	A	68	TYR	CD1-CG-CD2	5.47	126.30	118.10
1	A	33	ARG	N-CA-C	5.46	122.42	110.80
1	A	149	ARG	CD-NE-CZ	-5.45	116.77	124.40
1	A	17	HIS	N-CA-C	5.42	117.56	108.73
1	A	71	ALA	CB-CA-C	-5.41	101.41	110.56
1	A	10	PRO	O-C-N	5.37	129.55	123.00
1	A	142	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	A	261	ILE	N-CA-C	5.32	115.94	109.30
1	A	76	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	A	156	ARG	CD-NE-CZ	-5.23	117.08	124.40
1	A	292	LEU	O-C-N	-5.22	117.13	123.29
1	A	301	LYS	CA-C-N	-5.21	114.14	122.53
1	A	301	LYS	C-N-CA	-5.21	114.14	122.53
1	A	277	GLU	O-C-N	-5.19	115.69	122.59
1	A	257	MET	N-CA-C	5.18	118.15	110.48
1	A	64	LYS	CA-CB-CG	-5.16	103.78	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLY	CA-C-N	-5.16	112.19	120.64
1	A	35	GLY	C-N-CA	-5.16	112.19	120.64
1	A	319	GLU	CA-CB-CG	5.15	124.40	114.10
1	A	298	LEU	CB-CA-C	-5.11	103.09	110.96
1	A	343	LEU	CA-C-N	-5.09	113.46	120.28
1	A	343	LEU	C-N-CA	-5.09	113.46	120.28
1	A	323	LYS	N-CA-C	5.09	118.64	112.23
1	A	279	ALA	N-CA-C	5.07	121.59	110.80
1	A	315	MET	CA-C-O	5.07	124.86	119.34
1	A	54	LYS	N-CA-C	-5.03	100.08	108.23
1	A	7	PHE	O-C-N	-5.03	116.48	123.12
1	A	51	GLY	CA-C-N	-5.02	114.07	123.05
1	A	51	GLY	C-N-CA	-5.02	114.07	123.05
1	A	144	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	251	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	255	GLU	Peptide
1	A	282	ARG	Sidechain
1	A	352	ARG	Sidechain
1	A	81	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2789	0	2742	218	2
2	A	1	0	0	0	0
3	A	33	0	26	4	0
4	A	226	0	0	75	3
All	All	3049	0	2768	219	3

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 39.

All (219) 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:124:LEU:HA	4:A:1090:HOH:O	1.36	1.22
1:A:125:THR:HG22	4:A:1172:HOH:O	1.43	1.17
1:A:183:ALA:HB1	4:A:1010:HOH:O	1.41	1.17
1:A:175:GLN:C	1:A:176:THR:HG23	1.70	1.11
1:A:110:SER:HB3	4:A:1172:HOH:O	1.49	1.10
1:A:117:TRP:O	1:A:118:ASN:HB2	1.38	1.09
1:A:173:ARG:O	1:A:174:GLU:HB2	1.45	1.09
1:A:115:ILE:HB	4:A:1122:HOH:O	1.61	0.99
1:A:328:ASN:OD1	4:A:1199:HOH:O	1.79	0.99
1:A:117:TRP:O	1:A:118:ASN:CB	2.10	0.98
1:A:26:THR:HG23	1:A:81:ARG:HH11	1.30	0.97
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.47	0.93
1:A:134:ASN:O	1:A:138:GLN:HG3	1.68	0.93
1:A:124:LEU:HD23	4:A:1090:HOH:O	1.69	0.92
1:A:175:GLN:O	1:A:176:THR:HG23	1.72	0.90
1:A:235:ARG:HD3	1:A:334:PHE:CZ	2.07	0.89
1:A:323:LYS:HE3	4:A:1143:HOH:O	1.73	0.89
1:A:237:GLY:O	1:A:238:HIS:HB2	1.74	0.87
1:A:100:VAL:HG13	4:A:1182:HOH:O	1.74	0.86
1:A:100:VAL:CG1	4:A:1182:HOH:O	2.24	0.84
1:A:175:GLN:C	1:A:176:THR:CG2	2.44	0.84
1:A:319:GLU:HB2	4:A:1143:HOH:O	1.79	0.83
1:A:142:ARG:O	4:A:1085:HOH:O	1.96	0.82
1:A:222:ASN:O	1:A:226:GLU:HG2	1.78	0.82
1:A:294:THR:HG23	1:A:297:PRO:HD3	1.61	0.81
1:A:182:LEU:O	1:A:214:HIS:HB2	1.80	0.80
1:A:213:VAL:HB	1:A:233:THR:HG21	1.67	0.77
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.15	0.77
1:A:342:GLU:HG3	4:A:1171:HOH:O	1.84	0.76
1:A:235:ARG:NH1	1:A:334:PHE:CE2	2.54	0.76
1:A:278:HIS:HD2	1:A:280:VAL:H	1.35	0.75
1:A:218:VAL:HG13	1:A:218:VAL:O	1.87	0.75
1:A:213:VAL:CG2	1:A:233:THR:CG2	2.64	0.74
1:A:11:LYS:HG2	4:A:1075:HOH:O	1.87	0.73
1:A:278:HIS:CD2	1:A:280:VAL:H	2.06	0.73
1:A:46:LEU:HD21	4:A:1180:HOH:O	1.87	0.73
1:A:81:ARG:HD3	1:A:85:GLU:OE1	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:NH1	4:A:1090:HOH:O	2.20	0.72
1:A:128:GLU:OE1	4:A:1124:HOH:O	2.06	0.72
1:A:134:ASN:O	1:A:138:GLN:CG	2.38	0.71
1:A:174:GLU:OE2	4:A:1174:HOH:O	2.07	0.71
1:A:26:THR:HG23	1:A:81:ARG:NH1	2.04	0.70
1:A:120:ALA:CA	4:A:1068:HOH:O	2.40	0.70
1:A:277:GLU:HG2	4:A:1189:HOH:O	1.91	0.69
1:A:76:ARG:HG2	1:A:132:LEU:HD11	1.75	0.69
1:A:173:ARG:NH1	4:A:1047:HOH:O	2.26	0.69
1:A:213:VAL:CG2	1:A:233:THR:HG21	2.23	0.68
1:A:292:LEU:HD22	1:A:325:LEU:HD11	1.75	0.68
1:A:172:TYR:HB3	1:A:177:VAL:HG11	1.76	0.68
1:A:10:PRO:HB3	1:A:96:VAL:HG23	1.77	0.67
1:A:185:ASP:HB2	3:A:1001:FR9:H32	1.76	0.67
1:A:328:ASN:HA	4:A:1199:HOH:O	1.94	0.67
1:A:186:GLU:CG	1:A:186:GLU:O	2.43	0.67
1:A:123:ASP:OD1	4:A:1152:HOH:O	2.13	0.67
1:A:28:LEU:HD21	4:A:1190:HOH:O	1.94	0.66
1:A:110:SER:CB	4:A:1172:HOH:O	2.22	0.66
1:A:172:TYR:HB3	1:A:177:VAL:CG1	2.26	0.66
1:A:235:ARG:HG2	1:A:258:HIS:HB3	1.77	0.66
1:A:155:MET:SD	1:A:183:ALA:O	2.54	0.66
1:A:237:GLY:O	1:A:238:HIS:CB	2.44	0.65
1:A:68:TYR:CE2	4:A:1197:HOH:O	2.49	0.65
1:A:188:ILE:HG12	1:A:191:SER:HB3	1.78	0.65
1:A:213:VAL:CB	1:A:233:THR:HG21	2.27	0.65
1:A:52:MET:HE3	1:A:56:LEU:HB2	1.80	0.64
1:A:345:ASP:HB2	4:A:1225:HOH:O	1.97	0.64
1:A:246:THR:OG1	4:A:1215:HOH:O	2.15	0.64
1:A:277:GLU:HA	4:A:1112:HOH:O	1.96	0.64
1:A:213:VAL:HG23	1:A:233:THR:HG22	1.80	0.63
1:A:58:LEU:HB3	1:A:59:PRO:CD	2.23	0.62
1:A:27:ILE:HD13	4:A:1180:HOH:O	1.98	0.62
1:A:175:GLN:O	1:A:176:THR:CG2	2.44	0.62
1:A:29:TYR:CD1	1:A:29:TYR:C	2.79	0.60
1:A:13:GLU:OE1	1:A:16:VAL:HB	2.01	0.60
1:A:173:ARG:O	1:A:174:GLU:CB	2.30	0.60
1:A:52:MET:CE	1:A:56:LEU:HB2	2.32	0.60
1:A:235:ARG:NH1	1:A:334:PHE:CD2	2.71	0.59
1:A:182:LEU:O	1:A:183:ALA:HB2	2.02	0.59
1:A:76:ARG:CG	1:A:132:LEU:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TYR:O	1:A:205:VAL:HG23	2.03	0.58
1:A:68:TYR:CZ	4:A:1197:HOH:O	2.56	0.58
1:A:162:SER:OG	1:A:197:HIS:HD2	1.85	0.58
1:A:299:ILE:HG13	4:A:1197:HOH:O	2.04	0.58
1:A:124:LEU:CG	4:A:1090:HOH:O	2.50	0.58
1:A:28:LEU:HD23	4:A:1127:HOH:O	2.04	0.57
1:A:120:ALA:N	4:A:1068:HOH:O	2.36	0.57
1:A:239:GLY:O	1:A:242:THR:CG2	2.53	0.57
1:A:174:GLU:O	1:A:176:THR:N	2.32	0.57
1:A:239:GLY:O	1:A:242:THR:HG23	2.04	0.57
1:A:246:THR:HA	4:A:1215:HOH:O	2.04	0.57
1:A:7:PHE:CE2	4:A:1075:HOH:O	2.53	0.57
1:A:224:VAL:O	1:A:228:VAL:HG23	2.04	0.57
1:A:110:SER:C	4:A:1172:HOH:O	2.48	0.56
1:A:125:THR:CG2	4:A:1172:HOH:O	2.23	0.56
1:A:14:LEU:HB3	1:A:235:ARG:NH2	2.19	0.56
1:A:119:GLN:O	4:A:1122:HOH:O	2.18	0.56
1:A:98:VAL:HG13	1:A:148:VAL:HG13	1.88	0.56
1:A:100:VAL:HG11	4:A:1182:HOH:O	1.99	0.56
1:A:124:LEU:HD22	1:A:129:VAL:HG23	1.87	0.55
1:A:174:GLU:C	1:A:176:THR:H	2.15	0.55
1:A:243:LEU:HB3	4:A:1218:HOH:O	2.07	0.55
1:A:299:ILE:CG1	4:A:1197:HOH:O	2.55	0.55
1:A:113:GLU:HB2	4:A:1077:HOH:O	2.07	0.54
1:A:126:PRO:O	1:A:130:VAL:CG1	2.55	0.54
1:A:218:VAL:O	1:A:218:VAL:CG1	2.51	0.54
1:A:186:GLU:O	1:A:186:GLU:HG2	2.07	0.54
1:A:290:TYR:HH	1:A:317:PHE:HE2	1.55	0.54
1:A:158:GLN:HG2	1:A:161:TRP:CE2	2.44	0.53
1:A:27:ILE:HB	4:A:1180:HOH:O	2.07	0.53
1:A:120:ALA:HB2	4:A:1068:HOH:O	2.09	0.53
1:A:281:ILE:HD12	4:A:1200:HOH:O	2.08	0.53
1:A:235:ARG:NH1	1:A:334:PHE:CZ	2.74	0.52
1:A:48:ASN:HD22	1:A:301:LYS:HE2	1.74	0.52
1:A:24:PRO:CG	1:A:47:GLN:NE2	2.72	0.52
1:A:24:PRO:HG3	1:A:47:GLN:NE2	2.25	0.52
1:A:349:LYS:HD3	4:A:1156:HOH:O	2.09	0.52
1:A:61:PHE:CD1	3:A:1001:FR9:H2	2.45	0.51
1:A:124:LEU:CA	4:A:1090:HOH:O	2.19	0.51
1:A:172:TYR:O	1:A:177:VAL:HG13	2.10	0.51
1:A:321:GLU:O	1:A:325:LEU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASP:HA	4:A:1190:HOH:O	2.11	0.50
3:A:1001:FR9:H32	3:A:1001:FR9:O1	2.12	0.50
1:A:175:GLN:O	1:A:176:THR:CB	2.58	0.50
1:A:181:ASP:CG	1:A:182:LEU:N	2.70	0.50
1:A:131:SER:O	1:A:134:ASN:HB2	2.12	0.50
1:A:349:LYS:CD	4:A:1156:HOH:O	2.60	0.49
1:A:253:ARG:HG2	1:A:254:GLN:N	2.28	0.49
1:A:171:LYS:HB2	4:A:1133:HOH:O	2.11	0.49
1:A:58:LEU:HB2	4:A:1056:HOH:O	2.13	0.49
1:A:132:LEU:O	1:A:135:GLN:HB2	2.13	0.49
1:A:169:CYS:HA	1:A:177:VAL:HG21	1.94	0.49
1:A:179:ALA:HB2	1:A:210:HIS:HB2	1.94	0.49
1:A:156:ARG:HG2	1:A:182:LEU:HD22	1.93	0.48
1:A:226:GLU:O	1:A:230:THR:HB	2.13	0.48
1:A:266:SER:OG	1:A:278:HIS:HE1	1.96	0.48
1:A:184:GLY:O	1:A:185:ASP:HB3	2.13	0.48
1:A:54:LYS:HG2	1:A:55:PRO:HD2	1.94	0.48
1:A:185:ASP:HB2	3:A:1001:FR9:C32	2.43	0.48
1:A:124:LEU:CD2	4:A:1090:HOH:O	2.39	0.48
1:A:83:ALA:O	1:A:87:VAL:HG23	2.13	0.48
1:A:263:PRO:HD2	1:A:307:ASP:OD1	2.13	0.48
1:A:7:PHE:HE2	4:A:1075:HOH:O	1.93	0.48
1:A:129:VAL:O	1:A:133:VAL:HG23	2.14	0.47
1:A:256:ASN:HD22	1:A:256:ASN:N	2.11	0.47
1:A:113:GLU:CB	4:A:1077:HOH:O	2.60	0.47
1:A:166:VAL:HG11	1:A:200:ALA:O	2.14	0.47
1:A:299:ILE:HD11	4:A:1197:HOH:O	2.14	0.47
1:A:23:LYS:HE3	1:A:23:LYS:HB2	1.56	0.47
1:A:319:GLU:HG3	4:A:1115:HOH:O	2.13	0.47
1:A:10:PRO:HB3	1:A:96:VAL:CG2	2.43	0.47
1:A:174:GLU:C	1:A:176:THR:N	2.73	0.46
1:A:323:LYS:HB3	1:A:351:TYR:CE1	2.50	0.46
1:A:183:ALA:HA	1:A:184:GLY:HA2	1.69	0.46
1:A:183:ALA:HB2	1:A:214:HIS:CG	2.51	0.46
1:A:278:HIS:HD2	1:A:280:VAL:N	2.10	0.46
1:A:128:GLU:O	1:A:132:LEU:HD12	2.16	0.46
1:A:80:LYS:O	1:A:80:LYS:HG2	2.15	0.46
1:A:270:GLY:O	1:A:271:ALA:C	2.59	0.46
1:A:113:GLU:HG2	1:A:114:PRO:HA	1.97	0.46
1:A:192:SER:HB2	1:A:226:GLU:OE1	2.15	0.45
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:135:GLN:N	2.50	0.45
1:A:24:PRO:HG2	1:A:47:GLN:NE2	2.32	0.45
1:A:38:LEU:HD23	4:A:1127:HOH:O	2.16	0.45
1:A:117:TRP:HA	1:A:117:TRP:CE3	2.51	0.45
1:A:95:VAL:HG11	1:A:98:VAL:HB	1.99	0.45
1:A:120:ALA:CB	4:A:1068:HOH:O	2.64	0.45
1:A:24:PRO:HA	1:A:27:ILE:HD12	1.99	0.45
1:A:187:THR:HB	4:A:1132:HOH:O	2.16	0.45
1:A:331:LYS:HD2	4:A:1199:HOH:O	2.16	0.45
1:A:305:ASP:O	1:A:309:GLN:HB2	2.17	0.45
1:A:23:LYS:O	1:A:24:PRO:C	2.55	0.44
1:A:9:LYS:HB3	1:A:351:TYR:HE2	1.83	0.44
1:A:113:GLU:HA	1:A:114:PRO:HA	1.73	0.44
1:A:134:ASN:HD22	1:A:134:ASN:HA	1.55	0.44
1:A:323:LYS:HD3	1:A:351:TYR:CG	2.53	0.44
1:A:181:ASP:CG	1:A:182:LEU:H	2.26	0.44
1:A:27:ILE:CB	4:A:1180:HOH:O	2.64	0.43
1:A:126:PRO:O	1:A:130:VAL:HG12	2.18	0.43
1:A:176:THR:O	1:A:178:VAL:HG13	2.19	0.43
1:A:28:LEU:HD13	1:A:43:PRO:HD3	1.99	0.43
1:A:50:ILE:HD13	1:A:50:ILE:HG21	1.72	0.43
1:A:120:ALA:HA	4:A:1068:HOH:O	2.09	0.43
1:A:88:GLU:HB2	1:A:144:PHE:CE1	2.53	0.43
1:A:172:TYR:CB	1:A:177:VAL:HG11	2.46	0.43
1:A:45:GLU:HB3	4:A:1057:HOH:O	2.18	0.43
1:A:162:SER:OG	1:A:197:HIS:CD2	2.69	0.43
1:A:341:LYS:NZ	4:A:1226:HOH:O	2.51	0.43
1:A:32:LYS:HG3	4:A:1127:HOH:O	2.18	0.43
1:A:92:LYS:HG2	4:A:1201:HOH:O	2.18	0.43
1:A:117:TRP:O	1:A:118:ASN:CG	2.61	0.43
1:A:283:PHE:HB3	1:A:288:VAL:HB	2.01	0.43
1:A:64:LYS:HE2	4:A:1030:HOH:O	2.20	0.42
1:A:261:ILE:HD12	1:A:261:ILE:HG23	1.83	0.42
1:A:156:ARG:HD2	1:A:186:GLU:HA	2.01	0.42
1:A:337:GLU:HB3	4:A:1129:HOH:O	2.19	0.42
1:A:327:ILE:HD13	1:A:348:TYR:CE2	2.54	0.42
1:A:174:GLU:HB2	4:A:1174:HOH:O	2.19	0.42
1:A:186:GLU:HG3	1:A:223:VAL:HG11	2.00	0.42
1:A:273:LYS:HA	1:A:274:PRO:HD3	1.95	0.42
1:A:335:LEU:HD12	1:A:335:LEU:HA	1.83	0.42
1:A:168:LEU:O	1:A:172:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:CB	4:A:1174:HOH:O	2.67	0.41
1:A:284:LYS:NZ	4:A:1058:HOH:O	2.53	0.41
1:A:278:HIS:O	1:A:279:ALA:C	2.63	0.41
1:A:90:LYS:HA	1:A:90:LYS:HD2	1.61	0.41
1:A:57:THR:O	1:A:58:LEU:C	2.62	0.41
1:A:347:LEU:O	1:A:348:TYR:C	2.61	0.41
1:A:80:LYS:NZ	1:A:135:GLN:HB3	2.35	0.41
1:A:140:GLY:O	1:A:144:PHE:HB2	2.21	0.41
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.73	0.41
1:A:340:LYS:O	1:A:344:LEU:HD22	2.21	0.41
1:A:63:ALA:O	1:A:64:LYS:C	2.61	0.41
1:A:235:ARG:HD3	1:A:334:PHE:CE1	2.53	0.40
1:A:282:ARG:HH11	1:A:282:ARG:HD2	1.64	0.40
1:A:162:SER:O	1:A:166:VAL:HG22	2.21	0.40
1:A:127:ASP:HB2	4:A:1145:HOH:O	2.22	0.40
1:A:56:LEU:HD13	4:A:1050:HOH:O	2.21	0.40
1:A:58:LEU:CB	1:A:59:PRO:CD	2.94	0.40
1:A:69:MET:HE1	1:A:107:LEU:CD2	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1024:HOH:O	4:A:1222:HOH:O[4_565]	1.77	0.43
1:A:229:ASP:OD2	4:A:1024:HOH:O[3_644]	1.95	0.25
1:A:161:TRP:CH2	4:A:1017:HOH:O[6_465]	2.19	0.01

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%)	315 (91%)	22 (6%)	10 (3%)	3 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	174	GLU
1	A	175	GLN
1	A	256	ASN
1	A	277	GLU
1	A	25	GLU
1	A	37	ALA
1	A	43	PRO
1	A	238	HIS
1	A	176	THR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	FR9	A	1001	-	36,36,36	2.11	11 (30%)	44,49,49	2.16	12 (27%)

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	FR9	A	1001	-	-	3/24/24/24	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR9	O9-C8	-5.46	1.11	1.24
3	A	1001	FR9	C33-N1	-5.20	1.31	1.41
3	A	1001	FR9	C30-N22	-4.27	1.31	1.39
3	A	1001	FR9	C1-N2	4.22	1.47	1.37
3	A	1001	FR9	C34-C30	-3.86	1.33	1.39
3	A	1001	FR9	C8-N10	-3.09	1.24	1.33
3	A	1001	FR9	C5-N4	2.69	1.46	1.39
3	A	1001	FR9	C2-N3	-2.67	1.29	1.35
3	A	1001	FR9	C5-C8	-2.32	1.45	1.48
3	A	1001	FR9	C31-C29	-2.09	1.37	1.41
3	A	1001	FR9	O15-C14	2.04	1.51	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR9	O9-C8-C5	-6.56	113.94	120.25
3	A	1001	FR9	C1-N2-C3	-6.47	102.08	106.37
3	A	1001	FR9	C1-C5-N4	-4.75	104.43	109.78
3	A	1001	FR9	O15-C14-C13	3.39	124.62	111.51
3	A	1001	FR9	C5-C8-N10	3.23	119.56	116.28
3	A	1001	FR9	N2-C3-N4	2.88	116.29	112.21
3	A	1001	FR9	C11-C6-N3	-2.55	107.70	113.07
3	A	1001	FR9	C15-C10-C12	-2.36	116.64	119.87
3	A	1001	FR9	C13-N2-C1	2.28	130.05	126.14
3	A	1001	FR9	C18-C19-N22	-2.21	109.13	112.55
3	A	1001	FR9	C10-C15-C7	2.20	122.95	120.24
3	A	1001	FR9	O1-C2-N3	2.02	125.94	122.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

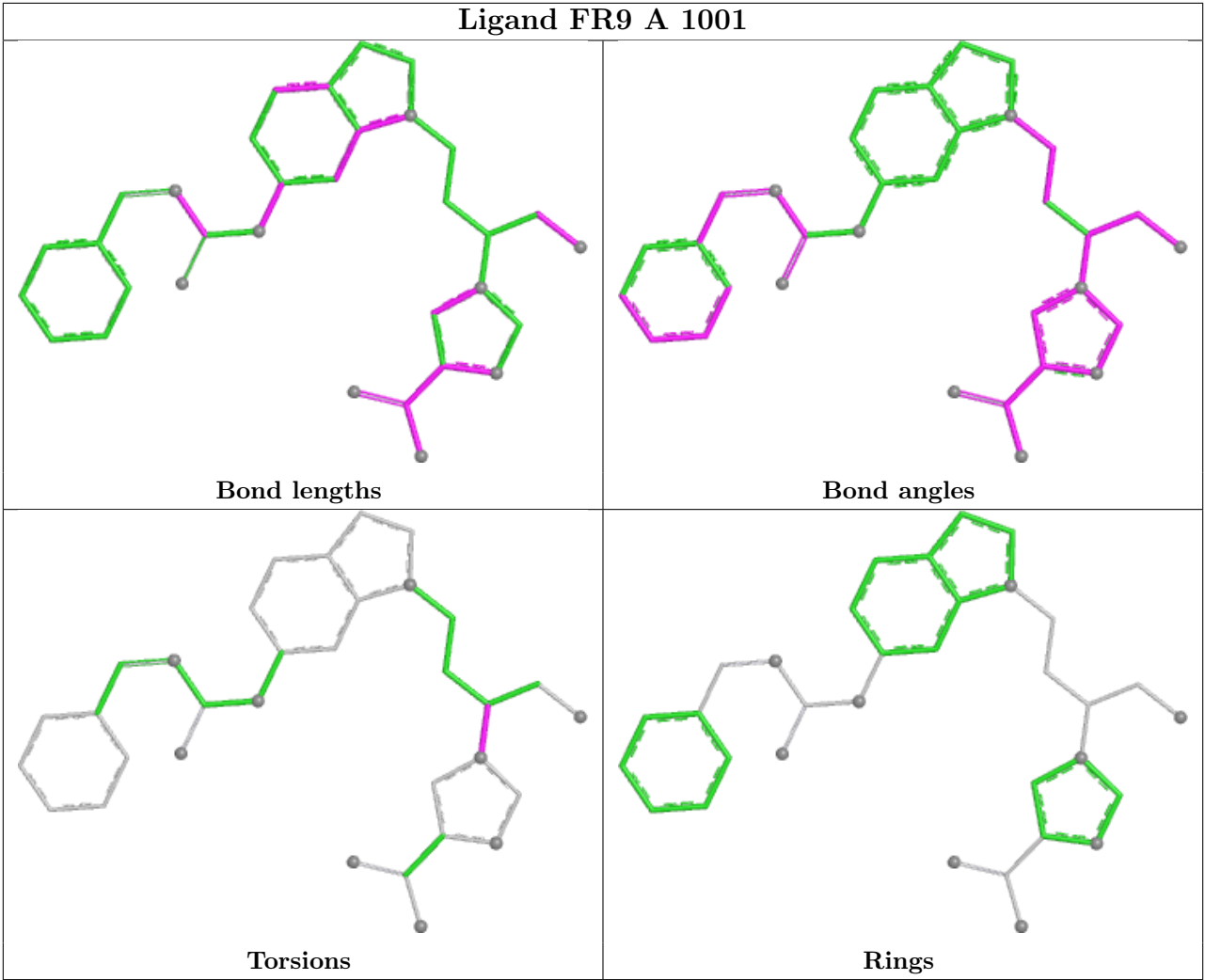
Mol	Chain	Res	Type	Atoms
3	A	1001	FR9	C18-C13-N2-C3
3	A	1001	FR9	C14-C13-N2-C1
3	A	1001	FR9	C18-C13-N2-C1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR9	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	337:GLU	C	338:ASP	N	1.09

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/356 (98%)	-0.04	7 (2%) 65 70	12, 28, 47, 58	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ALA	6.1
1	A	184	GLY	3.0
1	A	142	ARG	2.3
1	A	185	ASP	2.2
1	A	122	GLY	2.2
1	A	199	GLN	2.2
1	A	246	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

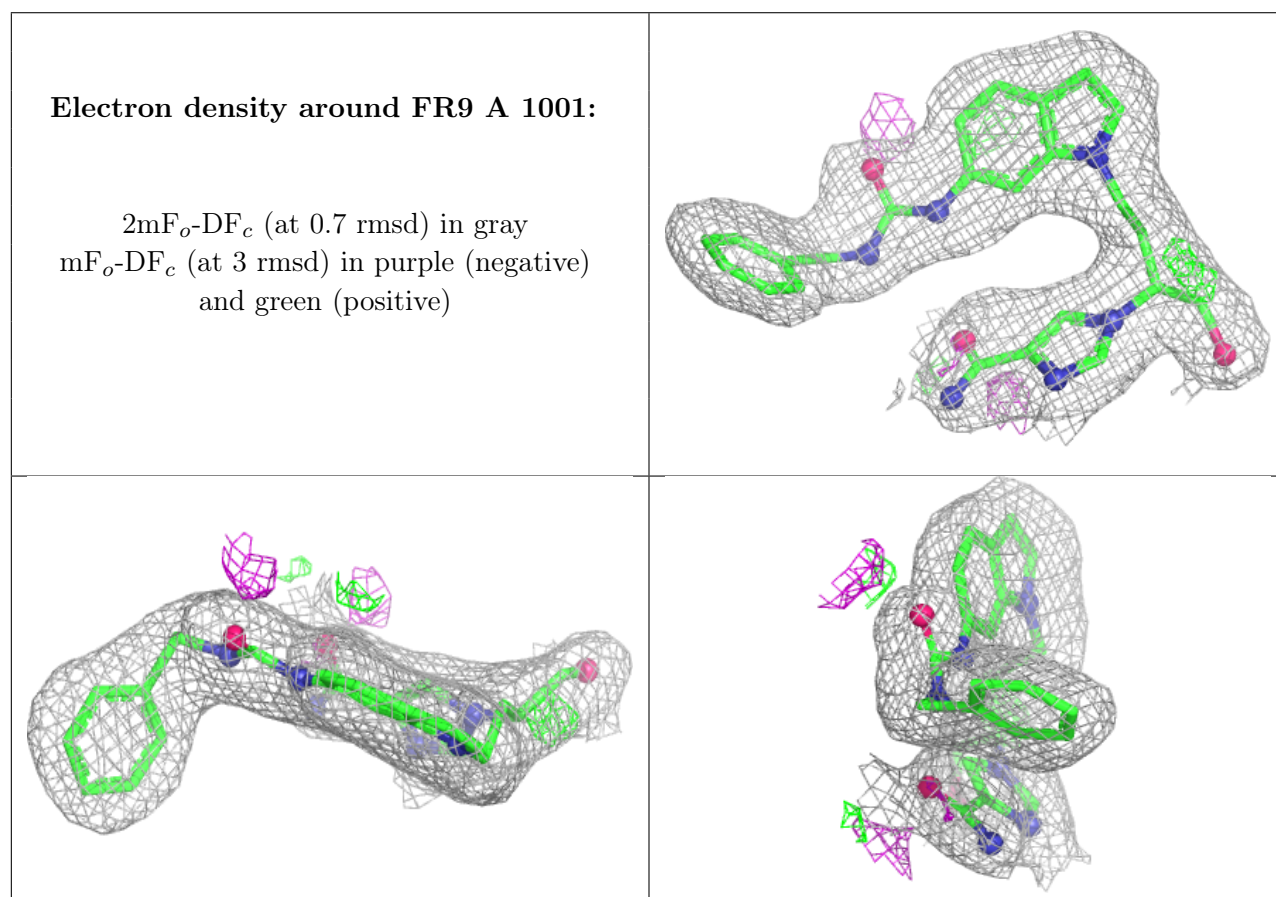
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FR9	A	1001	33/33	0.91	0.07	16,19,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	400	1/1	0.97	0.03	27,27,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.