



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:53 PM UTC

PDB ID : 1V79 / pdb_00001v79
Title : Crystal structures of adenosine deaminase complexed with potent inhibitors
Authors : Kinoshita, T.
Deposited on : 2003-12-14
Resolution : 2.50 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

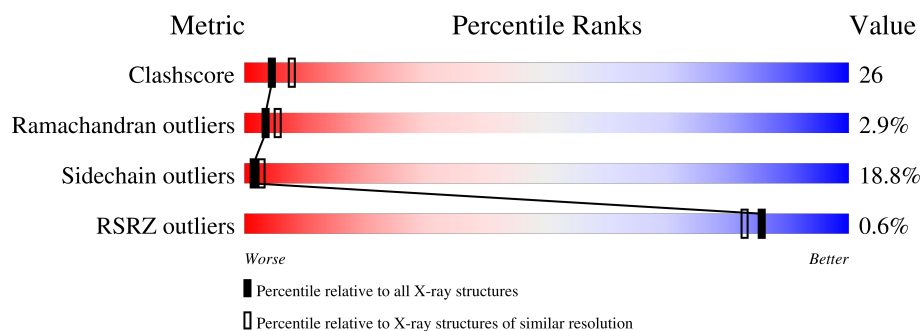
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 2958 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			

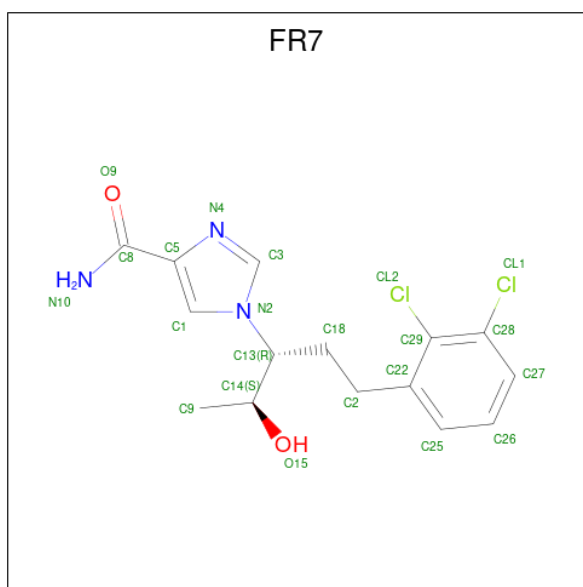
There are 15 discrepancies between the modelled and reference sequences:

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,2S)-1-[2-(2,3,-DICHLOROPHENYL)ETHYL]-2-HYDROXYPROPYL}-1H-IMIDAZOLE-4-CARBOXAMIDE (CCD ID: FR7) (formula: C₁₅H₁₇Cl₂N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			22	15	2	3	2		

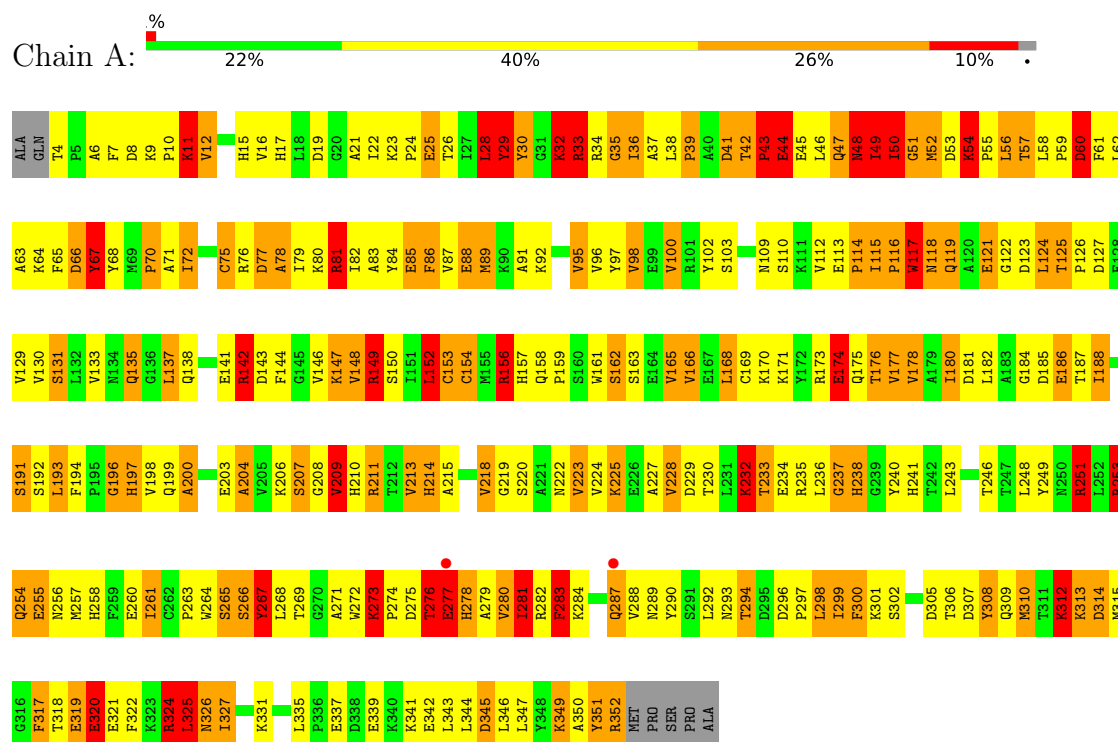
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		

3 Residue-property plots [i](#)

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	77.23Å 77.23Å 135.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50 12.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.50) 94.3 (12.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.63 (at 2.50Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.252 , 0.281 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 69.0	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	0.92	EDS
Total number of atoms	2958	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, FR7

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	1.95	48/2853 (1.7%)	3.06	405/3867 (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	0	18

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	ARG	CA-CB	-8.88	1.39	1.53
1	A	253	ARG	NE-CZ	8.04	1.41	1.33
1	A	174	GLU	N-CA	7.61	1.56	1.46
1	A	197	HIS	CG-ND1	-7.61	1.29	1.38
1	A	50	ILE	CA-C	-7.33	1.43	1.52
1	A	258	HIS	CG-ND1	-7.32	1.30	1.38
1	A	173	ARG	C-N	7.20	1.43	1.33
1	A	241	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	100	VAL	CB-CG1	-6.99	1.29	1.52
1	A	261	ILE	CA-C	-6.92	1.44	1.52
1	A	214	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	184	GLY	C-O	-6.33	1.15	1.23
1	A	173	ARG	NE-CZ	6.31	1.40	1.33
1	A	77	ASP	CA-CB	6.31	1.63	1.53
1	A	96	VAL	N-CA	6.27	1.52	1.46
1	A	277	GLU	CA-CB	6.21	1.64	1.53
1	A	264	TRP	NE1-CE2	6.13	1.44	1.37
1	A	173	ARG	CA-C	6.07	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	GLU	CG-CD	6.07	1.67	1.52
1	A	50	ILE	C-N	-6.00	1.26	1.33
1	A	95	VAL	CA-CB	-5.98	1.46	1.54
1	A	278	HIS	ND1-CE1	5.93	1.38	1.32
1	A	278	HIS	C-N	5.91	1.42	1.33
1	A	89	MET	CA-C	5.86	1.60	1.52
1	A	96	VAL	CA-CB	-5.81	1.48	1.54
1	A	30	TYR	CA-CB	-5.71	1.43	1.53
1	A	288	VAL	CA-CB	5.69	1.59	1.54
1	A	257	MET	CA-C	5.61	1.59	1.52
1	A	17	HIS	ND1-CE1	5.60	1.38	1.32
1	A	142	ARG	CD-NE	5.59	1.54	1.46
1	A	319	GLU	C-N	-5.56	1.26	1.33
1	A	275	ASP	N-CA	5.55	1.53	1.46
1	A	153	CYS	C-O	-5.49	1.17	1.24
1	A	165	VAL	CA-CB	-5.43	1.48	1.54
1	A	65	PHE	CA-C	5.43	1.60	1.52
1	A	352	ARG	NE-CZ	5.35	1.39	1.33
1	A	171	LYS	CA-C	-5.32	1.45	1.52
1	A	112	VAL	CA-C	5.28	1.59	1.52
1	A	157	HIS	CE1-NE2	5.28	1.37	1.32
1	A	174	GLU	CA-CB	5.23	1.62	1.53
1	A	238	HIS	ND1-CE1	5.17	1.37	1.32
1	A	60	ASP	CB-CG	5.15	1.65	1.52
1	A	177	VAL	C-O	-5.14	1.18	1.24
1	A	21	ALA	C-O	-5.13	1.18	1.23
1	A	12	VAL	C-O	-5.12	1.17	1.24
1	A	165	VAL	C-N	5.09	1.40	1.33
1	A	127	ASP	CA-C	5.08	1.59	1.52
1	A	324	ARG	NE-CZ	5.02	1.38	1.33

All (405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	26.04	138.64	112.60
1	A	77	ASP	CA-CB-CG	13.58	126.18	112.60
1	A	341	LYS	CA-CB-CG	-13.58	86.94	114.10
1	A	50	ILE	CA-C-N	-13.14	110.28	121.58
1	A	50	ILE	C-N-CA	-13.14	110.28	121.58
1	A	222	ASN	CA-CB-CG	-11.93	100.67	112.60
1	A	208	GLY	CA-C-N	-11.83	108.02	122.93
1	A	208	GLY	C-N-CA	-11.83	108.02	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	HIS	N-CA-C	11.76	124.18	111.36
1	A	314	ASP	N-CA-C	11.32	127.09	113.28
1	A	41	ASP	CA-CB-CG	-11.31	101.29	112.60
1	A	7	PHE	CA-CB-CG	11.29	125.09	113.80
1	A	119	GLN	CA-C-N	-11.27	104.86	120.87
1	A	119	GLN	C-N-CA	-11.27	104.86	120.87
1	A	313	LYS	N-CA-C	11.10	123.38	111.28
1	A	48	ASN	CA-C-N	10.84	133.94	120.72
1	A	48	ASN	C-N-CA	10.84	133.94	120.72
1	A	118	ASN	CA-C-N	-10.78	106.14	122.09
1	A	118	ASN	C-N-CA	-10.78	106.14	122.09
1	A	254	GLN	CB-CG-CD	-10.75	94.33	112.60
1	A	177	VAL	N-CA-C	10.53	122.78	108.89
1	A	351	TYR	CA-C-N	-10.46	102.88	121.70
1	A	351	TYR	C-N-CA	-10.46	102.88	121.70
1	A	51	GLY	CA-C-N	-10.32	106.00	122.73
1	A	51	GLY	C-N-CA	-10.32	106.00	122.73
1	A	251	ARG	NE-CZ-NH1	-10.24	111.26	121.50
1	A	37	ALA	CA-C-O	10.12	131.44	120.92
1	A	70	PRO	CA-C-N	-9.98	104.06	120.72
1	A	70	PRO	C-N-CA	-9.98	104.06	120.72
1	A	162	SER	N-CA-C	9.97	121.74	111.07
1	A	44	GLU	CB-CA-C	-9.62	91.27	110.42
1	A	276	THR	N-CA-CB	-9.61	95.08	110.46
1	A	166	VAL	CB-CA-C	-9.57	99.22	112.14
1	A	296	ASP	CA-CB-CG	9.34	121.94	112.60
1	A	269	THR	CA-C-N	-9.29	108.72	123.31
1	A	269	THR	C-N-CA	-9.29	108.72	123.31
1	A	33	ARG	CD-NE-CZ	-9.22	111.49	124.40
1	A	341	LYS	N-CA-C	9.15	122.41	111.33
1	A	84	TYR	N-CA-C	9.08	126.36	111.37
1	A	166	VAL	N-CA-CB	9.01	122.79	110.54
1	A	95	VAL	N-CA-CB	-8.92	98.26	110.56
1	A	224	VAL	CA-C-N	-8.76	106.09	120.72
1	A	224	VAL	C-N-CA	-8.76	106.09	120.72
1	A	223	VAL	CA-C-N	-8.76	109.53	120.56
1	A	223	VAL	C-N-CA	-8.76	109.53	120.56
1	A	207	SER	N-CA-C	8.75	122.08	110.88
1	A	235	ARG	CA-C-N	-8.75	110.66	122.99
1	A	235	ARG	C-N-CA	-8.75	110.66	122.99
1	A	49	ILE	N-CA-C	8.64	118.55	110.42
1	A	9	LYS	CA-C-N	-8.37	111.14	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	LYS	C-N-CA	-8.37	111.14	119.76
1	A	282	ARG	CA-C-N	-8.33	109.12	120.28
1	A	282	ARG	C-N-CA	-8.33	109.12	120.28
1	A	266	SER	N-CA-C	8.30	121.45	111.82
1	A	310	MET	N-CA-CB	8.26	122.39	110.16
1	A	35	GLY	CA-C-N	-8.23	111.14	122.91
1	A	35	GLY	C-N-CA	-8.23	111.14	122.91
1	A	254	GLN	N-CA-C	8.21	120.23	111.28
1	A	253	ARG	CD-NE-CZ	-8.18	112.94	124.40
1	A	52	MET	CA-C-N	-8.18	107.66	122.54
1	A	52	MET	C-N-CA	-8.18	107.66	122.54
1	A	233	THR	CB-CA-C	-8.14	95.06	109.62
1	A	175	GLN	CA-C-N	8.13	136.33	121.70
1	A	175	GLN	C-N-CA	8.13	136.33	121.70
1	A	173	ARG	CA-C-N	8.08	136.98	121.54
1	A	173	ARG	C-N-CA	8.08	136.98	121.54
1	A	194	PHE	CA-CB-CG	8.07	121.87	113.80
1	A	81	ARG	CD-NE-CZ	-8.05	113.13	124.40
1	A	253	ARG	CA-CB-CG	7.97	130.05	114.10
1	A	129	VAL	CA-C-N	-7.97	110.36	120.56
1	A	129	VAL	C-N-CA	-7.97	110.36	120.56
1	A	290	TYR	N-CA-C	7.95	121.25	109.24
1	A	277	GLU	CA-CB-CG	7.95	130.00	114.10
1	A	326	ASN	N-CA-C	7.93	120.00	111.36
1	A	95	VAL	CA-CB-CG2	-7.90	96.96	110.40
1	A	337	GLU	N-CA-C	7.86	120.54	111.11
1	A	327	ILE	CA-CB-CG1	7.86	123.75	110.40
1	A	228	VAL	CB-CA-C	-7.85	101.73	112.02
1	A	41	ASP	N-CA-C	7.76	124.58	113.02
1	A	254	GLN	OE1-CD-NE2	7.73	130.33	122.60
1	A	45	GLU	N-CA-C	-7.72	102.81	111.07
1	A	278	HIS	N-CA-C	7.71	122.05	110.64
1	A	71	ALA	N-CA-C	7.70	121.93	112.54
1	A	28	LEU	CB-CA-C	-7.69	98.50	110.81
1	A	290	TYR	CA-C-O	7.59	129.97	121.40
1	A	198	VAL	CA-C-O	7.57	129.20	121.17
1	A	287	GLN	CG-CD-NE2	-7.56	105.06	116.40
1	A	224	VAL	O-C-N	7.43	129.19	121.91
1	A	11	LYS	N-CA-C	7.41	121.56	109.85
1	A	310	MET	CA-CB-CG	7.40	128.90	114.10
1	A	49	ILE	N-CA-CB	-7.39	102.30	110.65
1	A	288	VAL	CA-C-N	-7.34	111.62	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	VAL	C-N-CA	-7.34	111.62	122.41
1	A	178	VAL	N-CA-C	7.30	121.38	113.43
1	A	173	ARG	N-CA-C	7.27	120.77	110.23
1	A	223	VAL	CA-CB-CG2	7.27	122.76	110.40
1	A	275	ASP	CA-CB-CG	-7.27	105.33	112.60
1	A	280	VAL	N-CA-C	7.26	118.03	110.62
1	A	114	PRO	N-CA-CB	-7.25	94.62	102.60
1	A	269	THR	CB-CA-C	-7.23	95.42	110.17
1	A	52	MET	N-CA-CB	-7.21	97.96	111.00
1	A	232	LYS	N-CA-C	7.21	121.33	111.39
1	A	123	ASP	CA-C-N	-7.18	112.87	122.42
1	A	123	ASP	C-N-CA	-7.18	112.87	122.42
1	A	176	THR	CA-C-N	-7.17	111.76	121.66
1	A	176	THR	C-N-CA	-7.17	111.76	121.66
1	A	166	VAL	O-C-N	7.16	128.82	121.87
1	A	79	ILE	CA-C-N	-7.14	110.71	120.28
1	A	79	ILE	C-N-CA	-7.14	110.71	120.28
1	A	320	GLU	N-CA-C	7.14	123.14	111.37
1	A	142	ARG	N-CA-C	7.10	119.92	111.33
1	A	163	SER	N-CA-C	7.07	119.84	111.71
1	A	275	ASP	CA-C-O	7.05	128.36	119.12
1	A	310	MET	CA-C-N	-7.05	108.70	120.68
1	A	310	MET	C-N-CA	-7.05	108.70	120.68
1	A	227	ALA	N-CA-C	7.04	119.56	111.11
1	A	313	LYS	CA-C-N	-7.02	109.00	122.06
1	A	313	LYS	C-N-CA	-7.02	109.00	122.06
1	A	43	PRO	CA-C-O	-7.01	107.85	120.60
1	A	223	VAL	N-CA-C	7.00	117.79	110.72
1	A	72	ILE	CB-CG1-CD1	-6.98	99.15	113.80
1	A	277	GLU	CB-CG-CD	6.96	124.43	112.60
1	A	75	CYS	N-CA-C	6.94	125.58	110.80
1	A	57	THR	CA-C-N	-6.93	110.73	121.62
1	A	57	THR	C-N-CA	-6.93	110.73	121.62
1	A	181	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	165	VAL	N-CA-C	6.92	117.62	110.36
1	A	135	GLN	N-CA-C	-6.91	103.68	111.07
1	A	289	ASN	N-CA-CB	-6.88	100.10	110.35
1	A	43	PRO	O-C-N	6.88	131.92	122.64
1	A	220	SER	N-CA-C	6.87	118.86	110.41
1	A	148	VAL	CA-C-N	-6.86	110.86	122.92
1	A	148	VAL	C-N-CA	-6.86	110.86	122.92
1	A	283	PHE	CG-CD2-CE2	6.83	132.32	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	VAL	CA-C-O	-6.81	113.95	121.17
1	A	274	PRO	CB-CA-C	6.81	121.17	110.49
1	A	89	MET	N-CA-CB	-6.80	100.14	110.01
1	A	258	HIS	CA-CB-CG	-6.80	107.00	113.80
1	A	171	LYS	O-C-N	6.79	129.15	122.09
1	A	78	ALA	CA-C-O	6.79	127.62	120.42
1	A	274	PRO	CA-C-N	-6.79	108.36	121.94
1	A	274	PRO	C-N-CA	-6.79	108.36	121.94
1	A	258	HIS	N-CA-C	6.79	120.55	109.76
1	A	209	VAL	CB-CA-C	6.77	120.05	110.84
1	A	325	LEU	CB-CA-C	6.77	122.02	110.79
1	A	32	LYS	CA-C-N	-6.75	110.05	120.31
1	A	32	LYS	C-N-CA	-6.75	110.05	120.31
1	A	124	LEU	CA-C-N	-6.73	111.58	122.48
1	A	124	LEU	C-N-CA	-6.73	111.58	122.48
1	A	153	CYS	N-CA-C	6.73	119.66	108.96
1	A	192	SER	CA-C-O	6.73	127.70	120.10
1	A	87	VAL	CA-C-O	6.72	128.30	121.17
1	A	149	ARG	N-CA-C	6.71	120.54	110.14
1	A	89	MET	CA-C-O	6.70	127.85	120.82
1	A	261	ILE	CA-C-N	-6.70	114.42	123.46
1	A	261	ILE	C-N-CA	-6.70	114.42	123.46
1	A	246	THR	N-CA-C	6.67	119.12	111.11
1	A	266	SER	CA-C-N	-6.67	111.77	120.44
1	A	266	SER	C-N-CA	-6.67	111.77	120.44
1	A	157	HIS	CA-CB-CG	-6.67	107.13	113.80
1	A	115	ILE	CA-C-N	-6.65	112.93	119.78
1	A	115	ILE	C-N-CA	-6.65	112.93	119.78
1	A	339	GLU	CA-C-O	6.65	127.56	119.31
1	A	169	CYS	CA-C-N	-6.62	109.34	121.52
1	A	169	CYS	C-N-CA	-6.62	109.34	121.52
1	A	352	ARG	CB-CA-C	6.57	122.58	110.10
1	A	122	GLY	CA-C-N	6.57	132.53	122.29
1	A	122	GLY	C-N-CA	6.57	132.53	122.29
1	A	112	VAL	N-CA-C	6.56	117.56	107.78
1	A	72	ILE	CA-C-O	6.55	126.45	120.30
1	A	123	ASP	N-CA-C	6.54	123.42	113.61
1	A	142	ARG	CD-NE-CZ	-6.54	115.25	124.40
1	A	283	PHE	CA-C-O	6.53	127.47	120.55
1	A	49	ILE	CA-C-N	-6.53	110.22	121.97
1	A	49	ILE	C-N-CA	-6.53	110.22	121.97
1	A	224	VAL	N-CA-C	6.53	116.68	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	CB-CG-CD	-6.52	96.30	111.30
1	A	314	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	288	VAL	CA-C-O	6.48	128.06	121.58
1	A	256	ASN	CA-CB-CG	-6.46	106.14	112.60
1	A	299	ILE	CA-C-O	6.45	127.22	120.25
1	A	199	GLN	CB-CA-C	6.44	123.04	110.67
1	A	25	GLU	CA-C-N	-6.44	109.87	121.14
1	A	25	GLU	C-N-CA	-6.44	109.87	121.14
1	A	344	LEU	N-CA-C	6.43	118.28	111.28
1	A	34	ARG	CB-CA-C	-6.42	100.47	111.46
1	A	281	ILE	N-CA-C	6.41	117.16	110.62
1	A	92	LYS	N-CA-C	6.40	120.35	112.54
1	A	141	GLU	N-CA-C	6.40	118.79	111.11
1	A	233	THR	N-CA-C	6.40	119.05	110.35
1	A	95	VAL	CA-CB-CG1	6.38	121.25	110.40
1	A	52	MET	CB-CA-C	6.35	121.93	109.35
1	A	255	GLU	CA-C-N	-6.34	112.76	122.08
1	A	255	GLU	C-N-CA	-6.34	112.76	122.08
1	A	188	ILE	CB-CG1-CD1	-6.34	100.49	113.80
1	A	200	ALA	N-CA-C	6.34	117.85	111.07
1	A	6	ALA	CA-C-N	-6.33	113.84	122.95
1	A	6	ALA	C-N-CA	-6.33	113.84	122.95
1	A	115	ILE	CA-CB-CG1	-6.31	99.67	110.40
1	A	243	LEU	N-CA-C	6.30	120.06	112.38
1	A	241	HIS	CA-CB-CG	-6.28	107.52	113.80
1	A	253	ARG	CA-C-O	6.27	127.20	120.24
1	A	53	ASP	N-CA-C	6.25	118.42	110.61
1	A	343	LEU	CA-C-N	-6.24	111.91	120.28
1	A	343	LEU	C-N-CA	-6.24	111.91	120.28
1	A	175	GLN	N-CA-C	6.23	124.07	110.80
1	A	91	ALA	CA-C-O	6.21	127.13	120.55
1	A	243	LEU	CA-C-N	-6.18	109.58	121.94
1	A	243	LEU	C-N-CA	-6.18	109.58	121.94
1	A	125	THR	N-CA-C	6.18	117.23	110.13
1	A	326	ASN	CA-CB-CG	-6.16	106.44	112.60
1	A	143	ASP	CA-C-N	-6.16	112.80	122.65
1	A	143	ASP	C-N-CA	-6.16	112.80	122.65
1	A	196	GLY	CA-C-N	-6.15	111.56	120.29
1	A	196	GLY	C-N-CA	-6.15	111.56	120.29
1	A	154	CYS	CA-C-O	6.14	127.95	121.19
1	A	230	THR	CA-C-N	-6.13	109.67	121.94
1	A	230	THR	C-N-CA	-6.13	109.67	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	LEU	CD1-CG-CD2	-6.13	97.32	110.80
1	A	96	VAL	N-CA-C	6.12	120.58	113.42
1	A	158	GLN	CA-CB-CG	6.09	126.29	114.10
1	A	66	ASP	CA-C-O	6.09	125.84	119.14
1	A	184	GLY	O-C-N	-6.08	114.79	122.70
1	A	142	ARG	CB-CG-CD	6.05	125.22	111.30
1	A	87	VAL	CA-C-N	-6.04	112.11	120.38
1	A	87	VAL	C-N-CA	-6.04	112.11	120.38
1	A	229	ASP	CA-C-N	-6.03	112.06	122.79
1	A	229	ASP	C-N-CA	-6.03	112.06	122.79
1	A	148	VAL	N-CA-C	6.02	116.68	107.77
1	A	37	ALA	N-CA-C	6.01	118.57	107.99
1	A	60	ASP	CB-CA-C	6.01	121.75	110.63
1	A	289	ASN	CB-CA-C	6.01	121.51	111.30
1	A	298	LEU	N-CA-C	6.01	117.50	111.07
1	A	310	MET	CB-CA-C	-6.00	100.65	110.85
1	A	339	GLU	N-CA-C	5.99	120.32	112.89
1	A	293	ASN	CA-C-N	-5.97	112.32	122.11
1	A	293	ASN	C-N-CA	-5.97	112.32	122.11
1	A	9	LYS	CB-CA-C	5.97	118.21	109.08
1	A	124	LEU	CA-C-O	5.96	126.96	120.58
1	A	175	GLN	CA-CB-CG	5.92	125.94	114.10
1	A	171	LYS	CA-C-O	-5.91	114.58	120.90
1	A	317	PHE	CA-C-N	-5.91	111.97	122.07
1	A	317	PHE	C-N-CA	-5.91	111.97	122.07
1	A	39	PRO	CB-CA-C	-5.90	101.83	111.56
1	A	48	ASN	N-CA-C	5.87	118.43	111.33
1	A	180	ILE	N-CA-C	5.84	117.41	108.71
1	A	265	SER	CB-CA-C	-5.83	98.82	110.42
1	A	346	LEU	N-CA-C	5.83	117.63	111.28
1	A	225	LYS	CA-C-N	-5.82	112.48	120.28
1	A	225	LYS	C-N-CA	-5.82	112.48	120.28
1	A	19	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	89	MET	CA-CB-CG	5.80	125.69	114.10
1	A	65	PHE	CA-C-N	-5.79	111.90	121.92
1	A	65	PHE	C-N-CA	-5.79	111.90	121.92
1	A	85	GLU	CB-CA-C	5.79	121.30	109.55
1	A	214	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	A	61	PHE	N-CA-C	5.76	118.78	111.69
1	A	21	ALA	CA-C-O	5.75	128.22	121.78
1	A	350	ALA	CA-C-N	-5.75	110.82	122.31
1	A	350	ALA	C-N-CA	-5.75	110.82	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CA-C-N	-5.74	113.18	122.82
1	A	182	LEU	C-N-CA	-5.74	113.18	122.82
1	A	15	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
1	A	116	PRO	CA-C-N	-5.73	114.69	122.82
1	A	116	PRO	C-N-CA	-5.73	114.69	122.82
1	A	8	ASP	CA-C-O	5.72	128.69	120.51
1	A	156	ARG	CA-C-N	-5.72	113.50	122.65
1	A	156	ARG	C-N-CA	-5.72	113.50	122.65
1	A	254	GLN	N-CA-CB	-5.71	101.72	110.12
1	A	224	VAL	CG1-CB-CG2	5.70	123.35	110.80
1	A	103	SER	CA-C-O	5.70	123.54	119.32
1	A	251	ARG	CA-C-N	-5.70	110.47	121.58
1	A	251	ARG	C-N-CA	-5.70	110.47	121.58
1	A	63	ALA	N-CA-C	5.69	118.26	111.71
1	A	147	LYS	N-CA-C	5.69	118.50	109.96
1	A	280	VAL	CA-C-N	-5.69	112.67	120.46
1	A	280	VAL	C-N-CA	-5.69	112.67	120.46
1	A	135	GLN	CB-CA-C	5.68	119.80	110.88
1	A	67	TYR	CA-C-N	-5.67	113.40	122.08
1	A	67	TYR	C-N-CA	-5.67	113.40	122.08
1	A	72	ILE	CA-C-N	-5.65	112.68	120.71
1	A	72	ILE	C-N-CA	-5.65	112.68	120.71
1	A	117	TRP	CB-CA-C	-5.63	103.21	112.06
1	A	243	LEU	CA-C-O	5.63	126.30	119.49
1	A	146	VAL	CA-C-N	-5.63	113.07	120.95
1	A	146	VAL	C-N-CA	-5.63	113.07	120.95
1	A	177	VAL	CA-C-N	-5.63	115.07	122.16
1	A	177	VAL	C-N-CA	-5.63	115.07	122.16
1	A	307	ASP	CA-C-O	5.62	126.73	120.82
1	A	29	TYR	CA-C-N	-5.62	111.30	121.14
1	A	29	TYR	C-N-CA	-5.62	111.30	121.14
1	A	307	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	277	GLU	CA-C-N	-5.60	112.29	121.97
1	A	277	GLU	C-N-CA	-5.60	112.29	121.97
1	A	324	ARG	CD-NE-CZ	-5.60	116.57	124.40
1	A	88	GLU	N-CA-CB	-5.59	101.67	110.06
1	A	98	VAL	CA-C-N	-5.58	115.18	123.11
1	A	98	VAL	C-N-CA	-5.58	115.18	123.11
1	A	42	THR	N-CA-CB	5.58	119.42	109.94
1	A	191	SER	N-CA-C	5.55	118.04	111.33
1	A	33	ARG	O-C-N	5.54	129.09	122.27
1	A	62	LEU	N-CA-C	5.54	118.08	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	VAL	CA-C-N	-5.54	115.08	122.72
1	A	16	VAL	C-N-CA	-5.54	115.08	122.72
1	A	170	LYS	CA-C-N	5.53	128.01	120.54
1	A	170	LYS	C-N-CA	5.53	128.01	120.54
1	A	234	GLU	CA-CB-CG	-5.53	103.04	114.10
1	A	211	ARG	N-CA-C	5.52	117.89	108.90
1	A	240	TYR	CA-C-O	5.51	126.61	120.82
1	A	306	THR	CB-CA-C	-5.51	101.99	110.81
1	A	10	PRO	CA-C-N	-5.51	113.56	122.81
1	A	10	PRO	C-N-CA	-5.51	113.56	122.81
1	A	131	SER	N-CA-C	5.50	117.72	111.11
1	A	119	GLN	N-CA-CB	5.50	119.14	110.23
1	A	349	LYS	N-CA-C	5.47	116.94	110.97
1	A	84	TYR	CA-C-N	-5.47	112.04	121.66
1	A	84	TYR	C-N-CA	-5.47	112.04	121.66
1	A	174	GLU	N-CA-C	5.47	122.44	110.80
1	A	234	GLU	CA-C-O	5.45	125.65	119.27
1	A	271	ALA	O-C-N	5.45	127.90	122.12
1	A	97	TYR	CA-C-O	5.44	126.61	119.98
1	A	315	MET	CA-C-O	5.43	125.16	119.51
1	A	79	ILE	CB-CG1-CD1	-5.43	102.40	113.80
1	A	42	THR	CA-C-O	5.43	126.40	119.67
1	A	88	GLU	CB-CG-CD	-5.42	103.39	112.60
1	A	309	GLN	CA-C-N	-5.41	112.61	120.29
1	A	309	GLN	C-N-CA	-5.41	112.61	120.29
1	A	288	VAL	N-CA-C	5.40	118.32	109.78
1	A	163	SER	CA-C-N	-5.40	112.50	120.28
1	A	163	SER	C-N-CA	-5.40	112.50	120.28
1	A	32	LYS	CA-CB-CG	5.38	124.86	114.10
1	A	86	PHE	CA-C-O	5.38	126.25	120.55
1	A	184	GLY	CA-C-O	5.38	129.93	120.57
1	A	29	TYR	N-CA-C	5.36	117.54	111.11
1	A	57	THR	CA-C-O	-5.35	115.40	121.72
1	A	54	LYS	CA-C-O	5.35	124.95	119.76
1	A	261	ILE	CB-CA-C	-5.35	104.28	110.91
1	A	89	MET	N-CA-C	5.35	116.79	111.07
1	A	175	GLN	N-CA-CB	-5.34	101.46	110.49
1	A	156	ARG	NE-CZ-NH2	-5.34	114.40	119.20
1	A	45	GLU	N-CA-CB	-5.33	102.28	110.01
1	A	251	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	276	THR	OG1-CB-CG2	5.33	119.95	109.30
1	A	60	ASP	N-CA-C	-5.32	105.59	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	LYS	CA-C-N	-5.31	115.44	122.98
1	A	147	LYS	C-N-CA	-5.31	115.44	122.98
1	A	267	TYR	CB-CA-C	5.31	119.22	110.88
1	A	42	THR	N-CA-C	5.31	117.92	109.64
1	A	218	VAL	CA-C-N	-5.31	114.53	120.53
1	A	218	VAL	C-N-CA	-5.31	114.53	120.53
1	A	193	LEU	CA-C-N	-5.29	113.45	120.65
1	A	193	LEU	C-N-CA	-5.29	113.45	120.65
1	A	273	LYS	CA-C-N	-5.29	114.81	120.47
1	A	273	LYS	C-N-CA	-5.29	114.81	120.47
1	A	350	ALA	N-CA-C	5.29	118.52	111.75
1	A	35	GLY	N-CA-C	5.25	125.63	113.18
1	A	327	ILE	CA-C-N	5.25	127.31	120.28
1	A	327	ILE	C-N-CA	5.25	127.31	120.28
1	A	349	LYS	CA-C-N	-5.24	112.73	120.38
1	A	349	LYS	C-N-CA	-5.24	112.73	120.38
1	A	116	PRO	CB-CA-C	5.23	117.93	111.23
1	A	306	THR	N-CA-CB	5.23	117.73	109.94
1	A	204	ALA	N-CA-C	5.23	118.44	111.75
1	A	237	GLY	N-CA-C	5.22	120.33	111.15
1	A	312	LYS	CA-C-O	5.22	127.97	120.51
1	A	66	ASP	CB-CA-C	5.21	118.78	109.29
1	A	341	LYS	CA-C-N	5.21	127.68	120.29
1	A	341	LYS	C-N-CA	5.21	127.68	120.29
1	A	199	GLN	N-CA-CB	-5.20	102.22	110.28
1	A	81	ARG	CB-CG-CD	5.19	123.24	111.30
1	A	214	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	241	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	300	PHE	N-CA-C	5.19	119.59	113.16
1	A	235	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	342	GLU	CA-C-N	-5.18	113.71	120.44
1	A	342	GLU	C-N-CA	-5.18	113.71	120.44
1	A	253	ARG	CG-CD-NE	5.18	123.39	112.00
1	A	60	ASP	CA-C-N	5.15	129.39	120.58
1	A	60	ASP	C-N-CA	5.15	129.39	120.58
1	A	279	ALA	N-CA-C	5.13	121.72	110.80
1	A	294	THR	OG1-CB-CG2	5.11	119.51	109.30
1	A	308	TYR	CA-C-N	-5.11	113.44	120.28
1	A	308	TYR	C-N-CA	-5.11	113.44	120.28
1	A	294	THR	N-CA-C	5.10	120.49	113.97
1	A	123	ASP	CB-CA-C	-5.09	101.14	109.99
1	A	345	ASP	CA-CB-CG	5.09	117.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LYS	CA-C-O	5.08	126.79	120.54
1	A	63	ALA	CA-C-O	5.07	125.83	120.10
1	A	123	ASP	CA-C-O	5.07	125.16	119.18
1	A	188	ILE	CA-C-O	5.06	127.20	120.98
1	A	267	TYR	CA-C-N	-5.06	113.71	120.54
1	A	267	TYR	C-N-CA	-5.06	113.71	120.54
1	A	57	THR	OG1-CB-CG2	-5.06	99.19	109.30
1	A	44	GLU	CB-CG-CD	-5.05	104.01	112.60
1	A	236	LEU	CA-C-N	-5.05	115.11	120.92
1	A	236	LEU	C-N-CA	-5.05	115.11	120.92
1	A	91	ALA	N-CA-C	5.05	116.78	111.28
1	A	153	CYS	CB-CA-C	-5.04	101.80	110.22
1	A	213	VAL	CA-C-N	-5.03	113.99	121.24
1	A	213	VAL	C-N-CA	-5.03	113.99	121.24
1	A	210	HIS	N-CA-C	5.02	116.76	110.24
1	A	77	ASP	CB-CA-C	5.01	119.20	110.68
1	A	30	TYR	CB-CG-CD1	-5.01	113.29	120.80
1	A	203	GLU	N-CA-C	5.01	116.82	111.36
1	A	331	LYS	CA-CB-CG	-5.01	104.09	114.10

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	TYR	Sidechain
1	A	149	ARG	Sidechain
1	A	153	CYS	Peptide
1	A	156	ARG	Sidechain
1	A	211	ARG	Sidechain
1	A	249	TYR	Sidechain
1	A	251	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	267	TYR	Sidechain
1	A	283	PHE	Sidechain
1	A	29	TYR	Sidechain
1	A	324	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	351	TYR	Sidechain
1	A	55	PRO	Peptide
1	A	67	TYR	Sidechain
1	A	68	TYR	Sidechain
1	A	81	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2789	0	2743	146	0
2	A	1	0	0	0	0
3	A	22	0	17	1	0
4	A	146	0	0	35	0
All	All	2958	0	2760	146	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 26.

All (146) 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:225:LYS:HA	4:A:1122:HOH:O	0.89	1.06
1:A:228:VAL:HG23	4:A:1122:HOH:O	1.56	1.02
1:A:284:LYS:HD2	1:A:321:GLU:HG3	1.43	0.98
1:A:75:CYS:SG	4:A:1095:HOH:O	2.24	0.94
1:A:36:ILE:HD12	4:A:1089:HOH:O	1.66	0.93
1:A:278:HIS:HD2	1:A:280:VAL:H	1.18	0.91
1:A:137:LEU:HD21	4:A:1030:HOH:O	1.74	0.87
1:A:137:LEU:HD11	4:A:1030:HOH:O	1.77	0.85
1:A:81:ARG:HB3	4:A:1105:HOH:O	1.79	0.83
1:A:214:HIS:HB2	4:A:1127:HOH:O	1.79	0.81
1:A:109:ASN:HB3	1:A:119:GLN:OE1	1.81	0.81
1:A:278:HIS:CD2	1:A:280:VAL:H	2.03	0.75
1:A:322:PHE:HA	1:A:325:LEU:HD13	1.69	0.74
1:A:283:PHE:CD2	4:A:1021:HOH:O	2.41	0.74
1:A:100:VAL:HG11	4:A:1030:HOH:O	1.88	0.73
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.23	0.72
1:A:36:ILE:HD13	1:A:70:PRO:HB2	1.70	0.71
1:A:47:GLN:OE1	1:A:301:LYS:HG2	1.90	0.70
1:A:138:GLN:HG2	1:A:142:ARG:HH21	1.55	0.70
1:A:80:LYS:HD2	4:A:1110:HOH:O	1.92	0.68
1:A:54:LYS:HD3	4:A:1083:HOH:O	1.93	0.68
1:A:267:TYR:CE1	1:A:268:LEU:HD23	2.29	0.68
1:A:33:ARG:HD3	4:A:1052:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:HA2	1:A:260:GLU:HB2	1.78	0.65
1:A:88:GLU:HG3	1:A:144:PHE:CE2	2.31	0.65
1:A:267:TYR:HE1	1:A:268:LEU:HD23	1.63	0.63
1:A:117:TRP:HH2	3:A:1001:FR7:H25	1.64	0.62
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.82	0.62
1:A:277:GLU:HB2	4:A:1125:HOH:O	1.99	0.62
1:A:284:LYS:HD3	1:A:317:PHE:CE1	2.35	0.62
1:A:310:MET:HB3	4:A:1123:HOH:O	2.00	0.61
1:A:23:LYS:HD3	1:A:85:GLU:OE2	2.01	0.61
1:A:133:VAL:HG12	1:A:137:LEU:HD22	1.82	0.60
1:A:320:GLU:HG2	4:A:1079:HOH:O	2.01	0.60
1:A:29:TYR:CE1	1:A:33:ARG:HD2	2.37	0.60
1:A:308:TYR:O	1:A:312:LYS:HB2	2.03	0.58
1:A:44:GLU:HG3	4:A:1138:HOH:O	2.02	0.58
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.85	0.58
1:A:174:GLU:O	1:A:176:THR:HA	2.02	0.58
1:A:313:LYS:HA	1:A:313:LYS:HE3	1.86	0.58
1:A:272:TRP:HE1	1:A:276:THR:HG22	1.68	0.58
1:A:81:ARG:HD3	1:A:85:GLU:OE1	2.03	0.58
1:A:78:ALA:O	1:A:82:ILE:HG23	2.04	0.57
1:A:319:GLU:HB2	4:A:1008:HOH:O	2.02	0.57
1:A:28:LEU:HD13	1:A:38:LEU:HD12	1.86	0.57
1:A:57:THR:HG23	1:A:60:ASP:HB2	1.85	0.57
1:A:138:GLN:O	1:A:142:ARG:HG2	2.05	0.56
1:A:327:ILE:CG2	4:A:1068:HOH:O	2.52	0.56
1:A:251:ARG:O	1:A:255:GLU:HG3	2.05	0.56
1:A:228:VAL:O	1:A:232:LYS:HA	2.07	0.55
1:A:272:TRP:NE1	1:A:276:THR:HG22	2.22	0.55
1:A:297:PRO:HA	1:A:302:SER:OG	2.07	0.55
1:A:159:PRO:HB2	1:A:196:GLY:HA3	1.88	0.55
1:A:261:ILE:HG13	4:A:1021:HOH:O	2.07	0.55
1:A:86:PHE:HZ	1:A:98:VAL:HG21	1.73	0.53
1:A:142:ARG:CB	4:A:1023:HOH:O	2.56	0.53
1:A:272:TRP:NE1	1:A:278:HIS:HA	2.23	0.53
1:A:345:ASP:OD1	1:A:349:LYS:HE3	2.08	0.53
1:A:85:GLU:O	1:A:89:MET:HB2	2.09	0.52
1:A:152:LEU:HD12	1:A:168:LEU:HB3	1.90	0.52
1:A:57:THR:O	1:A:58:LEU:C	2.49	0.52
1:A:49:ILE:C	1:A:51:GLY:H	2.18	0.52
1:A:318:THR:O	1:A:319:GLU:C	2.53	0.52
1:A:28:LEU:HA	1:A:38:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:O	1:A:85:GLU:HG2	2.10	0.51
1:A:292:LEU:HD13	1:A:325:LEU:HG	1.93	0.51
1:A:75:CYS:O	1:A:76:ARG:C	2.54	0.51
1:A:130:VAL:HG21	1:A:168:LEU:HG	1.93	0.51
1:A:23:LYS:O	1:A:24:PRO:C	2.54	0.50
1:A:29:TYR:O	1:A:33:ARG:HB2	2.12	0.50
1:A:186:GLU:CD	1:A:219:GLY:H	2.20	0.50
1:A:47:GLN:NE2	1:A:298:LEU:HD12	2.26	0.49
1:A:125:THR:HB	1:A:126:PRO:HD2	1.93	0.49
1:A:39:PRO:HG3	1:A:67:TYR:CD2	2.48	0.49
1:A:117:TRP:O	1:A:118:ASN:C	2.55	0.49
1:A:22:ILE:HD13	1:A:72:ILE:CD1	2.42	0.48
1:A:149:ARG:HH11	1:A:174:GLU:HG2	1.79	0.48
1:A:162:SER:HB3	1:A:200:ALA:CB	2.44	0.48
1:A:162:SER:HB3	1:A:200:ALA:HB2	1.94	0.48
1:A:267:TYR:O	1:A:268:LEU:C	2.52	0.48
1:A:261:ILE:HG22	1:A:263:PRO:HD3	1.95	0.48
1:A:22:ILE:O	1:A:298:LEU:HD13	2.13	0.48
1:A:76:ARG:HH11	1:A:76:ARG:HG3	1.79	0.47
1:A:305:ASP:CB	4:A:1115:HOH:O	2.63	0.47
1:A:313:LYS:HA	1:A:313:LYS:CE	2.44	0.47
1:A:116:PRO:O	1:A:117:TRP:C	2.56	0.46
1:A:44:GLU:O	1:A:48:ASN:CG	2.58	0.46
1:A:162:SER:O	1:A:165:VAL:HB	2.14	0.46
1:A:280:VAL:HG22	1:A:317:PHE:HZ	1.80	0.46
1:A:266:SER:OG	1:A:278:HIS:HE1	1.98	0.46
1:A:22:ILE:HD13	1:A:72:ILE:HD11	1.98	0.46
1:A:321:GLU:OE1	1:A:324:ARG:NE	2.48	0.46
1:A:327:ILE:HG21	4:A:1068:HOH:O	2.15	0.46
1:A:100:VAL:O	1:A:150:SER:HA	2.15	0.46
1:A:26:THR:O	1:A:30:TYR:HD2	1.98	0.46
1:A:98:VAL:HG13	1:A:148:VAL:HG13	1.98	0.46
1:A:204:ALA:HA	1:A:209:VAL:HG13	1.98	0.46
1:A:162:SER:OG	1:A:197:HIS:HD2	1.99	0.45
1:A:88:GLU:HG3	1:A:144:PHE:CD2	2.51	0.45
1:A:188:ILE:HG22	1:A:191:SER:HB3	1.97	0.45
1:A:133:VAL:O	1:A:137:LEU:HB2	2.16	0.45
1:A:72:ILE:HG21	1:A:72:ILE:HD13	1.72	0.45
1:A:310:MET:CB	4:A:1123:HOH:O	2.61	0.45
1:A:49:ILE:C	1:A:51:GLY:N	2.75	0.45
1:A:56:LEU:HD22	1:A:60:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:CZ	1:A:33:ARG:HD2	2.53	0.44
1:A:185:ASP:O	1:A:187:THR:N	2.51	0.44
1:A:281:ILE:HD13	4:A:1062:HOH:O	2.16	0.44
1:A:131:SER:HB3	1:A:135:GLN:HE21	1.83	0.44
1:A:57:THR:OG1	1:A:59:PRO:HD2	2.18	0.44
1:A:156:ARG:HD2	1:A:191:SER:OG	2.17	0.44
1:A:161:TRP:O	1:A:165:VAL:HG23	2.19	0.43
1:A:24:PRO:HG2	4:A:1143:HOH:O	2.19	0.43
1:A:49:ILE:HD11	4:A:1130:HOH:O	2.19	0.43
1:A:11:LYS:HB2	1:A:326:ASN:OD1	2.19	0.43
1:A:57:THR:HG23	1:A:60:ASP:CB	2.49	0.43
1:A:305:ASP:HB3	4:A:1115:HOH:O	2.19	0.43
1:A:117:TRP:O	1:A:119:GLN:N	2.52	0.42
1:A:52:MET:HB3	1:A:299:ILE:O	2.19	0.42
1:A:30:TYR:HE2	4:A:1105:HOH:O	2.03	0.42
1:A:149:ARG:HD3	1:A:178:VAL:HG13	2.00	0.42
1:A:278:HIS:CD2	1:A:278:HIS:C	2.97	0.42
1:A:42:THR:O	1:A:44:GLU:N	2.52	0.42
1:A:32:LYS:HD3	1:A:33:ARG:HA	2.01	0.42
1:A:113:GLU:HA	1:A:114:PRO:HA	1.64	0.42
1:A:310:MET:O	1:A:314:ASP:N	2.49	0.42
1:A:138:GLN:HG2	1:A:142:ARG:NH2	2.27	0.42
1:A:261:ILE:CG1	4:A:1021:HOH:O	2.66	0.42
1:A:100:VAL:CG1	4:A:1030:HOH:O	2.54	0.42
1:A:131:SER:O	1:A:135:GLN:HG3	2.20	0.42
1:A:186:GLU:OE1	1:A:215:ALA:HA	2.20	0.42
1:A:142:ARG:HB3	4:A:1023:HOH:O	2.18	0.41
1:A:261:ILE:HD11	4:A:1021:HOH:O	2.19	0.41
1:A:273:LYS:HB3	4:A:1091:HOH:O	2.19	0.41
1:A:43:PRO:O	1:A:44:GLU:OE1	2.38	0.41
1:A:319:GLU:O	1:A:322:PHE:HB2	2.20	0.41
1:A:29:TYR:CD1	1:A:29:TYR:C	2.99	0.41
1:A:32:LYS:O	1:A:33:ARG:C	2.62	0.41
1:A:268:LEU:HD12	1:A:300:PHE:HB3	2.02	0.41
1:A:313:LYS:HE3	1:A:313:LYS:CA	2.49	0.41
1:A:225:LYS:HB3	1:A:248:LEU:HD22	2.04	0.41
1:A:283:PHE:HD2	4:A:1021:HOH:O	1.92	0.41
1:A:284:LYS:CD	1:A:321:GLU:HG3	2.31	0.41
1:A:28:LEU:HD13	1:A:28:LEU:HA	1.82	0.40
1:A:312:LYS:HB3	1:A:313:LYS:H	1.68	0.40
1:A:154:CYS:SG	1:A:180:ILE:HD11	2.62	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%)	307 (88%)	30 (9%)	10 (3%)	3 5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLY
1	A	174	GLU
1	A	44	GLU
1	A	265	SER
1	A	50	ILE
1	A	121	GLU
1	A	186	GLU
1	A	277	GLU
1	A	238	HIS
1	A	43	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	304/309 (98%)	247 (81%)	57 (19%)	1 3

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	11	LYS
1	A	12	VAL
1	A	25	GLU
1	A	28	LEU
1	A	32	LYS
1	A	36	ILE
1	A	41	ASP
1	A	44	GLU
1	A	46	LEU
1	A	47	GLN
1	A	48	ASN
1	A	49	ILE
1	A	50	ILE
1	A	54	LYS
1	A	56	LEU
1	A	60	ASP
1	A	64	LYS
1	A	66	ASP
1	A	77	ASP
1	A	81	ARG
1	A	95	VAL
1	A	110	SER
1	A	115	ILE
1	A	117	TRP
1	A	121	GLU
1	A	124	LEU
1	A	137	LEU
1	A	142	ARG
1	A	147	LYS
1	A	152	LEU
1	A	166	VAL
1	A	168	LEU
1	A	174	GLU
1	A	177	VAL
1	A	193	LEU
1	A	206	LYS
1	A	207	SER
1	A	209	VAL
1	A	218	VAL
1	A	223	VAL
1	A	232	LYS
1	A	253	ARG

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Mol	Chain	Res	Type
1	A	254	GLN
1	A	267	TYR
1	A	273	LYS
1	A	276	THR
1	A	277	GLU
1	A	281	ILE
1	A	287	GLN
1	A	294	THR
1	A	312	LYS
1	A	320	GLU
1	A	325	LEU
1	A	335	LEU
1	A	347	LEU
1	A	352	ARG

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

Mol	Chain	Res	Type
1	A	134	ASN
1	A	135	GLN
1	A	138	GLN
1	A	197	HIS
1	A	199	GLN
1	A	210	HIS
1	A	250	ASN
1	A	278	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FR7	A	1001	-	22,23,23	1.80	7 (31%)	25,32,32	2.93	6 (24%)

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	FR7	A	1001	-	-	0/17/17/17	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR7	C1-N2	4.19	1.47	1.37
3	A	1001	FR7	O9-C8	-3.15	1.17	1.24
3	A	1001	FR7	C18-C13	2.99	1.57	1.53
3	A	1001	FR7	C3-N2	-2.51	1.31	1.35
3	A	1001	FR7	C5-N4	2.41	1.45	1.39
3	A	1001	FR7	C5-C8	2.11	1.51	1.48
3	A	1001	FR7	C1-C5	-2.07	1.34	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR7	O9-C8-C5	-8.45	112.13	120.25
3	A	1001	FR7	C5-C8-N10	8.11	124.52	116.28
3	A	1001	FR7	C1-N2-C3	-4.41	103.44	106.37
3	A	1001	FR7	O15-C14-C9	-4.13	97.32	109.68
3	A	1001	FR7	C1-C5-N4	-3.26	106.11	109.78
3	A	1001	FR7	C8-C5-N4	2.97	127.93	121.52

There are no chirality outliers.

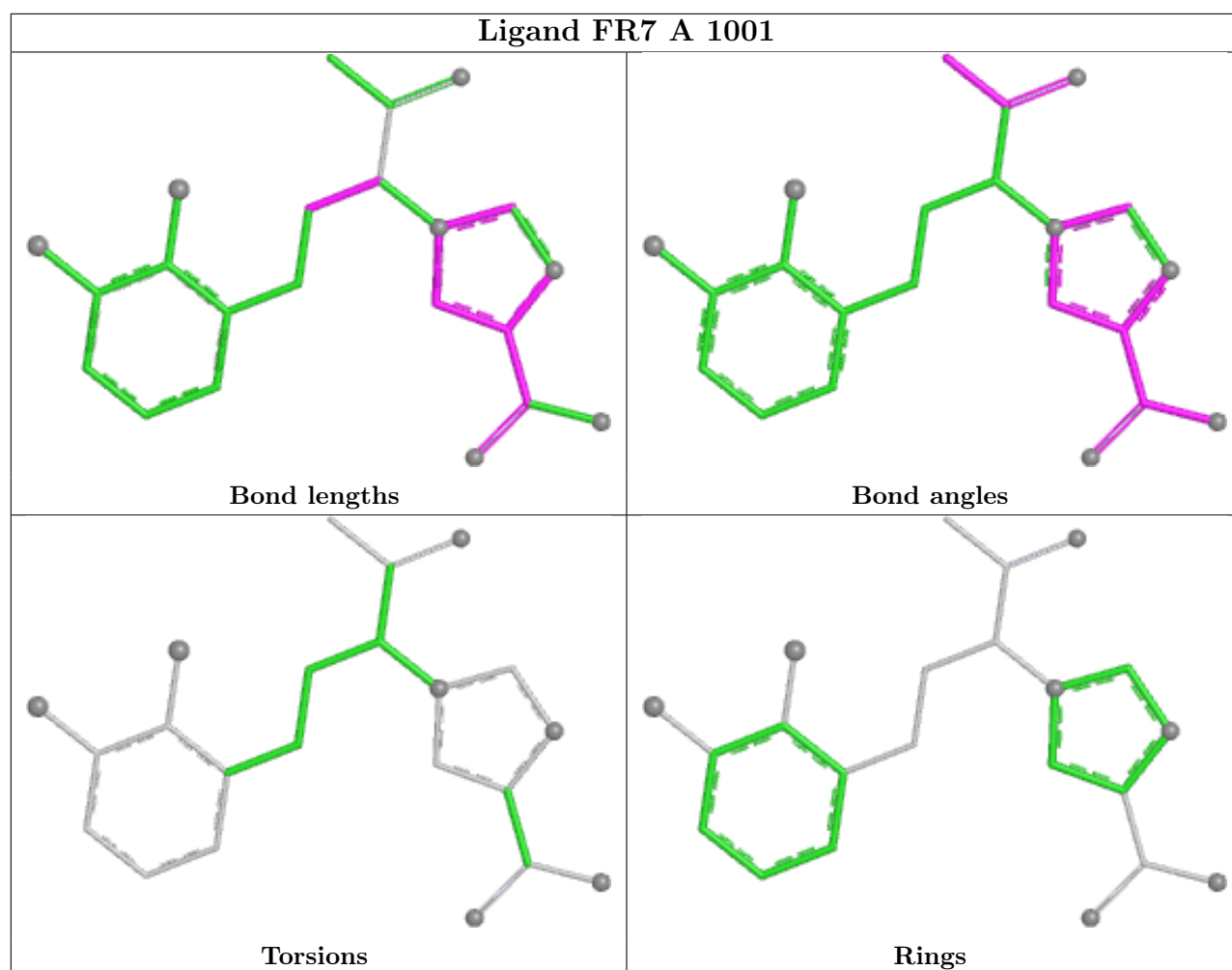
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	FR7	1	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 [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%)	-0.19	2 (0%) 85 83	5, 17, 34, 42	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	4.2
1	A	287	GLN	2.1

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.

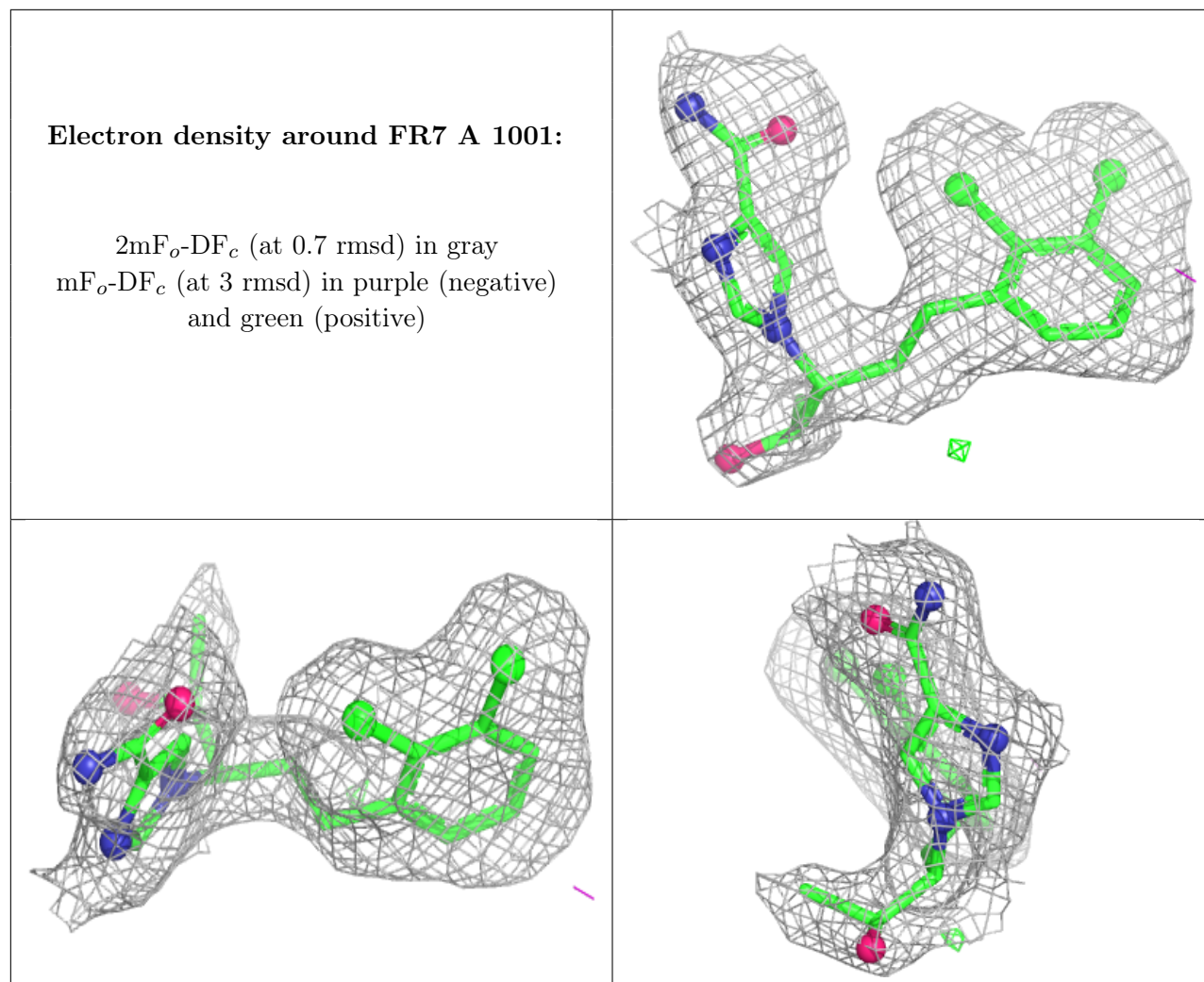
6.4 Ligands [i](#)

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	FR7	A	1001	22/22	0.96	0.07	8,18,23,30	0
2	ZN	A	400	1/1	0.99	0.04	19,19,19,19	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.