



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:04 am BST

PDB ID : 1V79  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

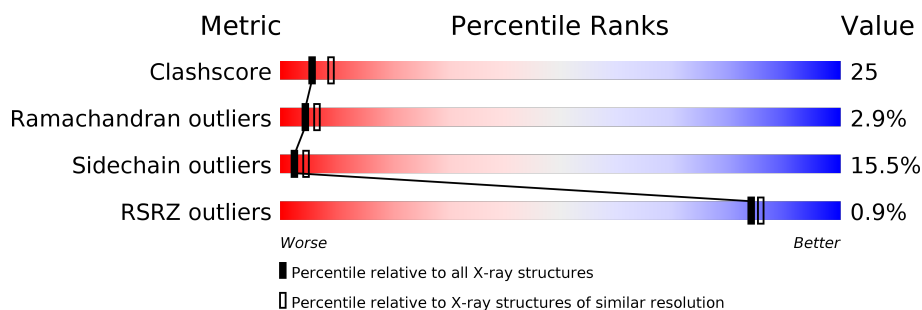
# 1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div></div> <div>41%36%15%6%</div> </div>

## 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			

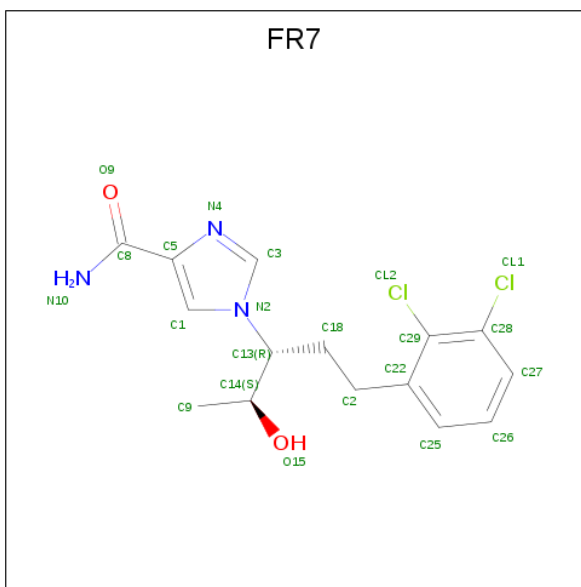
There are 15 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: FR7) (formula: C<sub>15</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub>).



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

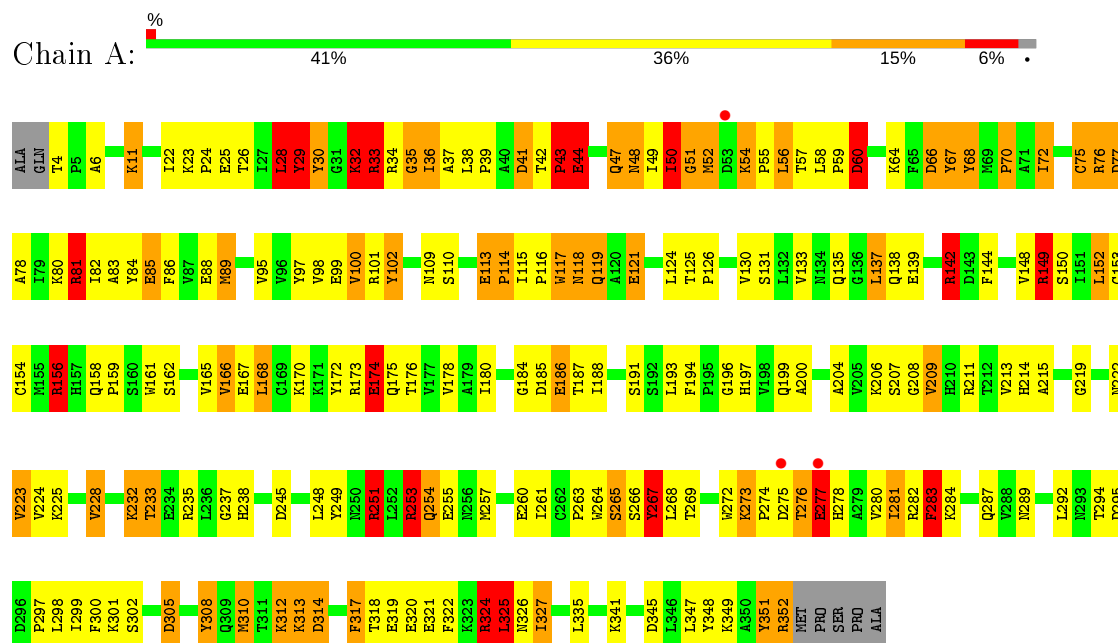
- Molecule 4 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	77.23 Å 77.23 Å 135.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50 25.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.50) 95.2 (25.29-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.63 (at 2.50 Å)	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 <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.52	19/2853 (0.7%)	2.30	128/3867 (3.3%)

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	18

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	VAL	CB-CG1	-11.13	1.29	1.52
1	A	277	GLU	CG-CD	10.19	1.67	1.51
1	A	113	GLU	CG-CD	7.30	1.62	1.51
1	A	253	ARG	NE-CZ	6.80	1.41	1.33
1	A	277	GLU	CB-CG	6.70	1.64	1.52
1	A	142	ARG	CA-CB	-6.64	1.39	1.53
1	A	174	GLU	CB-CG	6.55	1.64	1.52
1	A	167	GLU	CD-OE1	-6.36	1.18	1.25
1	A	267	TYR	CE2-CZ	6.35	1.46	1.38
1	A	60	ASP	CB-CG	6.28	1.65	1.51
1	A	139	GLU	CD-OE2	5.90	1.32	1.25
1	A	85	GLU	CD-OE2	-5.73	1.19	1.25
1	A	99	GLU	CD-OE1	-5.46	1.19	1.25
1	A	118	ASN	CB-CG	5.45	1.63	1.51
1	A	173	ARG	NE-CZ	5.34	1.40	1.33
1	A	174	GLU	CG-CD	5.19	1.59	1.51
1	A	184	GLY	C-O	-5.17	1.15	1.23
1	A	264	TRP	NE1-CE2	5.11	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CD-OE1	-5.07	1.20	1.25

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	NE-CZ-NH1	-18.08	111.26	120.30
1	A	30	TYR	CB-CG-CD1	-12.85	113.29	121.00
1	A	341	LYS	CA-CB-CG	-12.03	86.94	113.40
1	A	156	ARG	NE-CZ-NH2	-11.81	114.40	120.30
1	A	235	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	60	ASP	CA-CB-CG	11.47	138.64	113.40
1	A	102	TYR	CB-CG-CD1	-11.22	114.27	121.00
1	A	101	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	A	156	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	283	PHE	CG-CD2-CE2	10.47	132.32	120.80
1	A	235	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	44	GLU	CB-CA-C	-9.57	91.27	110.40
1	A	97	TYR	CB-CG-CD1	-9.55	115.27	121.00
1	A	95	VAL	CA-CB-CG2	-9.29	96.96	110.90
1	A	310	MET	CA-CB-CG	9.18	128.90	113.30
1	A	68	TYR	CB-CG-CD2	-9.12	115.53	121.00
1	A	60	ASP	CB-CG-OD2	9.05	126.44	118.30
1	A	33	ARG	CD-NE-CZ	-8.65	111.49	123.60
1	A	149	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	149	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	308	TYR	CB-CG-CD2	-8.14	116.12	121.00
1	A	276	THR	N-CA-CB	-8.01	95.08	110.30
1	A	223	VAL	CA-CB-CG2	7.91	122.76	110.90
1	A	224	VAL	CG1-CB-CG2	7.78	123.35	110.90
1	A	77	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	29	TYR	CB-CG-CD1	-7.61	116.43	121.00
1	A	253	ARG	CD-NE-CZ	-7.61	112.94	123.60
1	A	253	ARG	CA-CB-CG	7.57	130.05	113.40
1	A	277	GLU	CA-CB-CG	7.55	130.00	113.40
1	A	351	TYR	C-N-CA	-7.53	102.88	121.70
1	A	81	ARG	CD-NE-CZ	-7.48	113.13	123.60
1	A	251	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	267	TYR	CB-CG-CD1	-7.31	116.61	121.00
1	A	89	MET	CA-CB-CG	7.29	125.69	113.30
1	A	114	PRO	N-CA-CB	-7.23	94.62	103.30
1	A	70	PRO	C-N-CA	-7.06	104.06	121.70
1	A	52	MET	N-CA-CB	-7.02	97.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	VAL	CA-CB-CG1	6.90	121.25	110.90
1	A	84	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	283	PHE	CB-CG-CD2	6.84	125.59	120.80
1	A	119	GLN	C-N-CA	-6.74	104.86	121.70
1	A	327	ILE	CA-CB-CG1	6.71	123.75	111.00
1	A	254	GLN	CB-CG-CD	-6.64	94.33	111.60
1	A	194	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	A	310	MET	N-CA-CB	6.55	122.39	110.60
1	A	269	THR	C-N-CA	-6.46	108.72	122.30
1	A	295	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	166	VAL	CB-CA-C	-6.41	99.22	111.40
1	A	199	GLN	CB-CA-C	6.32	123.04	110.40
1	A	51	GLY	C-N-CA	-6.28	106.00	121.70
1	A	224	VAL	C-N-CA	-6.24	106.09	121.70
1	A	118	ASN	C-N-CA	-6.22	106.14	121.70
1	A	325	LEU	CB-CA-C	6.22	122.02	110.20
1	A	348	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	A	28	LEU	CB-CA-C	-6.16	98.50	110.20
1	A	283	PHE	CZ-CE2-CD2	-6.14	112.74	120.10
1	A	233	THR	CB-CA-C	-6.13	95.06	111.60
1	A	166	VAL	CG1-CB-CG2	6.11	120.68	110.90
1	A	173	ARG	C-N-CA	6.11	136.98	121.70
1	A	170	LYS	CD-CE-NZ	-6.10	97.66	111.70
1	A	352	ARG	CB-CA-C	6.09	122.58	110.40
1	A	308	TYR	CD1-CG-CD2	6.06	124.57	117.90
1	A	95	VAL	N-CA-CB	-6.02	98.26	111.50
1	A	269	THR	CB-CA-C	-5.99	95.42	111.60
1	A	142	ARG	CD-NE-CZ	-5.96	115.25	123.60
1	A	115	ILE	CA-CB-CG1	-5.96	99.67	111.00
1	A	52	MET	CA-CB-CG	5.96	123.43	113.30
1	A	314	ASP	N-CA-C	5.96	127.09	111.00
1	A	265	SER	CB-CA-C	-5.94	98.82	110.10
1	A	251	ARG	CB-CG-CD	-5.89	96.30	111.60
1	A	158	GLN	CA-CB-CG	5.86	126.29	113.40
1	A	175	GLN	C-N-CA	5.85	136.33	121.70
1	A	289	ASN	N-CA-CB	-5.83	100.10	110.60
1	A	77	ASP	CA-CB-CG	5.81	126.18	113.40
1	A	89	MET	N-CA-CB	-5.81	100.14	110.60
1	A	317	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	A	222	ASN	CA-CB-CG	-5.79	100.67	113.40
1	A	52	MET	CB-CA-C	5.77	121.93	110.40
1	A	43	PRO	O-C-N	5.76	131.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ILE	C-N-CA	-5.72	110.28	122.30
1	A	175	GLN	CA-CB-CG	5.70	125.94	113.40
1	A	30	TYR	CD1-CG-CD2	5.70	124.17	117.90
1	A	84	TYR	N-CA-C	5.69	126.36	111.00
1	A	60	ASP	CB-CA-C	5.68	121.75	110.40
1	A	352	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	66	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	52	MET	C-N-CA	-5.62	107.66	121.70
1	A	76	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	289	ASN	CB-CA-C	5.56	121.51	110.40
1	A	253	ARG	CG-CD-NE	5.52	123.39	111.80
1	A	305	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	41	ASP	CA-CB-CG	-5.51	101.29	113.40
1	A	283	PHE	CD1-CG-CD2	-5.50	111.15	118.30
1	A	208	GLY	C-N-CA	-5.47	108.02	121.70
1	A	85	GLU	CB-CA-C	5.45	121.30	110.40
1	A	97	TYR	CD1-CG-CD2	5.44	123.88	117.90
1	A	37	ALA	CA-C-O	5.40	131.44	120.10
1	A	75	CYS	N-CA-C	5.40	125.58	111.00
1	A	275	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	274	PRO	C-N-CA	-5.34	108.36	121.70
1	A	325	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	34	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	308	TYR	CG-CD2-CE2	-5.28	117.08	121.30
1	A	72	ILE	CB-CG1-CD1	-5.27	99.15	113.90
1	A	351	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	A	142	ARG	CB-CG-CD	5.24	125.22	111.60
1	A	32	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	310	MET	C-N-CA	-5.20	108.70	121.70
1	A	172	TYR	CB-CG-CD1	-5.19	117.88	121.00
1	A	245	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	184	GLY	CA-C-O	5.18	129.93	120.60
1	A	43	PRO	CA-C-O	-5.15	107.85	120.20
1	A	6	ALA	CB-CA-C	5.13	117.80	110.10
1	A	166	VAL	N-CA-CB	5.13	122.79	111.50
1	A	30	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	A	257	MET	CA-CB-CG	5.11	121.99	113.30
1	A	95	VAL	CG1-CB-CG2	5.09	119.04	110.90
1	A	228	VAL	CB-CA-C	-5.09	101.73	111.40
1	A	313	LYS	C-N-CA	-5.08	109.00	121.70
1	A	175	GLN	N-CA-CB	-5.08	101.46	110.60
1	A	30	TYR	CG-CD1-CE1	-5.06	117.25	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	41	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	282	ARG	C-N-CA	-5.03	109.12	121.70
1	A	41	ASP	N-CA-C	5.03	124.58	111.00
1	A	324	ARG	CD-NE-CZ	-5.03	116.57	123.60
1	A	35	GLY	N-CA-C	5.01	125.63	113.10
1	A	295	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	A	60	ASP	OD1-CG-OD2	-5.00	113.79	123.30

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	142	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	17	1	0
4	A	146	0	0	35	0
All	All	2958	0	2760	142	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 25.

All (142) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:ALA:HB1	1:A:137:LEU:HD13	1.85	0.58
1:A:44:GLU:HG3	4:A:1138:HOH:O	2.02	0.58
1:A:174:GLU:O	1:A:176:THR:HA	2.02	0.58
1:A:313:LYS:HE3	1:A:313:LYS:HA	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:142:ARG:CB	4:A:1023:HOH:O	2.56	0.53
1:A:86:PHE:HZ	1:A:98:VAL:HG21	1.73	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:28:LEU:HA	1:A:38:LEU:CD1	2.40	0.51
1:A:292:LEU:HD13	1:A:325:LEU:HG	1.93	0.51
1:A:81:ARG:O	1:A:85:GLU:HG2	2.10	0.51
1:A:130:VAL:HG21	1:A:168:LEU:HG	1.93	0.51
1:A:29:TYR:O	1:A:33:ARG:HB2	2.12	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:57:THR:O	1:A:58:LEU:C	2.49	0.49
1:A:39:PRO:HG3	1:A:67:TYR:CD2	2.48	0.49
1:A:22:ILE:HD13	1:A:72:ILE:CD1	2.42	0.48
1:A:162:SER:HB3	1:A:200:ALA:CB	2.44	0.48
1:A:149:ARG:HH11	1:A:174:GLU:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:HB3	1:A:200:ALA:HB2	1.94	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:267:TYR:O	1:A:268:LEU:C	2.52	0.48
1:A:305:ASP:CB	4:A:1115:HOH:O	2.63	0.47
1:A:313:LYS:CE	1:A:313:LYS:HA	2.44	0.47
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.79	0.47
1:A:49:ILE:C	1:A:51:GLY:H	2.18	0.47
1:A:318:THR:O	1:A:319:GLU:C	2.53	0.47
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:75:CYS:O	1:A:76:ARG:C	2.54	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:23:LYS:O	1:A:24:PRO:C	2.54	0.46
1:A:26:THR:O	1:A:30:TYR:HD2	1.98	0.46
1:A:204:ALA:HA	1:A:209:VAL:HG13	1.98	0.46
1:A:98:VAL:HG13	1:A:148: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:186:GLU:CD	1:A:219:GLY:H	2.20	0.45
1:A:133:VAL:O	1:A:137:LEU:HB2	2.16	0.45
1:A:310:MET:CB	4:A:1123:HOH:O	2.61	0.45
1:A:72:ILE:HG21	1:A:72:ILE:HD13	1.72	0.45
1:A:117:TRP:O	1:A:118:ASN:C	2.55	0.44
1:A:56:LEU:HD22	1:A:60:ASP:HB3	1.99	0.44
1:A:185:ASP:O	1:A:187:THR:N	2.51	0.44
1:A:29:TYR:CZ	1:A:33:ARG:HD2	2.53	0.44
1:A:116:PRO:O	1:A:117:TRP:C	2.56	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:156:ARG:HD2	1:A:191:SER:OG	2.17	0.44
1:A:57:THR:OG1	1:A:59:PRO:HD2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:ARG:HD3	1:A:178:VAL:HG13	2.00	0.42
1:A:30:TYR:HE2	4:A:1105:HOH:O	2.03	0.42
1:A:42:THR:O	1:A:44:GLU:N	2.52	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:32:LYS:HD3	1:A:33:ARG:HA	2.01	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:44:GLU:O	1:A:48:ASN:CG	2.58	0.41
1:A:319:GLU:O	1:A:322:PHE:HB2	2.20	0.41
1:A:43:PRO:O	1:A:44:GLU:OE1	2.38	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 ⓘ

### 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%)	307 (88%)	30 (9%)	10 (3%)	<b>4</b> <b>6</b>

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 ⓘ

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%)	257 (84%)	47 (16%)	<b>2</b> <b>4</b>

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	11	LYS
1	A	25	GLU
1	A	28	LEU
1	A	32	LYS
1	A	36	ILE
1	A	41	ASP
1	A	44	GLU
1	A	47	GLN
1	A	48	ASN
1	A	50	ILE

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Mol	Chain	Res	Type
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	110	SER
1	A	117	TRP
1	A	121	GLU
1	A	124	LEU
1	A	137	LEU
1	A	142	ARG
1	A	152	LEU
1	A	166	VAL
1	A	168	LEU
1	A	174	GLU
1	A	193	LEU
1	A	206	LYS
1	A	207	SER
1	A	209	VAL
1	A	223	VAL
1	A	232	LYS
1	A	253	ARG
1	A	254	GLN
1	A	267	TYR
1	A	273	LYS
1	A	277	GLU
1	A	281	ILE
1	A	287	GLN
1	A	294	THR
1	A	312	LYS
1	A	325	LEU
1	A	335	LEU
1	A	347	LEU
1	A	352	ARG

Some 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

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Mol	Chain	Res	Type
1	A	138	GLN
1	A	158	GLN
1	A	197	HIS
1	A	210	HIS
1	A	250	ASN
1	A	278	HIS

### 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 carbohydrates 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	FR7	A	1001	-	19,23,23	2.09	4 (21%)	20,32,32	3.03	3 (15%)

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	-	-	0/9/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR7	C1-N2	6.51	1.47	1.38
3	A	1001	FR7	O9-C8	-3.69	1.17	1.24
3	A	1001	FR7	C18-C13	2.71	1.57	1.53
3	A	1001	FR7	C5-N4	2.60	1.45	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR7	O9-C8-C5	-8.95	112.13	119.61
3	A	1001	FR7	C5-C8-N10	8.36	124.52	116.25
3	A	1001	FR7	O15-C14-C9	-4.19	97.32	109.74

There are no chirality outliers.

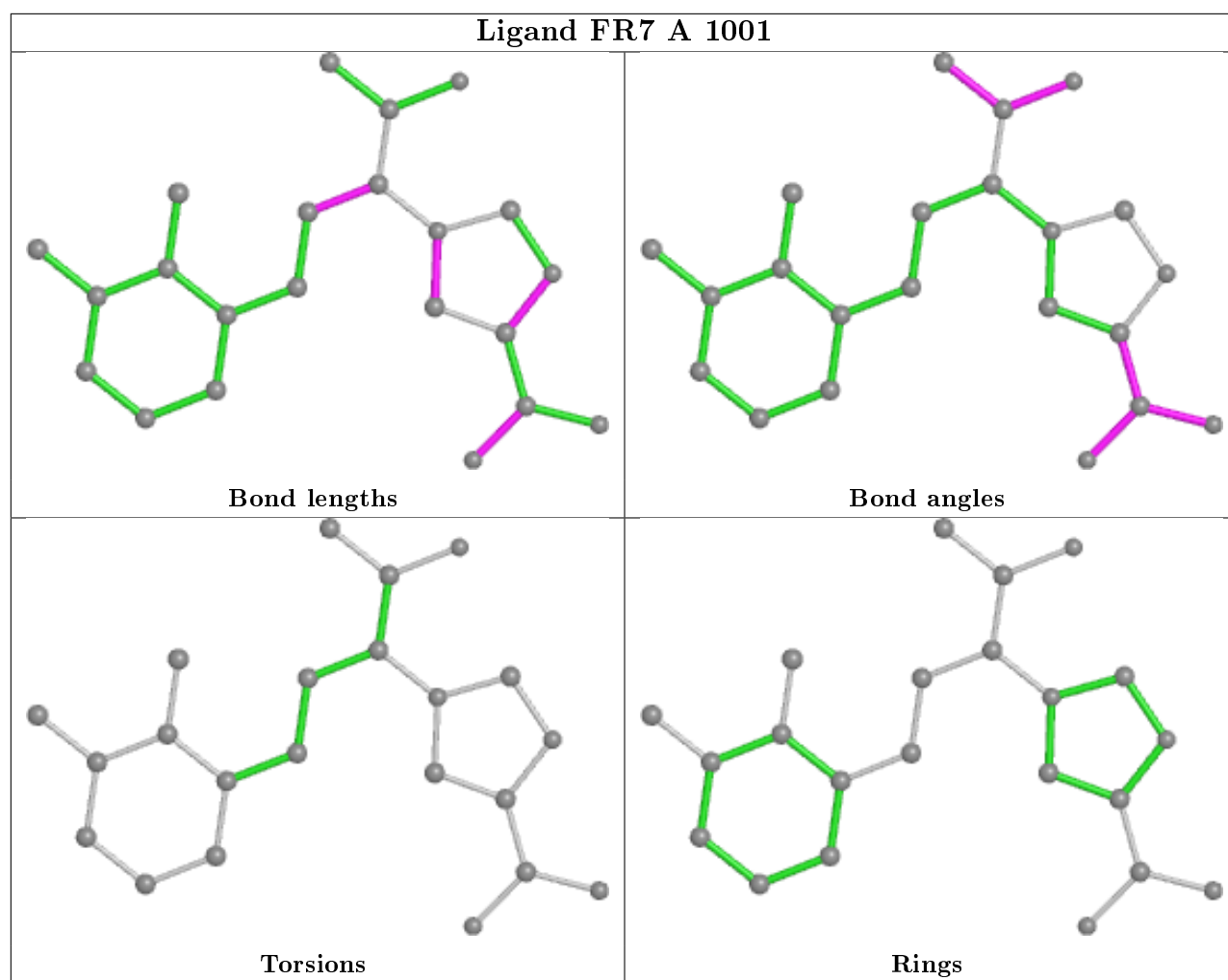
There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	349/356 (98%)	-0.32	3 (0%) 84 86	5, 17, 34, 42	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	3.3
1	A	275	ASP	3.1
1	A	53	ASP	2.4

### 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 carbohydrates in this entry.

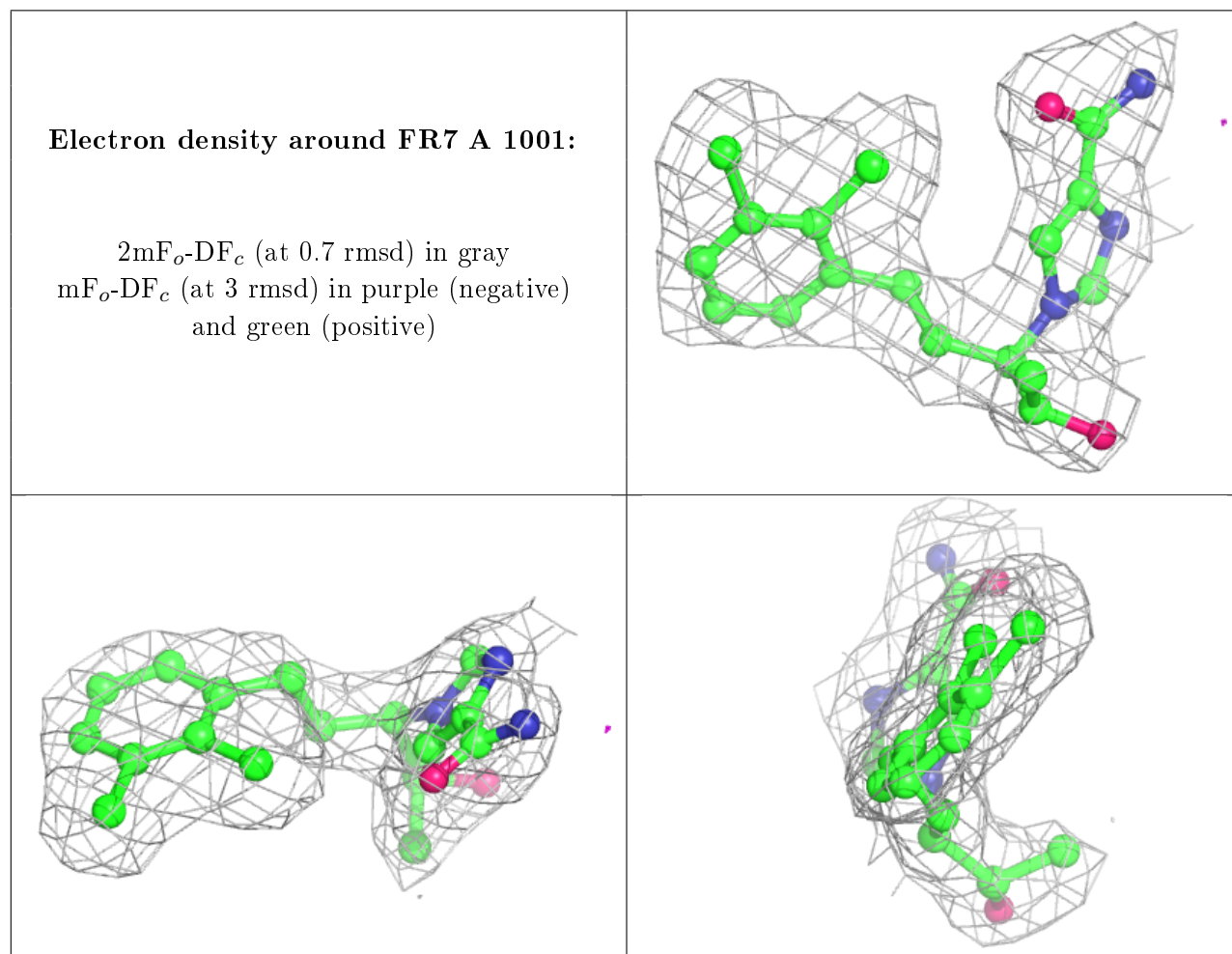
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	FR7	A	1001	22/22	0.95	0.15	8,18,23,30	0
2	ZN	A	400	1/1	0.99	0.10	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.