



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:07 am BST

PDB ID : 1O5R  
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](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

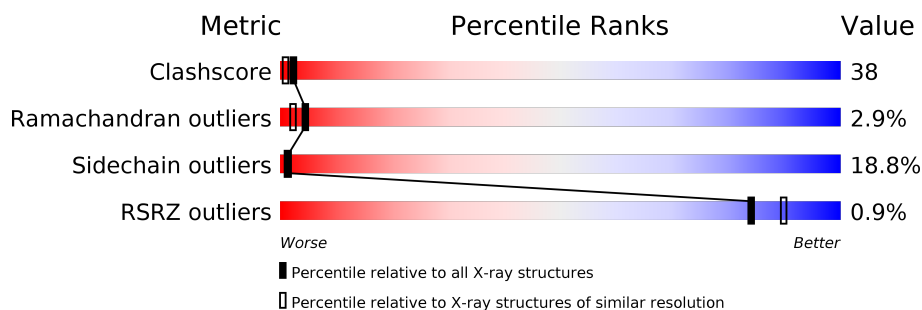
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 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>40%</div> <div>39%</div> <div>15%</div> <div>• •</div> </div>

## 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			

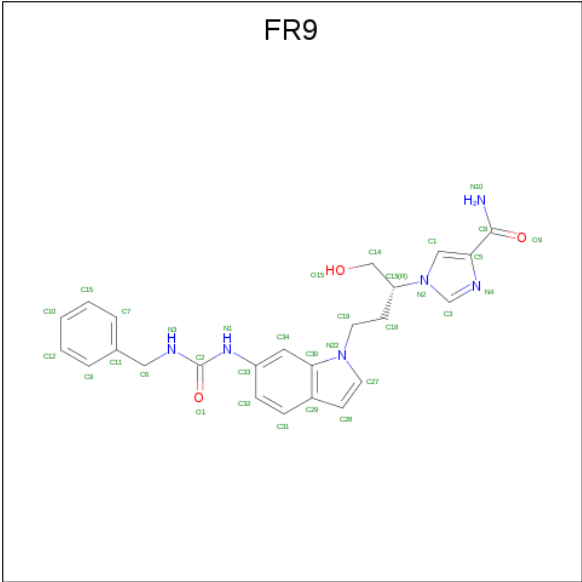
There are 15 discrepancies between the modelled and reference sequences:

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 (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)-3-(6-[(BENZYLAMINO)CARBONYL]AMINO)-1H-INDOL-1-YL)-1-(HYDROXYMETHYL)PROPYL]-1H-IMIDAZOLE-4-CARBOXAMIDE (three-letter code: FR9) (formula: C<sub>24</sub>H<sub>26</sub>N<sub>6</sub>O<sub>3</sub>).



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

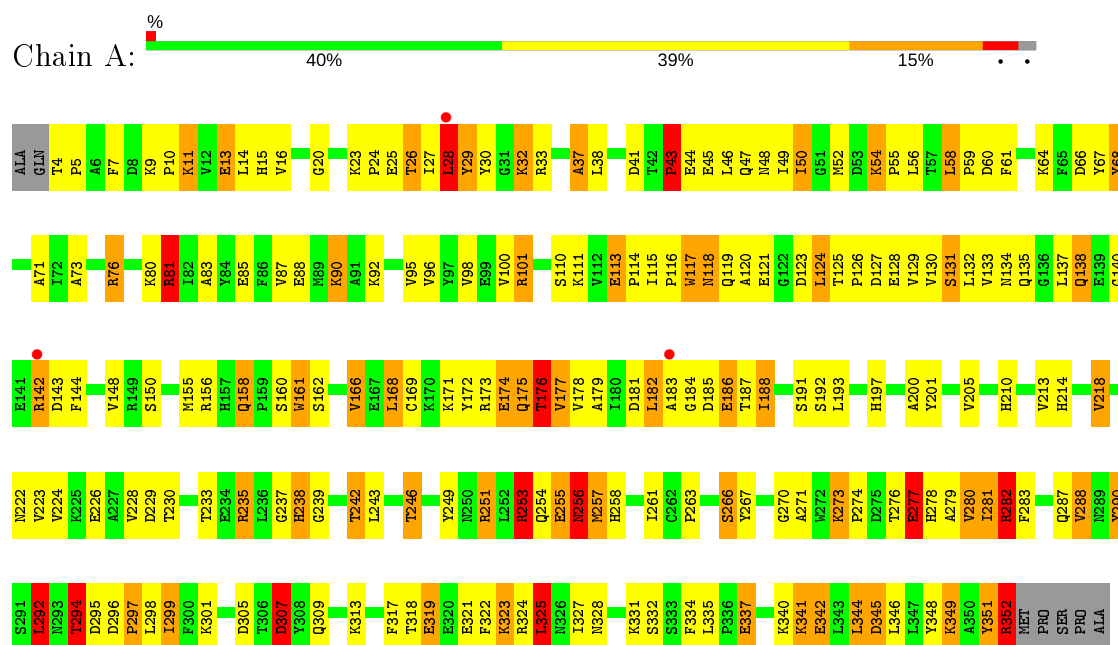
- Molecule 4 is water.

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 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, $\alpha$ , $\beta$ , $\gamma$	78.44Å 78.44Å 137.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.35 78.44 – 2.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.35) 99.0 (78.44-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.05Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.228 , 0.242 0.225 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 73.9	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	0.94	EDS
Total number of atoms	3049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 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	1.28	18/2853 (0.6%)	1.73	59/3867 (1.5%)

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	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	GLU	C-N	-10.82	1.09	1.34
1	A	13	GLU	CD-OE1	-8.83	1.16	1.25
1	A	161	TRP	NE1-CE2	8.77	1.49	1.37
1	A	117	TRP	NE1-CE2	8.56	1.48	1.37
1	A	13	GLU	CD-OE2	-6.59	1.18	1.25
1	A	292	LEU	C-O	-6.24	1.11	1.23
1	A	342	GLU	CG-CD	6.18	1.61	1.51
1	A	299	ILE	CB-CG1	-5.80	1.37	1.54
1	A	255	GLU	CD-OE1	-5.79	1.19	1.25
1	A	253	ARG	NE-CZ	5.72	1.40	1.33
1	A	342	GLU	CD-OE2	-5.31	1.19	1.25
1	A	20	GLY	N-CA	5.19	1.53	1.46
1	A	257	MET	CG-SD	-5.12	1.67	1.81
1	A	297	PRO	CA-C	5.11	1.63	1.52
1	A	287	GLN	C-O	-5.09	1.13	1.23
1	A	253	ARG	CB-CG	5.08	1.66	1.52
1	A	266	SER	CA-CB	-5.06	1.45	1.52
1	A	287	GLN	C-N	-5.01	1.22	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	TYR	CG-CD2-CE2	-13.65	110.38	121.30
1	A	307	ASP	CB-CG-OD2	11.66	128.79	118.30
1	A	282	ARG	CD-NE-CZ	-10.63	108.72	123.60
1	A	282	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	30	TYR	CB-CG-CD1	-9.00	115.60	121.00
1	A	73	ALA	C-N-CA	-8.83	103.77	122.30
1	A	249	TYR	CB-CG-CD1	-8.79	115.73	121.00
1	A	251	ARG	CD-NE-CZ	-8.45	111.78	123.60
1	A	67	TYR	CB-CG-CD2	-8.44	115.94	121.00
1	A	282	ARG	CA-CB-CG	-7.99	95.83	113.40
1	A	253	ARG	CB-CG-CD	7.91	132.15	111.60
1	A	15	HIS	CA-CB-CG	7.90	127.03	113.60
1	A	279	ALA	N-CA-CB	-7.78	99.21	110.10
1	A	246	THR	O-C-N	-7.75	110.30	122.70
1	A	68	TYR	CZ-CE2-CD2	7.65	126.69	119.80
1	A	68	TYR	CD1-CG-CD2	7.63	126.30	117.90
1	A	13	GLU	OE1-CD-OE2	-7.58	114.20	123.30
1	A	342	GLU	OE1-CD-OE2	-7.34	114.49	123.30
1	A	68	TYR	CB-CG-CD1	-7.33	116.60	121.00
1	A	30	TYR	CG-CD2-CE2	-7.10	115.62	121.30
1	A	28	LEU	CA-CB-CG	-7.00	99.20	115.30
1	A	30	TYR	CD1-CG-CD2	6.97	125.56	117.90
1	A	324	ARG	CD-NE-CZ	-6.96	113.86	123.60
1	A	267	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	A	325	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	277	GLU	CB-CG-CD	6.65	132.16	114.20
1	A	351	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	A	68	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	A	290	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	A	15	HIS	N-CA-CB	6.41	122.13	110.60
1	A	296	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	349	LYS	CG-CD-CE	6.30	130.80	111.90
1	A	28	LEU	CB-CG-CD2	-6.23	100.41	111.00
1	A	29	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	A	257	MET	CA-CB-CG	-6.14	102.85	113.30
1	A	307	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	325	LEU	CB-CA-C	5.96	121.53	110.20
1	A	257	MET	CG-SD-CE	-5.86	90.83	100.20
1	A	11	LYS	CB-CG-CD	5.85	126.81	111.60
1	A	295	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	71	ALA	CB-CA-C	-5.79	101.41	110.10
1	A	337	GLU	O-C-N	-5.77	113.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ASP	N-CA-C	5.63	126.21	111.00
1	A	294	THR	CA-CB-CG2	5.63	120.28	112.40
1	A	253	ARG	CA-C-O	5.50	131.66	120.10
1	A	324	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	44	GLU	C-N-CA	-5.48	108.00	121.70
1	A	32	LYS	C-N-CA	-5.42	108.15	121.70
1	A	256	ASN	N-CA-C	5.41	125.60	111.00
1	A	251	ARG	CB-CG-CD	5.40	125.65	111.60
1	A	26	THR	CA-CB-CG2	5.38	119.94	112.40
1	A	37	ALA	CB-CA-C	-5.31	102.14	110.10
1	A	253	ARG	O-C-N	-5.30	114.22	122.70
1	A	277	GLU	C-N-CA	-5.29	108.47	121.70
1	A	318	THR	C-N-CA	-5.24	108.60	121.70
1	A	288	VAL	CA-CB-CG1	5.22	118.74	110.90
1	A	235	ARG	CD-NE-CZ	-5.12	116.44	123.60
1	A	322	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	A	352	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	212	2
2	A	1	0	0	0	0
3	A	33	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	226	0	0	74	3
All	All	3049	0	2768	213	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 38.

All (213) 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: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:175:GLN:C	1:A:176:THR:HG23	1.70	1.07
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: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:175:GLN:C	1:A:176:THR:CG2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:173:ARG:NH1	4:A:1047:HOH:O	2.26	0.69
1:A:76:ARG:HG2	1:A:132:LEU:HD11	1.75	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:52:MET:HE3	1:A:56:LEU:HB2	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:VAL:O	1:A:218:VAL:CG1	2.51	0.58
1:A:76:ARG:CG	1:A:132:LEU:HD11	2.33	0.58
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:224:VAL:O	1:A:228:VAL:HG23	2.04	0.57
1:A:7:PHE:CE2	4:A:1075:HOH:O	2.53	0.57
1:A:125:THR:CG2	4:A:1172:HOH:O	2.23	0.56
1:A:119:GLN:O	4:A:1122:HOH:O	2.18	0.56
1:A:14:LEU:HB3	1:A:235:ARG:NH2	2.19	0.56
1:A:100:VAL:HG11	4:A:1182:HOH:O	1.99	0.56
1:A:98:VAL:HG13	1:A:148:VAL:HG13	1.88	0.56
1:A:29:TYR:C	1:A:29:TYR:CD1	2.79	0.55
1:A:124:LEU:HD22	1:A:129:VAL:HG23	1.87	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:186:GLU:HG2	1:A:186:GLU:O	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:110:SER:C	4:A:1172:HOH:O	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:CA	4:A:1090:HOH:O	2.19	0.51
1:A:61:PHE:CD1	3:A:1001:FR9:H2	2.45	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
1:A:41:ASP:HA	4:A:1190:HOH:O	2.11	0.50
1:A:174:GLU:C	1:A:176:THR:H	2.15	0.50
3:A:1001:FR9:O1	3:A:1001:FR9:H32	2.12	0.50
1:A:175:GLN:O	1:A:176:THR:CB	2.58	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: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:58:LEU:HB2	4:A:1056:HOH:O	2.13	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: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:113:GLU:HG2	1:A:114:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:HB2	1:A:226:GLU:OE1	2.15	0.45
1:A:132:LEU:O	1:A:135:GLN:N	2.50	0.45
1:A:83:ALA:HB1	1:A:137:LEU:HD13	1.99	0.45
1:A:181:ASP:CG	1:A:182:LEU:N	2.70	0.45
1:A:117:TRP:HA	1:A:117:TRP:CE3	2.51	0.45
1:A:38:LEU:HD23	4:A:1127:HOH:O	2.16	0.45
1:A:24:PRO:HG2	1:A:47:GLN:NE2	2.32	0.45
1:A:120:ALA:CB	4:A:1068:HOH:O	2.64	0.45
1:A:95:VAL:HG11	1:A:98:VAL:HB	1.99	0.45
1:A:187:THR:HB	4:A:1132:HOH:O	2.16	0.45
1:A:23:LYS:O	1:A:24:PRO:C	2.55	0.45
1:A:24:PRO:HA	1:A:27:ILE:HD12	1.99	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: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: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:120:ALA:HA	4:A:1068:HOH:O	2.09	0.43
1:A:28:LEU:HD13	1:A:43:PRO:HD3	1.99	0.43
1:A:50:ILE:HG21	1:A:50:ILE:HD13	1.72	0.43
1:A:172:TYR:CB	1:A:177:VAL:HG11	2.46	0.43
1:A:88:GLU:HB2	1:A:144:PHE:CE1	2.53	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:45:GLU:HB3	4:A:1057:HOH:O	2.18	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:283:PHE:HB3	1:A:288:VAL:HB	2.01	0.43
1:A:261:ILE:HD12	1:A:261:ILE:HG23	1.83	0.42
1:A:64:LYS:HE2	4:A:1030:HOH:O	2.20	0.42
1:A:156:ARG:HD2	1:A:186:GLU:HA	2.01	0.42
1:A:80:LYS:HZ2	1:A:135:GLN:HB3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HA	1:A:335:LEU:HD12	1.83	0.42
1:A:168:LEU:O	1:A:172:TYR:HB2	2.19	0.42
1:A:174:GLU:CB	4:A:1174:HOH:O	2.67	0.41
1:A:174:GLU:C	1:A:176:THR:N	2.73	0.41
1:A:90:LYS:HD2	1:A:90:LYS:HA	1.61	0.41
1:A:270:GLY:O	1:A:271:ALA:C	2.59	0.41
1:A:80:LYS:NZ	1:A:135:GLN:HB3	2.35	0.41
1:A:168:LEU:HA	1:A:168:LEU:HD12	1.73	0.41
1:A:140:GLY:O	1:A:144:PHE:HB2	2.21	0.41
1:A:340:LYS:O	1:A:344:LEU:HD22	2.21	0.41
1:A:235:ARG:HD3	1:A:334:PHE:CE1	2.53	0.40
1:A:282:ARG:HD2	1:A:282:ARG:HH11	1.64	0.40
1:A:116:PRO:O	1:A:117:TRP:HB2	2.21	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

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 [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%)	315 (91%)	22 (6%)	10 (3%)	<b>4</b> <b>2</b>

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 ⓘ

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%)	<b>1</b> <b>1</b>

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

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	PRO
1	A	28	LEU
1	A	33	ARG
1	A	43	PRO
1	A	49	ILE
1	A	50	ILE
1	A	54	LYS
1	A	58	LEU
1	A	60	ASP
1	A	66	ASP
1	A	76	ARG
1	A	81	ARG
1	A	90	LYS
1	A	101	ARG

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Mol	Chain	Res	Type
1	A	111	LYS
1	A	113	GLU
1	A	121	GLU
1	A	124	LEU
1	A	131	SER
1	A	138	GLN
1	A	142	ARG
1	A	143	ASP
1	A	150	SER
1	A	158	GLN
1	A	160	SER
1	A	166	VAL
1	A	168	LEU
1	A	176	THR
1	A	177	VAL
1	A	182	LEU
1	A	186	GLU
1	A	188	ILE
1	A	193	LEU
1	A	218	VAL
1	A	242	THR
1	A	253	ARG
1	A	256	ASN
1	A	257	MET
1	A	273	LYS
1	A	276	THR
1	A	280	VAL
1	A	281	ILE
1	A	292	LEU
1	A	294	THR
1	A	298	LEU
1	A	307	ASP
1	A	313	LYS
1	A	319	GLU
1	A	323	LYS
1	A	325	LEU
1	A	332	SER
1	A	341	LYS
1	A	344	LEU
1	A	345	ASP
1	A	346	LEU
1	A	352	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	48	ASN
1	A	134	ASN
1	A	197	HIS
1	A	256	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 carbohydrates 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	FR9	A	1001	-	32,36,36	2.75	11 (34%)	37,49,49	1.97	8 (21%)

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	-	-	0/16/24/24	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	C1-N2	6.57	1.47	1.38
3	A	1001	FR9	O9-C8	-6.53	1.11	1.24
3	A	1001	FR9	C30-N22	-6.39	1.31	1.39
3	A	1001	FR9	C33-N1	-5.19	1.31	1.41
3	A	1001	FR9	C8-N10	-4.49	1.24	1.33
3	A	1001	FR9	C5-C8	-3.93	1.45	1.50
3	A	1001	FR9	C34-C30	-3.66	1.33	1.40
3	A	1001	FR9	C5-N4	2.83	1.46	1.37
3	A	1001	FR9	C2-N3	-2.62	1.29	1.35
3	A	1001	FR9	C3-N4	-2.33	1.31	1.35
3	A	1001	FR9	O15-C14	2.03	1.51	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR9	O9-C8-C5	-6.78	113.94	119.61
3	A	1001	FR9	C1-N2-C13	4.74	130.05	125.53
3	A	1001	FR9	C5-C8-N10	3.35	119.56	116.25
3	A	1001	FR9	O15-C14-C13	2.91	124.62	112.42
3	A	1001	FR9	C34-C33-N1	-2.77	113.91	123.13
3	A	1001	FR9	C11-C6-N3	-2.50	107.70	113.05
3	A	1001	FR9	O9-C8-N10	2.49	126.11	122.58
3	A	1001	FR9	C5-C1-N2	2.27	110.28	107.91

There are no chirality outliers.

There are no torsion outliers.

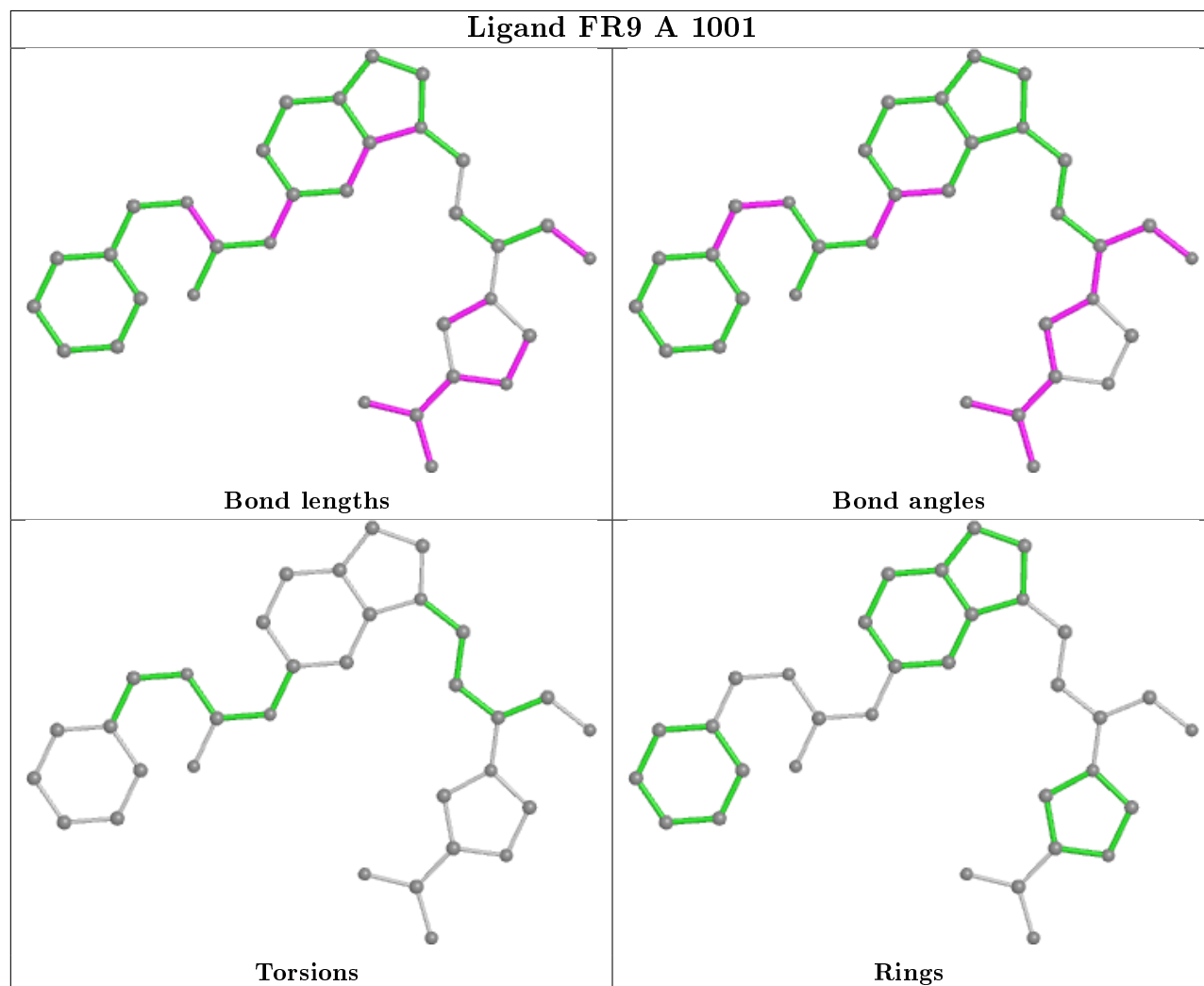
There are no ring outliers.

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 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%)	-0.30	3 (0%) 84 90	12, 28, 47, 58	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ALA	3.8
1	A	142	ARG	2.6
1	A	28	LEU	2.3

### 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.

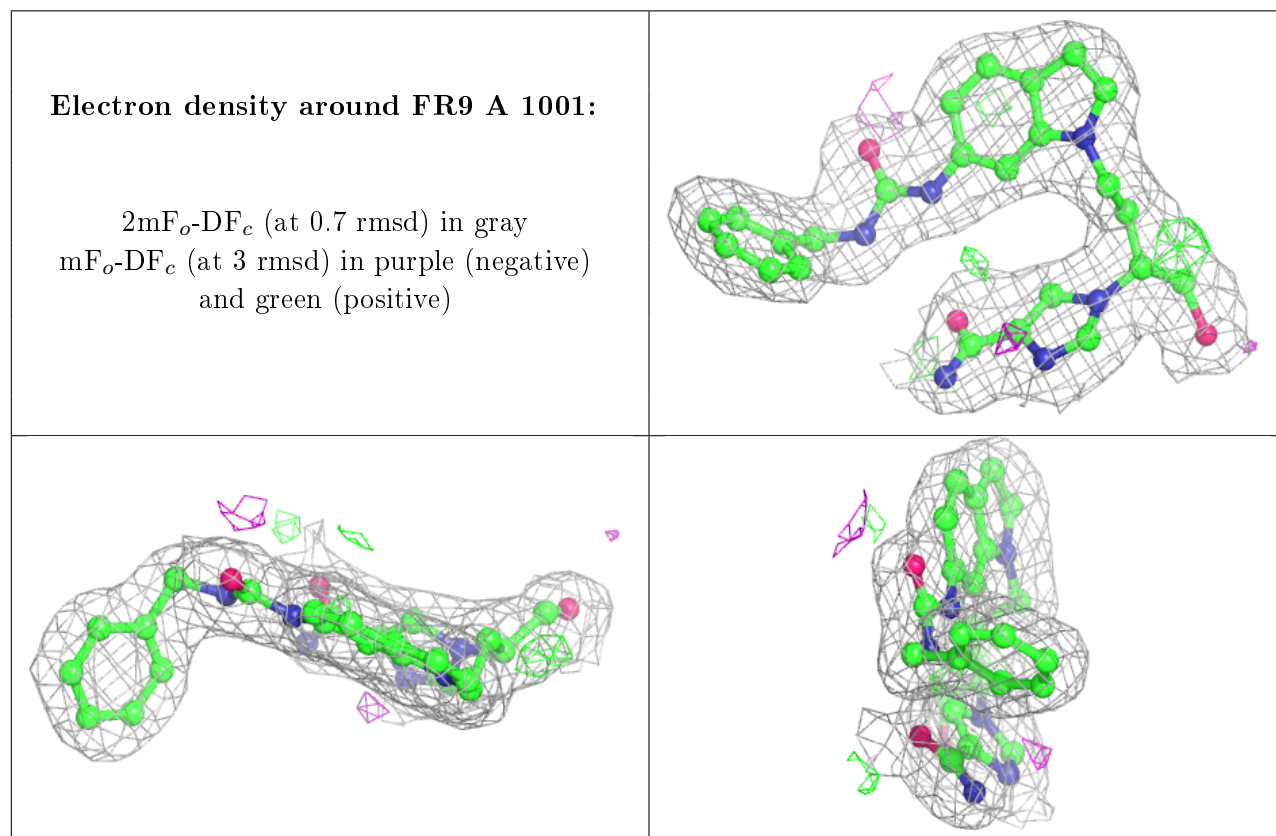
### 6.4 Ligands [i](#)

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	FR9	A	1001	33/33	0.94	0.10	16,19,25,26	0
2	ZN	A	400	1/1	0.98	0.11	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.