



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 02:35 AM EST

PDB ID : 1QXL  
Title : Crystal structure of Adenosine deaminase complexed with FR235380  
Authors : Kinoshita, T.  
Deposited on : 2003-09-08  
Resolution : 2.25 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

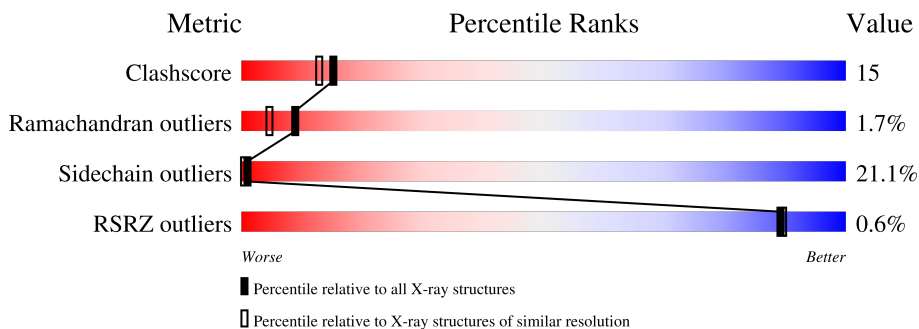
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2982 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
			Total	C	N	O	S			
1	A	349	2788	1773	470	533	12	0	0	0

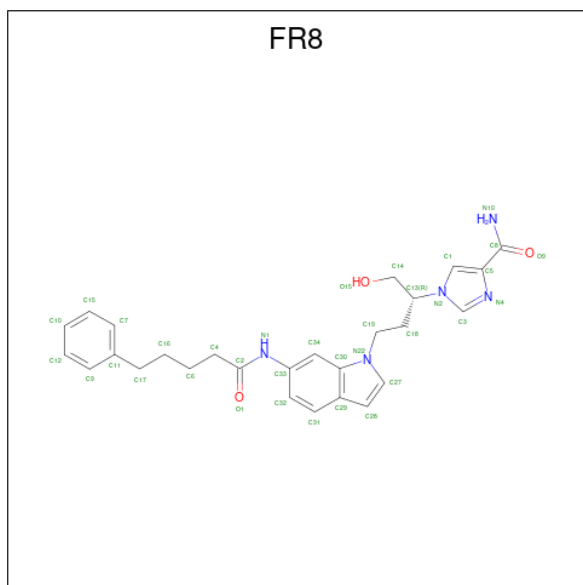
There are 16 discrepancies between the modelled and reference sequences:

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	47	LEU	GLN	conflict	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)-1-(HYDROXYMETHYL)-3-{6-[(5-PHENYLPENTANOYL)AMINO]-1H-INDOL-1-YL}PROPYL)-1H-IMIDAZOLE-4-CARBOXAMIDE (three-letter code: FR8) (formula: C<sub>27</sub>H<sub>31</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	35	27	5	3	0	0

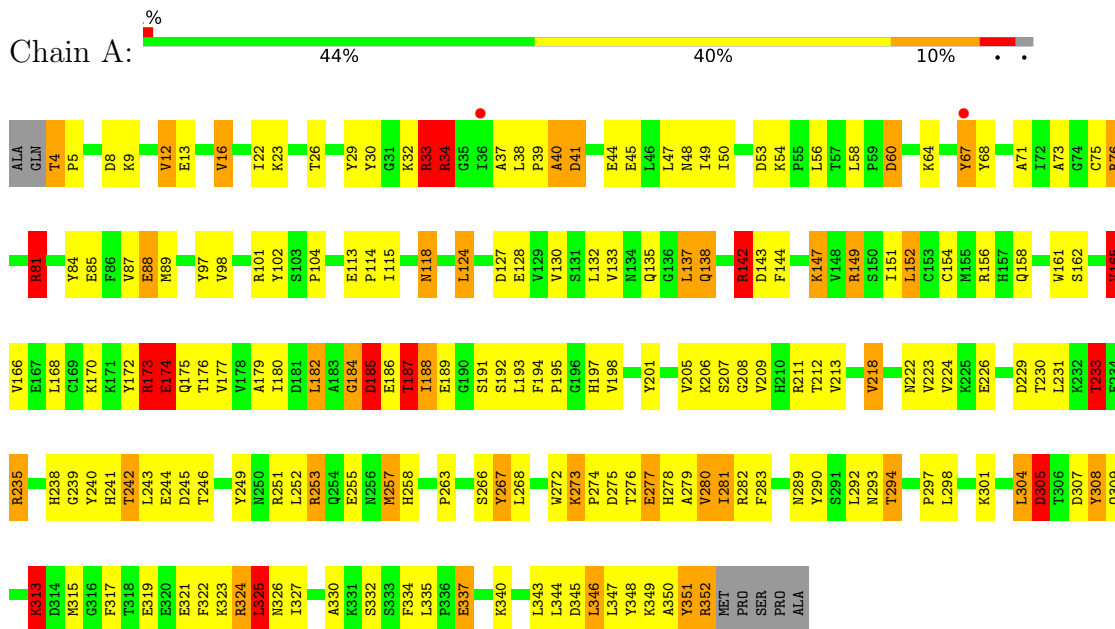
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	158	158	158	0	0

### 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, $\alpha$ , $\beta$ , $\gamma$	78.37Å 78.37Å 137.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.25 – 2.25 78.37 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (51.25-2.25) 97.3 (78.37-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.25Å)	Xtrriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.232 , 0.253 0.200 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FR8, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.14	5/2852 (0.2%)	2.03	100/3866 (2.6%)

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	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CD-OE2	10.32	1.37	1.25
1	A	294	THR	CB-OG1	6.10	1.55	1.43
1	A	189	GLU	CB-CG	5.85	1.63	1.52
1	A	185	ASP	N-CA	5.45	1.57	1.46
1	A	253	ARG	NE-CZ	5.33	1.40	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH1	-18.58	111.01	120.30
1	A	189	GLU	OE1-CD-OE2	14.63	140.86	123.30
1	A	235	ARG	NE-CZ-NH2	13.03	126.81	120.30
1	A	308	TYR	CB-CG-CD2	-10.47	114.72	121.00
1	A	282	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	A	172	TYR	CB-CG-CD2	-9.53	115.28	121.00
1	A	142	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	A	185	ASP	N-CA-CB	9.07	126.92	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	142	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	257	MET	CG-SD-CE	-8.50	86.61	100.20
1	A	253	ARG	CA-CB-CG	8.29	131.63	113.40
1	A	16	VAL	CG1-CB-CG2	8.26	124.11	110.90
1	A	251	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	A	60	ASP	CA-CB-CG	8.04	131.09	113.40
1	A	173	ARG	N-CA-CB	-7.69	96.75	110.60
1	A	205	VAL	CG1-CB-CG2	-7.62	98.70	110.90
1	A	149	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	84	TYR	CB-CG-CD1	-7.47	116.52	121.00
1	A	40	ALA	CB-CA-C	-7.26	99.21	110.10
1	A	279	ALA	N-CA-CB	-7.25	99.94	110.10
1	A	67	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	A	187	THR	CA-CB-CG2	6.96	122.15	112.40
1	A	352	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	A	325	LEU	CA-CB-CG	6.82	131.00	115.30
1	A	235	ARG	CB-CG-CD	-6.78	93.98	111.60
1	A	16	VAL	CB-CA-C	-6.76	98.56	111.40
1	A	304	LEU	CB-CA-C	-6.72	97.43	110.20
1	A	185	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	34	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	313	LYS	C-N-CA	-6.62	105.15	121.70
1	A	173	ARG	CG-CD-NE	-6.59	97.96	111.80
1	A	282	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	229	ASP	C-N-CA	-6.50	105.46	121.70
1	A	174	GLU	N-CA-C	6.45	128.42	111.00
1	A	201	TYR	CB-CG-CD2	-6.44	117.14	121.00
1	A	251	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	175	GLN	C-N-CA	6.30	137.44	121.70
1	A	12	VAL	CG1-CB-CG2	-6.26	100.88	110.90
1	A	305	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	A	240	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	84	TYR	CG-CD2-CE2	-6.17	116.36	121.30
1	A	294	THR	CA-CB-CG2	-6.15	103.80	112.40
1	A	198	VAL	CA-CB-CG1	6.07	120.00	110.90
1	A	165	VAL	CA-CB-CG2	5.99	119.89	110.90
1	A	189	GLU	CG-CD-OE1	-5.92	106.45	118.30
1	A	325	LEU	CB-CA-C	5.90	121.41	110.20
1	A	192	SER	N-CA-CB	5.89	119.34	110.50
1	A	175	GLN	N-CA-CB	-5.89	100.00	110.60
1	A	290	TYR	CB-CG-CD1	-5.86	117.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	CG-CD-NE	5.86	124.11	111.80
1	A	29	TYR	CB-CG-CD1	-5.86	117.49	121.00
1	A	325	LEU	N-CA-CB	-5.84	98.73	110.40
1	A	71	ALA	CB-CA-C	-5.82	101.36	110.10
1	A	182	LEU	CB-CG-CD2	5.78	120.83	111.00
1	A	182	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	283	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	A	351	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	138	GLN	C-N-CA	-5.74	107.36	121.70
1	A	194	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	A	32	LYS	C-N-CA	-5.71	107.42	121.70
1	A	198	VAL	CA-CB-CG2	5.71	119.47	110.90
1	A	253	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	211	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	280	VAL	CA-CB-CG1	5.53	119.20	110.90
1	A	84	TYR	CD1-CG-CD2	5.49	123.94	117.90
1	A	218	VAL	CA-CB-CG2	5.48	119.12	110.90
1	A	337	GLU	C-N-CA	-5.46	108.06	121.70
1	A	81	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	249	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	A	64	LYS	CA-CB-CG	-5.40	101.51	113.40
1	A	332	SER	CB-CA-C	-5.39	99.86	110.10
1	A	143	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	346	LEU	CB-CG-CD1	5.38	120.14	111.00
1	A	325	LEU	CB-CG-CD2	5.37	120.13	111.00
1	A	73	ALA	C-N-CA	-5.37	111.03	122.30
1	A	245	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	76	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	192	SER	CB-CA-C	-5.30	100.03	110.10
1	A	272	TRP	C-N-CA	-5.28	108.51	121.70
1	A	149	ARG	CD-NE-CZ	-5.27	116.22	123.60
1	A	233	THR	CB-CA-C	-5.25	97.42	111.60
1	A	324	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	87	VAL	C-N-CA	-5.23	108.62	121.70
1	A	102	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	348	TYR	CG-CD1-CE1	-5.22	117.12	121.30
1	A	175	GLN	O-C-N	-5.21	114.37	122.70
1	A	127	ASP	C-N-CA	-5.21	108.69	121.70
1	A	182	LEU	CD1-CG-CD2	5.16	125.99	110.50
1	A	68	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	A	277	GLU	C-N-CA	-5.13	108.87	121.70
1	A	294	THR	OG1-CB-CG2	5.12	121.79	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	CA-CB-CG	5.11	124.64	113.40
1	A	33	ARG	CD-NE-CZ	-5.08	116.48	123.60
1	A	60	ASP	N-CA-CB	5.07	119.73	110.60
1	A	184	GLY	C-N-CA	-5.07	109.02	121.70
1	A	98	VAL	CA-CB-CG2	5.04	118.46	110.90
1	A	64	LYS	CG-CD-CE	-5.02	96.83	111.90
1	A	293	ASN	C-N-CA	-5.02	109.14	121.70
1	A	22	ILE	CG1-CB-CG2	-5.02	100.36	111.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	149	ARG	Sidechain
1	A	173	ARG	Sidechain
1	A	235	ARG	Sidechain
1	A	267	TYR	Sidechain
1	A	308	TYR	Sidechain
1	A	33	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	351	TYR	Sidechain
1	A	352	ARG	Sidechain
1	A	4	THR	Peptide
1	A	41	ASP	Peptide
1	A	81	ARG	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2788	0	2746	84	0
2	A	1	0	0	0	0
3	A	35	0	31	0	0
4	A	158	0	0	6	0
All	All	2982	0	2777	84	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 15.

All (84) 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:239:GLY:O	1:A:242:THR:HG23	1.85	0.77
1:A:345:ASP:HB3	1:A:349:LYS:HZ2	1.49	0.76
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.66	0.75
1:A:185:ASP:OD1	1:A:187:THR:HB	1.87	0.75
1:A:278:HIS:CD2	1:A:280:VAL:HG12	2.21	0.75
1:A:278:HIS:CD2	1:A:280:VAL:H	2.05	0.73
1:A:281:ILE:HG22	1:A:317:PHE:HE1	1.59	0.67
1:A:88:GLU:HB3	1:A:144:PHE:CE2	2.31	0.66
1:A:113:GLU:HA	1:A:114:PRO:C	2.16	0.65
1:A:281:ILE:H	1:A:281:ILE:HD13	1.62	0.63
1:A:162:SER:HA	1:A:165:VAL:HG13	1.79	0.63
1:A:156:ARG:O	1:A:197:HIS:HE1	1.81	0.63
1:A:278:HIS:HD2	1:A:280:VAL:HG12	1.62	0.62
1:A:224:VAL:HG21	1:A:242:THR:HG22	1.81	0.61
1:A:132:LEU:HD13	4:A:1068:HOH:O	2.00	0.59
1:A:322:PHE:HA	1:A:325:LEU:HD13	1.84	0.59
1:A:350:ALA:HB3	4:A:1102:HOH:O	2.01	0.59
1:A:345:ASP:HB3	1:A:349:LYS:NZ	2.17	0.58
1:A:97:TYR:HD1	1:A:147:LYS:HG2	1.68	0.58
1:A:138:GLN:HB3	1:A:142:ARG:HH22	1.68	0.58
1:A:133:VAL:O	1:A:137:LEU:HB2	2.04	0.58
1:A:343:LEU:O	1:A:347:LEU:HD22	2.04	0.58
1:A:278:HIS:HD2	1:A:280:VAL:H	1.48	0.57
1:A:101:ARG:HA	1:A:151:ILE:O	2.05	0.56
1:A:281:ILE:HG21	1:A:315:MET:HB3	1.88	0.55
1:A:257:MET:HE3	1:A:258:HIS:N	2.23	0.54
1:A:38:LEU:H	1:A:38:LEU:HD22	1.72	0.54
1:A:133:VAL:HG12	1:A:137:LEU:HD22	1.90	0.53
1:A:104:PRO:HG3	1:A:152:LEU:HG	1.89	0.53
1:A:12:VAL:H	1:A:326:ASN:ND2	2.07	0.53
1:A:152:LEU:HD22	1:A:177:VAL:HG11	1.91	0.52
1:A:44:GLU:O	1:A:48:ASN:ND2	2.42	0.52
1:A:97:TYR:HD1	1:A:147:LYS:CG	2.21	0.52
1:A:154:CYS:SG	1:A:180:ILE:HD11	2.50	0.52
1:A:13:GLU:HA	4:A:1125:HOH:O	2.11	0.51
1:A:280:VAL:HG22	1:A:317:PHE:HZ	1.76	0.51
1:A:162:SER:OG	1:A:197:HIS:HD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:CD2	1:A:128:GLU:HG3	2.42	0.50
1:A:174:GLU:O	1:A:176:THR:HA	2.11	0.50
1:A:321:GLU:O	1:A:325:LEU:HB3	2.13	0.49
1:A:5:PRO:HA	1:A:305:ASP:OD1	2.13	0.48
1:A:273:LYS:HD3	1:A:274:PRO:HD2	1.95	0.48
1:A:128:GLU:O	1:A:132:LEU:HD12	2.14	0.48
1:A:208:GLY:HA2	4:A:1043:HOH:O	2.14	0.47
1:A:179:ALA:HB2	1:A:334:PHE:CD2	2.50	0.47
1:A:281:ILE:CG2	1:A:315:MET:HB3	2.46	0.46
1:A:188:ILE:HG13	1:A:191:SER:HB3	1.98	0.46
1:A:241:HIS:O	1:A:244:GLU:HG2	2.17	0.45
1:A:263:PRO:HD2	1:A:307:ASP:OD2	2.16	0.45
1:A:309:GLN:HE21	1:A:313:LYS:NZ	2.14	0.45
1:A:281:ILE:HG22	1:A:317:PHE:CE1	2.46	0.45
1:A:88:GLU:HB3	1:A:144:PHE:CD2	2.52	0.45
1:A:252:LEU:HD22	1:A:257:MET:HG3	1.98	0.45
1:A:257:MET:HE2	1:A:257:MET:HB3	1.76	0.44
1:A:124:LEU:HD23	1:A:128:GLU:HG3	1.99	0.44
1:A:97:TYR:CD1	1:A:147:LYS:HG2	2.51	0.44
1:A:97:TYR:HA	1:A:147:LYS:O	2.17	0.44
1:A:76:ARG:HA	4:A:1068:HOH:O	2.18	0.44
1:A:138:GLN:CB	1:A:142:ARG:HH22	2.30	0.43
1:A:158:GLN:HG2	1:A:161:TRP:CD2	2.53	0.43
1:A:330:ALA:O	1:A:340:LYS:HD3	2.18	0.43
1:A:170:LYS:O	1:A:173:ARG:HB2	2.19	0.43
1:A:30:TYR:O	1:A:34:ARG:HG3	2.19	0.42
1:A:44:GLU:H	1:A:44:GLU:HG3	1.53	0.42
1:A:50:ILE:HG22	1:A:67:TYR:HD1	1.83	0.42
1:A:81:ARG:O	1:A:85:GLU:HG3	2.19	0.42
1:A:213:VAL:HG23	1:A:233:THR:CG2	2.42	0.42
1:A:158:GLN:HG2	1:A:161:TRP:CE2	2.55	0.42
1:A:337:GLU:HG3	4:A:1113:HOH:O	2.20	0.42
1:A:50:ILE:HD13	1:A:50:ILE:HG21	1.60	0.42
1:A:267:TYR:CD2	1:A:267:TYR:C	2.93	0.42
1:A:23:LYS:HD2	1:A:89:MET:SD	2.60	0.42
1:A:9:LYS:HD3	1:A:9:LYS:HA	1.51	0.41
1:A:113:GLU:HA	1:A:114:PRO:O	2.19	0.41
1:A:212:THR:HA	1:A:233:THR:HG22	2.01	0.41
1:A:273:LYS:HA	1:A:274:PRO:HD3	1.92	0.41
1:A:184:GLY:O	1:A:185:ASP:CB	2.65	0.41
1:A:222:ASN:O	1:A:226:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HG23	1:A:297:PRO:HD3	2.03	0.41
1:A:323:LYS:O	1:A:327:ILE:HG12	2.20	0.41
1:A:170:LYS:HD2	1:A:207:SER:OG	2.20	0.40
1:A:273:LYS:O	1:A:275:ASP:N	2.53	0.40
1:A:38:LEU:HB3	1:A:39:PRO:HD2	2.03	0.40
1:A:266:SER:OG	1:A:278:HIS:HE1	2.05	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%)	323 (93%)	18 (5%)	6 (2%)	<b>9</b> <b>4</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	174	GLU
1	A	185	ASP
1	A	37	ALA
1	A	40	ALA
1	A	238	HIS

### 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%)	240 (79%)	64 (21%)	<b>1</b> <b>0</b>

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASP
1	A	16	VAL
1	A	26	THR
1	A	33	ARG
1	A	41	ASP
1	A	45	GLU
1	A	47	LEU
1	A	49	ILE
1	A	53	ASP
1	A	54	LYS
1	A	56	LEU
1	A	58	LEU
1	A	60	ASP
1	A	75	CYS
1	A	88	GLU
1	A	115	ILE
1	A	118	ASN
1	A	124	LEU
1	A	130	VAL
1	A	135	GLN
1	A	137	LEU
1	A	147	LYS
1	A	152	LEU
1	A	165	VAL
1	A	166	VAL
1	A	168	LEU
1	A	174	GLU
1	A	182	LEU
1	A	186	GLU
1	A	187	THR
1	A	188	ILE
1	A	193	LEU
1	A	195	PRO
1	A	206	LYS
1	A	209	VAL
1	A	218	VAL
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	230	THR
1	A	231	LEU
1	A	233	THR
1	A	242	THR
1	A	243	LEU
1	A	246	THR
1	A	253	ARG
1	A	255	GLU
1	A	268	LEU
1	A	273	LYS
1	A	276	THR
1	A	277	GLU
1	A	281	ILE
1	A	289	ASN
1	A	292	LEU
1	A	298	LEU
1	A	301	LYS
1	A	304	LEU
1	A	305	ASP
1	A	313	LYS
1	A	319	GLU
1	A	324	ARG
1	A	325	LEU
1	A	335	LEU
1	A	344	LEU
1	A	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	134	ASN
1	A	175	GLN
1	A	197	HIS
1	A	278	HIS
1	A	285	ASN
1	A	289	ASN
1	A	309	GLN
1	A	326	ASN

### 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 monosaccharides 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	FR8	A	1001	-	34,38,38	1.60	6 (17%)	39,51,51	1.18	3 (7%)

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	FR8	A	1001	-	-	2/18/26/26	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR8	C1-N2	6.01	1.46	1.38
3	A	1001	FR8	C33-N1	-3.18	1.35	1.41
3	A	1001	FR8	C5-N4	3.17	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FR8	C34-C30	-2.25	1.36	1.40
3	A	1001	FR8	C31-C29	-2.16	1.36	1.41
3	A	1001	FR8	C32-C33	2.02	1.42	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FR8	C18-C19-N22	-2.43	107.24	112.13
3	A	1001	FR8	C34-C33-N1	-2.32	115.39	123.13
3	A	1001	FR8	C5-C8-N10	2.09	118.32	116.25

There are no chirality outliers.

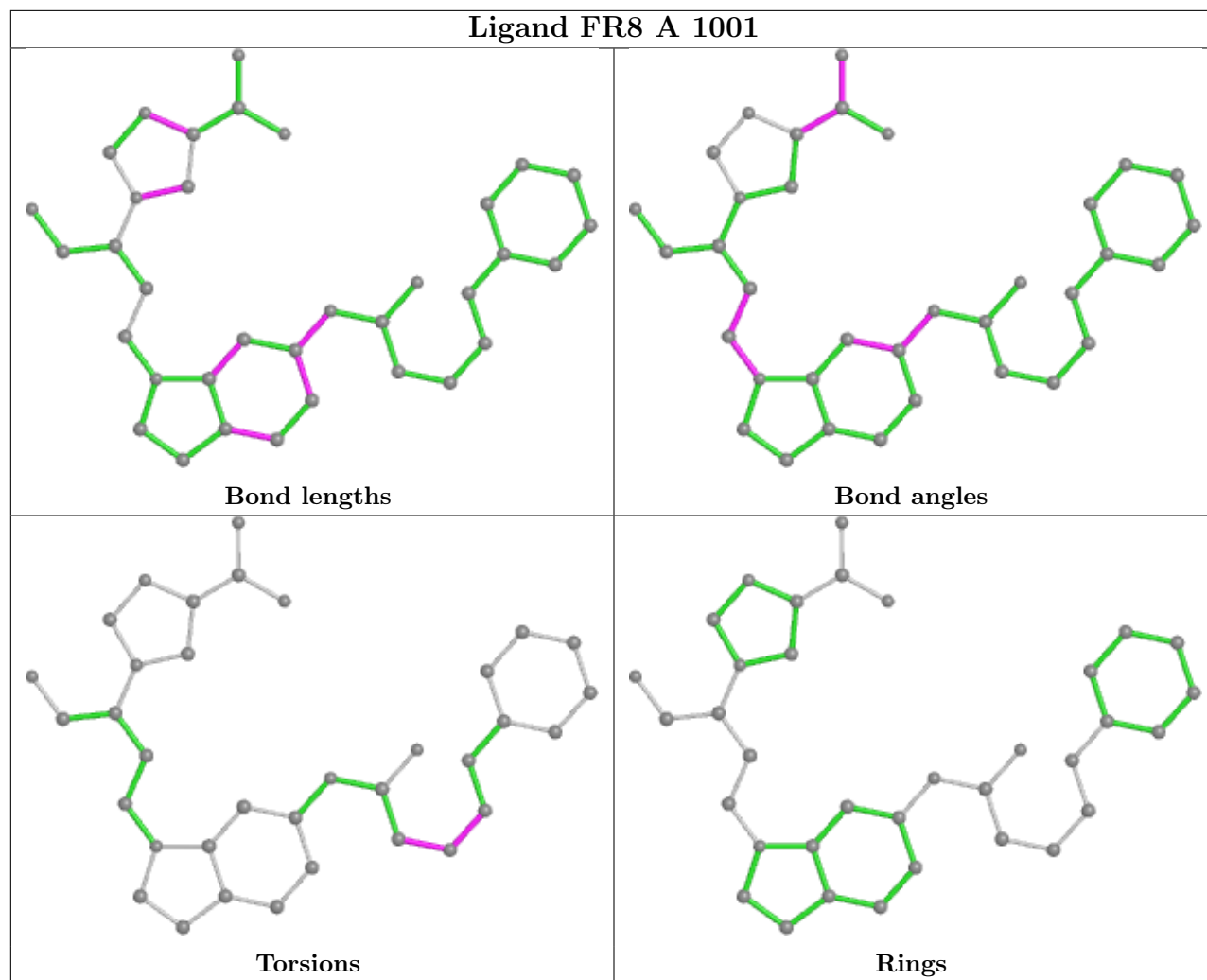
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FR8	C2-C4-C6-C16
3	A	1001	FR8	C17-C16-C6-C4

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.45	2 (0%) 89 89	13, 28, 50, 63	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ILE	2.6
1	A	67	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

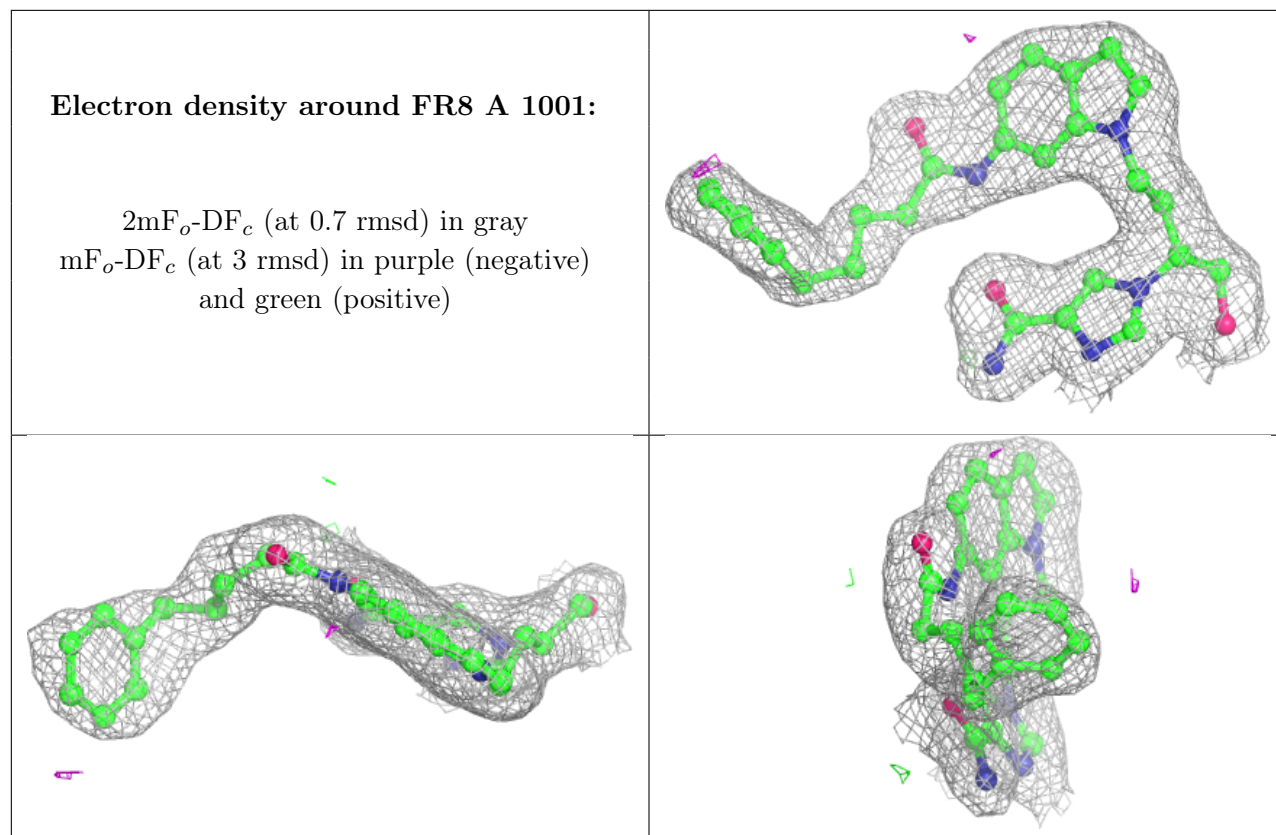
### 6.4 Ligands [i](#)

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	FR8	A	1001	35/35	0.96	0.09	17,23,39,40	0
2	ZN	A	400	1/1	1.00	0.11	23,23,23,23	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 [i](#)

There are no such residues in this entry.