



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:27 AM UTC

PDB ID : 9B98 / pdb\_00009b98  
Title : Crystal structure of the human PAD2 protein bound to small molecule  
Authors : Byrnes, L.J.; Vajdos, F.  
Deposited on : 2024-04-01  
Resolution : 2.00 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	:	4-5-2 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

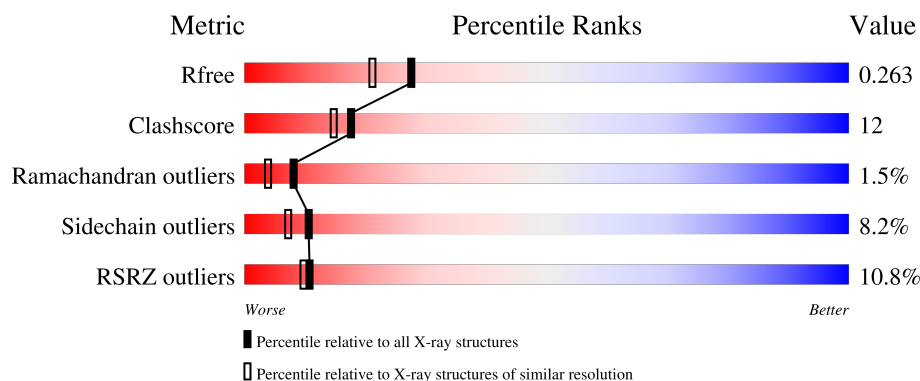
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	690	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	701	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5033 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 Protein-arginine deiminase type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4815	3097	797	897	24	0	2	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q9Y2J8
A	-19	GLY	-	expression tag	UNP Q9Y2J8
A	-18	HIS	-	expression tag	UNP Q9Y2J8
A	-17	HIS	-	expression tag	UNP Q9Y2J8
A	-16	HIS	-	expression tag	UNP Q9Y2J8
A	-15	HIS	-	expression tag	UNP Q9Y2J8
A	-14	HIS	-	expression tag	UNP Q9Y2J8
A	-13	HIS	-	expression tag	UNP Q9Y2J8
A	-12	HIS	-	expression tag	UNP Q9Y2J8
A	-11	HIS	-	expression tag	UNP Q9Y2J8
A	-10	HIS	-	expression tag	UNP Q9Y2J8
A	-9	HIS	-	expression tag	UNP Q9Y2J8
A	-8	SER	-	expression tag	UNP Q9Y2J8
A	-7	SER	-	expression tag	UNP Q9Y2J8
A	-6	GLY	-	expression tag	UNP Q9Y2J8
A	-5	HIS	-	expression tag	UNP Q9Y2J8
A	-4	ILE	-	expression tag	UNP Q9Y2J8
A	-3	GLU	-	expression tag	UNP Q9Y2J8
A	-2	GLY	-	expression tag	UNP Q9Y2J8
A	-1	ARG	-	expression tag	UNP Q9Y2J8
A	0	HIS	-	expression tag	UNP Q9Y2J8
A	666	SER	-	expression tag	UNP Q9Y2J8
A	667	ARG	-	expression tag	UNP Q9Y2J8
A	668	ARG	-	expression tag	UNP Q9Y2J8
A	669	SER	-	expression tag	UNP Q9Y2J8

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

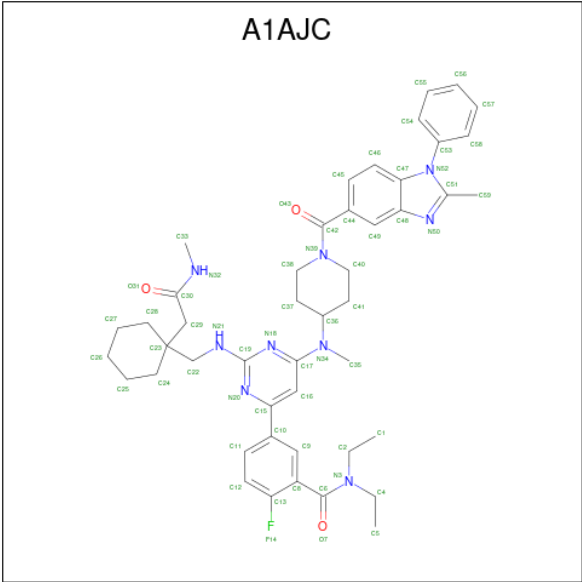


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		

- Molecule 4 is (5P)-N,N-diethyl-2-fluoro-5-(2-[(1-[2-(methylamino)-2-oxoethyl]cyclohexyl)methyl]amino]-6-{methyl[1-(2-methyl-1-phenyl-1H-1,3-benzimidazole-5-carbonyl)piperidin-4-yl]amino}pyrimidin-4-yl)benzamide (CCD ID: A1AJC) (formula: C<sub>46</sub>H<sub>56</sub>FN<sub>9</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			59	46	1	9	3		

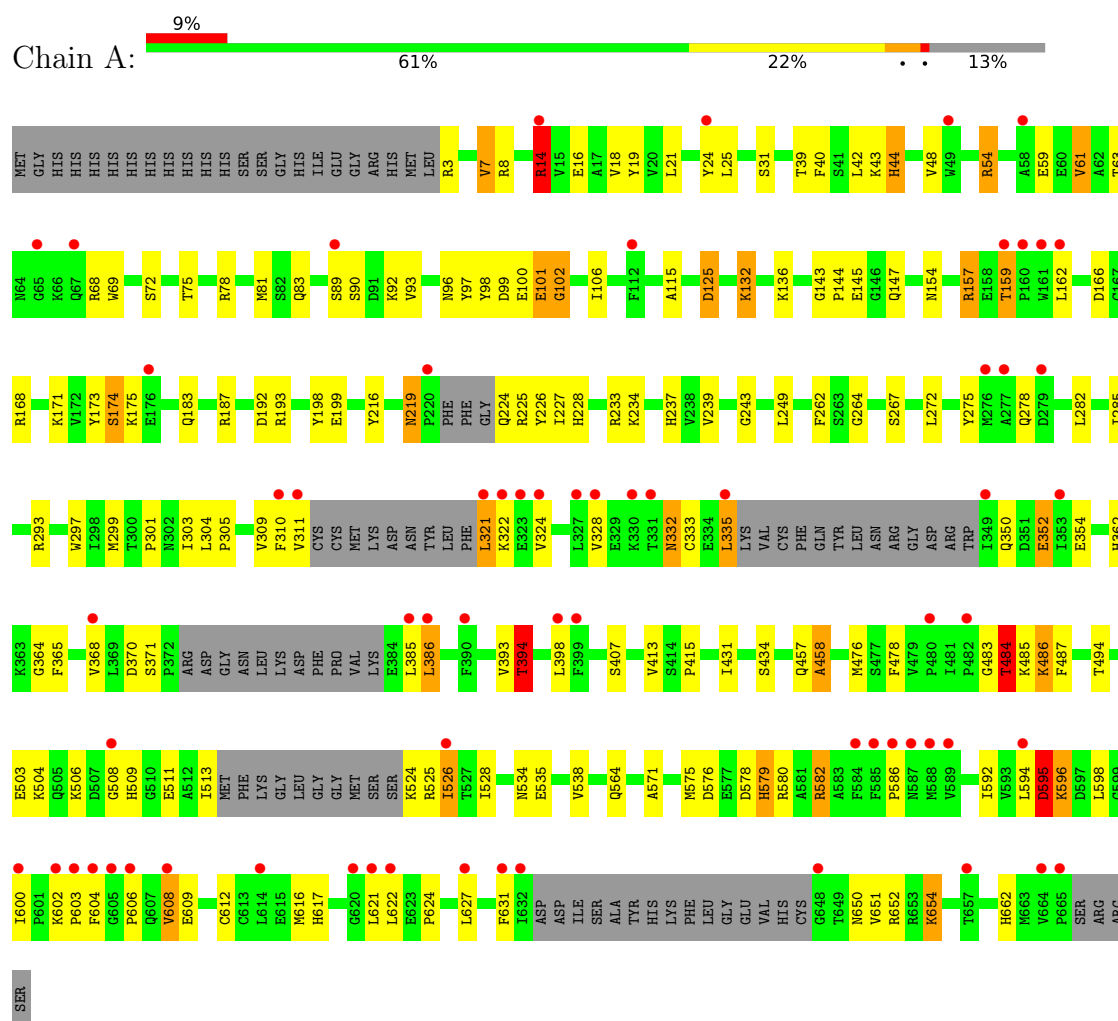
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	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: Protein-arginine deiminase type-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.71Å 52.78Å 76.59Å 90.00° 105.71° 90.00°	Depositor
Resolution (Å)	97.09 – 2.00 97.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	51.2 (97.09-2.00) 51.2 (97.09-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, $R_{free}$	0.186 , 0.258 0.195 , 0.263	Depositor DCC
$R_{free}$ test set	1358 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: A1AJC, CA, ACT

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	0.63	5/4930 (0.1%)	1.09	6/6686 (0.1%)

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	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	HIS	CE1-NE2	5.97	1.38	1.32
1	A	228	HIS	CE1-NE2	5.76	1.38	1.32
1	A	362	HIS	CE1-NE2	5.45	1.38	1.32
1	A	44	HIS	CE1-NE2	5.36	1.38	1.32
1	A	579	HIS	CE1-NE2	5.31	1.37	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	394	THR	CB-CA-C	-6.24	97.00	109.79
1	A	535	GLU	CB-CA-C	-5.71	101.14	110.85
1	A	125	ASP	CA-CB-CG	-5.64	106.96	112.60
1	A	484	THR	CA-C-N	5.24	131.13	121.70
1	A	484	THR	C-N-CA	5.24	131.13	121.70

There are no chirality outliers.



All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	3	ARG	Sidechain
1	A	54	ARG	Sidechain
1	A	580	ARG	Sidechain
1	A	652	ARG	Sidechain
1	A	8	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	4815	0	4795	119	0
2	A	8	0	6	3	0
3	A	5	0	0	0	0
4	A	59	0	0	0	0
5	A	146	0	0	20	0
All	All	5033	0	4801	120	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 12.

All (120) 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:136:LYS:HB2	5:A:901:HOH:O	1.58	1.04
2:A:701:ACT:H1	5:A:903:HOH:O	1.66	0.93
1:A:592:ILE:HB	5:A:934:HOH:O	1.68	0.92
1:A:147:GLN:HB3	5:A:901:HOH:O	1.78	0.82
1:A:272:LEU:HD23	1:A:285:ILE:HD11	1.65	0.78
1:A:434:SER:OG	5:A:801:HOH:O	2.04	0.76
1:A:168:ARG:HH11	1:A:168:ARG:HG3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HB3	5:A:927:HOH:O	1.89	0.72
1:A:352:GLU:OE2	5:A:802:HOH:O	2.08	0.71
1:A:159:THR:OG1	1:A:162:LEU:HD12	1.92	0.70
1:A:99:ASP:O	5:A:803:HOH:O	2.12	0.67
1:A:7:VAL:HG11	1:A:25:LEU:HD13	1.75	0.67
1:A:125:ASP:C	1:A:125:ASP:OD1	2.36	0.66
1:A:513:ILE:C	1:A:526:ILE:O	2.39	0.65
1:A:68:ARG:HG3	5:A:826:HOH:O	1.96	0.64
1:A:89:SER:O	1:A:90:SER:HB3	1.97	0.63
1:A:612:CYS:O	1:A:616:MET:HG2	1.98	0.63
1:A:272:LEU:CD2	1:A:285:ILE:HD11	2.28	0.63
1:A:171:LYS:HE2	5:A:847:HOH:O	1.98	0.63
1:A:99:ASP:HB3	1:A:106:ILE:HD13	1.82	0.62
1:A:234:LYS:HD3	5:A:837:HOH:O	1.99	0.61
1:A:40:PHE:HA	1:A:96:ASN:O	2.01	0.60
1:A:582:ARG:HH11	1:A:582:ARG:HG2	1.67	0.60
1:A:42:LEU:HD11	1:A:61:VAL:HG21	1.84	0.60
1:A:272:LEU:HD23	1:A:285:ILE:CD1	2.30	0.59
1:A:484:THR:HA	1:A:485:LYS:HB2	1.84	0.59
1:A:321:LEU:HD12	1:A:322:LYS:HG2	1.85	0.59
1:A:173:TYR:O	1:A:174:SER:CB	2.49	0.58
1:A:528:ILE:HG13	1:A:606:PRO:CB	2.35	0.57
1:A:19:TYR:HE1	1:A:21:LEU:HD23	1.69	0.57
1:A:370:ASP:HB3	1:A:394:THR:HG23	1.86	0.57
1:A:166:ASP:HB3	5:A:805:HOH:O	2.04	0.57
1:A:484:THR:HB	1:A:486:LYS:N	2.20	0.56
1:A:511:GLU:O	1:A:513:ILE:HD13	2.06	0.56
1:A:598:LEU:HD21	1:A:627:LEU:HD22	1.87	0.56
1:A:168:ARG:HG3	1:A:168:ARG:NH1	2.17	0.56
1:A:272:LEU:HD23	1:A:285:ILE:CG1	2.36	0.55
1:A:216:TYR:CD2	2:A:701:ACT:H2	2.42	0.54
1:A:219:ASN:HB2	1:A:224:GLN:HA	1.89	0.54
1:A:504:LYS:HB2	1:A:528:ILE:HD13	1.89	0.54
1:A:586:PRO:HD2	1:A:603:PRO:O	2.06	0.54
1:A:483:GLY:O	1:A:484:THR:HG23	2.08	0.53
1:A:596:LYS:HD3	1:A:596:LYS:H	1.73	0.53
1:A:154:ASN:ND2	5:A:805:HOH:O	2.41	0.52
1:A:528:ILE:HG13	1:A:606:PRO:HB3	1.90	0.52
1:A:494:THR:HA	1:A:571:ALA:O	2.10	0.52
1:A:39:THR:HA	1:A:69:TRP:O	2.09	0.52
1:A:192:ASP:HA	1:A:243:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLN:HG2	1:A:249:LEU:HD11	1.91	0.52
1:A:219:ASN:HB3	5:A:931:HOH:O	2.10	0.52
1:A:301:PRO:HD2	1:A:304:LEU:HD12	1.92	0.52
1:A:299:MET:HE3	1:A:354:GLU:OE2	2.10	0.51
1:A:68:ARG:HD3	1:A:98:TYR:CD1	2.46	0.50
1:A:534:ASN:O	1:A:538:VAL:HG23	2.10	0.50
1:A:484:THR:CA	1:A:485:LYS:HB2	2.41	0.50
1:A:328:VAL:HG21	1:A:335:LEU:HD11	1.93	0.50
1:A:503:GLU:HA	1:A:503:GLU:OE1	2.12	0.50
1:A:311:VAL:HG13	1:A:324:VAL:HG11	1.94	0.50
1:A:575:MET:CG	1:A:579:HIS:HA	2.42	0.49
1:A:7:VAL:CG1	1:A:25:LEU:HB3	2.42	0.49
1:A:582:ARG:HH11	1:A:582:ARG:CG	2.24	0.49
1:A:506:LYS:HG2	5:A:921:HOH:O	2.13	0.49
1:A:483:GLY:O	1:A:484:THR:OG1	2.28	0.49
1:A:101:GLU:O	1:A:102:GLY:C	2.57	0.48
1:A:144:PRO:HA	1:A:662:HIS:CD2	2.50	0.47
1:A:262:PHE:CZ	1:A:264:GLY:HA2	2.49	0.47
1:A:14:ARG:HH22	1:A:16:GLU:CG	2.27	0.47
1:A:143:GLY:HA2	1:A:662:HIS:O	2.14	0.47
1:A:305:PRO:HD2	1:A:654:LYS:HD2	1.97	0.47
1:A:159:THR:OG1	1:A:162:LEU:CD1	2.62	0.47
1:A:332:ASN:HD22	1:A:332:ASN:H	1.63	0.47
1:A:385:LEU:HD12	1:A:385:LEU:H	1.78	0.47
1:A:484:THR:CB	1:A:485:LYS:HB2	2.45	0.47
1:A:183:GLN:H	2:A:702:ACT:H2	1.81	0.46
1:A:303:ILE:HG12	1:A:415:PRO:HB3	1.97	0.46
1:A:14:ARG:HH12	1:A:16:GLU:HG3	1.80	0.46
1:A:578:ASP:O	1:A:579:HIS:HB2	2.15	0.46
1:A:304:LEU:HD13	1:A:654:LYS:O	2.16	0.46
1:A:509:HIS:CD2	1:A:608:VAL:HG21	2.51	0.46
1:A:157:ARG:NH2	1:A:386:LEU:O	2.48	0.45
1:A:299:MET:HE2	1:A:413:VAL:HG12	1.98	0.45
1:A:504:LYS:CB	1:A:528:ILE:HD13	2.47	0.45
1:A:476:MET:HE3	1:A:476:MET:HB2	1.87	0.45
1:A:81:MET:CE	1:A:115:ALA:HB2	2.47	0.45
1:A:173:TYR:O	1:A:174:SER:HB3	2.17	0.45
1:A:136:LYS:CB	5:A:901:HOH:O	2.38	0.44
1:A:19:TYR:CE1	1:A:81:MET:HB2	2.52	0.44
1:A:457:GLN:O	1:A:458:ALA:C	2.60	0.44
1:A:68:ARG:CG	5:A:826:HOH:O	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TRP:CZ3	1:A:299:MET:HG3	2.52	0.44
1:A:476:MET:HE1	1:A:478:PHE:CE2	2.53	0.44
1:A:328:VAL:HG13	1:A:333:CYS:HB2	1.99	0.43
1:A:592:ILE:HD12	5:A:934:HOH:O	2.18	0.43
1:A:44:HIS:CE1	1:A:63:THR:HG22	2.53	0.43
1:A:483:GLY:O	1:A:484:THR:CB	2.66	0.43
1:A:309:VAL:O	1:A:335:LEU:HA	2.19	0.43
1:A:509:HIS:CD2	1:A:608:VAL:HG11	2.53	0.43
1:A:506:LYS:C	1:A:508:GLY:H	2.27	0.43
1:A:199:GLU:OE2	1:A:275:TYR:OH	2.14	0.42
1:A:509:HIS:CE1	1:A:608:VAL:HG11	2.54	0.42
1:A:18:VAL:HG23	1:A:198:TYR:CE2	2.54	0.42
1:A:132:LYS:HG3	1:A:187:ARG:HH11	1.84	0.42
1:A:415:PRO:HG2	1:A:487:PHE:CG	2.54	0.41
1:A:385:LEU:HD12	1:A:385:LEU:N	2.35	0.41
1:A:594:LEU:O	1:A:595:ASP:CB	2.68	0.41
1:A:293:ARG:HD3	5:A:864:HOH:O	2.20	0.41
1:A:42:LEU:HD11	1:A:61:VAL:CG2	2.50	0.41
1:A:604:PHE:HB2	5:A:940:HOH:O	2.19	0.41
1:A:582:ARG:CG	1:A:582:ARG:NH1	2.82	0.41
1:A:525:ARG:C	1:A:526:ILE:HD13	2.45	0.41
1:A:48:VAL:HG11	1:A:93:VAL:CG2	2.51	0.41
1:A:54:ARG:HG3	1:A:75:THR:OG1	2.21	0.41
1:A:600:ILE:O	1:A:631:PHE:HA	2.21	0.41
1:A:24:TYR:CD2	1:A:78:ARG:HD2	2.56	0.41
1:A:97:TYR:O	1:A:106:ILE:HG12	2.21	0.40
1:A:598:LEU:HD12	1:A:622:LEU:HD13	2.03	0.40
1:A:132:LYS:HE3	1:A:187:ARG:HD3	2.03	0.40
1:A:364:GLY:O	1:A:365:PHE:HB3	2.22	0.40
1:A:175:LYS:HB3	1:A:226:TYR:OH	2.22	0.40
1:A:617:HIS:CE1	1:A:621:LEU:HD11	2.56	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	590/690 (86%)	541 (92%)	40 (7%)	9 (2%)	8 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	GLY
1	A	174	SER
1	A	484	THR
1	A	595	ASP
1	A	624	PRO
1	A	650	ASN
1	A	458	ALA
1	A	59	GLU
1	A	219	ASN

### 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	537/612 (88%)	493 (92%)	44 (8%)	10 7

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	14	ARG
1	A	31	SER
1	A	43	LYS
1	A	61	VAL
1	A	72	SER
1	A	83	GLN
1	A	92	LYS
1	A	100	GLU
1	A	101	GLU

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Mol	Chain	Res	Type
1	A	132	LYS
1	A	145	GLU
1	A	159	THR
1	A	227	ILE
1	A	239	VAL
1	A	267	SER
1	A	278	GLN
1	A	282	LEU
1	A	310	PHE
1	A	321	LEU
1	A	332	ASN
1	A	335	LEU
1	A	350	GLN
1	A	352	GLU
1	A	368	VAL
1	A	371	SER
1	A	386	LEU
1	A	393	VAL
1	A	394	THR
1	A	398	LEU
1	A	407	SER
1	A	431	ILE
1	A	486	LYS
1	A	524	LYS
1	A	526	ILE
1	A	564	GLN
1	A	582	ARG
1	A	595	ASP
1	A	596	LYS
1	A	602	LYS
1	A	608	VAL
1	A	609	GLU
1	A	651	VAL
1	A	654	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	224	GLN
1	A	237	HIS
1	A	278	GLN

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Mol	Chain	Res	Type
1	A	326	ASN
1	A	332	ASN
1	A	587	ASN
1	A	590	ASN
1	A	617	HIS
1	A	662	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\# Z  > 2$
4	A1AJC	A	708	-	63,65,65	0.36	0	87,93,93	0.58	0
2	ACT	A	702	-	3,3,3	1.02	0	3,3,3	0.70	0
2	ACT	A	701	-	3,3,3	1.03	0	3,3,3	0.78	0

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
4	A1AJC	A	708	-	-	0/49/69/69	0/7/7/7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

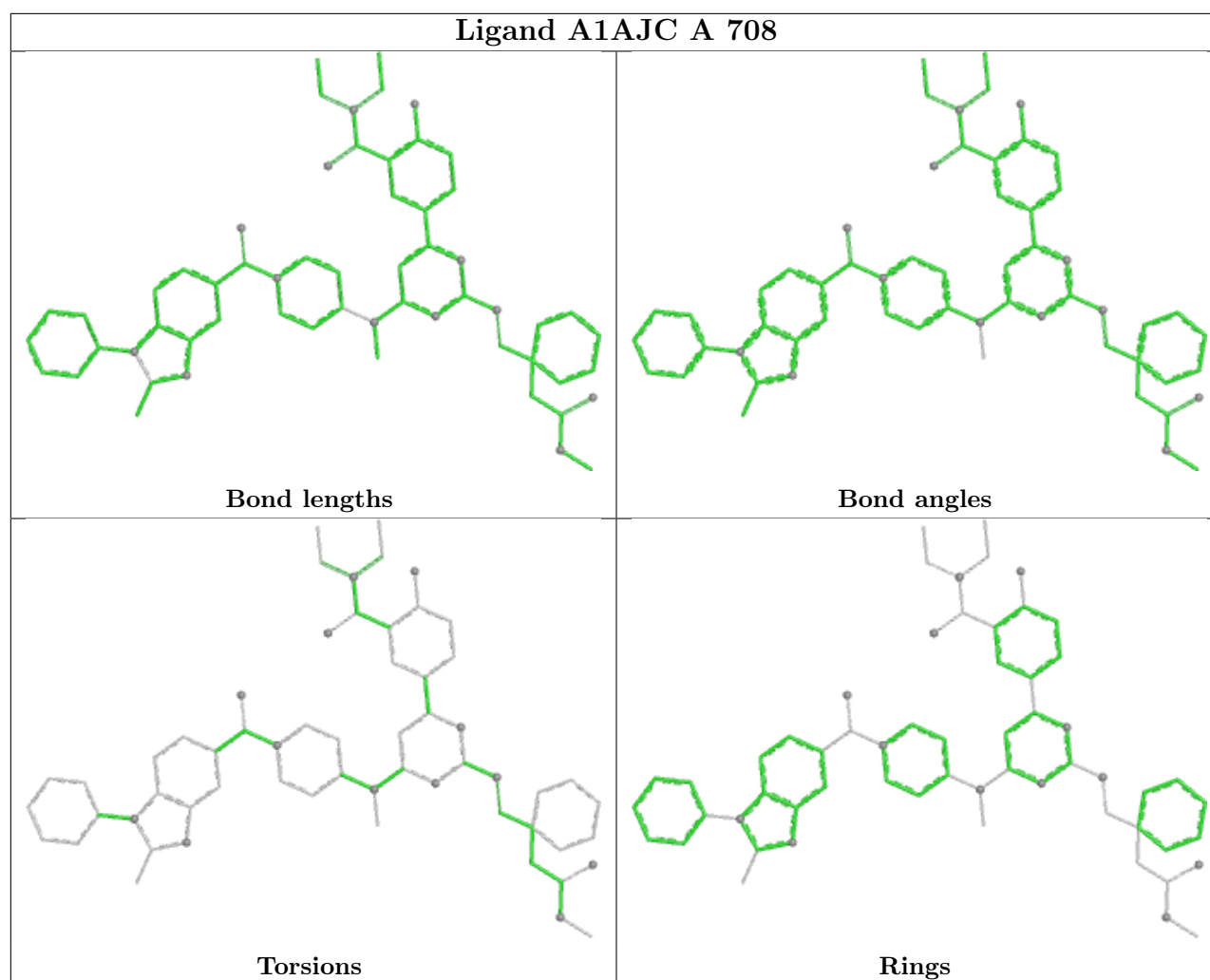
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	ACT	1	0
2	A	701	ACT	2	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

### 6.1 Protein, DNA and RNA chains

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	602/690 (87%)	0.62	65 (10%)	<b>11</b> <b>10</b>	19, 56, 110, 202	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	7.1
1	A	324	VAL	6.2
1	A	327	LEU	6.0
1	A	606	PRO	5.2
1	A	585	PHE	5.0
1	A	605	GLY	4.3
1	A	349	ILE	4.2
1	A	608	VAL	4.2
1	A	584	PHE	4.0
1	A	368	VAL	3.6
1	A	161	TRP	3.5
1	A	589	VAL	3.4
1	A	310	PHE	3.3
1	A	279	ASP	3.3
1	A	594	LEU	3.2
1	A	604	PHE	3.2
1	A	335	LEU	3.1
1	A	526	ILE	3.1
1	A	49	TRP	3.0
1	A	620	GLY	3.0
1	A	24	TYR	3.0
1	A	322	LYS	2.9
1	A	58	ALA	2.9
1	A	603	PRO	2.9
1	A	162	LEU	2.8
1	A	176	GLU	2.8
1	A	398	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	627	LEU	2.7
1	A	586	PRO	2.7
1	A	328	VAL	2.6
1	A	664	VAL	2.6
1	A	311	VAL	2.6
1	A	220	PRO	2.6
1	A	600	ILE	2.5
1	A	632	ILE	2.5
1	A	602	LYS	2.5
1	A	480	PRO	2.5
1	A	386	LEU	2.5
1	A	390	PHE	2.5
1	A	159	THR	2.5
1	A	665	PRO	2.5
1	A	508	GLY	2.5
1	A	587	ASN	2.5
1	A	588	MET	2.4
1	A	112	PHE	2.4
1	A	89	SER	2.4
1	A	277	ALA	2.4
1	A	67	GLN	2.3
1	A	614	LEU	2.3
1	A	65	GLY	2.3
1	A	621	LEU	2.3
1	A	331	THR	2.2
1	A	482	PRO	2.2
1	A	648	GLY	2.2
1	A	622	LEU	2.2
1	A	14	ARG	2.2
1	A	657	THR	2.2
1	A	276	MET	2.2
1	A	160	PRO	2.1
1	A	631	PHE	2.1
1	A	323	GLU	2.1
1	A	330	LYS	2.1
1	A	353	ILE	2.1
1	A	385	LEU	2.0
1	A	399	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

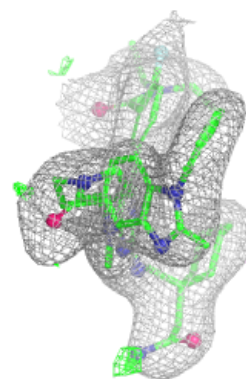
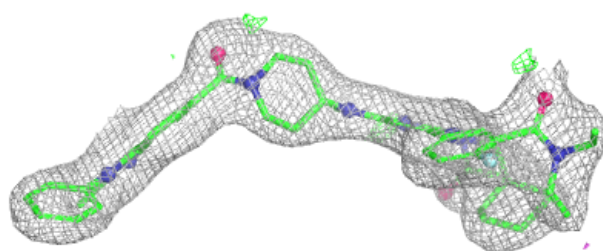
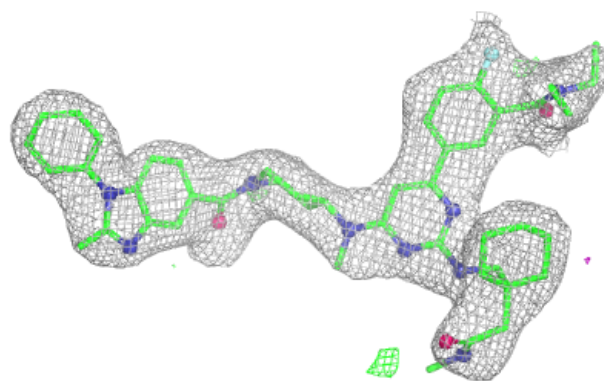
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	A	701	4/4	0.95	0.11	59,59,61,64	0
2	ACT	A	702	4/4	0.95	0.11	60,63,67,68	0
4	A1AJC	A	708	59/59	0.95	0.09	38,56,75,89	0
3	CA	A	703	1/1	0.96	0.05	57,57,57,57	0
3	CA	A	706	1/1	0.98	0.04	55,55,55,55	0
3	CA	A	704	1/1	0.99	0.02	41,41,41,41	0
3	CA	A	707	1/1	0.99	0.08	53,53,53,53	0
3	CA	A	705	1/1	0.99	0.03	54,54,54,54	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.

**Electron density around A1AJC A 708:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.