



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:33 PM UTC

PDB ID : 9B97 / pdb_00009b97
Title : Crystal structure of the human PAD2 protein bound to small molecule
Authors : Byrnes, L.J.; Vajdos, F.
Deposited on : 2024-04-01
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

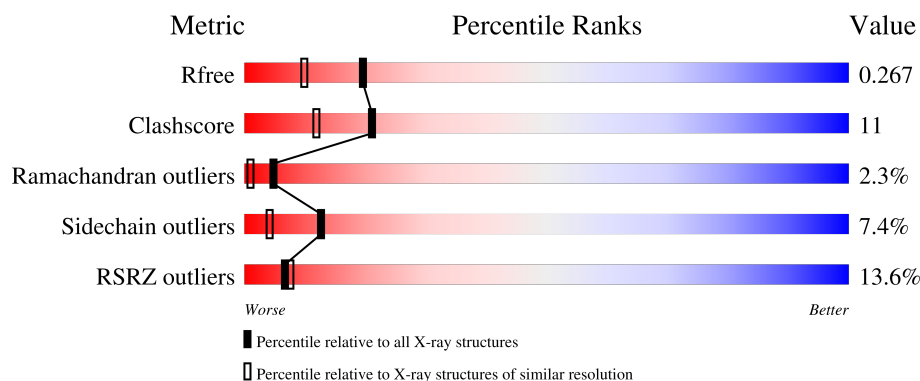
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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
4	ACT	A	705	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5244 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	626	5006	3218	829	929	30	0	3	0

There are 25 discrepancies between the modelled and reference sequences:

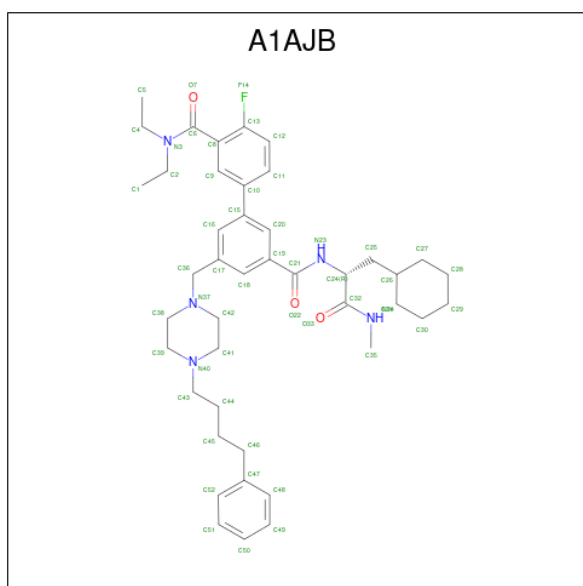
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q9Y2J8
A	-19	GLY	-	expression tag	UNP Q9Y2J8
A	-18	HIS	-	expression tag	UNP Q9Y2J8
A	-17	HIS	-	expression tag	UNP Q9Y2J8
A	-16	HIS	-	expression tag	UNP Q9Y2J8
A	-15	HIS	-	expression tag	UNP Q9Y2J8
A	-14	HIS	-	expression 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 (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			8	6	2			

- Molecule 3 is (1P)-N 3' -[(2S)-3-cyclohexyl-1-(methylamino)-1-oxopropan-2-yl]-N 3 ,N 3 -diethyl-4-fluoro-5'-{[4-(4-phenylbutyl)piperazin-1-yl]methyl}[1,1'-biphenyl]-3,3'-dicarboxamide (CCD ID: A1AJB) (formula: $C_{43}H_{58}FN_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			52	43	1	5	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

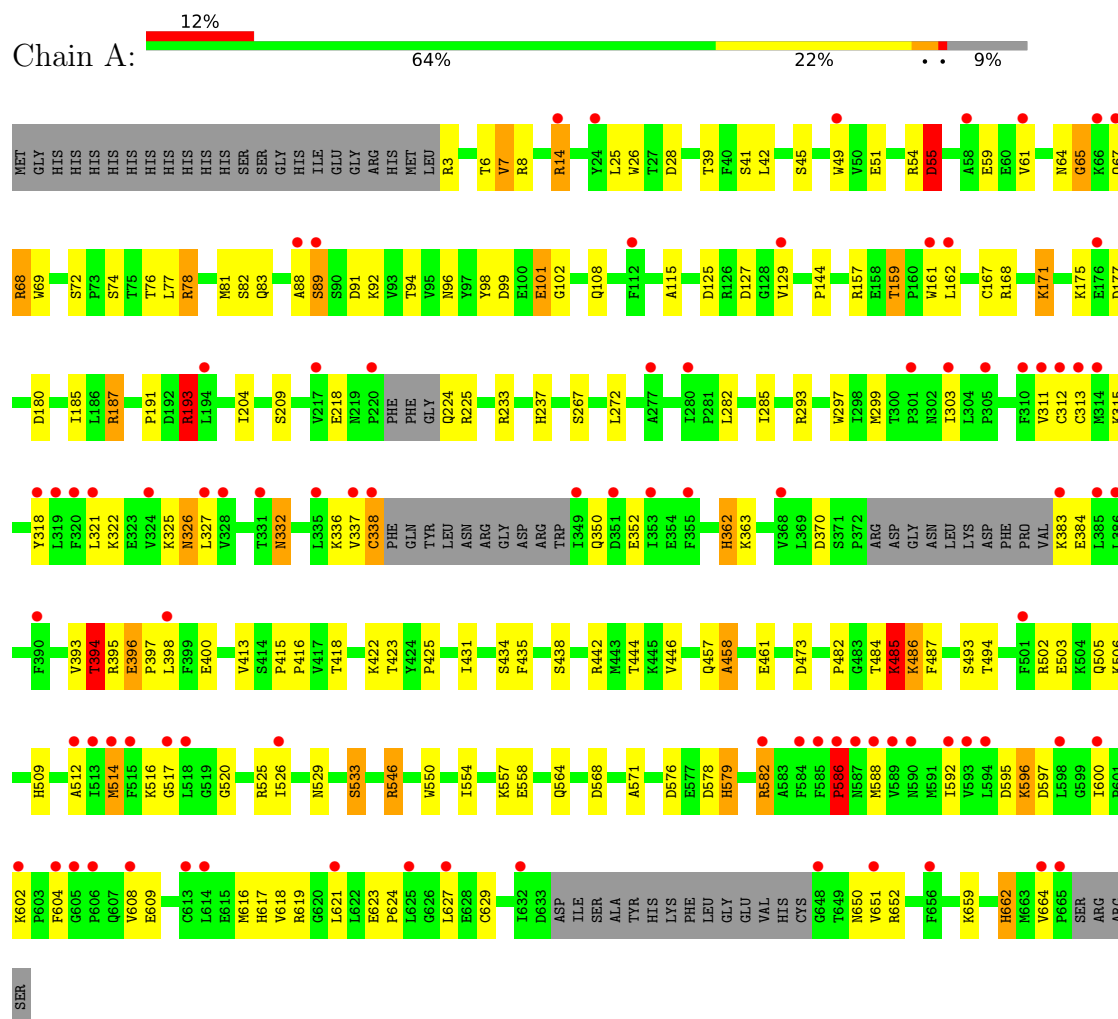
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total	O	0	0
			157	157		

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, α , β , γ	202.36Å 52.49Å 76.55Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	97.29 – 1.95 97.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	45.2 (97.29-1.95) 45.2 (97.29-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.186 , 0.267 0.194 , 0.267	Depositor DCC
R_{free} test set	1268 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AJB, CA, ACT, MPD

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	0.60	4/5129 (0.1%)	1.04	5/6950 (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	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	HIS	CE1-NE2	5.76	1.38	1.32
1	A	362	HIS	CE1-NE2	5.70	1.38	1.32
1	A	662	HIS	CE1-NE2	5.37	1.38	1.32
1	A	579	HIS	CE1-NE2	5.33	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	THR	CB-CA-C	6.84	117.76	110.17
1	A	473	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	394	THR	CB-CA-C	-5.79	99.35	110.24
1	A	485	LYS	CB-CA-C	5.55	120.64	110.10
1	A	576	ASP	CA-CB-CG	5.19	117.79	112.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	168	ARG	Sidechain
1	A	187	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	3	ARG	Sidechain
1	A	362	HIS	Peptide
1	A	395	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	525	ARG	Sidechain
1	A	546	ARG	Sidechain
1	A	652	ARG	Sidechain
1	A	68	ARG	Sidechain
1	A	78	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	5006	0	4995	110	0
2	A	8	0	14	2	0
3	A	52	0	0	1	0
4	A	16	0	12	3	0
5	A	5	0	0	0	0
6	A	157	0	0	12	0
All	All	5244	0	5021	111	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 11.

All (111) 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:167:CYS:SG	6:A:862:HOH:O	2.28	0.92
1:A:442[B]:ARG:HH11	1:A:442[B]:ARG:HG3	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD11	1:A:61:VAL:HG21	1.64	0.78
1:A:312:CYS:SG	1:A:312:CYS:O	2.40	0.77
1:A:161:TRP:HB3	6:A:949:HOH:O	1.87	0.73
1:A:484:THR:HA	1:A:485:LYS:HB3	1.71	0.72
1:A:99:ASP:O	6:A:801:HOH:O	2.06	0.72
1:A:550:TRP:CZ3	1:A:554:ILE:HD11	2.29	0.68
1:A:293:ARG:HD3	6:A:844:HOH:O	1.92	0.67
1:A:272:LEU:HD23	1:A:285:ILE:HD11	1.78	0.66
1:A:503:GLU:HA	1:A:503:GLU:OE1	1.95	0.65
1:A:159:THR:O	1:A:162:LEU:HG	1.98	0.63
1:A:442[B]:ARG:HG3	1:A:442[B]:ARG:NH1	2.13	0.63
1:A:39:THR:HG23	6:A:871:HOH:O	1.99	0.61
1:A:383:LYS:HG3	1:A:384:GLU:N	2.19	0.58
1:A:484:THR:HB	1:A:485:LYS:HG2	1.85	0.58
1:A:494:THR:HA	1:A:571:ALA:O	2.03	0.58
1:A:435:PHE:HA	2:A:701:MPD:H11	1.87	0.57
1:A:6:THR:OG1	1:A:26:TRP:NE1	2.36	0.57
1:A:322:LYS:O	1:A:326:ASN:HB2	2.05	0.56
1:A:125:ASP:C	1:A:125:ASP:OD1	2.48	0.55
1:A:484:THR:OG1	1:A:486:LYS:HB2	2.07	0.55
1:A:218:GLU:O	1:A:224:GLN:HB2	2.06	0.55
1:A:484:THR:HB	1:A:485:LYS:C	2.31	0.55
1:A:493:SER:HB2	1:A:568:ASP:HB3	1.89	0.55
1:A:54:ARG:O	1:A:55:ASP:C	2.50	0.54
1:A:96:ASN:ND2	1:A:108:GLN:HG2	2.22	0.54
1:A:332:ASN:HD22	1:A:332:ASN:H	1.56	0.54
1:A:600:ILE:HD12	1:A:629:CYS:HB3	1.90	0.54
1:A:180:ASP:OD1	1:A:363:LYS:NZ	2.41	0.54
1:A:272:LEU:CD2	1:A:285:ILE:HD11	2.36	0.54
1:A:299:MET:HE2	1:A:413:VAL:HG12	1.90	0.54
1:A:42:LEU:HD11	1:A:61:VAL:CG2	2.34	0.54
1:A:442[A]:ARG:HH21	1:A:461:GLU:CD	2.15	0.53
1:A:204:ILE:HD12	1:A:209:SER:HA	1.91	0.53
1:A:321:LEU:O	1:A:325:LYS:HB3	2.09	0.53
1:A:529:ASN:O	1:A:533:SER:OG	2.27	0.53
1:A:493:SER:CB	1:A:568:ASP:HB3	2.39	0.53
1:A:64:ASN:O	1:A:65:GLY:O	2.27	0.52
1:A:484:THR:HG22	1:A:485:LYS:HD3	1.91	0.52
1:A:482:PRO:HB3	1:A:596:LYS:HG3	1.92	0.52
1:A:193:ARG:CB	1:A:193:ARG:NH1	2.73	0.51
1:A:144:PRO:HA	1:A:662:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:SER:HA	3:A:702:A1AJB:C20	2.41	0.51
1:A:7:VAL:HG11	1:A:25:LEU:HD13	1.94	0.50
1:A:484:THR:HA	1:A:485:LYS:CB	2.40	0.50
1:A:81:MET:CE	1:A:115:ALA:HB2	2.42	0.50
1:A:370:ASP:O	1:A:394:THR:HG22	2.11	0.50
1:A:582:ARG:HG2	1:A:582:ARG:NH1	2.26	0.50
1:A:185:ILE:HG22	1:A:187:ARG:HG3	1.93	0.50
1:A:337:VAL:HG12	1:A:338:CYS:N	2.27	0.49
1:A:101:GLU:HG2	1:A:102:GLY:H	1.76	0.49
1:A:303:ILE:HD11	1:A:416:PRO:HD2	1.94	0.49
1:A:397:PRO:HG3	1:A:444:THR:HG21	1.95	0.49
1:A:68:ARG:HD2	6:A:871:HOH:O	2.13	0.49
1:A:578:ASP:O	1:A:579:HIS:HB2	2.13	0.49
1:A:81:MET:HE2	1:A:115:ALA:HB2	1.96	0.48
1:A:297:TRP:CZ3	1:A:299:MET:HG3	2.48	0.48
1:A:442[A]:ARG:HD2	4:A:705:ACT:H3	1.95	0.48
1:A:616:MET:HE2	1:A:619:ARG:HD2	1.95	0.47
1:A:514:MET:N	1:A:526:ILE:O	2.41	0.47
1:A:400:GLU:OE1	1:A:442[B]:ARG:NH1	2.48	0.47
1:A:41:SER:CB	1:A:67:GLN:O	2.64	0.46
1:A:506:LYS:HG2	6:A:923:HOH:O	2.16	0.46
1:A:39:THR:HA	1:A:69:TRP:O	2.16	0.45
1:A:415:PRO:HG2	1:A:487:PHE:CG	2.51	0.45
1:A:272:LEU:HD23	1:A:285:ILE:CG1	2.46	0.45
1:A:659:LYS:NZ	6:A:824:HOH:O	2.49	0.45
1:A:434:SER:O	4:A:705:ACT:H1	2.16	0.45
1:A:457:GLN:O	1:A:458:ALA:C	2.59	0.45
1:A:299:MET:HE2	1:A:413:VAL:CG1	2.47	0.45
1:A:509:HIS:O	1:A:512:ALA:HB3	2.16	0.45
1:A:350:GLN:HA	1:A:650:ASN:ND2	2.32	0.44
1:A:418:THR:HG23	1:A:422:LYS:O	2.17	0.44
1:A:51:GLU:OE1	1:A:78:ARG:NH1	2.50	0.44
1:A:509:HIS:CE1	1:A:608:VAL:HG13	2.52	0.44
1:A:193:ARG:NH1	1:A:193:ARG:HB2	2.32	0.44
1:A:442[A]:ARG:CZ	4:A:705:ACT:O	2.65	0.44
1:A:98:TYR:HB2	6:A:871:HOH:O	2.18	0.44
1:A:191:PRO:HG2	1:A:193:ARG:O	2.18	0.44
1:A:54:ARG:HA	1:A:74:SER:O	2.18	0.43
1:A:177:ASP:OD2	6:A:802:HOH:O	2.21	0.43
1:A:297:TRP:CH2	1:A:299:MET:HG3	2.53	0.43
1:A:39:THR:CG2	6:A:871:HOH:O	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLN:HG3	1:A:529:ASN:OD1	2.17	0.43
1:A:7:VAL:HG22	1:A:7:VAL:O	2.17	0.43
1:A:550:TRP:CH2	1:A:554:ILE:HD11	2.53	0.43
1:A:272:LEU:HD23	1:A:285:ILE:CD1	2.46	0.43
1:A:303:ILE:HD11	1:A:416:PRO:CD	2.49	0.43
1:A:484:THR:HB	1:A:486:LYS:N	2.33	0.43
1:A:550:TRP:CZ3	1:A:554:ILE:CD1	3.01	0.43
1:A:76:THR:C	1:A:77:LEU:HD23	2.43	0.43
1:A:586:PRO:HG2	1:A:602:LYS:O	2.19	0.42
1:A:623:GLU:HA	1:A:627:LEU:O	2.20	0.42
1:A:127:ASP:OD1	1:A:129:VAL:HB	2.19	0.42
1:A:327:LEU:HD11	1:A:597:ASP:HB3	2.02	0.42
1:A:588:MET:SD	1:A:618:VAL:HG21	2.59	0.42
1:A:617:HIS:CE1	1:A:621:LEU:HD11	2.55	0.42
1:A:423:THR:HG22	1:A:425:PRO:HD3	2.01	0.42
1:A:370:ASP:HB3	1:A:394:THR:HG23	2.01	0.42
1:A:49:TRP:HE1	1:A:82:SER:HB3	1.84	0.41
1:A:396:GLU:H	1:A:396:GLU:CD	2.29	0.41
1:A:486:LYS:HE2	1:A:487:PHE:H	1.85	0.41
1:A:89:SER:O	1:A:91:ASP:N	2.52	0.41
1:A:311:VAL:HG12	1:A:312:CYS:N	2.35	0.41
1:A:557:LYS:HE2	1:A:558:GLU:OE2	2.20	0.41
1:A:484:THR:CA	1:A:485:LYS:CB	2.99	0.41
1:A:171:LYS:HG3	6:A:936:HOH:O	2.20	0.40
1:A:204:ILE:CD1	1:A:209:SER:HA	2.50	0.40
2:A:701:MPD:HM1	2:A:701:MPD:O4	2.21	0.40
1:A:318:TYR:O	1:A:322:LYS:N	2.54	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	619/690 (90%)	570 (92%)	35 (6%)	14 (2%)	5 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLY
1	A	89	SER
1	A	88	ALA
1	A	609	GLU
1	A	55	ASP
1	A	59	GLU
1	A	315	LYS
1	A	595	ASP
1	A	604	PHE
1	A	624	PRO
1	A	520	GLY
1	A	517	GLY
1	A	458	ALA
1	A	586	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	559/612 (91%)	518 (93%)	41 (7%)	13 4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	14	ARG
1	A	28	ASP
1	A	45	SER
1	A	55	ASP
1	A	72	SER
1	A	83	GLN

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Mol	Chain	Res	Type
1	A	92	LYS
1	A	94	THR
1	A	101	GLU
1	A	171	LYS
1	A	175	LYS
1	A	193	ARG
1	A	225	ARG
1	A	267	SER
1	A	282	LEU
1	A	313	CYS
1	A	326	ASN
1	A	332	ASN
1	A	336	LYS
1	A	338	CYS
1	A	352	GLU
1	A	393	VAL
1	A	394	THR
1	A	396	GLU
1	A	398	LEU
1	A	431	ILE
1	A	446	VAL
1	A	485	LYS
1	A	486	LYS
1	A	514	MET
1	A	516	LYS
1	A	533	SER
1	A	546	ARG
1	A	564	GLN
1	A	582	ARG
1	A	586	PRO
1	A	592	ILE
1	A	596	LYS
1	A	651	VAL
1	A	664	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	224	GLN
1	A	302	ASN
1	A	332	ASN

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Mol	Chain	Res	Type
1	A	617	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	ACT	A	706	-	3,3,3	1.16	0	3,3,3	0.85	0
4	ACT	A	705	-	3,3,3	0.93	0	3,3,3	0.97	0
2	MPD	A	701	-	7,7,7	0.22	0	9,10,10	1.05	1 (11%)
3	A1AJB	A	702	-	56,56,56	0.33	0	75,75,75	0.64	1 (1%)
4	ACT	A	703	-	3,3,3	1.32	0	3,3,3	0.58	0
4	ACT	A	704	-	3,3,3	1.05	0	3,3,3	0.76	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
2	MPD	A	701	-	-	1/5/5/5	-
3	A1AJB	A	702	-	-	11/45/63/63	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	MPD	O2-C2-C1	-2.58	99.95	107.99
3	A	702	A1AJB	C32-C24-N23	2.53	117.95	111.11

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	MPD	C2-C3-C4-O4
3	A	702	A1AJB	C24-C32-N34-C35
3	A	702	A1AJB	O33-C32-N34-C35
3	A	702	A1AJB	N40-C43-C44-C45
3	A	702	A1AJB	C25-C24-C32-O33
3	A	702	A1AJB	C25-C24-C32-N34
3	A	702	A1AJB	N23-C24-C25-C26
3	A	702	A1AJB	C5-C4-N3-C6
3	A	702	A1AJB	C5-C4-N3-C2
3	A	702	A1AJB	N23-C24-C32-O33
3	A	702	A1AJB	N23-C24-C32-N34
3	A	702	A1AJB	C44-C45-C46-C47

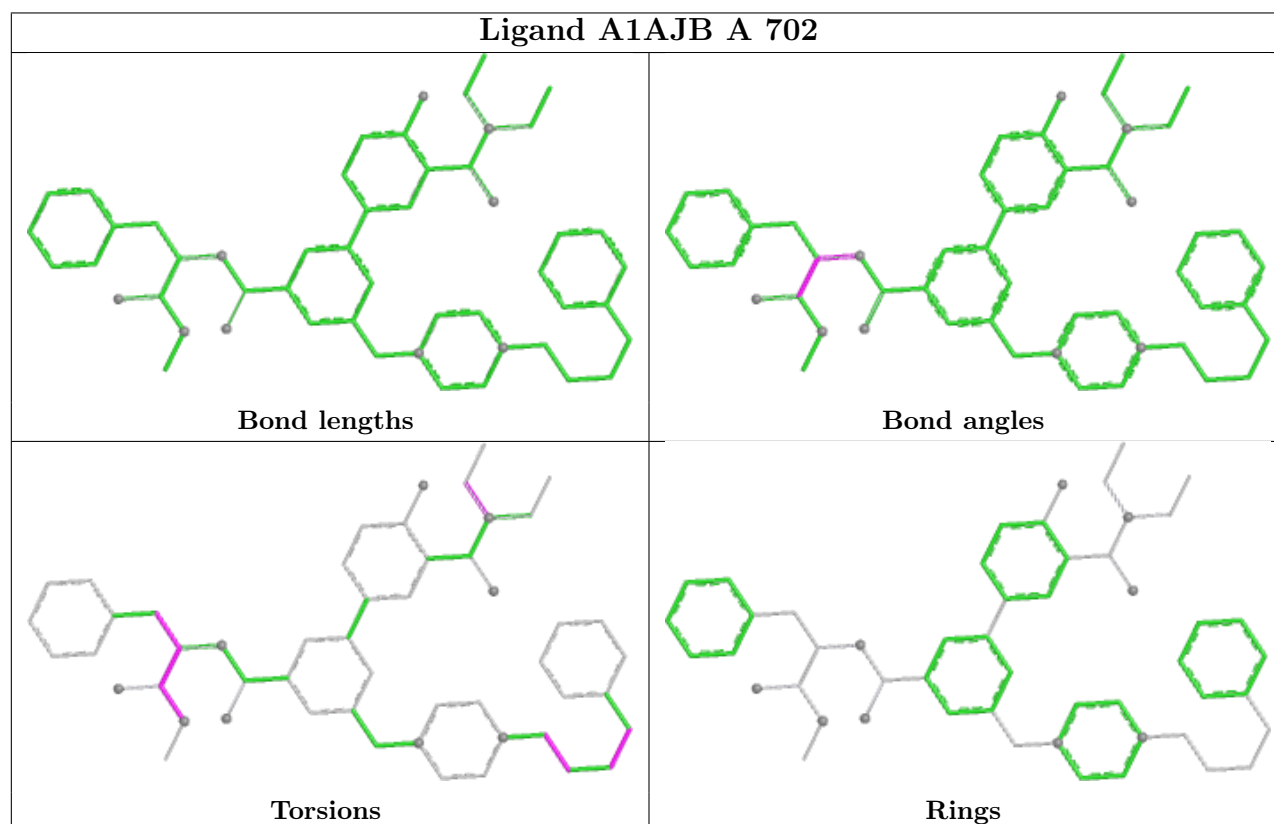
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	ACT	3	0
2	A	701	MPD	2	0
3	A	702	A1AJB	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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	626/690 (90%)	0.79	85 (13%) 7 7	16, 54, 133, 223	3 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	584	PHE	6.2
1	A	585	PHE	5.9
1	A	606	PRO	5.7
1	A	310	PHE	5.1
1	A	515	PHE	4.9
1	A	327	LEU	4.7
1	A	161	TRP	4.7
1	A	608	VAL	4.4
1	A	319	LEU	4.3
1	A	664	VAL	4.3
1	A	324	VAL	3.8
1	A	518	LEU	3.8
1	A	587	ASN	3.8
1	A	318	TYR	3.8
1	A	514	MET	3.7
1	A	589	VAL	3.7
1	A	311	VAL	3.6
1	A	337	VAL	3.6
1	A	614	LEU	3.5
1	A	335	LEU	3.5
1	A	632	ILE	3.4
1	A	162	LEU	3.4
1	A	49	TRP	3.4
1	A	303	ILE	3.2
1	A	194	LEU	3.2
1	A	613	CYS	3.2
1	A	321	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	220	PRO	3.1
1	A	627	LEU	3.1
1	A	586	PRO	3.1
1	A	604	PHE	3.1
1	A	513	ILE	3.1
1	A	383	LYS	3.1
1	A	592	ILE	3.0
1	A	598	LEU	3.0
1	A	621	LEU	3.0
1	A	526	ILE	3.0
1	A	355	PHE	3.0
1	A	398	LEU	2.9
1	A	665	PRO	2.9
1	A	386	LEU	2.9
1	A	320	PHE	2.8
1	A	588	MET	2.8
1	A	58	ALA	2.8
1	A	385	LEU	2.8
1	A	349	ILE	2.7
1	A	61	VAL	2.7
1	A	600	ILE	2.6
1	A	625	LEU	2.6
1	A	314	MET	2.6
1	A	390	PHE	2.5
1	A	605	GLY	2.5
1	A	590	ASN	2.5
1	A	277	ALA	2.5
1	A	331	THR	2.4
1	A	338	CYS	2.4
1	A	176	GLU	2.4
1	A	593	VAL	2.4
1	A	351	ASP	2.3
1	A	67	GLN	2.3
1	A	313	CYS	2.3
1	A	112	PHE	2.3
1	A	602	LYS	2.3
1	A	217	VAL	2.3
1	A	66	LYS	2.3
1	A	14	ARG	2.2
1	A	656	PHE	2.2
1	A	89	SER	2.2
1	A	368	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	517	GLY	2.2
1	A	280	ILE	2.2
1	A	582	ARG	2.2
1	A	651	VAL	2.2
1	A	648	GLY	2.2
1	A	305	PRO	2.2
1	A	24	TYR	2.1
1	A	353	ILE	2.1
1	A	301	PRO	2.1
1	A	312	CYS	2.1
1	A	501	PHE	2.1
1	A	129	VAL	2.1
1	A	594	LEU	2.1
1	A	88	ALA	2.1
1	A	512	ALA	2.1
1	A	328	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

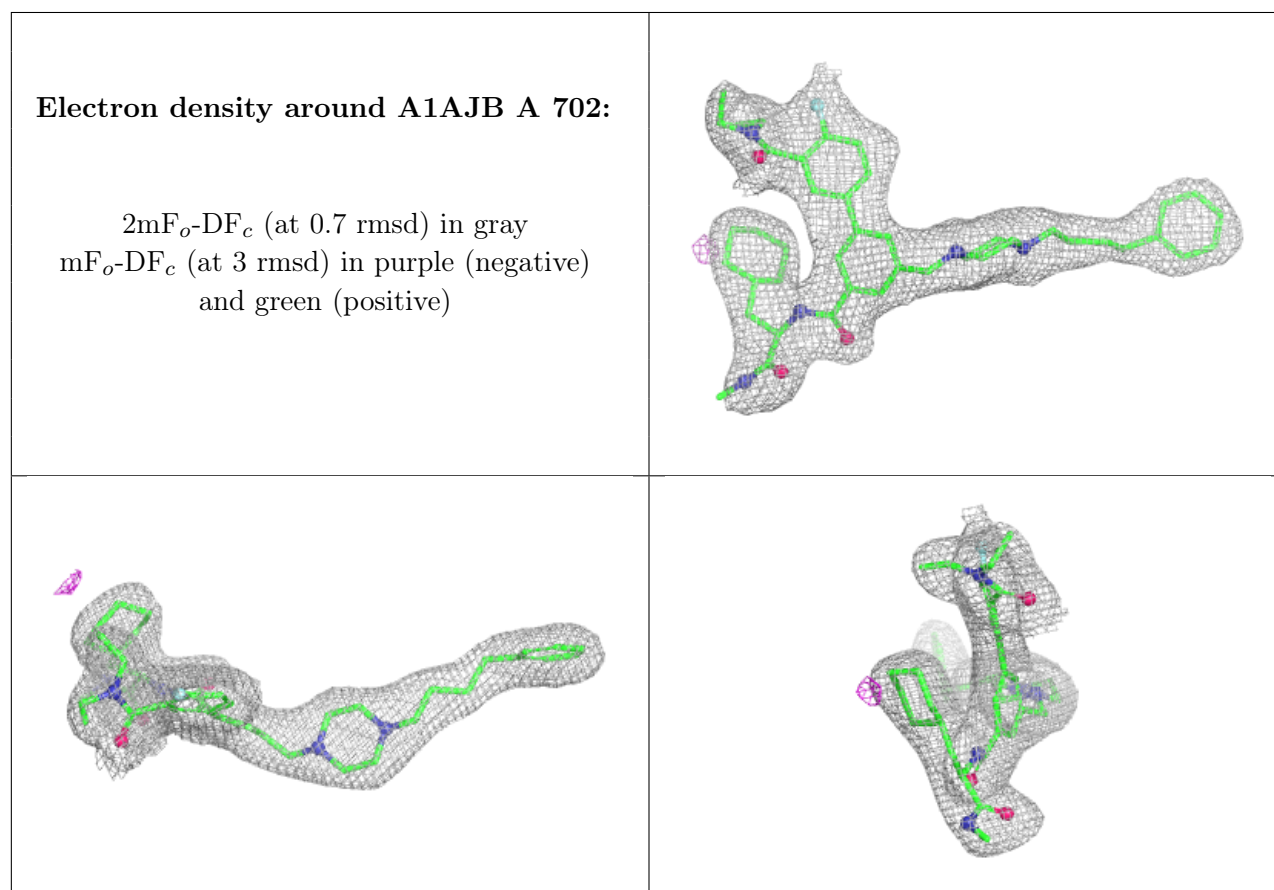
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	A	703	4/4	0.80	0.17	55,55,56,57	0
4	ACT	A	705	4/4	0.84	0.19	74,79,89,92	0
4	ACT	A	706	4/4	0.86	0.21	66,77,82,84	0
4	ACT	A	704	4/4	0.89	0.16	62,65,68,77	0
2	MPD	A	701	8/8	0.92	0.17	48,62,77,77	0
3	A1AJB	A	702	52/52	0.95	0.08	29,44,52,60	0
5	CA	A	707	1/1	0.95	0.05	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	710	1/1	0.97	0.04	55,55,55,55	0
5	CA	A	709	1/1	0.98	0.03	59,59,59,59	0
5	CA	A	711	1/1	0.98	0.09	60,60,60,60	0
5	CA	A	708	1/1	0.99	0.03	38,38,38,38	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.