



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 10:07 AM EDT

PDB ID : 9OVQ / pdb_00009ovq
Title : PAD2 with an inhibitor
Authors : Yamaguchi, M.
Deposited on : 2025-05-30
Resolution : 2.17 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

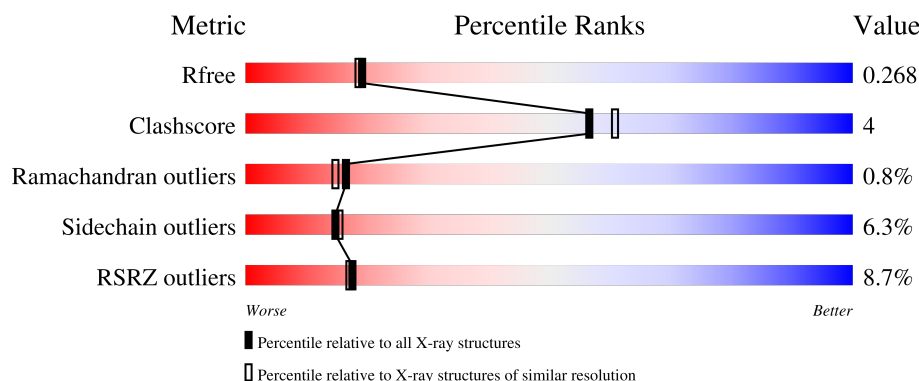
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.17 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	677	

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
3	CA	A	703	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4988 atoms, of which 26 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.

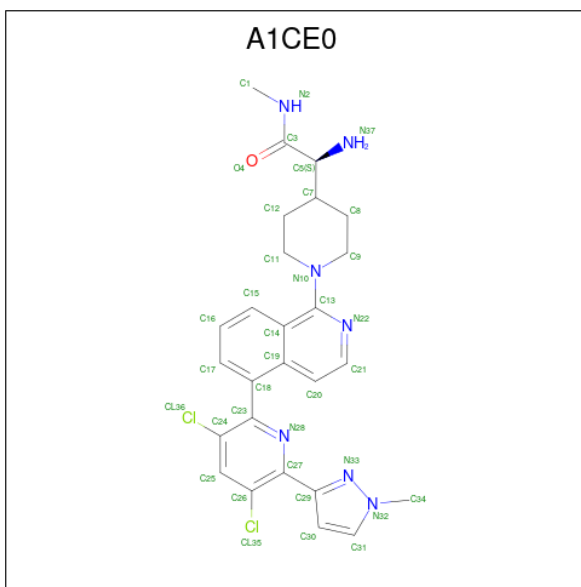
- Molecule 1 is a protein called Protein-arginine deiminase type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	7	0
			4867	3129	793	915	30			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9Y2J8
A	-6	PRO	-	expression tag	UNP Q9Y2J8
A	-5	LEU	-	expression tag	UNP Q9Y2J8
A	-4	GLY	-	expression tag	UNP Q9Y2J8
A	-3	SER	-	expression tag	UNP Q9Y2J8
A	-2	PRO	-	expression tag	UNP Q9Y2J8
A	-1	GLU	-	expression tag	UNP Q9Y2J8
A	0	PHE	-	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 (2S)-2-amino-2-(1-((5M)-5-[3,5-dichloro-6-(1-methyl-1H-pyrazol-3-yl)pyridin-2-yl]isoquinolin-1-yl)piperidin-4-yl)-N-methylacetamide (CCD ID: A1CE0) (formula: C₂₆H₂₇Cl₂N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	
			62	26	2	26	7	1	26

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca		
			4	4	0	0

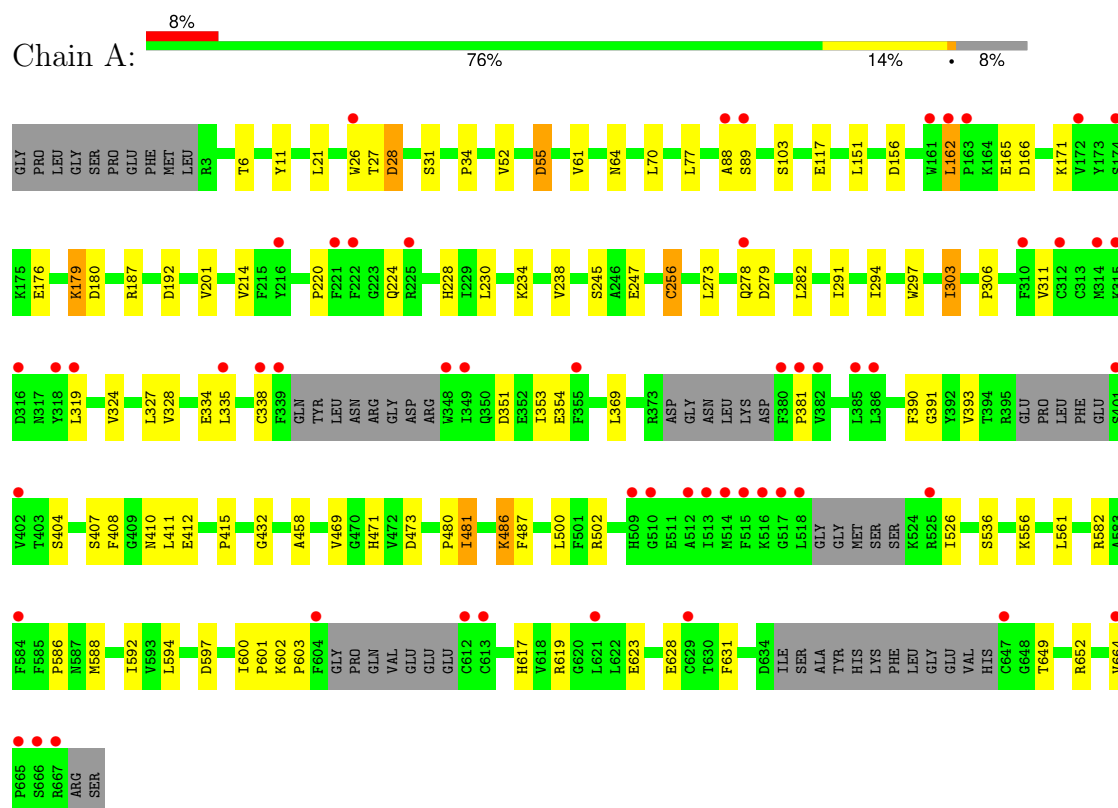
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O		
			55	55	0	0

3 Residue-property plots

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	201.94Å 51.25Å 76.31Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	30.51 – 2.17 30.51 – 2.17	Depositor EDS
% Data completeness (in resolution range)	49.9 (30.51-2.17) 49.9 (30.51-2.17)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.218 , 0.269 0.215 , 0.268	Depositor DCC
R_{free} test set	20836 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4988	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CE0, CA

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	0.73	0/4992	1.03	4/6784 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	481	ILE	N-CA-C	-5.60	101.61	107.60
1	A	166	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	180	ASP	CA-CB-CG	5.39	118.00	112.60
1	A	473	ASP	CA-CB-CG	5.31	117.91	112.60

There are no chirality outliers.

There are no planarity outliers.

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	4867	0	4720	43	0
2	A	36	26	0	0	0
3	A	4	0	0	0	0
4	A	55	0	0	1	0
All	All	4962	26	4720	43	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 4.

All (43) 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:220:PRO:HA	1:A:224:GLN:HG2	1.60	0.83
1:A:297:TRP:CE2	1:A:369:LEU:HD23	2.14	0.81
1:A:328:VAL:HG11	1:A:335:LEU:HB2	1.77	0.67
1:A:6:THR:OG1	1:A:26:TRP:NE1	2.29	0.65
1:A:228:HIS:ND1	1:A:234:LYS:NZ	2.45	0.64
1:A:303:ILE:HG12	1:A:415:PRO:HB3	1.82	0.62
1:A:481:ILE:HD12	1:A:486:LYS:HB3	1.81	0.62
1:A:556:LYS:HA	1:A:561:LEU:HB2	1.85	0.57
1:A:52:VAL:HG23	1:A:61:VAL:HG21	1.87	0.56
1:A:176:GLU:HA	1:A:179:LYS:HD3	1.88	0.55
1:A:311:VAL:HG22	1:A:649:THR:HG22	1.91	0.52
1:A:306:PRO:HG3	1:A:594:LEU:HA	1.93	0.51
1:A:297:TRP:NE1	1:A:369:LEU:HD23	2.27	0.50
1:A:586:PRO:HD2	1:A:603:PRO:HA	1.93	0.49
1:A:588:MET:HA	1:A:601:PRO:HD2	1.93	0.49
1:A:162:LEU:HD13	1:A:162:LEU:H	1.77	0.49
1:A:273:LEU:HB3	1:A:282:LEU:HB3	1.94	0.48
1:A:327:LEU:HD11	1:A:597:ASP:HB3	1.96	0.48
1:A:410:ASN:OD1	1:A:432:GLY:HA3	2.15	0.47
1:A:415:PRO:HG2	1:A:487:PHE:CG	2.52	0.45
1:A:303:ILE:HA	1:A:480:PRO:HG3	1.98	0.45
1:A:256:CYS:O	1:A:294:ILE:HG21	2.16	0.45
1:A:176:GLU:HA	1:A:179:LYS:CD	2.47	0.44
1:A:28:ASP:OD2	1:A:31:SER:HB2	2.18	0.44
1:A:311:VAL:HG21	1:A:324:VAL:HG11	1.99	0.44
1:A:214:VAL:HB	1:A:230:LEU:HB2	1.99	0.44
1:A:21:LEU:HD12	1:A:117:GLU:HB2	2.00	0.43
1:A:11:TYR:HE1	1:A:34:PRO:HA	1.83	0.43
1:A:27:THR:HB	1:A:77:LEU:HB2	2.00	0.43
1:A:469:VAL:HG12	1:A:471:HIS:CE1	2.53	0.43
1:A:619:ARG:O	1:A:623:GLU:HB2	2.18	0.43
1:A:354:GLU:HB2	1:A:408:PHE:CD1	2.54	0.43
1:A:6:THR:HG23	1:A:26:TRP:CE2	2.54	0.42
1:A:500:LEU:HD13	1:A:617:HIS:ND1	2.35	0.42
1:A:502:ARG:HD2	4:A:829:HOH:O	2.19	0.42
1:A:156:ASP:HA	1:A:391:GLY:HA2	2.02	0.42
1:A:600:ILE:O	1:A:631:PHE:HA	2.21	0.41
1:A:187:ARG:HG2	1:A:247:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:VAL:CG1	1:A:471:HIS:CE1	3.04	0.41
1:A:201:VAL:HG22	1:A:238:VAL:HG22	2.03	0.41
1:A:278:GLN:O	1:A:279:ASP:HB2	2.21	0.41
1:A:586:PRO:HG2	1:A:602:LYS:O	2.21	0.40
1:A:151:LEU:O	1:A:294:ILE:HA	2.21	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	615/677 (91%)	573 (93%)	37 (6%)	5 (1%)	16 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	381	PRO
1	A	88	ALA
1	A	55	ASP
1	A	458	ALA

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	531/600 (88%)	497 (94%)	34 (6%)	14	15

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	55	ASP
1	A	64	ASN
1	A	70	LEU
1	A	103	SER
1	A	162	LEU
1	A	165	GLU
1	A	171	LYS
1	A	179	LYS
1	A	192	ASP
1	A	245	SER
1	A	256	CYS
1	A	291	ILE
1	A	303	ILE
1	A	319	LEU
1	A	334	GLU
1	A	338	CYS
1	A	351	ASP
1	A	353	ILE
1	A	390	PHE
1	A	393	VAL
1	A	404	SER
1	A	407[A]	SER
1	A	407[B]	SER
1	A	411	LEU
1	A	412	GLU
1	A	486	LYS
1	A	526	ILE
1	A	536	SER
1	A	582	ARG
1	A	592	ILE
1	A	628	GLU
1	A	652	ARG
1	A	664	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	96	ASN
1	A	108	GLN
1	A	224	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are 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	$\# Z > 2$
2	A1CE0	A	701	-	38,40,40	0.68	1 (2%)	45,58,58	0.88	2 (4%)

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	A1CE0	A	701	-	-	3/19/32/32	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	A1CE0	C13-N22	2.52	1.36	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	A1CE0	C25-C26-C27	-3.09	118.76	121.88
2	A	701	A1CE0	C25-C24-C23	-2.85	118.99	121.88

There are no chirality outliers.

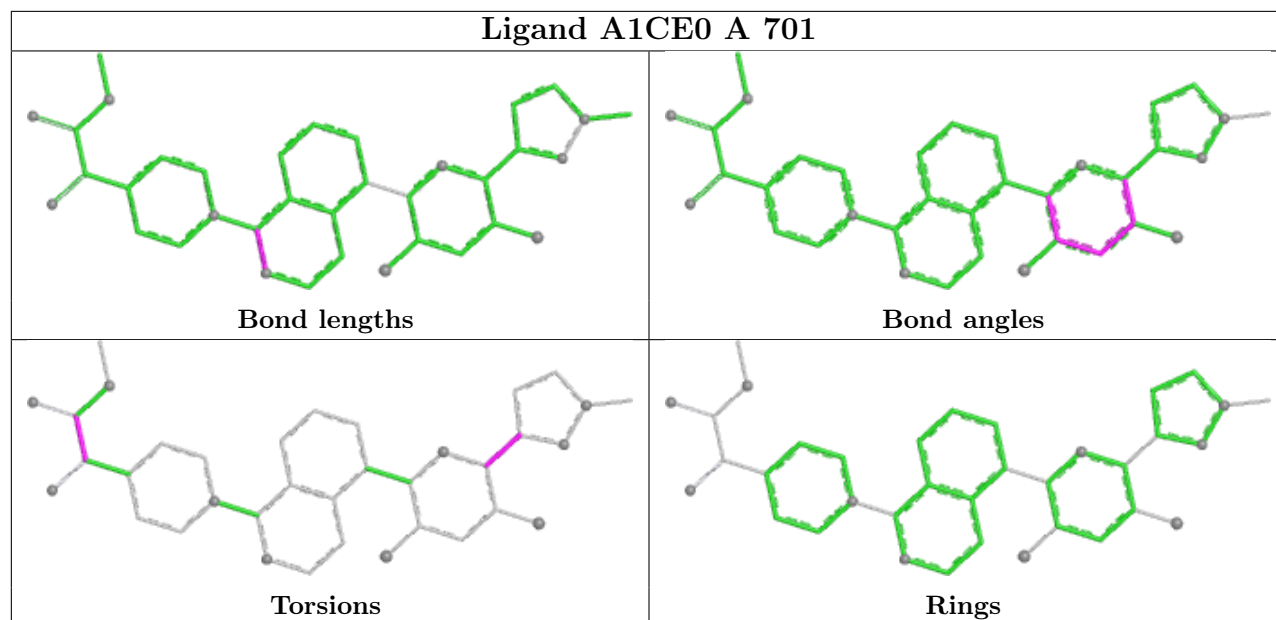
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	A1CE0	N28-C27-C29-C30
2	A	701	A1CE0	O4-C3-C5-N37
2	A	701	A1CE0	N2-C3-C5-C7

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 ⓘ

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	622/677 (91%)	0.57	54 (8%) 17 17	17, 47, 81, 103	7 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	LEU	5.3
1	A	161	TRP	4.8
1	A	604	PHE	4.5
1	A	612	CYS	4.3
1	A	382	VAL	4.1
1	A	380	PHE	3.9
1	A	163	PRO	3.8
1	A	162	LEU	3.8
1	A	515	PHE	3.7
1	A	318	TYR	3.6
1	A	222	PHE	3.5
1	A	319	LEU	3.5
1	A	385	LEU	3.4
1	A	221	PHE	3.3
1	A	647	CYS	3.3
1	A	310	PHE	3.2
1	A	667	ARG	3.1
1	A	316	ASP	3.0
1	A	664	VAL	2.9
1	A	513	ILE	2.9
1	A	348	TRP	2.8
1	A	621	LEU	2.8
1	A	355	PHE	2.7
1	A	666	SER	2.7
1	A	509	HIS	2.7
1	A	525	ARG	2.7
1	A	339	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	381	PRO	2.6
1	A	584	PHE	2.6
1	A	386	LEU	2.6
1	A	26	TRP	2.5
1	A	349	ILE	2.5
1	A	613	CYS	2.5
1	A	278	GLN	2.5
1	A	514	MET	2.4
1	A	312[A]	CYS	2.4
1	A	314	MET	2.4
1	A	335	LEU	2.4
1	A	88	ALA	2.4
1	A	665	PRO	2.3
1	A	338	CYS	2.3
1	A	517	GLY	2.2
1	A	516	LYS	2.2
1	A	401	SER	2.2
1	A	89	SER	2.1
1	A	629	CYS	2.1
1	A	225	ARG	2.1
1	A	512	ALA	2.1
1	A	315	LYS	2.1
1	A	216	TYR	2.1
1	A	172	VAL	2.1
1	A	402	VAL	2.1
1	A	510	GLY	2.0
1	A	174	SER	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.

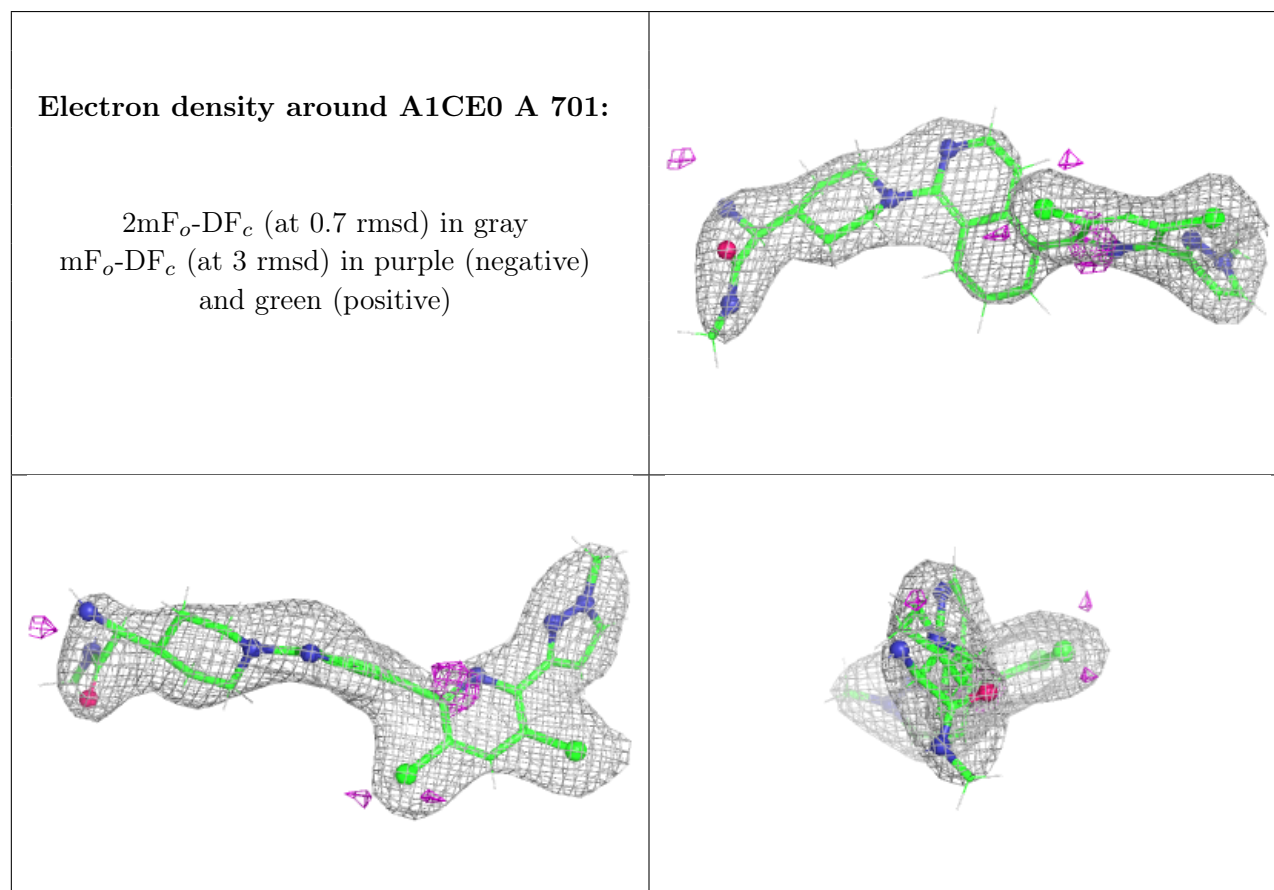
6.4 Ligands [i](#)

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
3	CA	A	703	1/1	0.28	0.51	70,70,70,70	0
3	CA	A	702	1/1	0.50	0.35	38,38,38,38	0
3	CA	A	704	1/1	0.91	0.09	78,78,78,78	0
2	A1CE0	A	701	36/36	0.92	0.10	51,53,55,55	26
3	CA	A	705	1/1	0.99	0.03	57,57,57,57	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.