



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:33 AM UTC

PDB ID : 3FDN / pdb_00003fdn
Title : Structure-based drug design of novel Aurora kinase A inhibitors: Structure basis for potency and specificity
Authors : Leou, J.S.; Wu, J.S.; Coumar, M.S.; Shukla, P.; Hsieh, H.P.; Wu, S.Y.
Deposited on : 2008-11-26
Resolution : 1.90 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

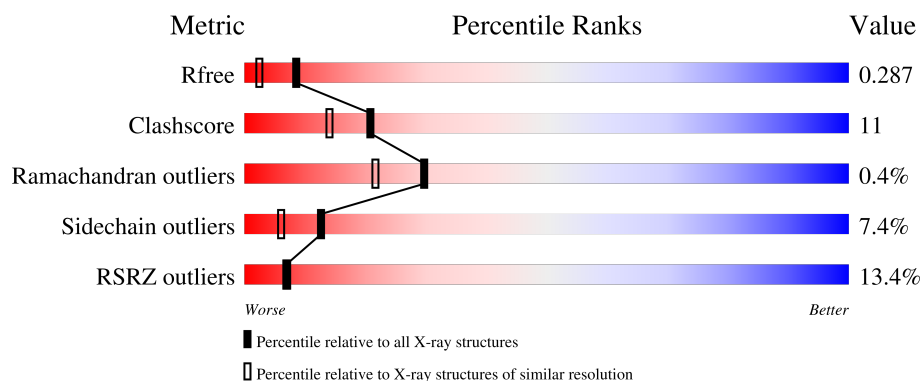
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	279	

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.

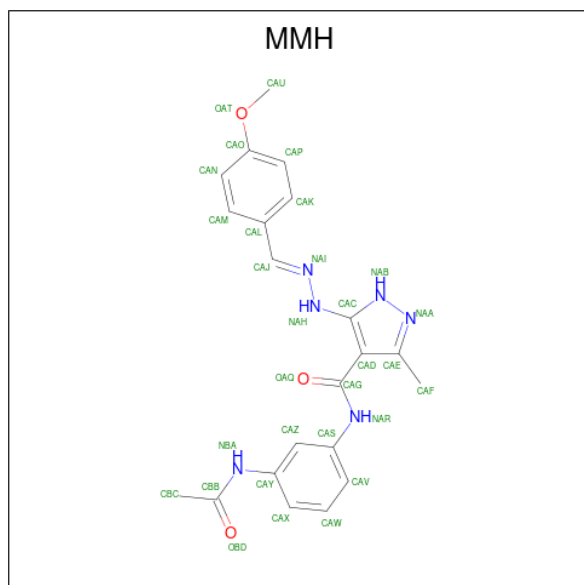
- Molecule 1 is a protein called Serine/threonine-protein kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2134	1372	374	381	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ASP	THR	engineered mutation	UNP O14965

- Molecule 2 is N-[3-(acetylamino)phenyl]-5-{(2E)-2-[(4-methoxyphenyl)methylidene]hydrazinyl}-3-methyl-1H-pyrazole-4-carboxamide (CCD ID: MMH) (formula: $C_{21}H_{22}N_6O_3$).



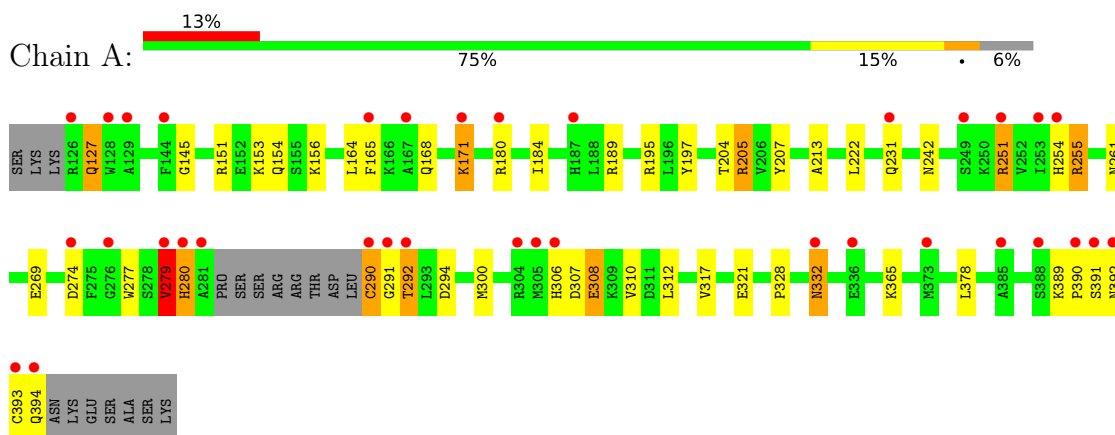
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total 199	O 199	0	0

i

- Molecule 1: Serine/threonine-protein kinase 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 81.61Å 169.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.90) 98.1 (30.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.287 0.233 , 0.287	Depositor DCC
R_{free} test set	1335 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2363	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: MMH

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	0.66	0/2187	0.87	3/2956 (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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	205	ARG	N-CA-C	6.15	118.30	109.14
1	A	279	VAL	N-CA-C	-5.12	105.85	110.82
1	A	153	LYS	N-CA-C	5.10	116.53	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	VAL	Peptide

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	2134	0	2129	46	0
2	A	30	0	22	3	0
3	A	199	0	0	6	0
All	All	2363	0	2151	48	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 (48) 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:290:CYS:HB2	1:A:291:GLY:HA3	1.02	0.98
1:A:290:CYS:CB	1:A:291:GLY:HA3	1.94	0.98
1:A:290:CYS:HB2	1:A:291:GLY:CA	1.93	0.97
1:A:332:ASN:HD22	1:A:332:ASN:N	1.67	0.90
1:A:332:ASN:ND2	1:A:332:ASN:H	1.71	0.83
1:A:213:ALA:H	2:A:1:MMH:HNAB	1.28	0.81
1:A:274:ASP:OD1	1:A:274:ASP:C	2.31	0.74
1:A:307:ASP:HB2	1:A:308:GLU:OE2	1.90	0.71
1:A:156:LYS:HE3	3:A:109:HOH:O	1.90	0.71
1:A:254:HIS:HD2	1:A:255:ARG:O	1.76	0.67
1:A:378:LEU:HD22	1:A:391:SER:HB2	1.75	0.67
1:A:168:GLN:HB2	3:A:472:HOH:O	1.95	0.66
1:A:332:ASN:N	1:A:332:ASN:ND2	2.28	0.64
1:A:145:GLY:HA2	3:A:425:HOH:O	1.99	0.62
1:A:274:ASP:OD1	1:A:274:ASP:O	2.19	0.59
1:A:254:HIS:CE1	1:A:274:ASP:OD1	2.58	0.56
1:A:168:GLN:HA	1:A:171:LYS:HD3	1.88	0.55
1:A:389:LYS:HE3	3:A:419:HOH:O	2.06	0.55
1:A:392:ASN:ND2	1:A:394:GLN:HB2	2.23	0.53
1:A:251:ARG:N	1:A:251:ARG:HD3	2.24	0.52
1:A:261:ASN:HB3	1:A:274:ASP:HB3	1.92	0.52
2:A:1:MMH:OAQ	2:A:1:MMH:HAV	2.10	0.51
1:A:393:CYS:HB3	1:A:394:GLN:HA	1.92	0.50
1:A:255:ARG:NE	1:A:300:MET:HE1	2.28	0.49
1:A:306:HIS:HB2	1:A:310:VAL:CG2	2.42	0.48
1:A:151:ARG:HH21	1:A:156:LYS:HD2	1.78	0.48
1:A:292:THR:HG22	1:A:294:ASP:H	1.78	0.48
1:A:222:LEU:HD21	1:A:321:GLU:HG2	1.96	0.48
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:HIS:HE1	1:A:274:ASP:OD1	1.97	0.48
1:A:392:ASN:HD22	1:A:394:GLN:HB2	1.79	0.47
1:A:195:ARG:HG2	1:A:197:TYR:CE1	2.49	0.47
1:A:242:ASN:HD22	1:A:389:LYS:NZ	2.13	0.47
1:A:180:ARG:HG3	1:A:180:ARG:HH11	1.80	0.45
1:A:165:PHE:HD1	1:A:205:ARG:CZ	2.28	0.45
1:A:254:HIS:CD2	1:A:255:ARG:O	2.64	0.45
1:A:378:LEU:HB3	1:A:391:SER:HB2	1.99	0.44
1:A:308:GLU:H	1:A:308:GLU:CD	2.23	0.44
1:A:180:ARG:NH2	3:A:77:HOH:O	2.50	0.44
1:A:255:ARG:HE	1:A:300:MET:HE1	1.83	0.44
2:A:1:MMH:HAZ	2:A:1:MMH:CAK	2.48	0.43
1:A:205:ARG:HG3	1:A:207:TYR:CZ	2.54	0.43
1:A:279:VAL:HG13	1:A:280:HIS:H	1.84	0.42
1:A:184:ILE:HG21	1:A:277:TRP:HB2	2.02	0.42
1:A:127:GLN:N	3:A:428:HOH:O	2.53	0.42
1:A:378:LEU:HD22	1:A:391:SER:CB	2.49	0.41
1:A:393:CYS:CB	1:A:394:GLN:HA	2.50	0.40
1:A:389:LYS:HG2	1:A:390:PRO:HD2	2.03	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	257/279 (92%)	248 (96%)	8 (3%)	1 (0%)	30 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ARG

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	229/247 (93%)	212 (93%)	17 (7%)	13 6

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	154	GLN
1	A	164	LEU
1	A	171	LYS
1	A	189	ARG
1	A	204	THR
1	A	231	GLN
1	A	251	ARG
1	A	269	GLU
1	A	279	VAL
1	A	280	HIS
1	A	290	CYS
1	A	292	THR
1	A	308	GLU
1	A	312	LEU
1	A	332	ASN
1	A	365	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	242	ASN
1	A	254	HIS
1	A	261	ASN
1	A	332	ASN
1	A	392	ASN
1	A	394	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 ⓘ

1 ligand is modelled in this entry.

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	MMH	A	1	-	31,32,32	2.84	9 (29%)	36,43,43	1.22	4 (11%)

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	MMH	A	1	-	-	3/19/20/20	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MMH	NAH-NAI	-11.21	1.24	1.38
2	A	1	MMH	NAB-NAA	-5.61	1.24	1.36
2	A	1	MMH	CAJ-NAI	4.14	1.33	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MMH	CAF-CAE	3.95	1.57	1.49
2	A	1	MMH	CAD-CAG	3.44	1.55	1.48
2	A	1	MMH	CAL-CAJ	-3.08	1.40	1.47
2	A	1	MMH	CAS-NAR	-3.05	1.35	1.41
2	A	1	MMH	CAY-NBA	-2.34	1.36	1.41
2	A	1	MMH	CAD-CAE	-2.24	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MMH	OBD-CBB-NBA	2.84	126.95	123.06
2	A	1	MMH	CAL-CAJ-NAI	2.68	125.55	121.19
2	A	1	MMH	OBD-CBB-CBC	-2.19	118.15	122.05
2	A	1	MMH	CAU-OAT-CAO	-2.13	112.93	117.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

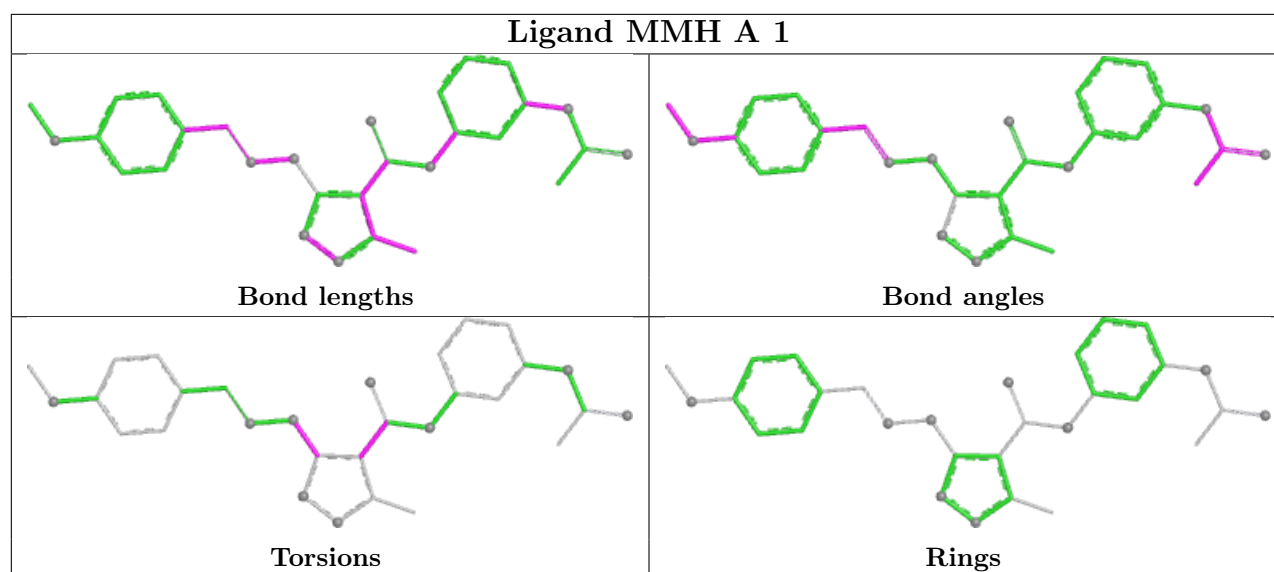
Mol	Chain	Res	Type	Atoms
2	A	1	MMH	NAB-CAC-NAH-NAI
2	A	1	MMH	CAC-CAD-CAG-OAQ
2	A	1	MMH	CAC-CAD-CAG-NAR

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MMH	3	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	261/279 (93%)	0.92	35 (13%) 7 7	23, 36, 60, 76	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	CYS	6.6
1	A	281	ALA	5.7
1	A	291	GLY	4.7
1	A	253	ILE	4.4
1	A	276	GLY	4.1
1	A	292	THR	3.9
1	A	306	HIS	3.9
1	A	165	PHE	3.8
1	A	332	ASN	3.7
1	A	304	ARG	3.5
1	A	290	CYS	3.3
1	A	180	ARG	3.3
1	A	280	HIS	3.1
1	A	126	ARG	2.9
1	A	390	PRO	2.8
1	A	336	GLU	2.8
1	A	279	VAL	2.8
1	A	187	HIS	2.7
1	A	305	MET	2.7
1	A	128	TRP	2.7
1	A	274	ASP	2.6
1	A	394	GLN	2.5
1	A	388	SER	2.5
1	A	391	SER	2.4
1	A	144	PHE	2.3
1	A	254	HIS	2.3
1	A	392	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	167	ALA	2.2
1	A	231	GLN	2.2
1	A	249	SER	2.2
1	A	251	ARG	2.1
1	A	129	ALA	2.1
1	A	385	ALA	2.1
1	A	171	LYS	2.0
1	A	373	MET	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](#)

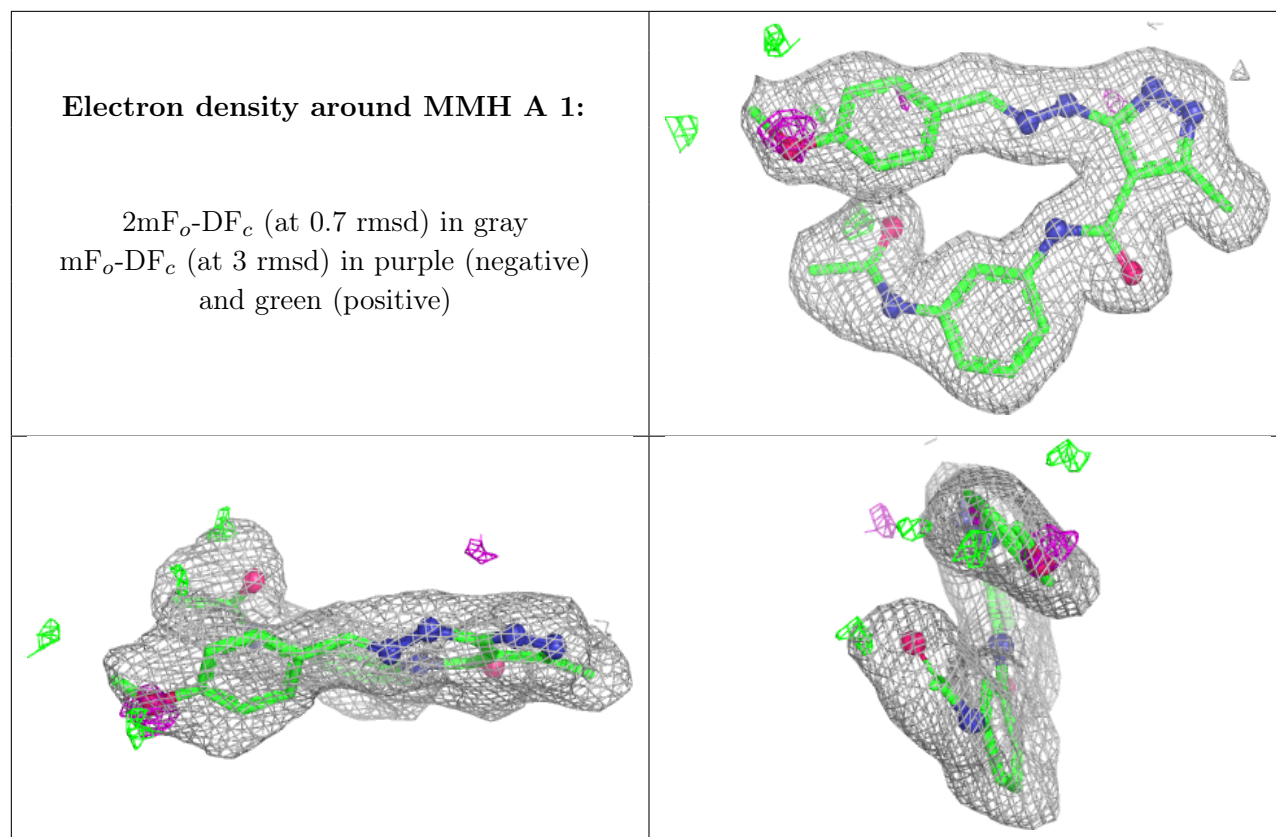
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	MMH	A	1	30/30	0.90	0.10	26,32,43,49	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.