



wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2025 – 04:05 pm BST

PDB ID : 9FBP / pdb_00009fbp
Title : Deletion mutant MmChi60
Authors : Rypniewski, W.; Bejger, M.; Biniek-Antosiak, K.
Deposited on : 2024-05-14
Resolution : 1.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

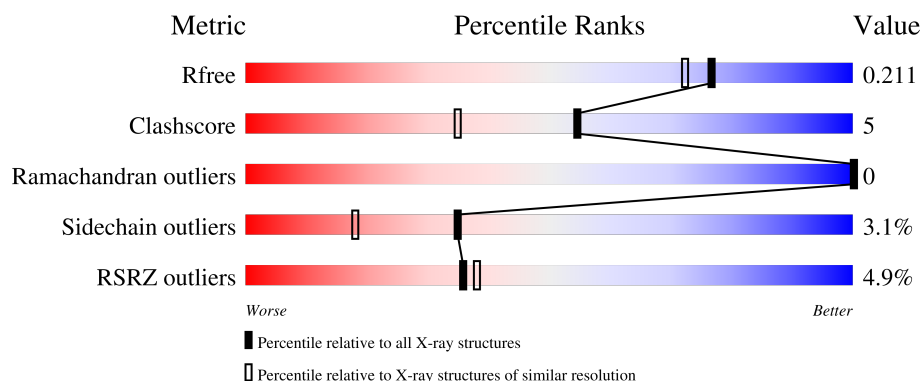
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	371	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
1	B	371	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6107 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 Chitinase 60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2941	1873	486	574	8			
1	B	371	Total	C	N	O	S	0	0	0
			2941	1873	486	574	8			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	VAL	-	expression tag	UNP B1VBB0
A	349	SER	-	expression tag	UNP B1VBB0
A	350	ASP	-	expression tag	UNP B1VBB0
A	351	ASP	-	expression tag	UNP B1VBB0
A	352	ASP	-	expression tag	UNP B1VBB0
A	353	TRP	-	expression tag	UNP B1VBB0
A	354	GLN	-	expression tag	UNP B1VBB0
A	355	VAL	-	expression tag	UNP B1VBB0
A	356	GLY	-	expression tag	UNP B1VBB0
A	357	SER	-	expression tag	UNP B1VBB0
A	358	THR	-	expression tag	UNP B1VBB0
A	359	TYR	-	expression tag	UNP B1VBB0
A	360	VAL	-	expression tag	UNP B1VBB0
A	361	LYS	-	expression tag	UNP B1VBB0
A	362	ASP	-	expression tag	UNP B1VBB0
A	363	ASP	-	expression tag	UNP B1VBB0
A	364	LYS	-	expression tag	UNP B1VBB0
A	365	VAL	-	expression tag	UNP B1VBB0
A	366	THR	-	expression tag	UNP B1VBB0
A	367	HIS	-	expression tag	UNP B1VBB0
A	368	ASN	-	expression tag	UNP B1VBB0
A	369	GLY	-	expression tag	UNP B1VBB0
A	370	ALA	-	expression tag	UNP B1VBB0
A	371	THR	-	expression tag	UNP B1VBB0
A	372	TRP	-	expression tag	UNP B1VBB0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	THR	-	expression tag	UNP B1VBB0
A	374	ALA	-	expression tag	UNP B1VBB0
A	375	GLN	-	expression tag	UNP B1VBB0
A	376	TRP	-	expression tag	UNP B1VBB0
A	377	TRP	-	expression tag	UNP B1VBB0
A	378	THR	-	expression tag	UNP B1VBB0
A	379	LYS	-	expression tag	UNP B1VBB0
A	380	GLY	-	expression tag	UNP B1VBB0
A	381	GLU	-	expression tag	UNP B1VBB0
A	382	GLU	-	expression tag	UNP B1VBB0
A	383	PRO	-	expression tag	UNP B1VBB0
A	384	GLY	-	expression tag	UNP B1VBB0
A	385	THR	-	expression tag	UNP B1VBB0
A	386	THR	-	expression tag	UNP B1VBB0
A	387	GLY	-	expression tag	UNP B1VBB0
A	388	GLU	-	expression tag	UNP B1VBB0
A	389	TRP	-	expression tag	UNP B1VBB0
A	390	GLY	-	expression tag	UNP B1VBB0
A	391	VAL	-	expression tag	UNP B1VBB0
A	392	TRP	-	expression tag	UNP B1VBB0
A	393	ARG	-	expression tag	UNP B1VBB0
B	348	VAL	-	expression tag	UNP B1VBB0
B	349	SER	-	expression tag	UNP B1VBB0
B	350	ASP	-	expression tag	UNP B1VBB0
B	351	ASP	-	expression tag	UNP B1VBB0
B	352	ASP	-	expression tag	UNP B1VBB0
B	353	TRP	-	expression tag	UNP B1VBB0
B	354	GLN	-	expression tag	UNP B1VBB0
B	355	VAL	-	expression tag	UNP B1VBB0
B	356	GLY	-	expression tag	UNP B1VBB0
B	357	SER	-	expression tag	UNP B1VBB0
B	358	THR	-	expression tag	UNP B1VBB0
B	359	TYR	-	expression tag	UNP B1VBB0
B	360	VAL	-	expression tag	UNP B1VBB0
B	361	LYS	-	expression tag	UNP B1VBB0
B	362	ASP	-	expression tag	UNP B1VBB0
B	363	ASP	-	expression tag	UNP B1VBB0
B	364	LYS	-	expression tag	UNP B1VBB0
B	365	VAL	-	expression tag	UNP B1VBB0
B	366	THR	-	expression tag	UNP B1VBB0
B	367	HIS	-	expression tag	UNP B1VBB0
B	368	ASN	-	expression tag	UNP B1VBB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	369	GLY	-	expression tag	UNP B1VBB0
B	370	ALA	-	expression tag	UNP B1VBB0
B	371	THR	-	expression tag	UNP B1VBB0
B	372	TRP	-	expression tag	UNP B1VBB0
B	373	THR	-	expression tag	UNP B1VBB0
B	374	ALA	-	expression tag	UNP B1VBB0
B	375	GLN	-	expression tag	UNP B1VBB0
B	376	TRP	-	expression tag	UNP B1VBB0
B	377	TRP	-	expression tag	UNP B1VBB0
B	378	THR	-	expression tag	UNP B1VBB0
B	379	LYS	-	expression tag	UNP B1VBB0
B	380	GLY	-	expression tag	UNP B1VBB0
B	381	GLU	-	expression tag	UNP B1VBB0
B	382	GLU	-	expression tag	UNP B1VBB0
B	383	PRO	-	expression tag	UNP B1VBB0
B	384	GLY	-	expression tag	UNP B1VBB0
B	385	THR	-	expression tag	UNP B1VBB0
B	386	THR	-	expression tag	UNP B1VBB0
B	387	GLY	-	expression tag	UNP B1VBB0
B	388	GLU	-	expression tag	UNP B1VBB0
B	389	TRP	-	expression tag	UNP B1VBB0
B	390	GLY	-	expression tag	UNP B1VBB0
B	391	VAL	-	expression tag	UNP B1VBB0
B	392	TRP	-	expression tag	UNP B1VBB0
B	393	ARG	-	expression tag	UNP B1VBB0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

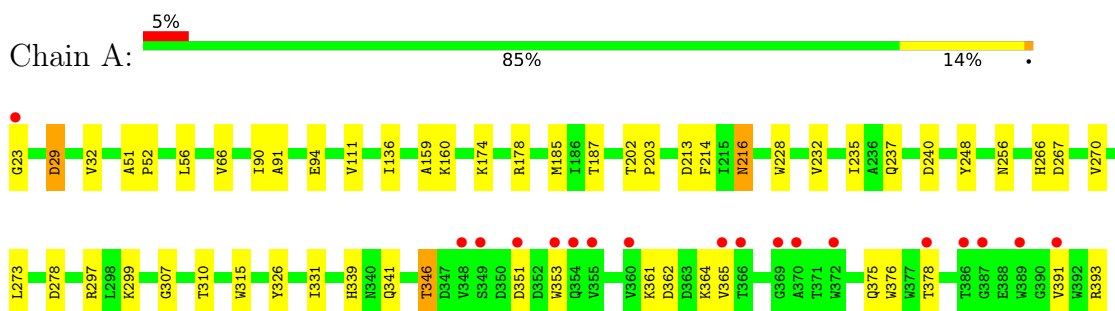
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	108	Total O 108 108	0	0
3	B	115	Total O 115 115	0	0

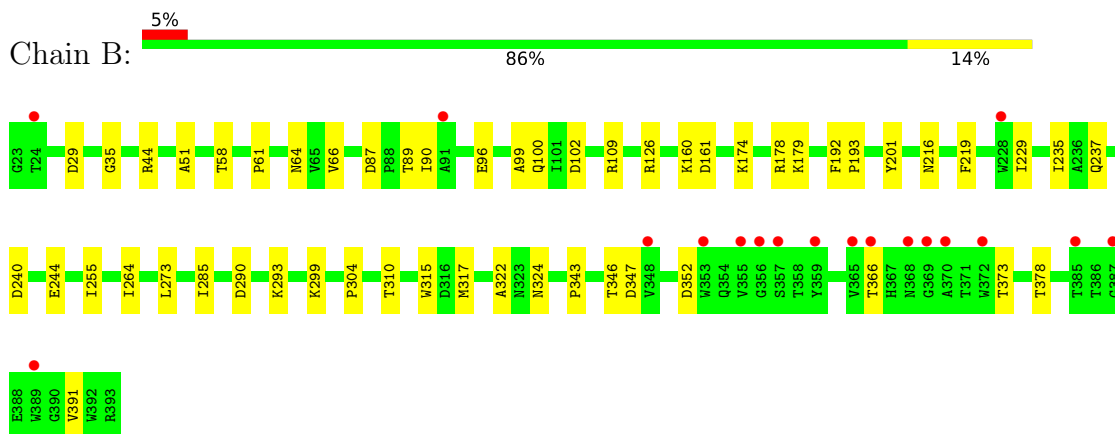
3 Residue-property plots

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: Chitinase 60



• Molecule 1: Chitinase 60



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.79Å 172.83Å 47.09Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	47.09 – 1.84 47.09 – 1.84	Depositor EDS
% Data completeness (in resolution range)	88.8 (47.09-1.84) 98.3 (47.09-1.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.154 , 0.219 0.169 , 0.211	Depositor DCC
R_{free} test set	2129 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.136 for h,-k,-l 0.022 for l,-k,h	Xtriage
Reported twinning fraction	0.532 for H, K, L 0.468 for -h,-k,l	Depositor
Outliers	0 of 60393 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6107	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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:
NA

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	0.70	0/3021	1.23	4/4122 (0.1%)
1	B	0.68	0/3021	1.15	3/4122 (0.1%)
All	All	0.69	0/6042	1.19	7/8244 (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	B	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	PRO	CB-CA-C	7.06	117.81	111.17
1	A	136	ILE	N-CA-CB	5.93	117.49	110.55
1	A	267	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	304	PRO	CB-CA-C	-5.52	104.78	111.46
1	B	219	PHE	CB-CA-C	5.18	118.08	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	126	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	2941	0	2764	30	0
1	B	2941	0	2764	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	108	0	0	6	0
3	B	115	0	0	3	0
All	All	6107	0	5528	54	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 5.

The worst 5 of 54 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:B:290:ASP:OD1	3:B:501:HOH:O	1.82	0.95
1:B:58:THR:HG22	1:B:317:MET:HE1	1.64	0.79
1:B:193:PRO:HB2	3:B:597:HOH:O	1.90	0.72
1:A:378:THR:HB	1:A:391:VAL:HG21	1.75	0.69
1:A:361:LYS:HG3	3:A:593:HOH:O	1.93	0.68

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	369/371 (100%)	356 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/371 (100%)	354 (96%)	15 (4%)	0	100	100
All	All	738/742 (100%)	710 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	306/306 (100%)	297 (97%)	9 (3%)	37	20
1	B	306/306 (100%)	296 (97%)	10 (3%)	33	16
All	All	612/612 (100%)	593 (97%)	19 (3%)	35	18

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	237	GLN
1	B	352	ASP
1	B	366	THR
1	B	346	THR
1	A	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	303	GLN
1	B	301	GLN
1	B	256	ASN
1	B	47	GLN
1	B	266	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	371/371 (100%)	0.17	18 (4%) 36 38	14, 23, 56, 67	0
1	B	371/371 (100%)	0.20	18 (4%) 36 38	13, 24, 48, 70	0
All	All	742/742 (100%)	0.18	36 (4%) 36 38	13, 24, 51, 70	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	GLY	4.8
1	B	372	TRP	4.6
1	B	389	TRP	4.3
1	A	348	VAL	4.1
1	B	24	THR	3.8

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](#)

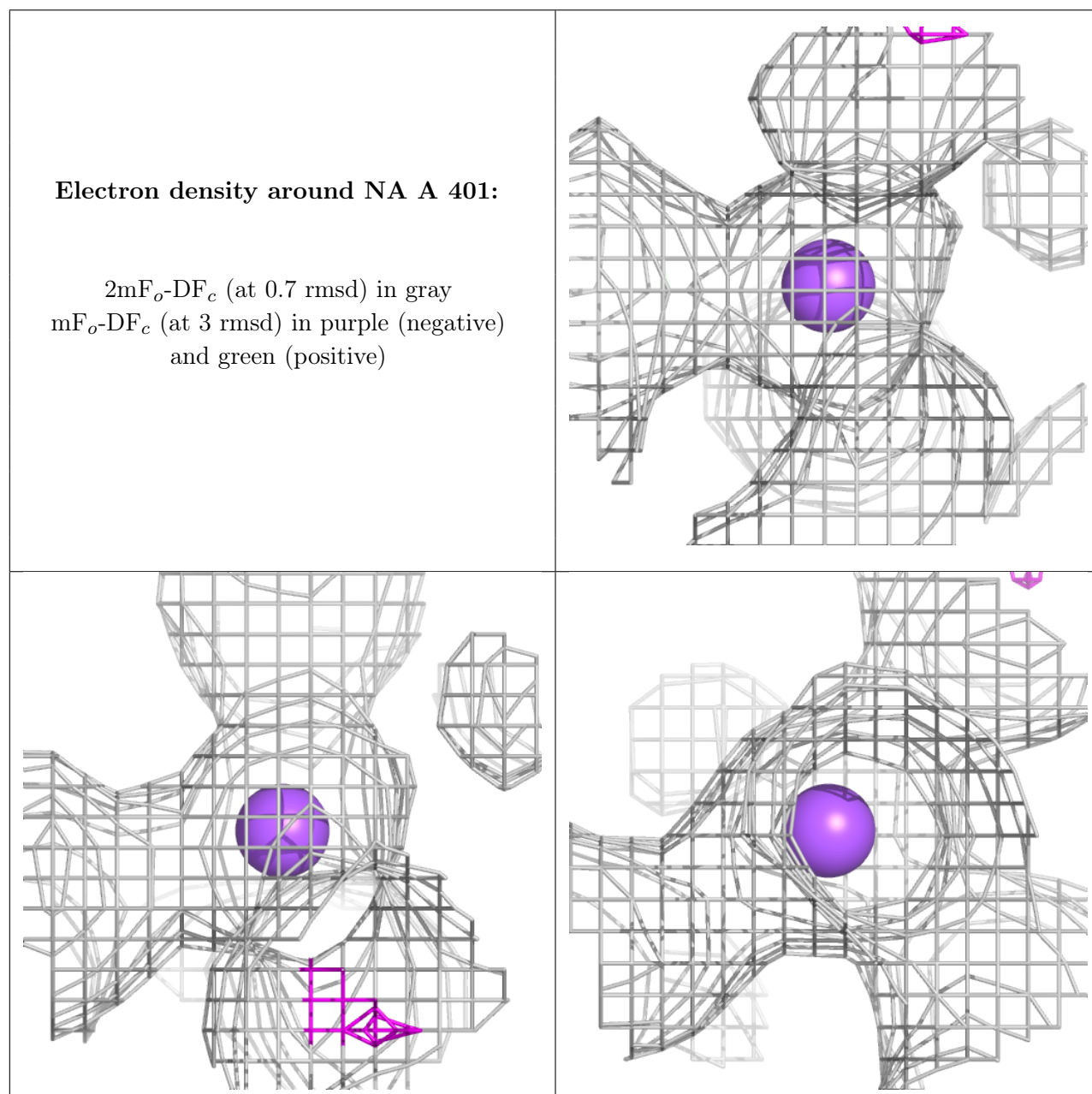
There are no monosaccharides in this entry.

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, 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.

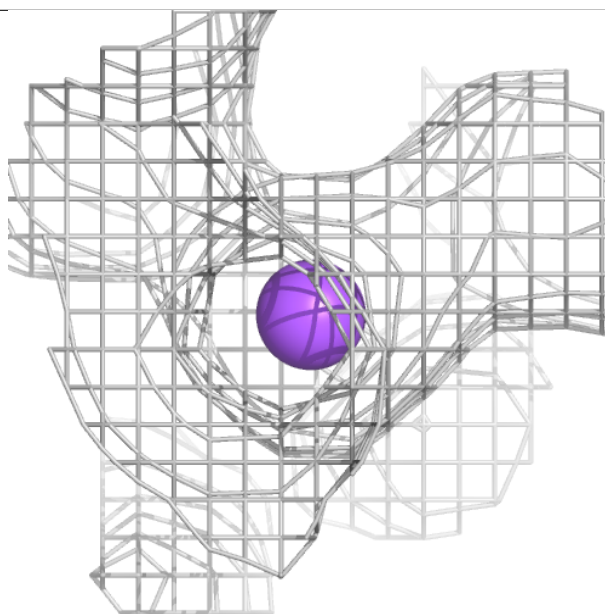
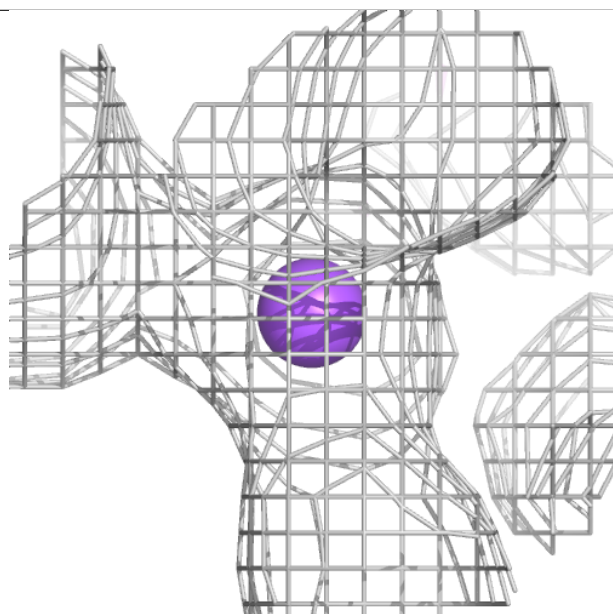
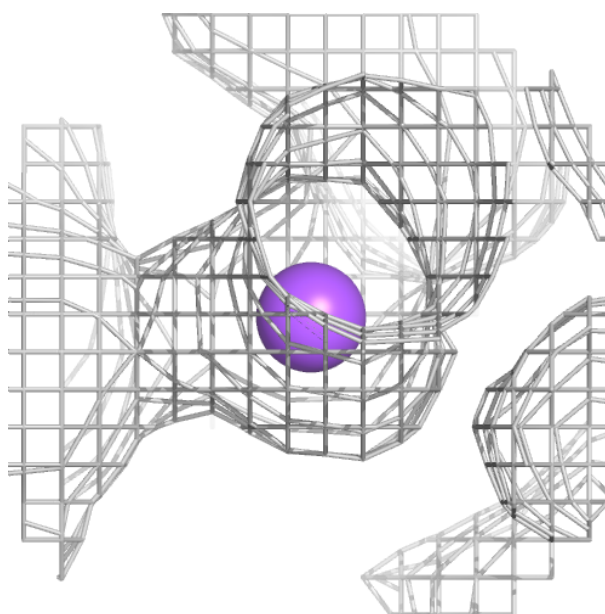
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	A	401	1/1	0.98	0.04	26,26,26,26	0
2	NA	B	401	1/1	0.98	0.06	24,24,24,24	0

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 NA B 401:

$2mF_o-DF_c$ (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.