



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 AM UTC

PDB ID : 6TG4 / pdb_00006tg4
Title : Tankyrase 2 in complex with an inhibitor (OM-1700)
Authors : Sowa, S.T.; Lehtio, L.
Deposited on : 2019-11-15
Resolution : 2.76 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

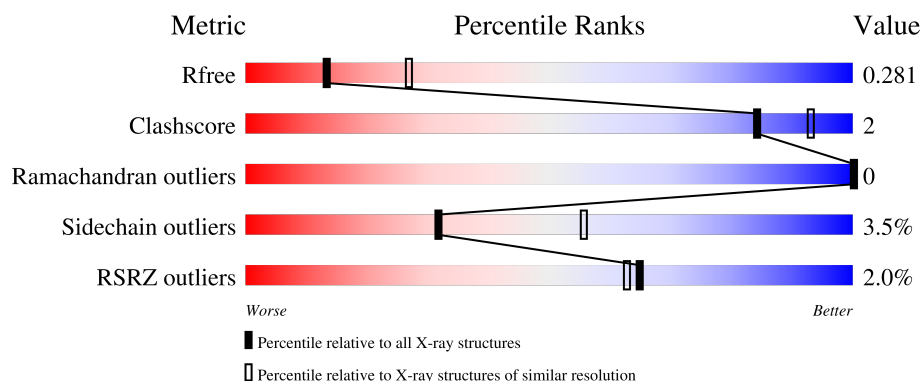
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	AAA	240	 2% 79% 6% 14%
1	BBB	240	 2% 73% 9% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6532 atoms, of which 3177 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 Tankyrase-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	206	Total	C	H	N	O	S	104	0	0
			3215	1032	1576	300	297	10			
1	BBB	200	Total	C	H	N	O	S	98	0	0
			3166	1015	1555	295	291	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	923	MET	-	initiating methionine	UNP Q9H2K2
AAA	924	HIS	-	expression tag	UNP Q9H2K2
AAA	925	HIS	-	expression tag	UNP Q9H2K2
AAA	926	HIS	-	expression tag	UNP Q9H2K2
AAA	927	HIS	-	expression tag	UNP Q9H2K2
AAA	928	HIS	-	expression tag	UNP Q9H2K2
AAA	929	HIS	-	expression tag	UNP Q9H2K2
AAA	930	SER	-	expression tag	UNP Q9H2K2
AAA	931	SER	-	expression tag	UNP Q9H2K2
AAA	932	GLY	-	expression tag	UNP Q9H2K2
AAA	933	VAL	-	expression tag	UNP Q9H2K2
AAA	934	ASP	-	expression tag	UNP Q9H2K2
AAA	935	LEU	-	expression tag	UNP Q9H2K2
AAA	936	GLY	-	expression tag	UNP Q9H2K2
AAA	937	THR	-	expression tag	UNP Q9H2K2
AAA	938	GLU	-	expression tag	UNP Q9H2K2
AAA	939	ASN	-	expression tag	UNP Q9H2K2
AAA	940	LEU	-	expression tag	UNP Q9H2K2
AAA	941	TYR	-	expression tag	UNP Q9H2K2
AAA	942	PHE	-	expression tag	UNP Q9H2K2
AAA	943	GLN	-	expression tag	UNP Q9H2K2
AAA	944	SER	-	expression tag	UNP Q9H2K2
AAA	945	MET	-	expression tag	UNP Q9H2K2
BBB	923	MET	-	initiating methionine	UNP Q9H2K2
BBB	924	HIS	-	expression tag	UNP Q9H2K2

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	925	HIS	-	expression tag	UNP Q9H2K2
BBB	926	HIS	-	expression tag	UNP Q9H2K2
BBB	927	HIS	-	expression tag	UNP Q9H2K2
BBB	928	HIS	-	expression tag	UNP Q9H2K2
BBB	929	HIS	-	expression tag	UNP Q9H2K2
BBB	930	SER	-	expression tag	UNP Q9H2K2
BBB	931	SER	-	expression tag	UNP Q9H2K2
BBB	932	GLY	-	expression tag	UNP Q9H2K2
BBB	933	VAL	-	expression tag	UNP Q9H2K2
BBB	934	ASP	-	expression tag	UNP Q9H2K2
BBB	935	LEU	-	expression tag	UNP Q9H2K2
BBB	936	GLY	-	expression tag	UNP Q9H2K2
BBB	937	THR	-	expression tag	UNP Q9H2K2
BBB	938	GLU	-	expression tag	UNP Q9H2K2
BBB	939	ASN	-	expression tag	UNP Q9H2K2
BBB	940	LEU	-	expression tag	UNP Q9H2K2
BBB	941	TYR	-	expression tag	UNP Q9H2K2
BBB	942	PHE	-	expression tag	UNP Q9H2K2
BBB	943	GLN	-	expression tag	UNP Q9H2K2
BBB	944	SER	-	expression tag	UNP Q9H2K2
BBB	945	MET	-	expression tag	UNP Q9H2K2

- Molecule 2 is a ligand with the chemical component id N8K but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for N8K. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	F	H	N	O	0	0
			57	25	1	23	6	2		
2	BBB	1	Total	C	F	H	N	O	0	0
			57	25	1	23	6	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Zn	0	0
			1	1		
3	BBB	1	Total	Zn	0	0
			1	1		

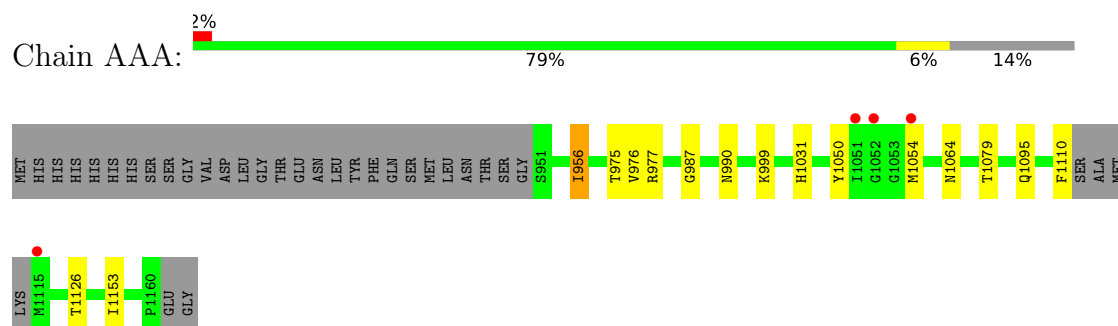
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	20	Total 20	O 20	0	0
4	BBB	15	Total 15	O 15	0	0

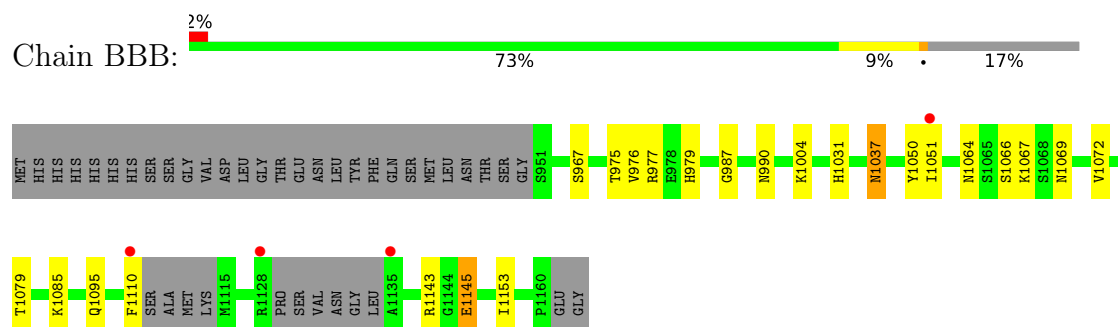
3 Residue-property plots [i](#)

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: Tankyrase-2



• Molecule 1: Tankyrase-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.68Å 77.90Å 149.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.46 – 2.76 37.46 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.46-2.76) 99.5 (37.46-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.230 , 0.281 0.230 , 0.281	Depositor DCC
R_{free} test set	670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.5	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	0.92	EDS
Total number of atoms	6532	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0017e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: N8K, ZN

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	AAA	1.00	0/1682	1.39	7/2268 (0.3%)
1	BBB	0.99	0/1652	1.40	5/2221 (0.2%)
All	All	0.99	0/3334	1.39	12/4489 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	1050	TYR	CA-C-N	5.77	128.04	120.60
1	AAA	1050	TYR	C-N-CA	5.77	128.04	120.60
1	BBB	987	GLY	CA-C-O	-5.64	118.07	122.52
1	BBB	1031	HIS	CA-C-N	5.62	125.47	121.65
1	BBB	1031	HIS	C-N-CA	5.62	125.47	121.65
1	AAA	987	GLY	CA-C-O	-5.42	118.24	122.52
1	AAA	1031	HIS	CA-C-N	5.35	125.29	121.65
1	AAA	1031	HIS	C-N-CA	5.35	125.29	121.65
1	BBB	1050	TYR	CA-C-N	5.16	127.06	120.56
1	BBB	1050	TYR	C-N-CA	5.16	127.06	120.56
1	AAA	1126	THR	CA-C-N	5.08	124.93	120.10
1	AAA	1126	THR	C-N-CA	5.08	124.93	120.10

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1639	1576	1550	5	0
1	BBB	1611	1555	1534	9	0
2	AAA	34	23	0	0	0
2	BBB	34	23	0	1	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	20	0	0	0	0
4	BBB	15	0	0	1	0
All	All	3355	3177	3084	15	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 2.

All (15) 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:AAA:1054:MET:HE2	1:AAA:1110:PHE:C	2.27	0.59
1:BBB:979:HIS:NE2	1:BBB:1066:SER:OG	2.31	0.58
1:BBB:976:VAL:O	1:BBB:977:ARG:NH1	2.45	0.49
1:AAA:975:THR:HB	1:AAA:1064:ASN:HA	1.96	0.48
1:BBB:975:THR:HB	1:BBB:1064:ASN:HA	1.96	0.47
1:BBB:1037:ASN:H	1:BBB:1037:ASN:ND2	2.12	0.47
1:BBB:1143:ARG:HB3	1:BBB:1145:GLU:OE1	2.17	0.45
1:BBB:979:HIS:CD2	1:BBB:1066:SER:HG	2.31	0.45
1:BBB:1069:ASN:O	1:BBB:1072:VAL:HG23	2.19	0.42
1:AAA:976:VAL:O	1:AAA:977:ARG:NH1	2.52	0.42
1:BBB:1079:THR:N	4:BBB:1302:HOH:O	2.53	0.41
1:BBB:1095:GLN:HA	1:BBB:1153:ILE:O	2.20	0.41
1:AAA:1095:GLN:HA	1:AAA:1153:ILE:O	2.21	0.41
1:AAA:956:ILE:HG23	1:AAA:999:LYS:HB3	2.01	0.41
2:BBB:1201:N8K:C20	2:BBB:1201:N8K:C10	3.00	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	AAA	202/240 (84%)	196 (97%)	6 (3%)	0	100	100
1	BBB	194/240 (81%)	189 (97%)	5 (3%)	0	100	100
All	All	396/480 (82%)	385 (97%)	11 (3%)	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	AAA	171/204 (84%)	168 (98%)	3 (2%)	51	71
1	BBB	169/204 (83%)	160 (95%)	9 (5%)	20	39
All	All	340/408 (83%)	328 (96%)	12 (4%)	32	56

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	956	ILE
1	AAA	990	ASN
1	AAA	1079	THR
1	BBB	967	SER
1	BBB	990	ASN
1	BBB	1004	LYS
1	BBB	1037	ASN
1	BBB	1051	ILE

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Mol	Chain	Res	Type
1	BBB	1067	LYS
1	BBB	1085	LYS
1	BBB	1110	PHE
1	BBB	1145	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 4 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 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 ⓘ

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	AAA	206/240 (85%)	0.23	4 (1%) 66 64	28, 44, 66, 85	0
1	BBB	200/240 (83%)	0.27	4 (2%) 65 63	33, 47, 76, 96	0
All	All	406/480 (84%)	0.25	8 (1%) 65 63	28, 45, 72, 96	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	1110	PHE	4.1
1	AAA	1052	GLY	3.1
1	AAA	1054	MET	2.8
1	BBB	1135	ALA	2.7
1	AAA	1115	MET	2.4
1	AAA	1051	ILE	2.3
1	BBB	1128	ARG	2.2
1	BBB	1051	ILE	2.1

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.

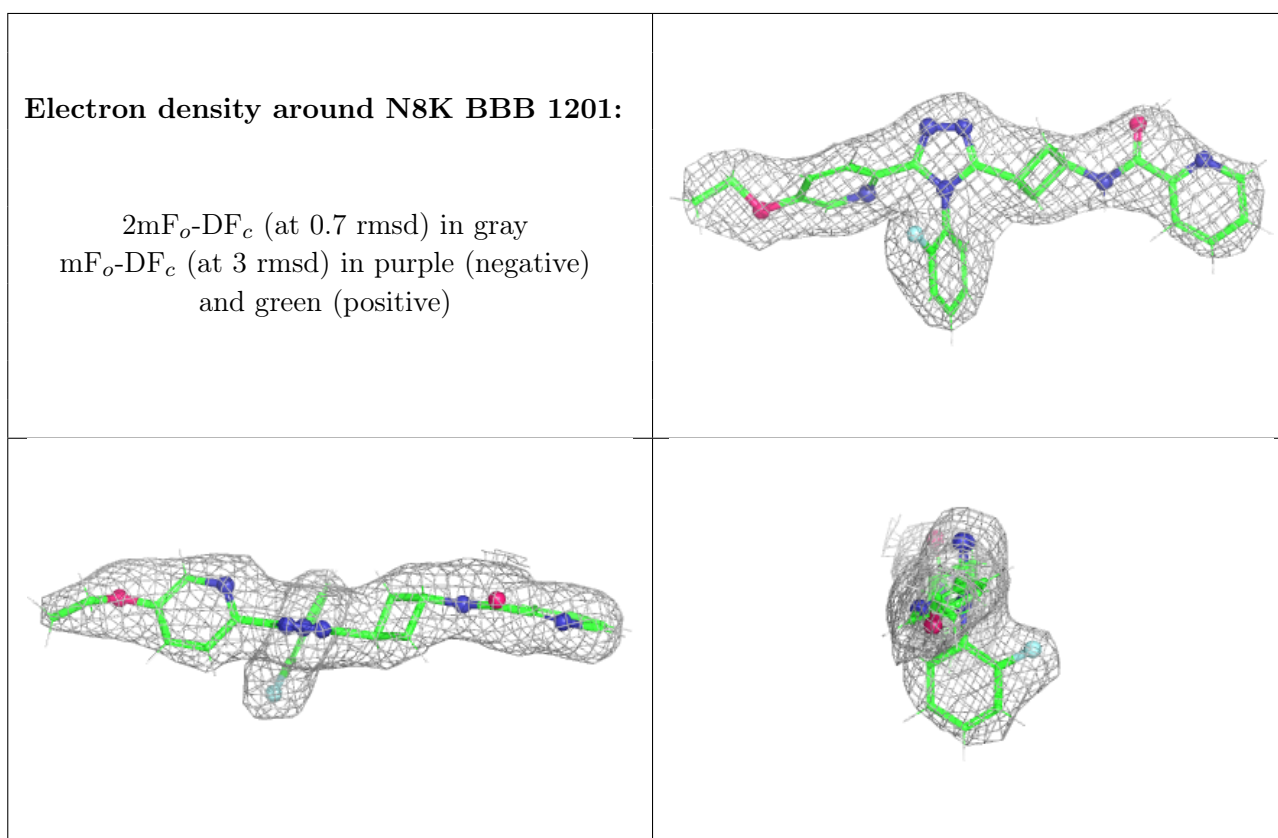
6.4 Ligands [i](#)

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.

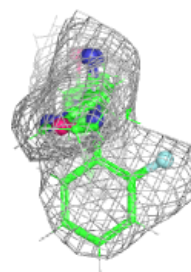
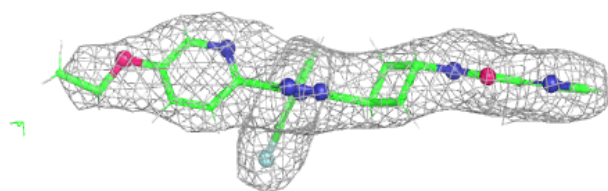
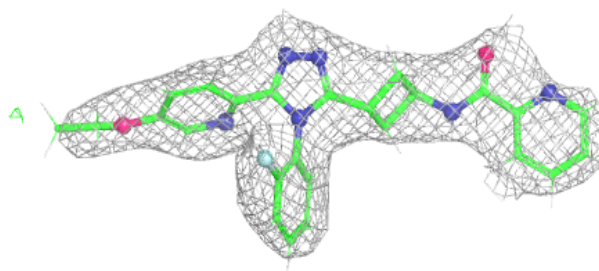
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	N8K	BBB	1201	34/34	0.93	0.09	37,44,52,53	0
2	N8K	AAA	1201	34/34	0.94	0.08	34,37,47,48	0
3	ZN	AAA	1202	1/1	1.00	0.01	41,41,41,41	0
3	ZN	BBB	1202	1/1	1.00	0.03	49,49,49,49	0

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.



Electron density around N8K AAA 1201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.