



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 01:03 pm GMT

PDB ID : 6YI0
Title : Human histidine triad nucleotide-binding protein 2 (hHINT2) refined to 1.65 Å in P41212 space group
Authors : Dolot, R.D.; Włodarczyk, A.; Bujacz, G.D.; Nawrot, B.C.
Deposited on : 2020-03-31
Resolution : 1.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

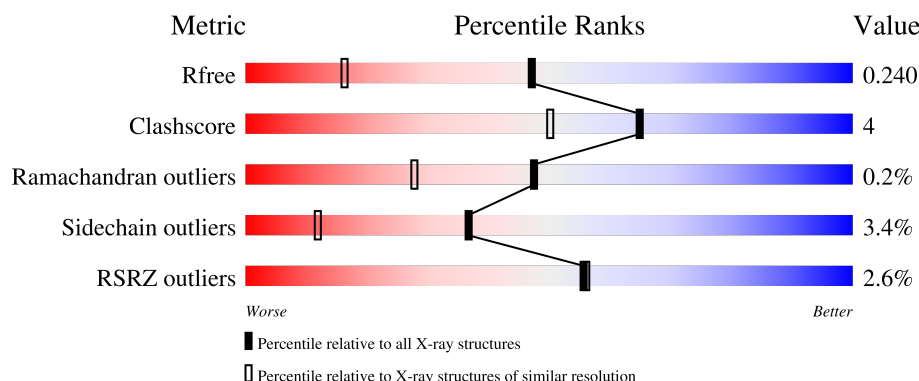
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	163	 66% 31%
1	BBB	163	 58% 37%
1	CCC	163	 56% 12% 31%
1	DDD	163	 50% 8% 40%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3806 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 Histidine triad nucleotide-binding protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	112	Total	C	N	O	S	0	4	0
			911	583	161	166	1			
1	BBB	102	Total	C	N	O	S	0	8	0
			861	550	152	158	1			
1	DDD	97	Total	C	N	O	S	0	1	0
			769	493	137	138	1			
1	CCC	112	Total	C	N	O	S	0	1	0
			883	567	156	159	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BBB	1	Total	Na	0	0
			1	1		

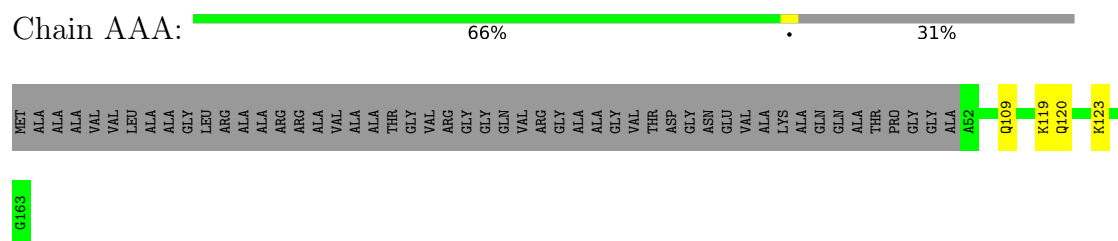
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	149	Total	O	0	0
			149	149		
3	BBB	125	Total	O	0	0
			125	125		
3	DDD	52	Total	O	0	0
			52	52		
3	CCC	55	Total	O	0	0
			55	55		

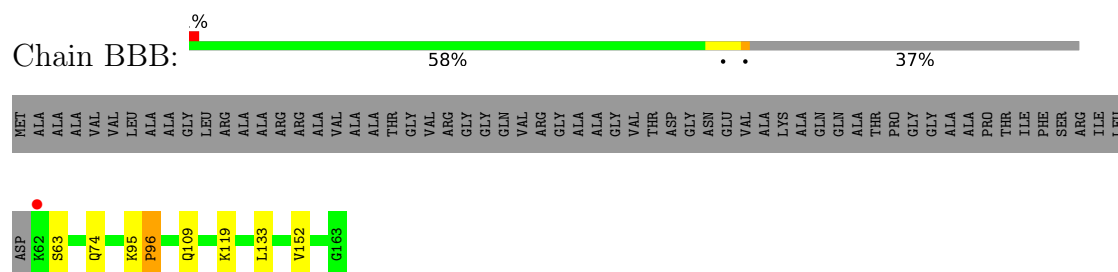
3 Residue-property plots

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.

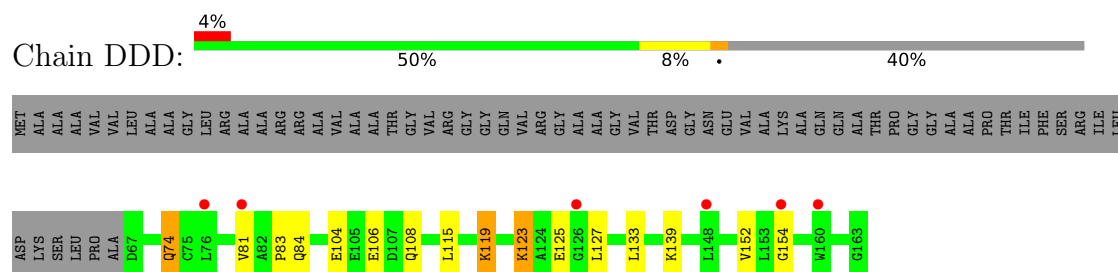
- Molecule 1: Histidine triad nucleotide-binding protein 2, mitochondrial



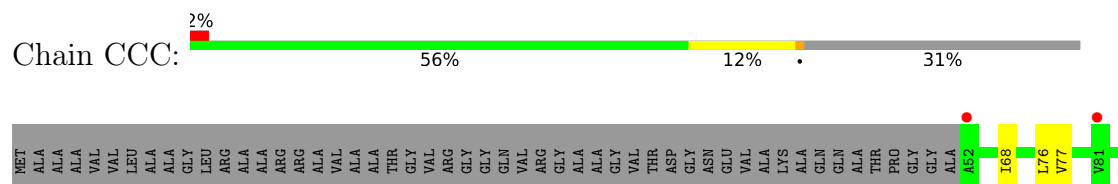
- Molecule 1: Histidine triad nucleotide-binding protein 2, mitochondrial



- Molecule 1: Histidine triad nucleotide-binding protein 2, mitochondrial



- Molecule 1: Histidine triad nucleotide-binding protein 2, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.94Å 76.94Å 140.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.04 – 1.65 40.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.04-1.65) 100.0 (40.00-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.184 , 0.233 0.191 , 0.240	Depositor DCC
R_{free} test set	2608 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.96	EDS
Total number of atoms	3806	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 29.39 % 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 1.5622e-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 [i](#)

5.1 Standard geometry [i](#)

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	AAA	0.69	0/932	0.87	0/1265
1	BBB	0.76	0/881	0.88	0/1195
1	CCC	0.68	0/904	0.81	0/1229
1	DDD	0.67	0/787	0.81	0/1068
All	All	0.70	0/3504	0.84	0/4757

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	911	0	918	3	0
1	BBB	861	0	857	5	0
1	CCC	883	0	891	14	0
1	DDD	769	0	772	14	0
2	BBB	1	0	0	0	0
3	AAA	149	0	0	1	0
3	BBB	125	0	0	1	0
3	CCC	55	0	0	0	0
3	DDD	52	0	0	1	0
All	All	3806	0	3438	28	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 (28) 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:120[A]:GLN:OE1	1:AAA:123:LYS:HE2	1.90	0.71
1:AAA:120[B]:GLN:NE2	3:AAA:202:HOH:O	2.26	0.68
1:CCC:113:HIS:O	1:CCC:117:VAL:HG23	2.03	0.59
1:DDD:123:LYS:O	1:DDD:125:GLU:O	2.22	0.58
1:DDD:127:LEU:HD22	1:DDD:154:GLY:HA3	1.86	0.56
1:CCC:90:LEU:HD22	1:CCC:90:LEU:N	2.21	0.55
1:CCC:68:ILE:HD12	1:CCC:76:LEU:HD11	1.90	0.54
1:CCC:98:PRO:HG2	1:CCC:102:GLN:OE1	2.08	0.54
1:DDD:108:GLN:HE21	1:CCC:109:GLN:HG3	1.73	0.52
1:BBB:95:LYS:HG3	1:BBB:96[A]:PRO:HD2	1.90	0.52
1:DDD:108:GLN:NE2	1:CCC:109:GLN:HG3	2.26	0.51
1:DDD:133:LEU:CD2	1:DDD:152:VAL:HG22	2.41	0.49
1:DDD:84:GLN:HE21	1:CCC:161:PRO:HB3	1.81	0.46
1:DDD:81:VAL:C	1:DDD:83:PRO:HD3	2.37	0.45
1:BBB:95:LYS:CG	1:BBB:96[A]:PRO:HD2	2.46	0.45
1:DDD:84:GLN:HG3	1:CCC:160:TRP:NE1	2.31	0.45
1:DDD:115:LEU:HD11	1:CCC:115:LEU:HD11	1.99	0.45
1:DDD:133:LEU:HD22	1:DDD:152:VAL:HG22	1.97	0.45
1:AAA:109:GLN:OE1	1:BBB:109:GLN:HG2	2.17	0.44
1:BBB:74[A]:GLN:NE2	3:BBB:303:HOH:O	2.33	0.44
1:DDD:74:GLN:NE2	3:DDD:204:HOH:O	2.49	0.43
1:BBB:133:LEU:HD22	1:BBB:152:VAL:HG22	2.02	0.42
1:CCC:116:LEU:O	1:CCC:120:GLN:HB2	2.21	0.41
1:DDD:84:GLN:HB3	1:CCC:161:PRO:HB3	2.03	0.41
1:DDD:104:GLU:HB3	1:DDD:106:GLU:OE1	2.20	0.41
1:DDD:119:LYS:HE2	1:CCC:103:ALA:O	2.22	0.40
1:CCC:77:VAL:HG11	1:CCC:121:THR:HG21	2.03	0.40
1:CCC:89:PHE:C	1:CCC:90:LEU:HD22	2.42	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	114/163 (70%)	113 (99%)	1 (1%)	0	100	100
1	BBB	108/163 (66%)	104 (96%)	2 (2%)	2 (2%)	8	0
1	CCC	111/163 (68%)	108 (97%)	3 (3%)	0	100	100
1	DDD	96/163 (59%)	94 (98%)	2 (2%)	0	100	100
All	All	429/652 (66%)	419 (98%)	8 (2%)	2 (0%)	47	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	96[A]	PRO
1	BBB	96[B]	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	AAA	98/120 (82%)	97 (99%)	1 (1%)	76	62
1	BBB	92/120 (77%)	90 (98%)	2 (2%)	52	27
1	CCC	94/120 (78%)	89 (95%)	5 (5%)	22	4
1	DDD	81/120 (68%)	77 (95%)	4 (5%)	25	5
All	All	365/480 (76%)	353 (97%)	12 (3%)	37	12

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

Mol	Chain	Res	Type
1	AAA	119	LYS
1	BBB	63	SER
1	BBB	119	LYS
1	DDD	74	GLN

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Mol	Chain	Res	Type
1	DDD	119	LYS
1	DDD	123	LYS
1	DDD	139	LYS
1	CCC	104	GLU
1	CCC	106	GLU
1	CCC	119	LYS
1	CCC	120	GLN
1	CCC	153	LEU

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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	112/163 (68%)	-0.31	0 100 100	17, 23, 31, 52	0
1	BBB	102/163 (62%)	-0.25	1 (0%) 82 85	16, 22, 32, 70	0
1	CCC	112/163 (68%)	0.47	4 (3%) 42 43	32, 47, 63, 74	0
1	DDD	97/163 (59%)	0.60	6 (6%) 20 19	29, 47, 66, 72	0
All	All	423/652 (64%)	0.12	11 (2%) 56 56	16, 33, 62, 74	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	154	GLY	3.7
1	BBB	62	LYS	3.6
1	DDD	126	GLY	3.3
1	DDD	81	VAL	3.1
1	CCC	124	ALA	2.7
1	CCC	139	LYS	2.4
1	DDD	76	LEU	2.3
1	DDD	148	LEU	2.1
1	CCC	52	ALA	2.1
1	DDD	160	TRP	2.1
1	CCC	81	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 monosaccharides in this entry.

6.4 Ligands

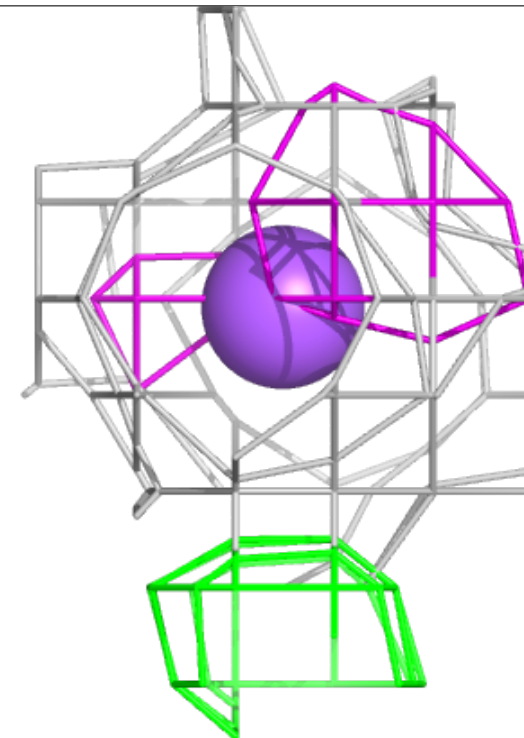
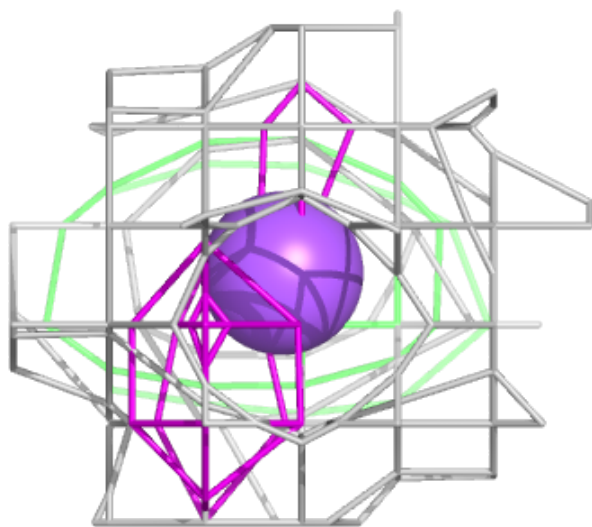
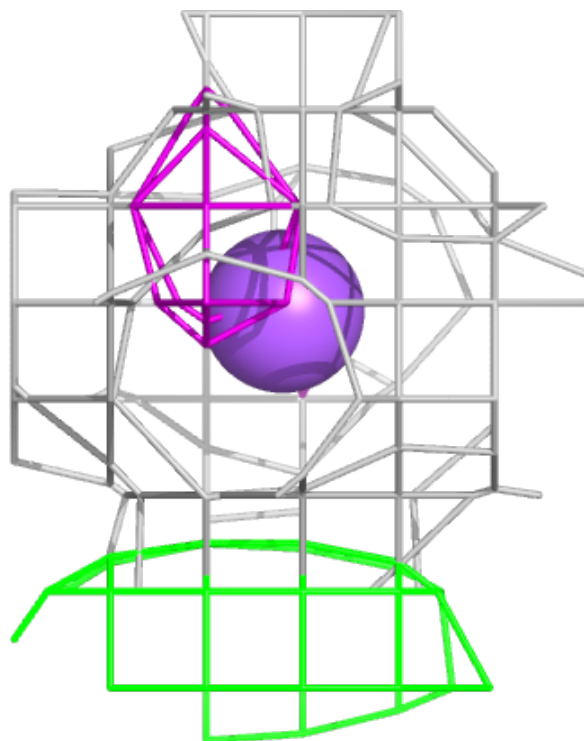
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BBB	201	1/1	0.98	0.06	23,23,23,23	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 BBB 201:

$2mF_o-DF_c$ (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.