



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 11:27 pm BST

PDB ID : 3MZ3
Title : Crystal structure of Co2+ HDAC8 complexed with M344
Authors : Dowling, D.P.; Gattis, S.G.; Fierke, C.A.; Christianson, D.W.
Deposited on : 2010-05-11
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

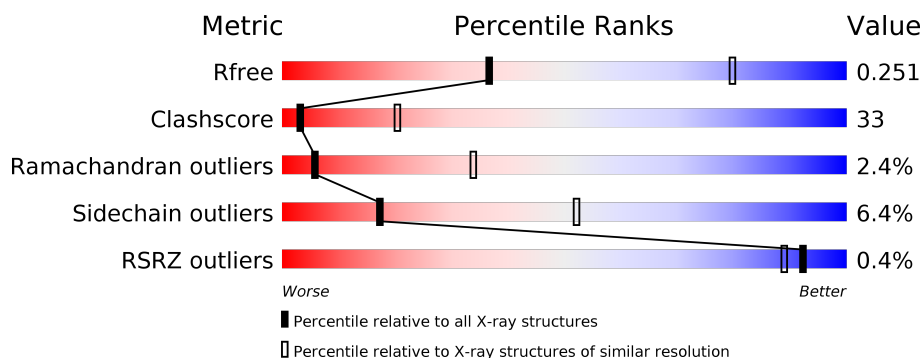
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	389	<div> <div></div> <div> <div></div> <div>44%</div> <div>43%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	389	<div> <div></div> <div> <div>43%</div> <div>43%</div> <div>5%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5647 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 Histone deacetylase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	17	0	0
			2785	1789	463	514	19			
1	B	356	Total	C	N	O	S	17	0	0
			2777	1785	462	511	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
A	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
A	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
A	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
A	382	GLY	-	EXPRESSION TAG	UNP Q9BY41
A	383	SER	-	EXPRESSION TAG	UNP Q9BY41
A	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	389	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
B	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
B	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
B	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
B	382	GLY	-	EXPRESSION TAG	UNP Q9BY41
B	383	SER	-	EXPRESSION TAG	UNP Q9BY41
B	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	389	HIS	-	EXPRESSION TAG	UNP Q9BY41

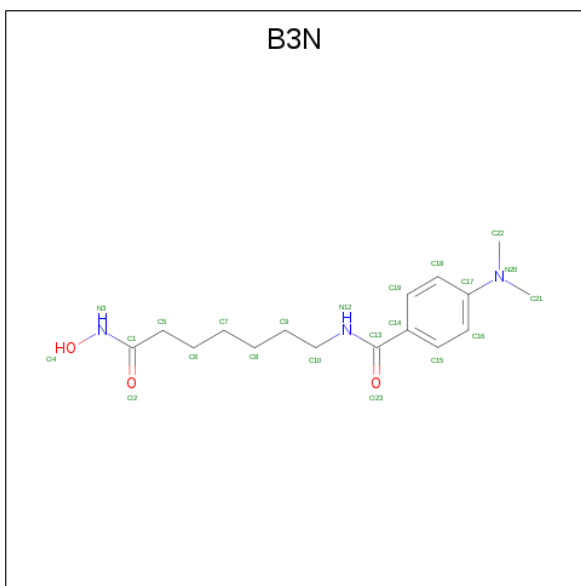
- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		

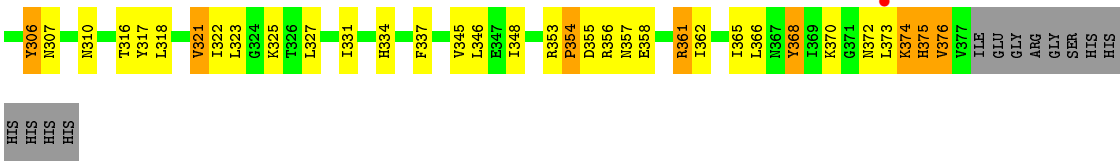
- Molecule 4 is 4-(dimethylamino)-N-[7-(hydroxyamino)-7-oxoheptyl]benzamide (three-letter code: B3N) (formula: C₁₆H₂₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	16	3	3		
4	B	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	20	Total 20	O 20	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.63Å 86.14Å 94.51Å 90.00° 94.07° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.37 – 3.19	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-3.20) 91.7 (49.37-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.19Å)	Xtriage
Refinement program	CNS 2.1	Depositor
R, R_{free}	0.204 , 0.256 0.205 , 0.251	Depositor DCC
R_{free} test set	729 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.953	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.5	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	0.93	EDS
Total number of atoms	5647	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: K, CO, B3N

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	0.41	0/2853	0.64	0/3869
1	B	0.42	0/2845	0.65	0/3858
All	All	0.42	0/5698	0.65	0/7727

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	TYR	Sidechain
1	B	306	TYR	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	2785	0	2752	186	0
1	B	2777	0	2748	185	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	22	0	24	4	0
4	B	22	0	24	4	0
5	A	15	0	0	1	0
5	B	20	0	0	1	0
All	All	5647	0	5548	367	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 33.

The worst 5 of 367 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:272:ASP:OD2	1:B:274:MET:HB2	1.69	0.93
1:A:272:ASP:OD2	1:A:274:MET:HB2	1.70	0.90
1:B:127:ILE:HG22	1:B:169:PHE:HE1	1.37	0.90
1:B:13:SER:HB2	1:B:15:VAL:HG12	1.53	0.89
1:A:127:ILE:HG22	1:A:169:PHE:HE1	1.37	0.88

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	353/389 (91%)	287 (81%)	57 (16%)	9 (2%)	5	32
1	B	352/389 (90%)	288 (82%)	56 (16%)	8 (2%)	6	34
All	All	705/778 (91%)	575 (82%)	113 (16%)	17 (2%)	6	34

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	354	PRO
1	A	356	ARG
1	B	21	SER
1	B	354	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	A	299/326 (92%)	280 (94%)	19 (6%)	17	52
1	B	298/326 (91%)	279 (94%)	19 (6%)	17	52
All	All	597/652 (92%)	559 (94%)	38 (6%)	17	52

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	B	36	LYS
1	B	361	ARG
1	B	21	SER
1	B	65	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	HIS
1	B	53	GLN
1	B	363	GLN
1	A	367	ASN
1	A	372	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
4	B3N	B	390	2	22,22,22	2.66	9 (40%)	26,27,27	1.13	1 (3%)
4	B3N	A	390	2	22,22,22	2.63	9 (40%)	26,27,27	1.11	2 (7%)

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
4	B3N	B	390	2	-	0/20/20/20	0/1/1/1
4	B3N	A	390	2	-	1/20/20/20	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	390	B3N	O4-N3	-6.43	1.23	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	390	B3N	O4-N3	-5.96	1.24	1.40
4	B	390	B3N	C16-C17	5.65	1.50	1.39
4	A	390	B3N	C16-C17	5.22	1.49	1.39
4	A	390	B3N	C19-C14	4.74	1.47	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	390	B3N	C18-C17-N20	-2.69	118.00	121.63
4	A	390	B3N	C18-C17-N20	-2.28	118.55	121.63
4	A	390	B3N	O2-C1-N3	-2.26	120.49	123.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

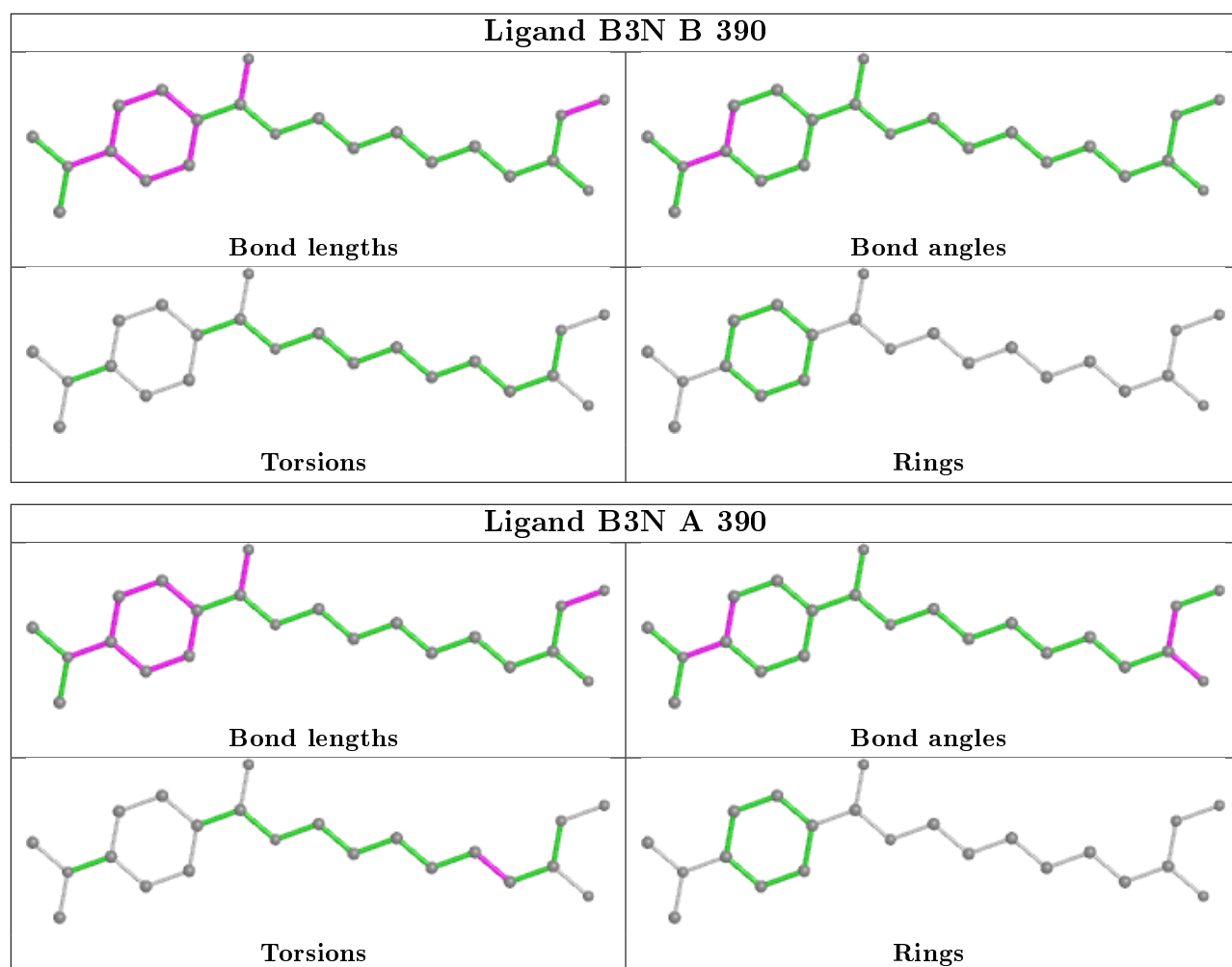
Mol	Chain	Res	Type	Atoms
4	A	390	B3N	C1-C5-C6-C7

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	390	B3N	4	0
4	A	390	B3N	4	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 [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	357/389 (91%)	-0.11	2 (0%) 89 83	45, 81, 109, 141	15 (4%)
1	B	356/389 (91%)	-0.08	1 (0%) 94 92	44, 81, 109, 127	15 (4%)
All	All	713/778 (91%)	-0.09	3 (0%) 92 89	44, 81, 109, 141	30 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ASP	2.7
1	A	373	LEU	2.4
1	B	373	LEU	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 carbohydrates 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	K	A	404	1/1	0.90	0.11	67,67,67,67	0
3	K	A	402	1/1	0.92	0.13	53,53,53,53	0

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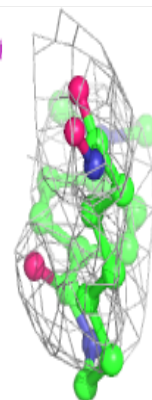
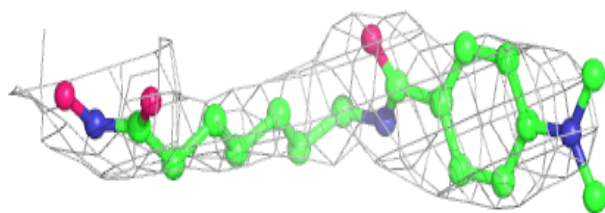
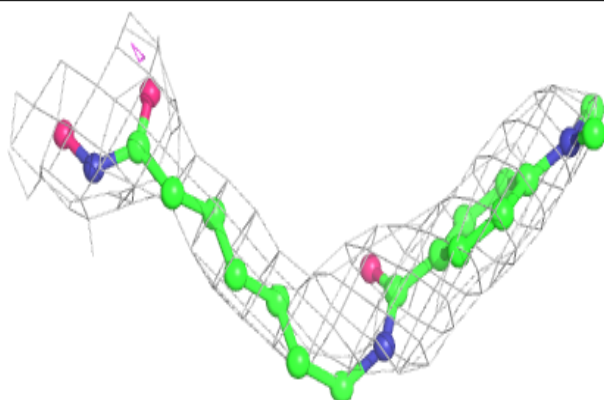
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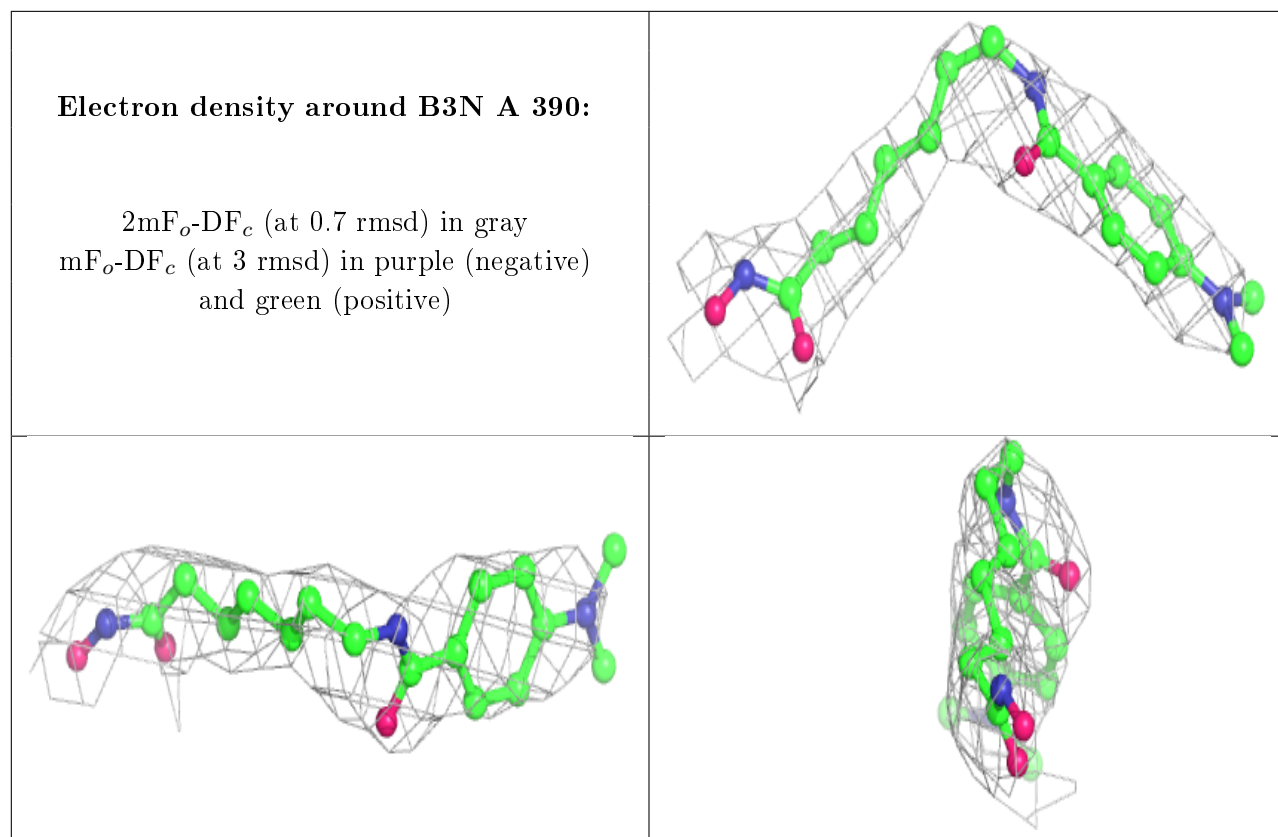
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	B	403	1/1	0.93	0.09	53,53,53,53	0
4	B3N	B	390	22/22	0.95	0.24	73,86,97,98	0
4	B3N	A	390	22/22	0.96	0.21	60,72,76,76	0
2	CO	B	401	1/1	0.97	0.10	70,70,70,70	0
3	K	B	405	1/1	0.97	0.06	72,72,72,72	0
2	CO	A	400	1/1	0.99	0.12	74,74,74,74	0

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 B3N B 390:

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.