Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 04:36 PM JST

PDB ID	:	7YQR
Title	:	Crystal Structure of Xcc NAMPT and its complex with NAM
Authors	:	Xu, G.L.; Ming, Z.H.
Deposited on	:	2022-08-08
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

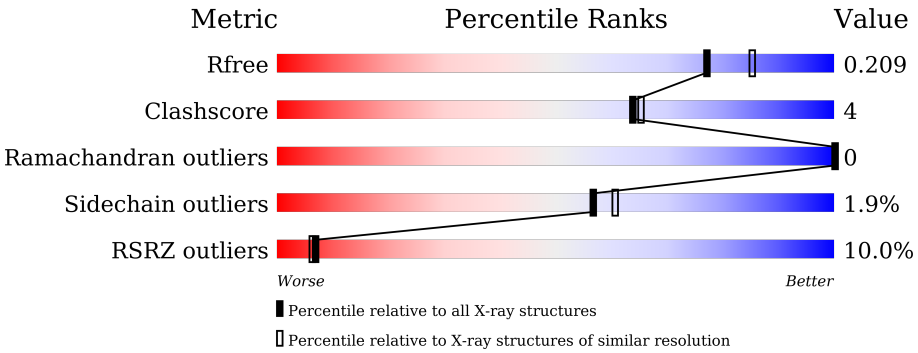
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	482	7% 88% 8%
1	B	482	12% 84% 10% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7608 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 Pre-B cell enhancing factor related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3615	2287	644	676	8			
1	B	458	Total	C	N	O	S	0	0	0
			3572	2259	635	670	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A0H2X5R2
A	-12	GLY	-	expression tag	UNP A0A0H2X5R2
A	-11	SER	-	expression tag	UNP A0A0H2X5R2
A	-10	SER	-	expression tag	UNP A0A0H2X5R2
A	-9	HIS	-	expression tag	UNP A0A0H2X5R2
A	-8	HIS	-	expression tag	UNP A0A0H2X5R2
A	-7	HIS	-	expression tag	UNP A0A0H2X5R2
A	-6	HIS	-	expression tag	UNP A0A0H2X5R2
A	-5	HIS	-	expression tag	UNP A0A0H2X5R2
A	-4	HIS	-	expression tag	UNP A0A0H2X5R2
A	-3	SER	-	expression tag	UNP A0A0H2X5R2
A	-2	GLN	-	expression tag	UNP A0A0H2X5R2
A	-1	GLY	-	expression tag	UNP A0A0H2X5R2
A	0	SER	-	expression tag	UNP A0A0H2X5R2
B	-13	MET	-	initiating methionine	UNP A0A0H2X5R2
B	-12	GLY	-	expression tag	UNP A0A0H2X5R2
B	-11	SER	-	expression tag	UNP A0A0H2X5R2
B	-10	SER	-	expression tag	UNP A0A0H2X5R2
B	-9	HIS	-	expression tag	UNP A0A0H2X5R2
B	-8	HIS	-	expression tag	UNP A0A0H2X5R2
B	-7	HIS	-	expression tag	UNP A0A0H2X5R2
B	-6	HIS	-	expression tag	UNP A0A0H2X5R2
B	-5	HIS	-	expression tag	UNP A0A0H2X5R2
B	-4	HIS	-	expression tag	UNP A0A0H2X5R2
B	-3	SER	-	expression tag	UNP A0A0H2X5R2

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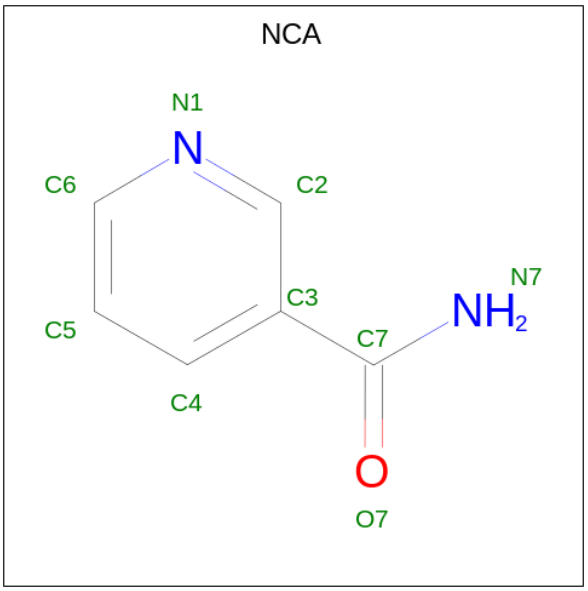
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP A0A0H2X5R2
B	-1	GLY	-	expression tag	UNP A0A0H2X5R2
B	0	SER	-	expression tag	UNP A0A0H2X5R2

- Molecule 2 is NICOTINAMIDE (three-letter code: NCA) (formula: $C_6H_6N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 6 2 1	0	0
2	A	1	Total C N O 9 6 2 1	0	0

- Molecule 3 is water.

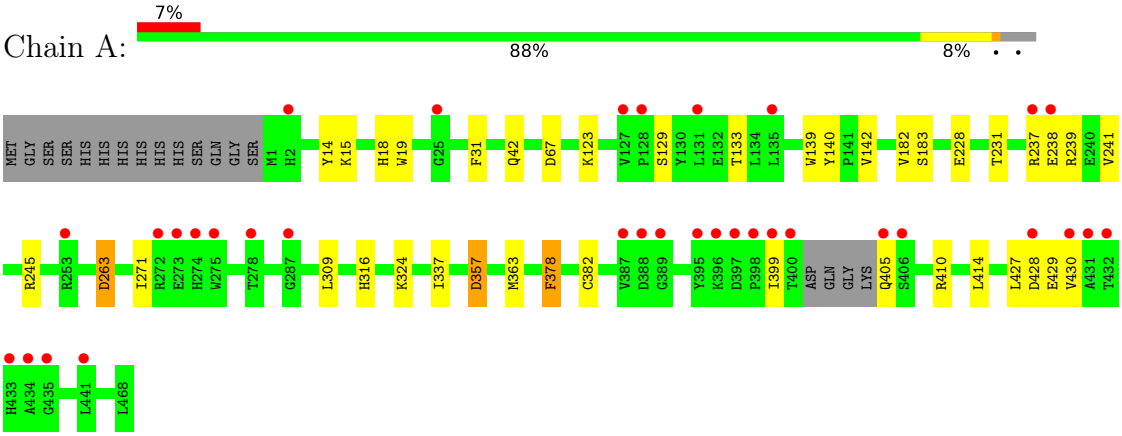
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	194	Total O 194 194	0	0
3	B	209	Total O 209 209	0	0

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.

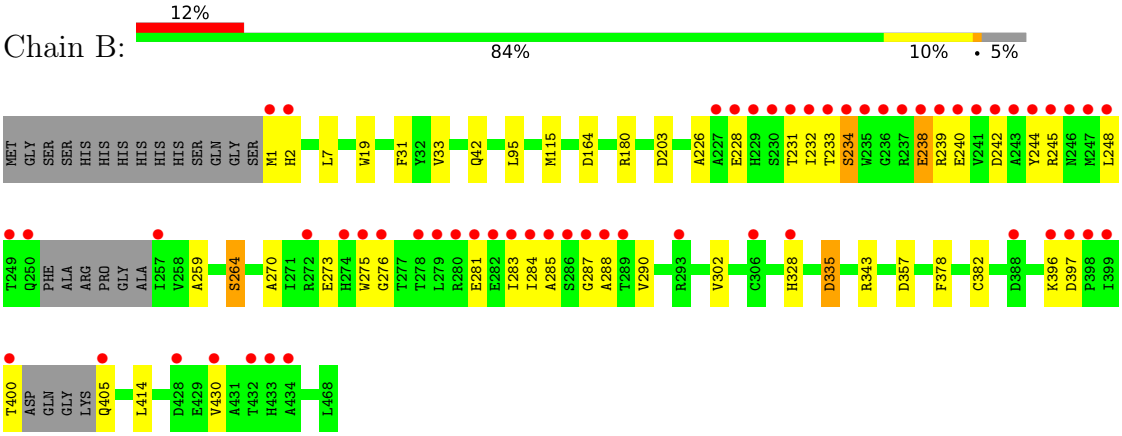
• Molecule 1: Pre-B cell enhancing factor related protein

Chain A:



• Molecule 1: Pre-B cell enhancing factor related protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	115.95Å 115.95Å 317.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.85 – 2.00 26.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.85-2.00) 100.0 (26.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.99Å)	Xtriage
Refinement program	PHENIX (1.15_3459: ???)	Depositor
R, R_{free}	0.187 , 0.209 0.187 , 0.209	Depositor DCC
R_{free} test set	4315 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NCA

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	0.37	0/3696	0.53	0/5033
1	B	0.38	0/3650	0.55	0/4969
All	All	0.37	0/7346	0.54	0/10002

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

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	3615	0	3556	27	0
1	B	3572	0	3513	36	0
2	A	18	0	12	0	0
3	A	194	0	0	3	1
3	B	209	0	0	5	1
All	All	7608	0	7081	60	1

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 (60) 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:400:THR:HB	1:B:405:GLN:HE21	1.29	0.96
1:B:242:ASP:HA	1:B:245:ARG:HG3	1.54	0.89
1:A:18:HIS:HE1	1:B:228:GLU:HG3	1.38	0.87
1:A:67:ASP:OD2	3:A:601:HOH:O	1.97	0.81
1:B:164:ASP:OD2	3:B:501:HOH:O	2.03	0.76
1:A:15:LYS:HE3	1:A:129:SER:O	1.86	0.74
1:B:283:ILE:HD12	1:B:290:VAL:HG21	1.67	0.74
1:B:233:THR:HG22	1:B:240:GLU:HG2	1.71	0.72
1:B:238:GLU:HG3	1:B:239:ARG:HG3	1.77	0.67
1:A:18:HIS:CE1	1:B:228:GLU:HG3	2.27	0.65
1:B:245:ARG:HA	1:B:248:LEU:HD12	1.79	0.65
1:A:428:ASP:OD1	3:A:602:HOH:O	2.15	0.63
1:B:7:LEU:HD21	1:B:95:LEU:HD11	1.82	0.62
1:B:288:ALA:O	3:B:502:HOH:O	2.16	0.61
1:B:231:THR:HA	1:B:234:SER:HB3	1.82	0.60
1:B:242:ASP:HA	1:B:245:ARG:CG	2.30	0.60
1:B:248:LEU:HD21	1:B:283:ILE:HD13	1.85	0.58
1:A:15:LYS:NZ	1:A:133:THR:H	2.03	0.55
1:A:14:TYR:OH	1:B:180:ARG:NH2	2.41	0.53
1:A:237:ARG:HH11	1:A:237:ARG:HG2	1.73	0.53
1:B:287:GLY:C	3:B:502:HOH:O	2.48	0.52
1:B:273:GLU:HB2	1:B:275:TRP:CD1	2.46	0.51
1:B:284:ILE:HG23	1:B:328:HIS:CE1	2.46	0.51
1:A:399:ILE:HD13	1:A:405:GLN:HB2	1.93	0.50
1:A:228:GLU:O	1:A:231:THR:HG22	2.11	0.49
1:A:271:ILE:HD13	1:A:309:LEU:HB3	1.96	0.48
1:B:284:ILE:HG23	1:B:328:HIS:NE2	2.28	0.48
1:A:15:LYS:HZ1	1:A:133:THR:H	1.63	0.47
1:A:337:ILE:HG22	1:A:363:MET:HG3	1.95	0.47
1:A:31:PHE:CE2	1:A:382:CYS:HB2	2.50	0.46
1:A:414:LEU:HD21	1:A:430:VAL:HG22	1.96	0.46
1:A:142:VAL:HG11	1:A:378:PHE:CZ	2.50	0.46
1:A:263:ASP:OD2	3:A:603:HOH:O	2.20	0.46
1:B:270:ALA:O	1:B:276:GLY:HA3	2.16	0.46
1:B:396:LYS:HG3	1:B:397:ASP:H	1.81	0.45
1:A:238:GLU:HG3	1:A:239:ARG:HG3	1.98	0.45
1:A:410:ARG:HB3	1:A:427:LEU:HD12	1.98	0.45
1:A:123:LYS:HD3	1:A:123:LYS:HA	1.74	0.45
1:B:226:ALA:HB2	1:B:259:ALA:HB3	1.99	0.45
1:B:240:GLU:HB3	1:B:244:TYR:HE1	1.82	0.44
1:A:316:HIS:CD2	1:A:324:LYS:HG2	2.52	0.44
1:A:429:GLU:HG2	1:A:429:GLU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LEU:HD21	1:B:430:VAL:HG22	1.98	0.44
1:A:182:VAL:HG22	1:A:183:SER:H	1.82	0.44
1:B:232:ILE:HG21	1:B:244:TYR:CG	2.53	0.44
1:B:264:SER:HB3	1:B:302:VAL:HG23	2.00	0.43
1:B:396:LYS:H	1:B:396:LYS:HG2	1.64	0.42
1:A:241:VAL:O	1:A:245:ARG:HG3	2.19	0.42
1:B:281:GLU:O	1:B:285:ALA:N	2.44	0.42
1:B:328:HIS:HD2	3:B:502:HOH:O	2.02	0.41
1:A:139:TRP:CE3	1:A:140:TYR:HA	2.56	0.41
1:B:240:GLU:O	1:B:244:TYR:HD1	2.04	0.41
1:B:33:VAL:HB	1:B:115:MET:HG3	2.02	0.41
1:B:343:ARG:NH2	3:B:504:HOH:O	2.32	0.41
1:A:337:ILE:CG2	1:A:363:MET:HG3	2.51	0.41
1:B:1:MET:CG	1:B:2:HIS:H	2.34	0.41
1:B:335:ASP:N	1:B:335:ASP:OD1	2.53	0.41
1:B:31:PHE:CE2	1:B:382:CYS:HB2	2.56	0.41
1:B:232:ILE:HD12	1:B:232:ILE:HG23	1.78	0.40
1:A:357:ASP:OD1	1:A:357:ASP:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:775:HOH:O	3:B:679:HOH:O[8_565]	1.69	0.51

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	460/482 (95%)	450 (98%)	10 (2%)	0	100	100
1	B	452/482 (94%)	442 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	912/964 (95%)	892 (98%)	20 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	376/391 (96%)	371 (99%)	5 (1%)	69 74
1	B	373/391 (95%)	364 (98%)	9 (2%)	49 51
All	All	749/782 (96%)	735 (98%)	14 (2%)	57 61

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TRP
1	A	42	GLN
1	A	263	ASP
1	A	357	ASP
1	A	378	PHE
1	B	19	TRP
1	B	42	GLN
1	B	203	ASP
1	B	234	SER
1	B	238	GLU
1	B	264	SER
1	B	335	ASP
1	B	357	ASP
1	B	378	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	317	GLN
1	A	449	GLN
1	B	405	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	NCA	A	502	-	9,9,9	2.81	3 (33%)	11,11,11	1.84	4 (36%)
2	NCA	A	501	-	9,9,9	2.64	3 (33%)	11,11,11	1.40	2 (18%)

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	NCA	A	502	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NCA	A	501	-	-	0/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NCA	C7-N7	7.12	1.46	1.33
2	A	501	NCA	C7-N7	6.81	1.46	1.33
2	A	502	NCA	C3-C7	2.75	1.54	1.50
2	A	502	NCA	O7-C7	-2.55	1.19	1.24
2	A	501	NCA	C3-C7	2.32	1.54	1.50
2	A	501	NCA	O7-C7	-2.16	1.20	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	NCA	C3-C7-N7	3.54	122.00	117.75
2	A	502	NCA	O7-C7-N7	-2.75	118.68	122.58
2	A	501	NCA	C3-C2-N1	-2.58	119.68	123.49
2	A	502	NCA	C6-N1-C2	2.55	121.25	116.85
2	A	502	NCA	C3-C2-N1	-2.51	119.78	123.49
2	A	501	NCA	C6-N1-C2	2.31	120.84	116.85

There are no chirality outliers.

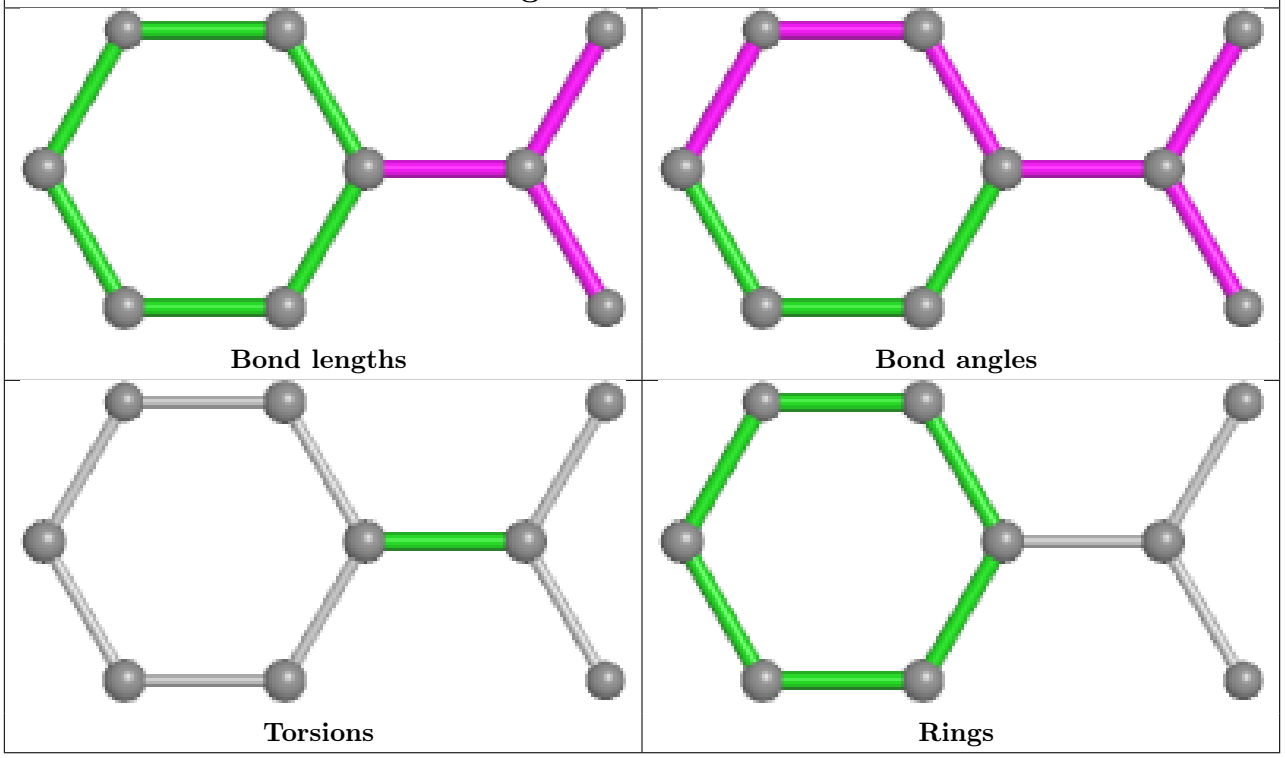
There are no torsion outliers.

There are no ring outliers.

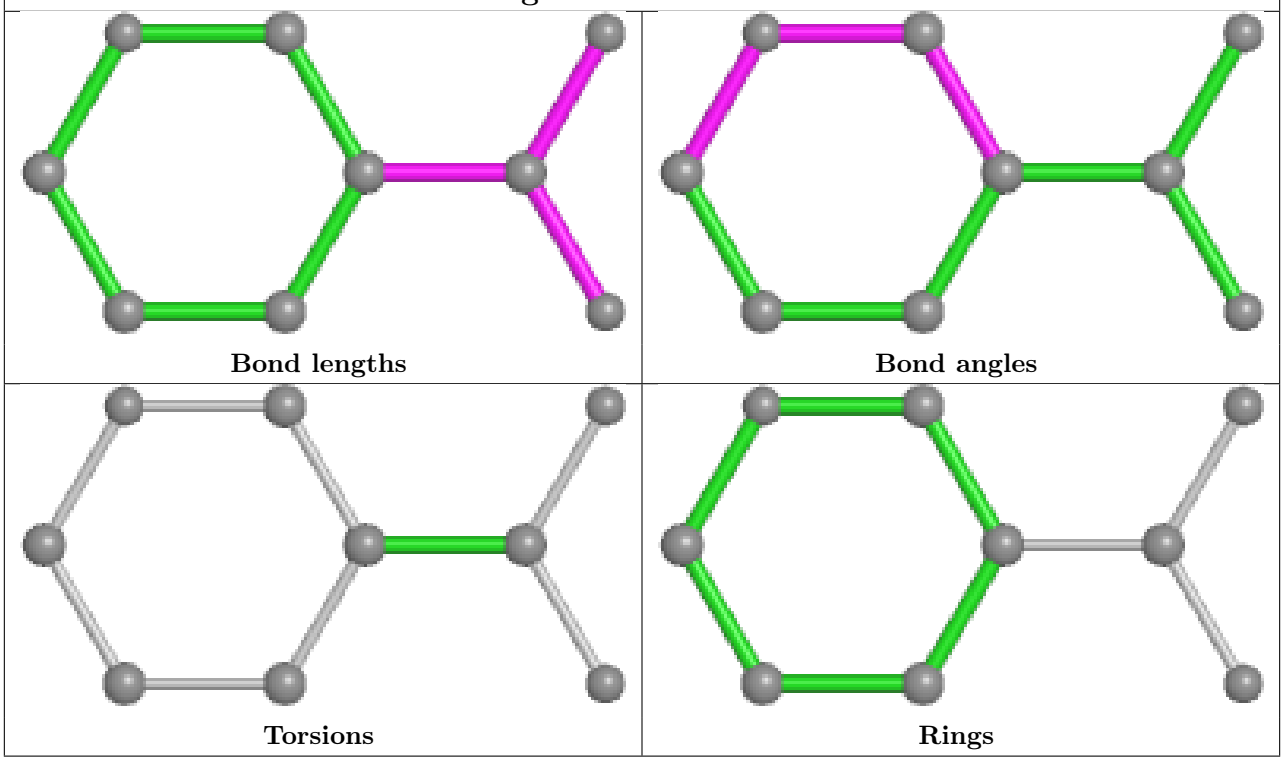
No monomer is involved in short contacts.

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 then 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.

Ligand NCA A 502



Ligand NCA A 501



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, 95^{th} 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	464/482 (96%)	0.21	34 (7%) 15 14	29, 42, 69, 87	0
1	B	458/482 (95%)	0.53	58 (12%) 3 3	29, 40, 96, 128	0
All	All	922/964 (95%)	0.37	92 (9%) 7 6	29, 41, 84, 128	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ILE	10.0
1	B	285	ALA	9.7
1	B	233	THR	9.5
1	B	244	TYR	9.2
1	B	248	LEU	8.7
1	B	241	VAL	8.6
1	B	400	THR	8.2
1	B	238	GLU	8.0
1	B	229	HIS	7.9
1	B	237	ARG	7.8
1	B	236	GLY	7.4
1	B	246	ASN	7.0
1	B	227	ALA	6.8
1	B	275	TRP	6.8
1	A	274	HIS	6.7
1	B	247	MET	6.7
1	B	235	TRP	6.6
1	B	231	THR	6.6
1	B	398	PRO	6.6
1	B	230	SER	6.6
1	B	274	HIS	6.4
1	A	430	VAL	6.4
1	B	239	ARG	6.1
1	A	431	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	249	THR	5.8
1	A	275	TRP	5.7
1	A	399	ILE	5.4
1	B	240	GLU	5.4
1	B	397	ASP	5.3
1	B	245	ARG	5.2
1	A	387	VAL	5.0
1	B	234	SER	4.9
1	B	405	GLN	4.5
1	B	396	LYS	4.5
1	B	288	ALA	4.5
1	A	405	GLN	4.4
1	B	250	GLN	4.4
1	B	281	GLU	4.4
1	B	232	ILE	4.2
1	B	388	ASP	4.2
1	A	237	ARG	4.2
1	A	397	ASP	4.1
1	B	283	ILE	4.1
1	A	432	THR	4.0
1	A	400	THR	3.9
1	B	282	GLU	3.8
1	A	396	LYS	3.8
1	A	273	GLU	3.7
1	B	286	SER	3.7
1	B	228	GLU	3.7
1	A	389	GLY	3.6
1	B	284	ILE	3.6
1	B	276	GLY	3.6
1	B	272	ARG	3.5
1	A	433	HIS	3.5
1	B	279	LEU	3.4
1	A	406	SER	3.4
1	A	434	ALA	3.3
1	B	280	ARG	3.2
1	A	398	PRO	3.1
1	A	238	GLU	3.1
1	B	287	GLY	3.1
1	B	242	ASP	3.1
1	A	428	ASP	3.1
1	B	257	ILE	3.0
1	B	243	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	395	TYR	2.9
1	B	432	THR	2.9
1	A	2	HIS	2.8
1	A	388	ASP	2.8
1	B	430	VAL	2.8
1	A	131	LEU	2.5
1	B	278	THR	2.5
1	B	434	ALA	2.5
1	B	289	THR	2.5
1	A	253	ARG	2.5
1	B	433	HIS	2.4
1	B	1	MET	2.4
1	A	128	PRO	2.3
1	A	441	LEU	2.2
1	B	428	ASP	2.2
1	B	328	HIS	2.2
1	B	293	ARG	2.2
1	A	287	GLY	2.2
1	A	25	GLY	2.1
1	A	127	VAL	2.1
1	A	272	ARG	2.1
1	B	306	CYS	2.1
1	A	135	LEU	2.1
1	A	435	GLY	2.1
1	B	2	HIS	2.0
1	A	278	THR	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 (i)

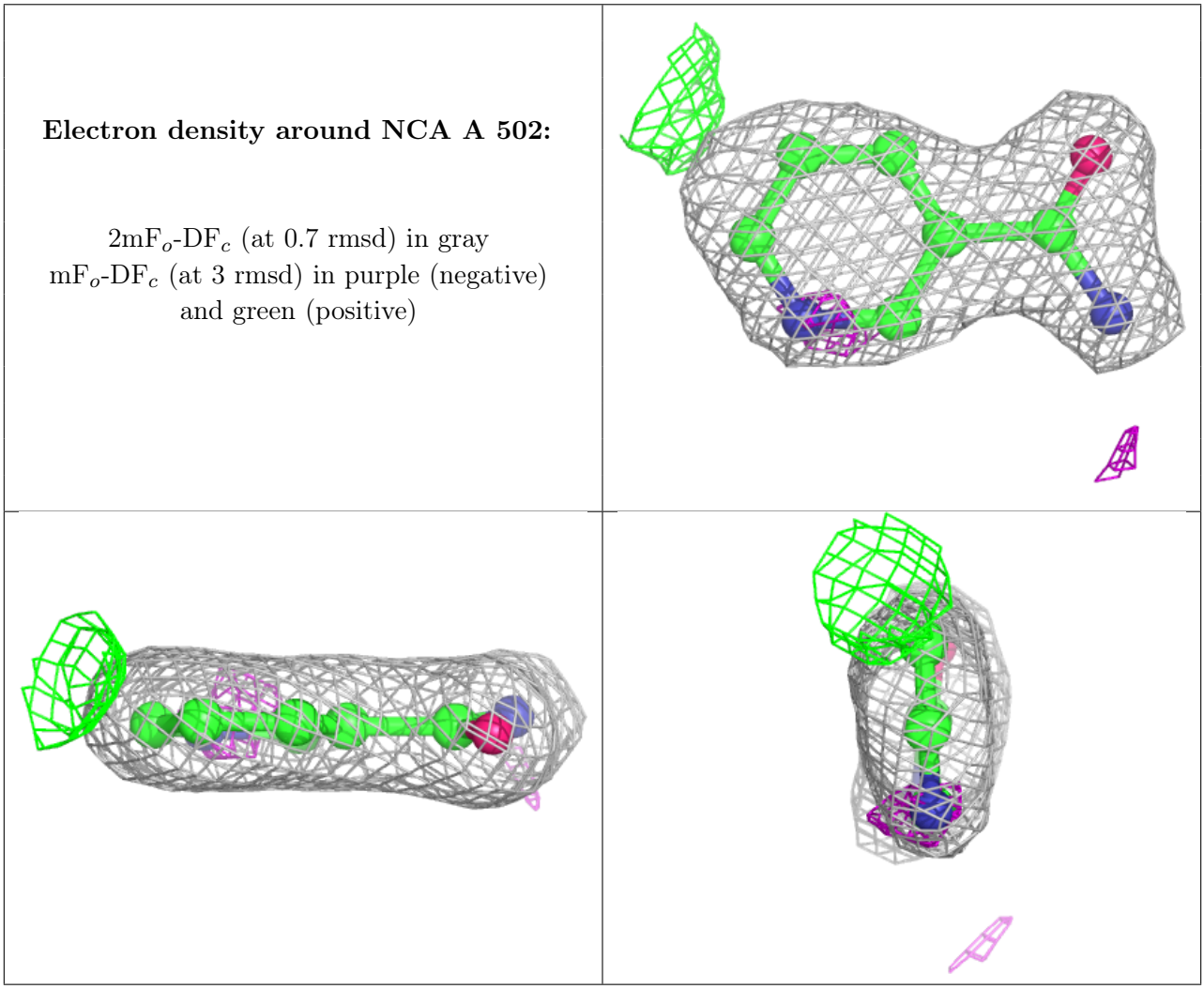
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NCA	A	502	9/9	0.94	0.12	39,42,46,49	0
2	NCA	A	501	9/9	0.96	0.12	37,42,45,47	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.

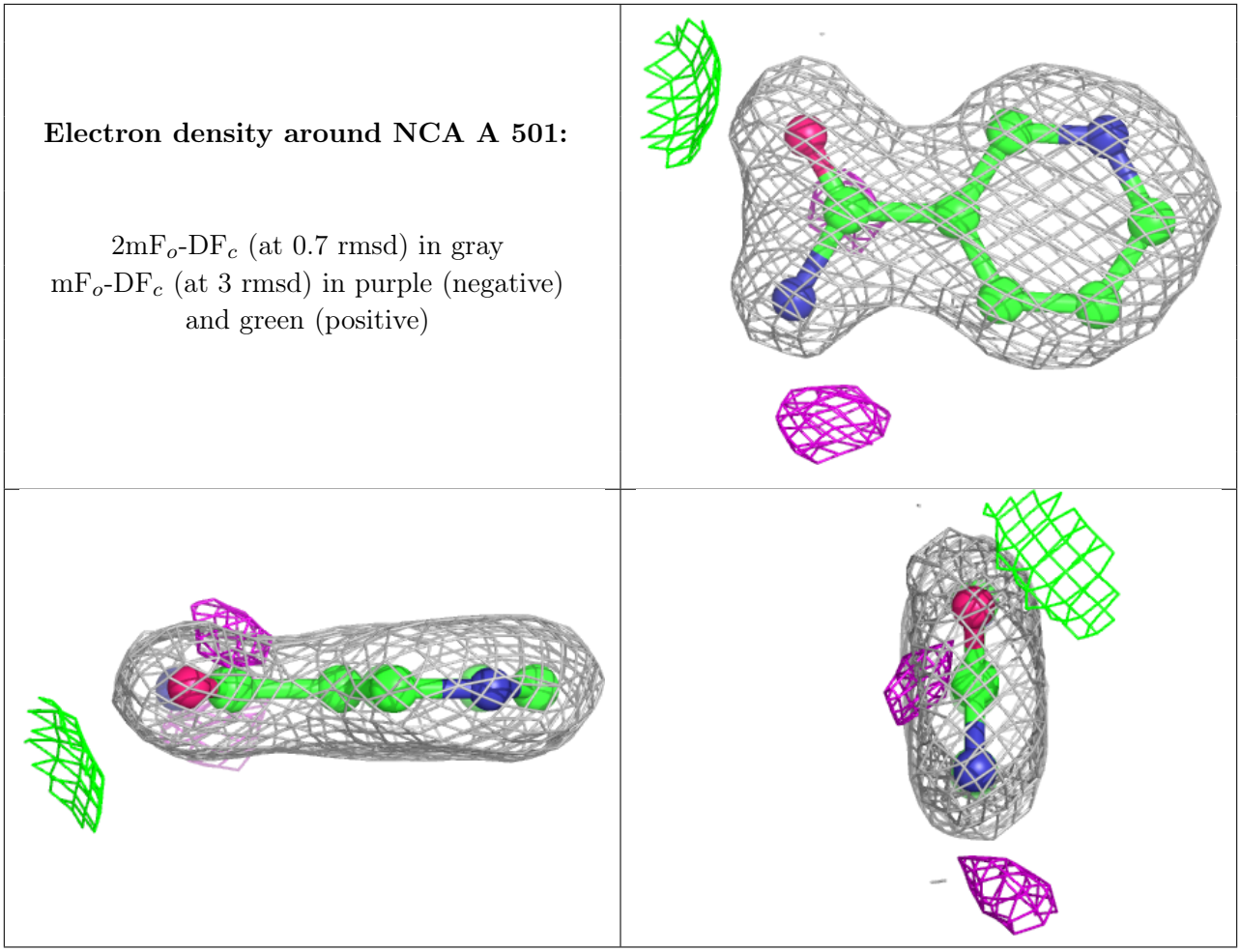
Electron density around NCA A 502:

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



Electron density around NCA A 501:

$2mF_o$-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.