wwPDB X-ray Structure Validation Summary Report (i)

Nov 11, 2020 – 12:07 PM GMT

PDB ID	:	7A54
Title	:	Two copies of the catalytic domain of NanA sialidase from Streptococcus pneumoniae juxtaposed in the P212121 space group, in complex with DANA
Authors	:	Bridot, C.; Bouckaert, J.
Deposited on	:	2020-08-20
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

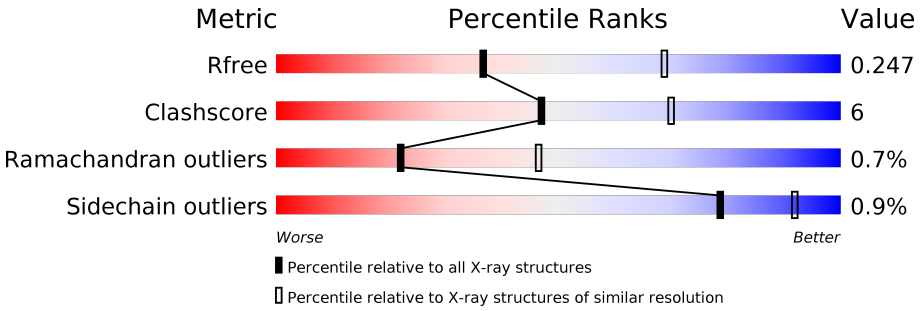
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	498	79% 15% • 5%
1	B	498	82% 12% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15032 atoms, of which 7268 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 Sialidase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	472	Total	C	H	N	O	S	0	0	0
			7347	2337	3616	659	723	12			
1	B	472	Total	C	H	N	O	S	0	0	0
			7350	2337	3620	659	722	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	MET	-	initiating methionine	UNP P62575
A	280	GLY	-	expression tag	UNP P62575
A	281	HIS	-	expression tag	UNP P62575
A	282	HIS	-	expression tag	UNP P62575
A	283	HIS	-	expression tag	UNP P62575
A	284	HIS	-	expression tag	UNP P62575
A	285	HIS	-	expression tag	UNP P62575
A	286	HIS	-	expression tag	UNP P62575
A	287	HIS	-	expression tag	UNP P62575
A	288	HIS	-	expression tag	UNP P62575
A	289	HIS	-	expression tag	UNP P62575
A	290	HIS	-	expression tag	UNP P62575
A	291	SER	-	expression tag	UNP P62575
A	292	SER	-	expression tag	UNP P62575
A	293	GLY	-	expression tag	UNP P62575
A	294	HIS	-	expression tag	UNP P62575
A	295	ILE	-	expression tag	UNP P62575
A	296	ASP	-	expression tag	UNP P62575
A	297	ASP	-	expression tag	UNP P62575
A	298	ASP	-	expression tag	UNP P62575
A	299	ASP	-	expression tag	UNP P62575
A	300	LYS	-	expression tag	UNP P62575
A	301	HIS	-	expression tag	UNP P62575
A	302	MET	-	expression tag	UNP P62575
B	279	MET	-	initiating methionine	UNP P62575

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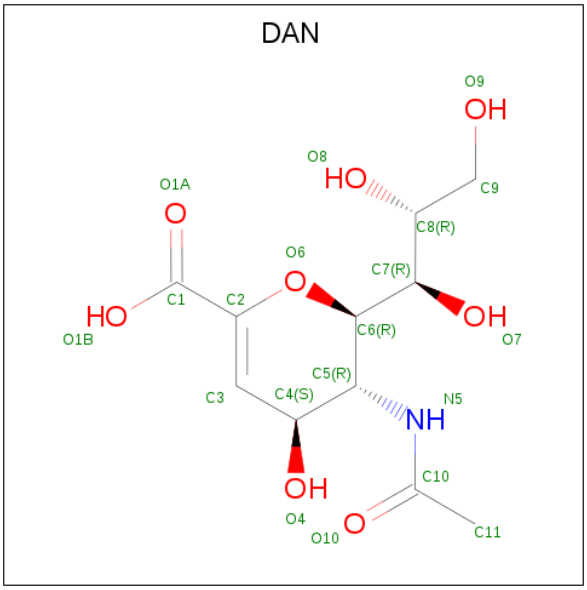
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	GLY	-	expression tag	UNP P62575
B	281	HIS	-	expression tag	UNP P62575
B	282	HIS	-	expression tag	UNP P62575
B	283	HIS	-	expression tag	UNP P62575
B	284	HIS	-	expression tag	UNP P62575
B	285	HIS	-	expression tag	UNP P62575
B	286	HIS	-	expression tag	UNP P62575
B	287	HIS	-	expression tag	UNP P62575
B	288	HIS	-	expression tag	UNP P62575
B	289	HIS	-	expression tag	UNP P62575
B	290	HIS	-	expression tag	UNP P62575
B	291	SER	-	expression tag	UNP P62575
B	292	SER	-	expression tag	UNP P62575
B	293	GLY	-	expression tag	UNP P62575
B	294	HIS	-	expression tag	UNP P62575
B	295	ILE	-	expression tag	UNP P62575
B	296	ASP	-	expression tag	UNP P62575
B	297	ASP	-	expression tag	UNP P62575
B	298	ASP	-	expression tag	UNP P62575
B	299	ASP	-	expression tag	UNP P62575
B	300	LYS	-	expression tag	UNP P62575
B	301	HIS	-	expression tag	UNP P62575
B	302	MET	-	expression tag	UNP P62575

- Molecule 2 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: DAN) (formula: $C_{11}H_{17}NO_8$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			36	11	16	1	8		
2	B	1	Total	C	H	N	O	0	0
			36	11	16	1	8		

- Molecule 3 is water.

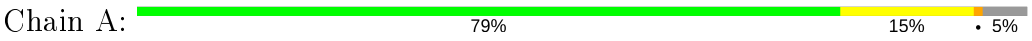
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		
3	B	120	Total	O	0	0
			120	120		

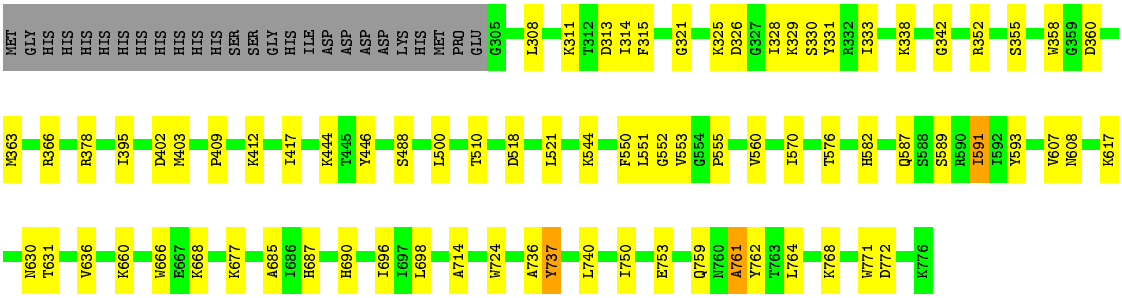
3 Residue-property plots (i)

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. 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. 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: Sialidase A

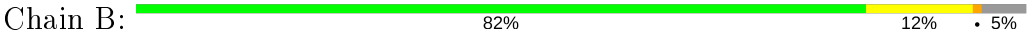
Chain A:

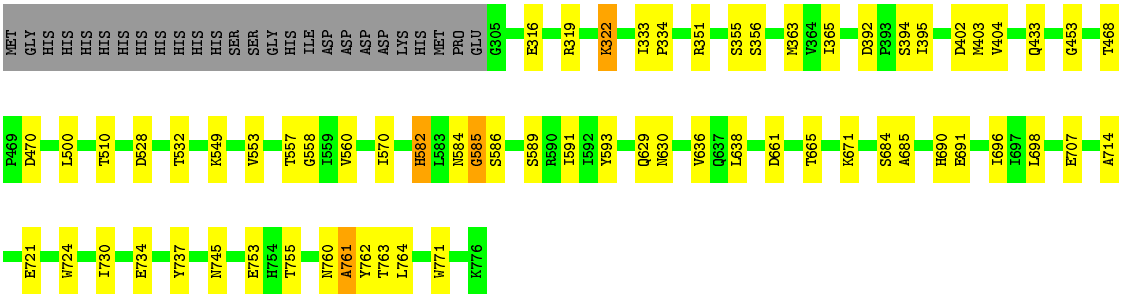




- Molecule 1: Sialidase A

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.87Å 96.19Å 220.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.27 – 2.70 48.10 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.27-2.70) 99.3 (48.10-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.206 , 0.247 0.206 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15032	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: DAN

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	0.32	0/3812	0.50	0/5147
1	B	0.40	1/3811 (0.0%)	0.53	1/5147 (0.0%)
All	All	0.36	1/7623 (0.0%)	0.52	1/10294 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	585	GLY	C-O	-14.88	0.99	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	585	GLY	C-N-CA	10.10	146.96	121.70

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	3731	3616	3649	48	0
1	B	3730	3620	3648	46	0
2	A	20	16	16	1	0
2	B	20	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	143	0	0	8	3
3	B	120	0	0	6	3
All	All	7764	7268	7329	92	4

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 6.

The worst 5 of 92 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:A:591:ILE:HG22	3:A:951:HOH:O	1.78	0.82
1:B:589:SER:N	1:B:630:ASN:OD1	2.16	0.77
1:B:500:LEU:O	1:B:510:THR:OG1	2.02	0.76
1:A:321:GLY:O	1:A:329:LYS:NZ	2.19	0.75
1:B:528:ASP:OD2	1:B:532:THR:HG22	1.88	0.74

All (4) 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:957:HOH:O	3:B:966:HOH:O[4_555]	1.90	0.30
3:A:930:HOH:O	3:A:962:HOH:O[3_554]	1.96	0.24
3:B:949:HOH:O	3:B:987:HOH:O[4_455]	2.01	0.19
3:A:935:HOH:O	3:B:993:HOH:O[4_555]	2.08	0.12

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	470/498 (94%)	438 (93%)	29 (6%)	3 (1%)	25 50
1	B	470/498 (94%)	437 (93%)	29 (6%)	4 (1%)	17 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	940/996 (94%)	875 (93%)	58 (6%)	7 (1%)	22 46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	761	ALA
1	B	586	SER
1	B	761	ALA
1	A	582	HIS
1	A	737	TYR

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	402/426 (94%)	397 (99%)	5 (1%)	71 88
1	B	402/426 (94%)	400 (100%)	2 (0%)	88 96
All	All	804/852 (94%)	797 (99%)	7 (1%)	78 92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	677	LYS
1	B	584	ASN
1	A	772	ASP
1	A	591	ILE
1	B	322	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	584	ASN
1	B	497	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 monosaccharides in this entry.

5.6 Ligand geometry

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	DAN	B	801	-	17,20,20	0.77	0	18,28,28	1.05	1 (5%)
2	DAN	A	801	-	17,20,20	0.78	0	18,28,28	1.06	1 (5%)

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	DAN	B	801	-	-	0/14/34/34	0/1/1/1
2	DAN	A	801	-	-	2/14/34/34	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	DAN	C11-C10-N5	2.28	119.96	116.10
2	A	801	DAN	C11-C10-N5	2.08	119.62	116.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	DAN	O8-C8-C9-O9
2	A	801	DAN	C7-C8-C9-O9

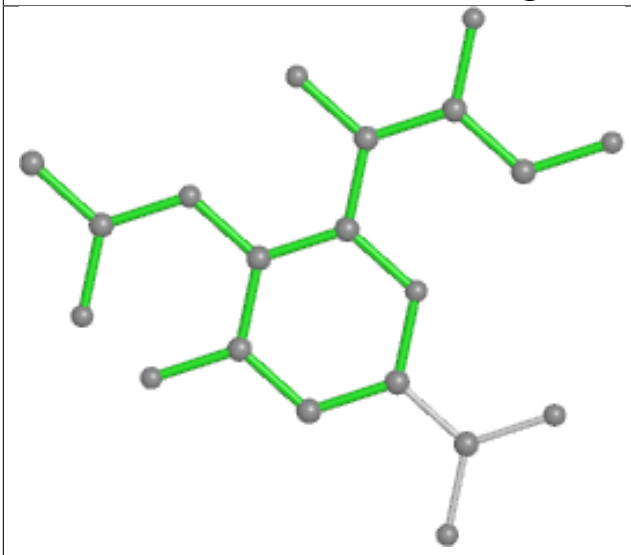
There are no ring outliers.

1 monomer is involved in 1 short contact:

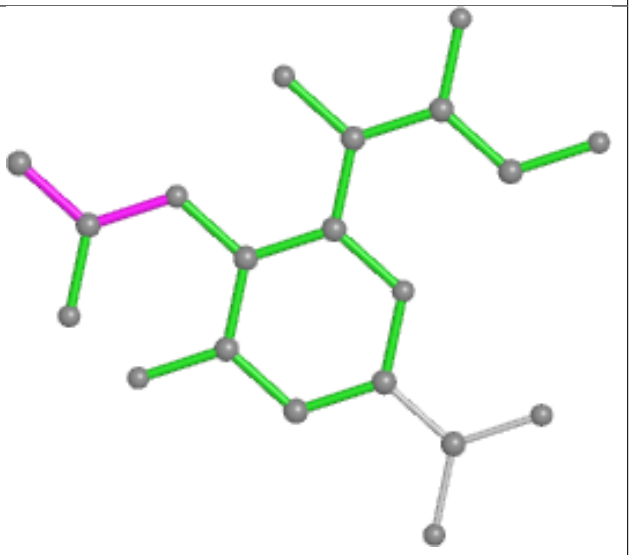
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	DAN	1	0

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 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.

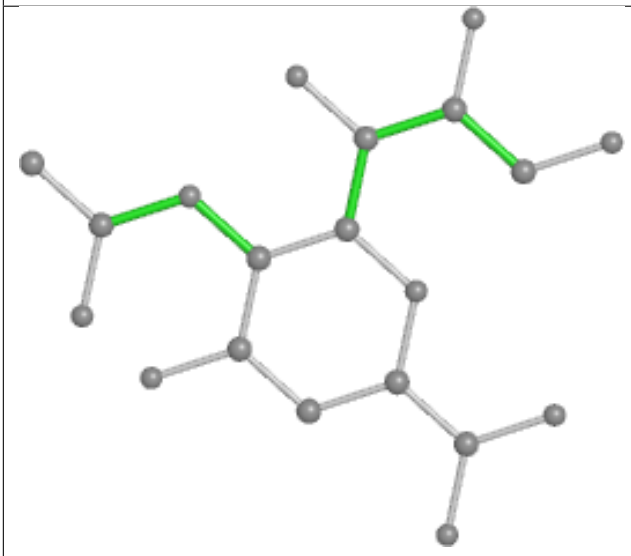
Ligand DAN B 801



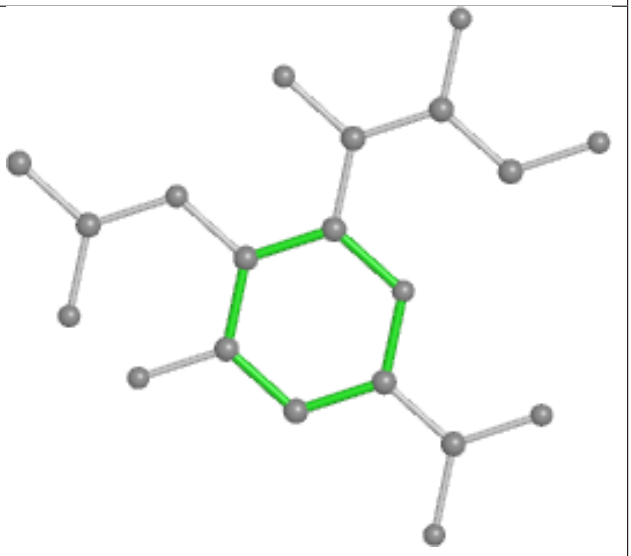
Bond lengths



Bond angles

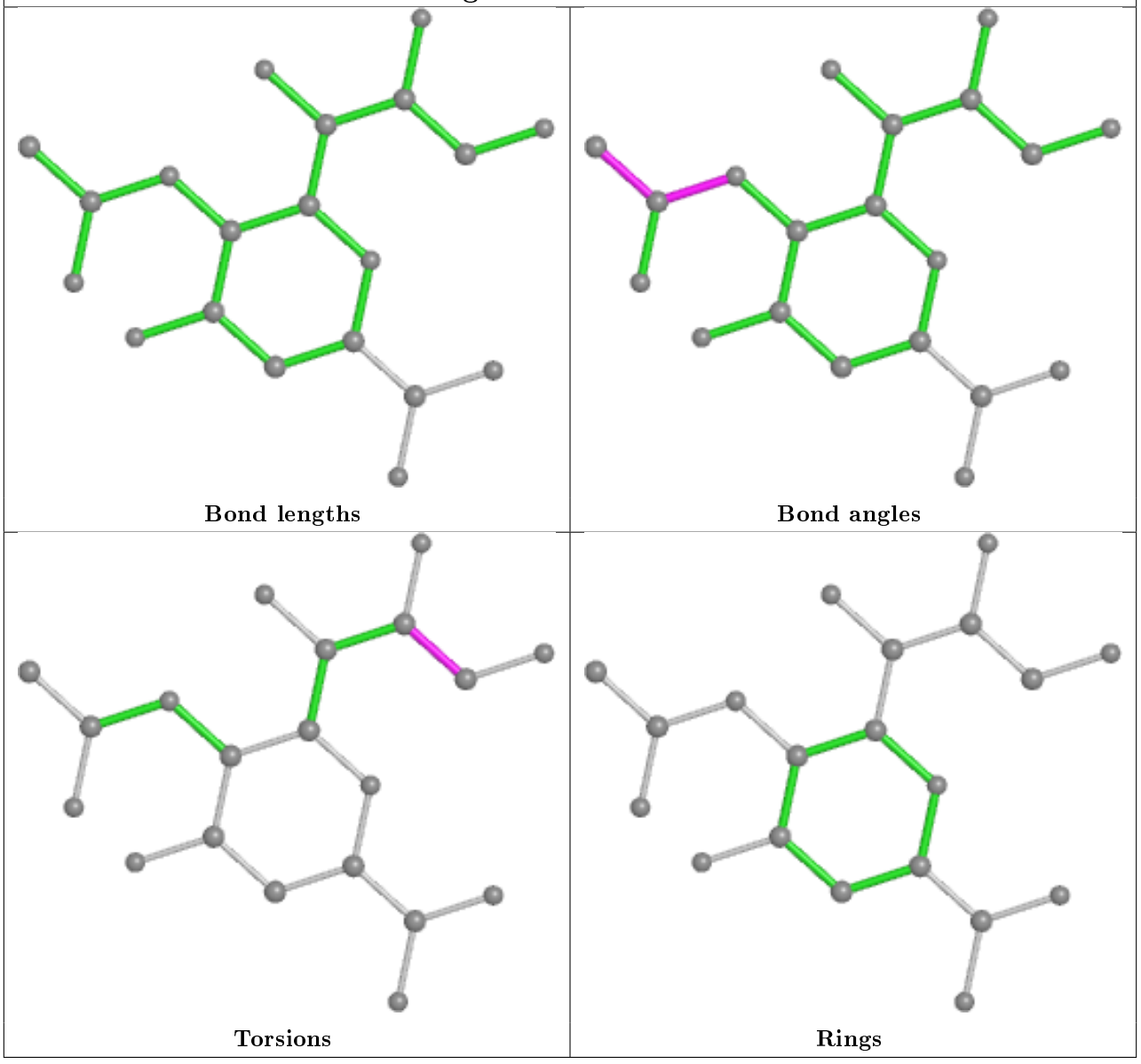


Torsions



Rings

Ligand DAN A 801



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

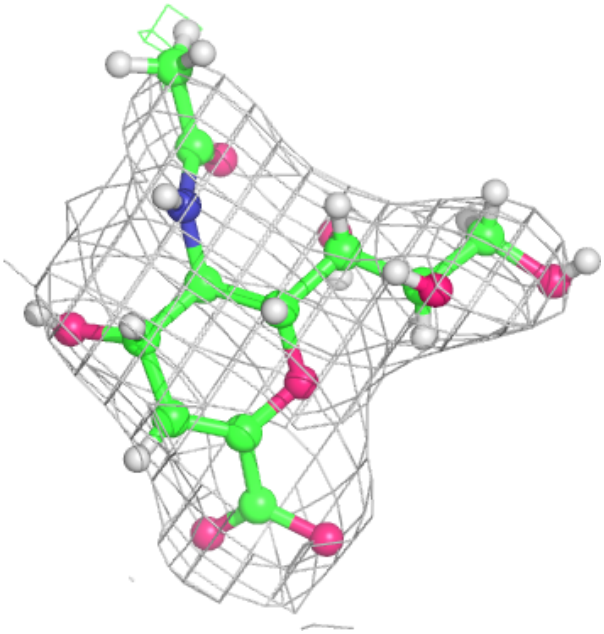
6.4 Ligands

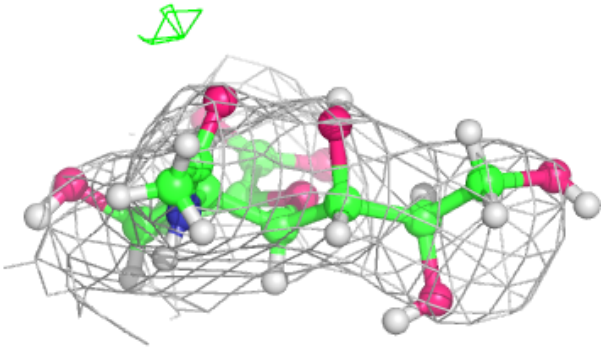
Unable to reproduce the depositors R factor - this section is therefore empty.

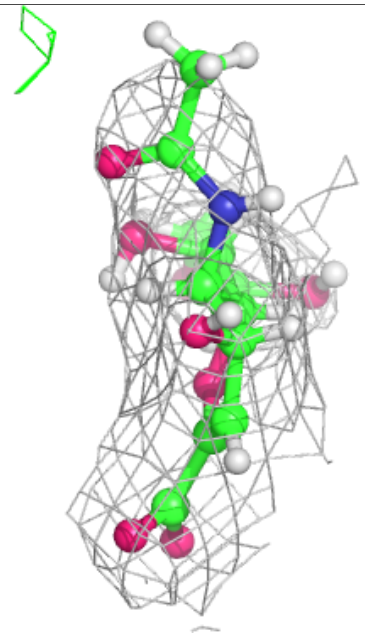
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DAN B 801:

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

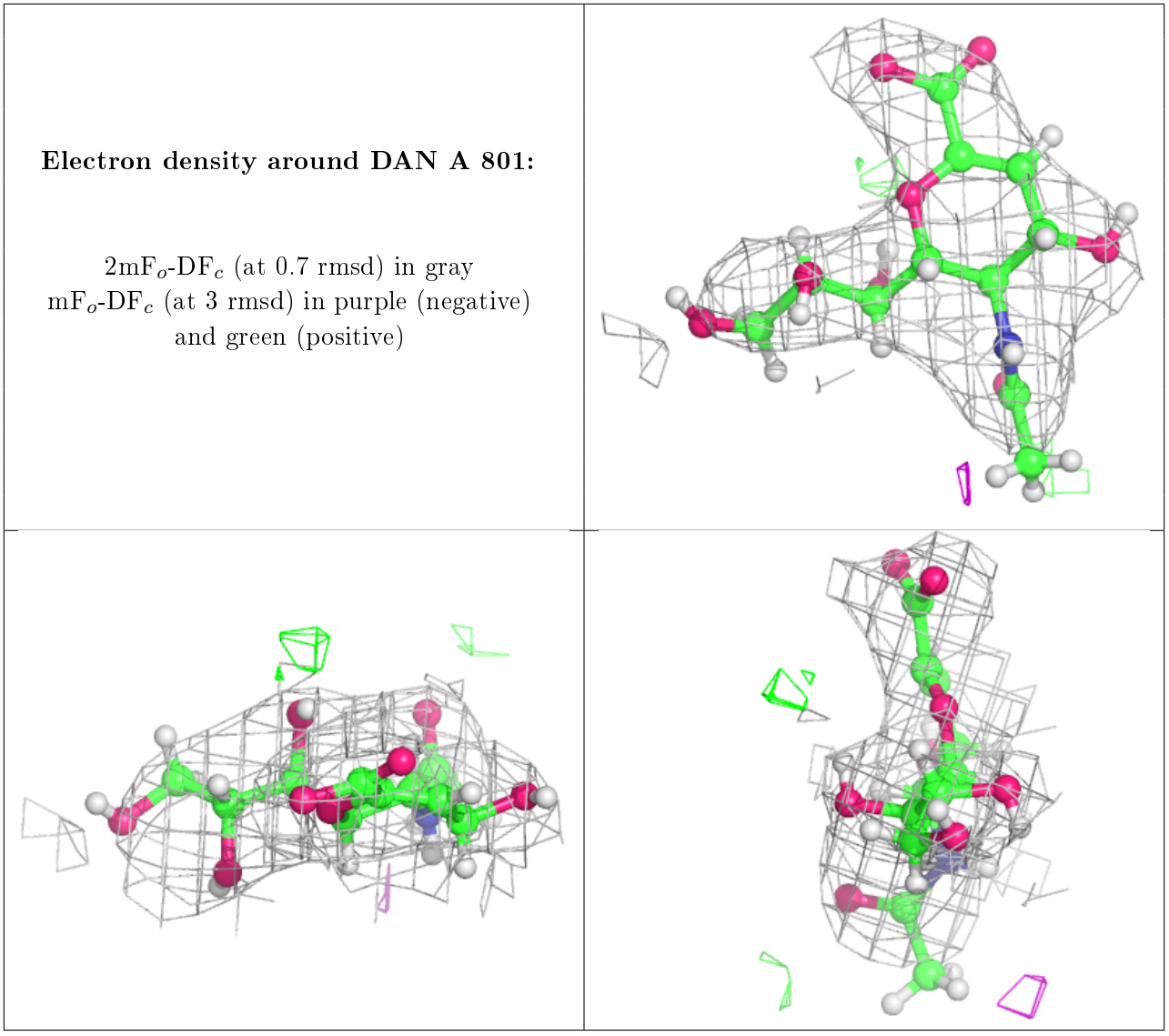






Electron density around DAN A 801:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.