Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 12:38 PM EDT

PDB ID	:	7S0I
Title	:	CRYSTAL STRUCTURE OF N1 NEURAMINIDASE FROM A/Michigan/45/2015(H1N1)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2021-08-30
Resolution	:	2.89 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:

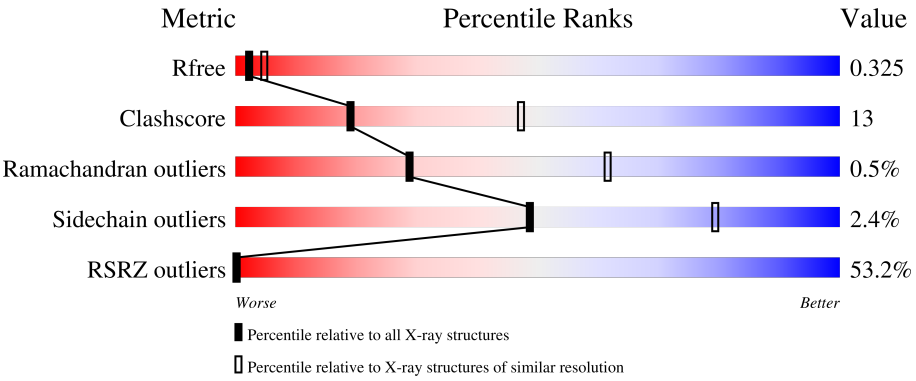
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	393	52% 72% 25%
2	B	4	25% 25% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	B	3	-	-	-	X
2	MAN	B	4	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3064 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2993	1881	513	577	22	0	0	0

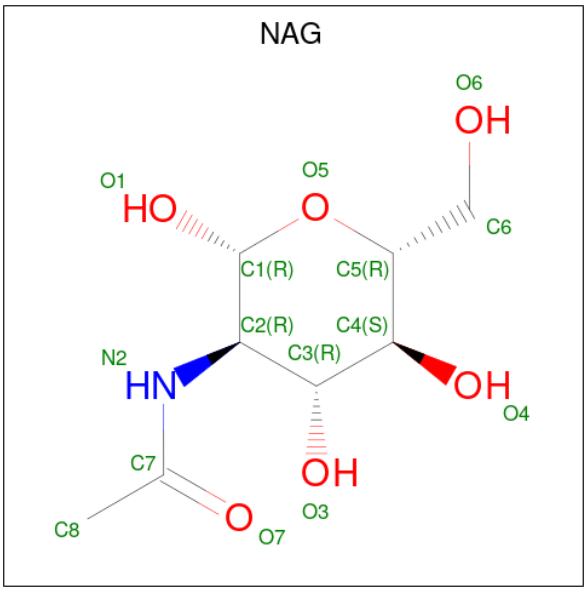
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP A0A0X9QTS2
A	78	SER	-	expression tag	UNP A0A0X9QTS2
A	79	PRO	-	expression tag	UNP A0A0X9QTS2
A	80	SER	-	expression tag	UNP A0A0X9QTS2
A	81	ARG	-	expression tag	UNP A0A0X9QTS2

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0

- Molecule 5 is water.

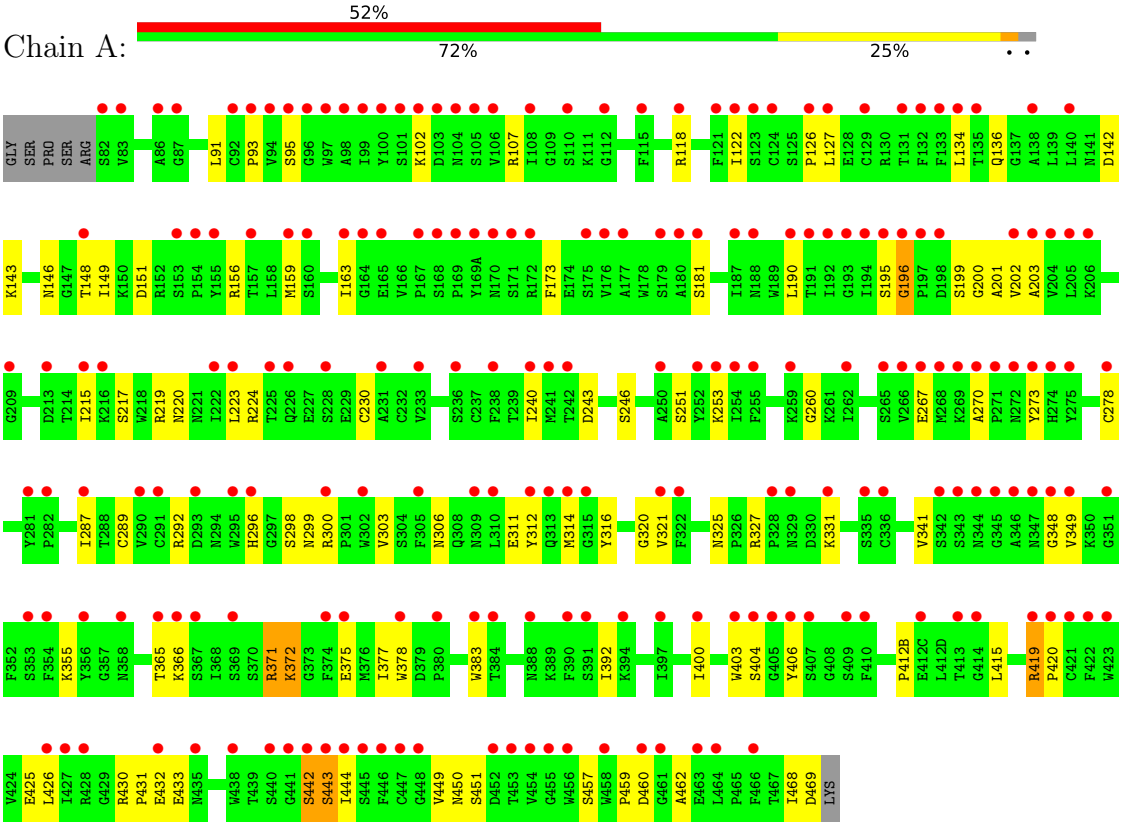
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0

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.

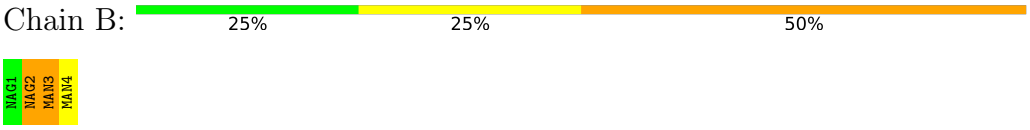
• Molecule 1: Neuraminidase

Chain A:



• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.13Å 92.13Å 104.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.07 – 2.89 46.07 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.0 (46.07-2.89) 91.2 (46.07-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.35	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.292 , 0.321 0.293 , 0.325	Depositor DCC
R_{free} test set	457 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 13.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	3064	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: CA, NAG, MAN

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	0.50	0/3075	0.78	1/4175 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	GLY	N-CA-C	-5.36	99.70	113.10

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	A	2993	0	2831	76	0
2	B	50	0	43	1	0
3	A	14	0	13	0	0
4	A	3	0	0	0	0
5	A	4	0	0	0	0
All	All	3064	0	2887	77	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 13.

All (77) 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:136:GLN:HE21	1:A:148:THR:HG22	1.13	1.14
1:A:403:TRP:O	1:A:426:LEU:HD12	1.49	1.11
1:A:136:GLN:NE2	1:A:148:THR:HG22	1.70	1.07
1:A:136:GLN:HE21	1:A:148:THR:CG2	1.81	0.93
1:A:136:GLN:NE2	1:A:148:THR:CG2	2.32	0.91
1:A:136:GLN:NE2	1:A:148:THR:CB	2.36	0.89
1:A:136:GLN:HE22	1:A:148:THR:HA	1.39	0.88
1:A:404:SER:HA	1:A:426:LEU:HD13	1.58	0.83
1:A:136:GLN:HE22	1:A:148:THR:CA	1.91	0.82
1:A:432:GLU:HG2	1:A:433:GLU:HG3	1.61	0.80
1:A:449:VAL:HG22	1:A:451:SER:H	1.47	0.80
1:A:136:GLN:NE2	1:A:148:THR:HB	2.04	0.73
1:A:403:TRP:O	1:A:426:LEU:CD1	2.34	0.72
1:A:136:GLN:HE22	1:A:148:THR:CB	2.04	0.69
1:A:196:GLY:HA3	1:A:201:ALA:HA	1.75	0.68
1:A:195:SER:O	1:A:202:VAL:N	2.25	0.68
1:A:406:TYR:HB2	1:A:425:GLU:OE2	1.96	0.66
1:A:300:ARG:HH22	1:A:349:VAL:HG23	1.61	0.65
1:A:219:ARG:NH2	1:A:251:SER:HB2	2.11	0.65
1:A:240:ILE:HG21	1:A:278:CYS:SG	2.37	0.64
1:A:298:SER:H	1:A:341:VAL:HG13	1.68	0.59
1:A:136:GLN:HG2	1:A:156:ARG:HE	1.69	0.58
1:A:196:GLY:CA	1:A:201:ALA:HA	2.34	0.57
1:A:375:GLU:OE1	1:A:377:ILE:HD11	2.04	0.57
1:A:102:LYS:HG3	1:A:444:ILE:HG22	1.86	0.57
1:A:349:VAL:HG12	1:A:371:ARG:NH1	2.19	0.57
1:A:201:ALA:HB3	1:A:223:LEU:HB3	1.87	0.56
1:A:299:ASN:OD1	1:A:341:VAL:HG12	2.04	0.56
1:A:190:LEU:HD13	1:A:260:GLY:HA2	1.86	0.56
1:A:366:LYS:HG2	1:A:375:GLU:OE2	2.05	0.56
1:A:91:LEU:HD22	1:A:420:PRO:HG3	1.88	0.56
1:A:142:ASP:OD1	1:A:143:LYS:N	2.38	0.56
1:A:126:PRO:HB2	1:A:127:LEU:HD22	1.89	0.54
1:A:107:ARG:HD2	1:A:460:ASP:O	2.08	0.54
1:A:325:ASN:OD1	1:A:371:ARG:HG3	2.07	0.53
1:A:366:LYS:HB3	1:A:400:ILE:HD12	1.90	0.53
1:A:199:SER:O	1:A:220:ASN:ND2	2.39	0.53
1:A:457:SER:O	1:A:459:PRO:HD3	2.09	0.52
1:A:93:PRO:O	1:A:450:ASN:ND2	2.38	0.52
1:A:468:ILE:O	1:A:469:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MET:HG2	1:A:173:PHE:HA	1.93	0.51
1:A:203:ALA:HB3	1:A:215:ILE:HG22	1.92	0.51
1:A:219:ARG:HB2	1:A:243:ASP:CG	2.31	0.51
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.11	0.50
1:A:430:ARG:HB3	1:A:431:PRO:HA	1.94	0.50
1:A:442:SER:OG	1:A:443:SER:N	2.44	0.50
1:A:118:ARG:NE	1:A:425:GLU:OE1	2.41	0.49
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.94	0.49
1:A:224:ARG:NH2	1:A:246:SER:OG	2.45	0.48
1:A:143:LYS:O	1:A:146:ASN:HB2	2.12	0.48
1:A:196:GLY:C	1:A:201:ALA:HA	2.34	0.48
1:A:289:CYS:HB2	1:A:303:VAL:HG13	1.95	0.48
1:A:95:SER:OG	1:A:450:ASN:HA	2.15	0.47
1:A:287:ILE:HD12	1:A:287:ILE:N	2.30	0.47
1:A:201:ALA:N	1:A:217:SER:OG	2.49	0.46
1:A:253:LYS:HG2	1:A:267:GLU:HA	1.96	0.46
1:A:378:TRP:HB3	1:A:392:ILE:HB	1.97	0.46
1:A:134:LEU:O	1:A:156:ARG:NH2	2.49	0.46
1:A:306:ASN:ND2	1:A:311:GLU:HB2	2.32	0.44
1:A:327:ARG:HH12	1:A:365:THR:HB	1.82	0.44
1:A:404:SER:HA	1:A:426:LEU:CD1	2.40	0.44
1:A:149:ILE:HD11	1:A:431:PRO:HG3	2.00	0.43
1:A:292:ARG:HH21	1:A:348:GLY:N	2.16	0.43
2:B:2:NAG:H4	2:B:3:MAN:H5	2.01	0.43
1:A:320:GLY:HA3	1:A:331:LYS:O	2.19	0.42
1:A:355:LYS:HE2	1:A:383:TRP:CD1	2.53	0.42
1:A:107:ARG:HG2	1:A:462:ALA:HB2	2.01	0.41
1:A:372:LYS:HB3	1:A:400:ILE:O	2.19	0.41
1:A:127:LEU:HD13	1:A:127:LEU:HA	1.85	0.41
1:A:419:ARG:HA	1:A:420:PRO:HD3	1.89	0.41
1:A:151:ASP:O	1:A:156:ARG:HD2	2.21	0.41
1:A:312:TYR:HD1	1:A:312:TYR:H	1.66	0.41
1:A:312:TYR:CD1	1:A:312:TYR:N	2.89	0.41
1:A:122:ILE:HD13	1:A:163:ILE:HD11	2.02	0.41
1:A:273:TYR:CD1	1:A:316:TYR:HE1	2.38	0.41
1:A:314:MET:HE3	1:A:314:MET:HB3	1.77	0.40
1:A:289:CYS:HB2	1:A:303:VAL:CG1	2.50	0.40

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	385/393 (98%)	370 (96%)	13 (3%)	2 (0%)	29 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	GLY
1	A	321	VAL

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	334/339 (98%)	326 (98%)	8 (2%)	49 79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	SER
1	A	230	CYS
1	A	296	HIS
1	A	371	ARG
1	A	372	LYS
1	A	419	ARG
1	A	442	SER
1	A	443	SER

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

Mol	Chain	Res	Type
1	A	136	GLN
1	A	296	HIS

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)

4 monosaccharides 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	NAG	B	1	2,1	14,14,15	0.26	0	17,19,21	0.62	0
2	NAG	B	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.64	0
2	MAN	B	3	2	11,11,12	0.92	1 (9%)	15,15,17	0.88	1 (6%)
2	MAN	B	4	2	11,11,12	1.03	1 (9%)	15,15,17	0.84	0

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	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.56	1.39	1.43
2	B	4	MAN	O5-C1	-2.33	1.40	1.43
2	B	3	MAN	C4-C3	2.08	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	MAN	O2-C2-C3	-2.17	105.79	110.14

There are no chirality outliers.

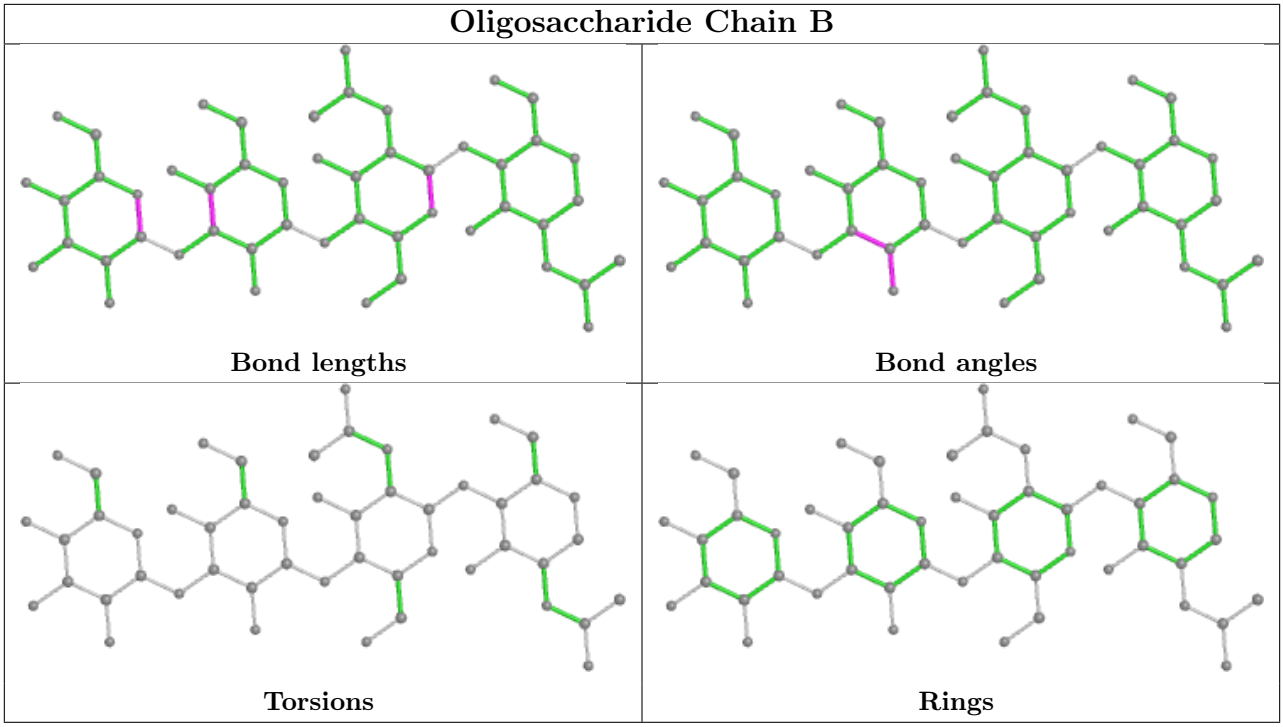
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	MAN	1	0
2	B	2	NAG	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 oligosaccharide.



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	NAG	A	501	1	14,14,15	0.61	0	17,19,21	0.95	0

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
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

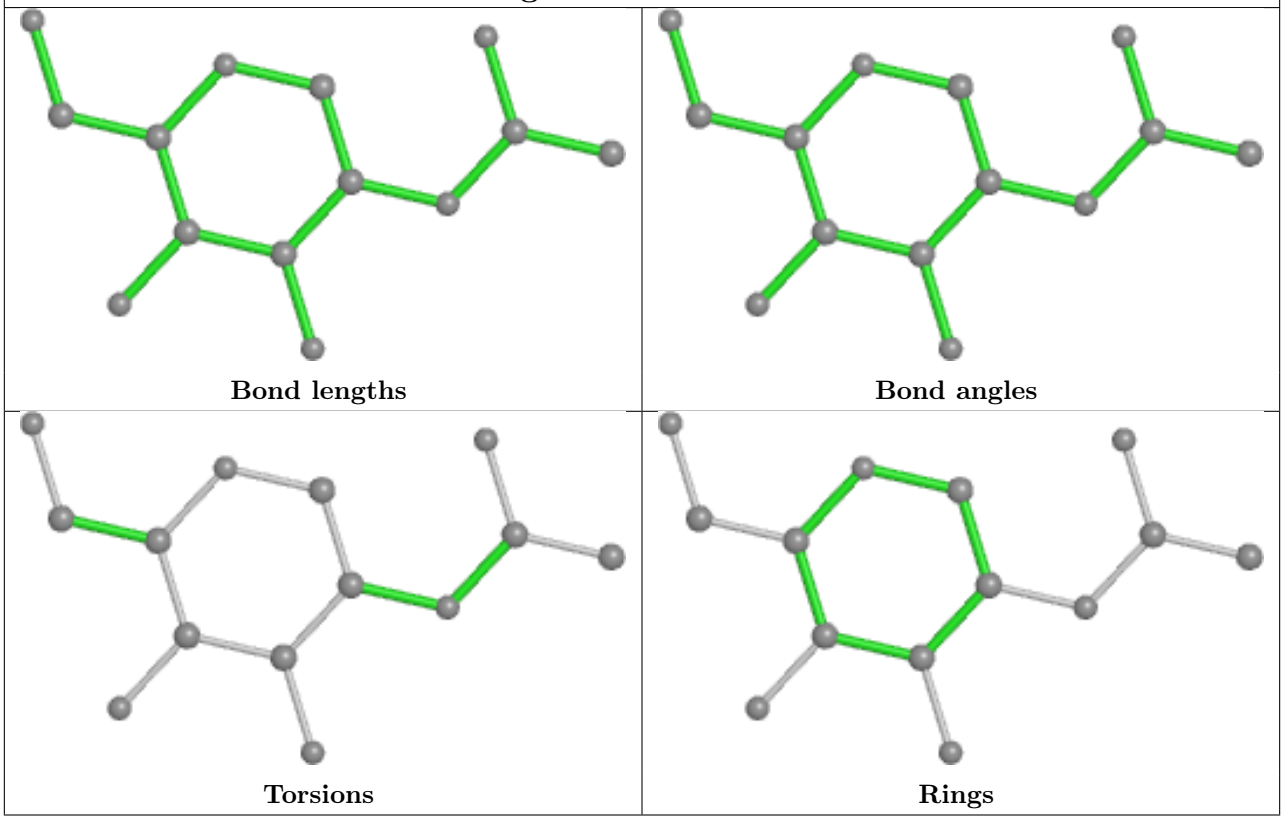
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 NAG 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	387/393 (98%)	2.17	206 (53%)	0	0	23, 34, 45, 77	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	9.4
1	A	254	ILE	5.5
1	A	192	ILE	5.3
1	A	312	TYR	5.3
1	A	193	GLY	5.2
1	A	97	TRP	5.1
1	A	441	GLY	5.1
1	A	181	SER	5.1
1	A	82	SER	4.9
1	A	268	MET	4.7
1	A	272	ASN	4.6
1	A	464	LEU	4.5
1	A	351	GLY	4.4
1	A	455	GLY	4.4
1	A	353	SER	4.2
1	A	291	CYS	4.1
1	A	131	THR	4.0
1	A	273	TYR	4.0
1	A	215	ILE	3.9
1	A	322	PHE	3.9
1	A	87	GLY	3.9
1	A	157	THR	3.9
1	A	191	THR	3.8
1	A	456	TRP	3.8
1	A	101	SER	3.8
1	A	405	GLY	3.8
1	A	175	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	3.7
1	A	196	GLY	3.7
1	A	344	ASN	3.7
1	A	461	GLY	3.7
1	A	253	LYS	3.7
1	A	99	ILE	3.6
1	A	100	TYR	3.6
1	A	205	LEU	3.6
1	A	460	ASP	3.6
1	A	336	CYS	3.6
1	A	265	SER	3.6
1	A	138	ALA	3.6
1	A	365	THR	3.6
1	A	310	LEU	3.5
1	A	122	ILE	3.5
1	A	349	VAL	3.4
1	A	447	CYS	3.4
1	A	410	PHE	3.4
1	A	432	GLU	3.3
1	A	266	VAL	3.3
1	A	202	VAL	3.3
1	A	153	SER	3.3
1	A	331	LYS	3.3
1	A	255	PHE	3.3
1	A	282	PRO	3.3
1	A	148	THR	3.3
1	A	195	SER	3.2
1	A	388	ASN	3.2
1	A	241	MET	3.2
1	A	281	TYR	3.2
1	A	404	SER	3.1
1	A	135	THR	3.1
1	A	354	PHE	3.1
1	A	171	SER	3.1
1	A	250	ALA	3.1
1	A	406	TYR	3.1
1	A	132	PHE	3.1
1	A	231	ALA	3.0
1	A	155	TYR	3.0
1	A	83	VAL	3.0
1	A	163	ILE	3.0
1	A	238	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	409	SER	2.9
1	A	124	CYS	2.9
1	A	440	SER	2.9
1	A	115	PHE	2.9
1	A	420	PRO	2.9
1	A	176	VAL	2.9
1	A	233	VAL	2.9
1	A	105	SER	2.8
1	A	328	PRO	2.8
1	A	275	TYR	2.8
1	A	203	ALA	2.8
1	A	172	ARG	2.8
1	A	414	GLY	2.8
1	A	375	GLU	2.8
1	A	242	THR	2.8
1	A	187	ILE	2.8
1	A	103	ASP	2.8
1	A	188	ASN	2.7
1	A	383	TRP	2.7
1	A	300	ARG	2.7
1	A	343	SER	2.7
1	A	413	THR	2.7
1	A	463	GLU	2.7
1	A	269	LYS	2.7
1	A	204	VAL	2.7
1	A	165	GLU	2.7
1	A	96	GLY	2.7
1	A	342	SER	2.7
1	A	448	GLY	2.7
1	A	110	SER	2.7
1	A	168	SER	2.7
1	A	209	GLY	2.7
1	A	374	PHE	2.7
1	A	223	LEU	2.7
1	A	321	VAL	2.6
1	A	86	ALA	2.6
1	A	118	ARG	2.6
1	A	347	ASN	2.6
1	A	167	PRO	2.6
1	A	121	PHE	2.6
1	A	427	ILE	2.6
1	A	421	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	445	SER	2.6
1	A	296	HIS	2.6
1	A	94	VAL	2.6
1	A	93	PRO	2.6
1	A	262	ILE	2.6
1	A	179	SER	2.6
1	A	252	TYR	2.6
1	A	403	TRP	2.6
1	A	108	ILE	2.5
1	A	278	CYS	2.5
1	A	104	ASN	2.5
1	A	197	PRO	2.5
1	A	443	SER	2.5
1	A	126	PRO	2.5
1	A	267	GLU	2.5
1	A	423	TRP	2.5
1	A	95	SER	2.5
1	A	228	SER	2.5
1	A	428	ARG	2.5
1	A	140	LEU	2.5
1	A	213	ASP	2.5
1	A	454	VAL	2.5
1	A	293	ASP	2.5
1	A	194	ILE	2.5
1	A	134	LEU	2.5
1	A	164	GLY	2.5
1	A	391	SER	2.4
1	A	442	SER	2.4
1	A	397	ILE	2.4
1	A	426	LEU	2.4
1	A	367	SER	2.4
1	A	302	TRP	2.4
1	A	378	TRP	2.4
1	A	123	SER	2.4
1	A	177	ALA	2.4
1	A	106	VAL	2.4
1	A	380	PRO	2.4
1	A	271	PRO	2.3
1	A	453	THR	2.3
1	A	407	SER	2.3
1	A	435	ASN	2.3
1	A	225	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	384	THR	2.3
1	A	335	SER	2.3
1	A	305	PHE	2.3
1	A	390	PHE	2.3
1	A	444	ILE	2.3
1	A	329	ASN	2.3
1	A	346	ALA	2.3
1	A	287	ILE	2.3
1	A	102	LYS	2.3
1	A	154	PRO	2.3
1	A	170	ASN	2.3
1	A	295	TRP	2.3
1	A	438	TRP	2.3
1	A	270	ALA	2.3
1	A	345	GLY	2.3
1	A	206	LYS	2.3
1	A	290	VAL	2.3
1	A	458	TRP	2.3
1	A	315	GLY	2.3
1	A	226	GLN	2.3
1	A	129	CYS	2.2
1	A	169(A)	TYR	2.2
1	A	198	ASP	2.2
1	A	190	LEU	2.2
1	A	133	PHE	2.2
1	A	240	ILE	2.2
1	A	314	MET	2.2
1	A	236	SER	2.2
1	A	92	CYS	2.2
1	A	127	LEU	2.2
1	A	356	TYR	2.2
1	A	259	LYS	2.2
1	A	274	HIS	2.2
1	A	309	ASN	2.1
1	A	169	PRO	2.1
1	A	366	LYS	2.1
1	A	419	ARG	2.1
1	A	422	PHE	2.1
1	A	180	ALA	2.1
1	A	358	ASN	2.1
1	A	369	SER	2.1
1	A	446	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	MET	2.1
1	A	466	PHE	2.1
1	A	313	GLN	2.1
1	A	160	SER	2.1
1	A	216	LYS	2.1
1	A	394	LYS	2.1
1	A	348	GLY	2.1
1	A	452	ASP	2.0
1	A	412(C)	GLU	2.0
1	A	400	ILE	2.0
1	A	222	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

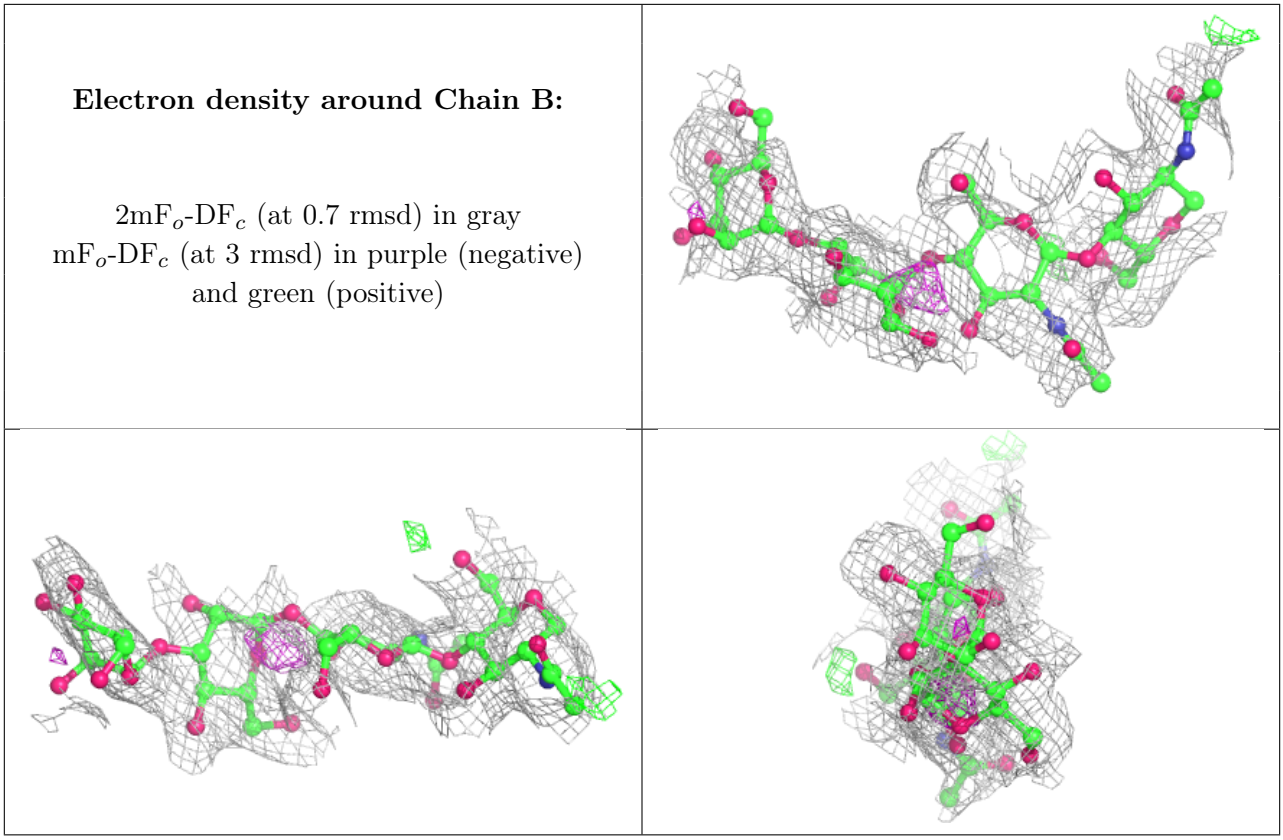
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

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	MAN	B	3	11/12	0.27	0.45	53,62,68,68	0
2	NAG	B	2	14/15	0.51	0.38	54,59,62,63	0
2	NAG	B	1	14/15	0.55	0.23	37,44,49,51	0
2	MAN	B	4	11/12	0.55	0.56	54,66,74,77	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

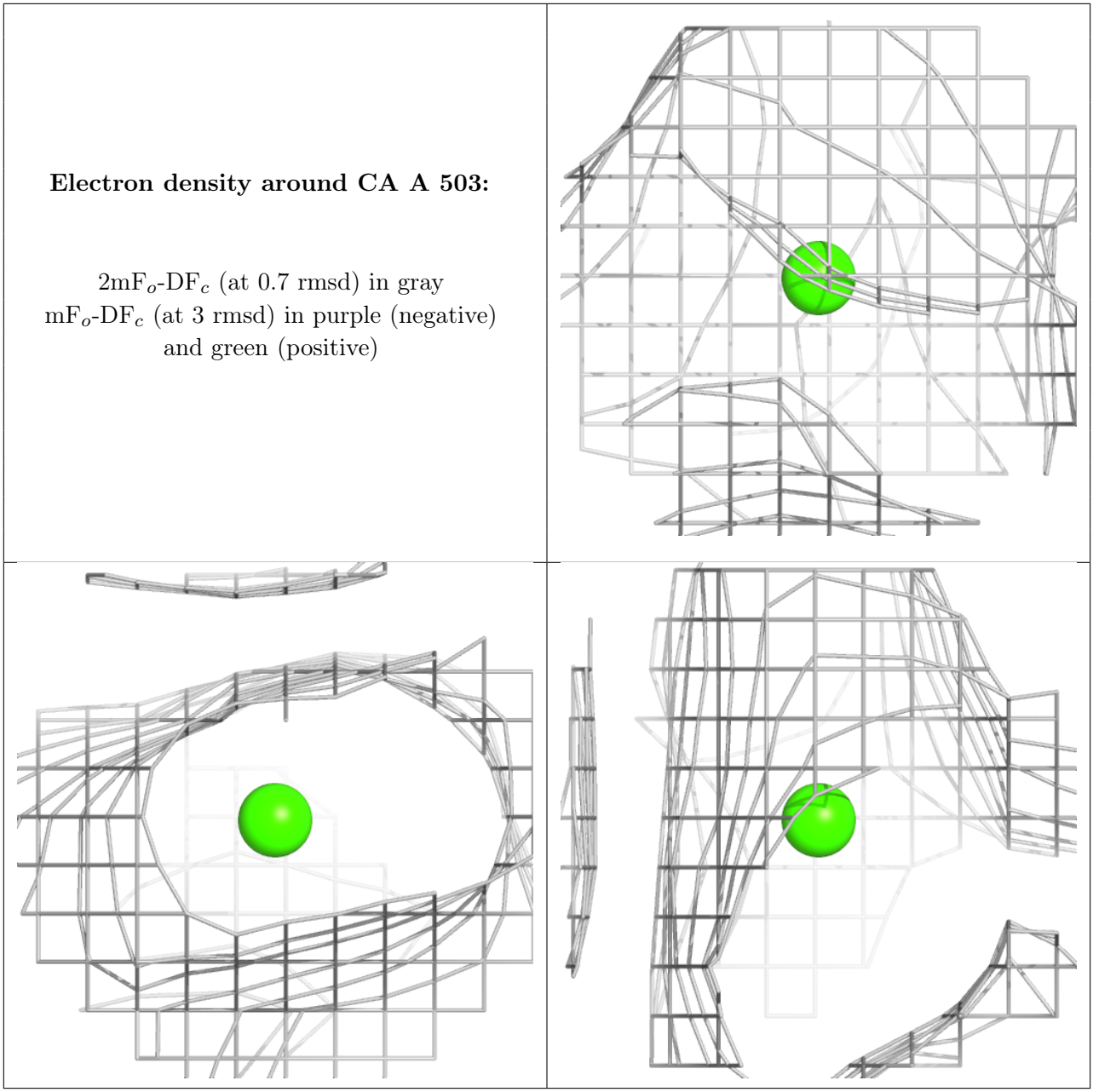
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	CA	A	503	1/1	0.55	0.24	31,31,31,31	0
3	NAG	A	501	14/15	0.59	0.29	54,64,67,67	0
4	CA	A	502	1/1	0.83	0.10	24,24,24,24	0
4	CA	A	504	1/1	0.90	0.49	41,41,41,41	1

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.

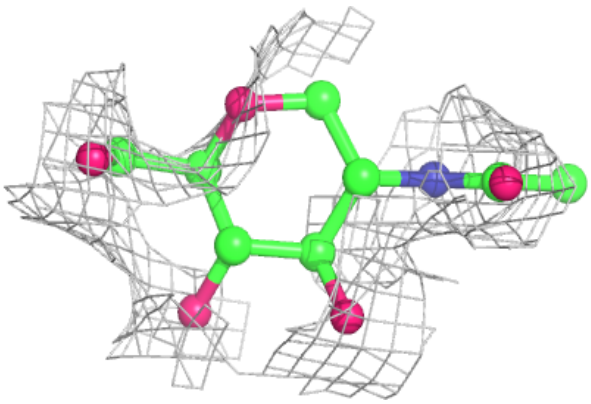
Electron density around CA A 503:

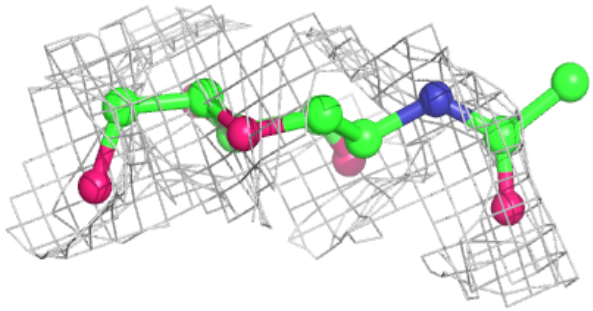
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAG A 501:

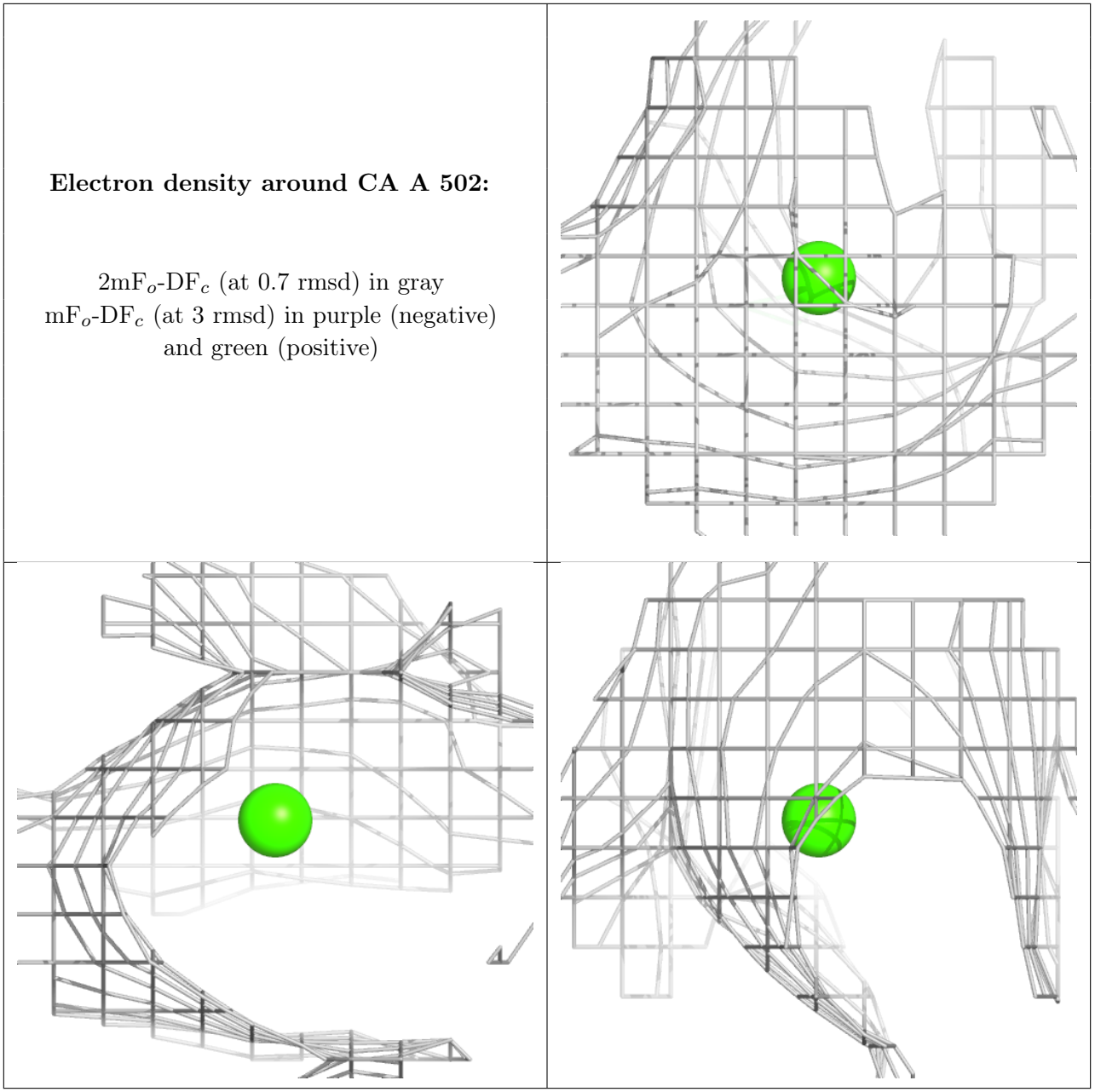
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





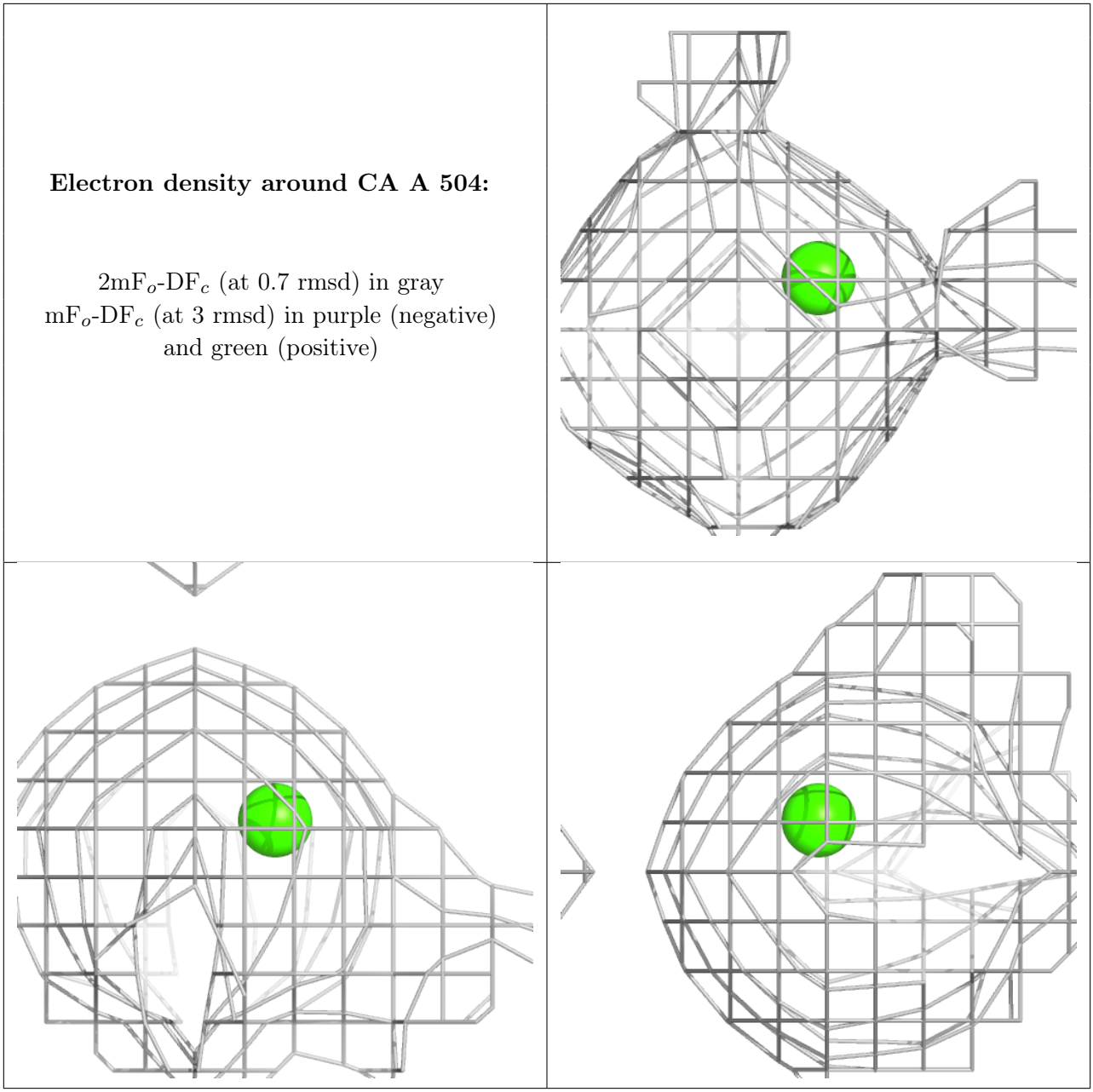
Electron density around CA A 502:

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



Electron density around CA A 504:

$2mF_o$-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.