Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:10 PM EDT

PDB ID	:	1INW
Title	:	A SIALIC ACID DERIVED PHOSPHONATE ANALOG INHIBITS DIFFERENT STRAINS OF INFLUENZA VIRUS NEURAMINIDASE WITH DIFFERENT EFFICIENCIES
Authors	:	White, C.L.; Janakiraman, M.N.; Laver, W.G.; Philippon, C.; Vasella, A.; Air, G.M.; Luo, M.
Deposited on	:	1994-09-26
Resolution	:	2.40 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 (1)) were used in the production of this report:

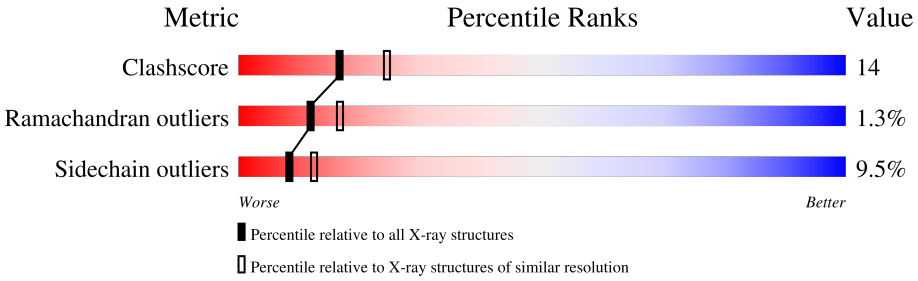
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	388	66% 29% .
2	B	5	100%

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 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4246 atoms, of which 1013 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.

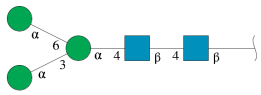
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	388	3745	1866	723	545	588	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

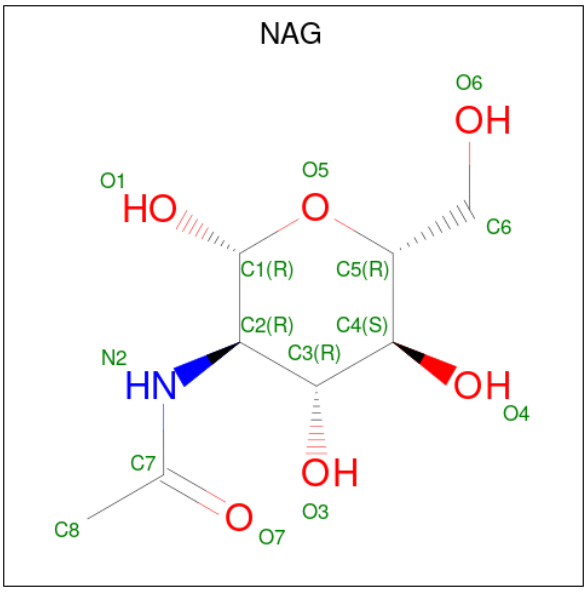
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



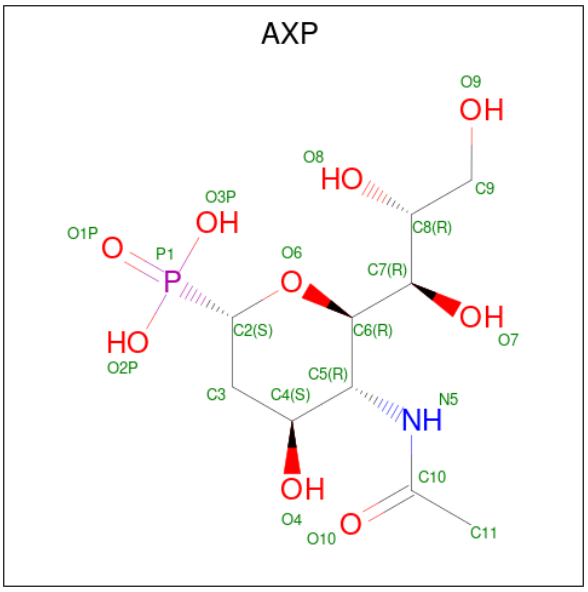
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	5	118	34	57	2	25	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is (1S)-4-acetamido-1,5-anhydro-2,4-dideoxy-1-phosphono-D-glycero-D-galacto-octitol (three-letter code: AXP) (formula: $C_{10}H_{20}NO_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			40	10	19	1	9	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

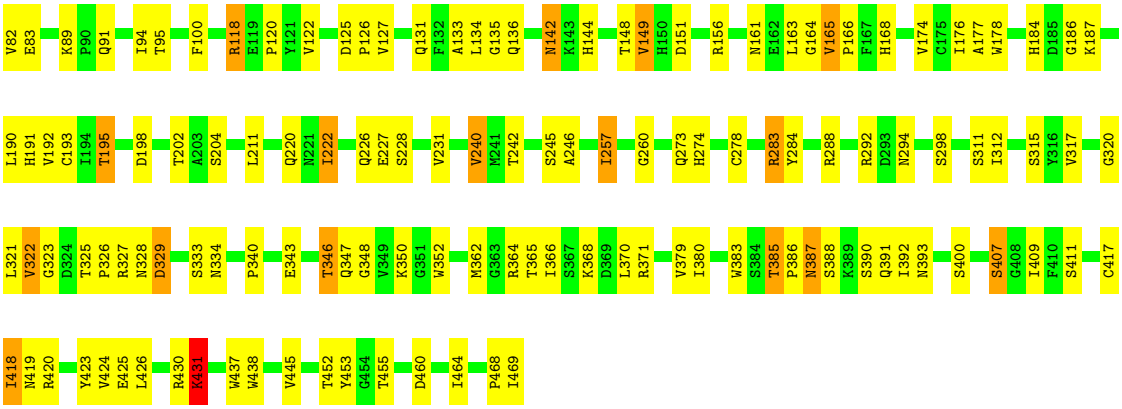
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	86	Total	H	O	7	0
			258	172	86		

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.

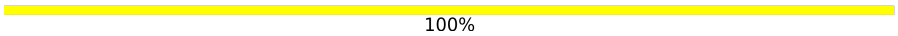
• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain A:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	122.08Å 141.67Å 141.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 21.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 65.4 (21.05-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.41Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , (Not available) 0.518 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 54.4	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	0.45	EDS
Total number of atoms	4246	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: MAN, NAG, AXP, CA

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	0.71	0/3092	0.89	3/4194 (0.1%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	431	LYS	N-CA-C	-5.76	95.45	111.00
1	A	292	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	323	GLY	N-CA-C	5.02	125.65	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	TYR	Sidechain

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	3022	723	2852	87	0
2	B	61	57	52	0	0
3	A	42	42	39	0	0
4	A	21	19	18	1	0
5	A	1	0	0	0	0
6	A	86	172	0	5	0
All	All	3233	1013	2961	87	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 14.

All (87) 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:431:LYS:HA	1:A:431:LYS:NZ	1.89	0.86
1:A:437:TRP:H	1:A:469:ILE:HG21	1.40	0.85
1:A:226:GLN:HE21	1:A:240:VAL:H	1.27	0.81
1:A:419:ASN:ND2	1:A:420:ARG:H	1.78	0.81
1:A:430:ARG:O	1:A:431:LYS:HB2	1.81	0.79
1:A:419:ASN:HD22	1:A:420:ARG:H	1.27	0.78
1:A:431:LYS:HA	1:A:431:LYS:HZ3	1.47	0.78
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.71	0.72
1:A:184:HIS:CD2	1:A:186:GLY:H	2.10	0.70
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.76	0.68
1:A:274:HIS:HD2	1:A:294:ASN:H	1.43	0.67
1:A:135:GLY:O	1:A:156:ARG:HD2	1.96	0.66
1:A:184:HIS:HD2	1:A:186:GLY:H	1.43	0.64
1:A:142:ASN:HD22	1:A:144:HIS:H	1.46	0.64
1:A:419:ASN:ND2	1:A:420:ARG:N	2.46	0.64
1:A:317:VAL:HG23	6:A:549:HOH:O	1.99	0.63
1:A:380:ILE:HB	1:A:390:SER:HB2	1.81	0.62
1:A:131:GLN:HE21	1:A:163:LEU:HD12	1.63	0.62
1:A:437:TRP:N	1:A:469:ILE:HG21	2.13	0.61
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.84	0.60
1:A:198:ASP:HB3	1:A:222:ILE:HG12	1.85	0.59
1:A:149:VAL:HG22	6:A:509:HOH:O	2.02	0.59
1:A:328:ASN:O	1:A:329:ASP:HB2	2.01	0.59
1:A:409:ILE:HD11	1:A:420:ARG:HD3	1.86	0.58
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.44	0.57
1:A:118:ARG:HD2	1:A:425:GLU:OE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:HD22	1:A:420:ARG:N	2.02	0.56
1:A:131:GLN:NE2	1:A:164:GLY:H	2.04	0.56
1:A:288:ARG:NH1	1:A:383:TRP:CZ2	2.73	0.55
1:A:437:TRP:HD1	1:A:469:ILE:CG2	2.20	0.55
1:A:166:PRO:O	1:A:168:HIS:HD2	1.89	0.55
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.37	0.54
1:A:95:THR:HG22	1:A:453:TYR:HE2	1.71	0.54
1:A:246:ALA:O	1:A:274:HIS:NE2	2.41	0.53
1:A:333:SER:HA	1:A:343:GLU:OE1	2.08	0.53
1:A:326:PRO:HA	1:A:368:LYS:O	2.09	0.52
1:A:468:PRO:O	1:A:469:ILE:HB	2.10	0.51
1:A:437:TRP:H	1:A:469:ILE:CG2	2.20	0.51
1:A:346:THR:O	1:A:347:GLN:HB2	2.11	0.51
1:A:391:GLN:HG2	1:A:392:ILE:N	2.27	0.49
1:A:228:SER:HB3	1:A:350:LYS:CE	2.42	0.49
1:A:347:GLN:HB3	6:A:573:HOH:O	2.12	0.49
1:A:190:LEU:HD11	1:A:257:ILE:HD11	1.95	0.48
1:A:366:ILE:HG21	1:A:400:SER:HB3	1.94	0.48
1:A:136:GLN:OE1	1:A:156:ARG:HD3	2.14	0.48
1:A:168:HIS:HB2	6:A:567:HOH:O	2.13	0.48
1:A:328:ASN:HB2	6:A:548:HOH:O	2.14	0.48
1:A:325:THR:O	1:A:348:GLY:HA2	2.14	0.48
1:A:321:LEU:HD12	1:A:379:VAL:HG22	1.94	0.47
1:A:320:GLY:HA3	1:A:387:ASN:HD22	1.79	0.47
1:A:385:THR:HA	1:A:386:PRO:HD2	1.81	0.46
1:A:174:VAL:HG11	1:A:191:HIS:CD2	2.51	0.46
1:A:283:ARG:O	1:A:284:TYR:C	2.53	0.46
1:A:418:ILE:HD11	1:A:420:ARG:NH2	2.31	0.45
1:A:245:SER:O	1:A:274:HIS:HE1	2.00	0.45
1:A:311:SER:C	1:A:312:ILE:HD13	2.37	0.45
1:A:392:ILE:HG12	1:A:393:ASN:N	2.30	0.45
1:A:198:ASP:HB3	1:A:222:ILE:CG1	2.46	0.45
1:A:365:THR:HG21	1:A:371:ARG:HA	1.99	0.45
1:A:321:LEU:O	1:A:322:VAL:HB	2.17	0.45
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.82	0.44
1:A:184:HIS:HD2	1:A:186:GLY:N	2.13	0.44
1:A:136:GLN:CD	1:A:156:ARG:HD3	2.39	0.43
1:A:452:THR:CG2	1:A:453:TYR:N	2.81	0.43
1:A:151:ASP:HB3	4:A:500:AXP:O4	2.19	0.43
1:A:362:MET:CE	1:A:364:ARG:HD3	2.49	0.43
1:A:82:VAL:O	1:A:187:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:NE2	1:A:240:VAL:H	2.04	0.43
1:A:120:PRO:HA	1:A:133:ALA:HA	2.00	0.42
1:A:464:ILE:HD12	1:A:464:ILE:HA	1.86	0.42
1:A:438:TRP:HD1	1:A:469:ILE:HD12	1.84	0.42
1:A:89:LYS:HB2	1:A:418:ILE:CG2	2.50	0.42
1:A:204:SER:HB3	1:A:211:LEU:HD11	2.02	0.42
1:A:298:SER:O	1:A:322:VAL:HG13	2.19	0.42
1:A:89:LYS:HB3	1:A:417:CYS:HA	2.01	0.42
1:A:176:ILE:HG22	1:A:195:THR:HG21	2.02	0.42
1:A:91:GLN:HG3	1:A:420:ARG:NH1	2.35	0.41
1:A:100:PHE:HB3	1:A:445:VAL:O	2.20	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.64	0.41
1:A:125:ASP:HB2	1:A:126:PRO:HD2	2.02	0.41
1:A:174:VAL:O	1:A:174:VAL:HG12	2.20	0.41
1:A:257:ILE:HD11	1:A:260:GLY:HA2	2.03	0.41
1:A:226:GLN:O	1:A:227:GLU:HB2	2.21	0.41
1:A:426:LEU:HD13	1:A:460:ASP:N	2.35	0.41
1:A:165:VAL:HA	1:A:166:PRO:HD2	1.94	0.41
1:A:100:PHE:HD2	1:A:445:VAL:CG2	2.34	0.40
1:A:352:TRP:HD1	1:A:407:SER:HG	1.69	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	386/388 (100%)	342 (89%)	39 (10%)	5 (1%)	12 17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP

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Mol	Chain	Res	Type
1	A	431	LYS
1	A	220	GLN
1	A	322	VAL
1	A	222	ILE

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	338/338 (100%)	306 (90%)	32 (10%)	8 12

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	94	ILE
1	A	118	ARG
1	A	122	VAL
1	A	127	VAL
1	A	134	LEU
1	A	142	ASN
1	A	148	THR
1	A	149	VAL
1	A	161	ASN
1	A	165	VAL
1	A	178	TRP
1	A	192	VAL
1	A	195	THR
1	A	202	THR
1	A	231	VAL
1	A	240	VAL
1	A	242	THR
1	A	257	ILE
1	A	283	ARG
1	A	315	SER
1	A	327	ARG

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Mol	Chain	Res	Type
1	A	346	THR
1	A	370	LEU
1	A	385	THR
1	A	387	ASN
1	A	388	SER
1	A	407	SER
1	A	418	ILE
1	A	424	VAL
1	A	431	LYS
1	A	455	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	142	ASN
1	A	168	HIS
1	A	184	HIS
1	A	226	GLN
1	A	274	HIS
1	A	334	ASN
1	A	356	ASN
1	A	358	ASN
1	A	387	ASN
1	A	393	ASN
1	A	419	ASN

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)

5 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	1.06	0	17,19,21	1.31	2 (11%)
2	NAG	B	2	2	14,14,15	0.97	1 (7%)	17,19,21	1.14	1 (5%)
2	MAN	B	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.27	2 (13%)
2	MAN	B	4	2	11,11,12	0.87	0	15,15,17	1.43	3 (20%)
2	MAN	B	5	2	11,11,12	0.84	1 (9%)	15,15,17	0.92	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	1/1/5/5	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	MAN	C4-C5	2.79	1.58	1.53
2	B	5	MAN	C4-C5	2.09	1.57	1.53
2	B	2	NAG	C4-C5	2.09	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-C2-N2	-2.66	105.95	110.49
2	B	4	MAN	C1-C2-C3	2.52	112.76	109.67
2	B	1	NAG	C1-O5-C5	2.46	115.52	112.19
2	B	3	MAN	O5-C1-C2	2.28	114.28	110.77
2	B	4	MAN	O2-C2-C1	2.28	113.81	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	O7-C7-C8	-2.18	118.00	122.06
2	B	3	MAN	C2-C3-C4	-2.08	107.29	110.89
2	B	4	MAN	O2-C2-C3	-2.05	106.02	110.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3	MAN	C1

All (1) torsion outliers are listed below:

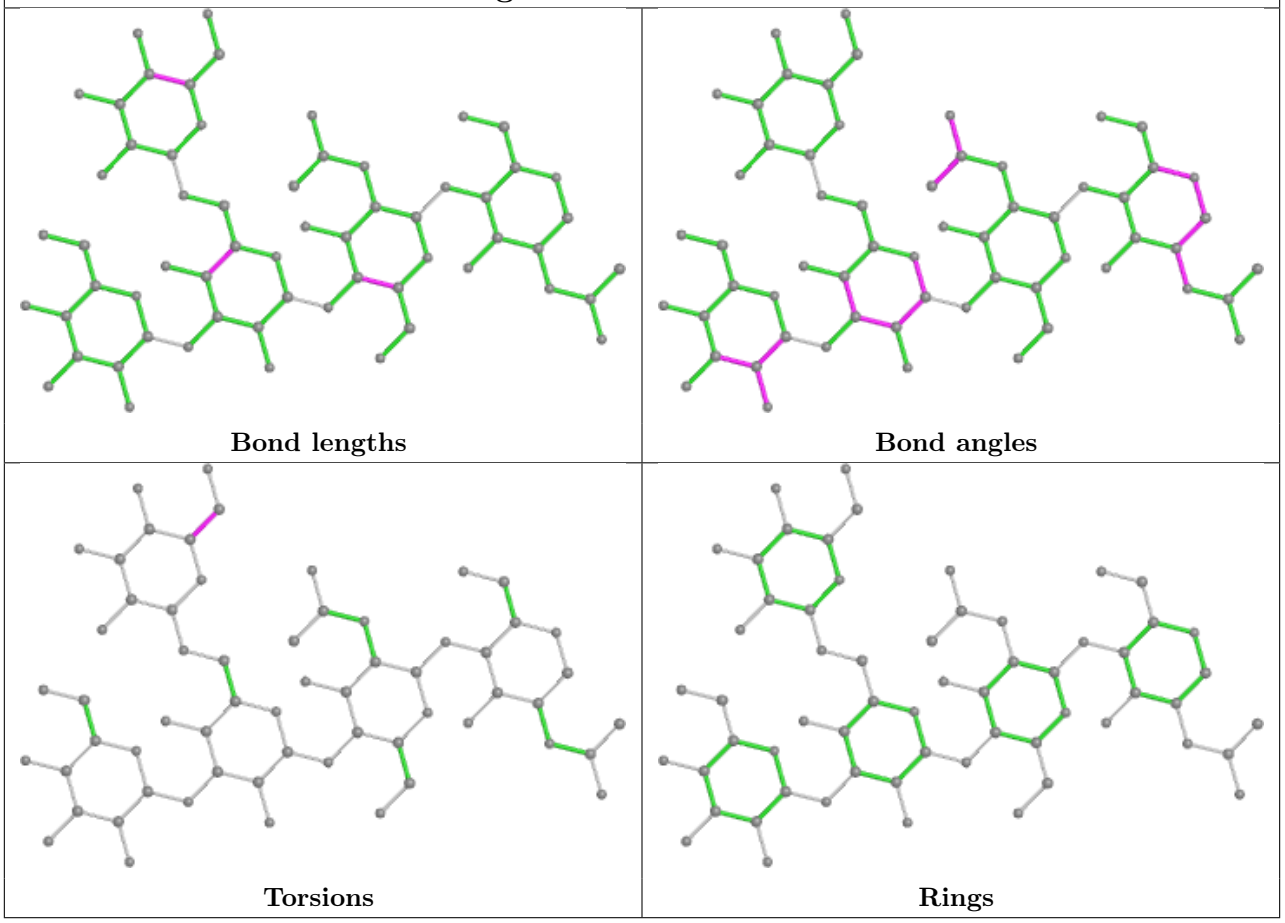
Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-C5-C6-O6

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 oligosaccharide.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	477(A)	1	14,14,15	0.95	1 (7%)	17,19,21	1.98	2 (11%)
3	NAG	A	470(A)	1	14,14,15	1.02	1 (7%)	17,19,21	1.39	1 (5%)
3	NAG	A	471(A)	1	14,14,15	1.13	2 (14%)	17,19,21	1.67	4 (23%)
4	AXP	A	500	-	18,21,21	1.90	5 (27%)	22,31,31	2.17	8 (36%)

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	477(A)	1	-	0/6/23/26	0/1/1/1
3	NAG	A	470(A)	1	-	2/6/23/26	0/1/1/1
3	NAG	A	471(A)	1	-	2/6/23/26	0/1/1/1
4	AXP	A	500	-	-	2/14/36/36	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	AXP	P1-O2P	-4.37	1.47	1.54
4	A	500	AXP	P1-O3P	-3.26	1.49	1.54
4	A	500	AXP	C8-C7	-3.08	1.47	1.53
3	A	471(A)	NAG	C2-N2	-2.57	1.41	1.46
3	A	477(A)	NAG	C1-C2	2.52	1.56	1.52
3	A	470(A)	NAG	C3-C2	-2.26	1.47	1.52
4	A	500	AXP	C6-C5	2.21	1.56	1.53
3	A	471(A)	NAG	C1-C2	-2.13	1.49	1.52
4	A	500	AXP	O6-C6	2.01	1.47	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	477(A)	NAG	C1-O5-C5	5.83	120.09	112.19
4	A	500	AXP	O3P-P1-O2P	-5.00	94.19	107.64
4	A	500	AXP	O3P-P1-O1P	-4.83	101.31	113.45
3	A	471(A)	NAG	C1-O5-C5	4.49	118.28	112.19
3	A	470(A)	NAG	C1-O5-C5	4.36	118.11	112.19
4	A	500	AXP	C3-C4-C5	3.51	115.70	111.46
3	A	477(A)	NAG	C3-C4-C5	-3.39	104.20	110.24
4	A	500	AXP	O4-C4-C5	-3.04	102.78	109.77
4	A	500	AXP	O6-C2-C3	2.85	114.51	110.59
4	A	500	AXP	O7-C7-C6	-2.45	104.19	109.50
3	A	471(A)	NAG	C1-C2-N2	2.42	114.63	110.49
4	A	500	AXP	O8-C8-C7	-2.28	103.55	109.10
4	A	500	AXP	O1P-P1-C2	2.17	118.24	113.34
3	A	471(A)	NAG	O5-C1-C2	-2.13	107.93	111.29
3	A	471(A)	NAG	O4-C4-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	AXP	C7-C8-C9-O9
4	A	500	AXP	O8-C8-C9-O9
3	A	471(A)	NAG	O5-C5-C6-O6
3	A	471(A)	NAG	C4-C5-C6-O6
3	A	470(A)	NAG	O5-C5-C6-O6
3	A	470(A)	NAG	C4-C5-C6-O6

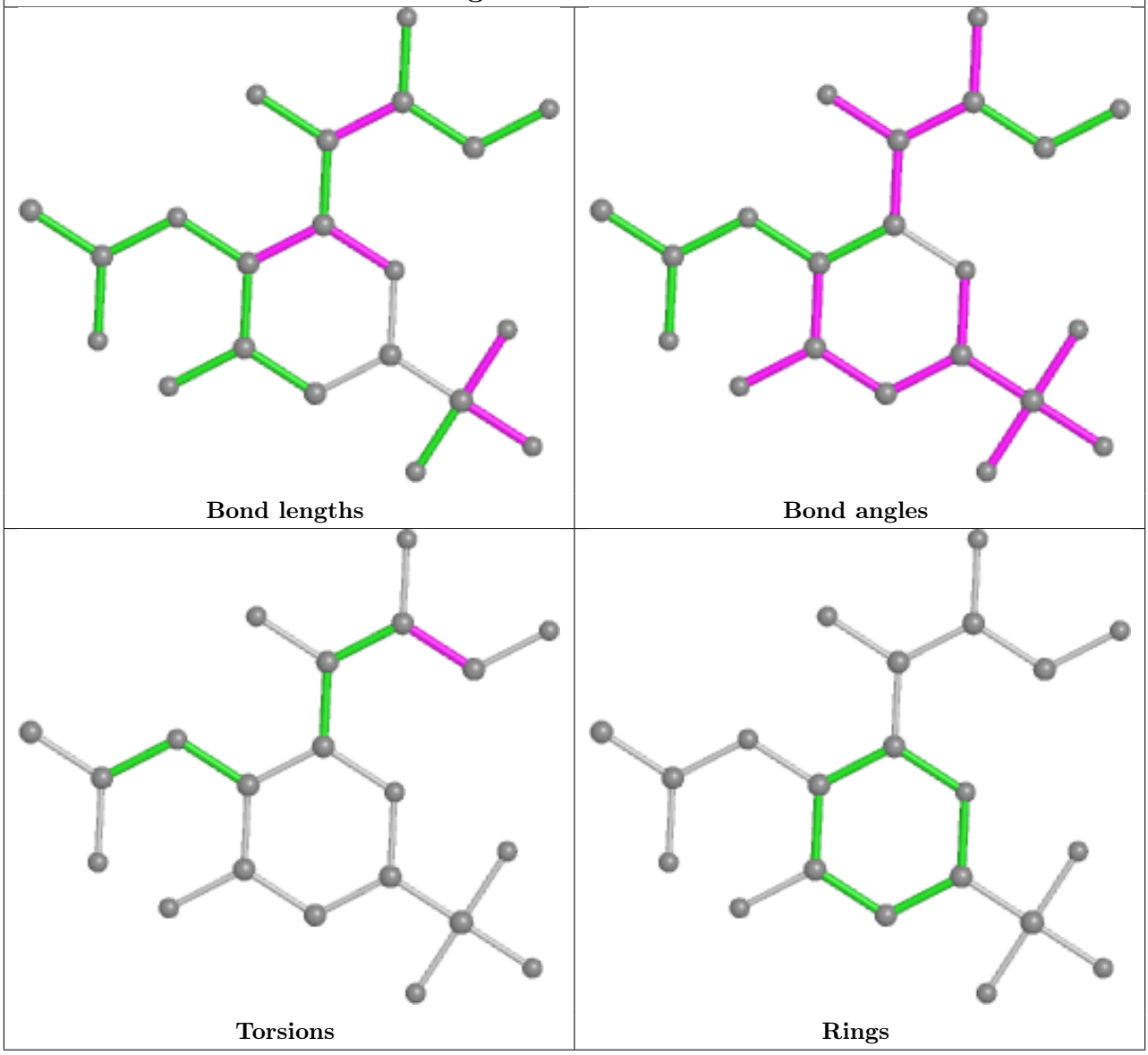
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	AXP	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 AXP A 500



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.

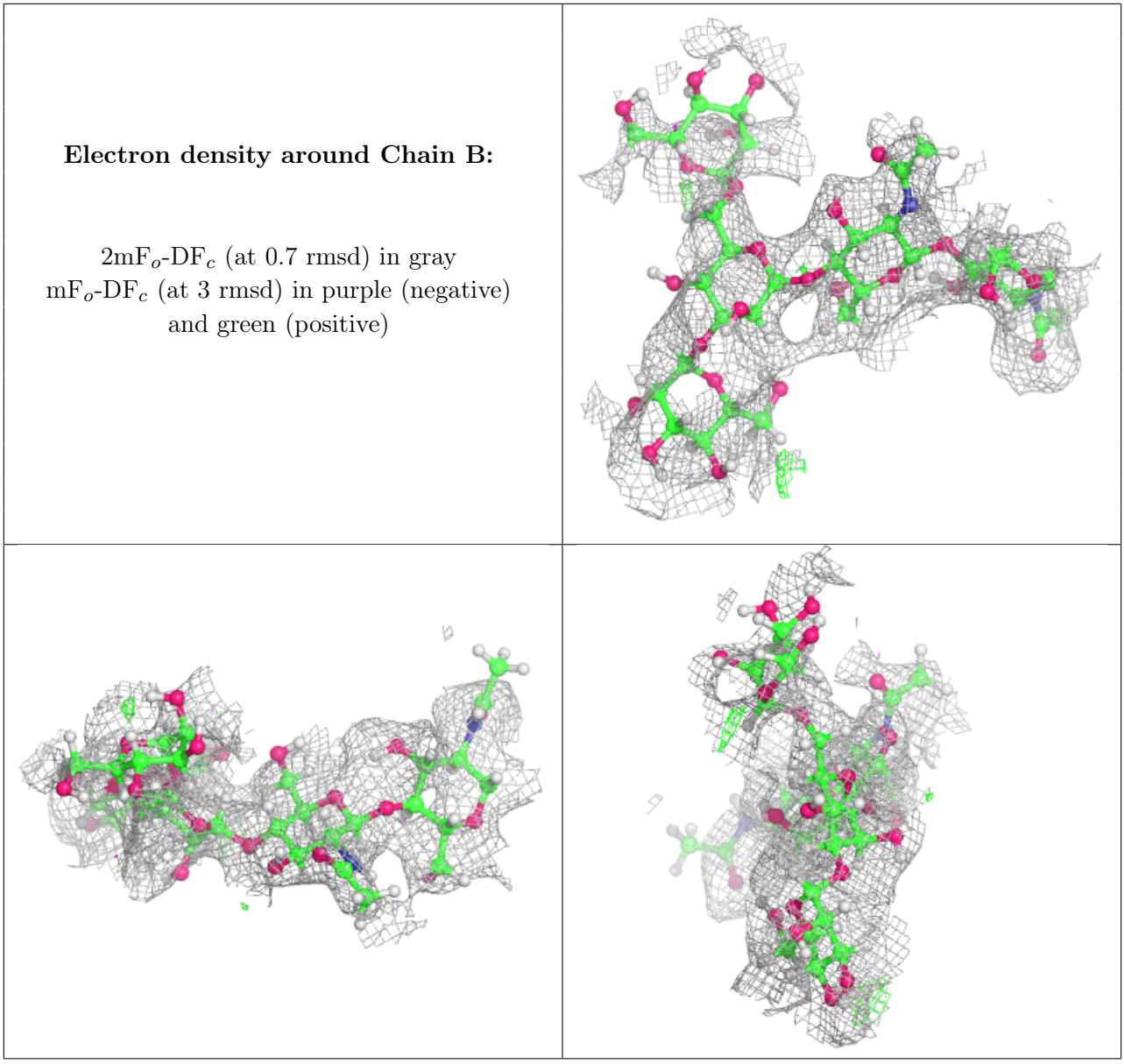
6.3 Carbohydrates

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

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.

Electron density around Chain B:

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



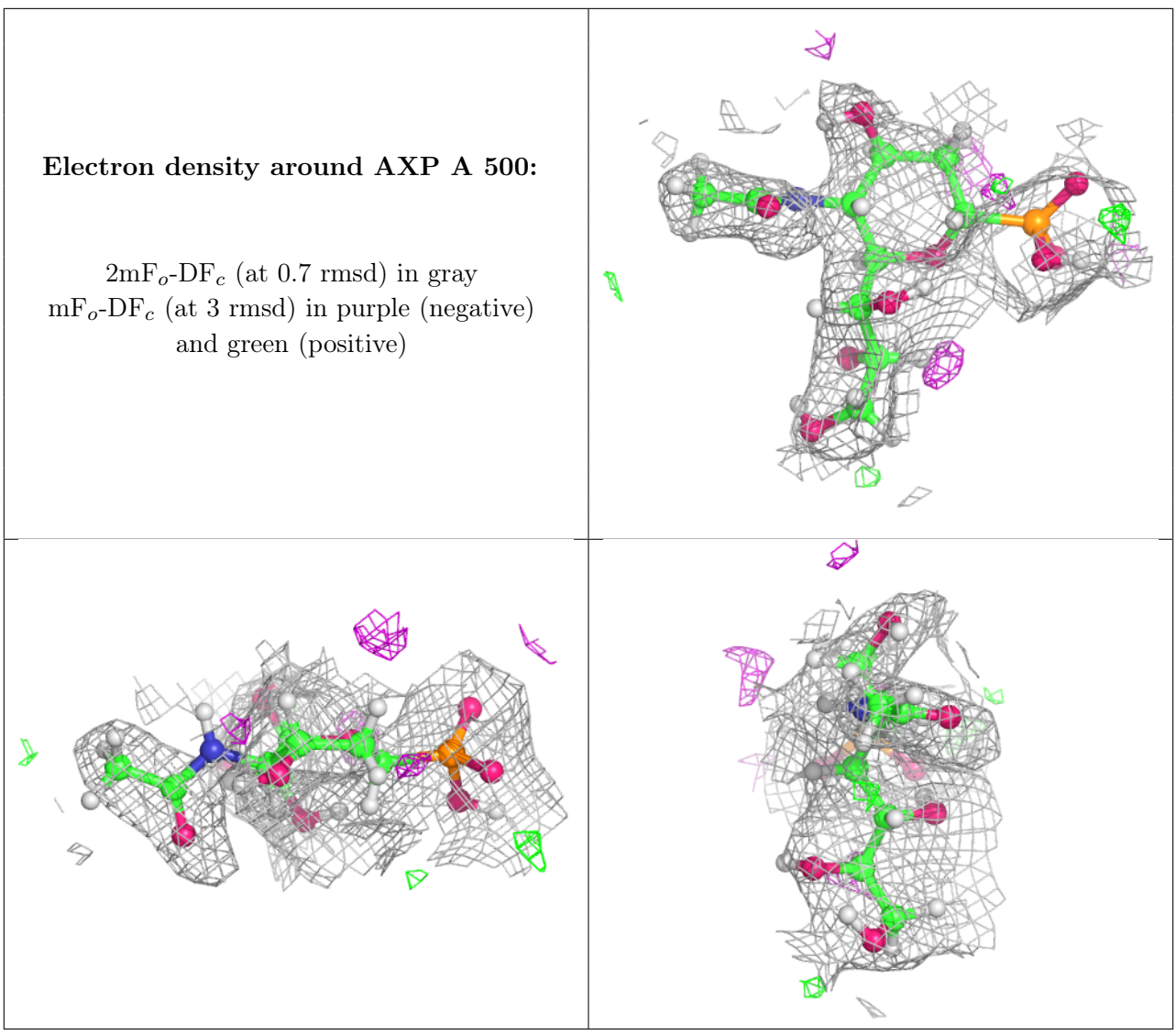
6.4 Ligands

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 AXP A 500:

$2mF_o$-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.