Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:10 AM BST

PDB ID	:	1OBB
Title	:	alpha-glucosidase A, AglA, from Thermotoga maritima in complex with maltose and NAD+
Authors	:	Lodge, J.A.; Maier, T.; Liebl, W.; Hoffmann, V.; Strater, N.
Deposited on	:	2003-01-29
Resolution	:	1.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

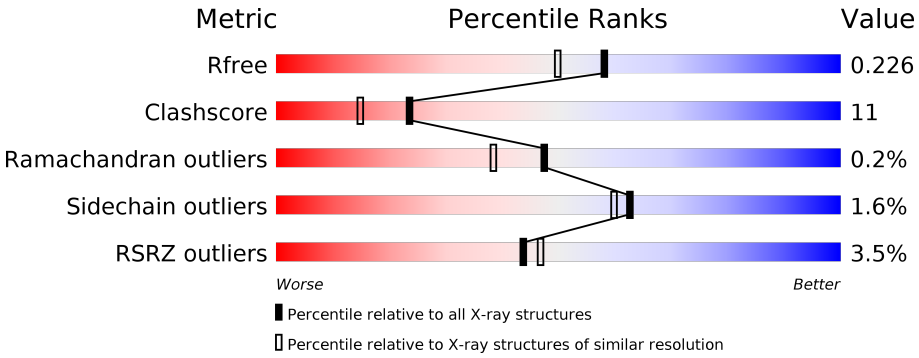
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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% 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	480	3% 84% 14%
1	B	480	4% 75% 24%
2	C	2	100%
2	D	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8523 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.

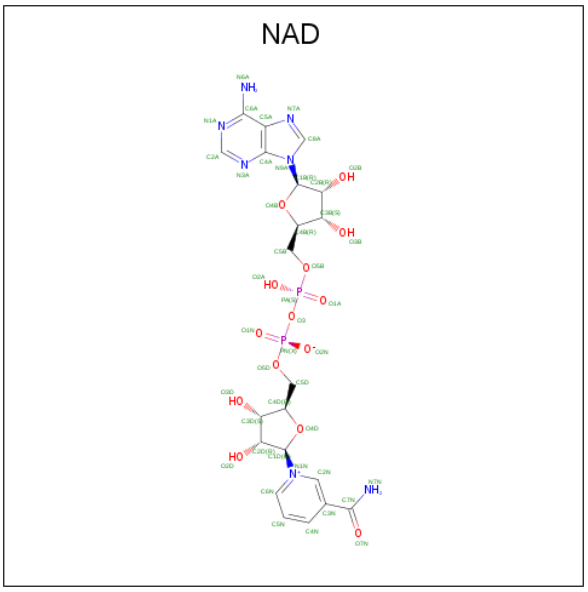
- Molecule 1 is a protein called ALPHA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	1	1
			3878	2491	652	722	13			
1	B	477	Total	C	N	O	S	0	1	1
			3865	2483	650	719	13			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

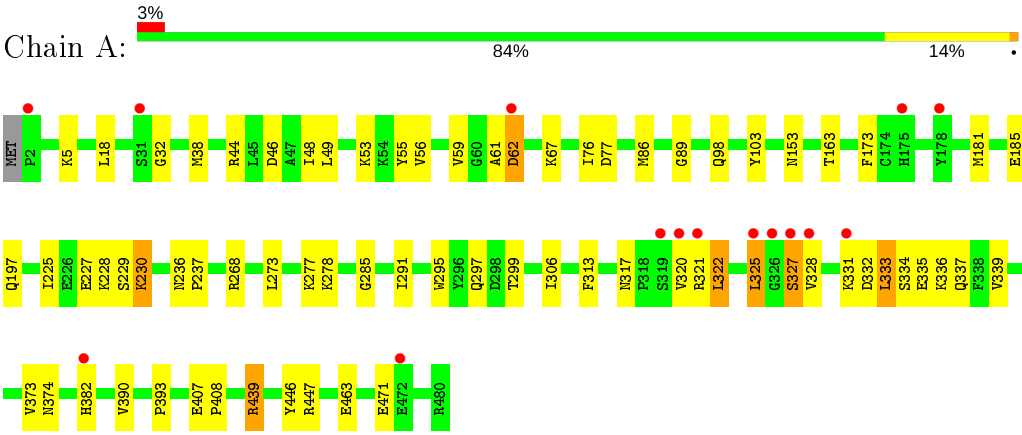
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	329	Total	O	0	0
			329	329		
4	B	317	Total	O	0	0
			317	317		

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.

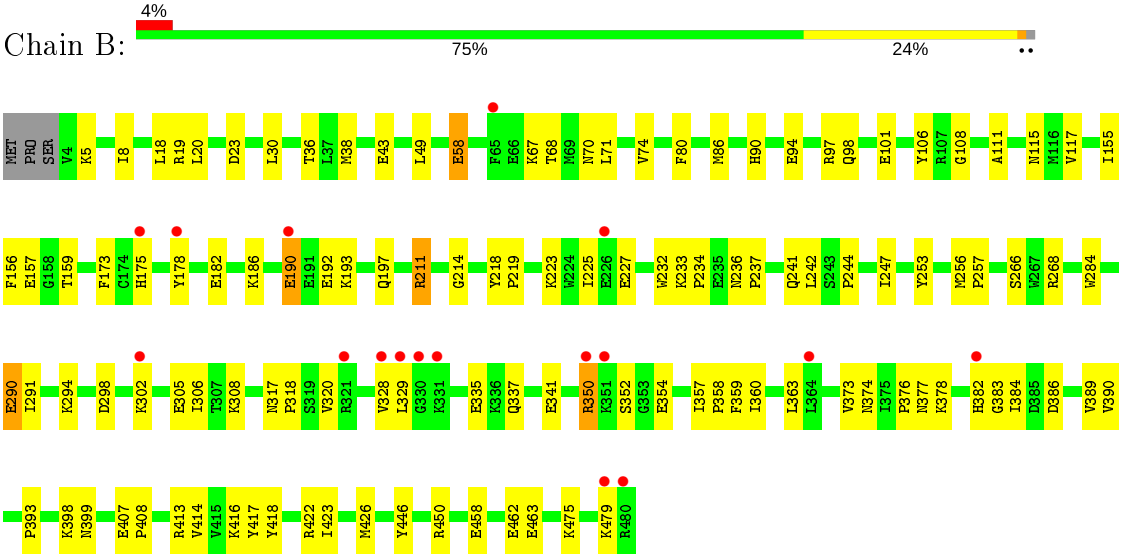
- Molecule 1: ALPHA-GLUCOSIDASE

Chain A:



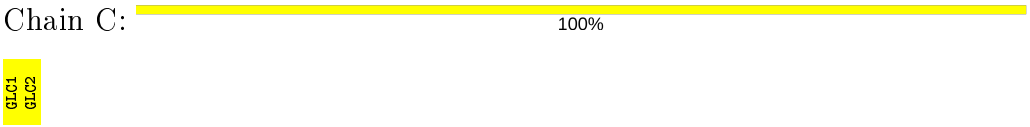
- Molecule 1: ALPHA-GLUCOSIDASE

Chain B:



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D: 100%

GLC1
GLC2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.00Å 85.70Å 83.60Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	17.65 – 1.90 17.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (17.65-1.90) 96.6 (17.64-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.235 0.188 , 0.226	Depositor DCC
R_{free} test set	2347 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8523	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4004e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CSD, GLC, NAD

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	0.61	2/3959 (0.1%)	0.73	3/5356 (0.1%)
1	B	0.69	2/3945 (0.1%)	0.77	6/5337 (0.1%)
All	All	0.65	4/7904 (0.1%)	0.75	9/10693 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211[A]	ARG	CD-NE	-15.22	1.20	1.46
1	B	211[B]	ARG	CD-NE	-15.22	1.20	1.46
1	A	439[A]	ARG	CA-CB	5.54	1.66	1.53
1	A	439[B]	ARG	CA-CB	5.54	1.66	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211[A]	ARG	CG-CD-NE	13.19	139.49	111.80
1	B	211[B]	ARG	CG-CD-NE	13.19	139.49	111.80
1	A	327	SER	N-CA-C	-5.80	95.35	111.00
1	B	211[A]	ARG	CB-CG-CD	5.37	125.56	111.60
1	B	211[B]	ARG	CB-CG-CD	5.37	125.56	111.60
1	B	211[A]	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	B	211[B]	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	A	439[A]	ARG	N-CA-CB	-5.11	101.41	110.60
1	A	439[B]	ARG	N-CA-CB	-5.11	101.41	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3878	0	3882	66	0
1	B	3865	0	3869	111	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	44	0	26	5	0
3	B	44	0	26	5	0
4	A	329	0	0	15	0
4	B	317	0	0	49	0
All	All	8523	0	7845	176	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 11.

All (176) 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:426:MET:HB2	4:B:2117:HOH:O	1.63	0.98
1:B:376:PRO:HB2	4:B:2220:HOH:O	1.66	0.94
1:B:417:TYR:N	4:B:2266:HOH:O	2.00	0.92
1:B:156:PHE:HE2	4:B:2271:HOH:O	1.57	0.86
1:B:290:GLU:OE1	1:B:291:ILE:HG13	1.76	0.86
1:A:49:LEU:HD11	1:A:67:LYS:HB2	1.57	0.85
1:A:190:GLU:HG3	4:A:2142:HOH:O	1.79	0.83
1:B:386:ASP:HA	4:B:2224:HOH:O	1.78	0.82
1:A:325:LEU:HD22	1:A:339:VAL:HG13	1.63	0.80
1:B:111:ALA:HB3	4:B:2071:HOH:O	1.82	0.78
1:B:106:TYR:HB3	4:B:2070:HOH:O	1.84	0.78
1:B:70:ASN:ND2	4:B:2037:HOH:O	2.15	0.78
1:B:43:GLU:HG2	1:B:308:LYS:HE2	1.67	0.75
1:B:290:GLU:OE2	4:B:2190:HOH:O	2.06	0.72
1:A:32:GLY:HA2	1:A:62:ASP:OD1	1.89	0.71
1:B:422:ARG:NH1	4:B:2271:HOH:O	2.22	0.71
1:B:86:MET:HE3	3:B:500:NAD:H3D	1.73	0.70
1:A:230:LYS:NZ	1:A:230:LYS:H	1.90	0.70
1:A:439[A]:ARG:NH2	4:A:2284:HOH:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:HG3	4:B:2271:HOH:O	1.90	0.70
1:B:422:ARG:O	4:B:2271:HOH:O	2.11	0.68
1:B:414:VAL:O	4:B:2266:HOH:O	2.12	0.68
1:B:156:PHE:CD2	4:B:2117:HOH:O	2.45	0.68
1:A:291:ILE:HG12	4:A:2197:HOH:O	1.92	0.67
1:B:115:ASN:OD1	4:B:2086:HOH:O	2.13	0.66
1:B:320:VAL:HG21	1:B:328:VAL:HG21	1.78	0.66
1:B:378:LYS:HG3	4:B:2220:HOH:O	1.95	0.66
1:B:414:VAL:C	4:B:2266:HOH:O	2.33	0.66
1:B:413:ARG:O	4:B:2266:HOH:O	2.13	0.66
1:A:321:ARG:HG3	1:A:321:ARG:HH11	1.60	0.65
1:B:458:GLU:O	1:B:462:GLU:HG3	1.96	0.65
1:B:19:ARG:HG2	1:B:19:ARG:HH11	1.62	0.65
1:A:325:LEU:HD23	1:A:342:VAL:CG1	2.27	0.64
1:B:253:TYR:OH	4:B:2164:HOH:O	2.12	0.64
1:B:232:TRP:O	1:B:233:LYS:HD3	1.97	0.64
1:B:156:PHE:CE2	4:B:2271:HOH:O	2.40	0.63
1:B:422:ARG:NH1	4:B:2117:HOH:O	2.31	0.63
1:B:157:GLU:OE2	4:B:2117:HOH:O	2.16	0.61
1:B:186:LYS:HD2	1:B:242:LEU:HD12	1.82	0.61
1:B:302:LYS:HE2	1:B:306:ILE:HD11	1.81	0.61
1:B:49:LEU:HD22	1:B:67:LYS:HB3	1.81	0.61
1:A:382:HIS:HD2	4:A:2264:HOH:O	1.82	0.61
1:A:49:LEU:CD1	1:A:67:LYS:HB2	2.28	0.61
1:B:384:ILE:HG12	4:B:2229:HOH:O	2.00	0.61
1:A:181:MET:O	1:A:185:GLU:HG3	2.01	0.60
1:A:173:PHE:CE1	1:A:373:VAL:HG12	2.35	0.60
1:B:173:PHE:CE1	1:B:373:VAL:HG12	2.37	0.60
1:A:55:TYR:O	1:A:59:VAL:HG22	2.02	0.59
1:B:329:LEU:HD13	1:B:335:GLU:HB3	1.84	0.59
1:B:211[A]:ARG:HG3	1:B:211[A]:ARG:HH11	1.66	0.59
1:A:317:ASN:O	1:A:320:VAL:HG12	2.02	0.59
1:B:302:LYS:HE3	1:B:305:GLU:OE1	2.02	0.59
1:A:230:LYS:HZ2	1:A:230:LYS:HB3	1.67	0.59
1:B:58:GLU:HG2	4:B:2028:HOH:O	2.03	0.58
1:A:227:GLU:C	1:A:230:LYS:HE2	2.24	0.58
1:B:350:ARG:HG3	4:B:2207:HOH:O	2.01	0.58
1:A:321:ARG:HG3	1:A:321:ARG:NH1	2.18	0.58
1:B:80:PHE:CE2	1:B:360:ILE:HG23	2.39	0.58
1:B:305:GLU:HG3	4:B:2195:HOH:O	2.03	0.57
1:A:163:THR:HA	4:A:2120:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HZ3	1:A:230:LYS:H	1.52	0.57
1:B:106:TYR:O	4:B:2071:HOH:O	2.17	0.57
1:A:76:ILE:O	1:A:77:ASP:HB2	2.05	0.56
1:B:294:LYS:CE	4:B:2192:HOH:O	2.52	0.56
1:A:331:LYS:HD2	1:A:331:LYS:N	2.22	0.54
1:A:447:ARG:NE	4:A:2296:HOH:O	2.40	0.54
1:A:407:GLU:HA	1:A:408:PRO:C	2.28	0.54
1:B:418:TYR:HA	4:B:2164:HOH:O	2.09	0.53
1:B:423:ILE:HG13	4:B:2267:HOH:O	2.09	0.53
1:A:5:LYS:HD3	1:A:77:ASP:HB3	1.90	0.53
1:A:273:LEU:HG	1:A:277:LYS:HE2	1.90	0.53
1:B:182:GLU:OE2	1:B:186:LYS:HE3	2.08	0.53
1:B:294:LYS:HE2	4:B:2192:HOH:O	2.07	0.53
1:B:190:GLU:OE2	1:B:193:LYS:HE2	2.10	0.52
1:B:418:TYR:N	4:B:2262:HOH:O	2.42	0.52
1:A:278:LYS:NZ	4:A:2187:HOH:O	2.43	0.51
1:B:155:ILE:HD13	4:B:2219:HOH:O	2.11	0.51
1:A:333:LEU:O	1:A:337:GLN:HG3	2.11	0.51
1:A:62:ASP:O	1:A:62:ASP:OD1	2.29	0.51
1:A:49:LEU:O	1:A:53:LYS:HE2	2.10	0.51
1:A:230:LYS:HD2	1:A:230:LYS:H	1.75	0.50
1:B:377:ASN:ND2	4:B:2224:HOH:O	2.43	0.50
1:B:5:LYS:HE3	1:B:36:THR:OG1	2.11	0.50
1:A:230:LYS:HD2	1:A:230:LYS:N	2.27	0.50
1:A:86:MET:HB2	3:A:500:NAD:H52N	1.94	0.49
1:B:422:ARG:NH2	4:B:2084:HOH:O	2.44	0.49
4:A:2296:HOH:O	1:B:266:SER:HB3	2.12	0.49
1:B:23:ASP:OD2	1:B:354:GLU:OE2	2.30	0.49
4:A:2284:HOH:O	1:B:268:ARG:NH1	2.44	0.49
1:A:339:VAL:HG12	4:A:2217:HOH:O	2.13	0.49
1:A:374:ASN:HA	1:A:390:VAL:O	2.12	0.49
1:B:108:GLY:O	4:B:2071:HOH:O	2.20	0.49
1:A:332:ASP:OD1	1:A:335:GLU:HG3	2.14	0.48
1:B:157:GLU:CD	4:B:2117:HOH:O	2.49	0.48
1:B:190:GLU:HB3	1:B:192:GLU:OE2	2.14	0.48
1:A:306:ILE:HD11	1:A:334:SER:OG	2.15	0.47
1:B:374:ASN:HA	1:B:390:VAL:O	2.15	0.47
1:A:268:ARG:HD2	1:B:446:TYR:CG	2.49	0.47
1:B:94:GLU:O	1:B:98:GLN:HG3	2.15	0.47
1:A:313:PHE:CE2	1:A:328:VAL:HG13	2.50	0.47
1:B:398:LYS:HG3	1:B:399:ASN:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LYS:N	4:B:2266:HOH:O	2.48	0.46
1:B:71:LEU:O	1:B:74:VAL:HG12	2.15	0.46
1:B:86:MET:HB2	3:B:500:NAD:H52N	1.96	0.46
1:A:173:PHE:HE1	1:A:373:VAL:HG12	1.81	0.46
1:A:230:LYS:CD	1:A:230:LYS:H	2.28	0.46
1:B:182:GLU:CG	1:B:186:LYS:HE3	2.45	0.46
3:A:500:NAD:H8A	4:A:2328:HOH:O	2.15	0.46
1:B:232:TRP:CH2	1:B:234:PRO:HD3	2.51	0.46
1:B:90:HIS:HE1	3:B:500:NAD:O1N	1.99	0.46
1:B:192:GLU:H	1:B:192:GLU:CD	2.20	0.45
1:B:19:ARG:HD3	1:B:352:SER:HB2	1.97	0.45
1:A:173:PHE:HZ	1:A:359:PHE:CD1	2.35	0.45
1:B:359:PHE:CE2	1:B:363:LEU:HD11	2.51	0.45
1:A:322:LEU:O	1:A:325:LEU:HG	2.16	0.45
1:A:56:VAL:HG13	1:A:61:ALA:HB3	1.99	0.45
1:B:86:MET:CE	3:B:500:NAD:H3D	2.42	0.45
1:B:223:LYS:HE3	1:B:227:GLU:OE2	2.17	0.45
1:B:298:ASP:OD1	4:B:2194:HOH:O	2.21	0.45
1:B:86:MET:HE3	4:B:2091:HOH:O	2.17	0.45
1:B:225:ILE:CD1	1:B:247:ILE:HD12	2.46	0.44
1:B:317:ASN:N	1:B:318:PRO:HD3	2.31	0.44
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.17	0.44
1:B:38:MET:HA	1:B:68:THR:O	2.18	0.44
1:A:18:LEU:HG	1:A:48:ILE:HD11	1.98	0.44
1:A:44:ARG:NH1	3:A:500:NAD:H3B	2.32	0.44
1:B:450:ARG:NH1	4:B:2071:HOH:O	2.43	0.44
1:B:159:THR:HG22	1:B:389:VAL:HG21	2.00	0.44
1:A:46:ASP:HB3	4:A:2026:HOH:O	2.18	0.43
1:B:117:VAL:HG23	4:B:2086:HOH:O	2.17	0.43
1:A:62:ASP:HA	4:A:2035:HOH:O	2.18	0.43
1:B:302:LYS:O	1:B:306:ILE:HG12	2.17	0.43
1:B:382:HIS:CD2	4:B:2225:HOH:O	2.71	0.43
1:B:86:MET:HE3	3:B:500:NAD:C3D	2.47	0.43
1:A:331:LYS:HB3	1:A:336:LYS:HE3	2.00	0.43
1:A:297:GLN:NE2	4:A:2200:HOH:O	2.50	0.43
1:B:407:GLU:HA	1:B:408:PRO:C	2.38	0.43
1:A:197:GLN:HG3	1:A:393:PRO:HG2	2.01	0.43
1:A:103:TYR:OH	1:A:463:GLU:OE2	2.21	0.43
1:B:117:VAL:N	4:B:2085:HOH:O	2.51	0.43
1:B:186:LYS:HD2	1:B:242:LEU:CD1	2.46	0.43
1:B:294:LYS:HB3	1:B:294:LYS:HE2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLN:HA	4:B:2155:HOH:O	2.18	0.42
1:B:211[A]:ARG:NH1	4:B:2141:HOH:O	2.52	0.42
1:A:446:TYR:CG	1:B:268:ARG:HD2	2.54	0.42
1:A:18:LEU:HG	1:A:48:ILE:CD1	2.50	0.42
1:B:383:GLY:O	1:B:384:ILE:HD13	2.20	0.42
1:B:418:TYR:CA	4:B:2164:HOH:O	2.66	0.42
1:A:38:MET:SD	3:A:500:NAD:H2A	2.60	0.42
1:A:225:ILE:HA	1:A:229:SER:HB3	2.01	0.42
1:A:325:LEU:CD1	1:A:325:LEU:O	2.68	0.42
1:B:237:PRO:HG3	1:B:284:TRP:CG	2.55	0.42
1:B:97:ARG:O	1:B:101:GLU:HG3	2.19	0.41
1:B:236:ASN:HB2	1:B:237:PRO:CD	2.50	0.41
1:B:256:MET:HE3	1:B:257:PRO:HD2	2.02	0.41
1:A:86:MET:HE2	1:A:89:GLY:HA2	2.02	0.41
1:A:236:ASN:HB2	1:A:237:PRO:CD	2.51	0.41
1:A:98:GLN:NE2	4:A:2063:HOH:O	2.52	0.41
1:A:228:LYS:C	1:A:230:LYS:HD2	2.41	0.41
1:A:295:TRP:O	1:A:299:THR:HG23	2.21	0.41
1:A:325:LEU:N	1:A:325:LEU:HD12	2.35	0.41
1:B:211[A]:ARG:CZ	4:B:2141:HOH:O	2.67	0.41
1:B:463:GLU:HG3	4:B:2299:HOH:O	2.20	0.41
1:B:211[B]:ARG:NH2	1:B:214:GLY:O	2.47	0.41
1:B:357:ILE:HB	1:B:358:PRO:HD3	2.02	0.41
1:A:277:LYS:HA	1:A:285:GLY:HA2	2.03	0.41
1:B:218:TYR:N	1:B:219:PRO:CD	2.84	0.41
1:B:475:LYS:HB2	1:B:475:LYS:NZ	2.36	0.41
1:B:8:ILE:HD13	1:B:20:LEU:HD12	2.03	0.41
1:A:153:ASN:ND2	3:A:500:NAD:O2D	2.54	0.41
1:B:290:GLU:OE1	1:B:291:ILE:N	2.50	0.40
1:B:175:HIS:NE2	1:B:178:TYR:CG	2.89	0.40
1:B:18:LEU:HA	1:B:18:LEU:HD23	1.83	0.40
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.92	0.40
1:B:197:GLN:HG3	1:B:393:PRO:HG2	2.02	0.40
1:B:225:ILE:HG12	1:B:247:ILE:HD12	2.03	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	477/480 (99%)	466 (98%)	10 (2%)	1 (0%)	47 38
1	B	475/480 (99%)	459 (97%)	15 (3%)	1 (0%)	47 38
All	All	952/960 (99%)	925 (97%)	25 (3%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	B	479	LYS

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	419/420 (100%)	413 (99%)	6 (1%)	67 65
1	B	417/420 (99%)	410 (98%)	7 (2%)	60 57
All	All	836/840 (100%)	823 (98%)	13 (2%)	62 60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	230	LYS
1	A	322	LEU
1	A	325	LEU

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	368	LYS
1	B	58	GLU
1	B	190	GLU
1	B	244	PRO
1	B	290	GLU
1	B	337	GLN
1	B	341	GLU
1	B	350	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	297	GLN
1	A	382	HIS
1	B	90	HIS
1	B	98	GLN
1	B	153	ASN
1	B	213	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSD	A	174	1	3,7,8	0.72	0	1,8,10	0.95	0
1	CSD	B	174	1	3,7,8	0.81	0	1,8,10	0.72	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
1	CSD	A	174	1	-	1/2/6/8	-
1	CSD	B	174	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	CSD	CA-CB-SG-OD1
1	B	174	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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	GLC	C	1	2	12,12,12	1.11	1 (8%)	17,17,17	1.73	4 (23%)
2	GLC	C	2	2	11,11,12	0.87	0	15,15,17	1.63	3 (20%)
2	GLC	D	1	2	12,12,12	1.06	1 (8%)	17,17,17	1.88	5 (29%)
2	GLC	D	2	2	11,11,12	0.89	0	15,15,17	1.49	3 (20%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	O5-C5	2.14	1.49	1.44
2	C	1	GLC	O5-C5	2.11	1.49	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C1-O5-C5	4.67	118.52	112.19
2	D	2	GLC	C1-O5-C5	3.94	117.53	112.19
2	D	1	GLC	O6-C6-C5	-3.76	98.38	111.29
2	D	1	GLC	C4-C3-C2	-3.54	104.65	110.82
2	C	1	GLC	C4-C3-C2	-3.50	104.72	110.82
2	D	1	GLC	O2-C2-C3	-3.43	102.42	110.35
2	C	1	GLC	O2-C2-C3	-3.27	102.79	110.35
2	C	1	GLC	O6-C6-C5	-3.16	100.44	111.29
2	C	2	GLC	O5-C5-C6	-2.71	102.95	107.20
2	D	2	GLC	C2-C3-C4	-2.51	106.55	110.89
2	D	1	GLC	C1-C2-C3	2.46	115.42	110.31
2	C	2	GLC	C2-C3-C4	-2.36	106.81	110.89
2	C	1	GLC	C1-C2-C3	2.22	114.92	110.31
2	D	1	GLC	O5-C5-C4	2.03	113.38	109.69
2	D	2	GLC	O5-C5-C6	-2.01	104.05	107.20

There are no chirality outliers.

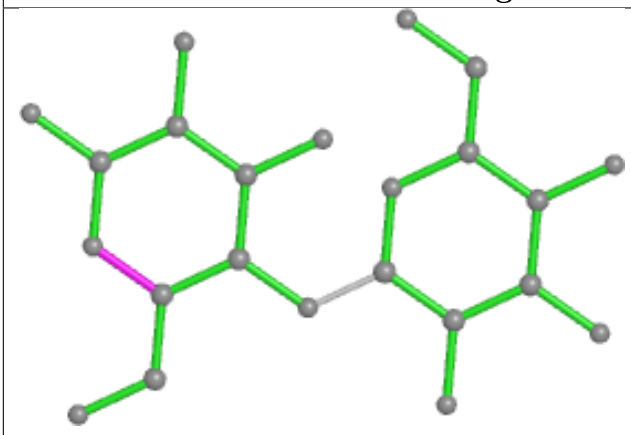
There are no torsion outliers.

There are no ring outliers.

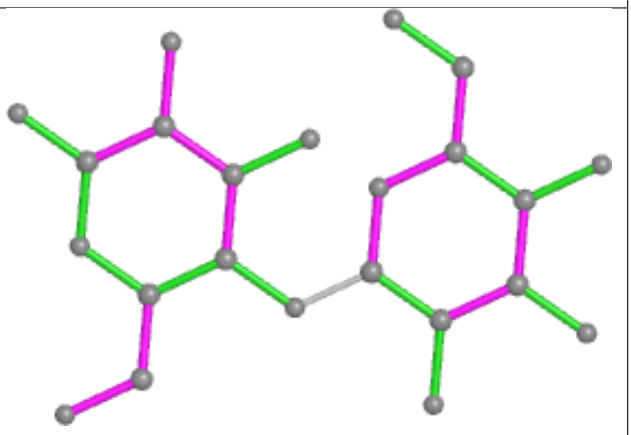
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

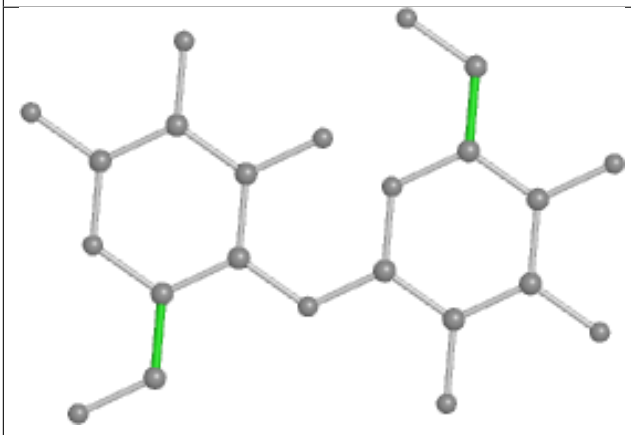
Oligosaccharide Chain C



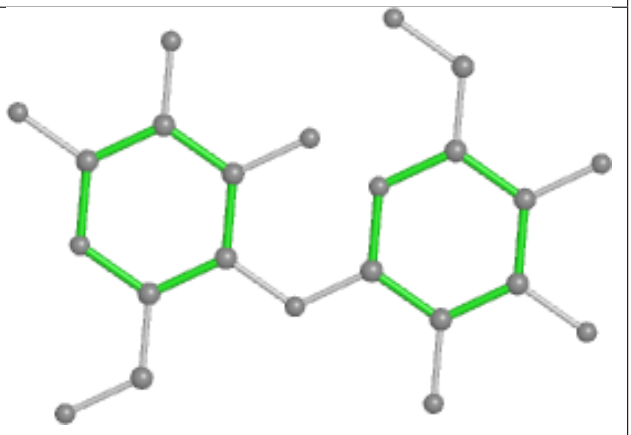
Bond lengths



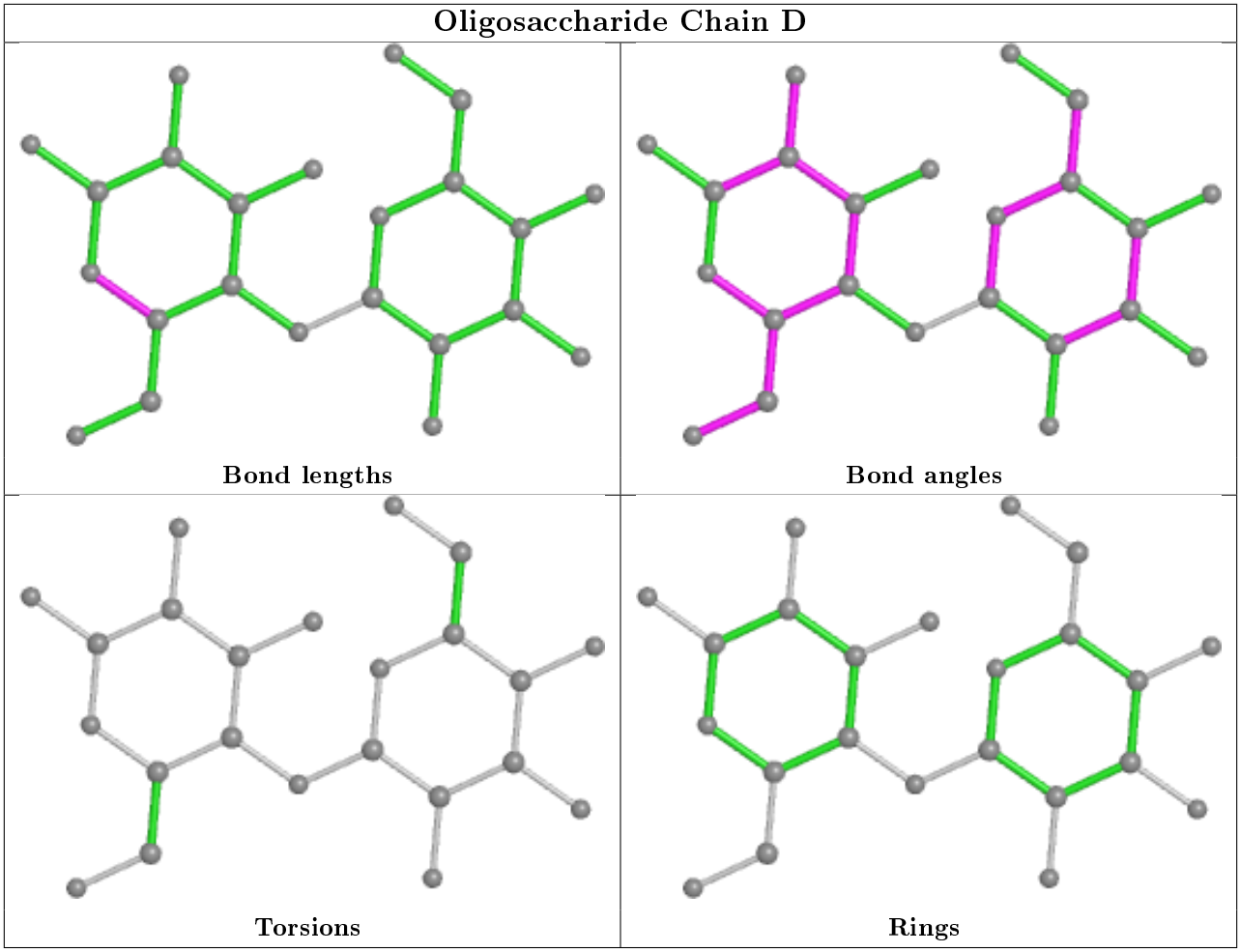
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
3	NAD	A	500	-	42,48,48	2.94	13 (30%)	50,73,73	1.49	9 (18%)
3	NAD	B	500	-	42,48,48	2.68	13 (30%)	50,73,73	1.48	8 (16%)

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	NAD	A	500	-	-	13/26/62/62	0/5/5/5
3	NAD	B	500	-	-	12/26/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	C2N-N1N	9.52	1.46	1.35
3	B	500	NAD	C2N-N1N	8.43	1.45	1.35
3	A	500	NAD	C4N-C3N	8.32	1.53	1.39
3	B	500	NAD	C4N-C3N	8.29	1.53	1.39
3	A	500	NAD	C2A-N3A	6.16	1.42	1.32
3	A	500	NAD	C5N-C4N	6.14	1.51	1.38
3	B	500	NAD	C5N-C4N	6.07	1.51	1.38
3	B	500	NAD	C2A-N3A	5.24	1.40	1.32
3	A	500	NAD	C4A-N3A	4.89	1.42	1.35
3	A	500	NAD	O4D-C1D	4.15	1.46	1.41
3	A	500	NAD	C6N-N1N	3.76	1.44	1.35
3	A	500	NAD	C2D-C1D	3.50	1.59	1.53
3	B	500	NAD	C6N-N1N	3.49	1.43	1.35
3	B	500	NAD	C4A-N3A	3.37	1.40	1.35
3	B	500	NAD	C2N-C3N	-3.26	1.33	1.39
3	B	500	NAD	O4D-C1D	3.21	1.45	1.41
3	A	500	NAD	C2N-C3N	-3.18	1.34	1.39
3	B	500	NAD	C3B-C4B	2.74	1.60	1.53
3	A	500	NAD	O4D-C4D	2.71	1.51	1.45
3	B	500	NAD	O4D-C4D	2.62	1.50	1.45
3	A	500	NAD	O4B-C4B	2.39	1.50	1.45
3	A	500	NAD	C6N-C5N	2.38	1.43	1.38
3	B	500	NAD	C2D-C1D	2.34	1.57	1.53
3	A	500	NAD	C3N-C7N	2.28	1.54	1.50
3	B	500	NAD	C3N-C7N	2.26	1.54	1.50
3	B	500	NAD	C6N-C5N	2.17	1.43	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	500	NAD	N3A-C2A-N1A	-4.49	121.66	128.68
3	A	500	NAD	N3A-C2A-N1A	-4.16	122.17	128.68
3	A	500	NAD	C2A-N1A-C6A	3.93	125.47	118.75
3	B	500	NAD	C2A-N1A-C6A	3.86	125.36	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	NAD	O4B-C1B-C2B	-3.77	101.42	106.93
3	B	500	NAD	O4D-C1D-C2D	-2.83	102.79	106.93
3	B	500	NAD	C5A-C6A-N1A	-2.44	114.83	120.35
3	A	500	NAD	C5A-C6A-N1A	-2.40	114.90	120.35
3	A	500	NAD	O4D-C1D-C2D	-2.39	103.44	106.93
3	B	500	NAD	C2N-N1N-C1D	-2.37	113.86	119.14
3	A	500	NAD	O2B-C2B-C3B	2.27	119.17	111.82
3	A	500	NAD	PA-O5B-C5B	-2.25	108.47	121.68
3	B	500	NAD	O2B-C2B-C3B	2.19	118.90	111.82
3	A	500	NAD	C3B-C2B-C1B	-2.14	97.75	100.98
3	B	500	NAD	C1B-N9A-C4A	-2.14	122.89	126.64
3	B	500	NAD	C3N-C7N-N7N	2.14	120.31	117.75
3	A	500	NAD	N6A-C6A-N1A	2.09	122.92	118.57

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	NAD	C5B-O5B-PA-O2A
3	A	500	NAD	C5D-O5D-PN-O3
3	A	500	NAD	C5D-O5D-PN-O1N
3	A	500	NAD	C5D-O5D-PN-O2N
3	A	500	NAD	O4D-C1D-N1N-C2N
3	B	500	NAD	C5D-O5D-PN-O3
3	B	500	NAD	C5D-O5D-PN-O1N
3	B	500	NAD	C5D-O5D-PN-O2N
3	B	500	NAD	O4D-C1D-N1N-C2N
3	B	500	NAD	O4D-C1D-N1N-C6N
3	B	500	NAD	C2D-C1D-N1N-C2N
3	B	500	NAD	C2D-C1D-N1N-C6N
3	A	500	NAD	O4B-C4B-C5B-O5B
3	B	500	NAD	O4B-C4B-C5B-O5B
3	B	500	NAD	C3B-C4B-C5B-O5B
3	A	500	NAD	C3B-C4B-C5B-O5B
3	A	500	NAD	PA-O3-PN-O1N
3	A	500	NAD	C5B-O5B-PA-O3
3	A	500	NAD	C5B-O5B-PA-O1A
3	B	500	NAD	O4D-C4D-C5D-O5D
3	A	500	NAD	PA-O3-PN-O2N
3	A	500	NAD	C2D-C1D-N1N-C2N
3	A	500	NAD	C2D-C1D-N1N-C6N
3	B	500	NAD	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	B	500	NAD	PA-O3-PN-O1N

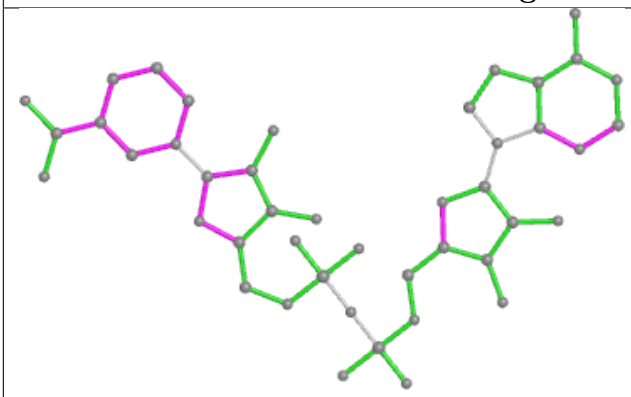
There are no ring outliers.

2 monomers are involved in 10 short contacts:

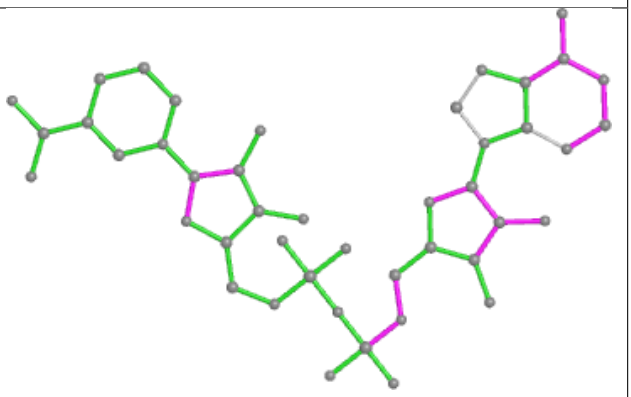
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAD	5	0
3	B	500	NAD	5	0

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.

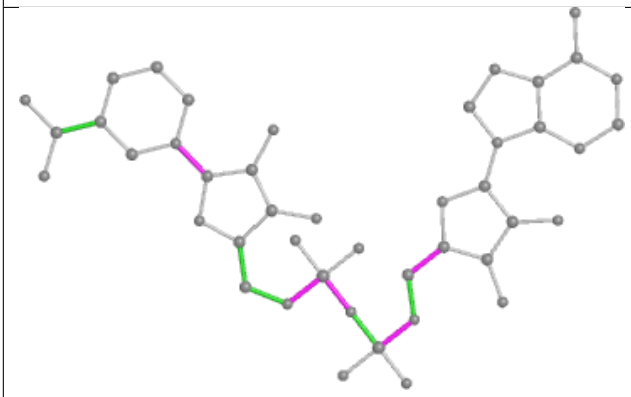
Ligand NAD A 500



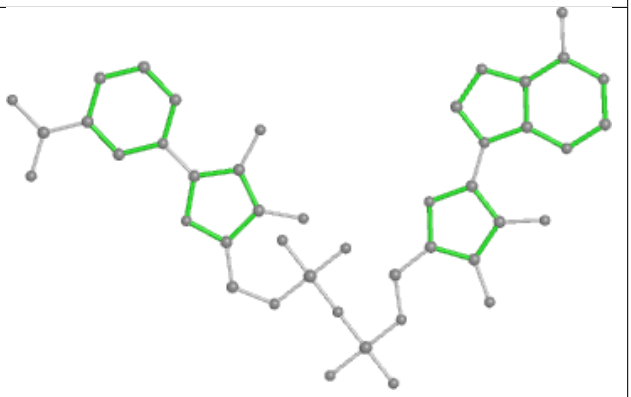
Bond lengths



Bond angles

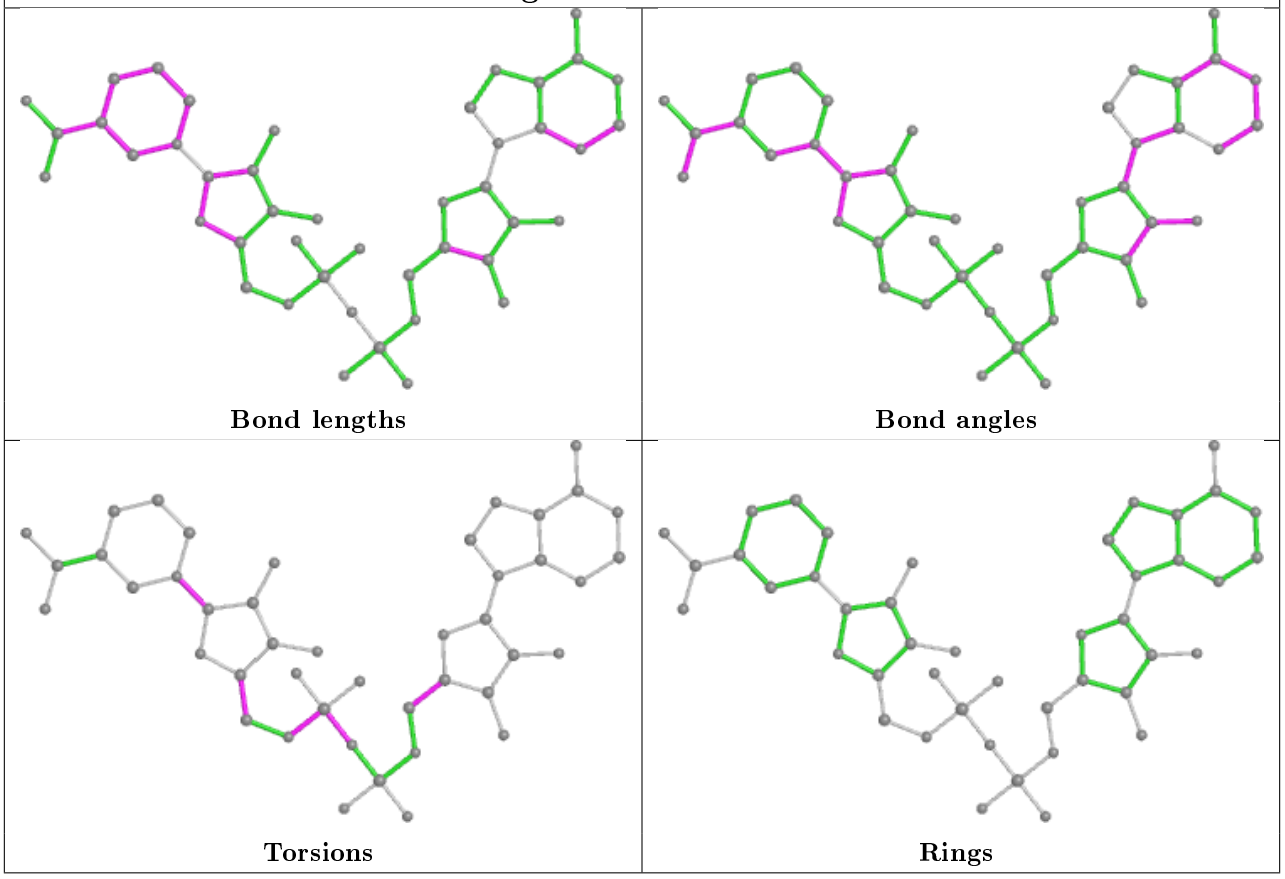


Torsions



Rings

Ligand NAD B 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	478/480 (99%)	0.00	16 (3%) 46 49	17, 29, 50, 70	0
1	B	476/480 (99%)	0.10	17 (3%) 42 45	18, 31, 49, 69	0
All	All	954/960 (99%)	0.05	33 (3%) 44 47	17, 30, 50, 70	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	480	ARG	7.1
1	A	178	TYR	6.9
1	B	331	LYS	4.9
1	B	178	TYR	4.7
1	A	325	LEU	4.5
1	B	329	LEU	4.0
1	B	351	LYS	3.8
1	A	326	GLY	3.8
1	A	319	SER	3.7
1	B	350	ARG	3.6
1	B	330	GLY	3.1
1	A	175	HIS	3.1
1	A	2	PRO	3.0
1	A	331	LYS	3.0
1	B	479	LYS	2.9
1	B	382	HIS	2.6
1	B	328	VAL	2.6
1	B	321	ARG	2.5
1	A	327	SER	2.4
1	B	175	HIS	2.4
1	B	65	PHE	2.4
1	B	302	LYS	2.3
1	A	328	VAL	2.3
1	A	62	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	382	HIS	2.2
1	B	364	LEU	2.2
1	A	321	ARG	2.2
1	A	472	GLU	2.2
1	A	31	SER	2.2
1	B	190	GLU	2.1
1	B	226	GLU	2.1
1	A	320	VAL	2.1
1	A	193	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSD	A	174	8/9	0.93	0.12	39,45,46,48	0
1	CSD	B	174	8/9	0.94	0.12	39,44,46,47	0

6.3 Carbohydrates (i)

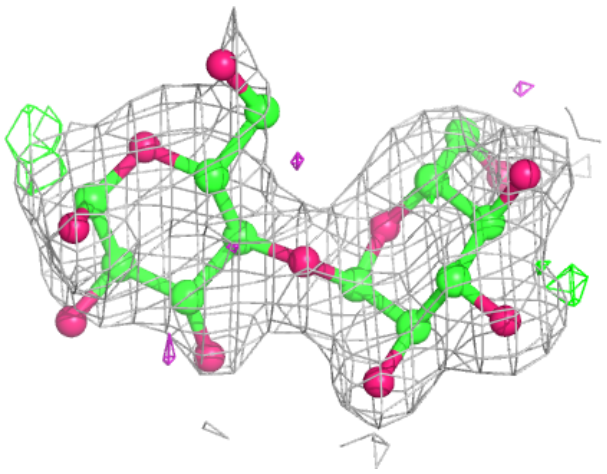
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

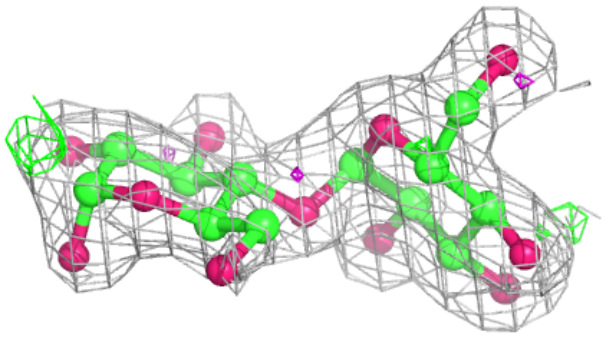
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	12/12	0.80	0.21	41,54,55,59	0
2	GLC	C	1	12/12	0.84	0.27	42,53,55,57	0
2	GLC	D	2	11/12	0.93	0.10	30,33,35,36	0
2	GLC	C	2	11/12	0.94	0.10	28,32,36,36	0

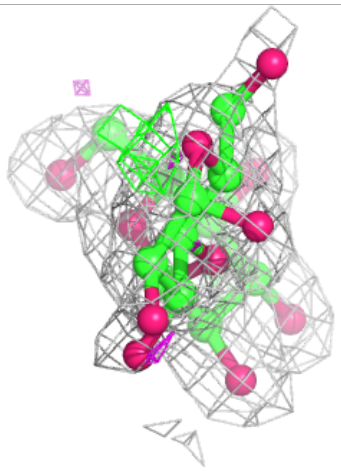
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

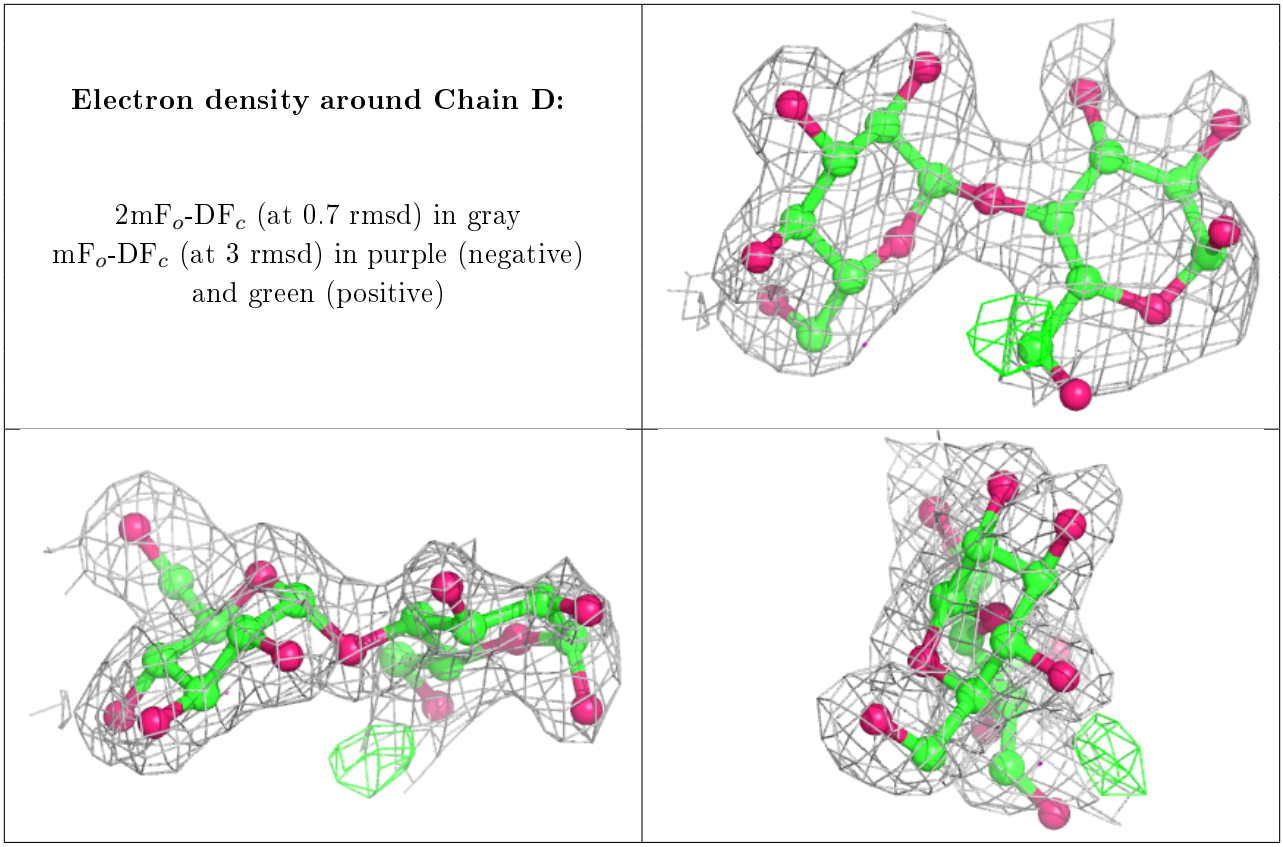






Electron density around Chain D:

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



6.4 Ligands

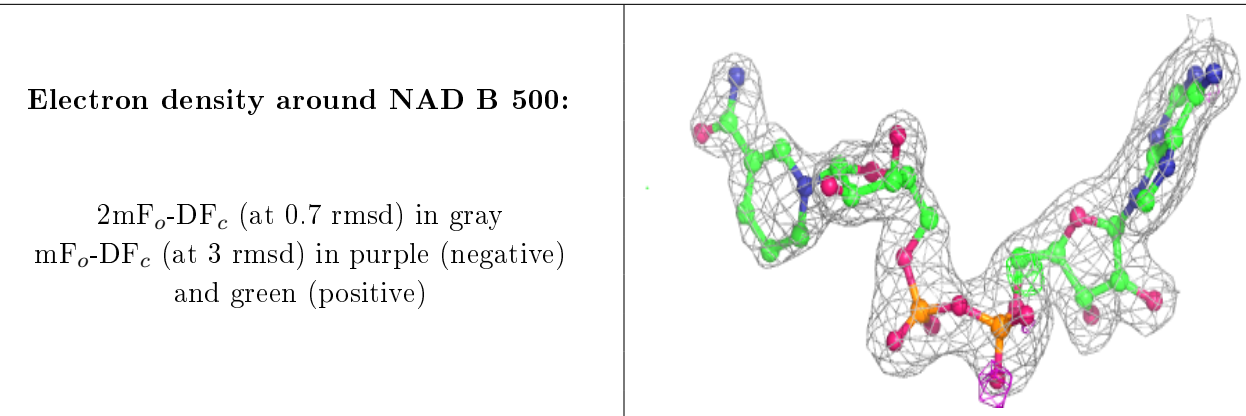
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

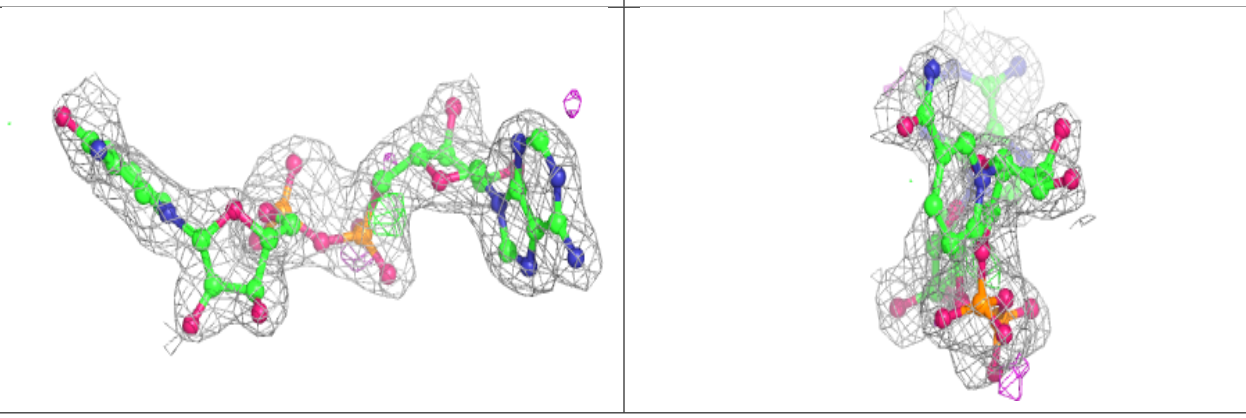
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAD	B	500	44/44	0.93	0.12	29,45,50,52	0
3	NAD	A	500	44/44	0.94	0.13	29,41,70,71	0

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 NAD B 500:

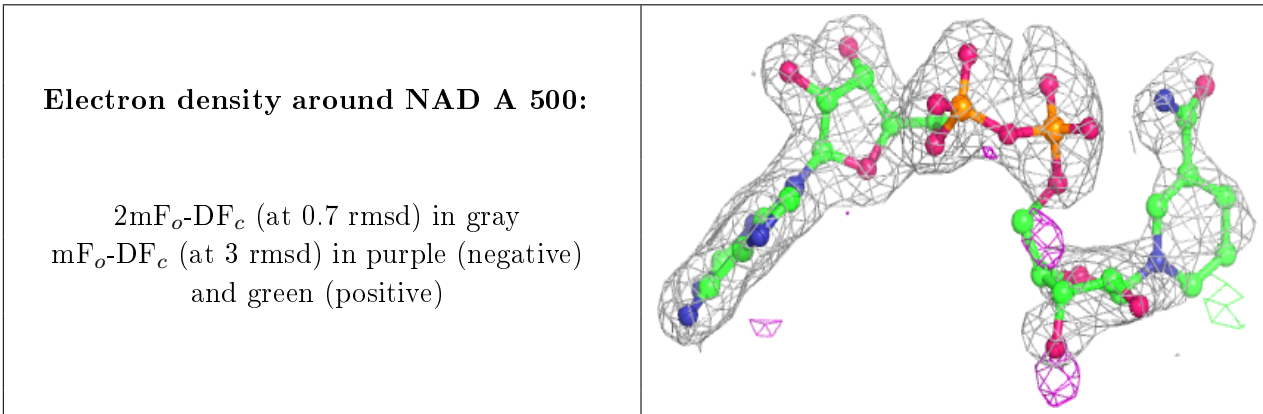
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

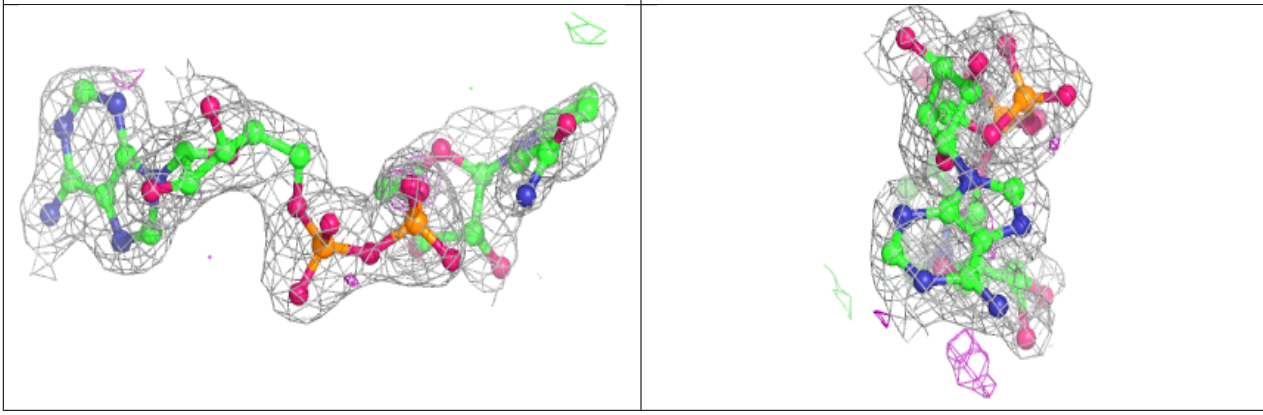




Electron density around NAD A 500:

$2mF_o$-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)

There are no such residues in this entry.