



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:53 PM EDT

PDB ID : 4DNS / pdb_00004dns
Title : Crystal structure of Bermuda grass isoallergen BG60 provides insight into the various cross-allergenicity of the pollen group 4 allergens
Authors : Huang, T.H.; Peng, H.J.; Su, S.N.; Liaw, S.H.
Deposited on : 2012-02-08
Resolution : 2.15 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

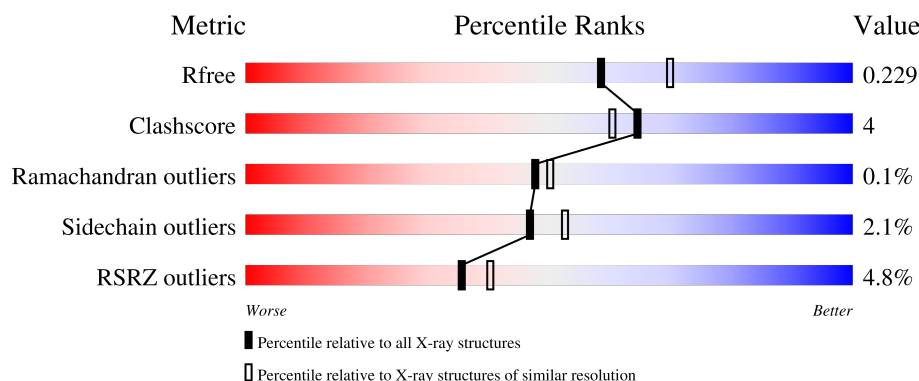
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	497	5% 88% 8% ..
1	B	497	5% 85% 12% ..
2	C	2	100%
2	D	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8048 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 FAD-linked oxidoreductase BG60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3778	2433	646	678	21			
1	B	485	Total	C	N	O	S	0	0	0
			3770	2429	645	675	21			

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



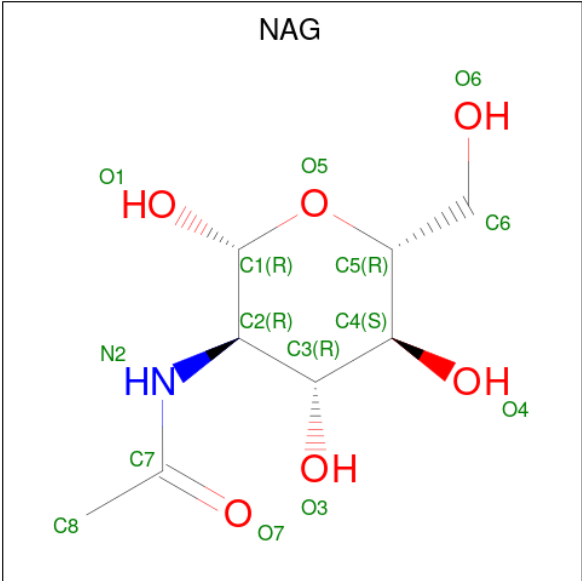
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

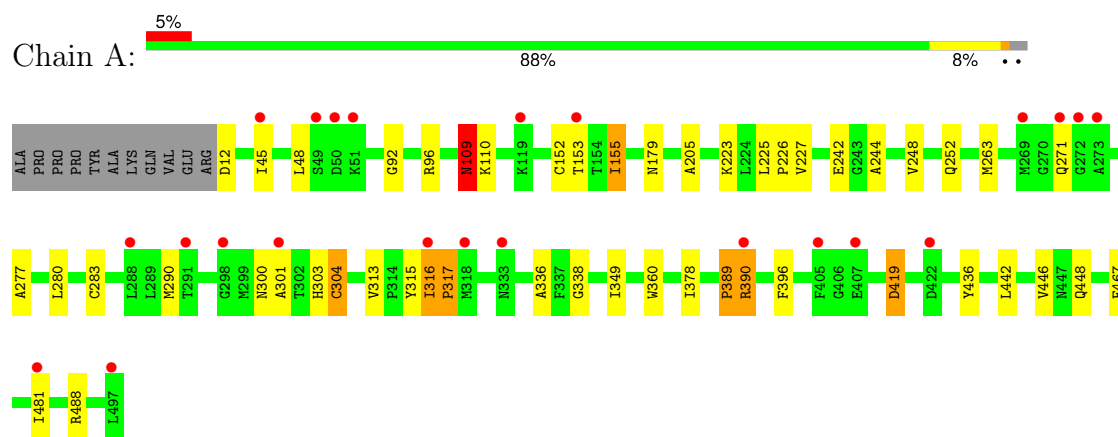
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		
5	B	152	Total	O	0	0
			152	152		

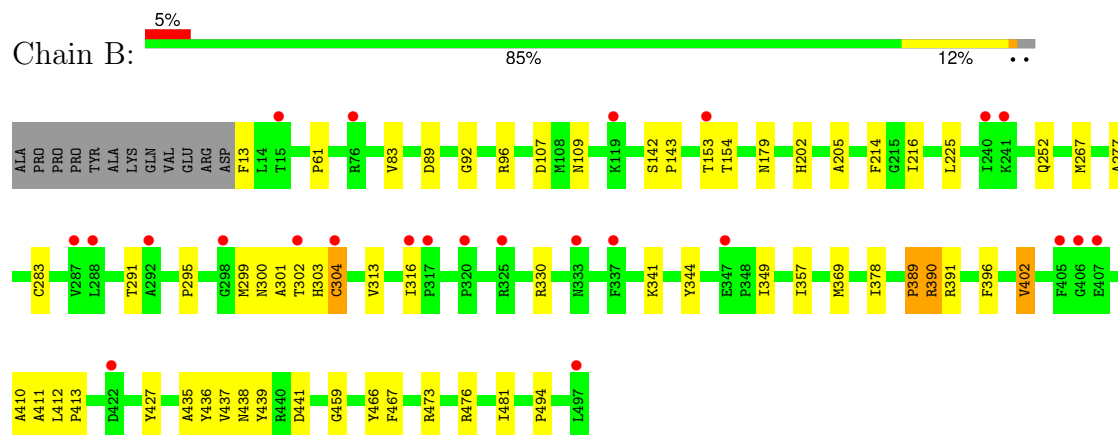
3 Residue-property plots

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.

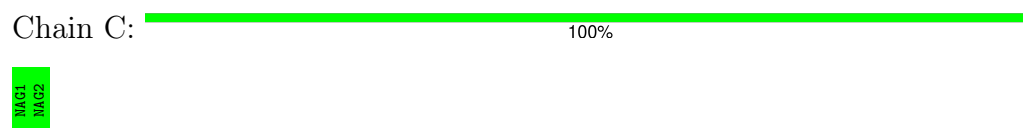
- Molecule 1: FAD-linked oxidoreductase BG60



- Molecule 1: FAD-linked oxidoreductase BG60



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.04Å 86.04Å 309.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.15) 96.2 (50.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.25 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.220 0.199 , 0.229	Depositor DCC
R_{free} test set	6381 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8048	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAG

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	0.73	1/3879 (0.0%)	1.11	19/5262 (0.4%)
1	B	0.74	1/3871 (0.0%)	1.10	15/5251 (0.3%)
All	All	0.74	2/7750 (0.0%)	1.10	34/10513 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	VAL	CA-CB	7.87	1.58	1.54
1	A	313	VAL	CA-CB	6.08	1.57	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ALA	N-CA-C	8.07	120.87	111.02
1	A	109	ASN	N-CA-C	7.02	120.73	111.75
1	B	109	ASN	N-CA-C	6.95	120.65	111.75
1	B	410	ALA	N-CA-C	6.93	120.21	111.69
1	A	227	VAL	N-CA-C	-6.56	103.81	109.19
1	A	277	ALA	N-CA-C	6.53	119.11	109.24
1	B	277	ALA	N-CA-C	6.32	119.32	109.52
1	B	153	THR	N-CA-C	6.17	118.00	111.28
1	A	315	TYR	CA-C-N	6.14	124.11	120.24
1	A	315	TYR	C-N-CA	6.14	124.11	120.24
1	B	205	ALA	N-CA-C	6.08	117.90	111.28
1	A	338	GLY	N-CA-C	5.86	119.87	110.90
1	B	304	CYS	N-CA-C	5.86	118.20	109.59
1	A	153	THR	N-CA-C	5.86	118.61	111.82
1	A	205	ALA	N-CA-C	5.75	117.55	111.28
1	A	336	ALA	N-CA-C	5.74	117.52	108.96
1	A	304	CYS	N-CA-C	5.70	118.52	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ILE	CB-CA-C	-5.66	108.35	114.35
1	A	488	ARG	N-CA-C	5.52	117.57	109.24
1	A	396	PHE	N-CA-C	5.50	117.21	108.79
1	B	437	VAL	N-CA-C	5.46	116.19	110.62
1	A	155	ILE	CB-CA-C	-5.45	103.22	111.33
1	B	154	THR	N-CA-C	5.43	119.77	113.20
1	A	313	VAL	CA-C-N	-5.39	114.20	119.64
1	A	313	VAL	C-N-CA	-5.39	114.20	119.64
1	B	396	PHE	N-CA-C	5.38	117.02	108.79
1	B	439	TYR	N-CA-C	-5.29	104.30	111.55
1	B	316	ILE	N-CA-C	5.22	120.17	108.88
1	B	301	ALA	N-CA-C	5.19	118.72	112.38
1	A	481	ILE	N-CA-C	5.14	115.81	110.82
1	A	301	ALA	N-CA-C	5.10	118.99	112.87
1	A	467	PHE	N-CA-C	5.01	121.13	113.61
1	B	467	PHE	N-CA-C	5.01	121.13	113.61
1	B	389	PRO	N-CA-C	5.01	123.27	114.75

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	3778	0	3783	24	0
1	B	3770	0	3779	32	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	53	0	29	0	0
3	B	53	0	29	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	158	0	0	4	0
5	B	152	0	0	4	0
All	All	8048	0	7696	56	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 4.

All (56) 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:390:ARG:HH11	1:B:390:ARG:HG2	1.29	0.97
1:A:283:CYS:HG	1:A:304:CYS:HG	1.19	0.87
1:A:316:ILE:HD11	5:A:665:HOH:O	1.76	0.85
1:B:283:CYS:HG	1:B:304:CYS:HG	1.26	0.82
1:A:252:GLN:HE22	1:A:349:ILE:H	1.36	0.73
1:B:390:ARG:HH11	1:B:390:ARG:CG	2.01	0.70
1:B:390:ARG:NH2	1:B:435:ALA:O	2.25	0.69
1:B:252:GLN:HE22	1:B:349:ILE:H	1.42	0.66
1:A:316:ILE:CD1	5:A:665:HOH:O	2.37	0.66
1:A:390:ARG:HH11	1:A:390:ARG:HB2	1.60	0.65
1:A:92:GLY:O	1:A:96:ARG:HG2	2.01	0.61
1:B:214:PHE:HD1	1:B:481:ILE:HD11	1.67	0.59
1:B:179:ASN:ND2	1:B:225:LEU:HD11	2.17	0.58
1:A:45:ILE:HG23	1:A:48:LEU:HD12	1.87	0.56
1:B:291:THR:O	1:B:295:PRO:HG3	2.07	0.54
1:B:349:ILE:HD12	1:B:427:TYR:HB3	1.90	0.54
1:A:179:ASN:ND2	1:A:225:LEU:HD11	2.23	0.53
1:A:226:PRO:HD3	5:B:623:HOH:O	2.07	0.53
1:A:442:LEU:HD22	1:A:446:VAL:HG12	1.91	0.53
1:B:252:GLN:NE2	1:B:349:ILE:H	2.06	0.52
1:B:390:ARG:CG	1:B:390:ARG:NH1	2.66	0.52
1:B:300:ASN:H	1:B:303:HIS:HD2	1.58	0.50
1:A:252:GLN:NE2	1:A:349:ILE:H	2.07	0.50
1:B:89:ASP:HB2	3:B:501:FAD:H52A	1.92	0.50
1:A:300:ASN:H	1:A:303:HIS:HD2	1.58	0.50
1:A:316:ILE:HB	1:A:317:PRO:HD3	1.93	0.50
1:A:390:ARG:HB2	1:A:390:ARG:NH1	2.27	0.49
1:B:92:GLY:O	1:B:96:ARG:HG2	2.14	0.48
1:B:330:ARG:NH1	5:B:678:HOH:O	2.46	0.48
1:A:390:ARG:NH2	5:A:613:HOH:O	2.46	0.47
1:A:390:ARG:NH2	1:A:436:TYR:HA	2.29	0.47
1:A:448:GLN:NE2	5:A:655:HOH:O	2.49	0.46
1:B:83:VAL:HG21	1:B:216:ILE:HG23	1.98	0.45
1:B:252:GLN:HE22	1:B:349:ILE:HG12	1.82	0.45
1:B:402:VAL:HG11	1:B:413:PRO:HB3	1.98	0.45
1:B:344:TYR:CZ	1:B:390:ARG:HG3	2.51	0.45
1:A:389:PRO:HG2	1:A:390:ARG:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ARG:HG2	1:B:390:ARG:NH1	2.09	0.44
1:A:152:CYS:HB2	1:A:155:ILE:HD11	1.99	0.44
1:B:357:ILE:HG22	1:B:369:MET:HE1	1.98	0.44
1:B:473:ARG:HG3	1:B:476:ARG:NH2	2.32	0.44
1:B:13:PHE:N	5:B:661:HOH:O	2.50	0.43
1:A:360:TRP:HZ3	1:A:419:ASP:HB3	1.84	0.42
1:B:390:ARG:NH2	1:B:466:TYR:O	2.52	0.42
1:B:202:HIS:HD2	5:B:619:HOH:O	2.02	0.42
1:B:459:GLY:HA3	1:B:494:PRO:HG3	2.01	0.42
1:B:300:ASN:OD1	1:B:302:THR:HG22	2.19	0.42
1:A:109:ASN:HD21	1:A:110:LYS:NZ	2.19	0.41
1:B:378:ILE:O	1:B:391:ARG:HD2	2.20	0.41
1:A:390:ARG:HD3	1:A:390:ARG:N	2.36	0.41
1:A:244:ALA:O	1:A:248:VAL:HG23	2.20	0.41
1:B:142:SER:HA	1:B:143:PRO:HD3	1.90	0.41
1:B:341:LYS:HG2	1:B:441:ASP:OD2	2.21	0.41
1:B:436:TYR:CE2	1:B:438:ASN:HB2	2.55	0.41
1:A:271:GLN:H	1:A:271:GLN:CD	2.28	0.41
1:B:61:PRO:HD2	1:B:107:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	484/497 (97%)	466 (96%)	17 (4%)	1 (0%)	43	44
1	B	483/497 (97%)	467 (97%)	16 (3%)	0	100	100
All	All	967/994 (97%)	933 (96%)	33 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	PRO

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	397/406 (98%)	386 (97%)	11 (3%)	38	40
1	B	396/406 (98%)	390 (98%)	6 (2%)	57	64
All	All	793/812 (98%)	776 (98%)	17 (2%)	47	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	109	ASN
1	A	223	LYS
1	A	242	GLU
1	A	263	MET
1	A	280	LEU
1	A	290	MET
1	A	378	ILE
1	A	389	PRO
1	A	390	ARG
1	A	419	ASP
1	B	267	MET
1	B	299	MET
1	B	389	PRO
1	B	390	ARG
1	B	402	VAL
1	B	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	179	ASN
1	A	202	HIS
1	A	221	GLN
1	A	252	GLN
1	A	271	GLN
1	A	303	HIS
1	A	397	ASN
1	A	438	ASN
1	B	179	ASN
1	B	252	GLN
1	B	303	HIS
1	B	438	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	C	1	2,1	14,14,15	0.59	0	17,19,21	0.75	0
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	0.61	0
2	NAG	D	1	2,1	14,14,15	0.61	0	17,19,21	0.91	2 (11%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	0.65	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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	-2.18	119.97	122.90
2	D	1	NAG	O5-C1-C2	-2.16	107.96	111.29

There are no chirality outliers.

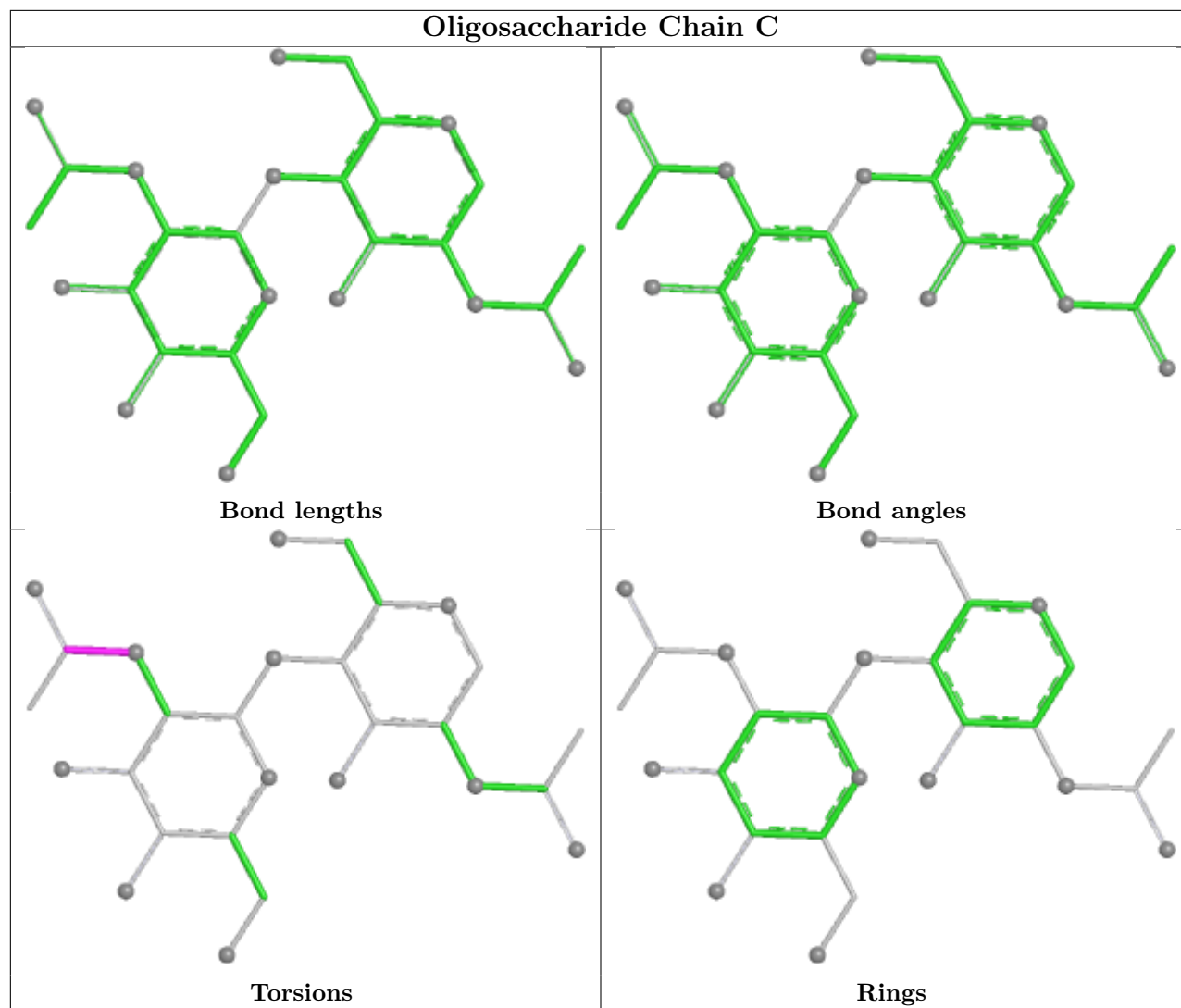
All (3) torsion outliers are listed below:

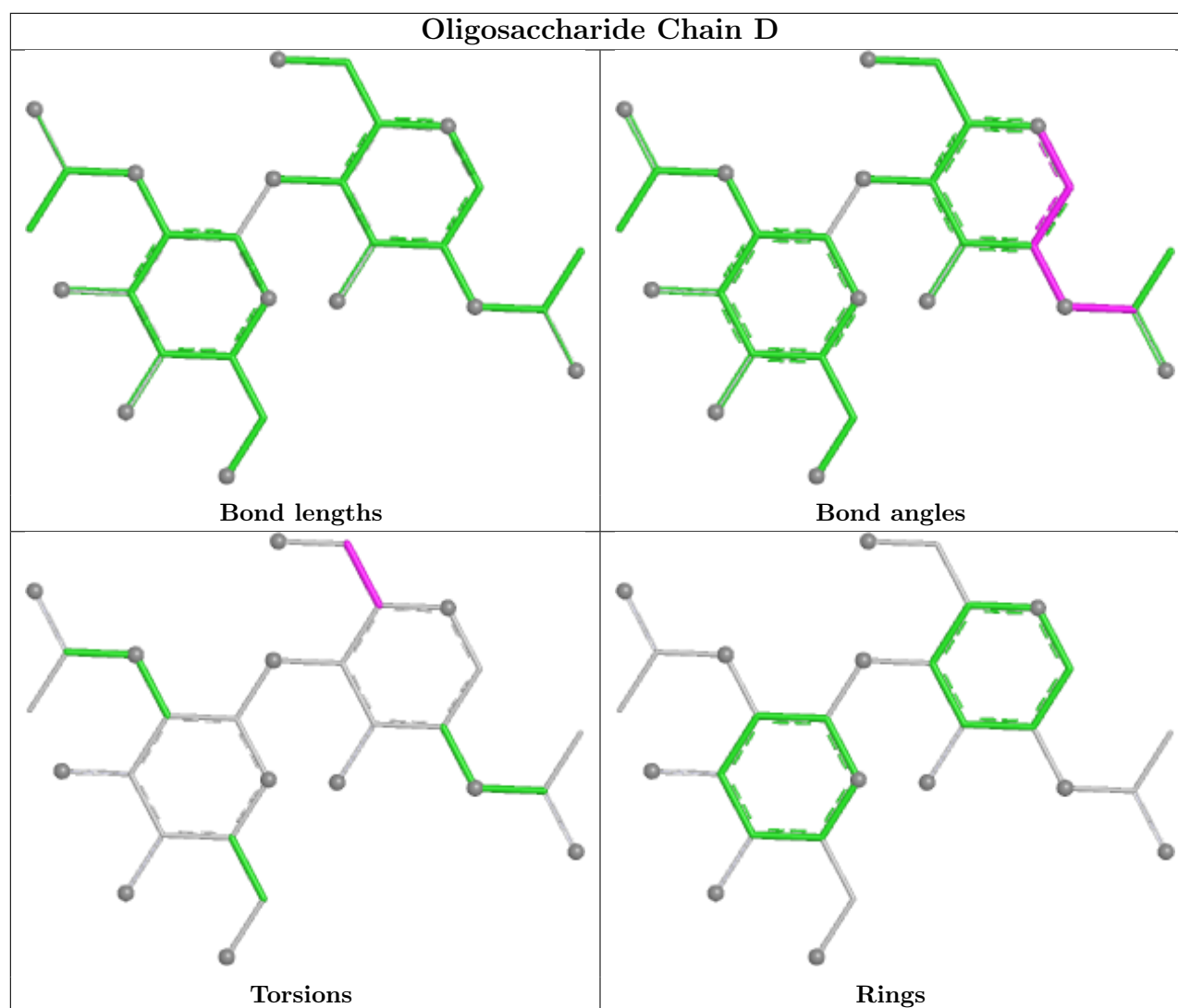
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

4 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	FAD	A	501	1	58,58,58	2.13	17 (29%)	85,89,89	1.24	7 (8%)
3	FAD	B	501	1	58,58,58	2.16	16 (27%)	85,89,89	1.22	7 (8%)
4	NAG	A	504	1	14,14,15	0.78	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	504	1	14,14,15	0.88	1 (7%)	17,19,21	0.56	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	FAD	A	501	1	-	8/34/50/50	0/6/6/6
3	FAD	B	501	1	-	10/34/50/50	0/6/6/6
4	NAG	A	504	1	-	4/6/23/26	0/1/1/1
4	NAG	B	504	1	-	5/6/23/26	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	FAD	C1'-C2'	6.17	1.61	1.52
3	B	501	FAD	C1'-C2'	6.03	1.61	1.52
3	B	501	FAD	C9A-C5X	5.54	1.50	1.41
3	A	501	FAD	C9A-C5X	5.35	1.49	1.41
3	A	501	FAD	C4A-N3A	4.65	1.43	1.34
3	A	501	FAD	C4'-C3'	4.58	1.61	1.53
3	B	501	FAD	C4'-C3'	4.57	1.61	1.53
3	B	501	FAD	C4A-N3A	4.56	1.42	1.34
3	B	501	FAD	C4X-N5	4.55	1.40	1.30
3	B	501	FAD	C9A-N10	4.45	1.48	1.41
3	A	501	FAD	C4X-N5	4.08	1.39	1.30
3	A	501	FAD	C9A-N10	3.82	1.47	1.41
3	B	501	FAD	C10-N10	3.75	1.45	1.37
3	A	501	FAD	C8-C7	3.48	1.49	1.40
3	B	501	FAD	C9-C8	3.37	1.44	1.39
3	B	501	FAD	C10-N1	3.35	1.40	1.33
3	A	501	FAD	C9-C8	3.33	1.44	1.39
3	A	501	FAD	C10-N10	3.33	1.44	1.37
3	B	501	FAD	C8-C7	3.32	1.48	1.40
3	A	501	FAD	PA-O3P	-3.17	1.56	1.59
3	A	501	FAD	P-O3P	-3.13	1.56	1.59
3	B	501	FAD	C7M-C7	2.85	1.56	1.51
3	A	501	FAD	C6-C5X	2.71	1.44	1.40
3	B	501	FAD	C6-C5X	2.68	1.44	1.40
3	B	501	FAD	PA-O3P	-2.68	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	FAD	C10-N1	2.67	1.38	1.33
3	A	501	FAD	C7M-C7	2.59	1.55	1.51
3	A	501	FAD	C5'-C4'	-2.45	1.48	1.51
3	B	501	FAD	C5'-C4'	-2.26	1.48	1.51
3	B	501	FAD	P-O3P	-2.25	1.57	1.59
3	A	501	FAD	C5A-C6A	2.12	1.46	1.41
3	B	501	FAD	C5A-C6A	2.08	1.46	1.41
4	B	504	NAG	C1-C2	2.03	1.55	1.52
3	A	501	FAD	C2'-C3'	-2.02	1.49	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	FAD	C2'-C1'-N10	4.01	129.16	110.20
3	A	501	FAD	C2'-C1'-N10	4.00	129.12	110.20
3	B	501	FAD	O4B-C1B-N9A	3.13	114.10	108.09
3	A	501	FAD	O4B-C1B-N9A	3.05	113.94	108.09
3	A	501	FAD	C4X-C10-N10	3.02	120.80	116.48
3	A	501	FAD	O3'-C3'-C4'	2.90	115.52	108.93
3	B	501	FAD	C4X-C10-N10	2.81	120.50	116.48
3	B	501	FAD	O3'-C3'-C4'	2.80	115.30	108.93
3	A	501	FAD	C1B-N9A-C8A	2.39	132.41	127.09
3	B	501	FAD	C1B-N9A-C8A	2.29	132.18	127.09
3	B	501	FAD	O3B-C3B-C4B	2.11	117.15	111.08
3	A	501	FAD	O4B-C4B-C3B	-2.04	101.11	105.15
3	A	501	FAD	C9A-N10-C10	-2.04	117.64	120.75
3	B	501	FAD	C9A-N10-C10	-2.01	117.69	120.75

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	FAD	N10-C1'-C2'-O2'
3	B	501	FAD	N10-C1'-C2'-O2'
3	B	501	FAD	N10-C1'-C2'-C3'
3	B	501	FAD	C3'-C4'-C5'-O5'
4	A	504	NAG	C8-C7-N2-C2
4	A	504	NAG	O7-C7-N2-C2
4	B	504	NAG	C8-C7-N2-C2
4	B	504	NAG	O7-C7-N2-C2
4	B	504	NAG	O5-C5-C6-O6
4	A	504	NAG	O5-C5-C6-O6

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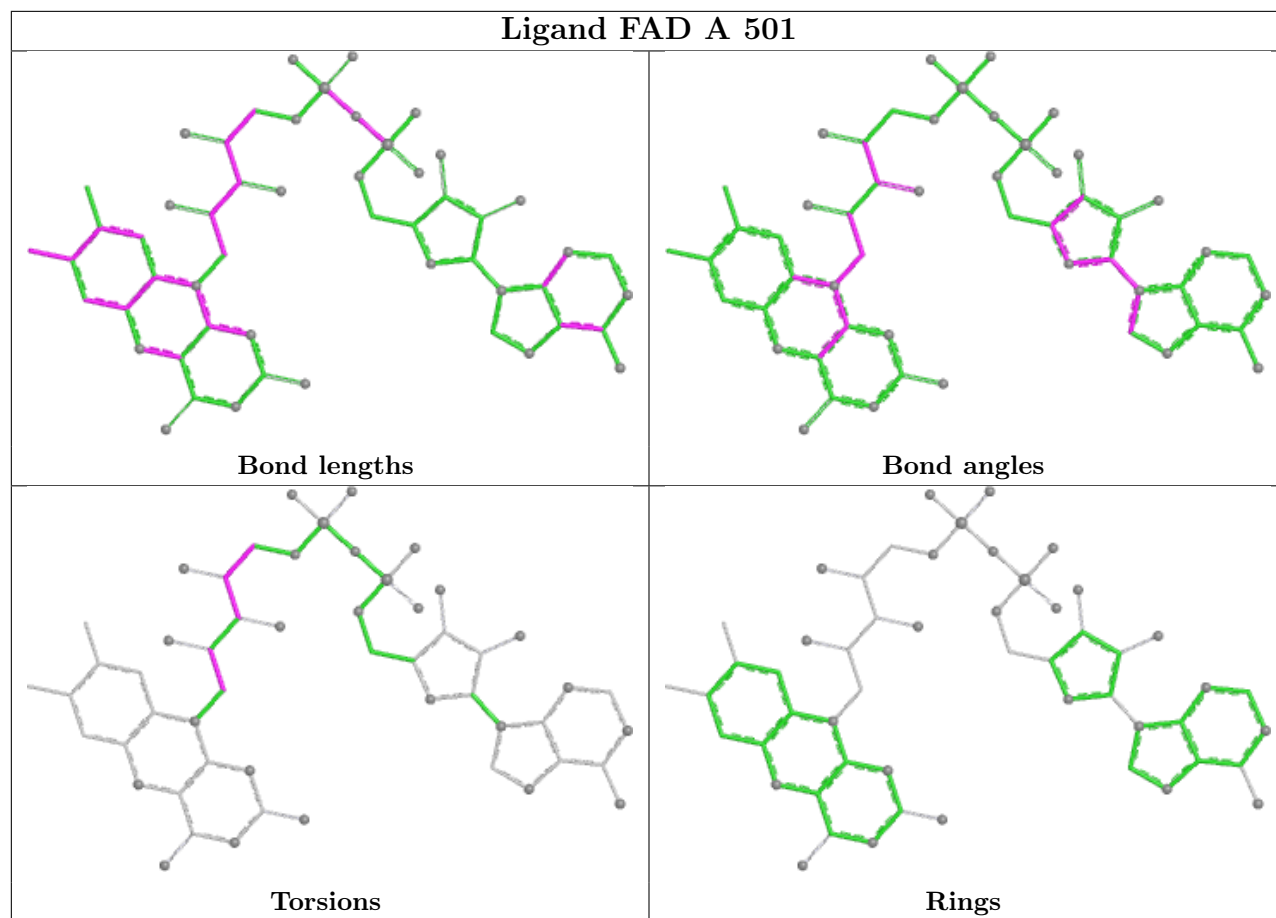
Mol	Chain	Res	Type	Atoms
4	A	504	NAG	C4-C5-C6-O6
4	B	504	NAG	C4-C5-C6-O6
3	A	501	FAD	O3'-C3'-C4'-C5'
3	A	501	FAD	O3'-C3'-C4'-O4'
3	A	501	FAD	O4'-C4'-C5'-O5'
3	B	501	FAD	O4'-C4'-C5'-O5'
3	B	501	FAD	O3'-C3'-C4'-C5'
3	A	501	FAD	C2'-C3'-C4'-O4'
3	A	501	FAD	C3'-C4'-C5'-O5'
3	B	501	FAD	O3'-C3'-C4'-O4'
3	A	501	FAD	C2'-C3'-C4'-C5'
4	B	504	NAG	C3-C2-N2-C7
3	B	501	FAD	C2'-C3'-C4'-C5'
3	B	501	FAD	PA-O3P-P-O1P
3	A	501	FAD	N10-C1'-C2'-C3'
3	B	501	FAD	C2'-C3'-C4'-O4'
3	B	501	FAD	PA-O3P-P-O2P

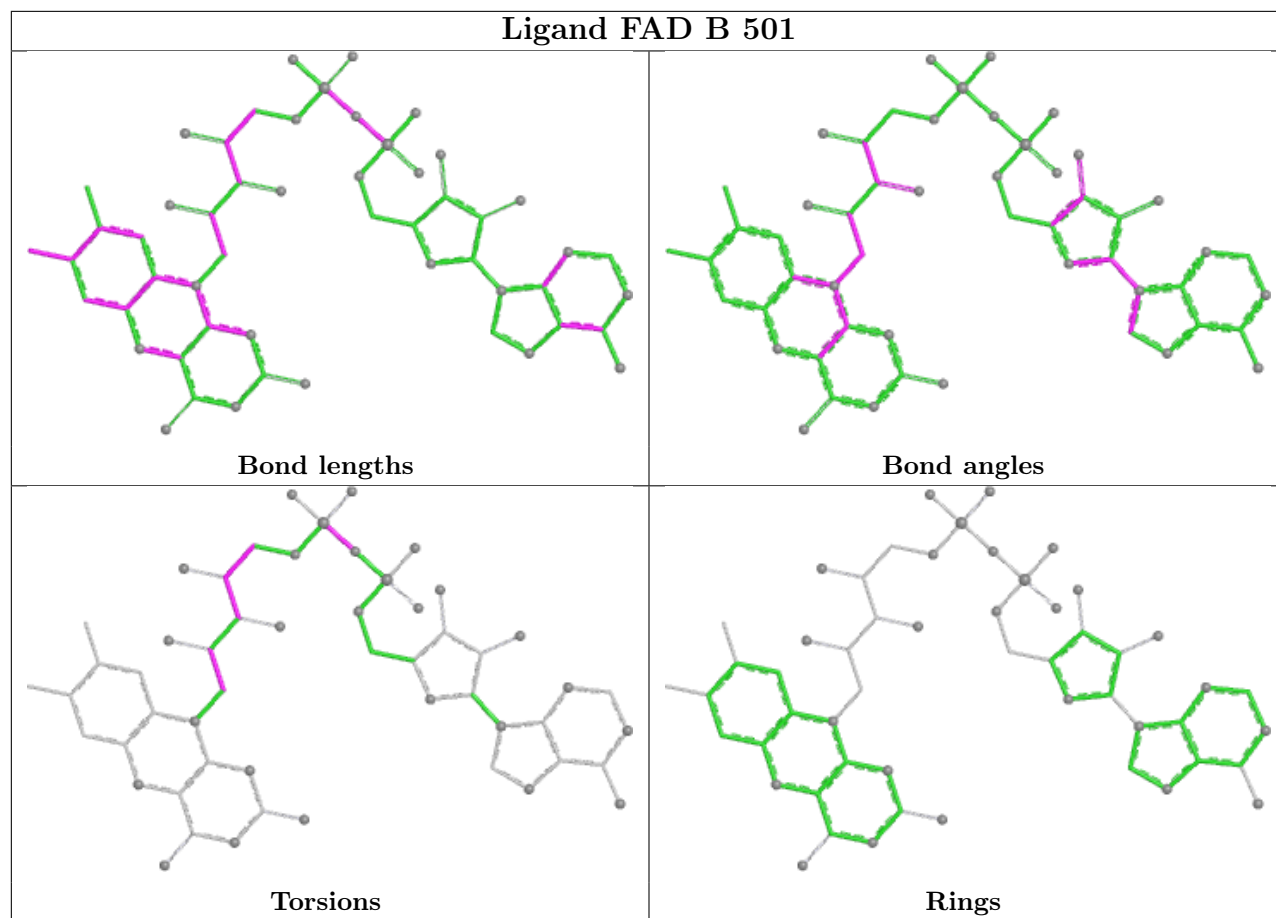
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	FAD	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 than 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.





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, 95th 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	486/497 (97%)	0.28	23 (4%) 36 41	10, 21, 39, 50	0
1	B	485/497 (97%)	0.32	24 (4%) 35 39	10, 23, 41, 49	0
All	All	971/994 (97%)	0.30	47 (4%) 35 40	10, 22, 40, 50	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	PHE	6.5
1	A	288	LEU	4.9
1	B	405	PHE	4.6
1	B	422	ASP	3.9
1	A	316	ILE	3.8
1	B	288	LEU	3.7
1	A	481	ILE	3.6
1	B	15	THR	3.6
1	B	153	THR	3.4
1	B	325	ARG	3.3
1	A	153	THR	3.3
1	B	302	THR	3.3
1	B	298	GLY	3.3
1	A	50	ASP	3.2
1	B	406	GLY	3.2
1	B	347	GLU	3.2
1	A	271	GLN	3.0
1	A	298	GLY	3.0
1	A	422	ASP	3.0
1	A	291	THR	2.9
1	B	292	ALA	2.8
1	B	333	ASN	2.7
1	A	407	GLU	2.6
1	A	269	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	240	ILE	2.5
1	B	241	LYS	2.4
1	A	390	ARG	2.3
1	A	119	LYS	2.3
1	A	45	ILE	2.3
1	B	317	PRO	2.3
1	A	301	ALA	2.3
1	A	318	MET	2.3
1	B	287	VAL	2.3
1	A	333	ASN	2.3
1	B	76	ARG	2.2
1	A	273	ALA	2.2
1	B	497	LEU	2.2
1	A	49	SER	2.2
1	B	304	CYS	2.2
1	A	51	LYS	2.2
1	B	119	LYS	2.2
1	B	316	ILE	2.1
1	A	272	GLY	2.1
1	B	337	PHE	2.1
1	A	497	LEU	2.1
1	B	320	PRO	2.0
1	B	407	GLU	2.0

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

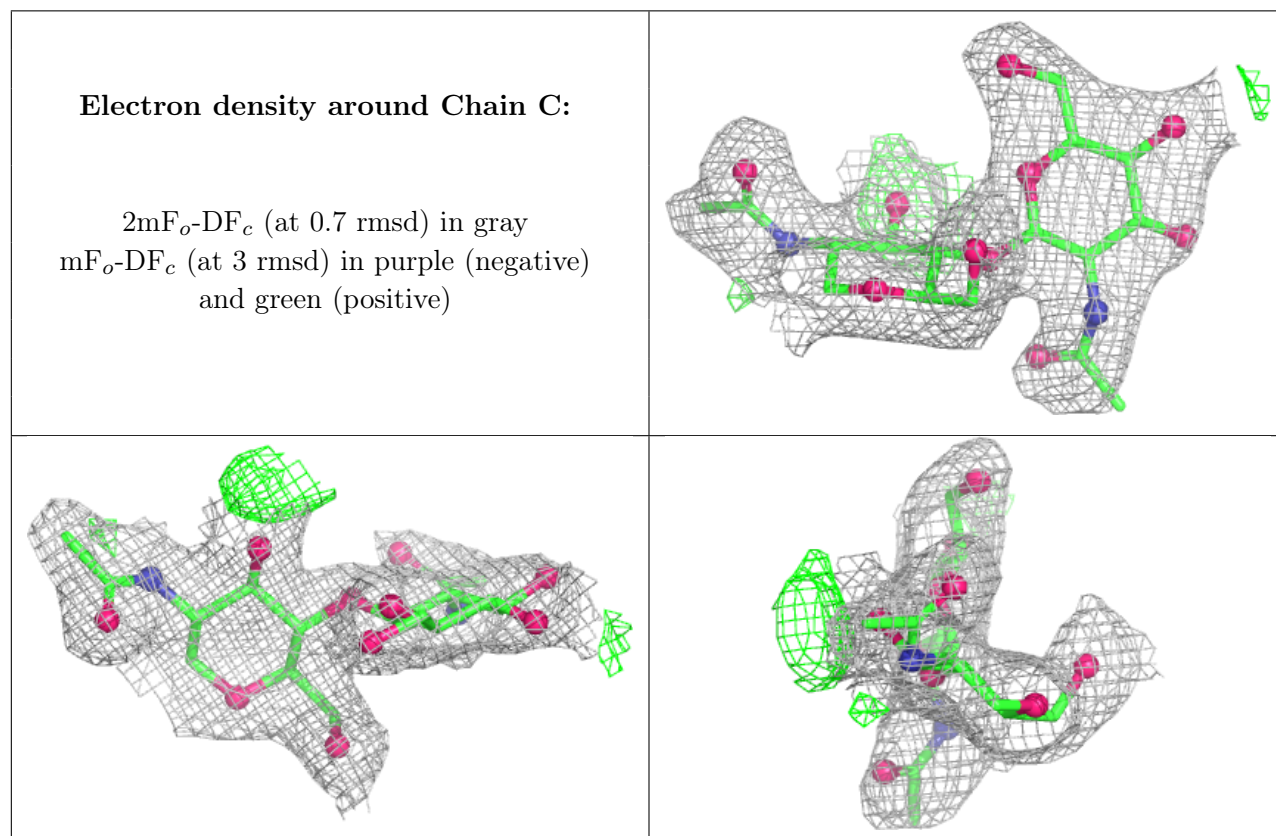
There are no non-standard protein/DNA/RNA residues in this entry.

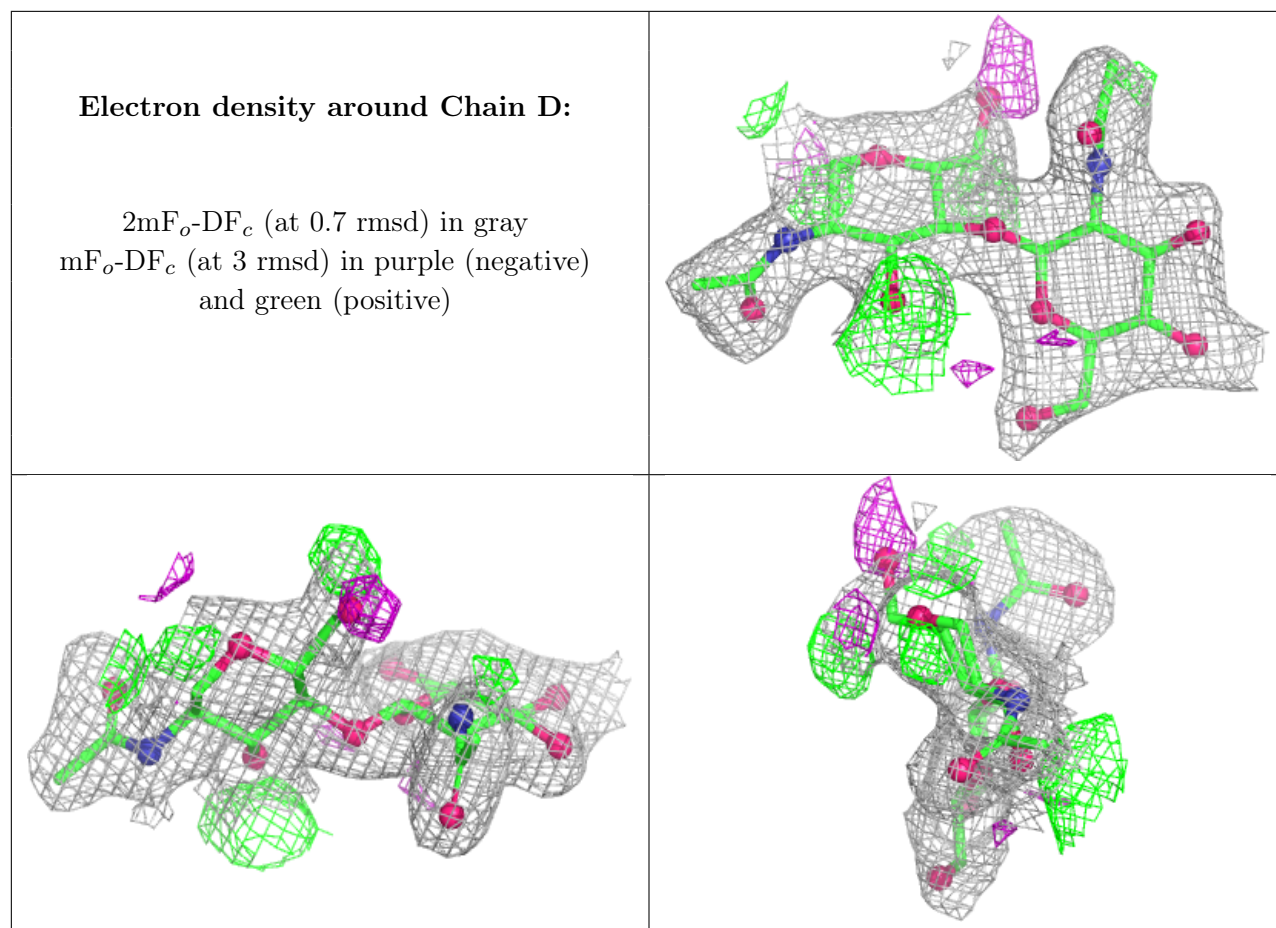
6.3 Carbohydrates [i](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.83	0.12	34,38,40,42	0
2	NAG	C	2	14/15	0.84	0.12	33,37,40,40	0
2	NAG	D	1	14/15	0.85	0.11	24,26,31,38	0
2	NAG	C	1	14/15	0.93	0.07	17,21,24,28	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](#)

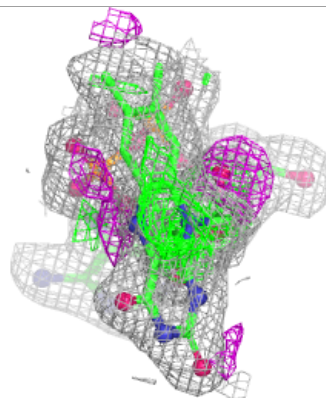
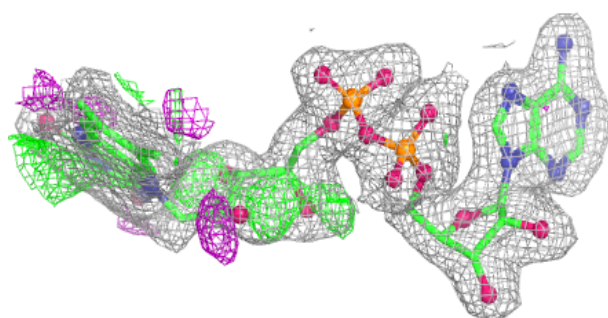
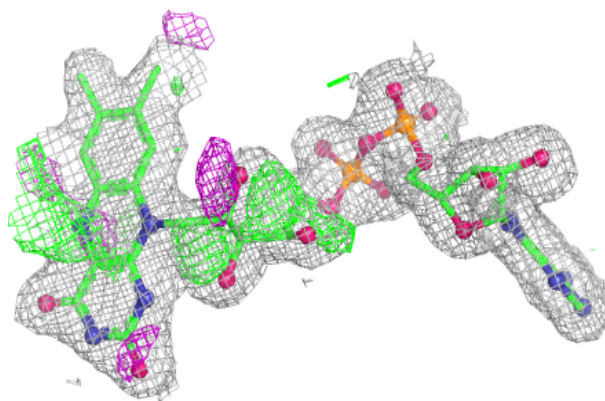
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	504	14/15	0.55	0.16	48,50,54,55	0
4	NAG	B	504	14/15	0.56	0.16	48,50,52,52	0
3	FAD	A	501	53/53	0.94	0.08	8,13,19,21	0
3	FAD	B	501	53/53	0.94	0.08	8,14,22,23	0

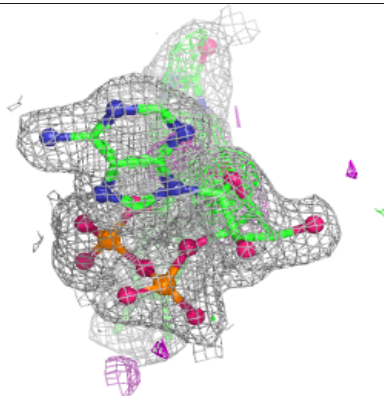
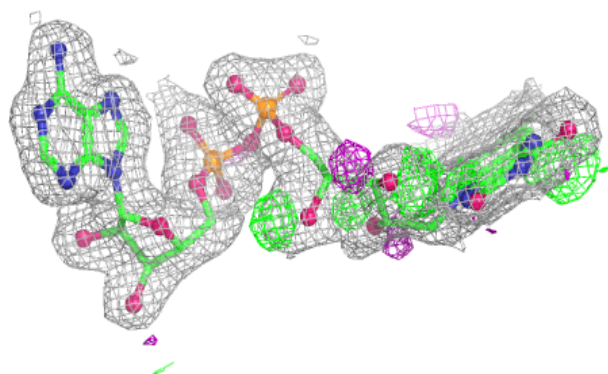
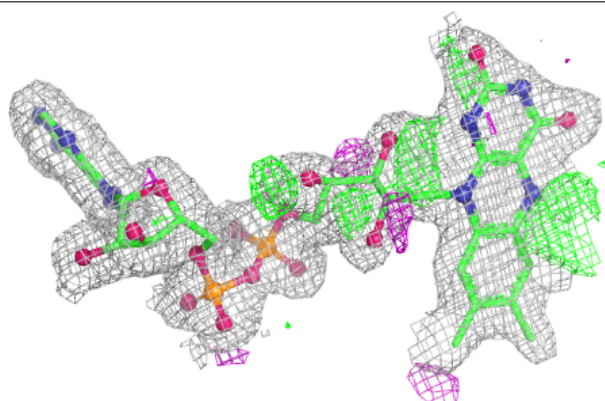
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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 FAD B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.