



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 AM UTC

PDB ID : 6E9N / pdb_00006e9n
Title : E. coli D-galactonate:proton symporter in the inward open form
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Deposited on : 2018-08-01
Resolution : 2.92 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

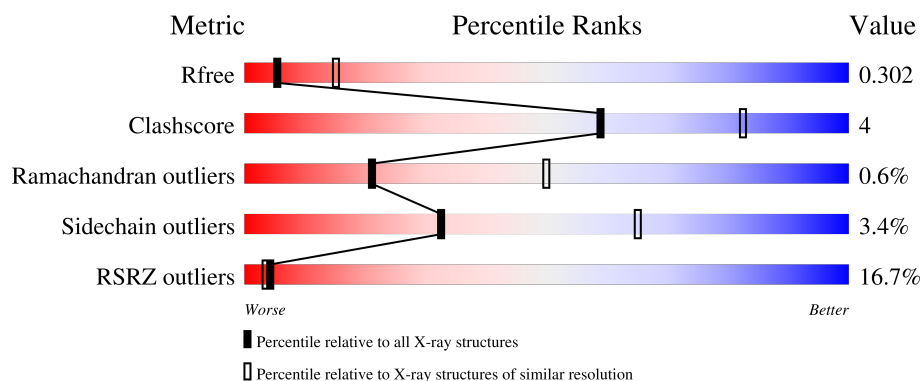
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	460	17% 78% 10% 11%
1	B	460	13% 76% 12% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6472 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 D-galactonate transport.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3177	2125	508	527	17			
1	B	409	Total	C	N	O	S	0	0	0
			3177	2125	508	527	17			

There are 30 discrepancies between the modelled and reference sequences:

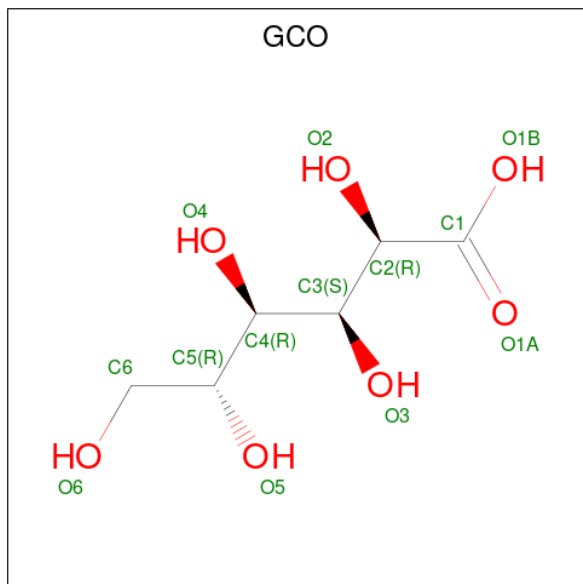
Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	-	expression tag	UNP J7QAK3
A	447	LEU	-	expression tag	UNP J7QAK3
A	448	VAL	-	expression tag	UNP J7QAK3
A	449	PRO	-	expression tag	UNP J7QAK3
A	450	ARG	-	expression tag	UNP J7QAK3
A	451	GLY	-	expression tag	UNP J7QAK3
A	452	SER	-	expression tag	UNP J7QAK3
A	453	GLY	-	expression tag	UNP J7QAK3
A	454	SER	-	expression tag	UNP J7QAK3
A	455	HIS	-	expression tag	UNP J7QAK3
A	456	HIS	-	expression tag	UNP J7QAK3
A	457	HIS	-	expression tag	UNP J7QAK3
A	458	HIS	-	expression tag	UNP J7QAK3
A	459	HIS	-	expression tag	UNP J7QAK3
A	460	HIS	-	expression tag	UNP J7QAK3
B	446	SER	-	expression tag	UNP J7QAK3
B	447	LEU	-	expression tag	UNP J7QAK3
B	448	VAL	-	expression tag	UNP J7QAK3
B	449	PRO	-	expression tag	UNP J7QAK3
B	450	ARG	-	expression tag	UNP J7QAK3
B	451	GLY	-	expression tag	UNP J7QAK3
B	452	SER	-	expression tag	UNP J7QAK3
B	453	GLY	-	expression tag	UNP J7QAK3
B	454	SER	-	expression tag	UNP J7QAK3
B	455	HIS	-	expression tag	UNP J7QAK3

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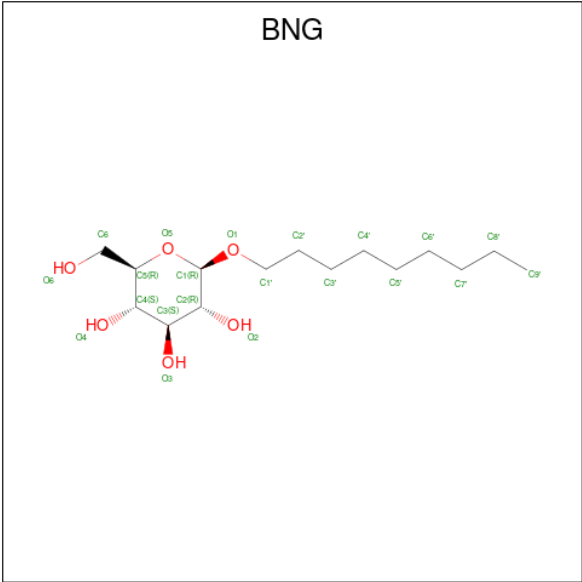
Chain	Residue	Modelled	Actual	Comment	Reference
B	456	HIS	-	expression tag	UNP J7QAK3
B	457	HIS	-	expression tag	UNP J7QAK3
B	458	HIS	-	expression tag	UNP J7QAK3
B	459	HIS	-	expression tag	UNP J7QAK3
B	460	HIS	-	expression tag	UNP J7QAK3

- Molecule 2 is D-gluconic acid (CCD ID: GCO) (formula: $C_6H_{12}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: $C_{15}H_{30}O_6$).

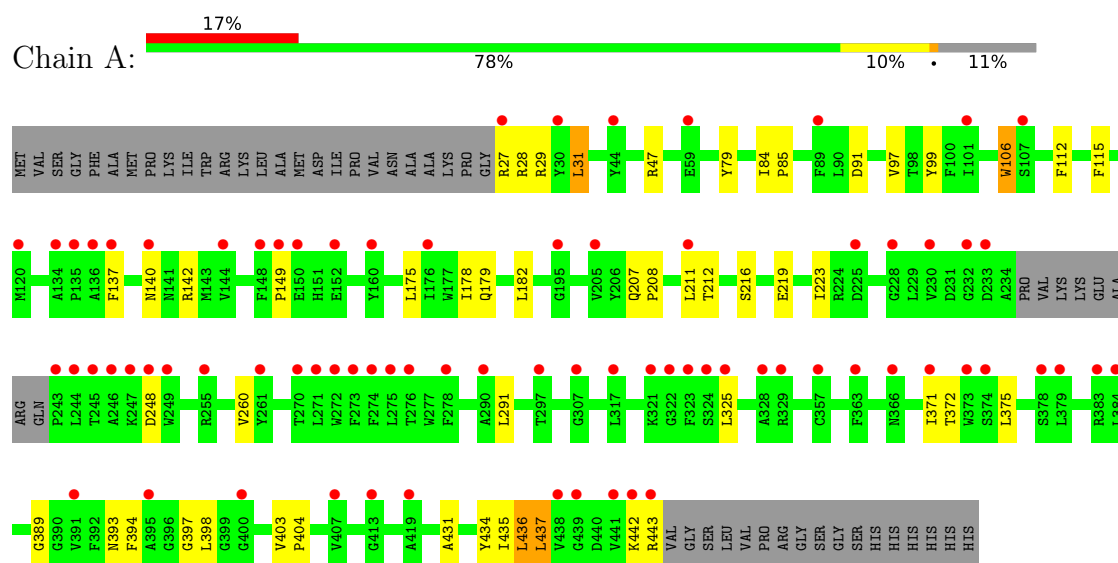


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		

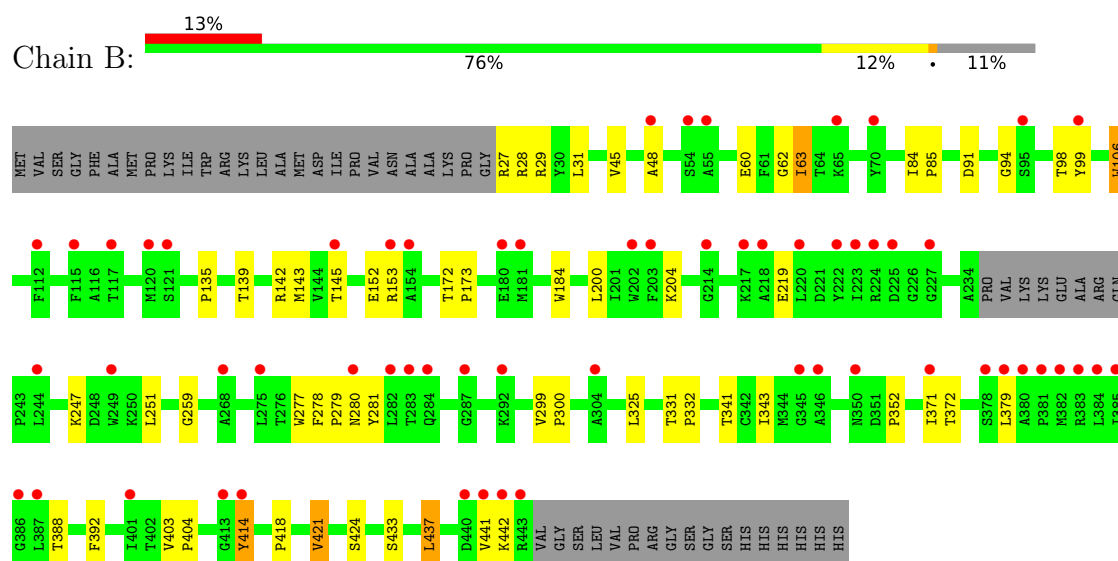
3 Residue-property plots

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: D-galactonate transport



• Molecule 1: D-galactonate transport



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.70Å 107.63Å 103.21Å 90.00° 108.32° 90.00°	Depositor
Resolution (Å)	48.28 – 2.92 48.28 – 2.92	Depositor EDS
% Data completeness (in resolution range)	60.5 (48.28-2.92) 60.5 (48.28-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.243 , 0.297 0.251 , 0.302	Depositor DCC
R_{free} test set	1256 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 8.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

5.1 Standard geometry

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

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	0.12	0/3270	0.29	0/4451
1	B	0.12	0/3270	0.28	0/4451
All	All	0.12	0/6540	0.28	0/8902

There are no bond length outliers.

There are no bond angle outliers.

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	3177	0	3238	28	0
1	B	3177	0	3238	31	0
2	A	13	0	11	2	0
3	A	42	0	60	1	0
3	B	63	0	90	0	0
All	All	6472	0	6637	57	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 (57) 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:60:GLU:OE1	1:B:184:TRP:NE1	2.23	0.71
1:B:91:ASP:OD1	1:B:142:ARG:NH2	2.28	0.66
1:B:247:LYS:O	1:B:251:LEU:N	2.32	0.62
1:B:28:ARG:N	1:B:219:GLU:OE2	2.33	0.61
1:A:115:PHE:O	1:B:204:LYS:NZ	2.38	0.56
1:A:137:PHE:HB2	2:A:501:GCO:H62	1.89	0.55
1:A:435:ILE:HG23	1:A:436:LEU:HD23	1.88	0.54
1:A:47:ARG:NH2	1:A:79:TYR:OH	2.40	0.54
1:B:94:GLY:O	1:B:98:THR:OG1	2.20	0.53
1:A:91:ASP:OD1	1:A:142:ARG:NH2	2.41	0.52
1:A:371:ILE:HA	3:A:502:BNG:H4	1.92	0.52
1:A:389:GLY:O	1:A:393:ASN:ND2	2.43	0.52
1:A:372:THR:O	1:A:375:LEU:N	2.43	0.51
1:A:442:LYS:O	1:A:443:ARG:HB2	2.11	0.51
1:B:139:THR:O	1:B:143:MET:N	2.41	0.50
1:B:29:ARG:NH1	1:B:152:GLU:OE1	2.42	0.50
1:B:277:TRP:O	1:B:281:TYR:N	2.43	0.49
1:B:27:ARG:N	1:B:219:GLU:OE2	2.45	0.49
1:B:388:THR:O	1:B:392:PHE:N	2.41	0.49
1:A:178:ILE:O	1:A:182:LEU:N	2.46	0.47
1:B:84:ILE:N	1:B:85:PRO:HD2	2.29	0.47
1:B:62:GLY:O	1:B:63:ILE:C	2.57	0.47
1:A:137:PHE:HB2	2:A:501:GCO:C6	2.45	0.47
1:A:112:PHE:CZ	1:B:200:LEU:HB2	2.49	0.46
1:B:278:PHE:HB3	1:B:279:PRO:HD3	1.99	0.45
1:A:28:ARG:HH11	1:A:31:LEU:HB3	1.81	0.45
1:B:331:THR:HB	1:B:332:PRO:HD3	1.99	0.45
1:B:341:THR:O	1:B:424:SER:OG	2.31	0.44
1:B:45:VAL:O	1:B:48:ALA:N	2.51	0.44
1:A:106:TRP:CD1	1:A:106:TRP:C	2.95	0.44
1:B:259:GLY:HA2	1:B:437:LEU:HD12	2.00	0.44
1:A:84:ILE:N	1:A:85:PRO:CD	2.81	0.44
1:B:106:TRP:C	1:B:106:TRP:CD1	2.95	0.44
1:B:259:GLY:O	1:B:433:SER:OG	2.36	0.44
1:A:394:PHE:O	1:A:398:LEU:N	2.49	0.43
1:A:137:PHE:O	1:A:140:ASN:N	2.52	0.43
1:A:27:ARG:N	1:A:219:GLU:OE2	2.51	0.43
1:B:84:ILE:HG23	1:B:85:PRO:HD3	2.01	0.43
1:B:172:THR:N	1:B:173:PRO:CD	2.82	0.42
1:B:299:VAL:HB	1:B:300:PRO:HD3	2.00	0.42
1:A:208:PRO:O	1:A:212:THR:OG1	2.31	0.42
1:A:84:ILE:HG12	1:A:85:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HG2	1:A:223:ILE:HD11	2.02	0.42
1:A:248:ASP:OD1	1:A:248:ASP:N	2.53	0.42
1:A:393:ASN:O	1:A:397:GLY:N	2.42	0.42
1:A:403:VAL:CG1	1:A:404:PRO:HD3	2.50	0.42
1:A:431:ALA:O	1:A:435:ILE:HG22	2.20	0.42
1:B:414:TYR:CD2	1:B:414:TYR:N	2.87	0.42
1:B:418:PRO:O	1:B:421:VAL:N	2.50	0.41
1:B:403:VAL:N	1:B:404:PRO:CD	2.83	0.41
1:A:84:ILE:CG1	1:A:85:PRO:HD3	2.50	0.41
1:B:145:THR:HA	1:B:153:ARG:HE	1.85	0.41
1:B:379:LEU:HA	1:B:442:LYS:O	2.21	0.40
1:A:175:LEU:O	1:A:179:GLN:N	2.42	0.40
1:A:436:LEU:HB2	1:A:437:LEU:HD23	2.04	0.40
1:B:343:ILE:HG22	1:B:424:SER:OG	2.21	0.40
1:B:135:PRO:O	1:B:139:THR:HG23	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	405/460 (88%)	383 (95%)	21 (5%)	1 (0%)	43	71
1	B	405/460 (88%)	389 (96%)	12 (3%)	4 (1%)	12	37
All	All	810/920 (88%)	772 (95%)	33 (4%)	5 (1%)	21	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	VAL
1	B	63	ILE
1	B	352	PRO

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Mol	Chain	Res	Type
1	A	149	PRO
1	B	371	ILE

5.3.2 Protein sidechains ⓘ

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	325/366 (89%)	312 (96%)	13 (4%)	28	61
1	B	325/366 (89%)	316 (97%)	9 (3%)	38	70
All	All	650/732 (89%)	628 (97%)	22 (3%)	32	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	97	VAL
1	A	99	TYR
1	A	106	TRP
1	A	207	GLN
1	A	211	LEU
1	A	216	SER
1	A	260	VAL
1	A	291	LEU
1	A	325	LEU
1	A	434	TYR
1	A	436	LEU
1	A	437	LEU
1	B	31	LEU
1	B	99	TYR
1	B	106	TRP
1	B	280	ASN
1	B	325	LEU
1	B	372	THR
1	B	414	TYR
1	B	421	VAL

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Mol	Chain	Res	Type
1	B	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GCO	A	501	-	12,12,12	0.99	0	15,16,16	1.13	1 (6%)
3	BNG	B	502	-	21,21,21	1.06	2 (9%)	26,26,26	0.84	0
3	BNG	A	502	-	21,21,21	1.06	1 (4%)	26,26,26	0.91	1 (3%)
3	BNG	B	503	-	21,21,21	1.15	2 (9%)	26,26,26	0.93	2 (7%)
3	BNG	B	501	-	21,21,21	1.03	2 (9%)	26,26,26	1.16	3 (11%)
3	BNG	A	503	-	21,21,21	1.10	2 (9%)	26,26,26	0.83	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	GCO	A	501	-	-	14/18/18/18	-
3	BNG	B	502	-	-	5/12/32/32	0/1/1/1
3	BNG	A	502	-	-	10/12/32/32	0/1/1/1
3	BNG	B	503	-	-	8/12/32/32	0/1/1/1
3	BNG	B	501	-	-	4/12/32/32	0/1/1/1
3	BNG	A	503	-	-	8/12/32/32	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	BNG	O5-C1	3.52	1.50	1.41
3	A	503	BNG	O5-C1	3.49	1.50	1.41
3	B	502	BNG	O5-C1	3.35	1.50	1.41
3	A	502	BNG	O5-C1	3.34	1.50	1.41
3	B	501	BNG	O5-C1	3.31	1.50	1.41
3	B	503	BNG	O1-C1	-2.17	1.36	1.40
3	B	502	BNG	O1-C1	-2.11	1.36	1.40
3	A	503	BNG	O1-C1	-2.03	1.36	1.40
3	B	501	BNG	O1-C1	-2.01	1.36	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	BNG	C1-C2-C3	2.66	115.60	110.01
3	B	503	BNG	O5-C5-C4	2.43	114.07	109.70
3	B	503	BNG	C1'-O1-C1	2.31	117.63	113.68
3	B	501	BNG	C1-O5-C5	-2.29	109.24	113.72
2	A	501	GCO	O1B-C1-C2	2.26	119.58	113.31
3	A	502	BNG	C1-O5-C5	-2.20	109.42	113.72
3	B	501	BNG	C4-C3-C2	2.10	114.51	110.83

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GCO	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	501	GCO	C1-C2-C3-O3
2	A	501	GCO	O2-C2-C3-C4
2	A	501	GCO	O2-C2-C3-O3
2	A	501	GCO	O5-C5-C6-O6
3	A	503	BNG	C2'-C1'-O1-C1
3	B	502	BNG	C2-C1-O1-C1'
3	B	502	BNG	O5-C1-O1-C1'
3	B	503	BNG	O5-C1-O1-C1'
2	A	501	GCO	O1A-C1-C2-O2
2	A	501	GCO	O1B-C1-C2-O2
2	A	501	GCO	C4-C5-C6-O6
3	A	503	BNG	O5-C5-C6-O6
3	B	503	BNG	O5-C5-C6-O6
3	A	503	BNG	C4-C5-C6-O6
3	A	502	BNG	O5-C1-O1-C1'
3	A	502	BNG	C2-C1-O1-C1'
3	B	503	BNG	C2-C1-O1-C1'
3	B	503	BNG	C2'-C3'-C4'-C5'
3	A	502	BNG	O1-C1'-C2'-C3'
3	A	503	BNG	C5'-C6'-C7'-C8'
3	B	501	BNG	C5'-C6'-C7'-C8'
3	B	502	BNG	C4'-C5'-C6'-C7'
3	A	503	BNG	C3'-C4'-C5'-C6'
3	B	501	BNG	C1'-C2'-C3'-C4'
3	B	503	BNG	C4-C5-C6-O6
3	A	503	BNG	C2-C1-O1-C1'
3	A	502	BNG	C1'-C2'-C3'-C4'
2	A	501	GCO	O1A-C1-C2-C3
3	B	501	BNG	O5-C5-C6-O6
3	A	502	BNG	O5-C5-C6-O6
2	A	501	GCO	O1B-C1-C2-C3
2	A	501	GCO	O3-C3-C4-O4
3	A	503	BNG	C1'-C2'-C3'-C4'
3	B	503	BNG	C4'-C5'-C6'-C7'
3	B	503	BNG	C5'-C6'-C7'-C8'
3	B	503	BNG	C2'-C1'-O1-C1
3	A	503	BNG	O1-C1'-C2'-C3'
3	A	502	BNG	C4'-C5'-C6'-C7'
3	B	502	BNG	C1'-C2'-C3'-C4'
2	A	501	GCO	O3-C3-C4-C5
2	A	501	GCO	C2-C3-C4-C5
3	B	502	BNG	O1-C1'-C2'-C3'

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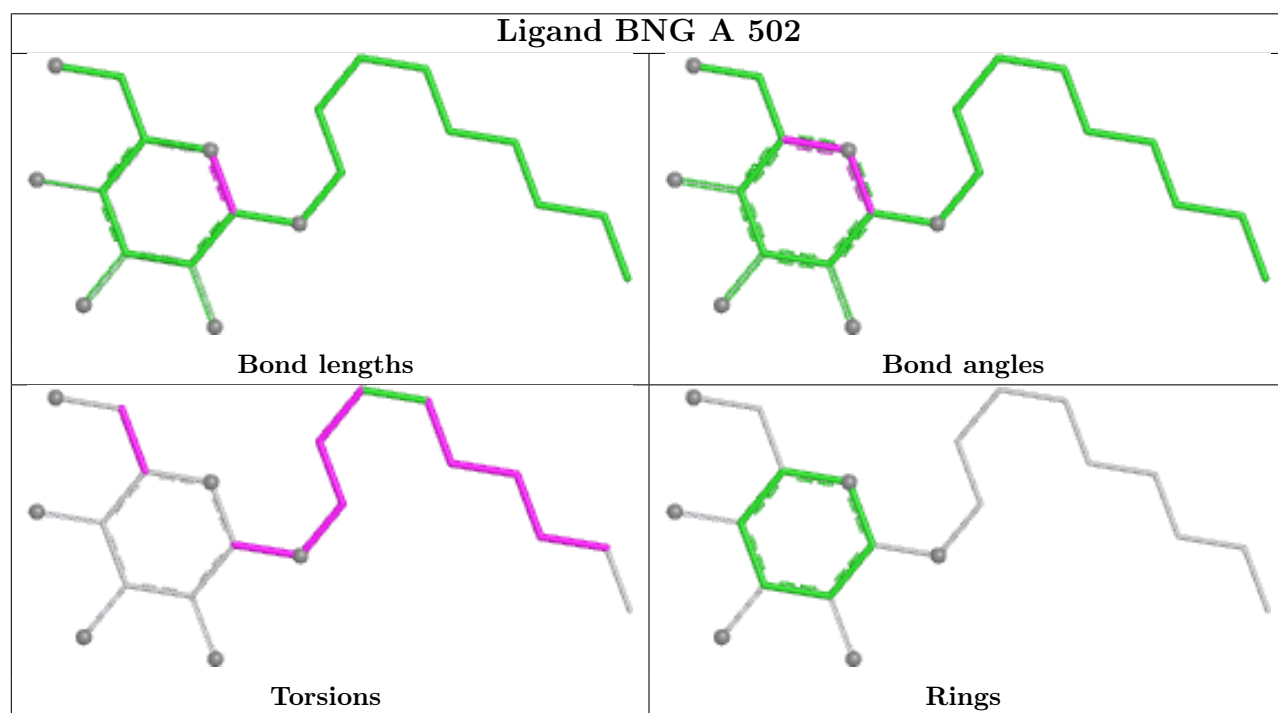
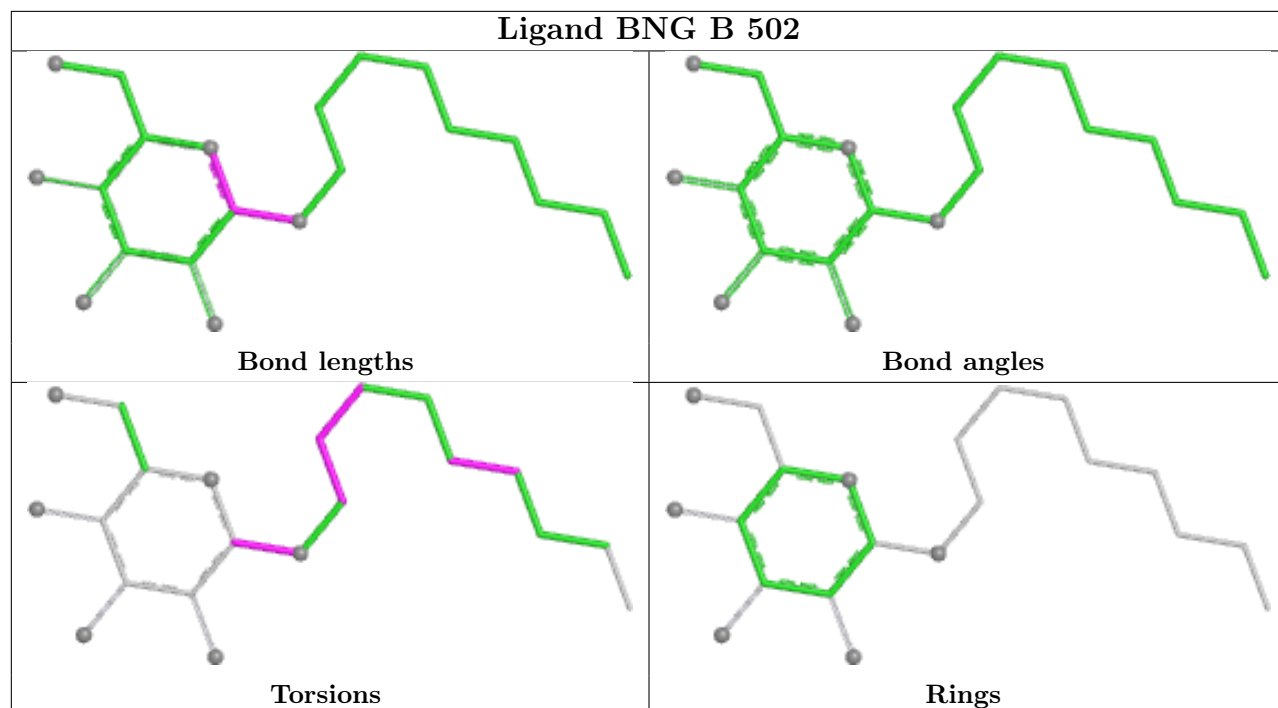
Mol	Chain	Res	Type	Atoms
3	A	502	BNG	C6'-C7'-C8'-C9'
2	A	501	GCO	C2-C3-C4-O4
3	A	502	BNG	C3'-C4'-C5'-C6'
3	A	502	BNG	C2'-C1'-O1-C1
3	B	501	BNG	C6'-C7'-C8'-C9'
3	A	502	BNG	C5'-C6'-C7'-C8'

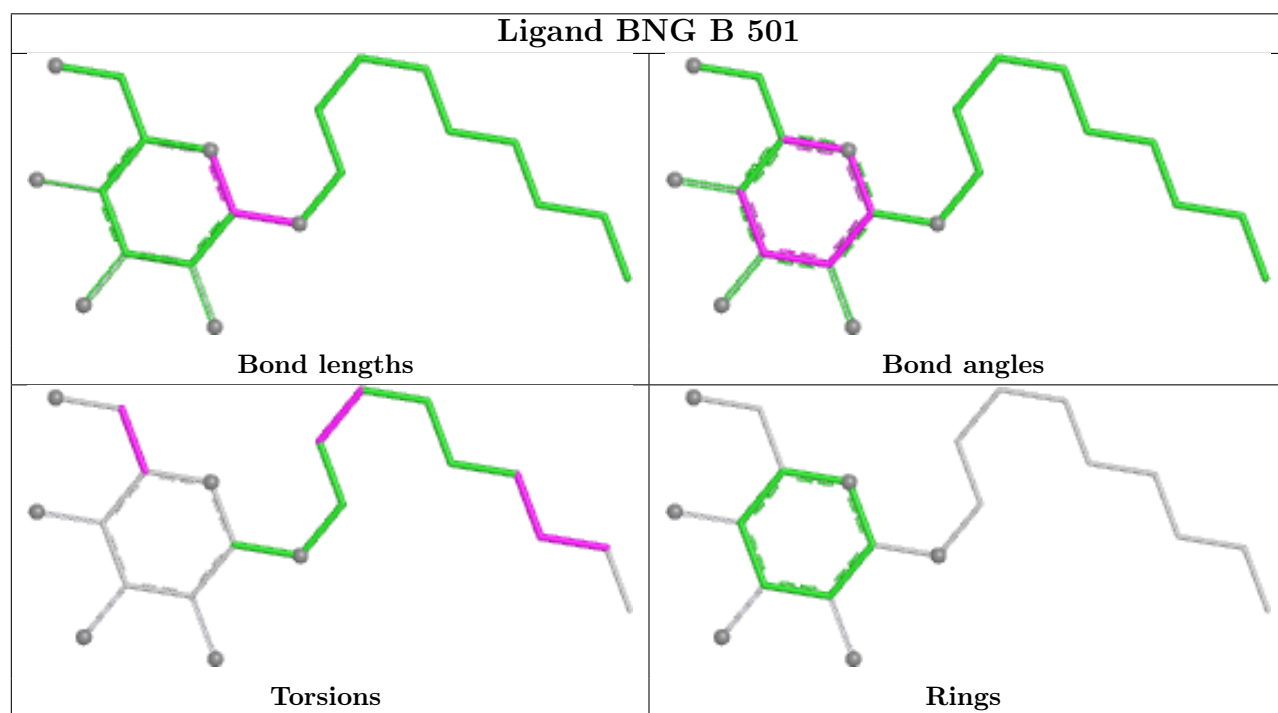
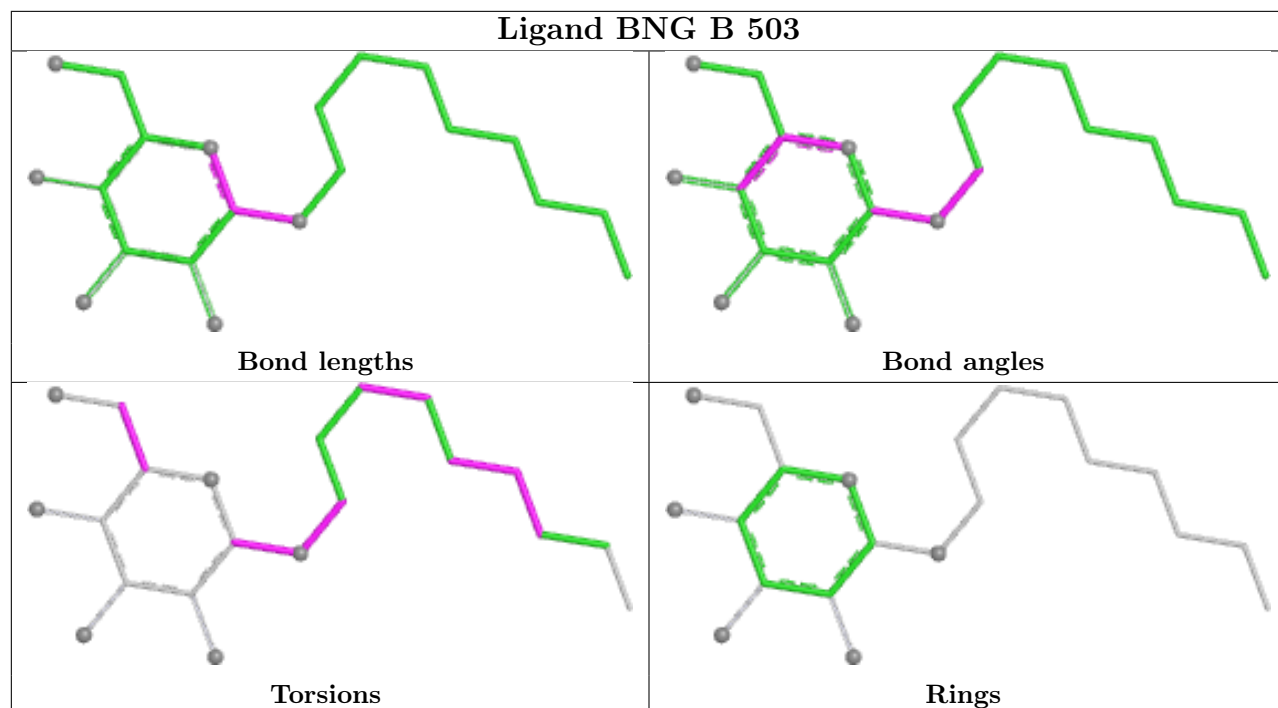
There are no ring outliers.

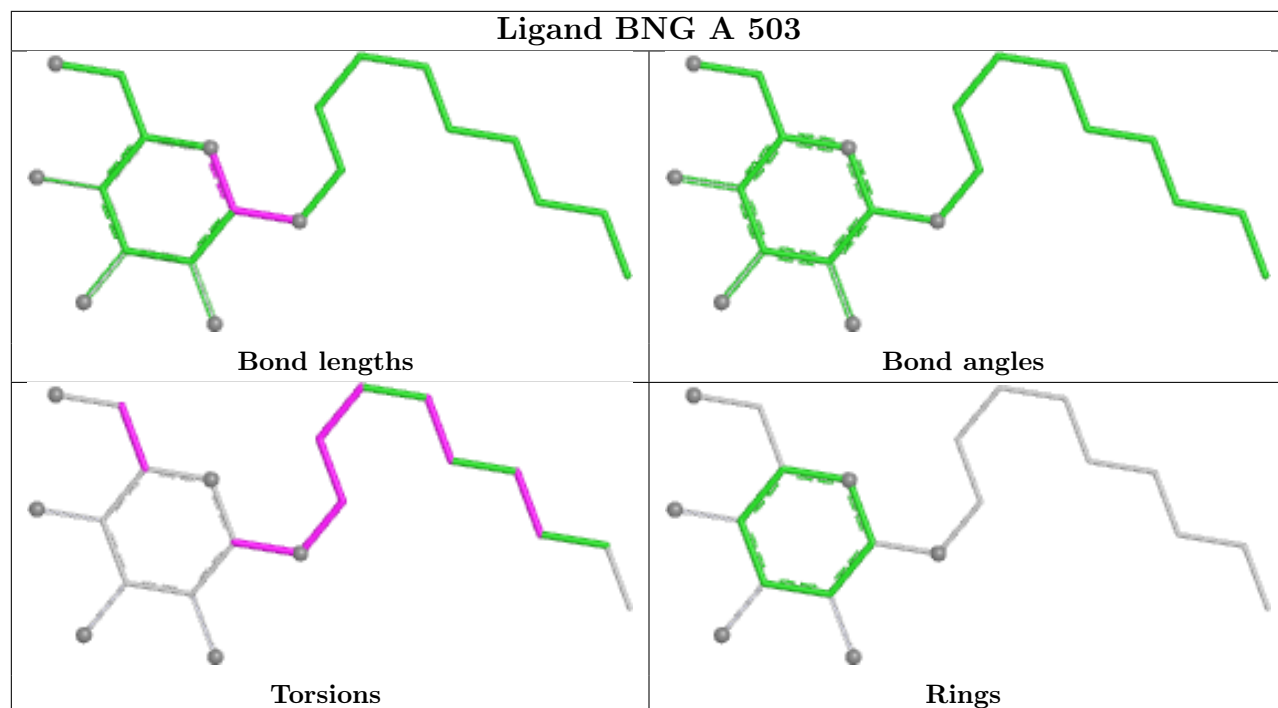
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GCO	2	0
3	A	502	BNG	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	409/460 (88%)	1.17	77 (18%) 3 3	24, 50, 100, 153	0
1	B	409/460 (88%)	1.00	60 (14%) 6 4	25, 56, 86, 127	0
All	All	818/920 (88%)	1.09	137 (16%) 4 3	24, 54, 94, 153	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	PRO	10.7
1	A	244	LEU	9.8
1	A	245	THR	7.4
1	A	248	ASP	6.4
1	A	272	TRP	6.1
1	B	382	MET	6.1
1	A	273	PHE	5.6
1	B	345	GLY	5.5
1	A	249	TRP	5.5
1	B	379	LEU	5.5
1	B	217	LYS	5.1
1	B	441	VAL	5.1
1	A	378	SER	5.1
1	A	325	LEU	4.7
1	B	225	ASP	4.7
1	A	152	GLU	4.7
1	A	441	VAL	4.7
1	A	274	PHE	4.6
1	B	443	ARG	4.5
1	A	144	VAL	4.4
1	A	323	PHE	4.3
1	B	65	LYS	4.2
1	A	363	PHE	4.2
1	B	383	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	101	ILE	4.1
1	A	275	LEU	4.0
1	A	148	PHE	3.9
1	A	246	ALA	3.9
1	B	112	PHE	3.9
1	A	324	SER	3.7
1	B	442	LYS	3.7
1	A	278	PHE	3.7
1	B	180	GLU	3.6
1	A	270	THR	3.6
1	B	371	ILE	3.6
1	B	386	GLY	3.5
1	A	205	VAL	3.4
1	B	214	GLY	3.4
1	B	346	ALA	3.4
1	B	218	ALA	3.3
1	B	440	ASP	3.3
1	B	292	LYS	3.2
1	B	381	PRO	3.2
1	B	181	MET	3.2
1	B	117	THR	3.2
1	B	120	MET	3.2
1	A	44	TYR	3.1
1	B	414	TYR	3.1
1	A	329	ARG	3.1
1	A	383	ARG	3.1
1	A	384	LEU	3.1
1	A	255	ARG	3.1
1	B	380	ALA	3.1
1	A	30	TYR	3.1
1	A	195	GLY	3.1
1	A	225	ASP	3.0
1	A	321	LYS	3.0
1	B	202	TRP	3.0
1	B	387	LEU	2.9
1	B	222	TYR	2.9
1	B	385	ILE	2.9
1	B	384	LEU	2.9
1	A	400	GLY	2.8
1	A	442	LYS	2.8
1	B	70	TYR	2.8
1	B	287	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	373	TRP	2.8
1	A	160	TYR	2.8
1	A	233	ASP	2.8
1	A	317	LEU	2.7
1	A	379	LEU	2.7
1	A	150	GLU	2.7
1	A	228	GLY	2.6
1	B	280	ASN	2.6
1	A	271	LEU	2.6
1	A	27	ARG	2.6
1	A	261	TYR	2.6
1	A	107	SER	2.6
1	B	153	ARG	2.6
1	A	232	GLY	2.6
1	A	371	ILE	2.6
1	A	419	ALA	2.5
1	A	247	LYS	2.5
1	A	176	ILE	2.5
1	A	357	CYS	2.5
1	A	443	ARG	2.5
1	B	54	SER	2.5
1	A	391	VAL	2.5
1	B	244	LEU	2.4
1	B	249	TRP	2.4
1	A	328	ALA	2.4
1	B	350	ASN	2.4
1	A	407	VAL	2.4
1	A	89	PHE	2.4
1	A	413	GLY	2.3
1	B	227	GLY	2.3
1	B	55	ALA	2.3
1	B	224	ARG	2.3
1	A	439	GLY	2.3
1	A	374	SER	2.3
1	B	283	THR	2.3
1	B	99	TYR	2.3
1	B	378	SER	2.3
1	A	366	ASN	2.2
1	B	284	GLN	2.2
1	B	145	THR	2.2
1	B	401	ILE	2.2
1	A	230	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	MET	2.2
1	B	203	PHE	2.2
1	A	135	PRO	2.2
1	A	322	GLY	2.2
1	B	115	PHE	2.2
1	B	282	LEU	2.2
1	B	48	ALA	2.2
1	B	121	SER	2.2
1	A	297	THR	2.1
1	A	307	GLY	2.1
1	B	413	GLY	2.1
1	A	136	ALA	2.1
1	B	304	ALA	2.1
1	A	438	VAL	2.1
1	A	134	ALA	2.1
1	A	290	ALA	2.1
1	B	154	ALA	2.1
1	B	268	ALA	2.1
1	B	223	ILE	2.1
1	A	140	ASN	2.1
1	B	275	LEU	2.1
1	A	137	PHE	2.1
1	B	95	SER	2.1
1	A	149	PRO	2.1
1	A	276	THR	2.1
1	A	395	ALA	2.1
1	A	211	LEU	2.0
1	B	220	LEU	2.0
1	A	59	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

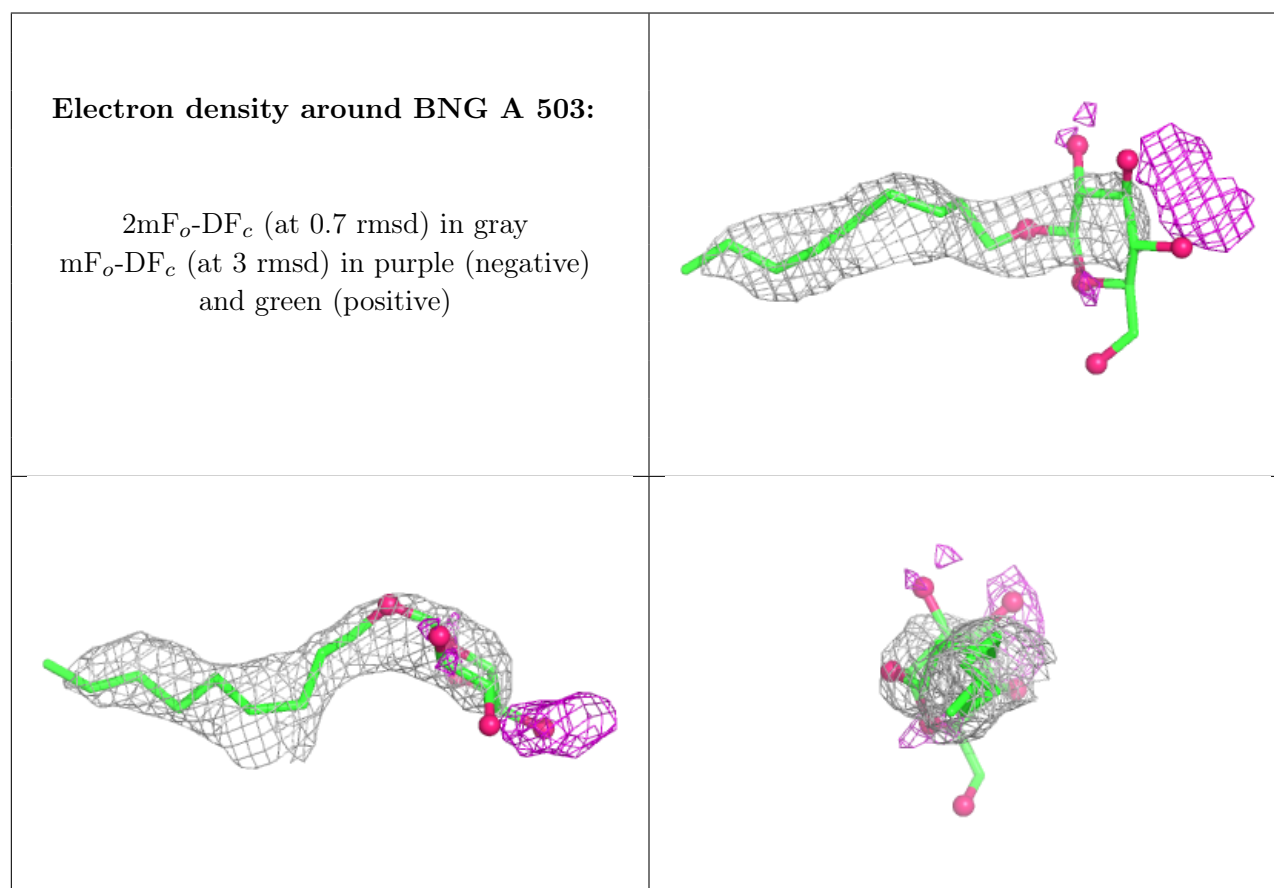
There are no oligosaccharides in this entry.

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, 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.

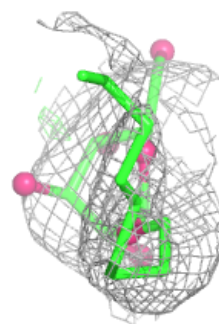
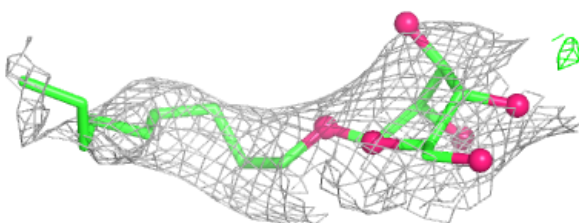
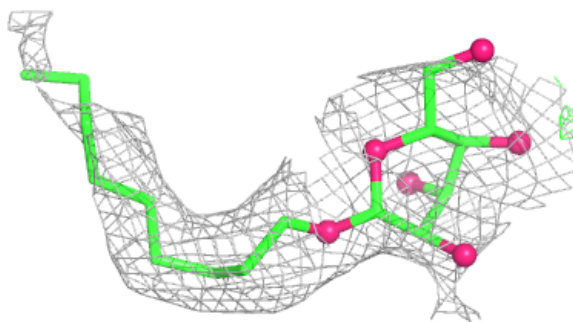
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GCO	A	501	13/13	0.59	0.20	69,91,98,105	0
3	BNG	A	503	21/21	0.64	0.23	37,58,95,103	0
3	BNG	B	501	21/21	0.76	0.18	45,66,78,104	0
3	BNG	B	502	21/21	0.76	0.17	69,83,98,100	0
3	BNG	B	503	21/21	0.76	0.24	45,77,102,105	0
3	BNG	A	502	21/21	0.77	0.23	46,79,97,110	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.

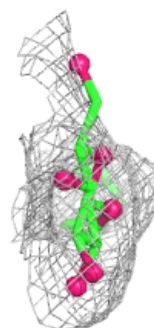
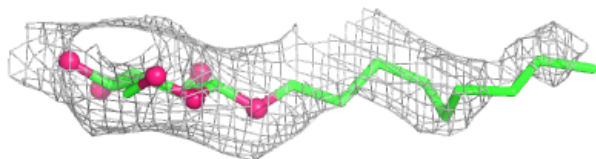


Electron density around BNG B 501:

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

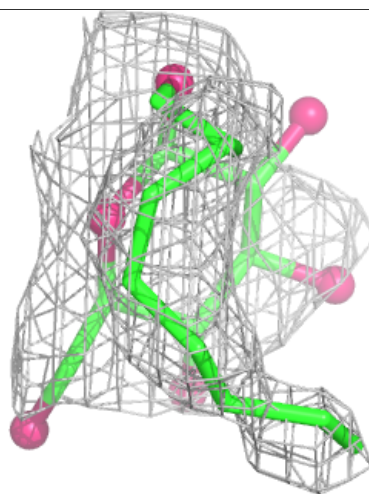
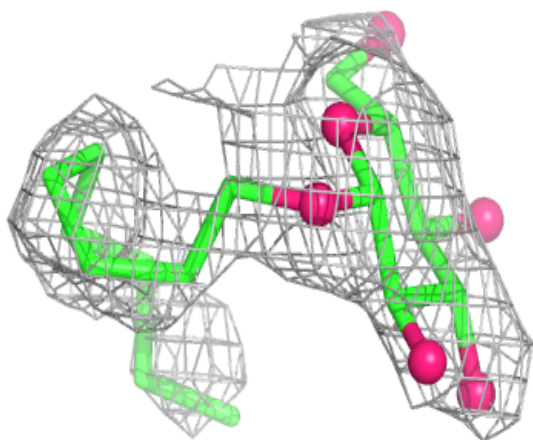
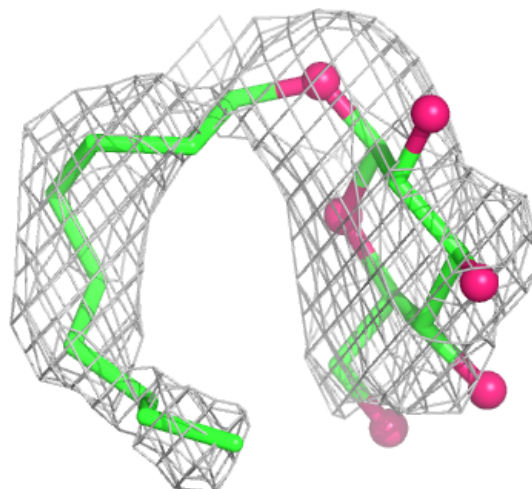
**Electron density around BNG B 502:**

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



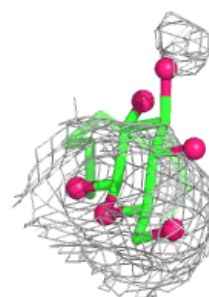
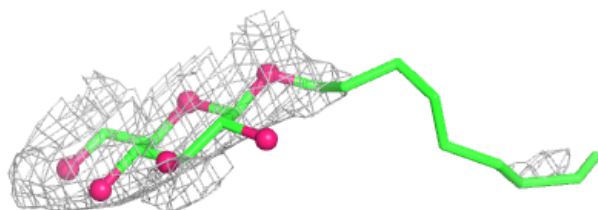
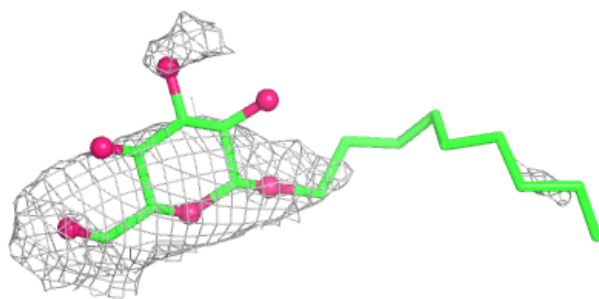
Electron density around BNG B 503:

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



Electron density around BNG A 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.