



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:06 AM UTC

PDB ID : 6RQ7 / pdb_00006rq7
Title : Gadolinium MRI contrast compound binding in human plasma glycoprotein afamin - resurrection of highly anisotropic data
Authors : Rupp, B.; Bowler, M.W.; Naschberger, A.; Juyoux, P.; vonVelsen, J.
Deposited on : 2019-05-15
Resolution : 2.69 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

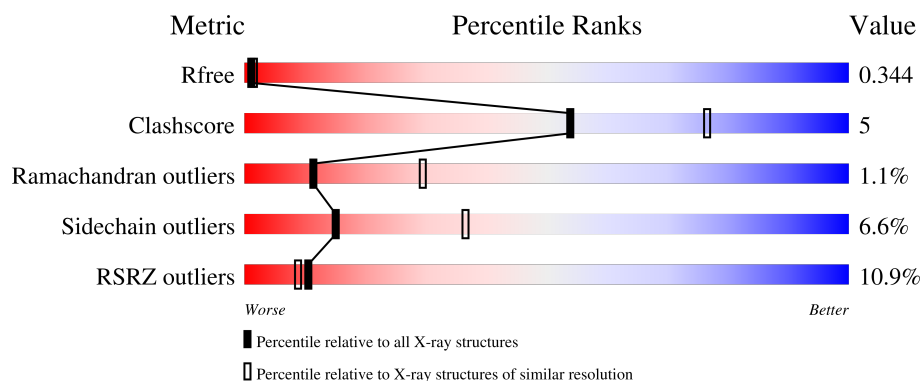
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	B	586	9% 67% 14% • 18%
2	A	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4018 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 Afamin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	479	Total	C	N	O	S	0	1	0
			3875	2462	649	731	33			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	579	LYS	-	expression tag	UNP P43652
B	580	GLY	-	expression tag	UNP P43652
B	581	GLU	-	expression tag	UNP P43652
B	582	ASN	-	expression tag	UNP P43652
B	583	LEU	-	expression tag	UNP P43652
B	584	TYR	-	expression tag	UNP P43652
B	585	PHE	-	expression tag	UNP P43652
B	586	GLN	-	expression tag	UNP P43652

- 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	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd) (labeled as "Ligand of Interest" by depositor).

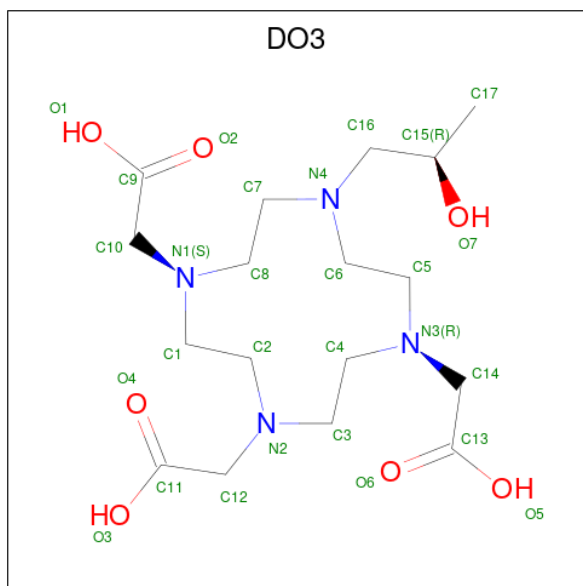
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Gd	0	0
			3	3		

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 10-((2R)-2-HYDROXYPROPYL)-1,4,7,10-TETRAAZACYCLODODECANE 1,4,7-TRIACETIC ACID (CCD ID: DO3) (formula: $C_{17}H_{32}N_4O_7$).

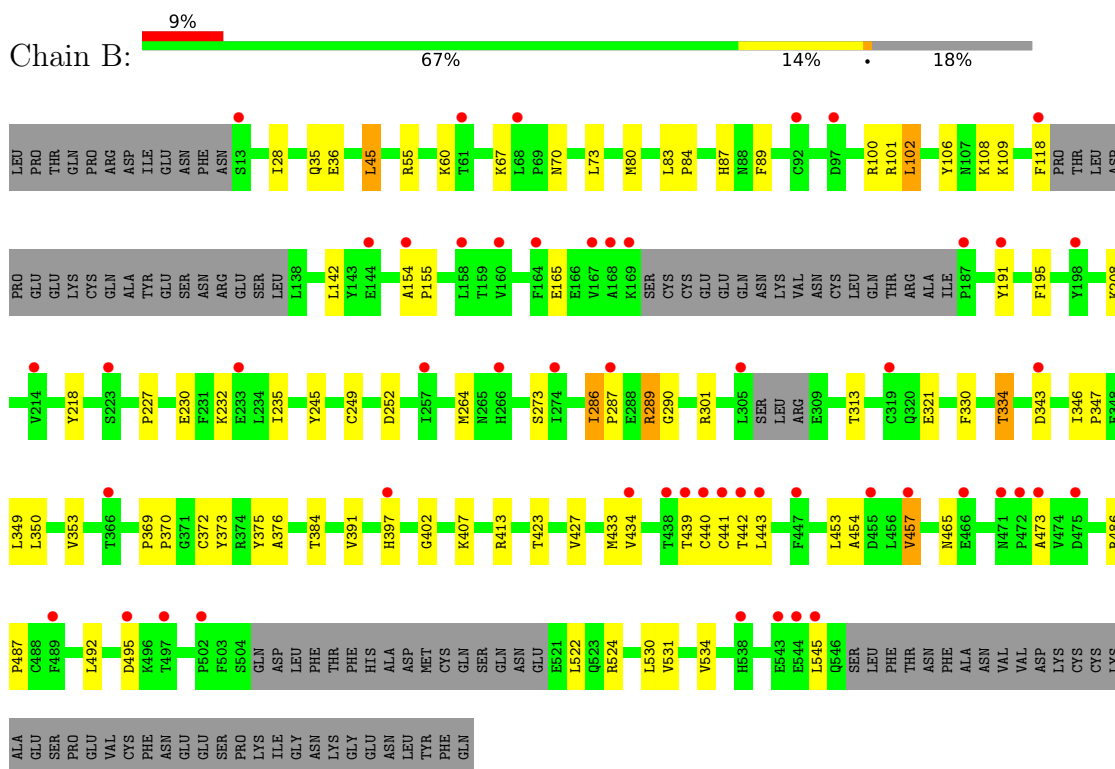


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 28	C 17	N 4	O 7	28	0
5	B	1	Total 28	C 17	N 4	O 7	28	0
5	B	1	Total 28	C 17	N 4	O 7	28	0

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: Afamin



- 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.35Å 109.73Å 48.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.24 – 2.69 75.24 – 2.69	Depositor EDS
% Data completeness (in resolution range)	59.6 (75.24-2.69) 59.8 (75.24-2.69)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.263 , 0.335 0.267 , 0.344	Depositor DCC
R_{free} test set	482 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4018	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: GD, DO3, 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	B	0.98	0/3956	1.56	1/5330 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	GLY	CA-C-O	-5.58	118.12	122.52

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	B	3875	0	3796	38	0
2	A	28	0	25	0	0
3	B	3	0	0	0	0
4	B	28	0	26	0	0
5	B	84	0	85	0	0
All	All	4018	0	3932	38	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 5.

All (38) 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:441:CYS:O	1:B:441:CYS:SG	2.55	0.63
1:B:334:THR:HG22	1:B:353:VAL:HG21	1.90	0.54
1:B:423:THR:O	1:B:427:VAL:HG23	2.08	0.54
1:B:370:PRO:HA	1:B:373:TYR:CE2	2.46	0.49
1:B:330:PHE:O	1:B:334:THR:HG23	2.12	0.49
1:B:433:MET:SD	1:B:457:VAL:HG21	2.53	0.49
1:B:454:ALA:O	1:B:457:VAL:HG22	2.13	0.48
1:B:35:GLN:HE22	1:B:109:LYS:H	1.62	0.47
1:B:346:ILE:HB	1:B:347:PRO:HD3	1.97	0.47
1:B:154:ALA:HB3	1:B:155:PRO:HD3	1.96	0.46
1:B:218:TYR:HH	1:B:245:TYR:HH	1.63	0.46
1:B:334:THR:HG22	1:B:353:VAL:CG2	2.46	0.45
1:B:413:ARG:NH1	1:B:492:LEU:O	2.49	0.45
1:B:83:LEU:HB3	1:B:84:PRO:HD3	1.97	0.45
1:B:264:MET:HG3	1:B:290:GLY:HA2	1.99	0.44
1:B:534:VAL:HG22	1:B:545:LEU:HD13	1.99	0.44
1:B:84:PRO:HA	1:B:89:PHE:CE2	2.53	0.43
1:B:102:LEU:HD22	1:B:106:TYR:CE2	2.54	0.43
1:B:313:THR:HG22	1:B:376:ALA:HB3	1.99	0.43
1:B:486:ARG:N	1:B:487:PRO:HD2	2.32	0.43
1:B:530:LEU:O	1:B:534:VAL:HG23	2.19	0.43
1:B:80:MET:SD	1:B:83:LEU:HD22	2.58	0.43
1:B:349:LEU:O	1:B:353:VAL:HG23	2.19	0.43
1:B:439:THR:O	1:B:440:CYS:SG	2.77	0.42
1:B:36:GLU:HB2	1:B:87:HIS:ND1	2.35	0.42
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.91	0.42
1:B:289:ARG:HH21	1:B:289:ARG:HB3	1.85	0.42
1:B:423:THR:HA	1:B:531:VAL:HG11	2.02	0.42
1:B:369:PRO:O	1:B:372:CYS:SG	2.78	0.42
1:B:28:ILE:HD11	1:B:142:LEU:HD22	2.02	0.42
1:B:191:TYR:CE2	1:B:195:PHE:CE1	3.08	0.41
1:B:108:LYS:O	1:B:465:ASN:ND2	2.52	0.41
1:B:334:THR:CG2	1:B:353:VAL:HG21	2.51	0.41
1:B:286:ILE:HA	1:B:287:PRO:HA	1.84	0.41
1:B:522:LEU:HD13	1:B:522:LEU:C	2.46	0.41
1:B:70:ASN:HD22	1:B:101:ARG:HD2	1.87	0.40
1:B:227:PRO:HG3	1:B:301:ARG:HG2	2.03	0.40
1:B:245:TYR:O	1:B:249:CYS:SG	2.79	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	B	470/586 (80%)	412 (88%)	53 (11%)	5 (1%)	11	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	THR
1	B	165	GLU
1	B	473	ALA
1	B	252	ASP
1	B	495	ASP

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	B	441/542 (81%)	412 (93%)	29 (7%)	15	36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	LEU
1	B	55	ARG
1	B	60	LYS
1	B	67	LYS
1	B	73	LEU
1	B	100	ARG

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	118	PHE
1	B	208	LYS
1	B	230	GLU
1	B	232	LYS
1	B	235	ILE
1	B	273	SER
1	B	286	ILE
1	B	289	ARG
1	B	321	GLU
1	B	334	THR
1	B	343	ASP
1	B	350	LEU
1	B	375	TYR
1	B	384	THR
1	B	391	VAL
1	B	397	HIS
1	B	407	LYS
1	B	434	VAL
1	B	443	LEU
1	B	453	LEU
1	B	457	VAL
1	B	524	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	B	35	GLN
1	B	70	ASN
1	B	74	GLN
1	B	85	GLN
1	B	99	GLN
1	B	107	ASN
1	B	224	GLN
1	B	291	GLN
1	B	295	ASN
1	B	297	ASN
1	B	317	ASN
1	B	320	GLN
1	B	532	ASN
1	B	546	GLN

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 ⓘ

2 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	A	1	2,1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	A	2	2	14,14,15	0.33	0	17,19,21	0.72	1 (5%)

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	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	O5-C1-C2	-2.20	107.88	111.29

There are no chirality outliers.

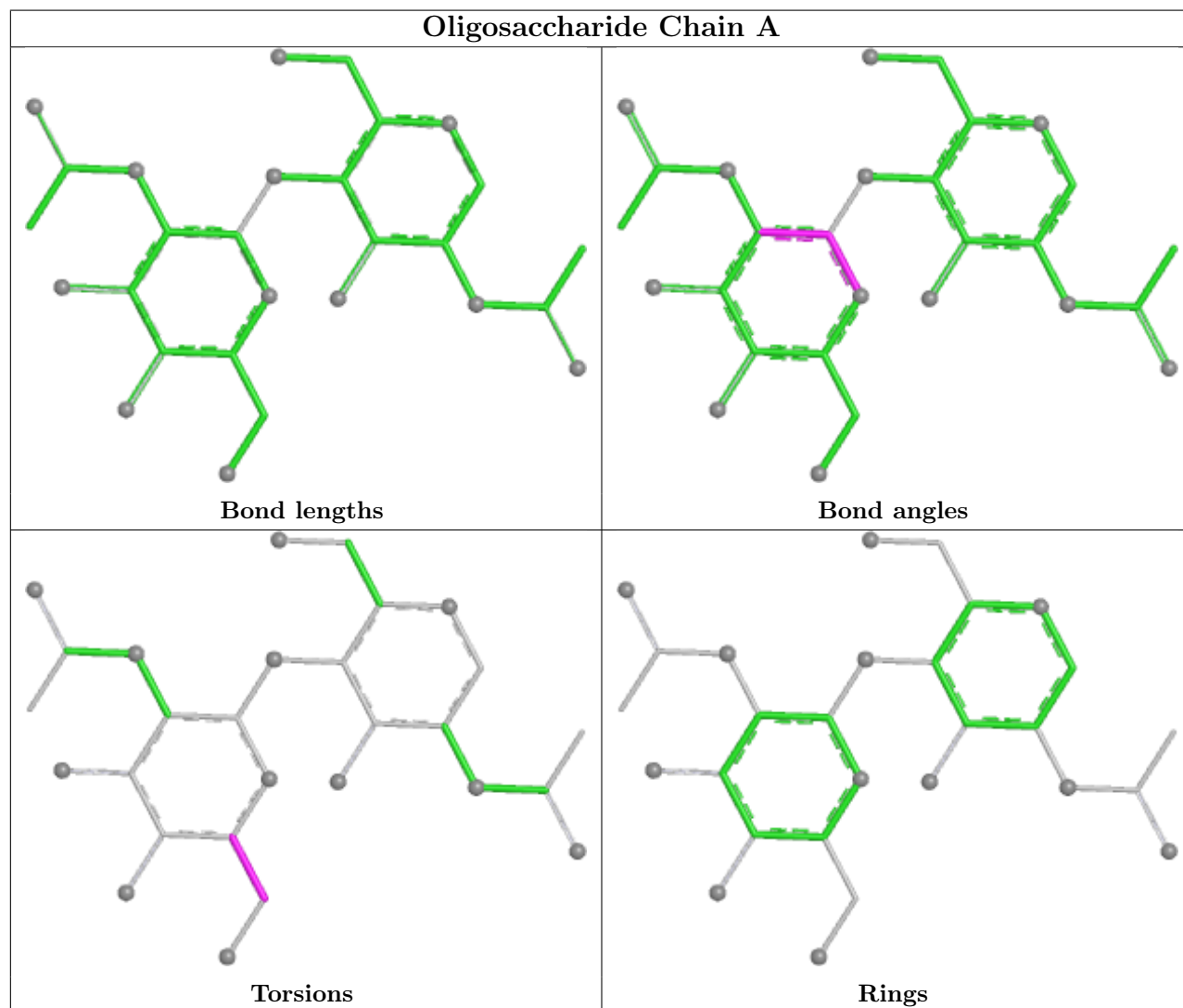
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	NAG	O5-C5-C6-O6
2	A	2	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](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DO3	B	810	3	28,28,28	0.70	0	36,36,36	0.60	0
4	NAG	B	807	1	14,14,15	0.44	0	17,19,21	0.48	0
5	DO3	B	809	3	28,28,28	0.70	0	36,36,36	0.60	0
4	NAG	B	804	1	14,14,15	0.34	0	17,19,21	0.67	0
5	DO3	B	808	3	28,28,28	0.71	0	36,36,36	0.61	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
5	DO3	B	810	3	-	12/36/36/36	0/1/1/1
4	NAG	B	807	1	-	0/6/23/26	0/1/1/1
5	DO3	B	809	3	-	11/36/36/36	0/1/1/1
4	NAG	B	804	1	-	4/6/23/26	0/1/1/1
5	DO3	B	808	3	-	7/36/36/36	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	808	DO3	O3-C11-C12-N2
5	B	809	DO3	O5-C13-C14-N3
5	B	809	DO3	O6-C13-C14-N3
5	B	809	DO3	C17-C15-C16-N4
5	B	809	DO3	C1-C2-N2-C12
4	B	804	NAG	O5-C5-C6-O6
5	B	808	DO3	O4-C11-C12-N2
5	B	810	DO3	O5-C13-C14-N3
5	B	810	DO3	O6-C13-C14-N3
5	B	809	DO3	C5-C6-N4-C16
4	B	804	NAG	C4-C5-C6-O6

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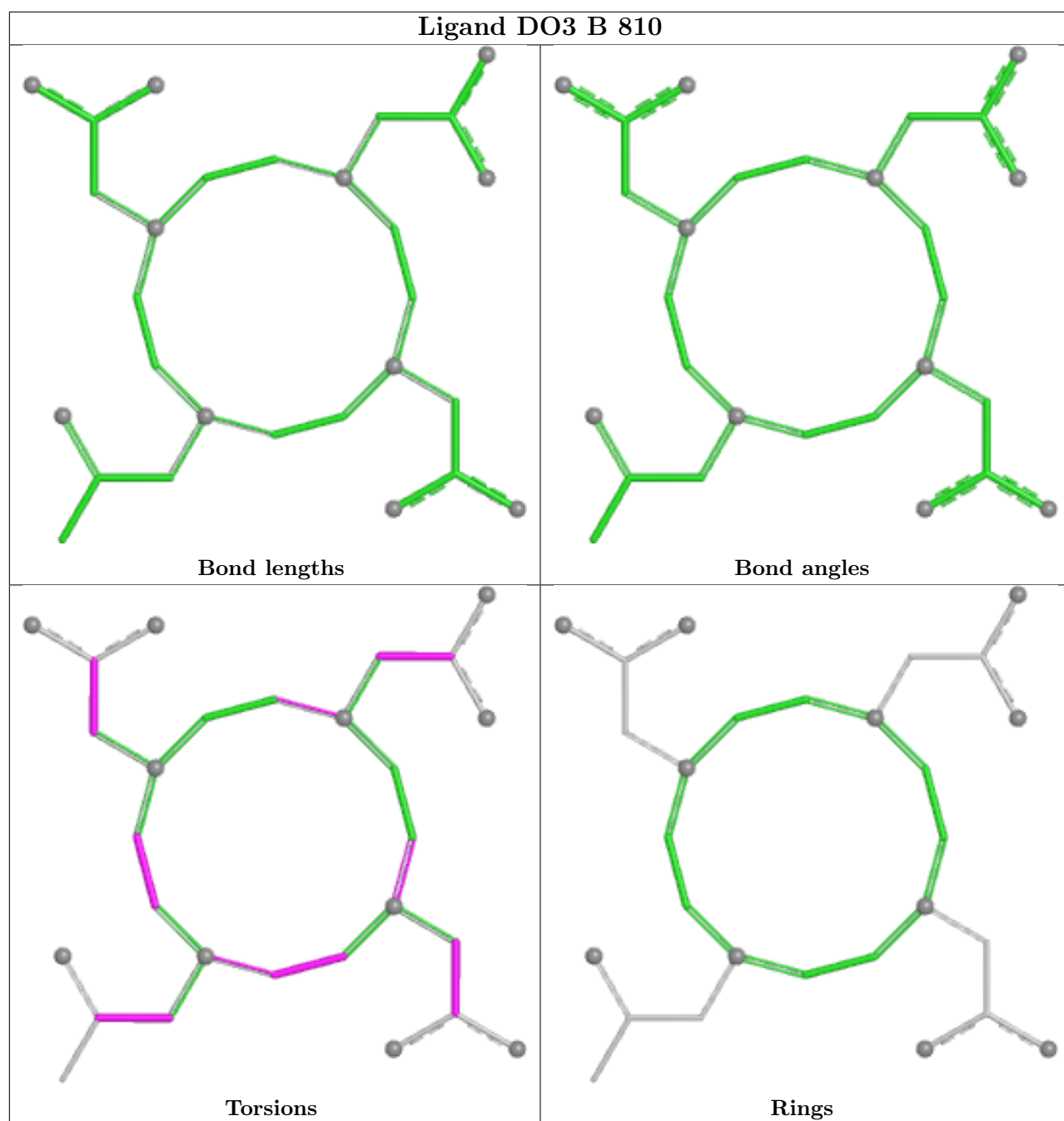
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Mol	Chain	Res	Type	Atoms
4	B	804	NAG	C8-C7-N2-C2
4	B	804	NAG	O7-C7-N2-C2
5	B	808	DO3	C11-C12-N2-C3
5	B	810	DO3	N3-C5-C6-N4
5	B	810	DO3	C5-C6-N4-C16
5	B	809	DO3	N1-C1-C2-N2
5	B	810	DO3	N1-C10-C9-O2
5	B	810	DO3	N1-C10-C9-O1
5	B	810	DO3	N4-C7-C8-N1
5	B	808	DO3	O7-C15-C16-N4
5	B	809	DO3	O7-C15-C16-N4
5	B	810	DO3	O7-C15-C16-N4
5	B	808	DO3	N1-C10-C9-O2
5	B	809	DO3	C7-C8-N1-C10
5	B	809	DO3	C7-C8-N1-C1
5	B	808	DO3	C9-C10-N1-C8
5	B	808	DO3	N1-C10-C9-O1
5	B	810	DO3	C3-C4-N3-C14
5	B	809	DO3	C4-C3-N2-C2
5	B	810	DO3	C3-C4-N3-C5
5	B	810	DO3	C1-C2-N2-C12
5	B	809	DO3	C13-C14-N3-C4
5	B	810	DO3	O4-C11-C12-N2

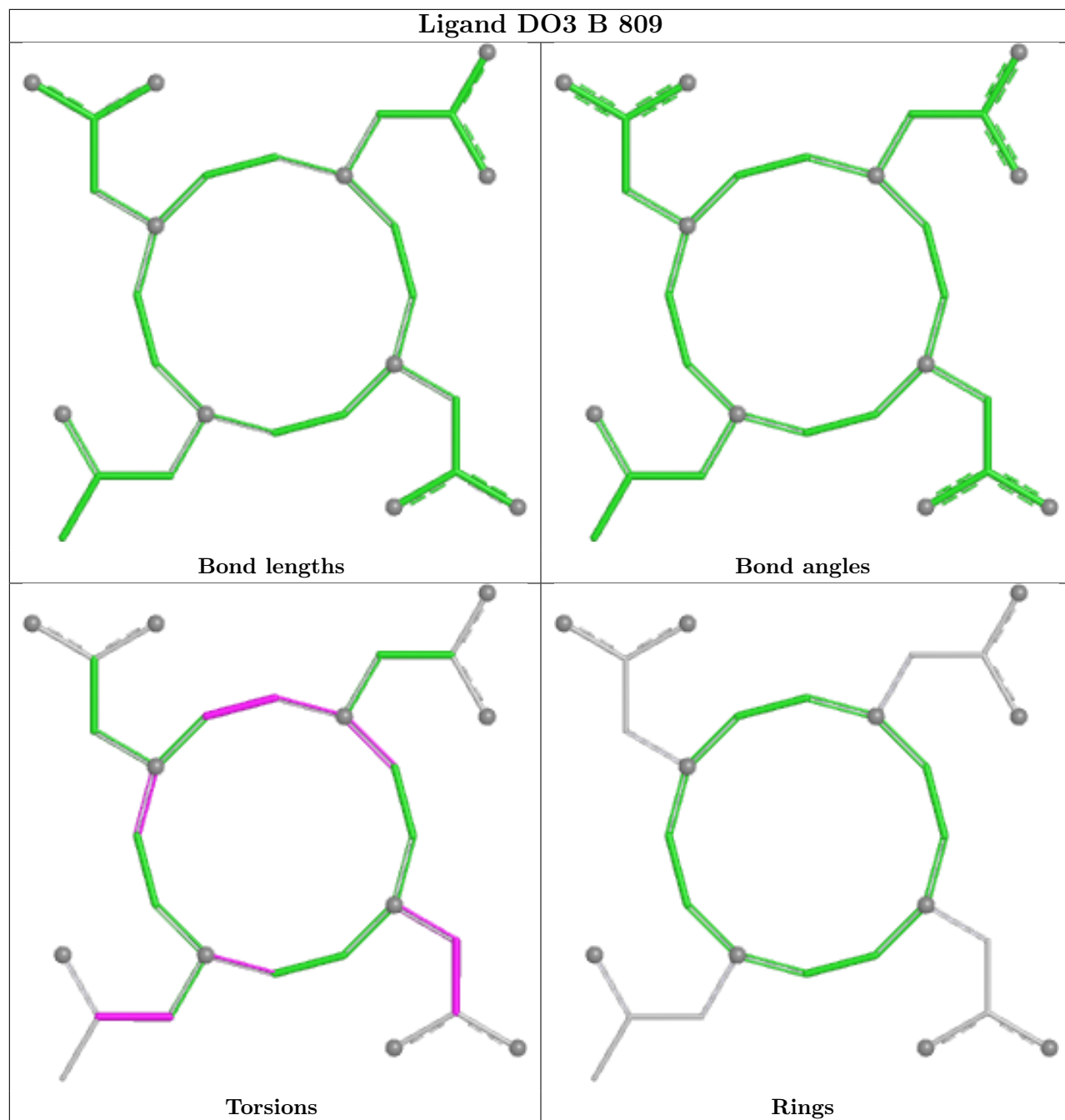
There are no ring outliers.

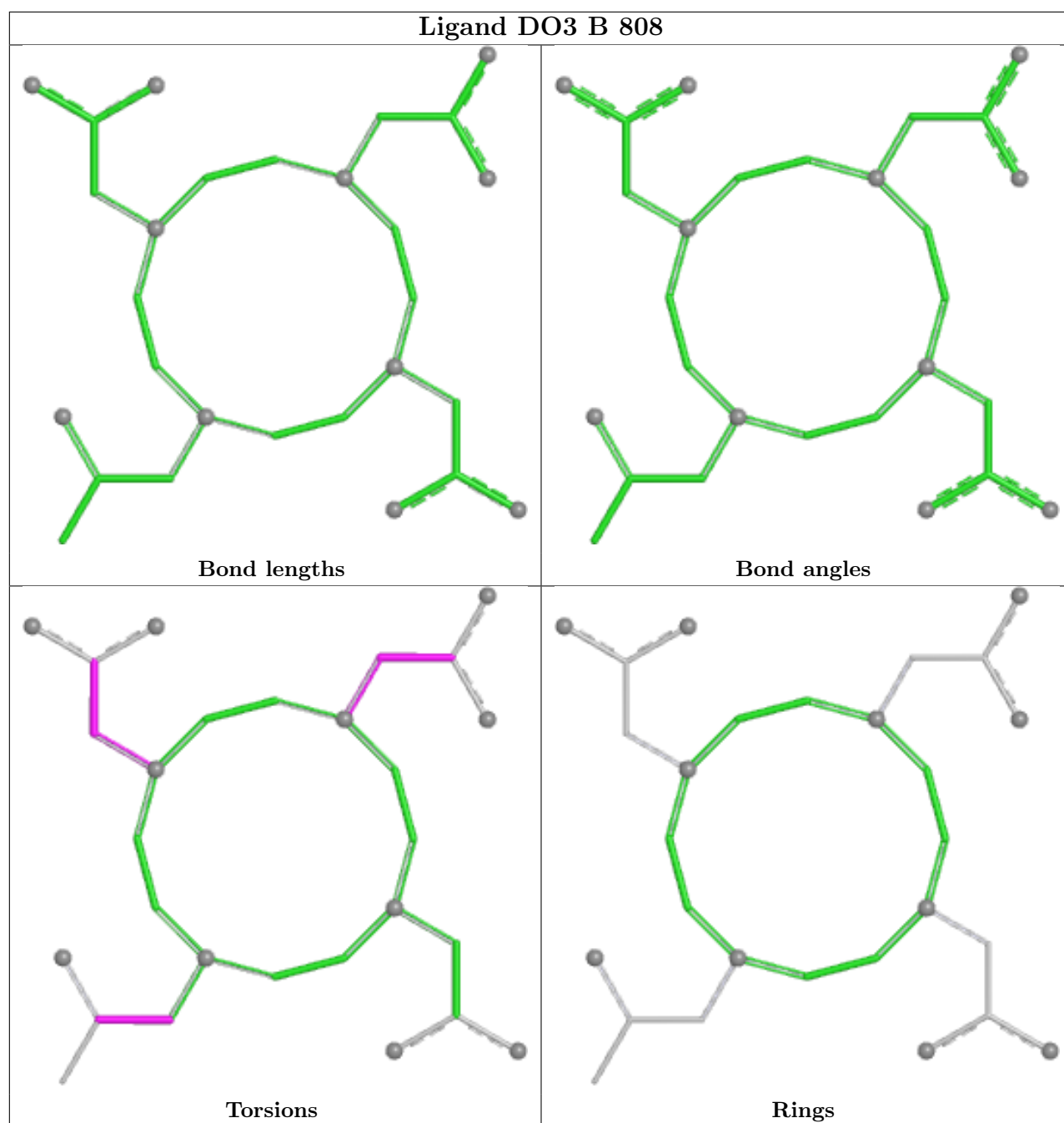
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



Ligand DO3 B 809





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	B	479/586 (81%)	0.90	52 (10%) 10 9	29, 59, 93, 120	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	ASP	4.9
1	B	287	PRO	4.7
1	B	438	THR	3.6
1	B	198[A]	TYR	3.6
1	B	158	LEU	3.5
1	B	439	THR	3.4
1	B	440	CYS	3.4
1	B	543	GLU	3.4
1	B	97	ASP	3.2
1	B	472	PRO	3.1
1	B	164	PHE	2.9
1	B	61	THR	2.9
1	B	447	PHE	2.8
1	B	471	ASN	2.8
1	B	497	THR	2.7
1	B	442	THR	2.6
1	B	68	LEU	2.5
1	B	475	ASP	2.5
1	B	167	VAL	2.5
1	B	168	ALA	2.5
1	B	13	SER	2.5
1	B	160	VAL	2.5
1	B	169	LYS	2.4
1	B	457	VAL	2.4
1	B	473	ALA	2.4
1	B	366	THR	2.4
1	B	274	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	397	HIS	2.4
1	B	466	GLU	2.4
1	B	214	VAL	2.4
1	B	266	HIS	2.4
1	B	118	PHE	2.4
1	B	144	GLU	2.3
1	B	92	CYS	2.3
1	B	441	CYS	2.3
1	B	544	GLU	2.3
1	B	495	ASP	2.3
1	B	502	PRO	2.3
1	B	305	LEU	2.3
1	B	489	PHE	2.3
1	B	319	CYS	2.2
1	B	191	TYR	2.2
1	B	187	PRO	2.2
1	B	443	LEU	2.2
1	B	154	ALA	2.1
1	B	434	VAL	2.1
1	B	233	GLU	2.1
1	B	223	SER	2.1
1	B	545	LEU	2.1
1	B	538	HIS	2.1
1	B	343	ASP	2.1
1	B	257	ILE	2.0

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

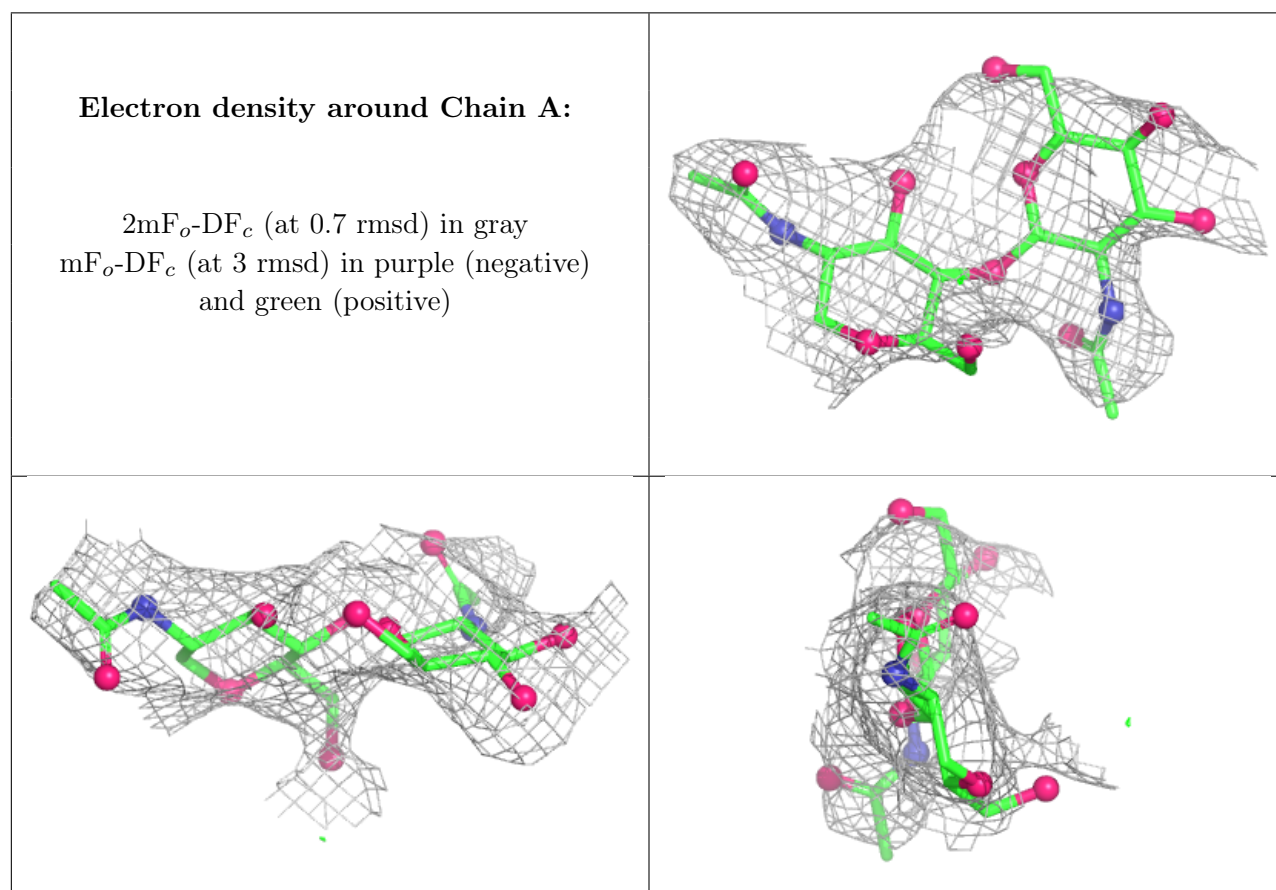
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	A	1	14/15	-	-	70,73,94,96	0
2	NAG	A	2	14/15	-	-	79,93,98,105	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.



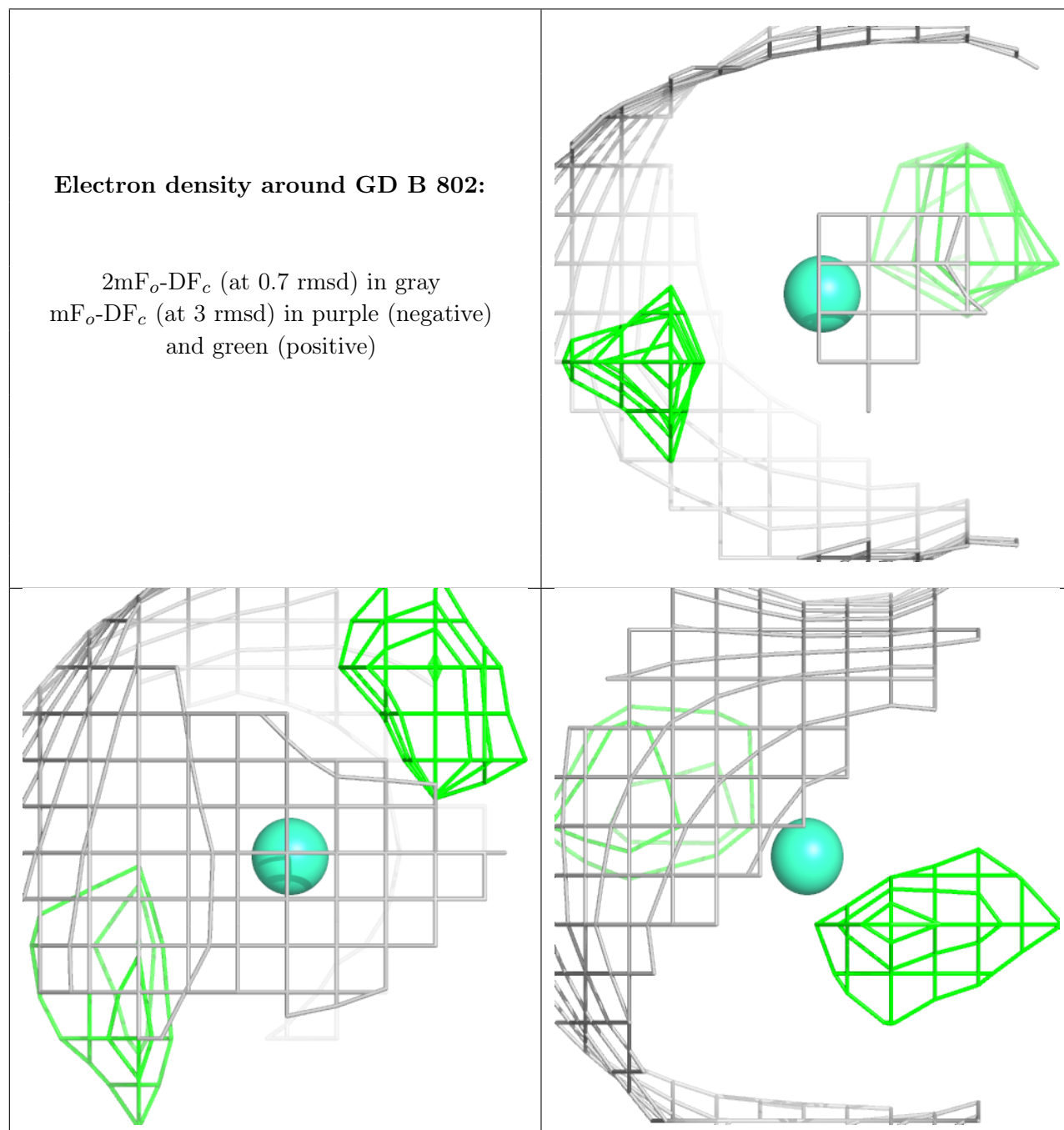
6.4 Ligands [i](#)

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	B	804	14/15	0.63	0.18	77,96,105,106	0
4	NAG	B	807	14/15	0.72	0.11	63,66,73,85	0
3	GD	B	802	1/1	0.92	0.09	109,109,109,109	1
3	GD	B	801	1/1	0.97	0.04	101,101,101,101	1
3	GD	B	803	1/1	0.97	0.03	97,97,97,97	1
5	DO3	B	808	28/28	-	-	110,130,143,150	28
5	DO3	B	809	28/28	-	-	76,84,96,99	28
5	DO3	B	810	28/28	-	-	74,88,105,107	28

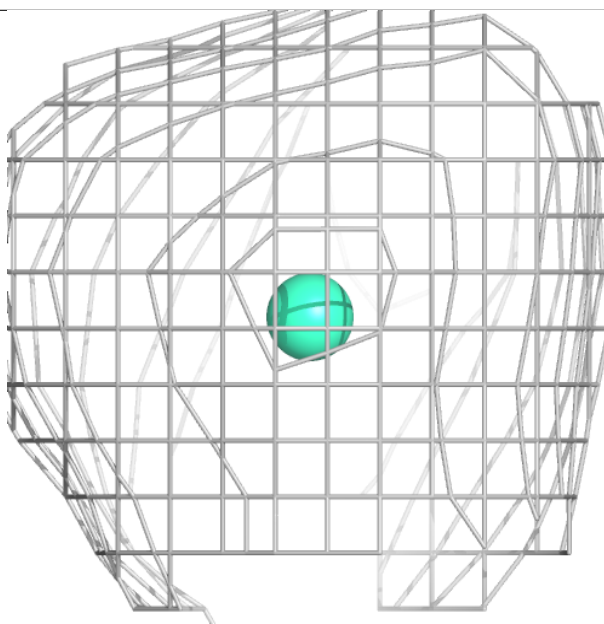
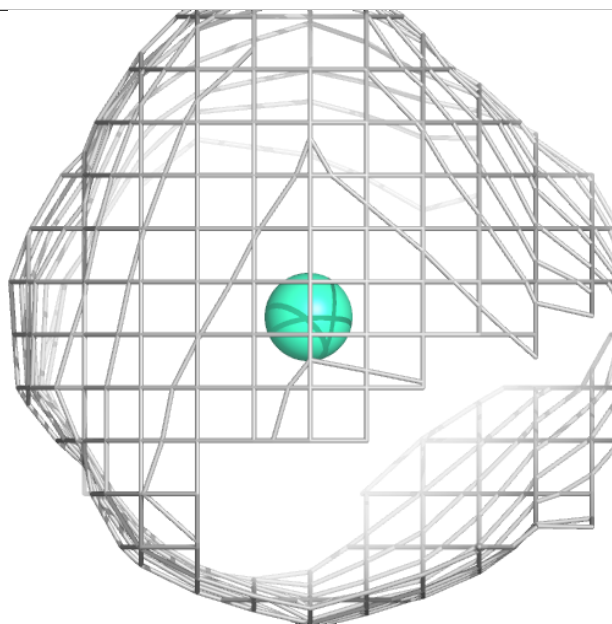
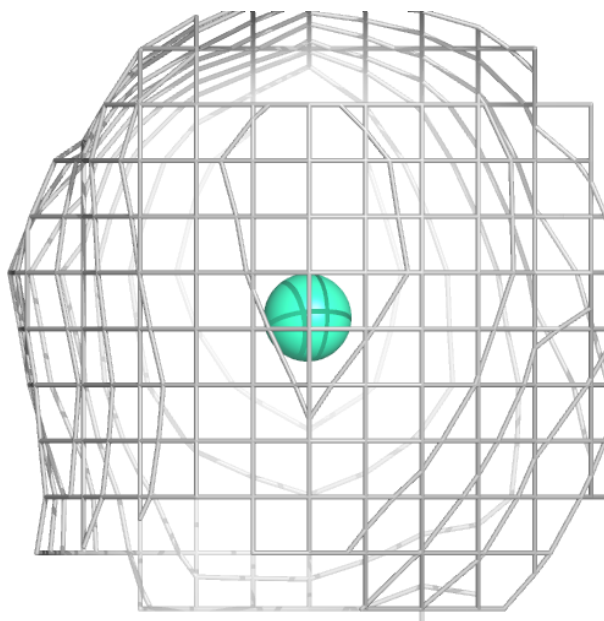
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



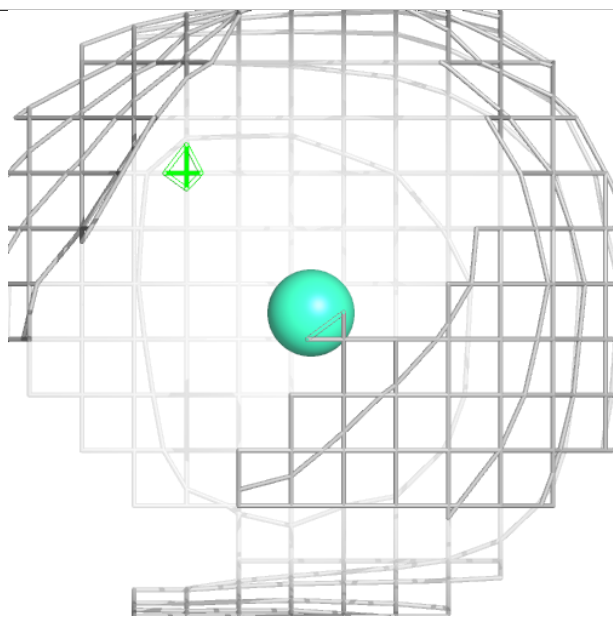
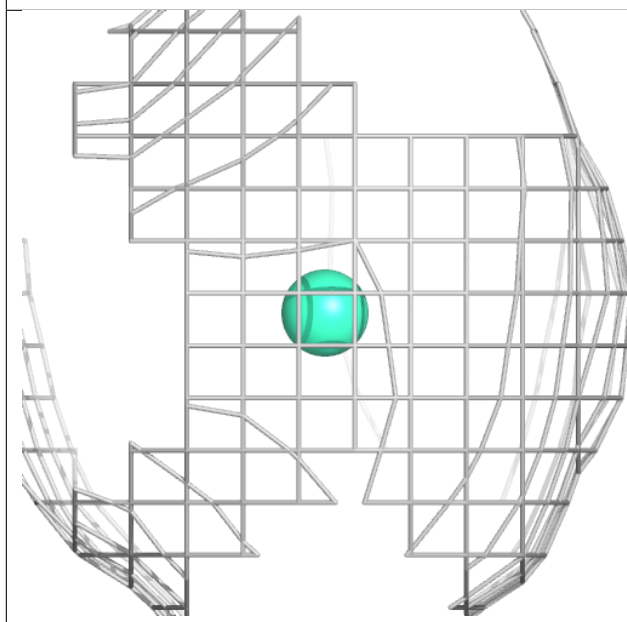
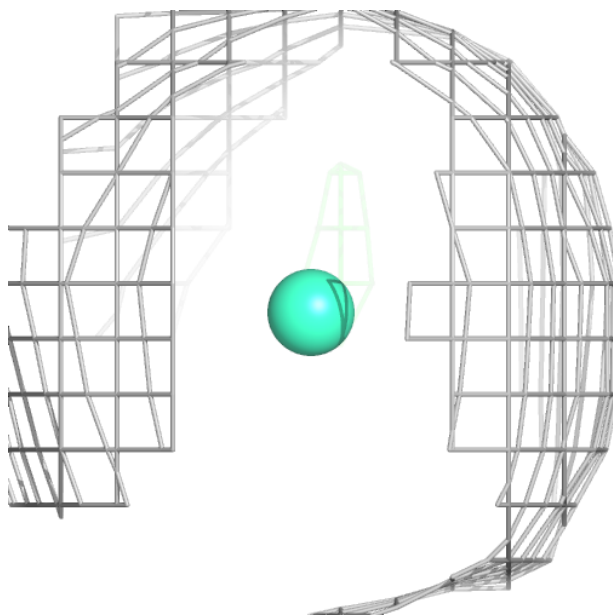
Electron density around GD B 801:

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



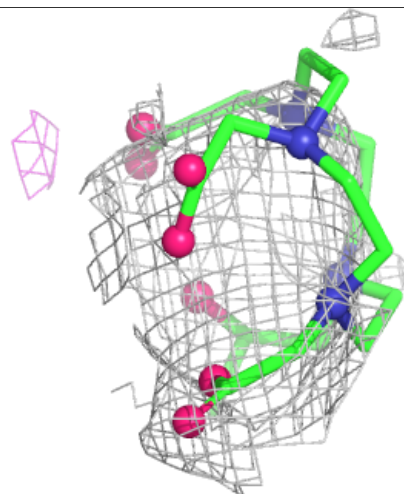
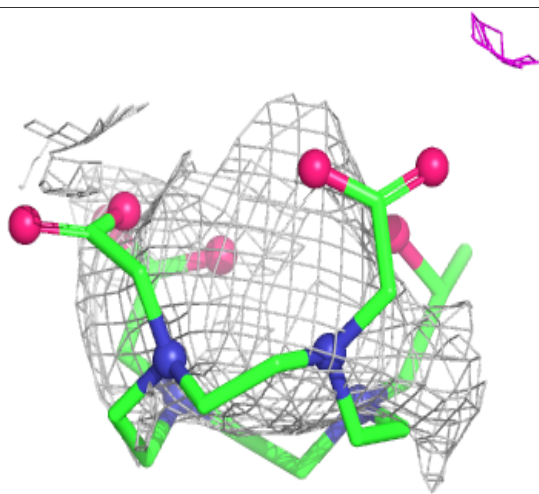
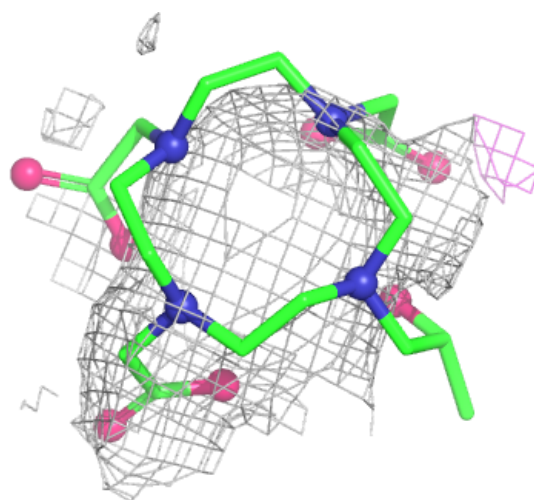
Electron density around GD B 803:

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



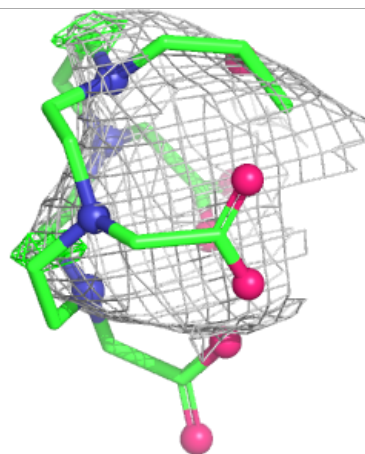
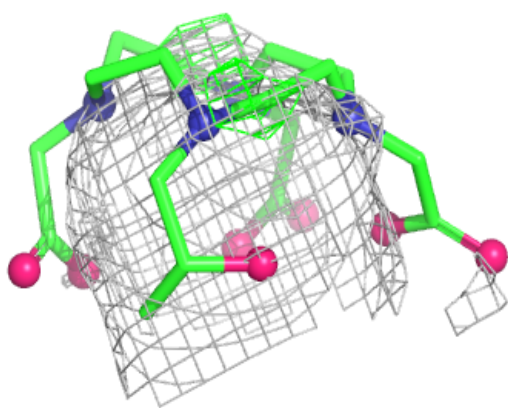
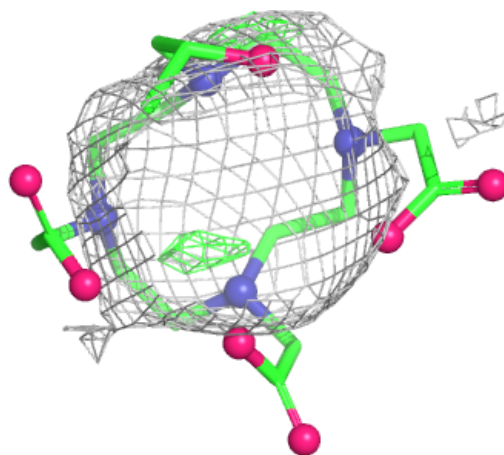
Electron density around DO3 B 808:

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



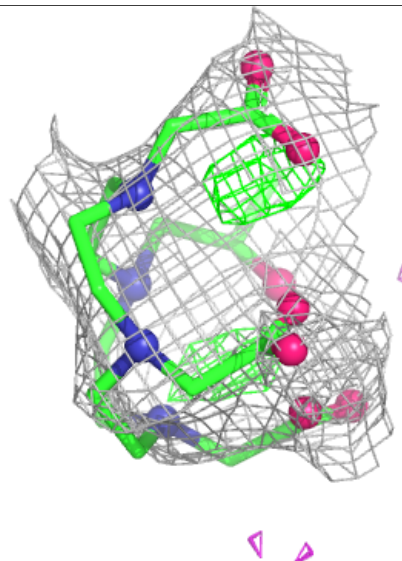
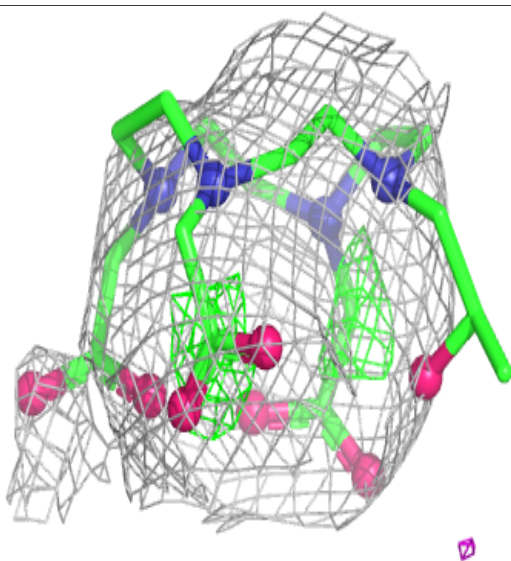
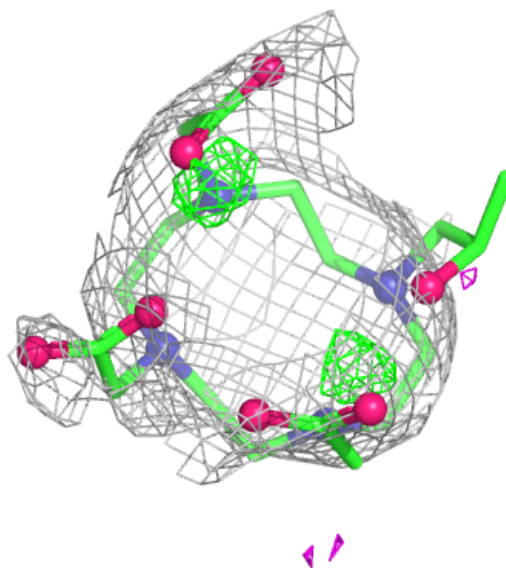
Electron density around DO3 B 809:

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



Electron density around DO3 B 810:

$2mF_o-DF_c$ (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.