Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 02:37 PM EDT

PDB ID	:	2Z63
Title	:	Crystal structure of the TV8 hybrid of human TLR4 and hagfish VLRB.61
Authors	:	Kim, H.M.; Park, B.S.; Lee, J.-O.
Deposited on	:	2007-07-22
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

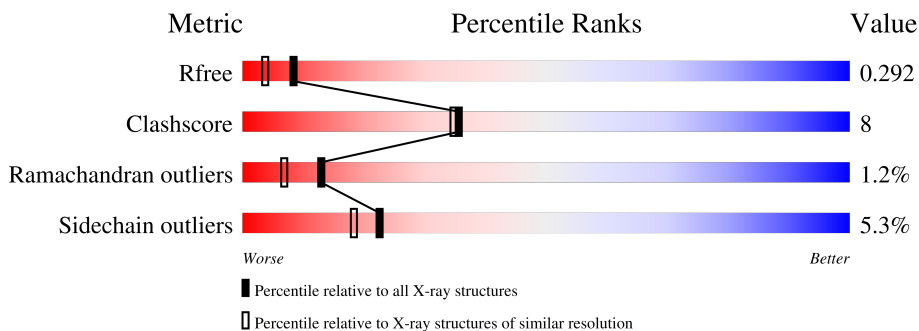|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	Percentile Ranks	Value
Rfree		0.292
Clashscore		8
Ramachandran outliers		1.2%
Sidechain outliers		5.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	570	78% 20% •
2	B	3	67% 33%
3	C	2	50% 50%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4894 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 Toll-like receptor 4, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total 4536	C 2901	N 754	O 858	S 23	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	ALA	-	SEE REMARK 999	UNP O00206
A	529	SER	-	SEE REMARK 999	UNP O00206

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
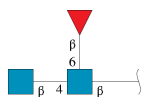
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
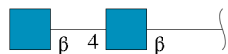
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total 292	O 292	0	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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Toll-like receptor 4, Variable lymphocyte receptor B

Chain A:

78%   20%   •
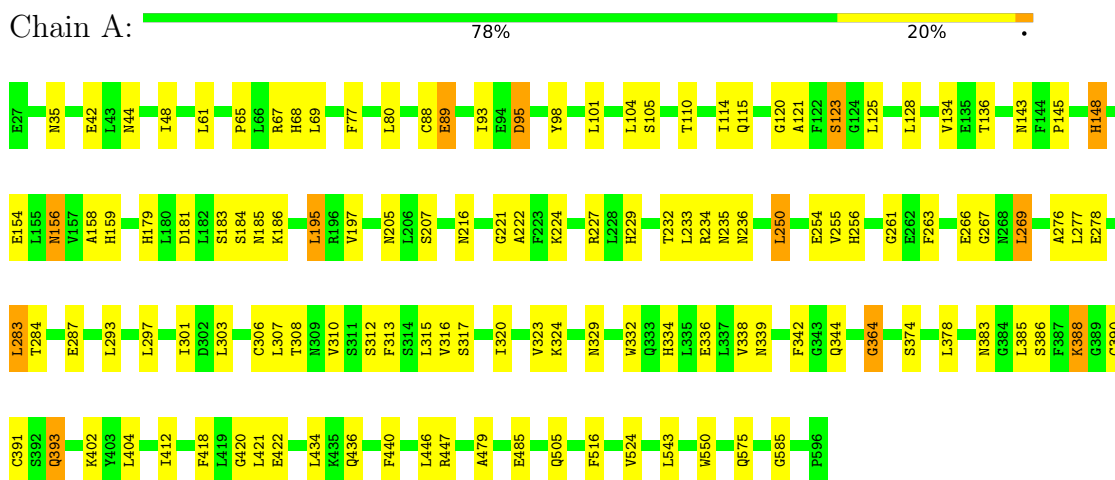
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose

Chain B:

67%   33%
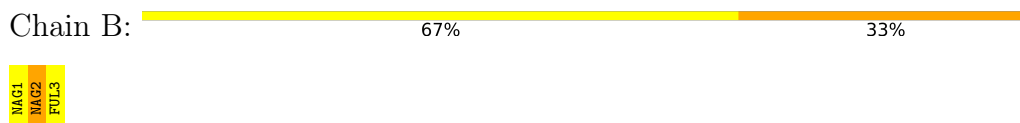
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain C:

50%   50%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	88.14Å　　88.14Å　　92.20Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	20.00　－　2.00 38.16　－　2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-2.00) 95.8 (38.16-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.250　,　0.298 0.251　,　0.292	Depositor DCC
R_{free} test set	2623 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.6	EDS
L-test for twinning[2]	$< |L| > = 0.32, < L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.237 for -h,-k,l 0.387 for h,-h-k,-l 0.218 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4894	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FUL, 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	0.53	0/4631	0.66	1/6269 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	LEU	CA-CB-CG	5.84	128.73	115.30

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	4536	0	4504	72	0
2	B	38	0	34	1	0
3	C	28	0	25	1	0
4	A	292	0	0	9	0
All	All	4894	0	4563	74	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 8.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HD22	1:A:404:LEU:HD12	1.55	0.89
1:A:418:PHE:HB3	4:A:1187:HOH:O	1.76	0.82
1:A:235:ASN:HD21	1:A:263:PHE:H	1.32	0.77
1:A:378:LEU:HD22	1:A:404:LEU:CD1	2.13	0.76
1:A:479:ALA:HB1	4:A:1041:HOH:O	1.85	0.75
1:A:269:LEU:H	1:A:269:LEU:HD12	1.53	0.74
1:A:221:GLY:HA2	1:A:224:LYS:HE3	1.71	0.73
1:A:77:PHE:HB3	1:A:80:LEU:HG	1.70	0.73
1:A:421:LEU:HB2	4:A:1187:HOH:O	1.91	0.70
1:A:388:LYS:H	1:A:388:LYS:HD2	1.59	0.68
1:A:195:LEU:HD11	1:A:222:ALA:O	1.94	0.67
1:A:229:HIS:O	1:A:256:HIS:HB3	1.95	0.65
3:C:1:NAG:H3	3:C:1:NAG:H83	1.78	0.65
1:A:159:HIS:HA	1:A:184:SER:O	1.97	0.64
1:A:221:GLY:CA	1:A:224:LYS:HE3	2.27	0.64
1:A:317:SER:HA	1:A:339:ASN:O	1.97	0.64
1:A:516:PHE:HB3	1:A:543:LEU:HD21	1.78	0.63
1:A:154:GLU:HG3	1:A:179:HIS:HB3	1.83	0.60
1:A:585:GLY:HA2	4:A:1227:HOH:O	2.02	0.59
1:A:320:ILE:HG23	1:A:323:VAL:HG23	1.84	0.58
1:A:197:VAL:HG13	4:A:1092:HOH:O	2.02	0.58
2:B:2:NAG:H82	2:B:3:FUL:H3	1.87	0.57
1:A:447:ARG:NH2	4:A:1031:HOH:O	2.38	0.57
1:A:233:LEU:HA	1:A:236:ASN:HD21	1.70	0.56
1:A:383:ASN:HB2	1:A:385:LEU:HG	1.88	0.55
1:A:297:LEU:HD13	1:A:303:LEU:HD13	1.88	0.55
1:A:235:ASN:ND2	1:A:263:PHE:H	2.02	0.55
1:A:344:GLN:HA	1:A:364:GLY:HA3	1.89	0.54
1:A:316:VAL:HG22	1:A:338:VAL:HG22	1.90	0.53
1:A:393:GLN:HG3	1:A:420:GLY:HA3	1.89	0.53
1:A:391:CYS:O	1:A:418:PHE:HA	2.09	0.53
1:A:148:HIS:H	1:A:148:HIS:CD2	2.27	0.53
1:A:67:ARG:HA	1:A:89:GLU:O	2.09	0.52
1:A:67:ARG:HB3	1:A:68:HIS:HD2	1.75	0.52
1:A:436:GLN:NE2	1:A:436:GLN:HA	2.24	0.51
1:A:44:ASN:ND2	4:A:1116:HOH:O	2.44	0.51
1:A:80:LEU:HB3	1:A:104:LEU:CD1	2.41	0.51
1:A:386:SER:HB2	1:A:388:LYS:NZ	2.26	0.51
1:A:93:ILE:HG22	1:A:121:ALA:HB1	1.93	0.50
1:A:179:HIS:ND1	1:A:207:SER:HB2	2.26	0.50
1:A:61:LEU:O	1:A:88:CYS:SG	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HB3	1:A:283:LEU:HD11	1.95	0.48
1:A:98:TYR:HB3	1:A:101:LEU:HD12	1.94	0.47
1:A:156:ASN:HA	1:A:181:ASP:HB3	1.95	0.47
1:A:254:GLU:HA	1:A:284:THR:HB	1.97	0.47
1:A:125:LEU:HD13	1:A:128:LEU:HD22	1.96	0.47
1:A:227:ARG:HA	1:A:254:GLU:O	2.15	0.46
1:A:386:SER:HB2	1:A:388:LYS:HZ1	1.80	0.46
1:A:524:VAL:HG13	1:A:550:TRP:HZ3	1.79	0.46
1:A:114:ILE:HD12	1:A:136:THR:HB	1.99	0.45
1:A:505:GLN:HB2	4:A:1041:HOH:O	2.15	0.45
1:A:422:GLU:H	1:A:422:GLU:CD	2.20	0.45
1:A:287:GLU:HG2	1:A:312:SER:HB3	1.97	0.45
1:A:342:PHE:C	1:A:344:GLN:H	2.20	0.45
1:A:393:GLN:CG	1:A:420:GLY:HA3	2.46	0.44
1:A:232:THR:HG22	1:A:234:ARG:HG3	2.00	0.44
1:A:334:HIS:HE1	1:A:336:GLU:HB2	1.82	0.44
1:A:110:THR:HG23	1:A:134:VAL:HB	1.99	0.43
1:A:310:VAL:HG12	1:A:332:TRP:CD1	2.53	0.43
1:A:143:ASN:O	1:A:145:PRO:HD3	2.19	0.43
1:A:185:ASN:HB3	1:A:186:LYS:H	1.67	0.43
1:A:205:ASN:OD1	1:A:229:HIS:HB2	2.18	0.43
1:A:234:ARG:HA	1:A:261:GLY:O	2.19	0.43
1:A:306:CYS:HB2	4:A:1150:HOH:O	2.19	0.42
1:A:390:CYS:HA	1:A:391:CYS:HA	1.90	0.42
1:A:313:PHE:HE2	1:A:315:LEU:HG	1.85	0.42
1:A:313:PHE:CE2	1:A:315:LEU:HG	2.55	0.41
1:A:120:GLY:O	1:A:123:SER:HB2	2.20	0.41
1:A:158:ALA:HA	1:A:183:SER:O	2.20	0.41
1:A:48:ILE:H	1:A:48:ILE:HD12	1.85	0.41
1:A:436:GLN:NE2	1:A:440:PHE:HE1	2.18	0.41
1:A:412:ILE:HB	1:A:434:LEU:HD23	2.02	0.41
1:A:233:LEU:CA	1:A:236:ASN:ND2	2.84	0.40
1:A:95:ASP:HA	1:A:120:GLY: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	568/570 (100%)	520 (92%)	41 (7%)	7 (1%)	13 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	276	ALA
1	A	35	ASN
1	A	42	GLU
1	A	65	PRO
1	A	267	GLY
1	A	364	GLY

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	526/526 (100%)	498 (95%)	28 (5%)	22 18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	95	ASP
1	A	105	SER
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	123	SER
1	A	148	HIS
1	A	156	ASN
1	A	195	LEU
1	A	216	ASN
1	A	250	LEU
1	A	255	VAL
1	A	266	GLU
1	A	269	LEU
1	A	277	LEU
1	A	278	GLU
1	A	293	LEU
1	A	301	ILE
1	A	307	LEU
1	A	308	THR
1	A	324	LYS
1	A	329	ASN
1	A	374	SER
1	A	388	LYS
1	A	393	GLN
1	A	402	LYS
1	A	446	LEU
1	A	485	GLU
1	A	575	GLN

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

Mol	Chain	Res	Type
1	A	91	GLN
1	A	156	ASN
1	A	216	ASN
1	A	235	ASN
1	A	236	ASN
1	A	268	ASN
1	A	329	ASN
1	A	393	GLN
1	A	426	HIS
1	A	436	GLN
1	A	484	GLN
1	A	510	GLN
1	A	523	GLN
1	A	547	GLN

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Mol	Chain	Res	Type
1	A	578	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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	B	1	1,2	14,14,15	0.60	0	17,19,21	1.09	2 (11%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
2	FUL	B	3	2	10,10,11	0.61	0	14,14,16	0.76	0
3	NAG	C	1	1,3	14,14,15	0.70	0	17,19,21	1.74	3 (17%)
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	O5-C1-C2	-4.27	104.55	111.29
3	C	1	NAG	C2-N2-C7	3.12	127.34	122.90
3	C	1	NAG	O5-C5-C6	2.76	111.53	107.20
2	B	1	NAG	O5-C5-C6	2.69	111.42	107.20
2	B	2	NAG	C1-O5-C5	2.06	114.99	112.19
2	B	1	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
3	C	1	NAG	C3-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
2	B	2	NAG	1	0
2	B	3	FUL	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 oligosaccharide.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings
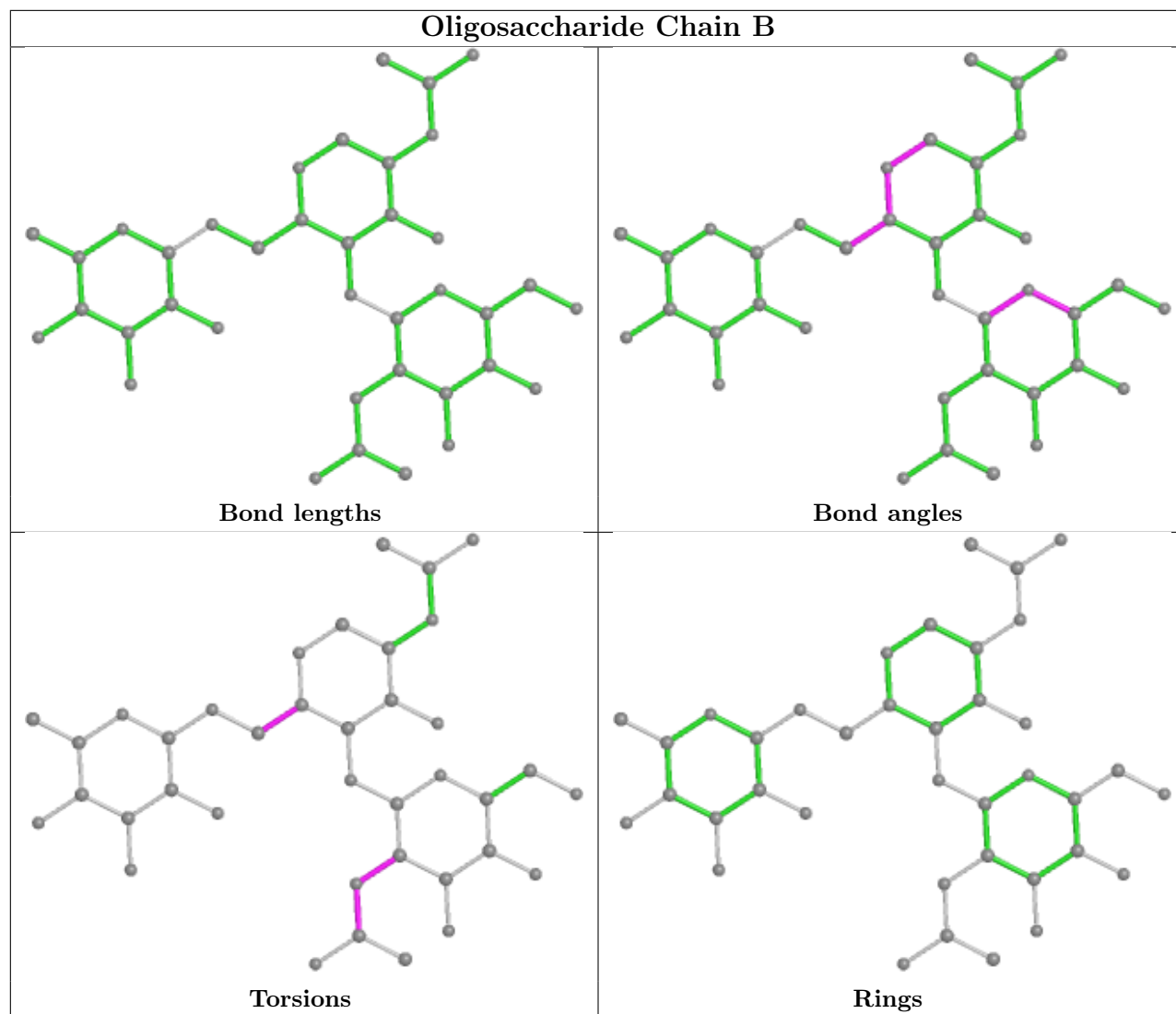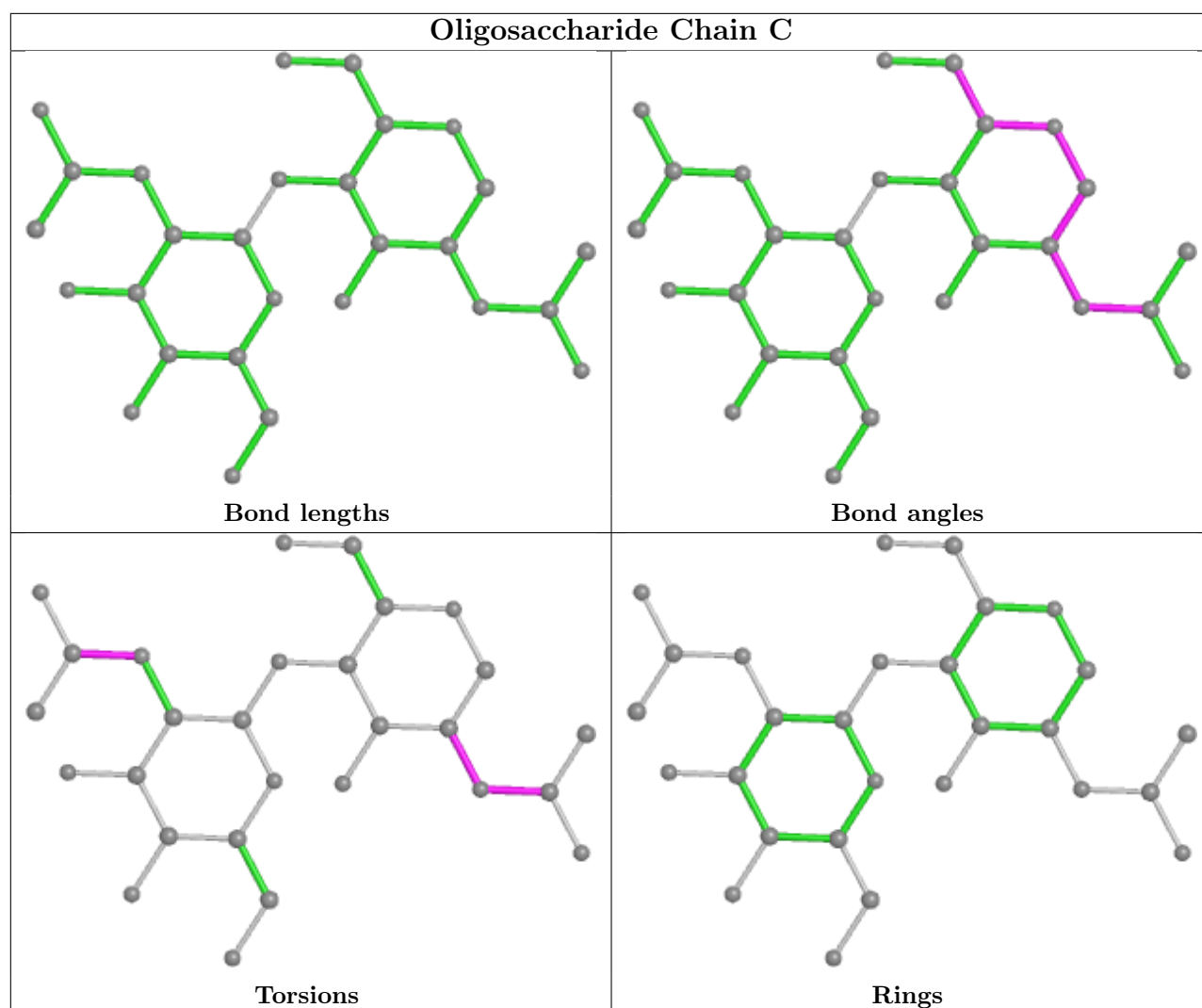
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

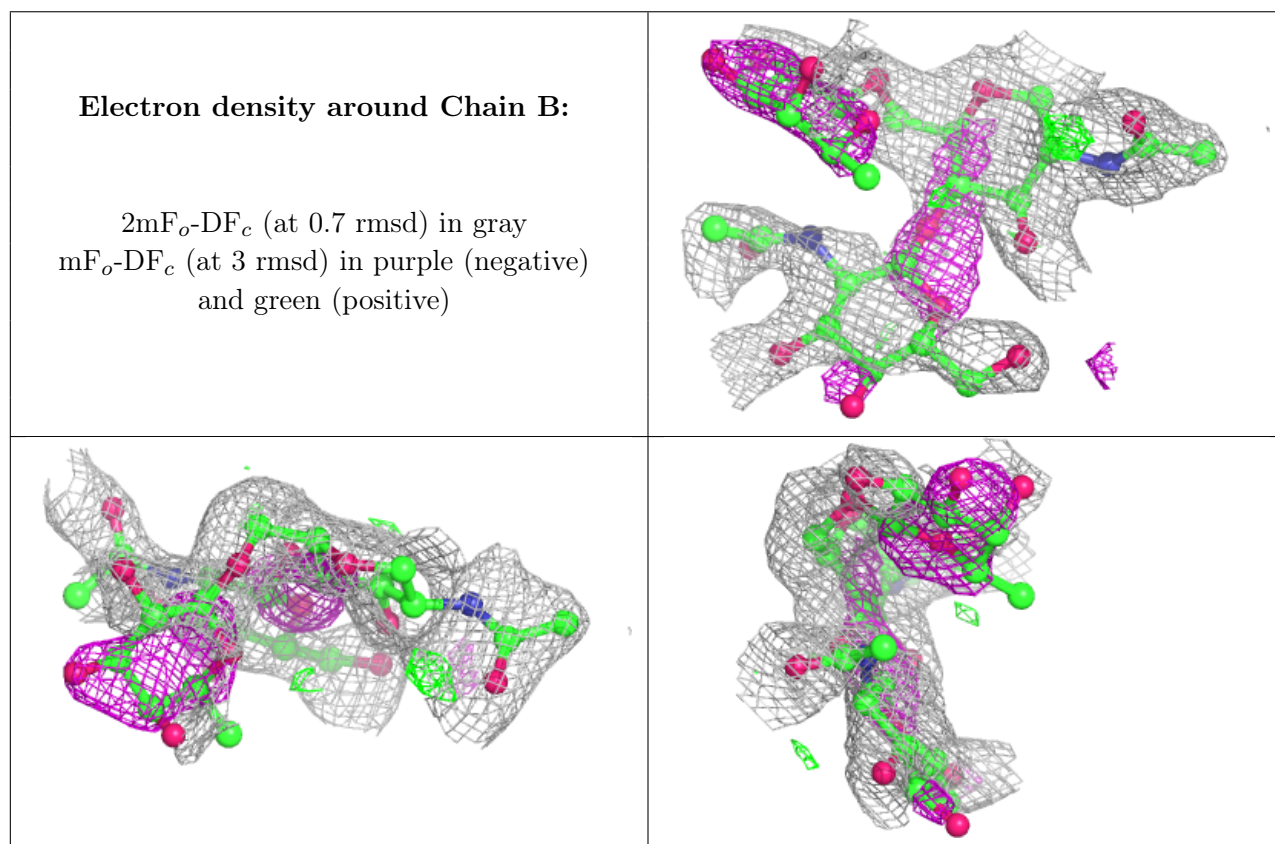Unable to reproduce the depositors R factor - this section is therefore empty.

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

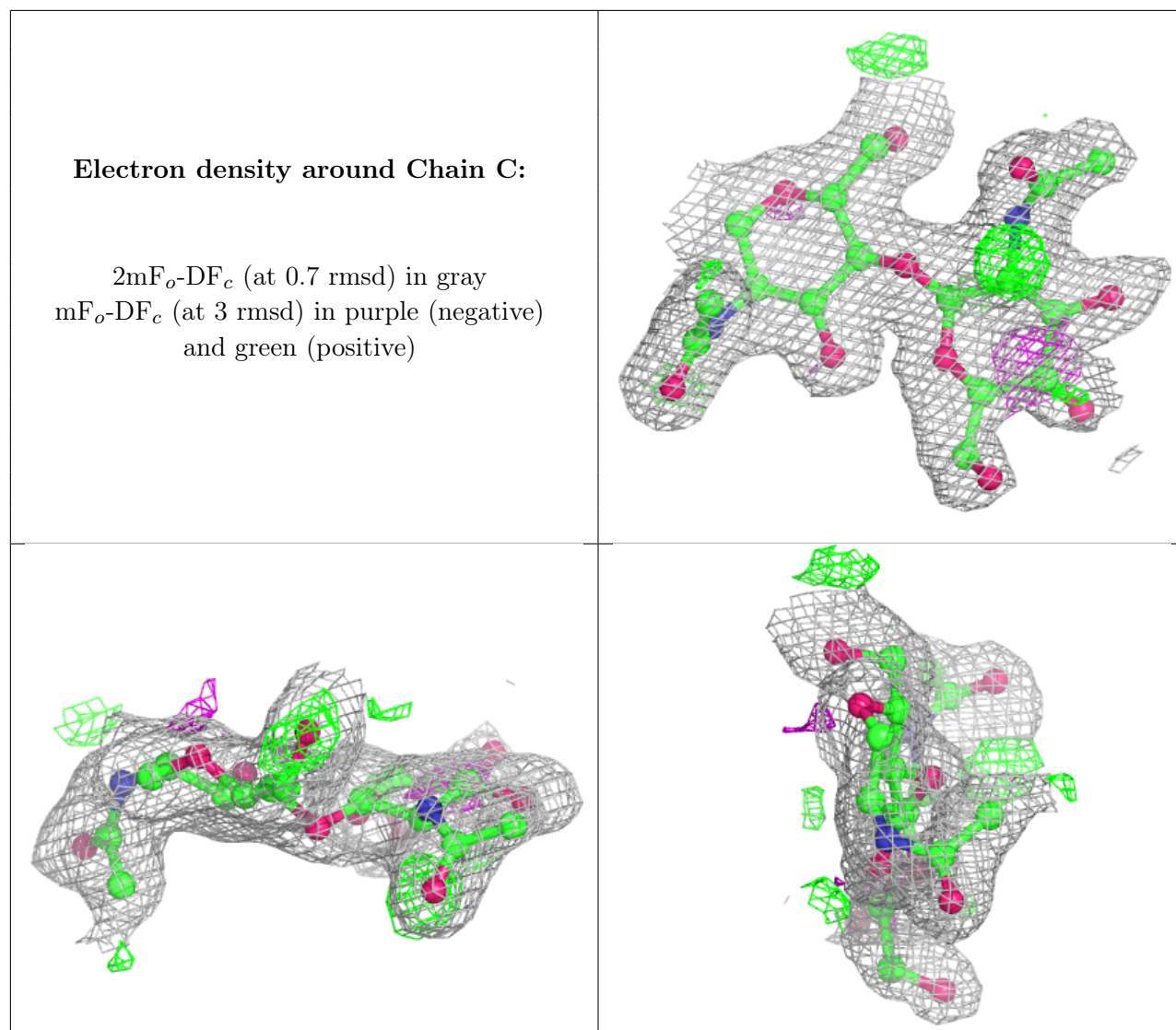Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

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

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

Electron density around Chain B:

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

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)

6.4 Ligands (i)

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

6.5 Other polymers (i)

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