



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2024 – 09:52 PM EDT

PDB ID : 3WN5
Title : Crystal structure of asymmetrically engineered Fc variant in complex with FcγRIIIa
Authors : Kadono, S.; Mimoto, F.; Katada, H.; Igawa, T.; Kamikawa, T.; Hattori, K.
Deposited on : 2013-12-05
Resolution : 2.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

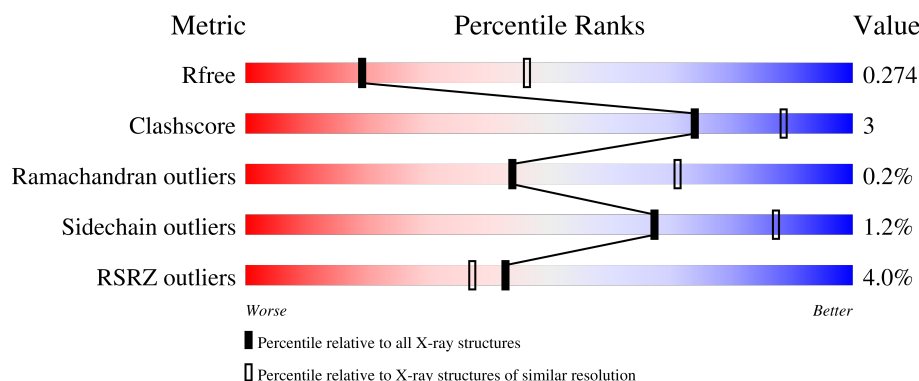
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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.





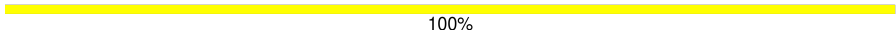
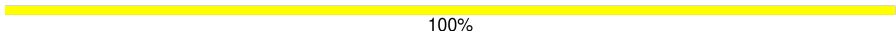

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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	230	
1	D	230	
2	B	230	
2	E	230	
3	C	197	

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Mol	Chain	Length	Quality of chain
3	F	197	 80% 6% 14%
4	G	9	 44% 44% 11%
4	H	9	 11% 89%
4	L	9	 56% 44%
5	I	5	 60% 40%
6	J	2	 100%
6	M	2	 100%
7	K	8	 50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9947 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1664	1057	277	323	7			
1	D	212	Total	C	N	O	S	0	0	0
			1646	1046	274	319	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	CYS	engineered mutation	UNP P01857
A	270	GLU	ASP	engineered mutation	UNP P01857
A	326	ASP	LYS	engineered mutation	UNP P01857
A	330	LYS	ALA	engineered mutation	UNP P01857
A	334	GLU	LYS	engineered mutation	UNP P01857
A	356	CYS	ASP	engineered mutation	UNP P01857
A	366	SER	THR	engineered mutation	UNP P01857
A	368	ALA	LEU	engineered mutation	UNP P01857
A	407	VAL	TYR	engineered mutation	UNP P01857
D	220	SER	CYS	engineered mutation	UNP P01857
D	270	GLU	ASP	engineered mutation	UNP P01857
D	326	ASP	LYS	engineered mutation	UNP P01857
D	330	LYS	ALA	engineered mutation	UNP P01857
D	334	GLU	LYS	engineered mutation	UNP P01857
D	356	CYS	ASP	engineered mutation	UNP P01857
D	366	SER	THR	engineered mutation	UNP P01857
D	368	ALA	LEU	engineered mutation	UNP P01857
D	407	VAL	TYR	engineered mutation	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1664	1065	271	320	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	210	Total	C	N	O	S	0	0	0
			1644	1056	267	313	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	SER	CYS	engineered mutation	UNP P01857
B	234	TYR	LEU	engineered mutation	UNP P01857
B	235	TYR	LEU	engineered mutation	UNP P01857
B	236	TRP	GLY	engineered mutation	UNP P01857
B	239	MET	SER	engineered mutation	UNP P01857
B	268	ASP	HIS	engineered mutation	UNP P01857
B	298	ALA	SER	engineered mutation	UNP P01857
B	327	ASP	ALA	engineered mutation	UNP P01857
B	349	CYS	TYR	engineered mutation	UNP P01857
B	366	TRP	THR	engineered mutation	UNP P01857
E	220	SER	CYS	engineered mutation	UNP P01857
E	234	TYR	LEU	engineered mutation	UNP P01857
E	235	TYR	LEU	engineered mutation	UNP P01857
E	236	TRP	GLY	engineered mutation	UNP P01857
E	239	MET	SER	engineered mutation	UNP P01857
E	268	ASP	HIS	engineered mutation	UNP P01857
E	298	ALA	SER	engineered mutation	UNP P01857
E	327	ASP	ALA	engineered mutation	UNP P01857
E	349	CYS	TYR	engineered mutation	UNP P01857
E	366	TRP	THR	engineered mutation	UNP P01857

- Molecule 3 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	169	Total	C	N	O	S	0	0	0
			1358	867	232	255	4			
3	F	170	Total	C	N	O	S	0	0	0
			1354	862	230	258	4			

There are 20 discrepancies between the modelled and reference sequences:

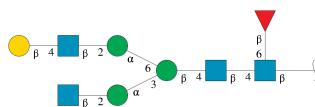
Chain	Residue	Modelled	Actual	Comment	Reference
C	35	GLN	ASN	engineered mutation	UNP P08637
C	71	GLN	ASN	engineered mutation	UNP P08637
C	155	VAL	PHE	SEE REMARK 999	UNP P08637
C	166	GLN	ASN	engineered mutation	UNP P08637

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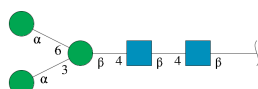
Chain	Residue	Modelled	Actual	Comment	Reference
C	188	HIS	-	expression tag	UNP P08637
C	189	HIS	-	expression tag	UNP P08637
C	190	HIS	-	expression tag	UNP P08637
C	191	HIS	-	expression tag	UNP P08637
C	192	HIS	-	expression tag	UNP P08637
C	193	HIS	-	expression tag	UNP P08637
F	35	GLN	ASN	engineered mutation	UNP P08637
F	71	GLN	ASN	engineered mutation	UNP P08637
F	155	VAL	PHE	SEE REMARK 999	UNP P08637
F	166	GLN	ASN	engineered mutation	UNP P08637
F	188	HIS	-	expression tag	UNP P08637
F	189	HIS	-	expression tag	UNP P08637
F	190	HIS	-	expression tag	UNP P08637
F	191	HIS	-	expression tag	UNP P08637
F	192	HIS	-	expression tag	UNP P08637
F	193	HIS	-	expression tag	UNP P08637

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



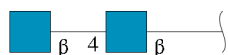
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	0	0	0
			110	62	4	44			
4	H	9	Total	C	N	O	0	0	0
			110	62	4	44			
4	L	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



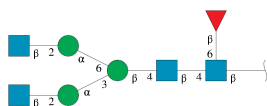
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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
7	K	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 8 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	I	0	0
			2	2		
8	B	3	Total	I	0	0
			3	3		
8	C	2	Total	I	0	0
			2	2		
8	D	1	Total	I	0	0
			1	1		
8	E	4	Total	I	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	4	Total I 4 4	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total C N O 14 8 1 5	0	0

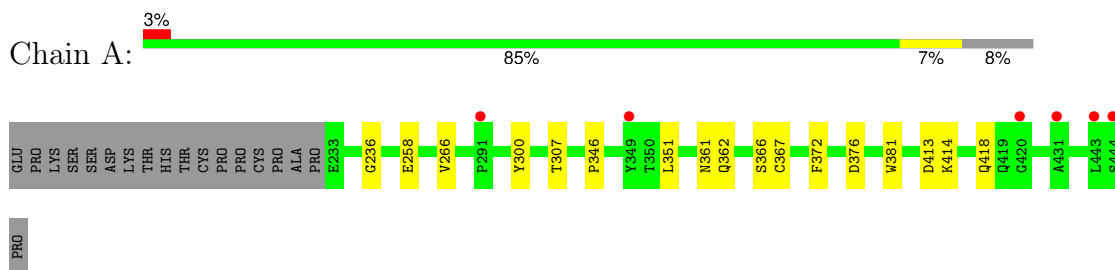
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	7	Total O 7 7	0	0
10	B	11	Total O 11 11	0	0
10	C	6	Total O 6 6	0	0
10	D	4	Total O 4 4	0	0
10	E	3	Total O 3 3	0	0
10	F	10	Total O 10 10	0	0

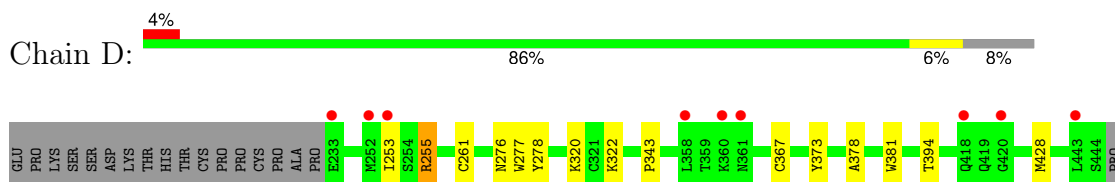
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

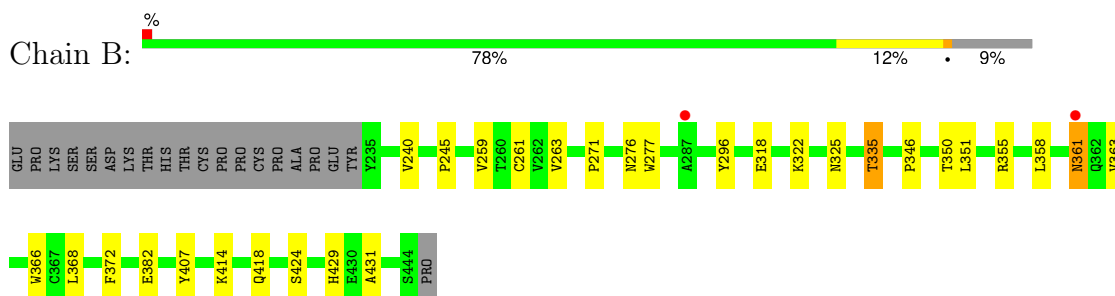
- Molecule 1: Ig gamma-1 chain C region



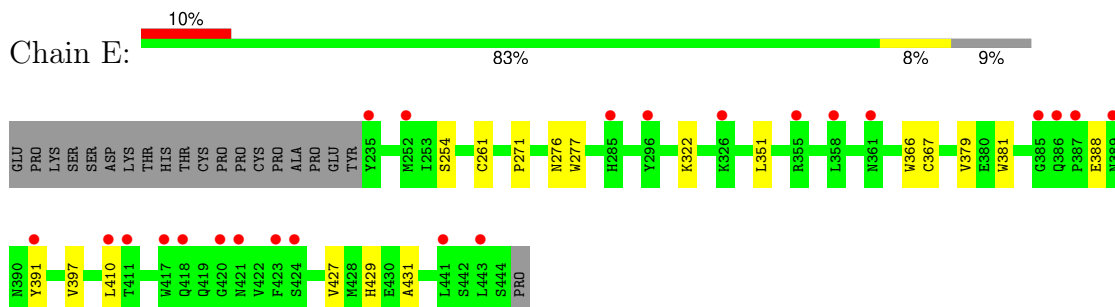
- Molecule 1: Ig gamma-1 chain C region



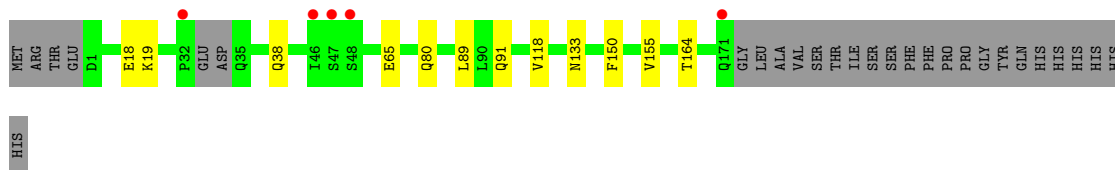
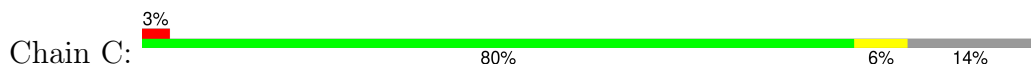
- Molecule 2: Ig gamma-1 chain C region



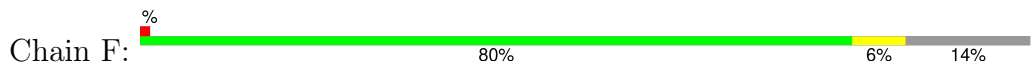
- Molecule 2: Ig gamma-1 chain C region



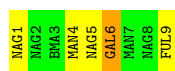
- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A



- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A



- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

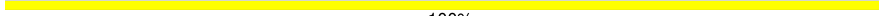


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  60% 40%

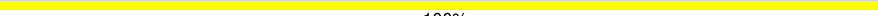


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.03Å 72.49Å 163.48Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	25.00 – 2.78 25.00 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.78) 97.9 (25.00-2.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.274 0.236 , 0.274	Depositor DCC
R_{free} test set	2186 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l 0.016 for -k,-h,-l 0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: GAL, FUL, IOD, MAN, NAG, BMA

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	0.28	0/1709	0.46	0/2334
1	D	0.28	0/1691	0.46	0/2313
2	B	0.28	0/1713	0.46	0/2343
2	E	0.28	0/1693	0.44	0/2318
3	C	0.30	0/1395	0.49	0/1897
3	F	0.29	0/1391	0.48	0/1895
All	All	0.28	0/9592	0.46	0/13100

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	1664	0	1594	8	0
1	D	1646	0	1567	11	0
2	B	1664	0	1580	16	0
2	E	1644	0	1547	11	0
3	C	1358	0	1299	7	0
3	F	1354	0	1273	4	0
4	G	110	0	94	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	110	0	94	2	0
4	L	110	0	94	0	0
5	I	61	0	52	0	0
6	J	28	0	25	0	0
6	M	28	0	25	0	0
7	K	99	0	85	0	0
8	A	2	0	0	0	0
8	B	3	0	0	1	0
8	C	2	0	0	0	0
8	D	1	0	0	0	0
8	E	4	0	0	1	0
8	F	4	0	0	1	0
9	F	14	0	13	0	0
10	A	7	0	0	0	0
10	B	11	0	0	0	0
10	C	6	0	0	0	0
10	D	4	0	0	0	0
10	E	3	0	0	0	0
10	F	10	0	0	0	0
All	All	9947	0	9342	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 3.

The worst 5 of 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:D:255:ARG:HG2	1:D:255:ARG:HH11	1.47	0.80
1:D:255:ARG:HH11	1:D:255:ARG:CG	2.04	0.71
2:B:296:TYR:H	4:H:9:FUL:H61	1.57	0.69
3:F:152:ARG:HB3	3:F:161:SER:HB3	1.75	0.68
2:E:351:LEU:HB2	2:E:366:TRP:HB2	1.81	0.61

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	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
1	D	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
2	B	208/230 (90%)	201 (97%)	6 (3%)	1 (0%)	25	52
2	E	208/230 (90%)	201 (97%)	6 (3%)	1 (0%)	25	52
3	C	165/197 (84%)	162 (98%)	3 (2%)	0	100	100
3	F	166/197 (84%)	162 (98%)	4 (2%)	0	100	100
All	All	1167/1314 (89%)	1130 (97%)	35 (3%)	2 (0%)	44	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	PRO
2	E	271	PRO

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	190/214 (89%)	188 (99%)	2 (1%)	70	88
1	D	187/214 (87%)	186 (100%)	1 (0%)	86	95
2	B	188/215 (87%)	184 (98%)	4 (2%)	48	77
2	E	181/215 (84%)	181 (100%)	0	100	100
3	C	150/178 (84%)	149 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	148/178 (83%)	143 (97%)	5 (3%)	32 63
All	All	1044/1214 (86%)	1031 (99%)	13 (1%)	67 87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	255	ARG
3	F	43	GLU
3	F	159	ASN
3	F	46	ILE
3	F	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	429	HIS
3	F	108	HIS
3	F	69	GLN
3	C	171	GLN
2	E	418	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 ⓘ

44 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
4	NAG	G	1	4,1	14,14,15	0.47	0	17,19,21	1.18	2 (11%)
4	NAG	G	2	4	14,14,15	0.57	0	17,19,21	0.83	0
4	BMA	G	3	4	11,11,12	0.44	0	15,15,17	0.72	0
4	MAN	G	4	4	11,11,12	0.54	0	15,15,17	0.91	1 (6%)
4	NAG	G	5	4	14,14,15	0.53	0	17,19,21	0.72	0
4	GAL	G	6	4	11,11,12	0.58	0	15,15,17	1.14	1 (6%)
4	MAN	G	7	4	11,11,12	0.55	0	15,15,17	0.80	0
4	NAG	G	8	4	14,14,15	0.46	0	17,19,21	0.74	0
4	FUL	G	9	4	10,10,11	0.64	0	14,14,16	1.43	2 (14%)
4	NAG	H	1	4,2	14,14,15	0.58	0	17,19,21	0.97	1 (5%)
4	NAG	H	2	4	14,14,15	0.50	0	17,19,21	0.88	0
4	BMA	H	3	4	11,11,12	0.55	0	15,15,17	1.13	2 (13%)
4	MAN	H	4	4	11,11,12	0.53	0	15,15,17	0.80	1 (6%)
4	NAG	H	5	4	14,14,15	0.58	0	17,19,21	1.20	1 (5%)
4	GAL	H	6	4	11,11,12	0.58	0	15,15,17	0.66	0
4	MAN	H	7	4	11,11,12	0.48	0	15,15,17	1.54	3 (20%)
4	NAG	H	8	4	14,14,15	0.60	0	17,19,21	1.06	1 (5%)
4	FUL	H	9	4	10,10,11	0.42	0	14,14,16	0.81	0
5	NAG	I	1	3,5	14,14,15	0.48	0	17,19,21	1.94	2 (11%)
5	NAG	I	2	5	14,14,15	0.49	0	17,19,21	0.80	0
5	BMA	I	3	5	11,11,12	0.44	0	15,15,17	0.75	0
5	MAN	I	4	5	11,11,12	0.58	0	15,15,17	0.90	0
5	MAN	I	5	5	11,11,12	0.57	0	15,15,17	1.16	2 (13%)
6	NAG	J	1	3,6	14,14,15	0.48	0	17,19,21	0.95	1 (5%)
6	NAG	J	2	6	14,14,15	0.44	0	17,19,21	0.90	1 (5%)
7	NAG	K	1	1,7	14,14,15	0.51	0	17,19,21	1.07	1 (5%)
7	NAG	K	2	7	14,14,15	0.52	0	17,19,21	0.70	0
7	BMA	K	3	7	11,11,12	0.42	0	15,15,17	1.09	2 (13%)
7	MAN	K	4	7	11,11,12	0.51	0	15,15,17	0.80	1 (6%)
7	NAG	K	5	7	14,14,15	0.48	0	17,19,21	0.72	0
7	MAN	K	6	7	11,11,12	0.58	0	15,15,17	0.80	1 (6%)
7	NAG	K	7	7	14,14,15	0.50	0	17,19,21	0.73	0
7	FUL	K	8	7	10,10,11	0.45	0	14,14,16	0.56	0
4	NAG	L	1	4,2	14,14,15	0.43	0	17,19,21	1.33	1 (5%)
4	NAG	L	2	4	14,14,15	0.47	0	17,19,21	0.82	0
4	BMA	L	3	4	11,11,12	0.45	0	15,15,17	0.75	0
4	MAN	L	4	4	11,11,12	0.55	0	15,15,17	0.89	1 (6%)
4	NAG	L	5	4	14,14,15	0.53	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	L	6	4	11,11,12	0.62	0	15,15,17	0.61	0
4	MAN	L	7	4	11,11,12	0.47	0	15,15,17	1.13	1 (6%)
4	NAG	L	8	4	14,14,15	0.58	0	17,19,21	1.08	1 (5%)
4	FUL	L	9	4	10,10,11	0.48	0	14,14,16	0.60	0
6	NAG	M	1	3,6	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
6	NAG	M	2	6	14,14,15	0.48	0	17,19,21	0.89	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
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	NAG	G	5	4	-	2/6/23/26	0/1/1/1
4	GAL	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
4	NAG	G	8	4	-	0/6/23/26	0/1/1/1
4	FUL	G	9	4	-	-	0/1/1/1
4	NAG	H	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	NAG	H	5	4	-	0/6/23/26	0/1/1/1
4	GAL	H	6	4	-	0/2/19/22	0/1/1/1
4	MAN	H	7	4	-	0/2/19/22	0/1/1/1
4	NAG	H	8	4	-	0/6/23/26	0/1/1/1
4	FUL	H	9	4	-	-	0/1/1/1
5	NAG	I	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
6	NAG	J	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
7	NAG	K	5	7	-	0/6/23/26	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
7	NAG	K	7	7	-	0/6/23/26	0/1/1/1
7	FUL	K	8	7	-	-	0/1/1/1
4	NAG	L	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	MAN	L	4	4	-	0/2/19/22	0/1/1/1
4	NAG	L	5	4	-	2/6/23/26	0/1/1/1
4	GAL	L	6	4	-	2/2/19/22	0/1/1/1
4	MAN	L	7	4	-	0/2/19/22	0/1/1/1
4	NAG	L	8	4	-	1/6/23/26	0/1/1/1
4	FUL	L	9	4	-	-	0/1/1/1
6	NAG	M	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-O5-C5	5.75	119.89	112.19
4	L	1	NAG	C1-O5-C5	4.14	117.73	112.19
4	H	5	NAG	C4-C3-C2	3.67	116.40	111.02
5	I	1	NAG	C2-N2-C7	3.63	127.77	122.90
4	G	6	GAL	C1-O5-C5	3.54	116.94	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

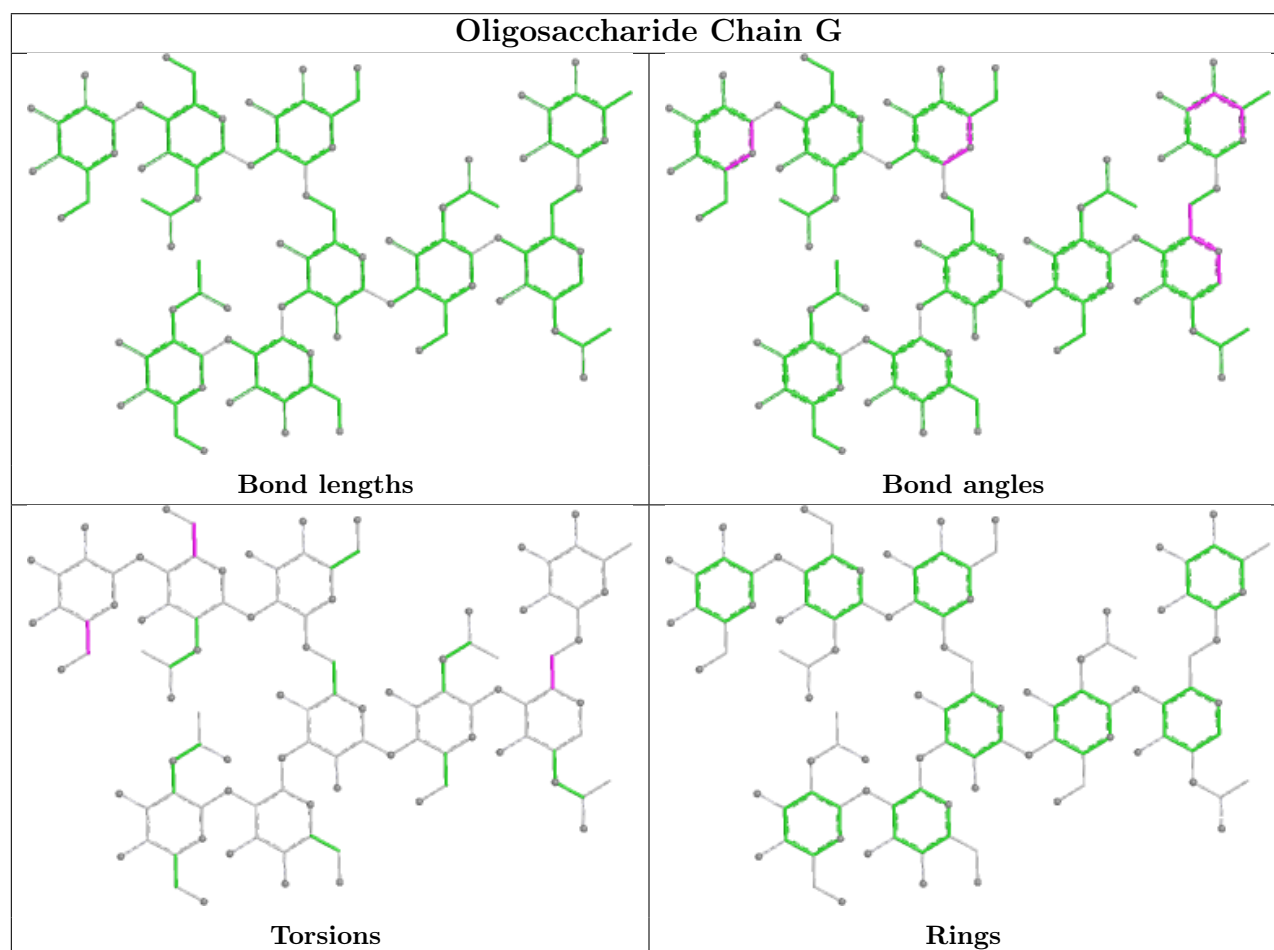
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	L	6	GAL	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	L	6	GAL	C4-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6

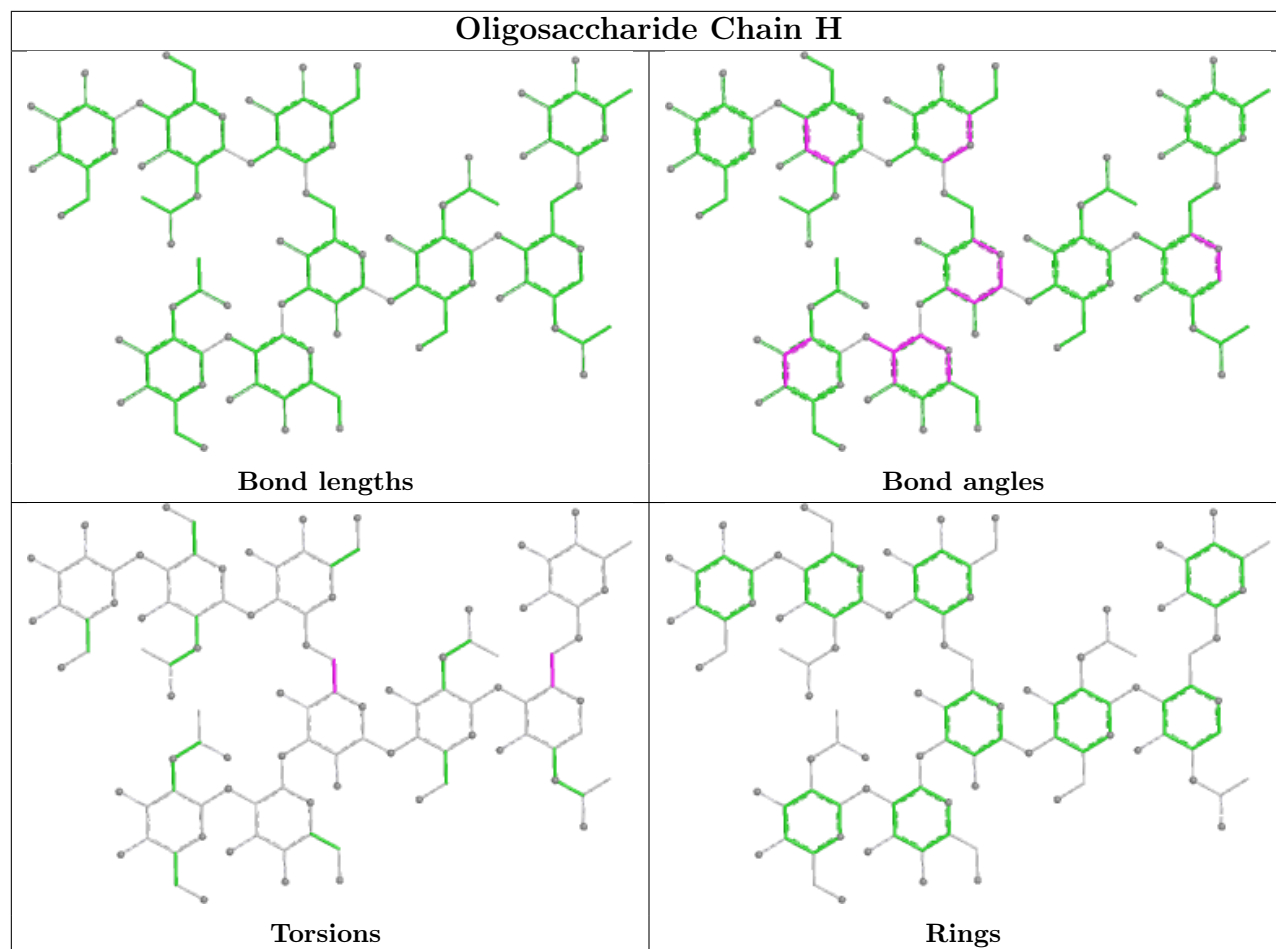
There are no ring outliers.

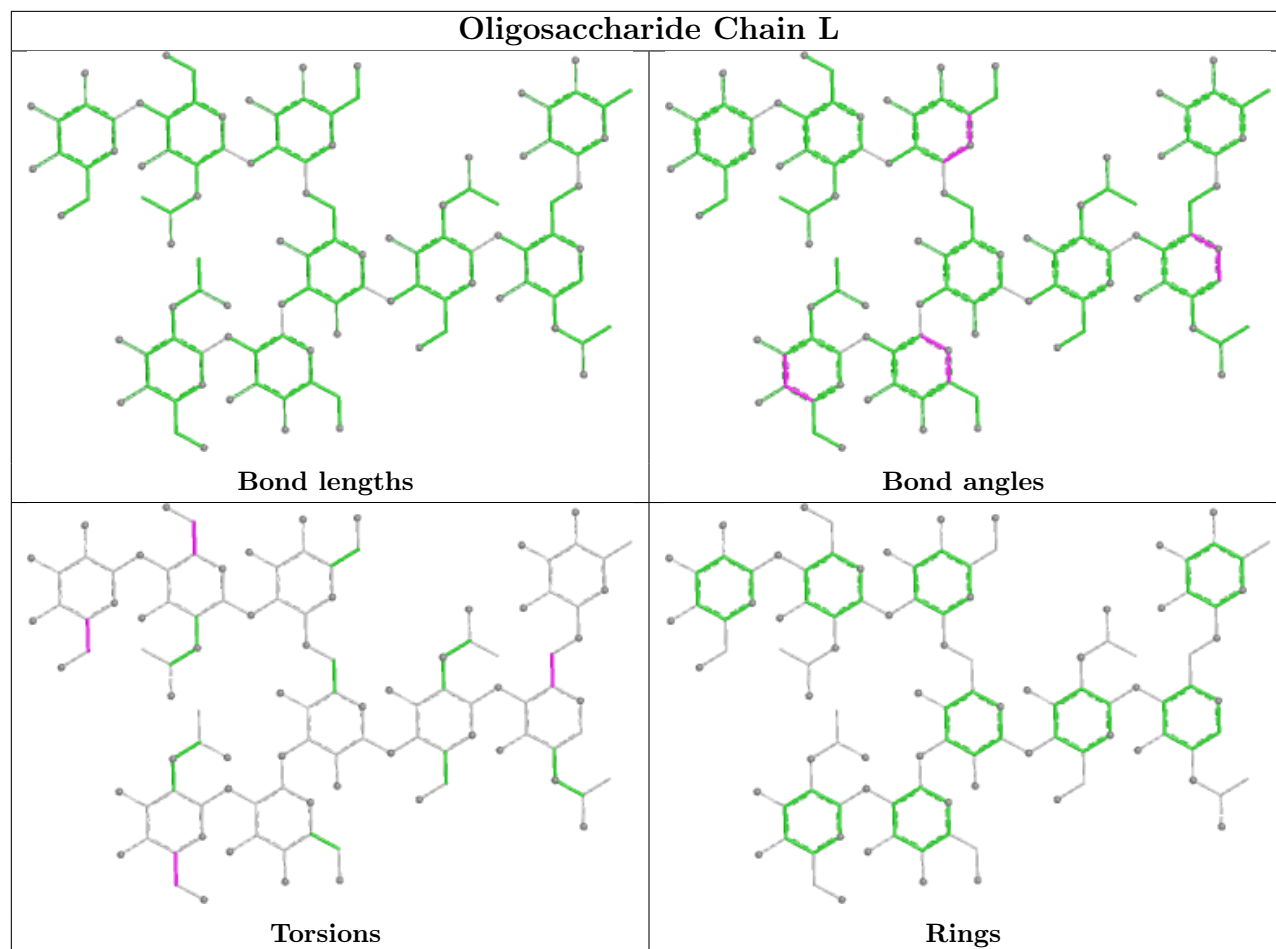
4 monomers are involved in 3 short contacts:

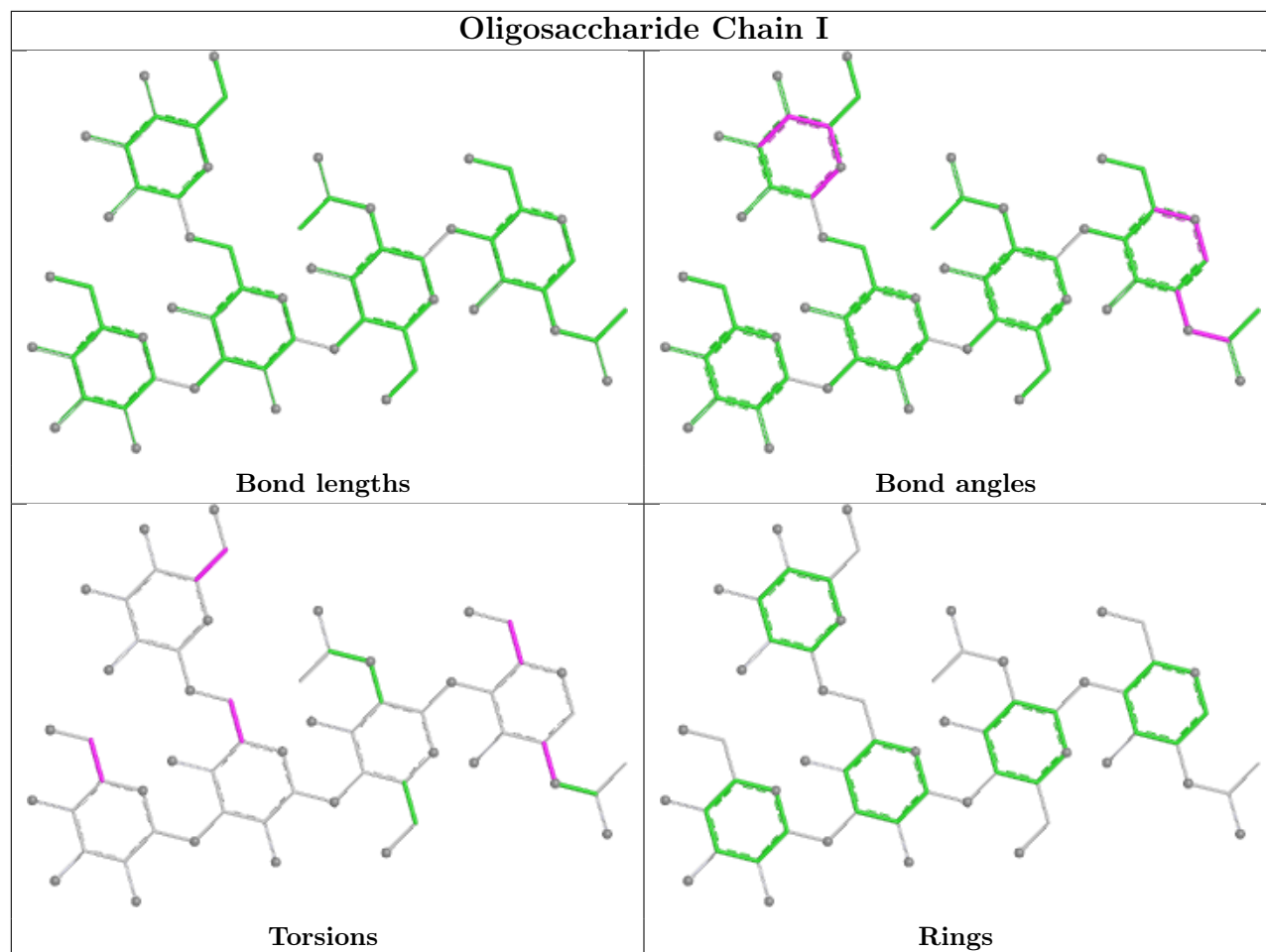
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	G	6	GAL	1	0
4	H	9	FUL	2	0
4	G	5	NAG	1	0

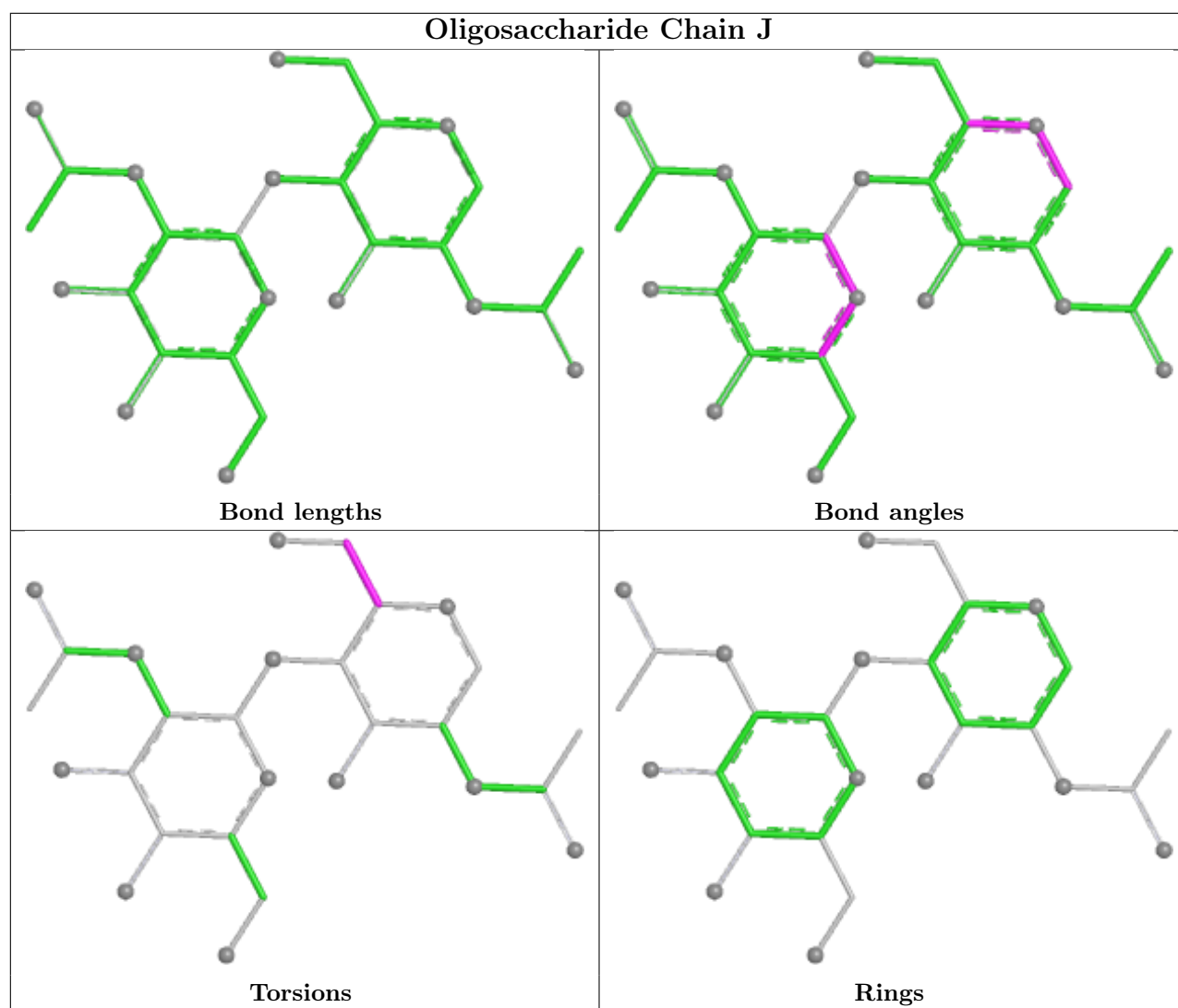
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

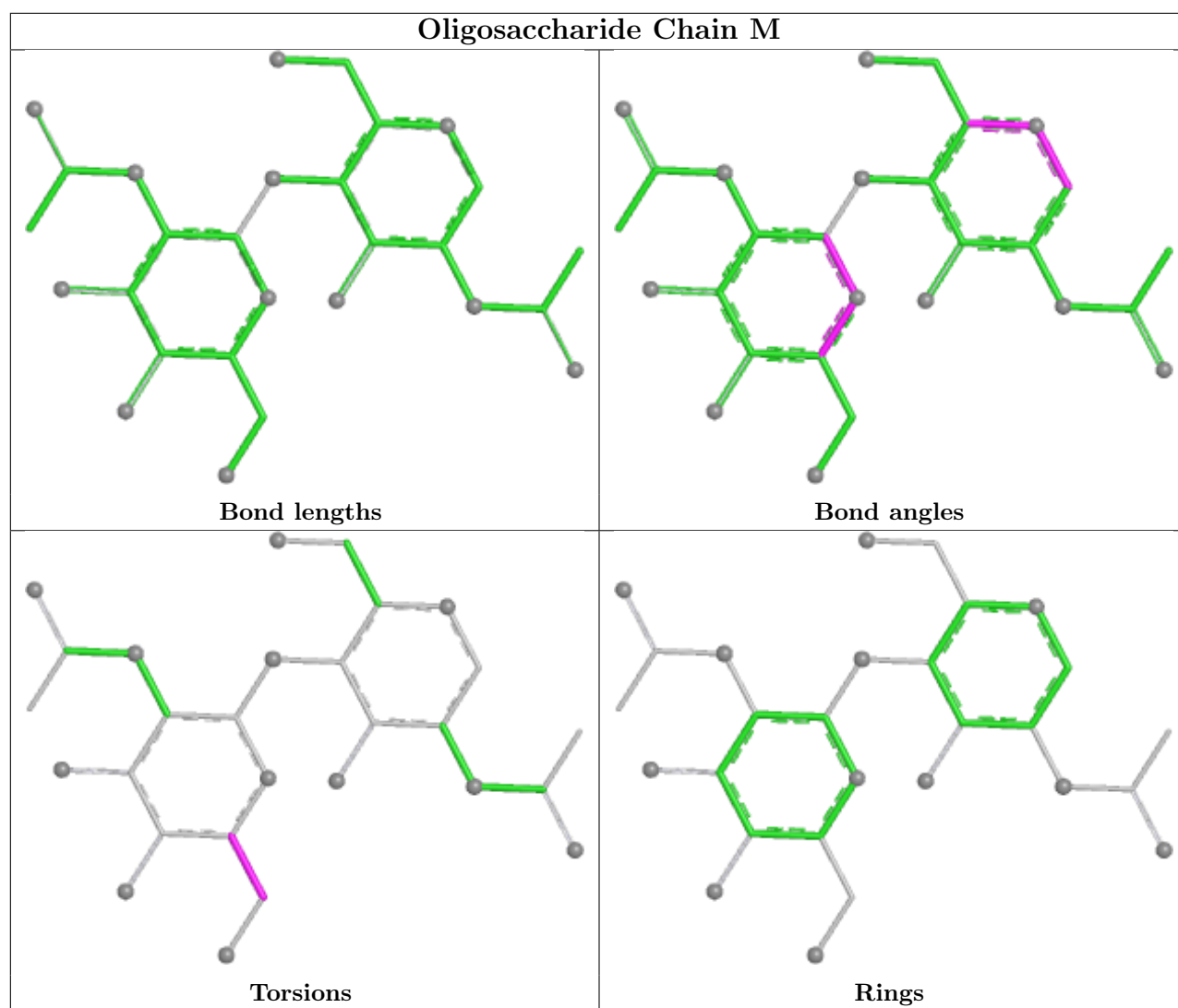


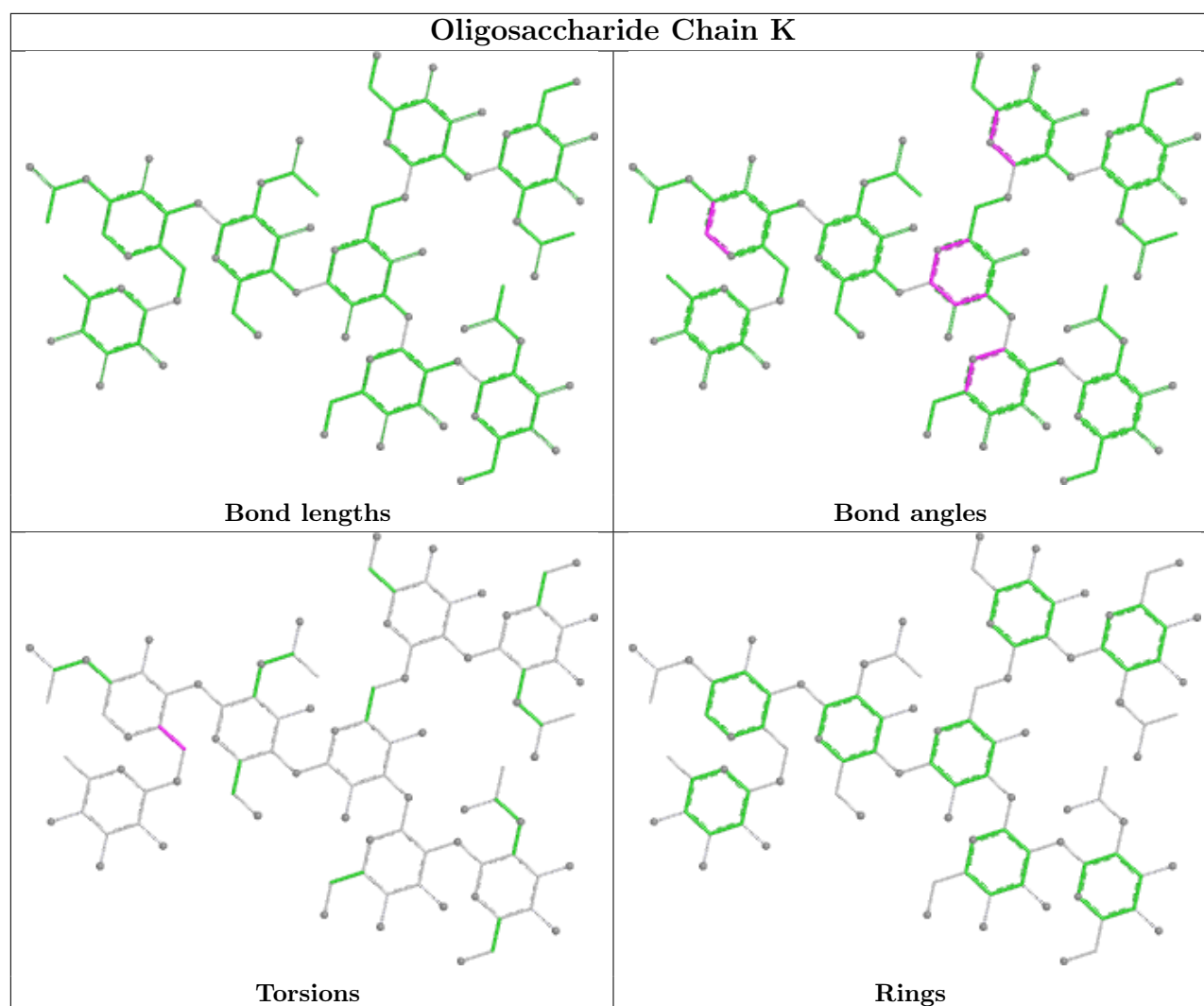












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 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	$\# Z > 2$
9	NAG	F	201	3	14,14,15	0.51	0	17,19,21	0.78	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
9	NAG	F	201	3	-	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(°)
9	F	201	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	201	NAG	C4-C5-C6-O6
9	F	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	212/230 (92%)	0.09	6 (2%) 55 49	38, 52, 68, 79	0
1	D	212/230 (92%)	0.27	9 (4%) 41 36	37, 57, 84, 98	0
2	B	210/230 (91%)	0.07	2 (0%) 79 75	31, 48, 77, 94	0
2	E	210/230 (91%)	0.72	23 (10%) 12 10	44, 70, 111, 121	0
3	C	169/197 (85%)	-0.05	5 (2%) 52 47	30, 44, 73, 98	0
3	F	170/197 (86%)	-0.00	2 (1%) 76 72	30, 45, 68, 94	0
All	All	1183/1314 (90%)	0.20	47 (3%) 43 37	30, 53, 85, 121	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	47	SER	4.2
1	D	420	GLY	4.2
2	E	443	LEU	4.0
2	E	391	TYR	3.9
2	E	386	GLN	3.7

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.

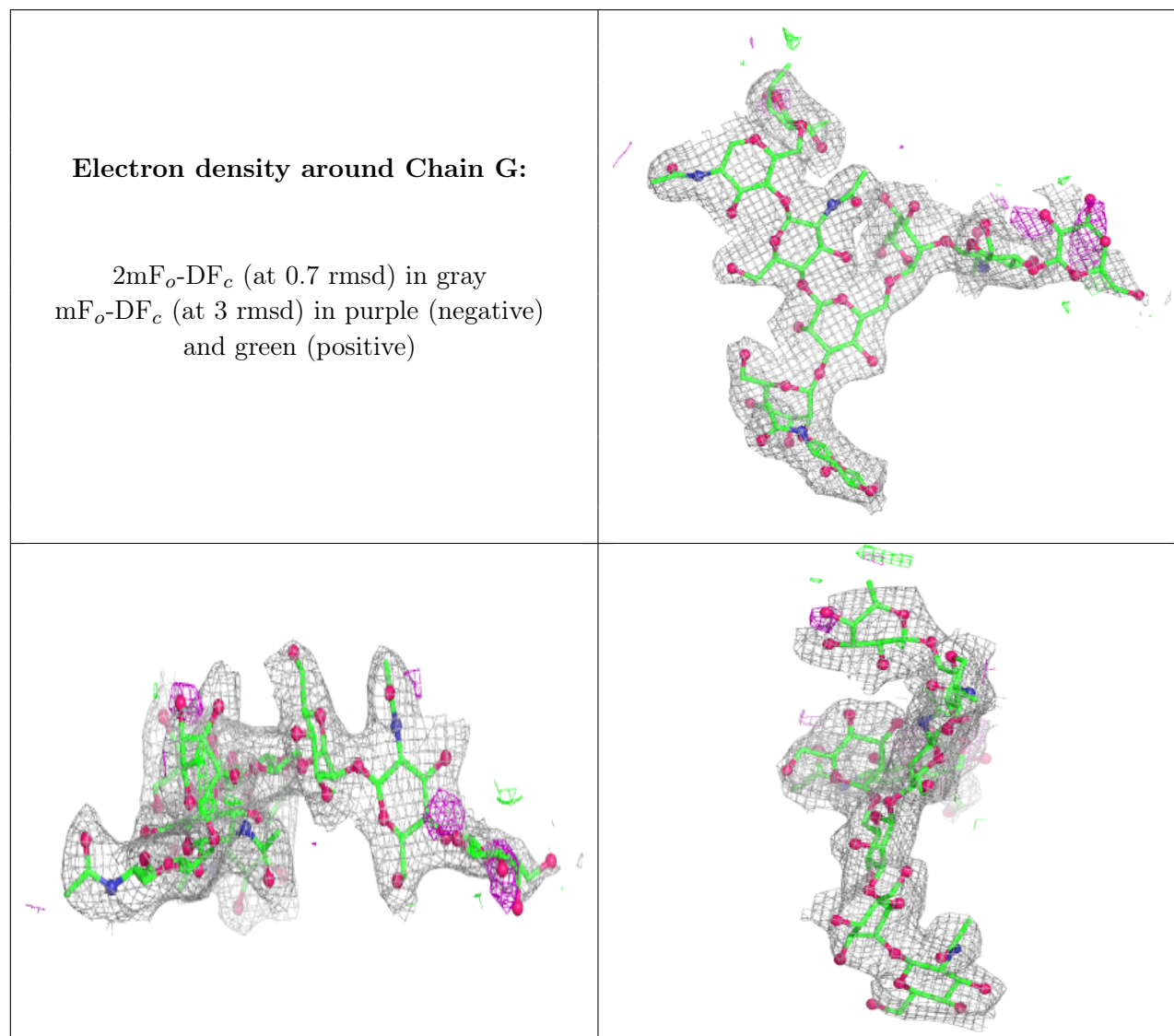
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FUL	L	9	10/11	0.55	0.20	75,78,79,79	0
4	GAL	G	6	11/12	0.58	0.28	77,83,85,86	0
5	MAN	I	5	11/12	0.58	0.14	84,86,90,93	0
4	NAG	H	8	14/15	0.64	0.19	88,91,93,93	0
4	FUL	H	9	10/11	0.64	0.18	63,65,66,67	0
5	MAN	I	4	11/12	0.66	0.14	82,84,86,87	0
4	NAG	L	8	14/15	0.66	0.20	96,100,107,108	0
6	NAG	J	2	14/15	0.73	0.14	65,68,71,72	0
4	MAN	H	7	11/12	0.74	0.12	68,72,75,83	0
6	NAG	M	2	14/15	0.76	0.14	65,69,71,71	0
7	FUL	K	8	10/11	0.79	0.14	59,60,61,62	0
4	GAL	L	6	11/12	0.80	0.14	64,66,67,67	0
7	NAG	K	5	14/15	0.81	0.14	71,74,75,76	0
7	MAN	K	4	11/12	0.82	0.11	62,64,65,68	0
4	FUL	G	9	10/11	0.82	0.13	46,47,48,51	0
4	NAG	H	5	14/15	0.82	0.12	67,68,70,72	0
4	MAN	L	7	11/12	0.84	0.11	76,80,82,89	0
4	MAN	G	7	11/12	0.86	0.10	51,53,55,55	0
4	MAN	H	4	11/12	0.87	0.12	62,63,64,65	0
5	NAG	I	1	14/15	0.87	0.10	47,49,53,54	0
4	NAG	G	8	14/15	0.87	0.11	52,53,56,59	0
4	GAL	H	6	11/12	0.88	0.11	73,74,76,78	0
7	NAG	K	7	14/15	0.88	0.11	54,56,58,58	0
4	BMA	L	3	11/12	0.88	0.11	60,63,65,71	0
4	BMA	H	3	11/12	0.89	0.10	57,59,61,67	0
6	NAG	J	1	14/15	0.89	0.12	57,60,63,65	0
5	BMA	I	3	11/12	0.89	0.09	71,74,78,80	0
4	NAG	L	5	14/15	0.89	0.11	56,59,61,62	0
4	MAN	G	4	11/12	0.90	0.09	53,54,55,56	0
4	NAG	G	5	14/15	0.90	0.10	55,58,62,68	0
7	NAG	K	1	14/15	0.91	0.10	49,51,54,59	0
4	MAN	L	4	11/12	0.91	0.08	55,58,59,60	0
5	NAG	I	2	14/15	0.91	0.09	51,57,61,67	0
4	NAG	L	1	14/15	0.91	0.12	61,64,68,72	0
4	BMA	G	3	11/12	0.91	0.09	44,46,50,51	0
4	NAG	L	2	14/15	0.93	0.09	55,60,61,63	0
6	NAG	M	1	14/15	0.93	0.09	46,49,53,58	0
4	NAG	H	1	14/15	0.94	0.10	45,50,56,61	0
7	NAG	K	2	14/15	0.95	0.10	47,50,53,53	0
7	MAN	K	6	11/12	0.95	0.07	47,48,49,52	0
7	BMA	K	3	11/12	0.95	0.07	49,52,54,58	0
4	NAG	H	2	14/15	0.95	0.09	50,54,56,57	0
4	NAG	G	1	14/15	0.96	0.06	43,44,45,46	0

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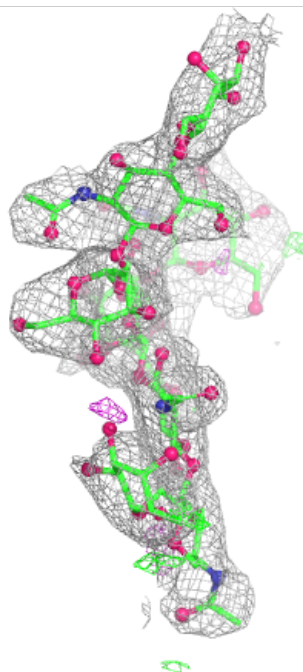
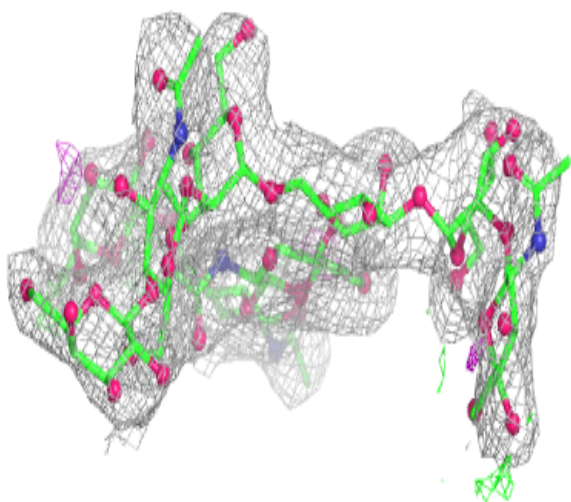
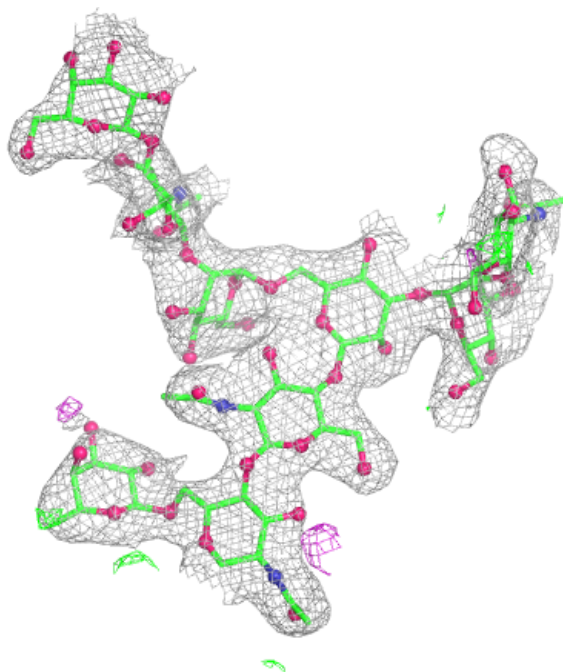
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	G	2	14/15	0.96	0.08	42,43,44,44	0

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



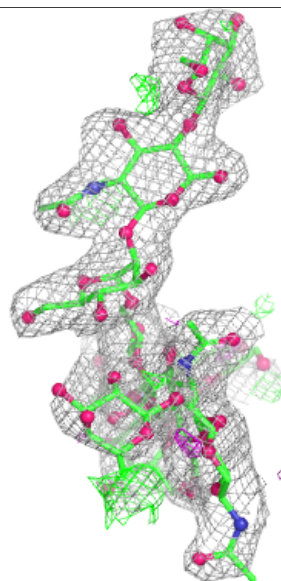
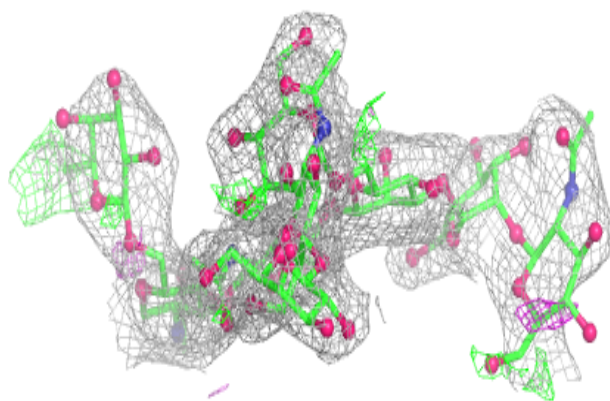
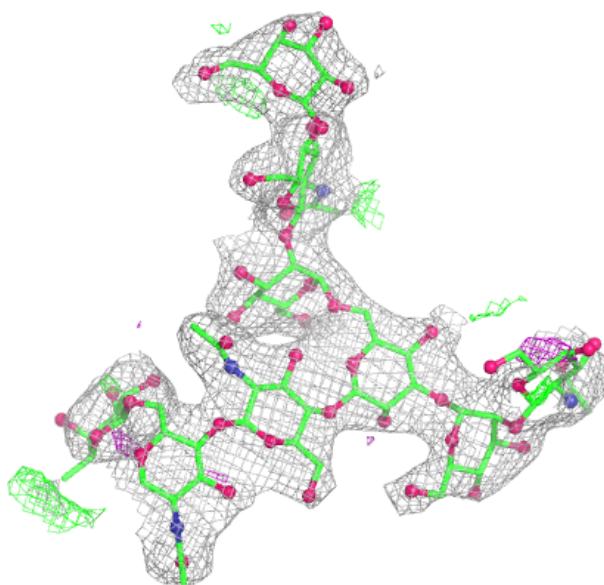
Electron density around Chain H:

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



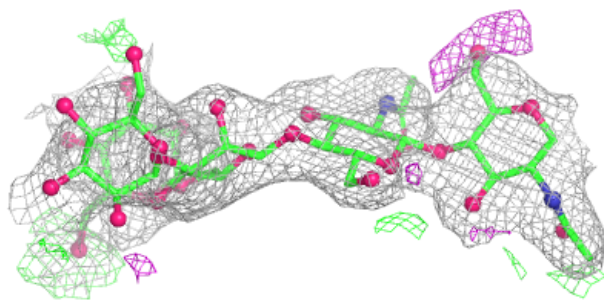
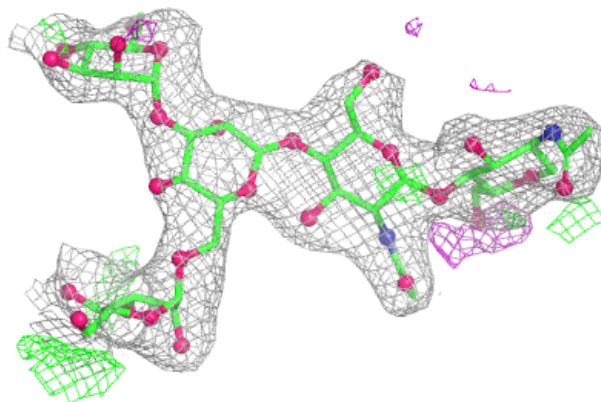
Electron density around Chain L:

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



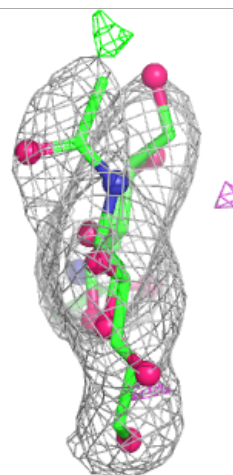
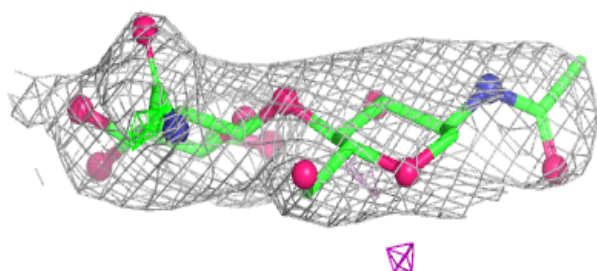
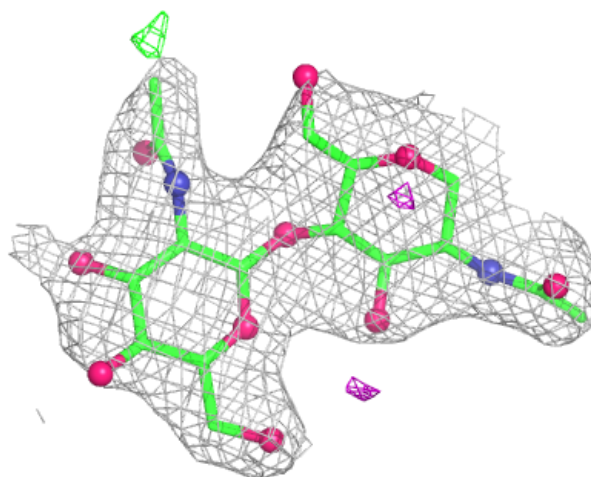
Electron density around Chain I:

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



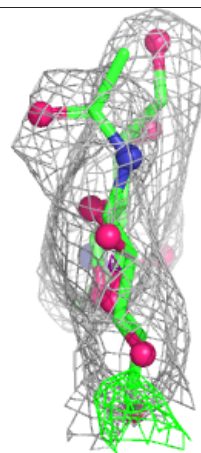
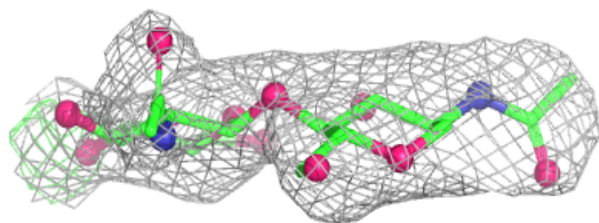
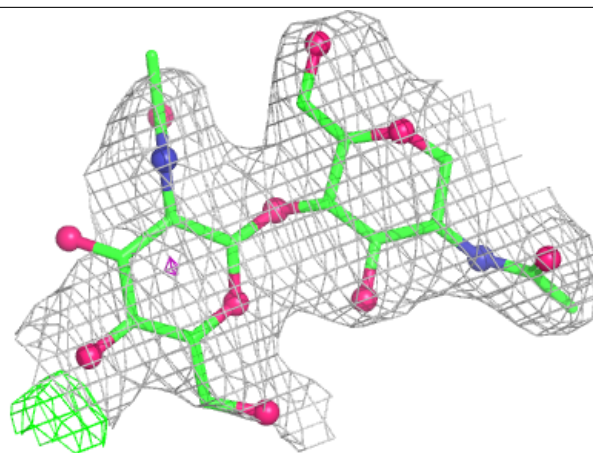
Electron density around Chain J:

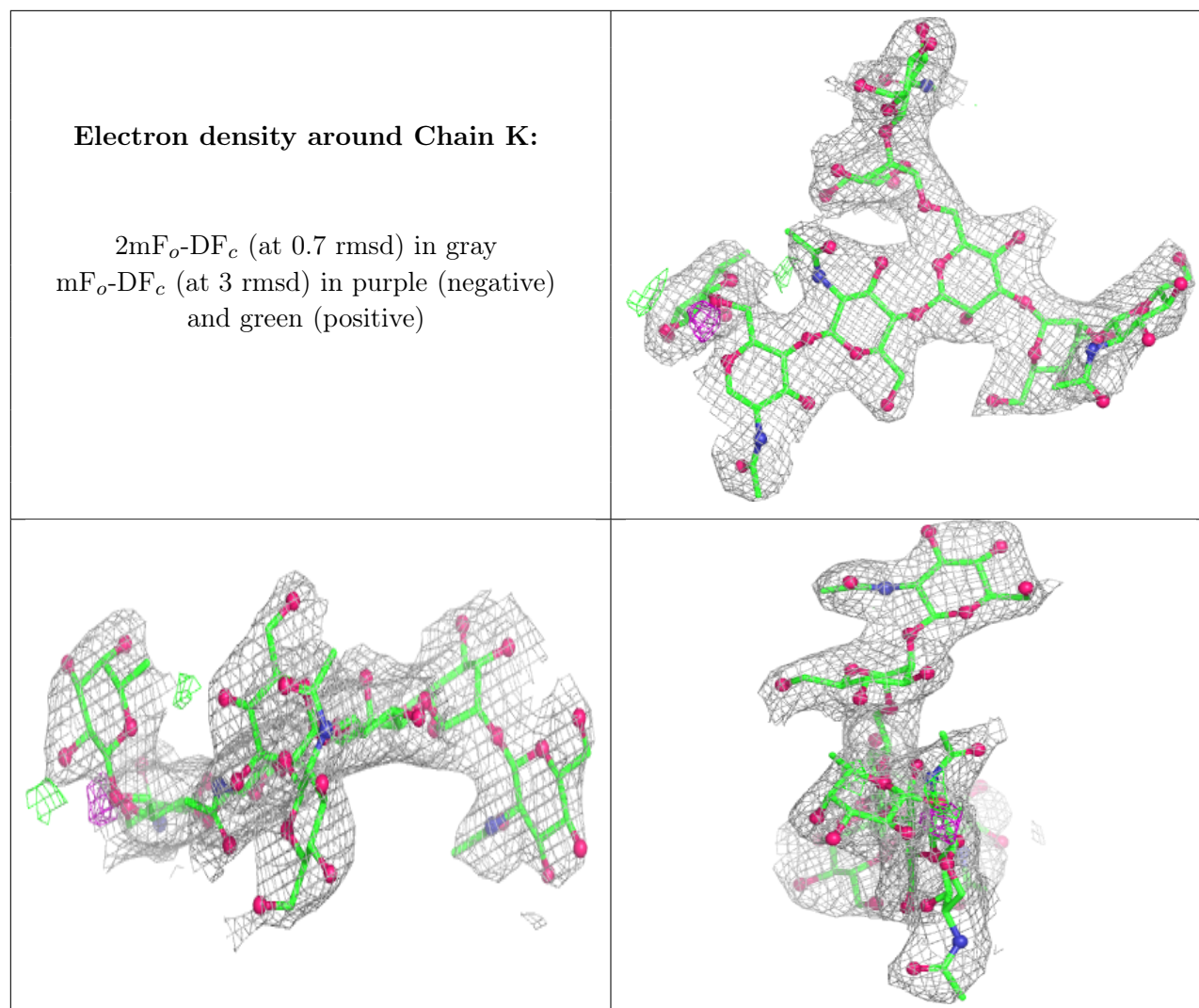
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

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





6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
9	NAG	F	201	14/15	0.66	0.15	64,74,77,78	0
8	IOD	D	1009	1/1	0.85	0.11	86,86,86,86	1
8	IOD	A	1010	1/1	0.93	0.07	71,71,71,71	1
8	IOD	F	207	1/1	0.95	0.05	81,81,81,81	1
8	IOD	B	1012	1/1	0.95	0.09	80,80,80,80	1
8	IOD	C	209	1/1	0.96	0.13	91,91,91,91	0
8	IOD	A	1011	1/1	0.97	0.04	75,75,75,75	1
8	IOD	E	1011	1/1	0.97	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	IOD	E	1012	1/1	0.98	0.15	93,93,93,93	0
8	IOD	E	1013	1/1	0.98	0.12	99,99,99,99	0
8	IOD	F	206	1/1	0.98	0.04	58,58,58,58	1
8	IOD	E	1010	1/1	0.98	0.05	102,102,102,102	0
8	IOD	B	1011	1/1	0.98	0.08	83,83,83,83	0
8	IOD	F	205	1/1	1.00	0.09	68,68,68,68	0
8	IOD	B	1010	1/1	1.00	0.03	49,49,49,49	0
8	IOD	C	208	1/1	1.00	0.01	36,36,36,36	0
8	IOD	F	204	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.