WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 06:16 PM JST

PDB ID	:	5XMH
Title	:	Crystal structure of an IgM rheumatoid factor YES8c in complex with IgG1 Fc
Authors	:	Shiroishi, M.; Shimokawa, K.; Lee, J.M.; Kusakabe, M.; Ueda, T.
Deposited on	:	2017-05-15
Resolution	:	2.80 Å(reported)

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 2.80 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 | | 0.272
Clashscore | | 4
Ramachandran outliers | | 0.8%
Sidechain outliers | | 2.7%
RSRZ outliers | | 2.2%

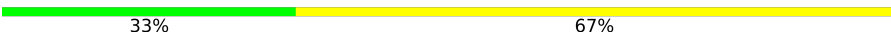Worse — Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
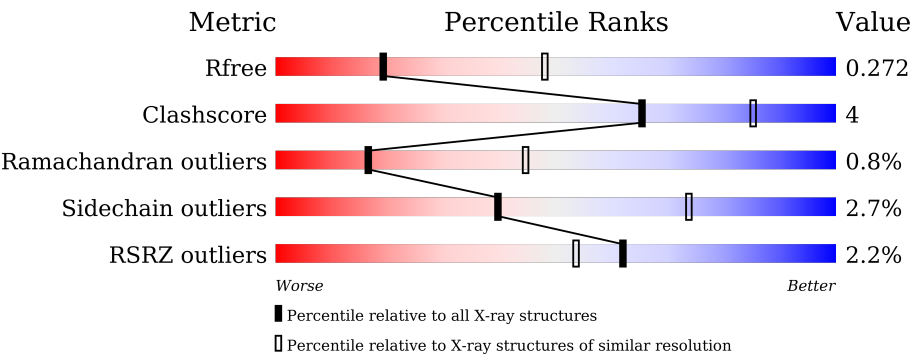
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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% 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	208	92% 8%
1	B	208	2% 89% 10%
2	C	216	% 44% 6% 50%
2	L	216	90% 9%
3	D	226	48% 7% 46%
3	H	226	7% 77% 19%

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Mol	Chain	Length	Quality of chain
4	E	8	50% 38% 12%
5	F	6	33% 67%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8222 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1619	1031	271	311	6			
1	B	207	Total	C	N	O	S	0	0	0
			1547	987	258	296	6			

- Molecule 2 is a protein called YES8c light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1606	1005	268	329	4			
2	C	107	Total	C	N	O	S	0	0	0
			791	498	131	160	2			

- Molecule 3 is a protein called YES8c heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1538	981	252	300	5			
3	D	123	Total	C	N	O	S	0	0	0
			883	565	144	171	3			

- Molecule 4 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
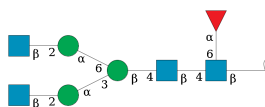
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	8	Total 99	C 56	N 4	O 39	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
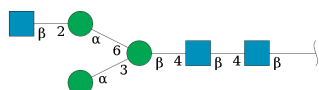
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total 75	C 42	N 3	O 30	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total 19	O 19	0	0
6	B	9	Total 9	O 9	0	0
6	L	18	Total 18	O 18	0	0
6	H	13	Total 13	O 13	0	0
6	D	2	Total 2	O 2	0	0
6	C	3	Total 3	O 3	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 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: Immunoglobulin gamma-1 heavy chain

Chain A:
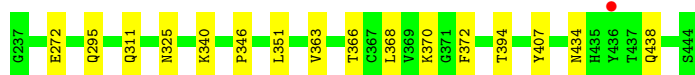
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain B:
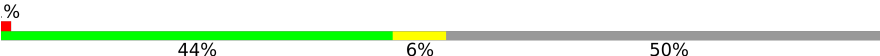
- Molecule 2: YES8c light chain

Chain L:

- Molecule 2: YES8c light chain

Chain C:
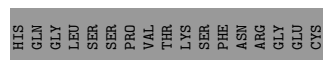
- Molecule 3: YES8c heavy chain

Chain H:
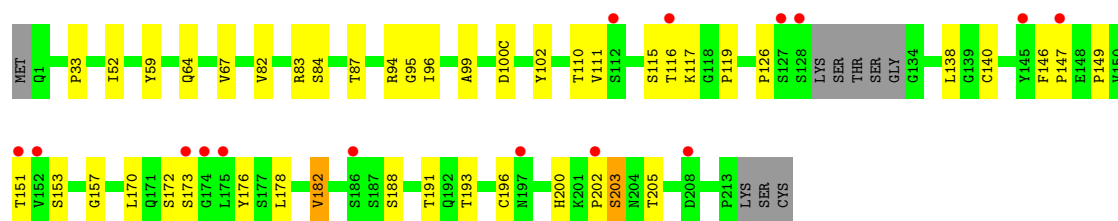
• Molecule 3: YES8c heavy chain

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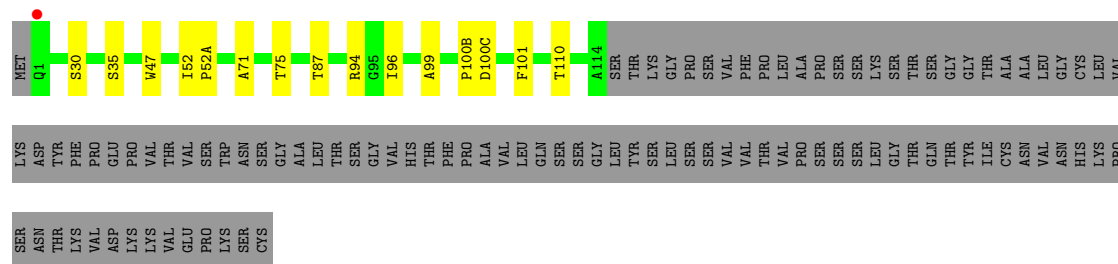
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:
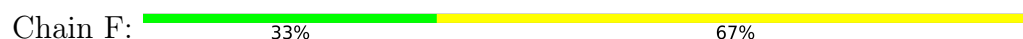
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	189.90Å 189.90Å 79.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.80 19.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.90-2.80) 99.2 (19.90-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.220 , 0.272 0.222 , 0.272	Depositor DCC
R_{free} test set	2044 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 21.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8222	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: MAN, NAG, FUC, 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	0.25	0/1665	0.44	0/2280
1	B	0.25	0/1591	0.44	0/2186
2	C	0.26	0/810	0.46	0/1103
2	L	0.26	0/1642	0.46	0/2239
3	D	0.25	0/905	0.47	0/1233
3	H	0.27	0/1578	0.49	0/2165
All	All	0.26	0/8191	0.46	0/11206

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	1619	0	1526	9	0
1	B	1547	0	1392	10	0
2	C	791	0	732	6	0
2	L	1606	0	1496	9	0
3	D	883	0	799	10	0
3	H	1538	0	1412	21	0
4	E	99	0	85	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	75	0	64	0	0
6	A	19	0	0	0	0
6	B	9	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	H	13	0	0	1	0
6	L	18	0	0	0	0
All	All	8222	0	7506	58	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.

The worst 5 of 58 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)
2:L:108:ARG:NH1	2:L:109:THR:O	2.21	0.74
1:A:272:GLU:O	1:A:325:ASN:ND2	2.22	0.71
3:H:126:PRO:HG3	3:H:138:LEU:HB3	1.73	0.71
2:L:189:HIS:O	2:L:211:ARG:NH1	2.27	0.68
3:H:94:ARG:HB2	3:H:95:GLY:HA3	1.79	0.64

There are no symmetry-related clashes.

5.3   Torsion angles   (i)

5.3.1   Protein backbone   (i)

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	206/208 (99%)	198 (96%)	7 (3%)	1 (0%)	25	56
1	B	205/208 (99%)	199 (97%)	5 (2%)	1 (0%)	25	56
2	C	105/216 (49%)	102 (97%)	3 (3%)	0	100	100
2	L	212/216 (98%)	203 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	121/226 (54%)	113 (93%)	8 (7%)	0	100	100
3	H	213/226 (94%)	194 (91%)	13 (6%)	6 (3%)	4	14
All	All	1062/1300 (82%)	1009 (95%)	45 (4%)	8 (1%)	16	44

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	116	THR
1	A	340	LYS
3	H	157	GLY
3	H	188	SER
3	H	203	SER

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	180/194 (93%)	178 (99%)	2 (1%)	70	90
1	B	159/194 (82%)	155 (98%)	4 (2%)	42	75
2	C	82/187 (44%)	78 (95%)	4 (5%)	21	52
2	L	172/187 (92%)	168 (98%)	4 (2%)	45	78
3	D	82/187 (44%)	81 (99%)	1 (1%)	67	89
3	H	153/187 (82%)	146 (95%)	7 (5%)	23	55
All	All	828/1136 (73%)	806 (97%)	22 (3%)	40	74

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	182	VAL
3	D	75	THR
3	H	196	CYS
2	C	69	THR
2	L	33	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	325	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 ⓘ

14 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	E	1	4,1	14,14,15	0.25	0	17,19,21	0.63	1 (5%)
4	NAG	E	2	4	14,14,15	0.41	0	17,19,21	0.41	0
4	BMA	E	3	4	11,11,12	0.93	0	15,15,17	1.01	1 (6%)
4	MAN	E	4	4	11,11,12	0.78	0	15,15,17	1.12	1 (6%)
4	NAG	E	5	4	14,14,15	0.18	0	17,19,21	0.44	0
4	MAN	E	6	4	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
4	NAG	E	7	4	14,14,15	0.24	0	17,19,21	0.56	0
4	FUC	E	8	4	10,10,11	0.72	0	14,14,16	0.94	0
5	NAG	F	1	5,1	14,14,15	0.82	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	F	2	5	14,14,15	0.18	0	17,19,21	0.51	0
5	BMA	F	3	5	11,11,12	0.63	0	15,15,17	1.02	1 (6%)
5	MAN	F	4	5	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
5	NAG	F	5	5	14,14,15	0.26	0	17,19,21	0.46	0
5	MAN	F	6	5	11,11,12	0.85	0	15,15,17	1.00	1 (6%)

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	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	NAG	E	5	4	-	4/6/23/26	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
4	NAG	E	7	4	-	4/6/23/26	0/1/1/1
4	FUC	E	8	4	-		0/1/1/1
5	NAG	F	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	NAG	F	5	5	-	4/6/23/26	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	O5-C1	-2.76	1.39	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	4	MAN	O2-C2-C3	-3.09	103.95	110.14
5	F	4	MAN	O2-C2-C3	-2.68	104.77	110.14
5	F	4	MAN	C1-O5-C5	2.55	115.64	112.19
4	E	6	MAN	O2-C2-C3	-2.48	105.17	110.14
5	F	1	NAG	C3-C4-C5	2.45	114.61	110.24

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	5	NAG	C4-C5-C6-O6
4	E	5	NAG	O5-C5-C6-O6
5	F	5	NAG	O5-C5-C6-O6
4	E	5	NAG	C4-C5-C6-O6

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| Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
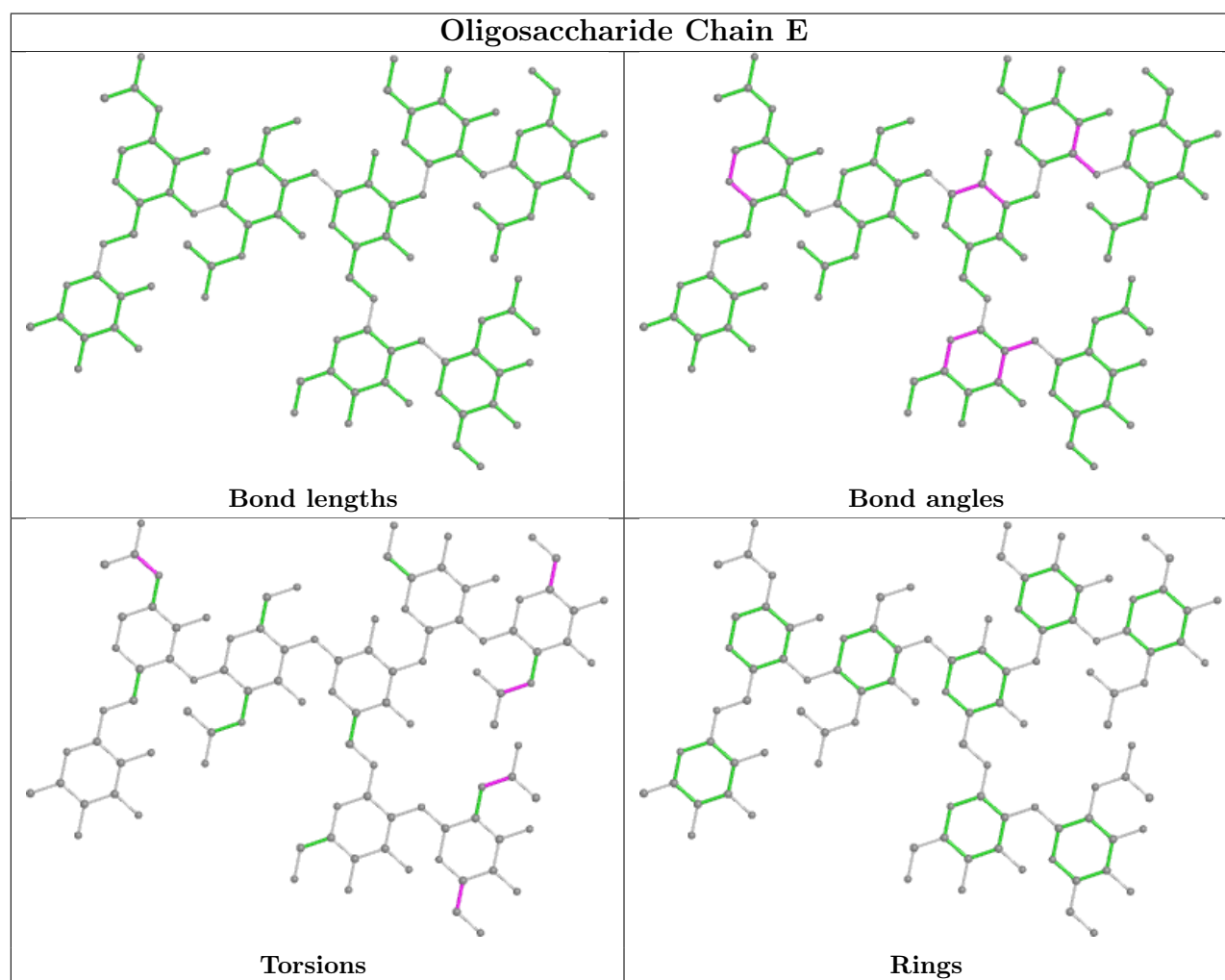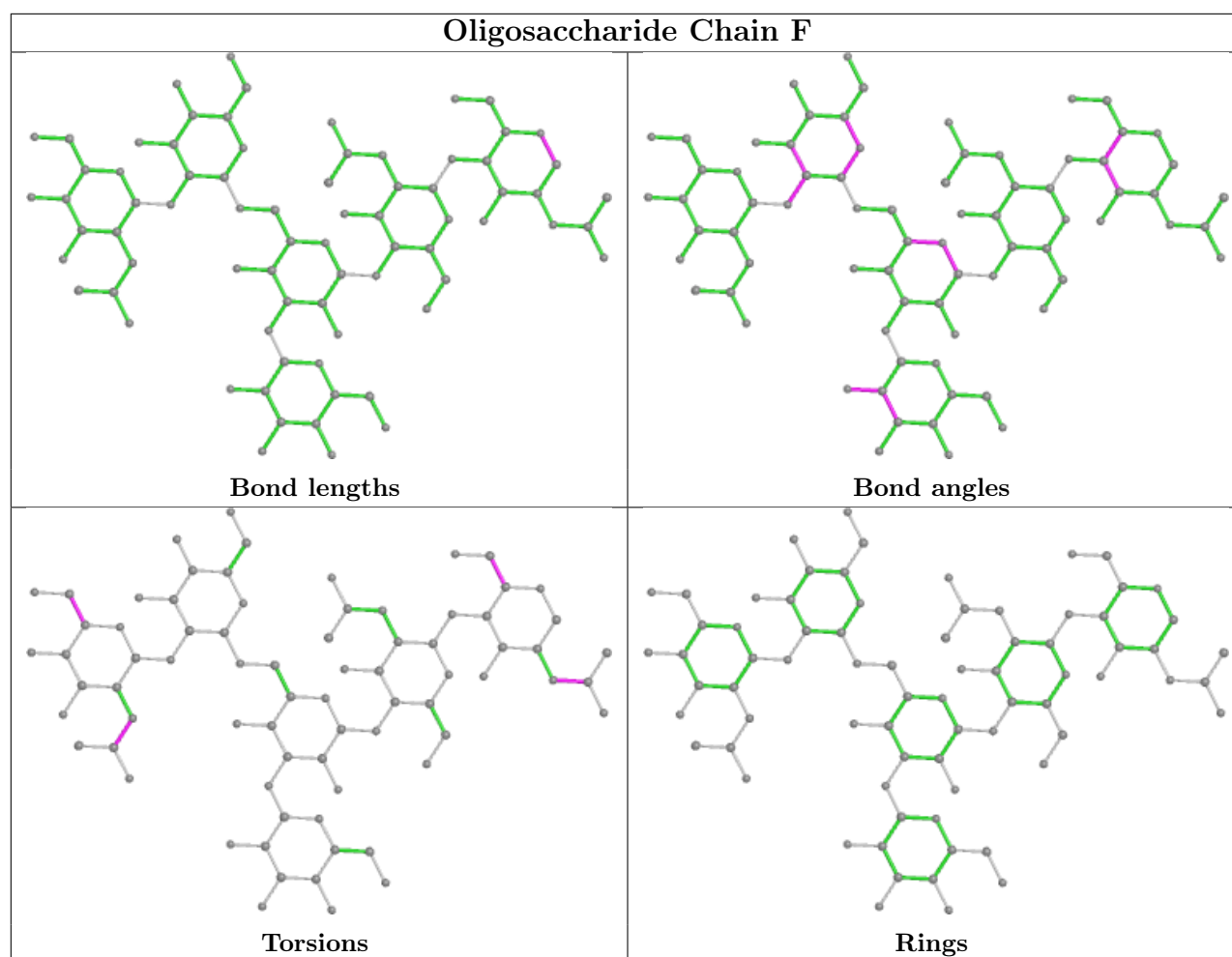
5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	208/208 (100%)	-0.24	1 (0%)	87	83	35, 46, 73, 81	0
1	B	207/208 (99%)	0.03	5 (2%)	59	51	36, 53, 89, 99	0
2	C	107/216 (49%)	0.03	2 (1%)	66	58	48, 56, 68, 71	0
2	L	214/216 (99%)	-0.44	0	100	100	30, 40, 59, 67	0
3	D	123/226 (54%)	0.10	1 (0%)	82	77	49, 58, 75, 85	0
3	H	217/226 (96%)	0.20	15 (6%)	24	18	35, 49, 82, 89	0
All	All	1076/1300 (82%)	-0.07	24 (2%)	62	53	30, 51, 78, 99	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	208	ASP	6.0
3	H	145	TYR	4.7
1	B	296	TYR	3.5
3	H	112	SER	3.4
3	H	175	LEU	2.8

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 ⓘ

SUGAR-RSR INFOmissingINFO

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.