WORLD WIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 03:01 AM EDT

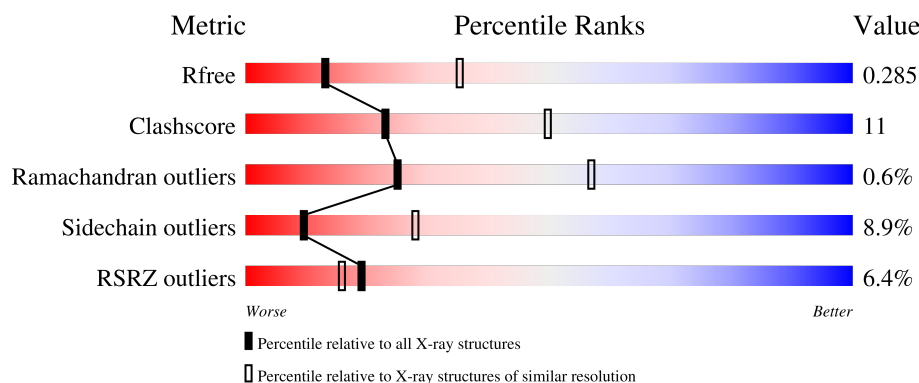|		
PDB ID	:	4J4P
Title	:	The complex of human IgE-Fc with two bound Fab fragments
Authors	:	Drinkwater, N.; Sutton, B.J.
Deposited on	:	2013-02-07
Resolution	:	2.91 Å(reported)

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 2.91 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		0.285
Clashscore		11
Ramachandran outliers		0.6%
Sidechain outliers		8.9%
RSRZ outliers		6.4%

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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	323	% — 66% 29% · ·
1	B	323	3% — 67% 27% · ·
2	C	249	12% — 61% 24% · 11%
2	H	249	% — 59% 25% 5% · 10%
3	D	235	20% — 69% 21% · 9%

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Mol	Chain	Length	Quality of chain
3	L	235	62% 28% · 9%
4	E	5	20% 60% 20%
4	F	5	80% 20%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11702 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 epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total 2461	C 1535	N 438	O 477	S 11	6	0	0
1	B	317	Total 2480	C 1548	N 441	O 480	S 11	6	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	engineered mutation	UNP P01854
A	371	GLN	ASN	engineered mutation	UNP P01854
B	265	GLN	ASN	engineered mutation	UNP P01854
B	371	GLN	ASN	engineered mutation	UNP P01854

- Molecule 2 is a protein called Immunoglobulin G Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total 1715	C 1081	N 288	O 339	S 7	0	0	0
2	C	222	Total 1701	C 1074	N 286	O 335	S 6	6	0	0

- Molecule 3 is a protein called Immunoglobulin G Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total 1591	C 993	N 262	O 332	S 4	0	0	0
3	D	215	Total 1591	C 993	N 262	O 332	S 4	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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.
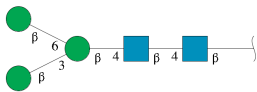
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total 61	C 34	N 2	O 25	0	0	0
4	F	5	Total 61	C 34	N 2	O 25	0	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	8	Total 8	O 8	0	0
5	H	9	Total 9	O 9	0	0
5	L	2	Total 2	O 2	0	0
5	C	5	Total 5	O 5	0	0
5	D	6	Total 6	O 6	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: Ig epsilon chain C region
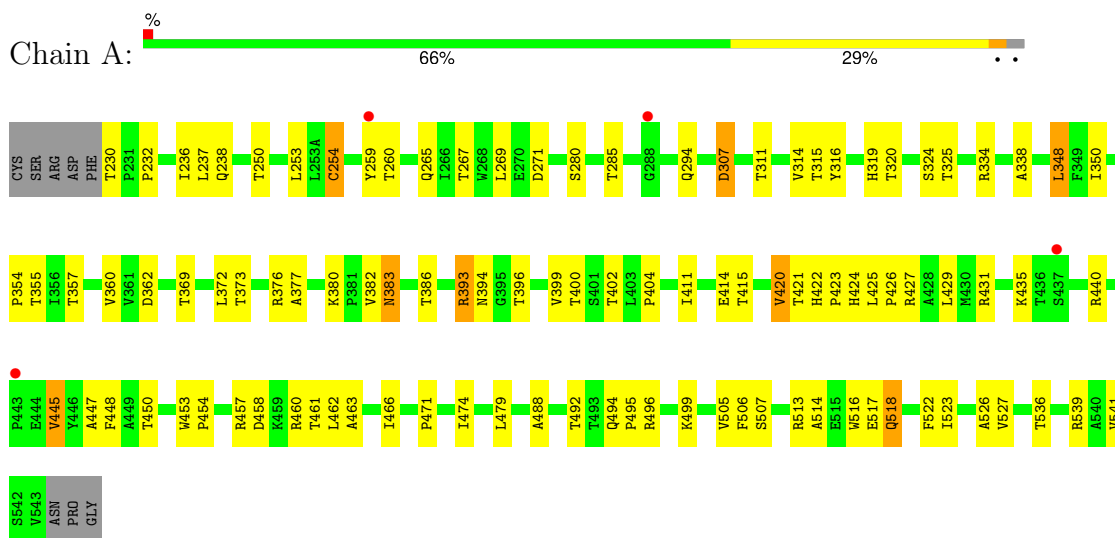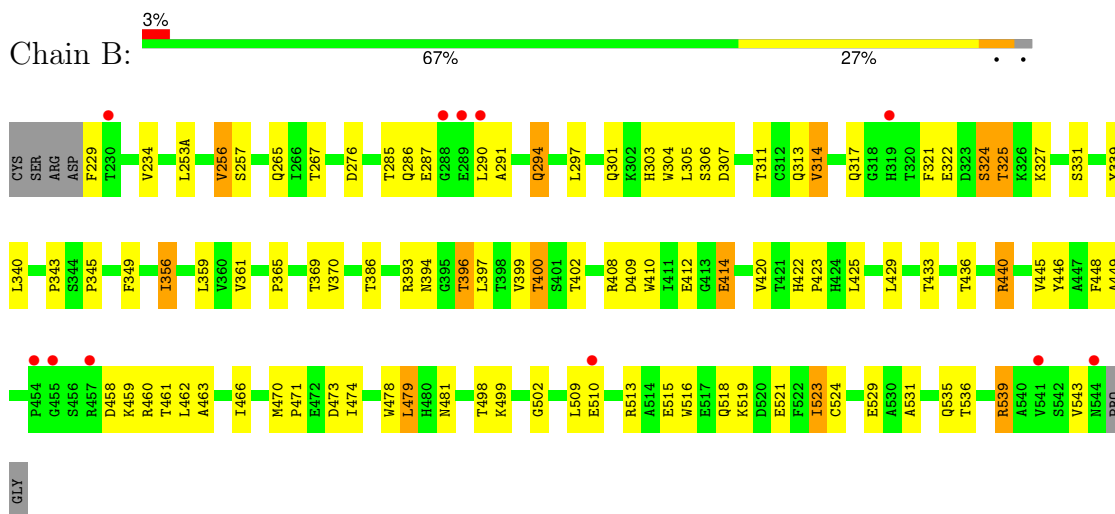
Chain A:

- Molecule 1: Ig epsilon chain C region

Chain B:

- Molecule 2: Immunoglobulin G Fab Fragment Heavy Chain

Chain H:

• Molecule 2: Immunoglobulin G Fab Fragment Heavy Chain
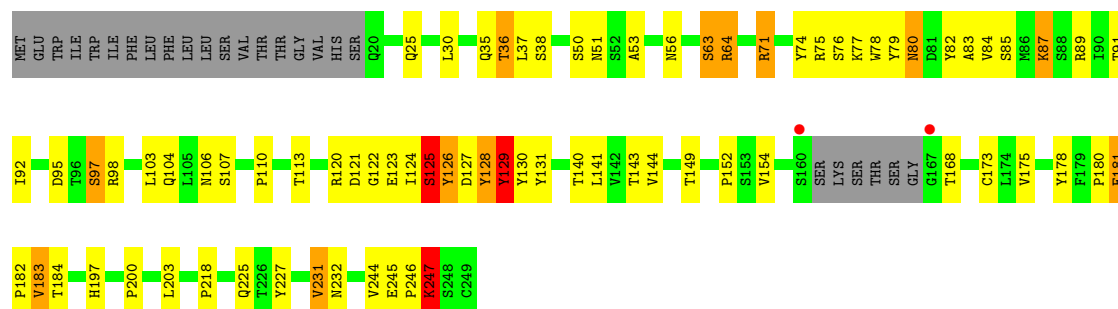
Chain C:
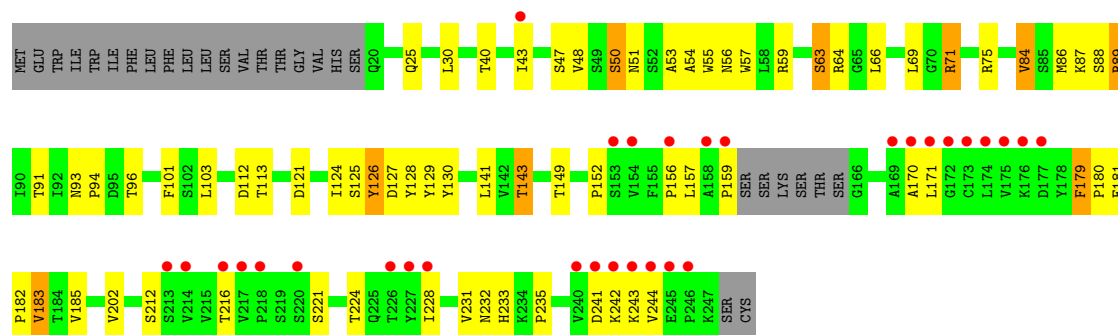
• Molecule 3: Immunoglobulin G Fab Fragment Light Chain
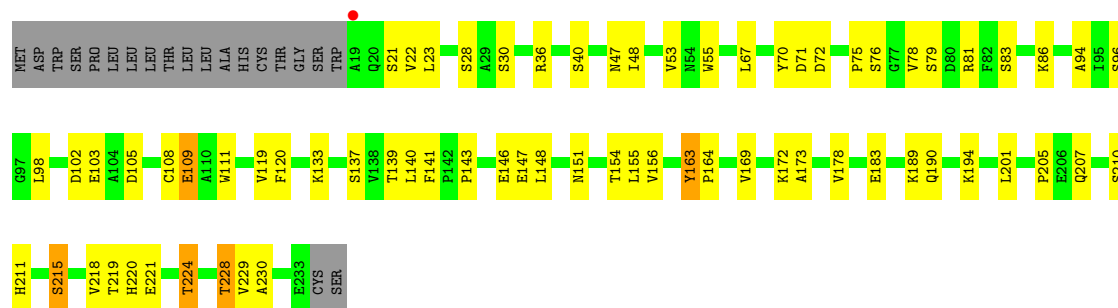
Chain L:

• Molecule 3: Immunoglobulin G Fab Fragment Light Chain

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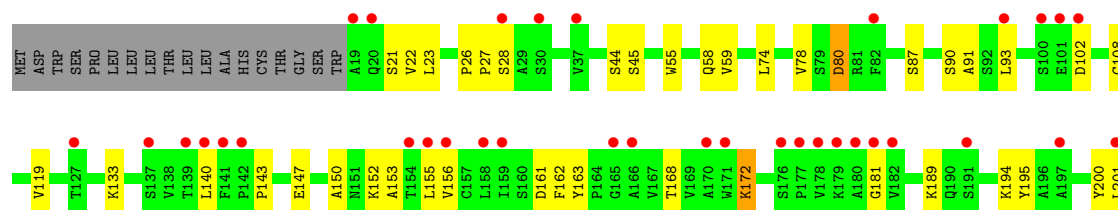
• Molecule 4: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyrano se

• Molecule 4: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyrano se
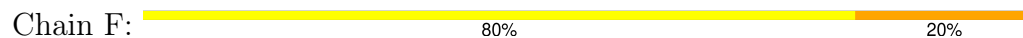
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.59Å 100.81Å 219.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.02 – 2.91 67.02 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (67.02-2.91) 99.7 (67.02-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.236 , 0.284 0.238 , 0.285	Depositor DCC
R_{free} test set	2115 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	87.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 59.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11702	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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 $< |L| >$, $< L^2 >$ 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: 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	0.51	0/2521	0.72	2/3436 (0.1%)
1	B	0.47	0/2541	0.68	1/3463 (0.0%)
2	C	0.46	0/1745	0.71	0/2383
2	H	0.60	0/1759	0.85	1/2402 (0.0%)
3	D	0.49	1/1629 (0.1%)	0.62	0/2226
3	L	0.56	0/1629	0.77	0/2226
All	All	0.51	1/11824 (0.0%)	0.72	4/16136 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	H	0	4
3	D	0	1
3	L	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	215	SER	CB-OG	11.26	1.56	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
2	H	84	VAL	N-CA-C	-6.22	94.22	111.00
1	A	334	ARG	N-CA-C	-5.29	96.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	518	GLN	N-CA-C	-5.16	97.08	111.00
1	B	414	GLU	N-CA-C	5.12	124.82	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	124	ILE	Peptide
2	H	181	GLU	Peptide
2	H	247	LYS	Peptide
2	H	83	ALA	Peptide
3	L	163	TYR	Peptide

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	2461	0	2408	60	0
1	B	2480	0	2423	59	0
2	C	1701	0	1648	38	0
2	H	1715	0	1660	44	0
3	D	1591	0	1530	31	0
3	L	1591	0	1530	41	0
4	E	61	0	52	2	0
4	F	61	0	52	2	0
5	A	11	0	0	0	0
5	B	8	0	0	0	0
5	C	5	0	0	0	0
5	D	6	0	0	0	0
5	H	9	0	0	0	0
5	L	2	0	0	1	0
All	All	11702	0	11303	261	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 11.

The worst 5 of 261 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:232:PRO:HB3	1:A:259:TYR:HB3	1.58	0.86
2:H:125:SER:OG	2:H:126:TYR:N	2.09	0.81
1:B:460:ARG:HH22	1:B:543:VAL:HG21	1.45	0.81
3:L:133:LYS:HD2	3:L:221:GLU:HG3	1.63	0.79
3:L:172:LYS:HB2	3:L:215:SER:HB2	1.66	0.78

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	313/323 (97%)	299 (96%)	13 (4%)	1 (0%)	41	70
1	B	315/323 (98%)	298 (95%)	17 (5%)	0	100	100
2	C	218/249 (88%)	198 (91%)	18 (8%)	2 (1%)	17	46
2	H	220/249 (88%)	197 (90%)	17 (8%)	6 (3%)	5	18
3	D	213/235 (91%)	194 (91%)	19 (9%)	0	100	100
3	L	213/235 (91%)	199 (93%)	14 (7%)	0	100	100
All	All	1492/1614 (92%)	1385 (93%)	98 (7%)	9 (1%)	25	57

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	125	SER
2	H	182	PRO
2	H	183	VAL
2	C	182	PRO
2	C	183	VAL

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	279/286 (98%)	253 (91%)	26 (9%)	9	25
1	B	281/286 (98%)	260 (92%)	21 (8%)	13	36
2	C	193/219 (88%)	173 (90%)	20 (10%)	7	20
2	H	196/219 (90%)	169 (86%)	27 (14%)	3	10
3	D	180/198 (91%)	172 (96%)	8 (4%)	28	60
3	L	180/198 (91%)	166 (92%)	14 (8%)	12	33
All	All	1309/1406 (93%)	1193 (91%)	116 (9%)	9	28

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	98	ARG
3	D	80	ASP
2	H	200	PRO
3	D	58	GLN
2	C	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	286	GLN
1	B	422	HIS
1	B	484	GLN
2	H	225	GLN
2	C	233	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 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	1,4	14,14,15	0.57	0	17,19,21	2.41	6 (35%)
4	NAG	E	2	4	14,14,15	0.65	0	17,19,21	1.36	4 (23%)
4	BMA	E	3	4	11,11,12	0.70	0	15,15,17	2.07	5 (33%)
4	BMA	E	4	4	11,11,12	0.49	0	15,15,17	1.13	2 (13%)
4	BMA	E	5	4	11,11,12	0.59	0	15,15,17	0.91	0
4	NAG	F	1	1,4	14,14,15	1.07	1 (7%)	17,19,21	0.65	0
4	NAG	F	2	4	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
4	BMA	F	3	4	11,11,12	1.70	3 (27%)	15,15,17	1.59	4 (26%)
4	BMA	F	4	4	11,11,12	1.51	3 (27%)	15,15,17	1.37	2 (13%)
4	BMA	F	5	4	11,11,12	1.47	2 (18%)	15,15,17	1.30	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	BMA	F	4	4	-	0/2/19/22	0/1/1/1
4	BMA	F	5	4	-	0/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	BMA	C4-C5	3.52	1.60	1.53
4	F	1	NAG	O5-C1	-3.50	1.37	1.43
4	F	4	BMA	C2-C3	2.89	1.56	1.52
4	F	3	BMA	C2-C3	2.83	1.56	1.52
4	F	4	BMA	C1-C2	2.67	1.58	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	7.76	122.58	112.19
4	E	3	BMA	O5-C5-C6	4.42	116.26	107.66
4	E	3	BMA	O3-C3-C2	4.17	118.57	110.05
4	F	3	BMA	O3-C3-C2	3.96	118.14	110.05
4	F	2	NAG	C1-O5-C5	3.73	117.18	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	4	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	2	0
4	F	2	NAG	2	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

Oligosaccharide Chain F — Bond lengths, Bond angles, Torsions, Rings
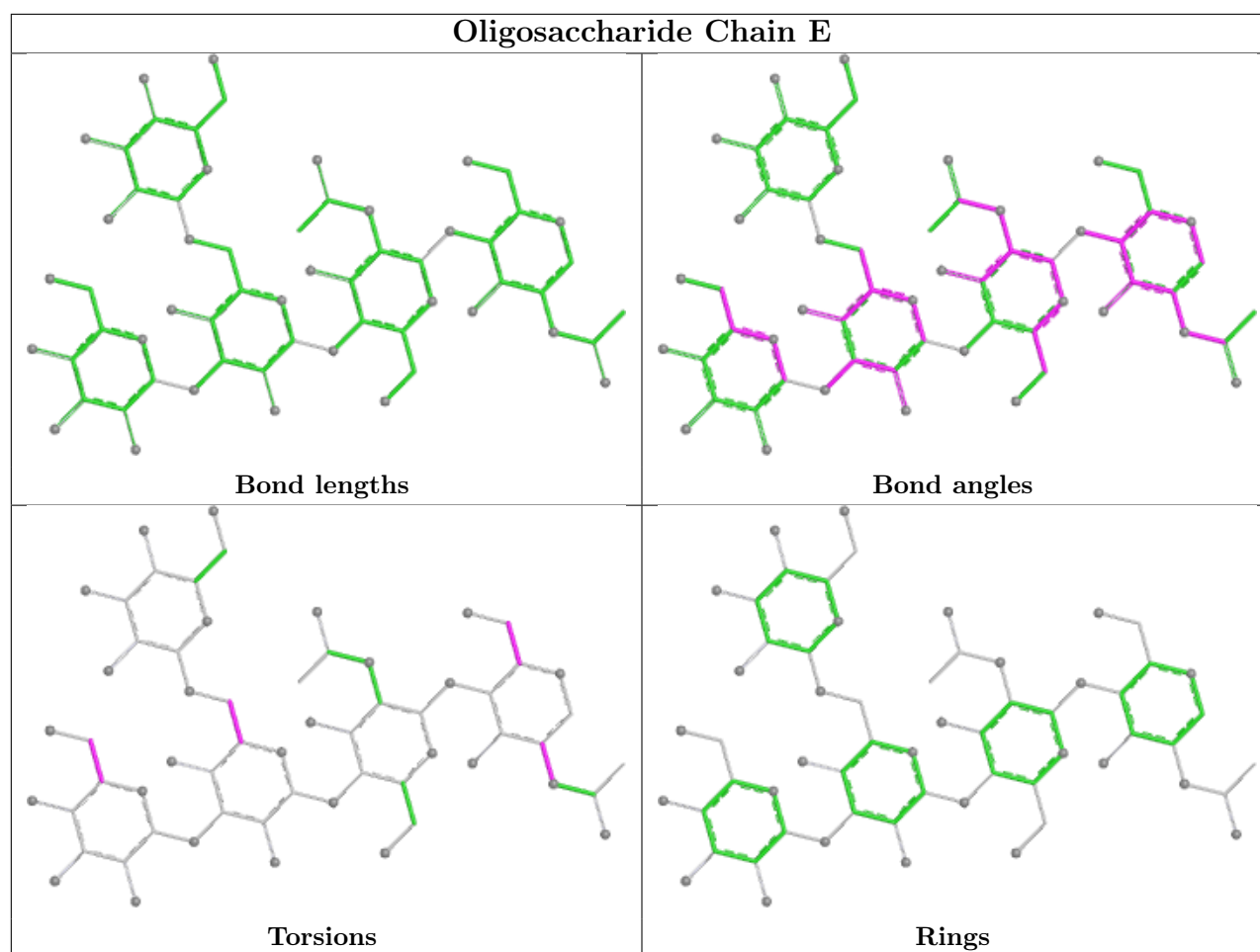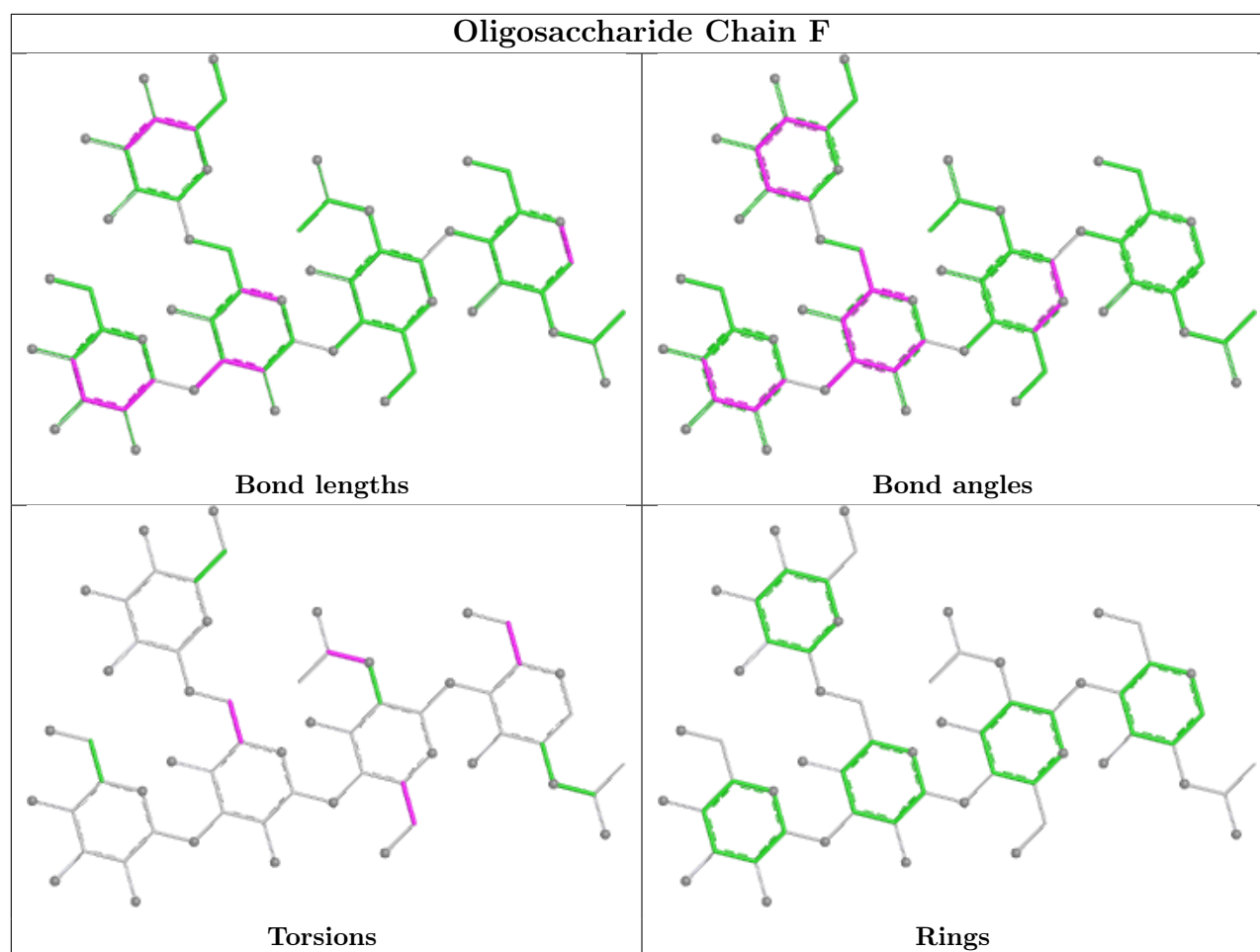
5.6 Ligand geometry ⓘ

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 ⓘ

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	315/323 (97%)	-0.01	4 (1%)	77	77	58, 92, 132, 142	4 (1%)
1	B	317/323 (98%)	0.07	11 (3%)	44	40	65, 94, 164, 193	6 (1%)
2	C	222/249 (89%)	0.78	31 (13%)	2	2	63, 102, 214, 225	5 (2%)
2	H	224/249 (89%)	-0.01	2 (0%)	84	84	50, 80, 159, 189	2 (0%)
3	D	215/235 (91%)	0.91	47 (21%)	0	0	64, 139, 199, 211	0
3	L	215/235 (91%)	-0.05	1 (0%)	91	91	53, 85, 123, 159	0
All	All	1508/1614 (93%)	0.25	96 (6%)	19	16	50, 93, 186, 225	17 (1%)

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	169	ALA	6.9
3	L	19	ALA	6.6
2	C	159	PRO	6.6
3	D	203	LEU	6.6
2	C	245	GLU	6.4

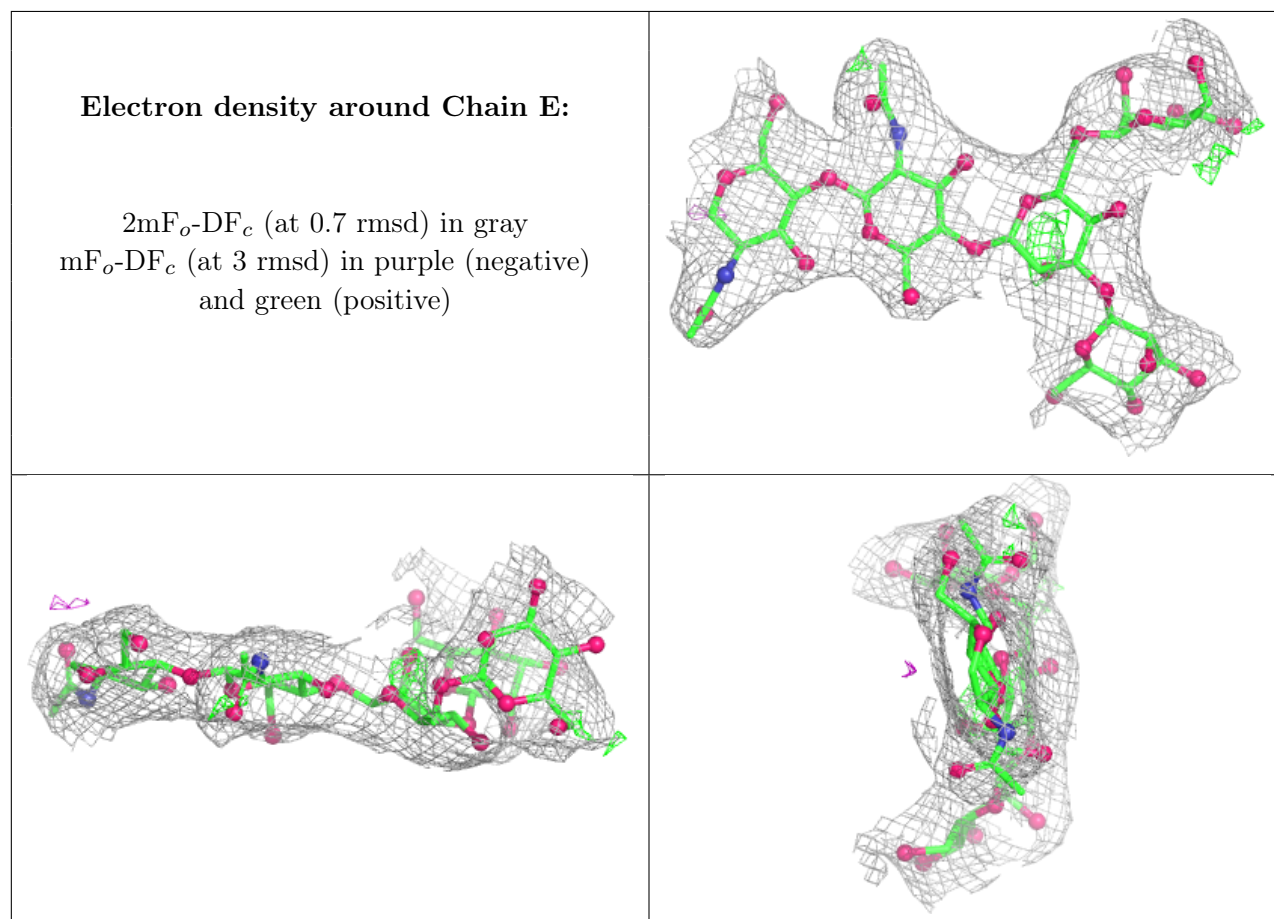## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

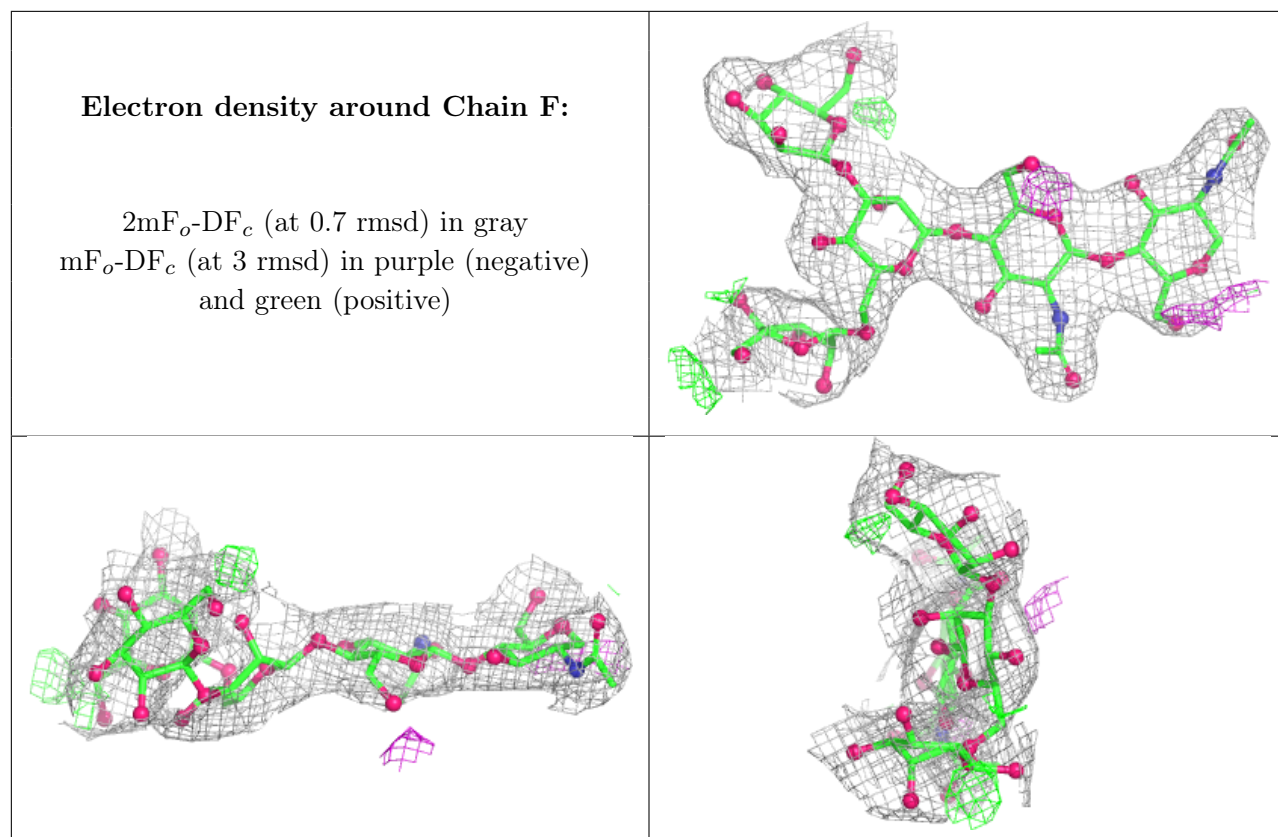There are no non-standard protein/DNA/RNA residues in this entry.

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	F	4	11/12	0.82	0.22	129,132,140,142	0
4	BMA	F	3	11/12	0.83	0.20	110,114,120,123	0
4	BMA	E	5	11/12	0.86	0.20	117,126,139,140	0
4	BMA	F	5	11/12	0.86	0.19	117,127,129,129	0
4	BMA	E	3	11/12	0.90	0.26	97,101,112,115	0
4	BMA	E	4	11/12	0.90	0.24	120,131,135,138	0
4	NAG	F	1	14/15	0.91	0.22	80,92,96,102	0
4	NAG	F	2	14/15	0.93	0.23	94,101,105,107	0
4	NAG	E	1	14/15	0.96	0.21	70,76,82,86	0
4	NAG	E	2	14/15	0.97	0.25	79,85,89,90	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 E:

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

Electron density around Chain F:

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

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.