Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:22 PM BST

PDB ID	:	5HBV
Title	:	Complex structure of Fab35 and mouse nAChR alpha1
Authors	:	Noridomi, K.; Watanabe, G.; Hansen, M.N.; Han, G.W.; Chen, L.
Deposited on	:	2016-01-02
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

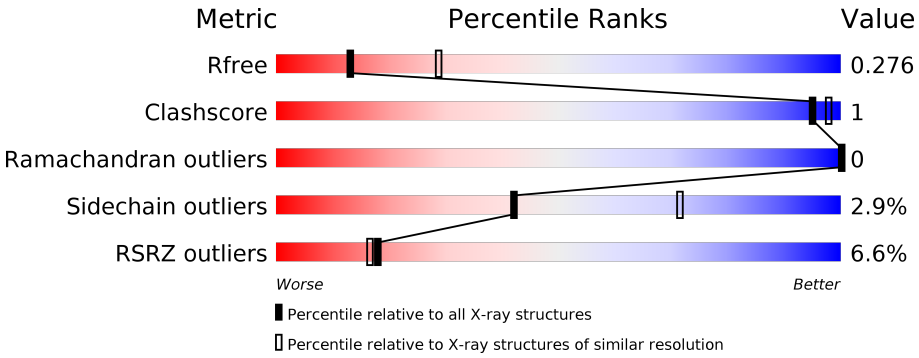
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	74	3% 99% .
2	B	212	2% 98% .
3	C	213	% 91% 8% .
4	D	219	17% 92% 7%
5	E	9	33% 67%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5705 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 Alpha-bungarotoxin isoform V31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			547	337	94	105	11			

- Molecule 2 is a protein called Acetylcholine receptor subunit alpha 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1738	1118	288	325	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LYS	-	expression tag	UNP P04756
B	1	SER	-	expression tag	UNP P04756
B	8	GLU	VAL	engineered mutation	UNP P04756
B	149	ARG	TRP	engineered mutation	UNP P04756
B	155	ALA	VAL	engineered mutation	UNP P04756

- Molecule 3 is a protein called Fab35, Light Chain.

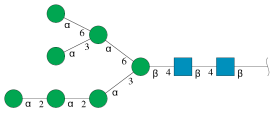
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1623	1016	267	334	6			

- Molecule 4 is a protein called Fab35, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	219	Total	C	N	O	S	0	0	0
			1646	1034	278	325	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyr

anose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deox
y-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 6 is water.

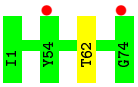
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	27	Total	O	0	0
			27	27		
6	C	8	Total	O	0	0
			8	8		
6	D	8	Total	O	0	0
			8	8		

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.

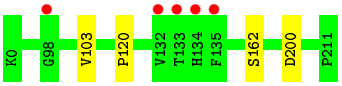
• Molecule 1: Alpha-bungarotoxin isoform V31

Chain A:



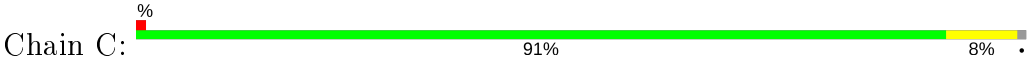
• Molecule 2: Acetylcholine receptor subunit alpha 1

Chain B:



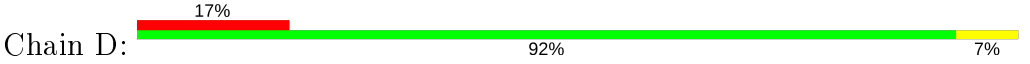
• Molecule 3: Fab35, Light Chain

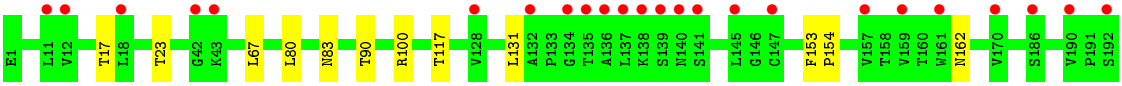
Chain C:

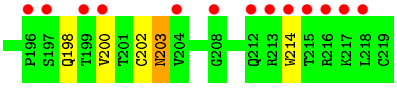


• Molecule 4: Fab35, Heavy Chain

Chain D:







• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	159.91Å 42.02Å 137.58Å 90.00° 116.46° 90.00°	Depositor
Resolution (Å)	50.01 – 2.70 45.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.01-2.70) 99.5 (45.40-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.227 , 0.268 0.232 , 0.276	Depositor DCC
R_{free} test set	1117 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5705	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: BMA, NAG, MAN

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	0.41	0/561	0.61	0/763
2	B	0.38	0/1788	0.63	0/2439
3	C	0.37	0/1655	0.59	0/2250
4	D	0.40	0/1687	0.58	0/2308
All	All	0.39	0/5691	0.60	0/7760

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	547	0	525	0	0
2	B	1738	0	1676	1	0
3	C	1623	0	1580	6	0
4	D	1646	0	1588	7	0
5	E	105	0	88	0	0
6	A	3	0	0	0	0
6	B	27	0	0	0	0
6	C	8	0	0	0	0
6	D	8	0	0	0	0
All	All	5705	0	5457	13	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 1.

All (13) 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)
3:C:132:VAL:HG11	4:D:131:LEU:HD13	1.81	0.62
4:D:90:THR:HG23	4:D:117:THR:HA	1.84	0.59
4:D:67:LEU:HD22	4:D:80:LEU:HD11	1.90	0.54
3:C:21:LEU:HD22	3:C:101:THR:HG21	1.91	0.52
4:D:203:ASN:HD22	4:D:214:TRP:HB3	1.77	0.49
3:C:192:THR:HB	3:C:207:SER:HB3	1.95	0.49
2:B:103:VAL:HG12	2:B:120:PRO:HB2	1.95	0.47
4:D:17:THR:HG22	4:D:83:ASN:CB	2.45	0.46
3:C:141:ARG:HD2	3:C:162:VAL:HG11	2.01	0.42
4:D:17:THR:HG22	4:D:83:ASN:HB3	2.01	0.41
3:C:149:ILE:HD13	3:C:188:HIS:CD2	2.56	0.41
4:D:153:PHE:HA	4:D:154:PRO:HA	1.91	0.40
3:C:149:ILE:HG22	3:C:191:TYR:CE1	2.57	0.40

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	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
2	B	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
3	C	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
4	D	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
All	All	708/718 (99%)	676 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	65/66 (98%)	64 (98%)	1 (2%)	65	86
2	B	194/196 (99%)	192 (99%)	2 (1%)	76	91
3	C	186/189 (98%)	178 (96%)	8 (4%)	29	57
4	D	185/191 (97%)	178 (96%)	7 (4%)	33	62
All	All	630/642 (98%)	612 (97%)	18 (3%)	42	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
2	B	162	SER
2	B	200	ASP
3	C	83	LEU
3	C	90	GLN
3	C	92	ILE
3	C	99	THR
3	C	107	ARG
3	C	155	ARG
3	C	177	THR
3	C	192	THR
4	D	23	THR
4	D	100	ARG
4	D	162	ASN
4	D	198	GLN
4	D	200	VAL
4	D	202	CYS
4	D	203	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	38	GLN

Continued on next page...

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Mol	Chain	Res	Type
4	D	203	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

9 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	$\#\|Z\| > 2$
5	NAG	E	1	2,5	14,14,15	0.18	0	17,19,21	0.91	0
5	NAG	E	2	5	14,14,15	0.33	0	17,19,21	0.86	1 (5%)
5	BMA	E	3	5	11,11,12	0.39	0	15,15,17	0.90	0
5	MAN	E	4	5	11,11,12	0.41	0	15,15,17	1.44	1 (6%)
5	MAN	E	5	5	11,11,12	0.44	0	15,15,17	0.92	1 (6%)
5	MAN	E	6	5	11,11,12	0.36	0	15,15,17	1.22	2 (13%)
5	MAN	E	7	5	11,11,12	0.41	0	15,15,17	0.90	0
5	MAN	E	8	5	11,11,12	0.33	0	15,15,17	1.09	1 (6%)
5	MAN	E	9	5	11,11,12	0.57	0	15,15,17	0.97	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
5	NAG	E	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	1/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	2/2/19/22	0/1/1/1
5	MAN	E	8	5	-	0/2/19/22	0/1/1/1
5	MAN	E	9	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	4	MAN	C1-O5-C5	3.67	117.16	112.19
5	E	9	MAN	C1-O5-C5	2.89	116.11	112.19
5	E	6	MAN	C1-O5-C5	2.78	115.96	112.19
5	E	8	MAN	C1-O5-C5	2.54	115.63	112.19
5	E	6	MAN	C3-C4-C5	2.32	114.39	110.24
5	E	2	NAG	C1-O5-C5	2.21	115.19	112.19
5	E	5	MAN	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

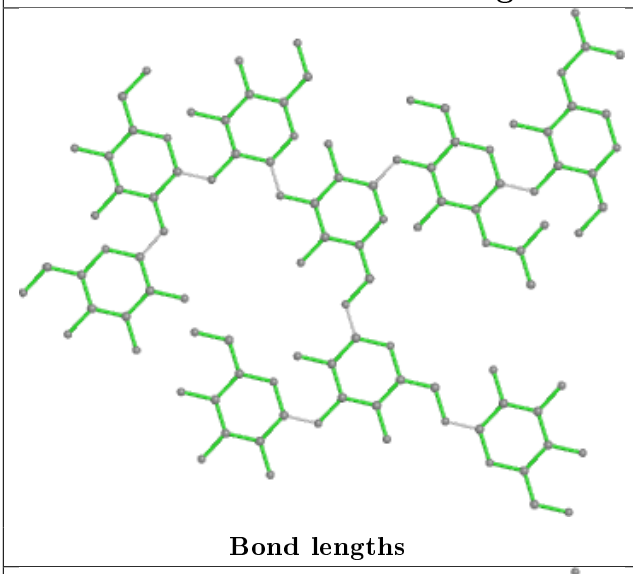
Mol	Chain	Res	Type	Atoms
5	E	9	MAN	C4-C5-C6-O6
5	E	7	MAN	O5-C5-C6-O6
5	E	9	MAN	O5-C5-C6-O6
5	E	7	MAN	C4-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6

There are no ring outliers.

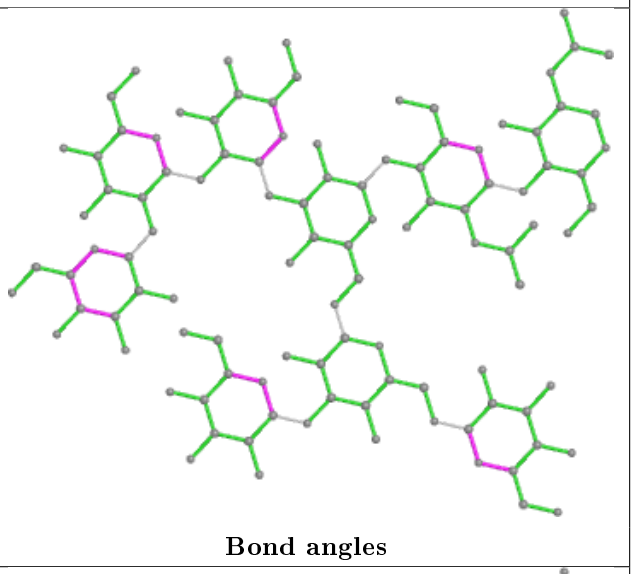
No monomer is involved in short contacts.

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

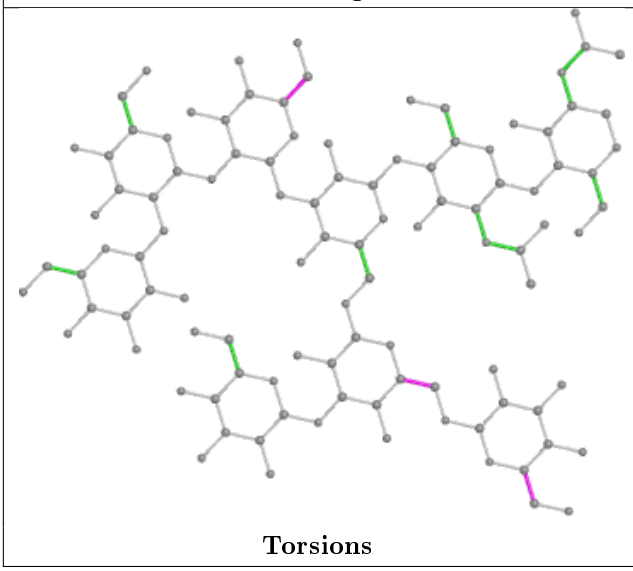
Oligosaccharide Chain E



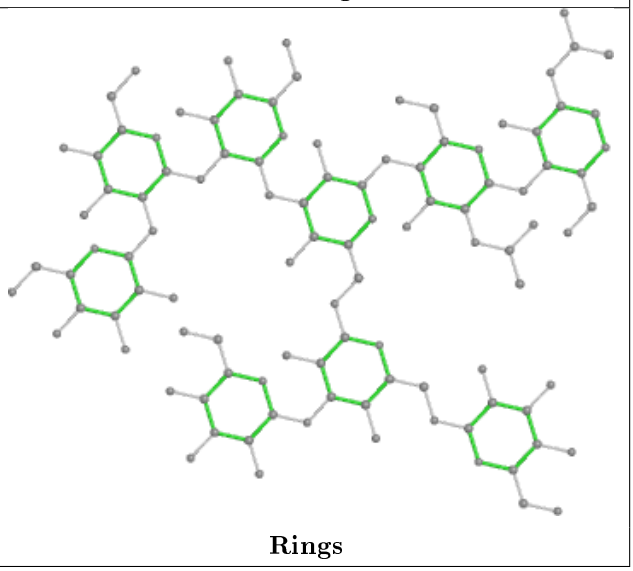
Bond lengths



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, 95^{th} 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	74/74 (100%)	0.35	2 (2%) 54 55	41, 57, 93, 112	0
2	B	212/212 (100%)	0.20	5 (2%) 59 60	34, 46, 80, 143	0
3	C	211/213 (99%)	0.35	3 (1%) 75 77	42, 68, 105, 135	0
4	D	219/219 (100%)	1.07	37 (16%) 1 1	41, 95, 146, 161	0
All	All	716/718 (99%)	0.53	47 (6%) 18 16	34, 65, 127, 161	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	HIS	7.3
4	D	204	VAL	7.0
4	D	137	LEU	7.0
4	D	214	TRP	6.7
3	C	124	LEU	6.6
4	D	197	SER	6.5
4	D	135	THR	5.7
4	D	161	TRP	5.6
4	D	213	ARG	5.3
4	D	196	PRO	5.2
4	D	199	THR	4.7
4	D	190	VAL	4.4
4	D	145	LEU	4.4
4	D	212	GLN	4.4
4	D	136	ALA	3.9
2	B	133	THR	3.9
4	D	192	SER	3.8
2	B	135	PHE	3.7
4	D	134	GLY	3.6
1	A	54	TYR	3.4
4	D	159	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	125	ALA	3.4
4	D	132	ALA	3.3
4	D	140	ASN	3.2
2	B	132	VAL	3.1
4	D	200	VAL	3.0
4	D	147	CYS	3.0
4	D	215	THR	3.0
4	D	208	GLY	2.9
4	D	128	VAL	2.9
1	A	74	GLY	2.9
4	D	216	ARG	2.9
4	D	157	VAL	2.8
4	D	11	LEU	2.8
4	D	18	LEU	2.7
4	D	217	LYS	2.7
4	D	12	VAL	2.7
4	D	170	VAL	2.6
4	D	42	GLY	2.6
2	B	98	GLY	2.6
4	D	186	SER	2.5
4	D	218	LEU	2.4
4	D	138	LYS	2.4
4	D	139	SER	2.4
4	D	141	SER	2.3
4	D	43	LYS	2.2
3	C	211	ASN	2.1

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, 95^{th} 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(Å^2)	Q<0.9
5	MAN	E	6	11/12	0.64	0.36	118,130,133,134	0
5	MAN	E	9	11/12	0.68	0.29	81,89,91,91	0

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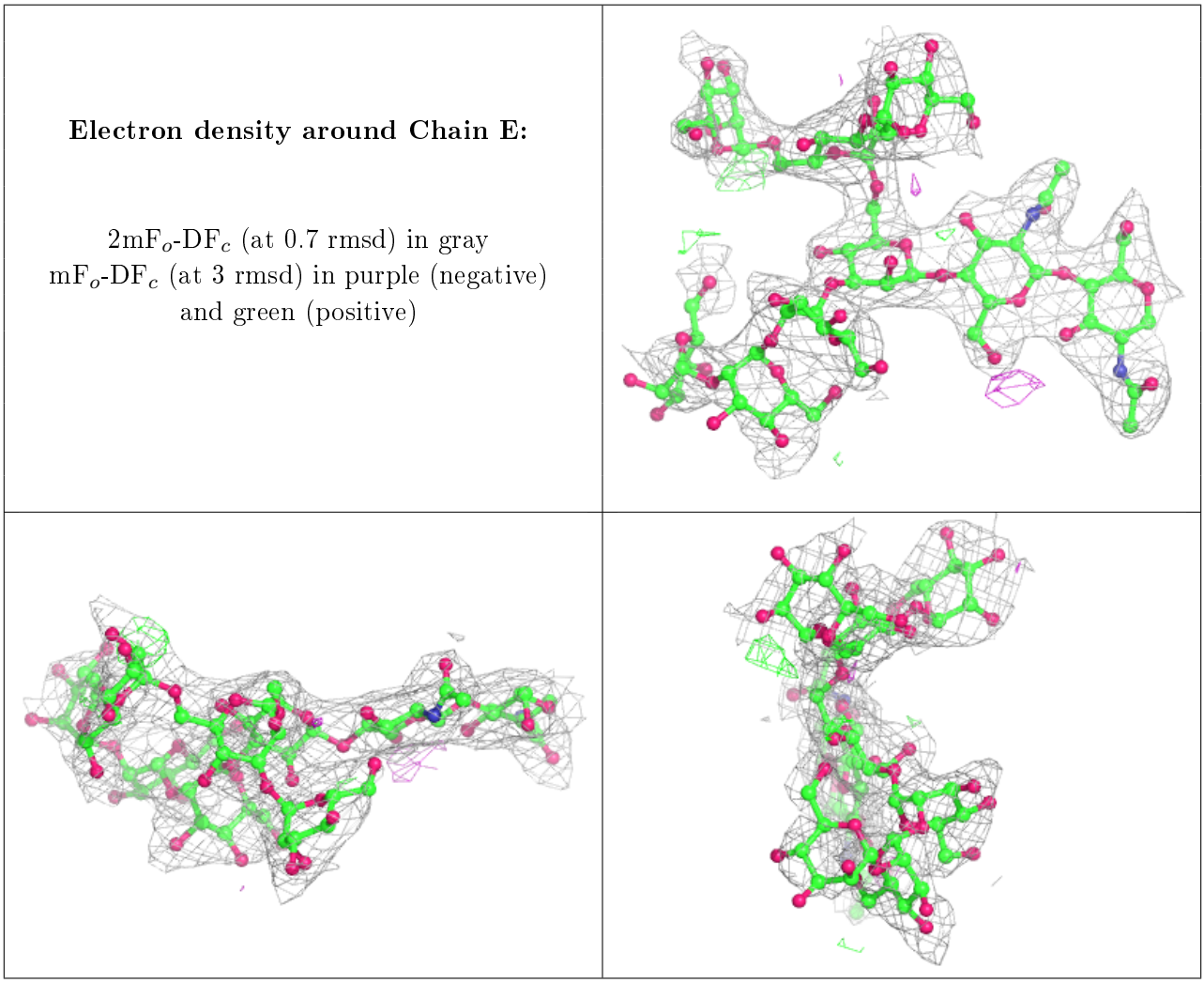
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	E	5	11/12	0.74	0.20	103,109,114,123	0
5	MAN	E	4	11/12	0.90	0.14	86,89,94,101	0
5	MAN	E	8	11/12	0.94	0.14	68,70,78,81	0
5	NAG	E	2	14/15	0.96	0.14	41,46,49,52	0
5	MAN	E	7	11/12	0.96	0.19	66,71,79,85	0
5	BMA	E	3	11/12	0.96	0.14	57,62,66,74	0
5	NAG	E	1	14/15	0.97	0.15	42,42,45,48	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:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-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 (i)

There are no such residues in this entry.