wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 10:17 PM EDT

PDB ID	:	2GH0
Title	:	Growth factor/receptor complex
Authors	:	Wang, X.Q.
Deposited on	:	2006-03-24
Resolution	:	1.92 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 (i) 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 (i)) were used in the production of this report:

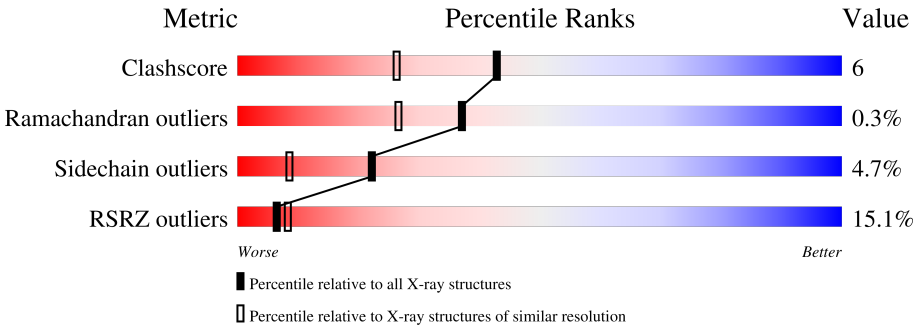
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.92 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))
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	C	101	5% 85% 12%
1	D	101	15% 92% 5%
2	A	213	18% 75% 16% 6%
2	B	213	15% 77% 13% 7%
3	E	5	60% 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4881 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 artemin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	100	Total	C	N	O	S	0	0	0
			758	463	153	134	8			
1	D	99	Total	C	N	O	S	0	0	0
			750	459	152	131	8			

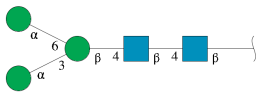
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASP	-	cloning artifact	UNP Q5T4W7
C	121	PRO	-	cloning artifact	UNP Q5T4W7
D	120	ASP	-	cloning artifact	UNP Q5T4W7
D	121	PRO	-	cloning artifact	UNP Q5T4W7

- Molecule 2 is a protein called GDNF family receptor alpha-3.

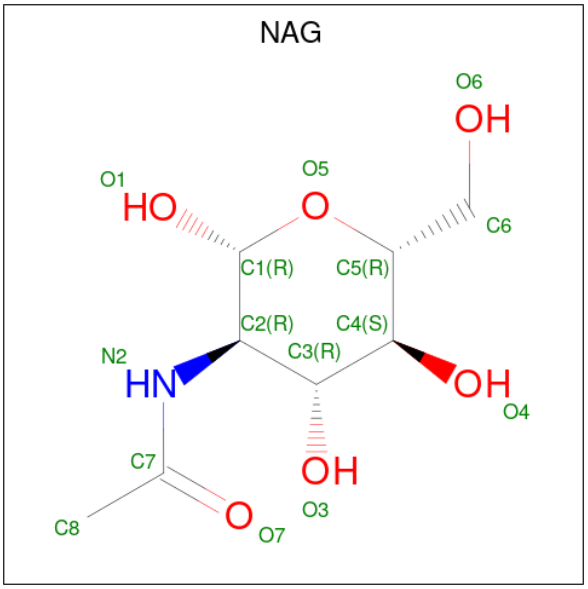
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	200	Total	C	N	O	S	0	0	0
			1535	946	284	280	25			
2	B	199	Total	C	N	O	S	0	0	0
			1527	942	283	277	25			

- Molecule 3 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
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

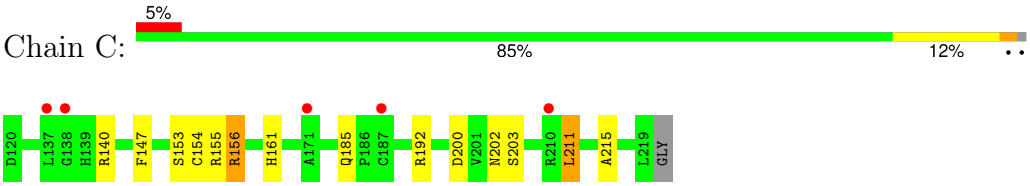
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	35	Total O 35 35	0	0
5	D	26	Total O 26 26	0	0
5	A	111	Total O 111 111	0	0
5	B	64	Total O 64 64	0	0

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.

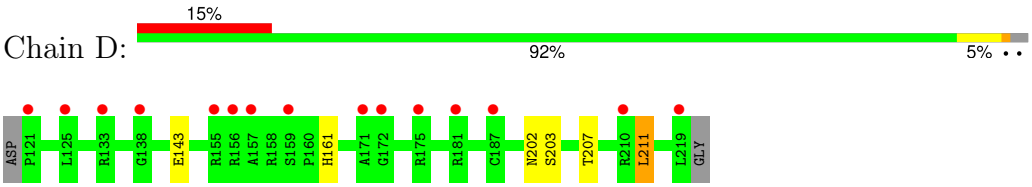
• Molecule 1: artemin

Chain C:



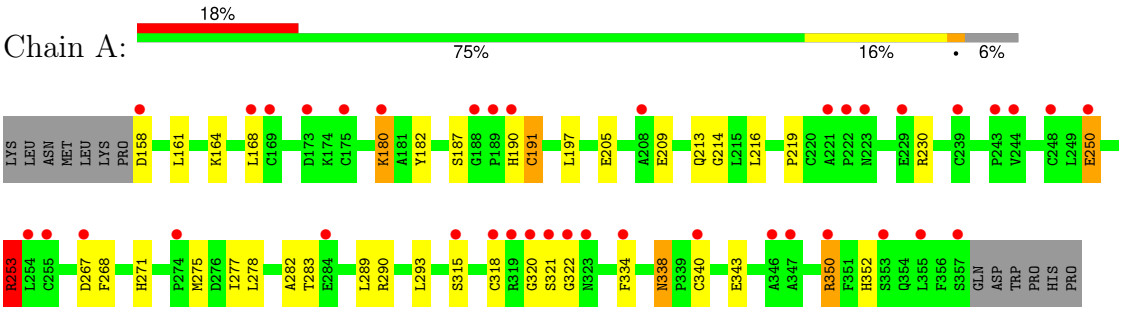
• Molecule 1: artemin

Chain D:



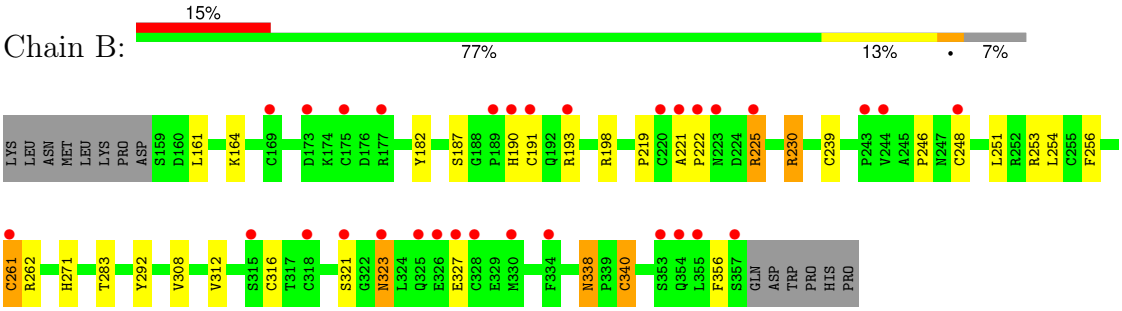
• Molecule 2: GDNF family receptor alpha-3

Chain A:



• Molecule 2: GDNF family receptor alpha-3

Chain B:



• Molecule 3: 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-glucopyra

nose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.68Å 41.46Å 119.86Å 90.00° 103.56° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 50.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.92) 94.2 (50.00-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.82 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.263 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4881	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C	0.86	0/774	0.85	0/1048
1	D	0.72	0/766	0.86	0/1036
2	A	1.14	9/1565 (0.6%)	0.97	7/2115 (0.3%)
2	B	0.86	1/1557 (0.1%)	0.85	3/2104 (0.1%)
All	All	0.94	10/4662 (0.2%)	0.89	10/6303 (0.2%)

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	A	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	322	GLY	C-N	12.33	1.62	1.34
2	A	180	LYS	CE-NZ	7.95	1.69	1.49
2	A	350	ARG	CG-CD	7.10	1.69	1.51
2	A	250	GLU	CD-OE2	6.03	1.32	1.25
2	A	320	GLY	C-O	5.85	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	230	ARG	NE-CZ-NH2	-12.06	114.27	120.30
2	A	230	ARG	NE-CZ-NH2	-9.55	115.53	120.30
2	B	230	ARG	NE-CZ-NH1	8.16	124.38	120.30
2	A	253	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	230	ARG	NE-CZ-NH1	6.14	123.37	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	187	SER	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	C	758	0	755	13	0
1	D	750	0	752	6	0
2	A	1535	0	1490	17	0
2	B	1527	0	1486	22	0
3	E	61	0	51	2	0
4	B	14	0	13	0	0
5	A	111	0	0	1	0
5	B	64	0	0	1	0
5	C	35	0	0	1	0
5	D	26	0	0	1	0
All	All	4881	0	4547	56	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 6.

The worst 5 of 56 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:A:180:LYS:CE	2:A:180:LYS:NZ	1.68	1.54
2:B:292:TYR:OH	2:B:312:VAL:HG21	1.43	1.14
2:B:323:ASN:HD22	2:B:323:ASN:H	1.23	0.84
1:C:154:CYS:H	1:C:185:GLN:NE2	1.88	0.71
2:B:292:TYR:OH	2:B:312:VAL:CG2	2.32	0.70

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	C	98/101 (97%)	97 (99%)	1 (1%)	0	100 100
1	D	97/101 (96%)	93 (96%)	4 (4%)	0	100 100
2	A	198/213 (93%)	190 (96%)	6 (3%)	2 (1%)	13 4
2	B	197/213 (92%)	189 (96%)	8 (4%)	0	100 100
All	All	590/628 (94%)	569 (96%)	19 (3%)	2 (0%)	37 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	190	HIS
2	A	191	CYS

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	C	84/84 (100%)	82 (98%)	2 (2%)	44 28
1	D	83/84 (99%)	82 (99%)	1 (1%)	67 59
2	A	172/185 (93%)	162 (94%)	10 (6%)	17 5
2	B	171/185 (92%)	160 (94%)	11 (6%)	14 4
All	All	510/538 (95%)	486 (95%)	24 (5%)	22 8

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	190	HIS
2	B	253	ARG
2	B	248	CYS
2	B	254	LEU
2	A	197	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	271	HIS
2	B	323	ASN
2	B	338	ASN
2	A	271	HIS
2	A	323	ASN

5.3.3 RNA (i)

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)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	1.11	1 (7%)	17,19,21	2.14	6 (35%)
3	NAG	E	2	3	14,14,15	1.21	2 (14%)	17,19,21	1.86	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	E	3	3	11,11,12	1.60	3 (27%)	15,15,17	3.09	7 (46%)
3	MAN	E	4	3	11,11,12	2.73	5 (45%)	15,15,17	1.93	5 (33%)
3	MAN	E	5	3	11,11,12	0.74	1 (9%)	15,15,17	2.30	5 (33%)

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	MAN	O4-C4	6.50	1.59	1.43
3	E	3	BMA	O5-C1	3.04	1.48	1.43
3	E	2	NAG	O5-C5	-2.88	1.37	1.43
3	E	3	BMA	O3-C3	-2.86	1.35	1.43
3	E	4	MAN	O3-C3	2.86	1.50	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3	BMA	O3-C3-C4	-7.25	93.28	110.38
3	E	3	BMA	C1-O5-C5	-5.61	104.67	112.19
3	E	1	NAG	O5-C1-C2	-4.72	103.99	111.29
3	E	2	NAG	C4-C3-C2	-4.60	104.28	111.02
3	E	5	MAN	C1-O5-C5	4.46	118.16	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

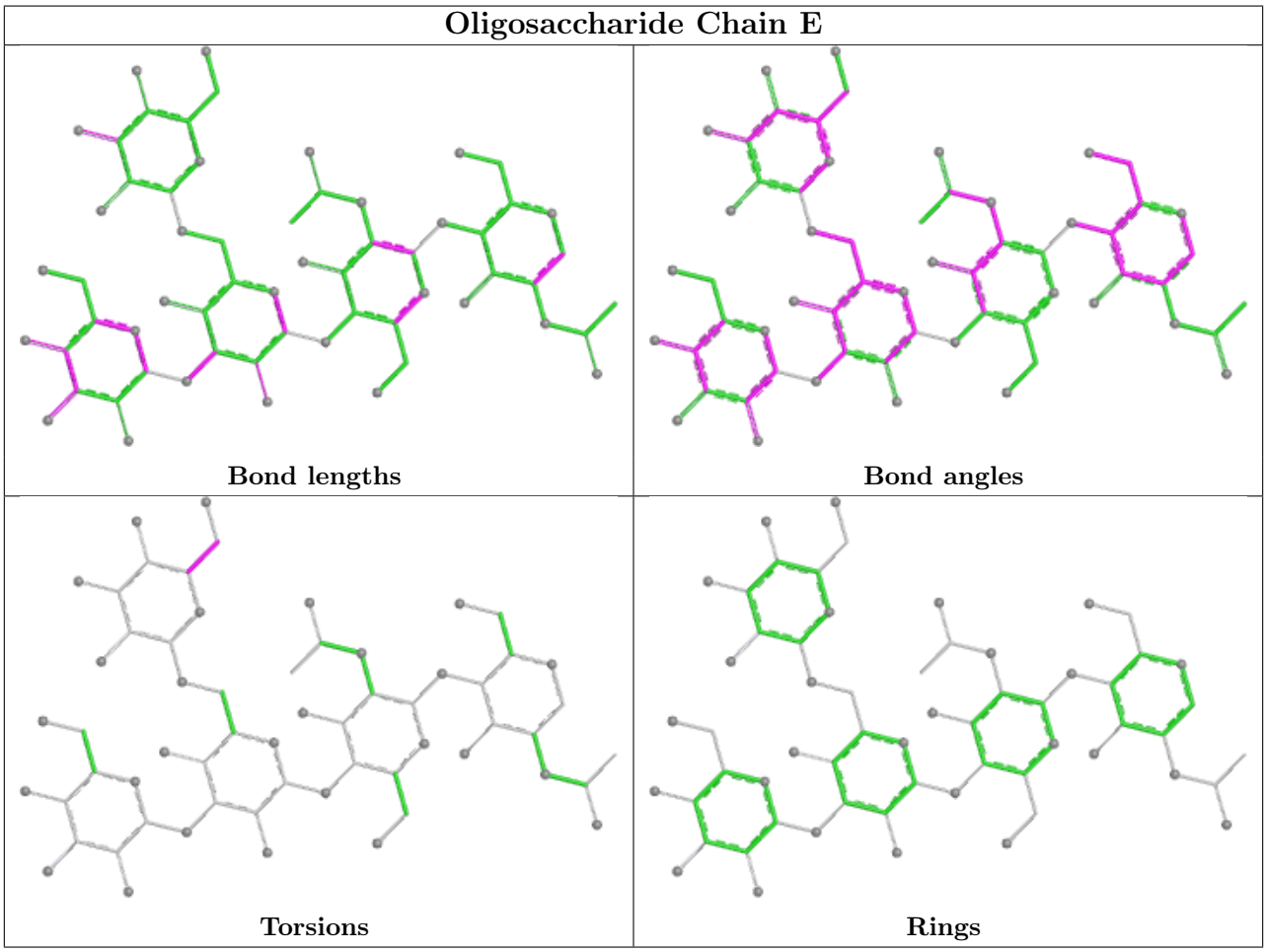
Mol	Chain	Res	Type	Atoms
3	E	5	MAN	O5-C5-C6-O6
3	E	5	MAN	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	BMA	2	0
3	E	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.



5.6 Ligand geometry (i)

1 ligand is 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	B	1100	2	14,14,15	0.67	0	17,19,21	1.18	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	B	1100	2	-	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(^{o})	Ideal(^{o})
4	B	1100	NAG	C1-O5-C5	3.40	116.74	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1100	NAG	O5-C5-C6-O6
4	B	1100	NAG	C4-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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	322:GLY	C	323:ASN	N	1.62

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	C	100/101 (99%)	0.71	5 (5%)	35	40	22, 33, 43, 47	0
1	D	99/101 (98%)	1.19	15 (15%)	6	8	29, 38, 54, 58	0
2	A	200/213 (93%)	1.24	39 (19%)	4	4	31, 36, 48, 56	0
2	B	199/213 (93%)	1.13	31 (15%)	6	7	27, 36, 48, 55	0
All	All	598/628 (95%)	1.11	90 (15%)	6	8	22, 36, 49, 58	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	354	GLN	5.8
2	B	190	HIS	5.4
2	A	267	ASP	5.3
2	B	222	PRO	5.3
1	D	187	CYS	5.0

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, 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
3	MAN	E	5	11/12	0.82	0.12	37,42,49,49	0
3	MAN	E	4	11/12	0.83	0.15	37,49,55,58	0

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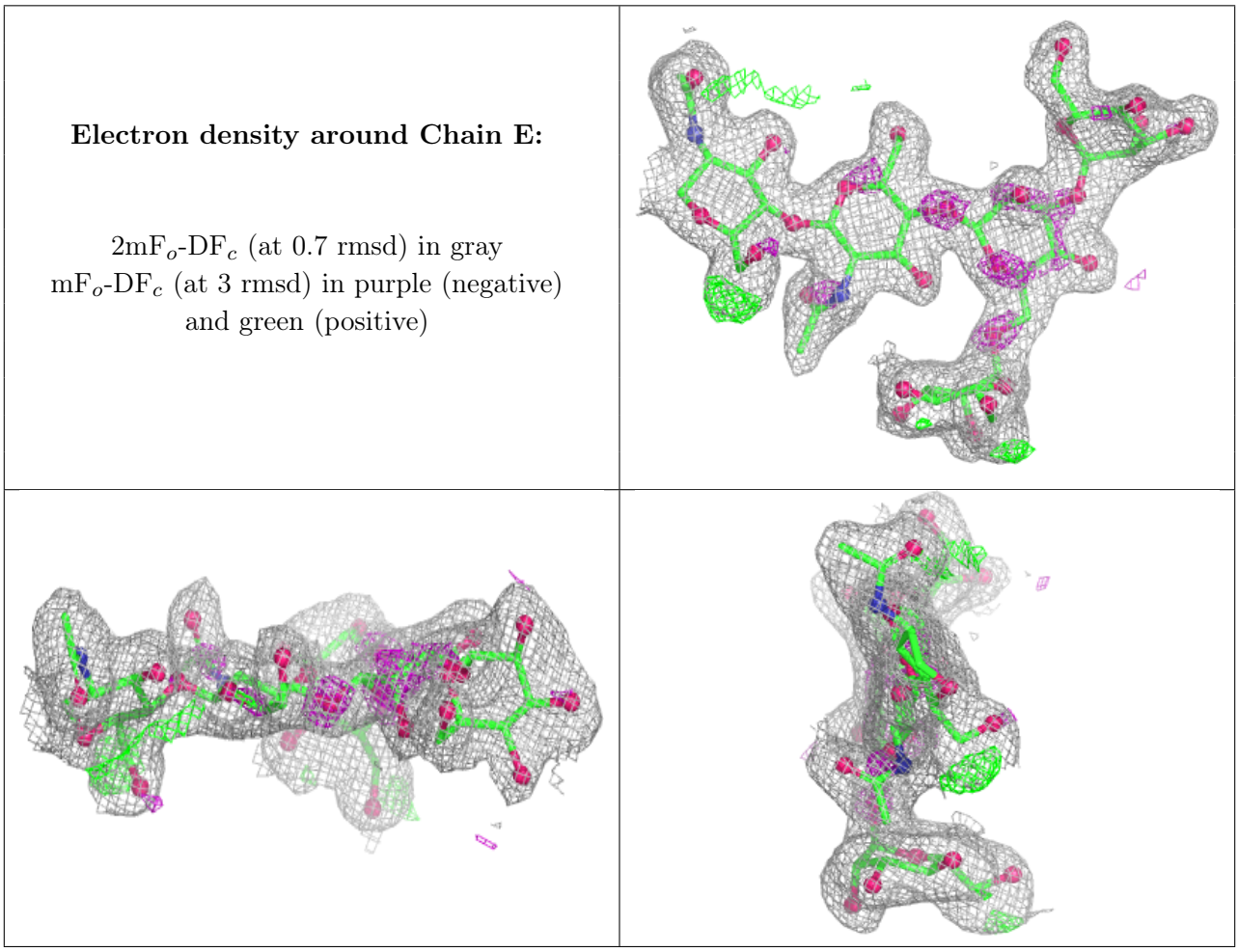
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	1	14/15	0.91	0.10	30,32,37,41	0
3	BMA	E	3	11/12	0.91	0.13	23,32,36,37	0
3	NAG	E	2	14/15	0.92	0.12	24,31,38,39	0

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.



6.4 Ligands

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(Å^2)	Q<0.9
4	NAG	B	1100	14/15	0.83	0.12	39,47,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.