wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 02:07 PM EDT

PDB ID	:	8GF2
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies eCR3022.20 and CC12.3
Authors	:	Yuan, M.; Zhu, X.; Wilson, I.A.
Deposited on	:	2023-03-07
Resolution	:	2.85 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 (1)) were used in the production of this report:

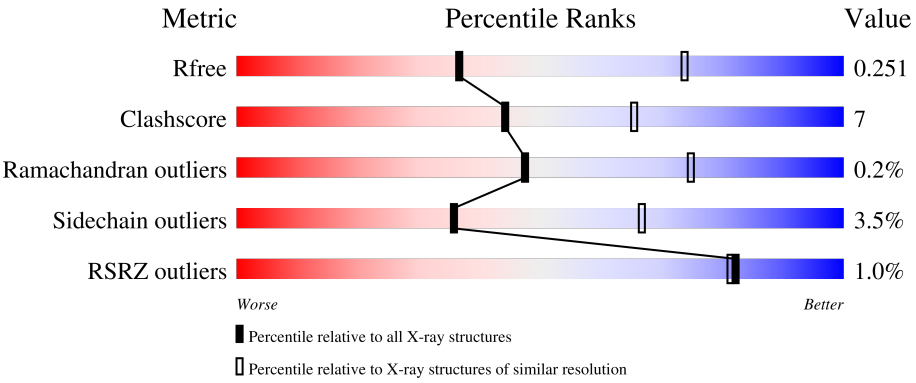
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	231	2% 65% 16% 17%
1	B	231	72% 11% 16%
2	C	220	79% 17%
2	E	220	3% 79% 20%
3	D	215	77% 20%

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Mol	Chain	Length	Quality of chain
3	F	215	85% 14%
4	H	222	% 83% 14%
4	X	222	82% 15%
5	L	221	% 84% 14%
5	Y	221	% 82% 16%
6	G	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16286 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1529	983	254	284	8			
1	B	193	Total	C	N	O	S	0	0	0
			1537	987	256	286	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
B	542	SER	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CC12.3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	0	0	0
			1600	1016	264	314	6			
2	E	220	Total	C	N	O	S	0	0	0
			1645	1040	272	326	7			

- Molecule 3 is a protein called CC12.3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1622	1014	277	327	4			
3	F	213	Total	C	N	O	S	0	0	0
			1635	1021	279	331	4			

- Molecule 4 is a protein called eCR3022.20 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1626	1036	265	317	8			
4	X	217	Total	C	N	O	S	0	0	0
			1623	1034	264	316	9			

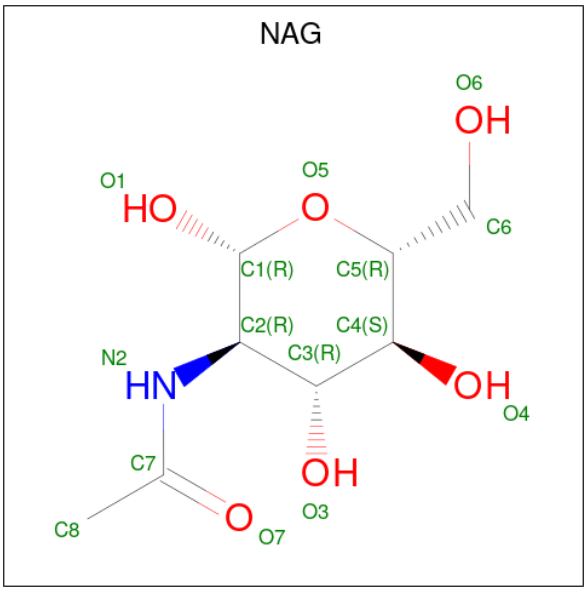
- Molecule 5 is a protein called eCR3022.20 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	221	Total	C	N	O	S	0	0	0
			1717	1080	283	349	5			
5	Y	220	Total	C	N	O	S	0	0	0
			1710	1077	282	346	5			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

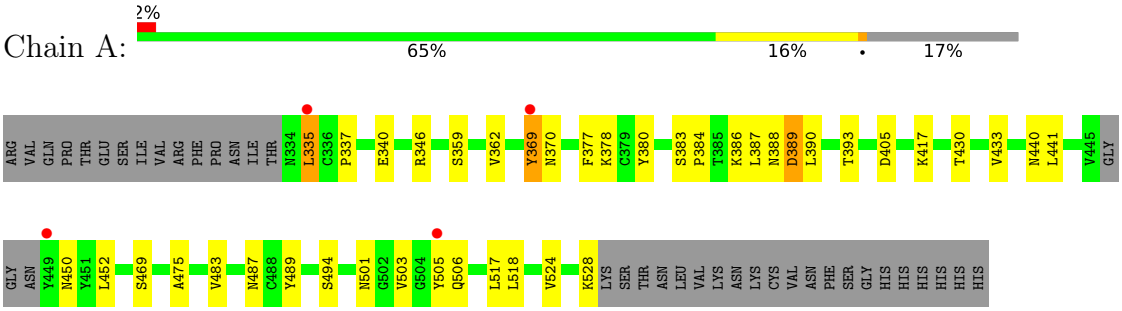


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

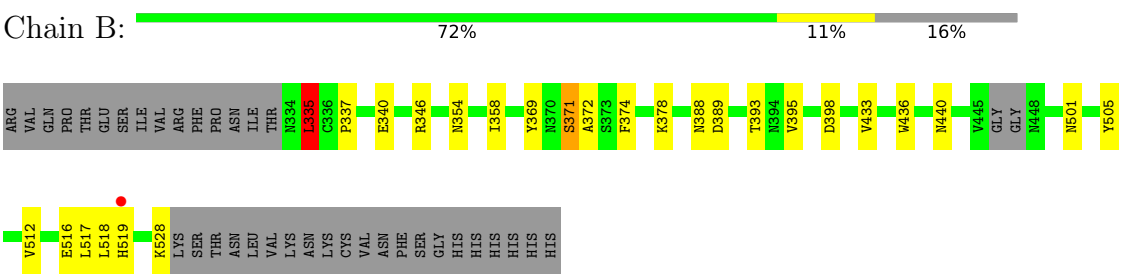
3 Residue-property plots (i)

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.

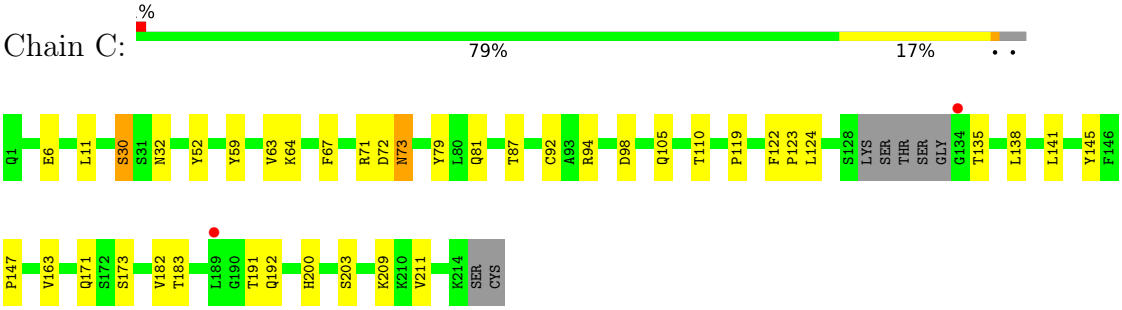
• Molecule 1: Spike protein S1



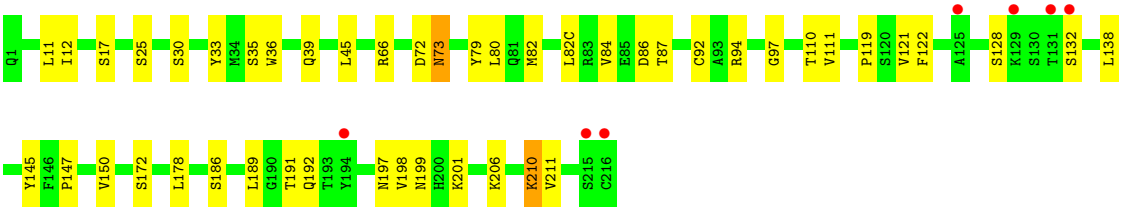
• Molecule 1: Spike protein S1



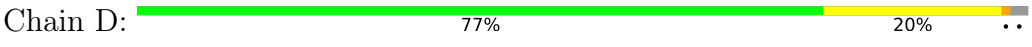
• Molecule 2: CC12.3 Fab heavy chain

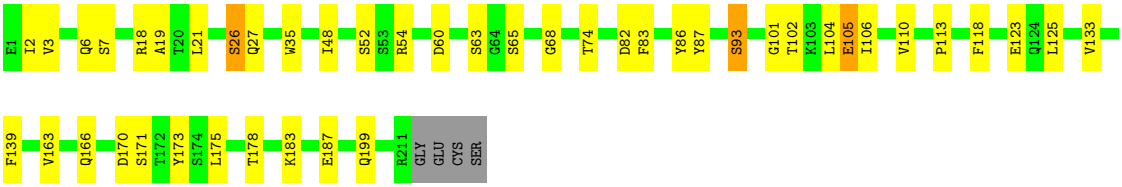


• Molecule 2: CC12.3 Fab heavy chain

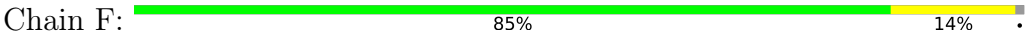


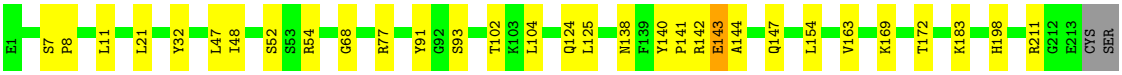
• Molecule 3: CC12.3 Fab light chain



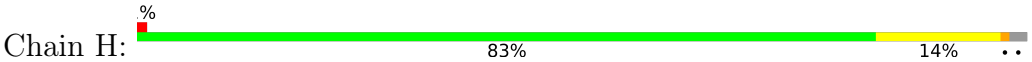


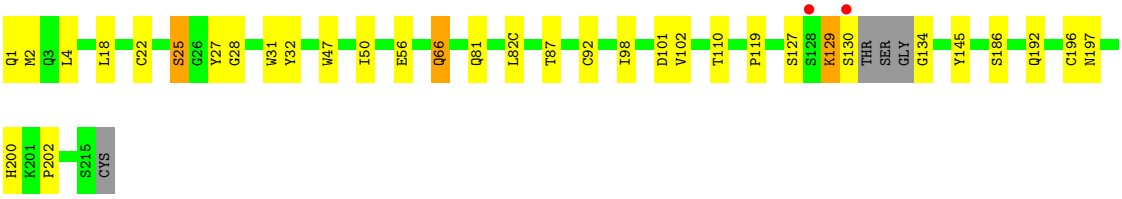
• Molecule 3: CC12.3 Fab light chain



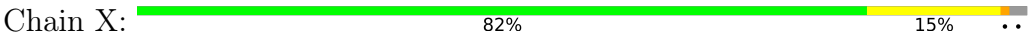


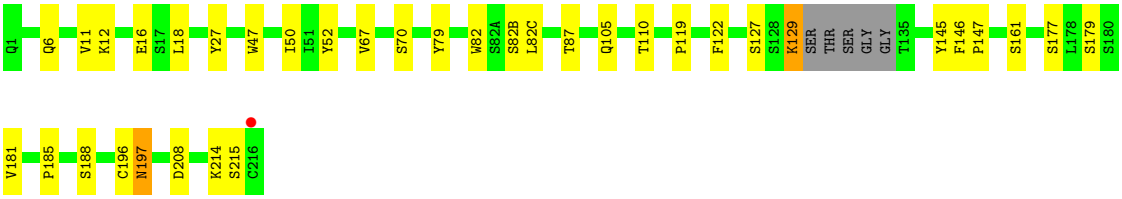
• Molecule 4: eCR3022.20 Fab heavy chain



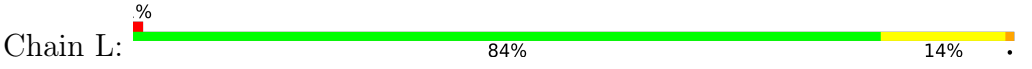


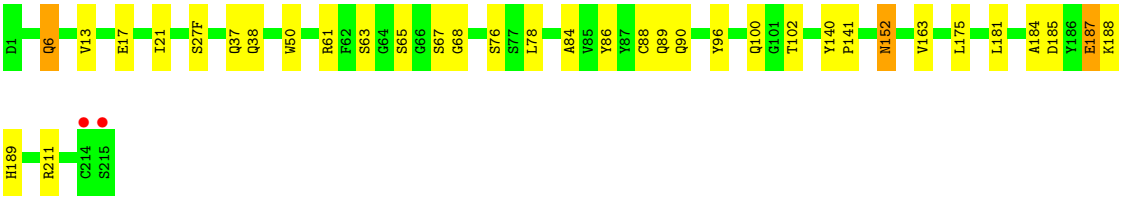
• Molecule 4: eCR3022.20 Fab heavy chain



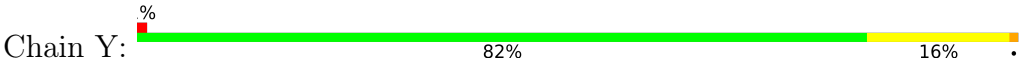


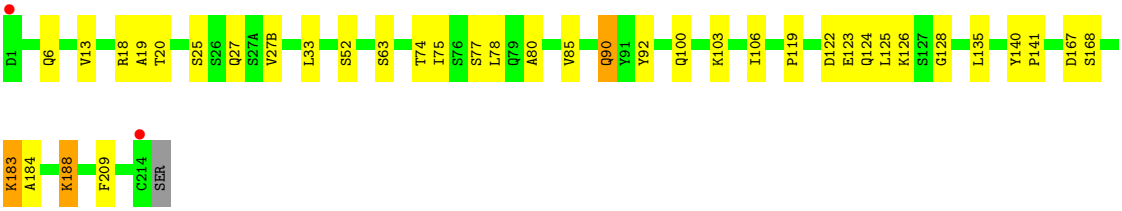
• Molecule 5: eCR3022.20 Fab light chain





• Molecule 5: eCR3022.20 Fab light chain





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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	157.57Å 161.22Å 230.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 2.85 46.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.83-2.85) 99.1 (46.83-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.209 , 0.252 0.210 , 0.251	Depositor DCC
R_{free} test set	3440 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16286	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: NAG

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	0.33	0/1572	0.57	2/2138 (0.1%)
1	B	0.32	0/1580	0.58	2/2149 (0.1%)
2	C	0.28	0/1639	0.53	0/2231
2	E	0.28	0/1685	0.51	0/2292
3	D	0.31	0/1657	0.61	2/2249 (0.1%)
3	F	0.33	0/1670	0.62	2/2266 (0.1%)
4	H	0.30	0/1669	0.56	1/2272 (0.0%)
4	X	0.27	0/1666	0.50	0/2267
5	L	0.31	1/1757 (0.1%)	0.53	2/2389 (0.1%)
5	Y	0.34	1/1750 (0.1%)	0.60	4/2381 (0.2%)
All	All	0.31	2/16645 (0.0%)	0.56	15/22634 (0.1%)

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
4	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	183	LYS	CD-CE	5.34	1.64	1.51
5	L	187	GLU	CG-CD	-5.09	1.44	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	105	GLU	CA-CB-CG	8.72	132.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	169	LYS	CD-CE-NZ	-8.26	92.70	111.70
5	Y	188	LYS	CB-CG-CD	-7.01	93.38	111.60
1	A	483	VAL	CG1-CB-CG2	6.90	121.94	110.90
5	L	181	LEU	CB-CG-CD2	6.45	121.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	66	GLN	Peptide

5.2 Too-close contacts (i)

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	1529	0	1452	25	0
1	B	1537	0	1458	19	0
2	C	1600	0	1560	27	0
2	E	1645	0	1604	23	0
3	D	1622	0	1583	36	0
3	F	1635	0	1592	19	0
4	H	1626	0	1601	20	0
4	X	1623	0	1597	21	0
5	L	1717	0	1662	21	0
5	Y	1710	0	1656	22	0
6	G	28	0	25	0	0
7	A	14	0	13	0	0
All	All	16286	0	15803	213	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 7.

The worst 5 of 213 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:F:141:PRO:HB2	3:F:143:GLU:OE1	1.43	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:ILE:HD11	3:D:171:SER:HB3	1.33	1.11
3:D:83:PHE:CD1	3:D:106:ILE:HG22	1.99	0.96
3:D:83:PHE:CG	3:D:106:ILE:HG22	2.02	0.95
2:E:121:VAL:HG21	2:E:198:VAL:HG11	1.51	0.91

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	188/231 (81%)	174 (93%)	13 (7%)	1 (0%)	29	57
1	B	189/231 (82%)	172 (91%)	16 (8%)	1 (0%)	29	57
2	C	209/220 (95%)	202 (97%)	7 (3%)	0	100	100
2	E	218/220 (99%)	209 (96%)	8 (4%)	1 (0%)	29	57
3	D	209/215 (97%)	198 (95%)	10 (5%)	1 (0%)	29	57
3	F	211/215 (98%)	205 (97%)	5 (2%)	1 (0%)	29	57
4	H	214/222 (96%)	206 (96%)	8 (4%)	0	100	100
4	X	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
5	L	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
5	Y	218/221 (99%)	212 (97%)	6 (3%)	0	100	100
All	All	2088/2218 (94%)	1997 (96%)	86 (4%)	5 (0%)	47	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	SER
1	A	450	ASN
2	E	132	SER

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Mol	Chain	Res	Type
3	F	68	GLY
3	D	68	GLY

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	167/203 (82%)	157 (94%)	10 (6%)	19	45
1	B	168/203 (83%)	164 (98%)	4 (2%)	49	77
2	C	180/186 (97%)	177 (98%)	3 (2%)	60	83
2	E	186/186 (100%)	177 (95%)	9 (5%)	25	55
3	D	183/186 (98%)	175 (96%)	8 (4%)	28	58
3	F	184/186 (99%)	181 (98%)	3 (2%)	62	84
4	H	182/185 (98%)	174 (96%)	8 (4%)	28	58
4	X	182/185 (98%)	175 (96%)	7 (4%)	33	64
5	L	196/196 (100%)	189 (96%)	7 (4%)	35	66
5	Y	195/196 (100%)	190 (97%)	5 (3%)	46	75
All	All	1823/1912 (95%)	1759 (96%)	64 (4%)	36	67

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	X	196	CYS
5	Y	33	LEU
4	H	129	LYS
4	H	92	CYS
5	Y	52	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	147	GLN

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Mol	Chain	Res	Type
3	F	27	GLN
2	E	73	ASN
1	B	360	ASN
2	E	199	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)

2 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	$\#\|Z\| > 2$
6	NAG	G	1	1,6	14,14,15	0.27	0	17,19,21	0.44	0
6	NAG	G	2	6	14,14,15	0.20	0	17,19,21	0.45	0

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
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

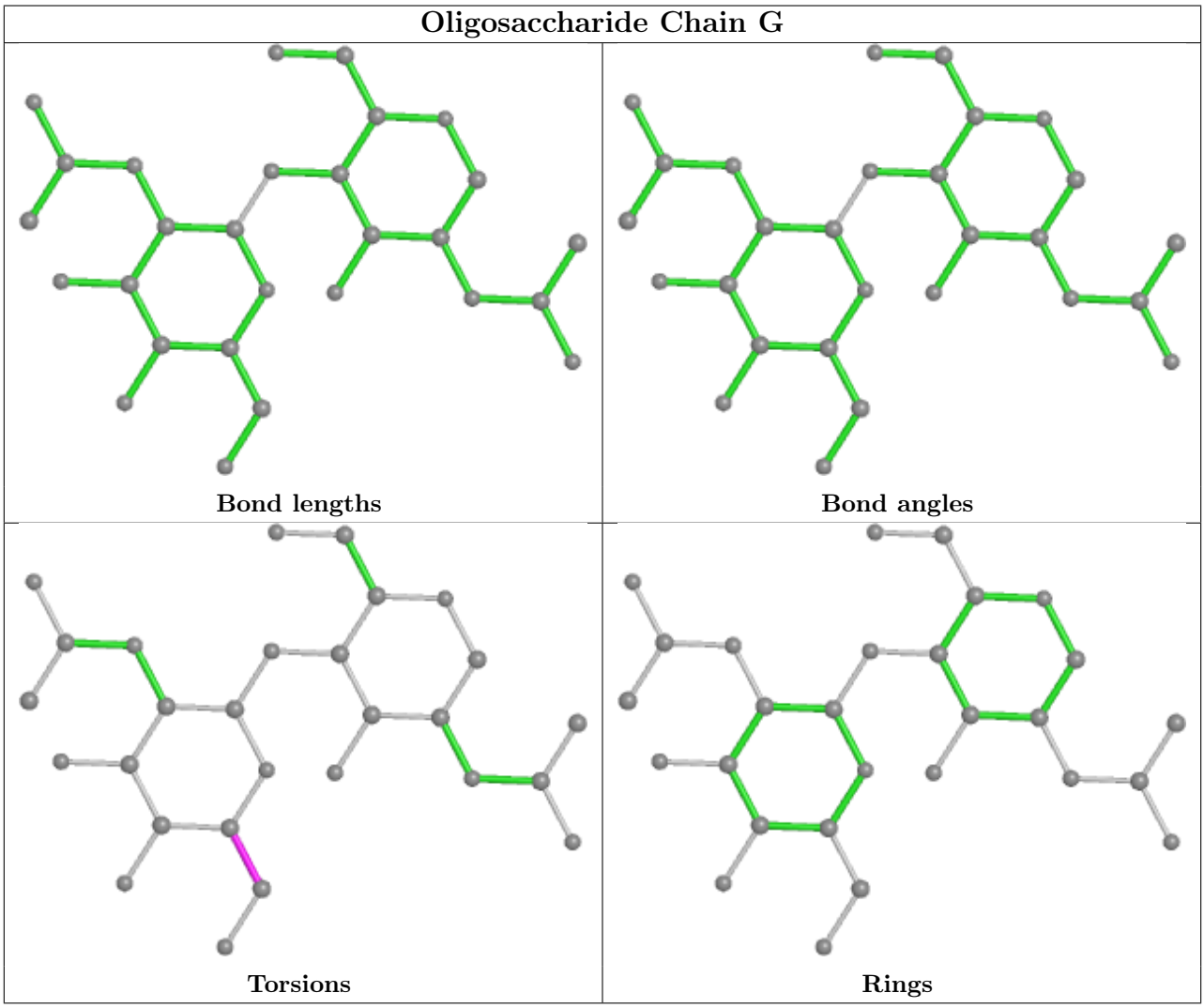
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	2	NAG	C4-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.



5.6 Ligand geometry

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	$\#\|Z\| > 2$
7	NAG	A	601	1	14,14,15	0.33	0	17,19,21	0.44	0

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
7	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	192/231 (83%)	0.04	4 (2%) 63 60	39, 62, 109, 133	0
1	B	193/231 (83%)	-0.07	1 (0%) 91 90	32, 52, 98, 127	0
2	C	213/220 (96%)	-0.03	2 (0%) 84 84	37, 57, 95, 108	0
2	E	220/220 (100%)	-0.02	7 (3%) 47 42	32, 56, 106, 167	0
3	D	211/215 (98%)	-0.03	0 100 100	38, 60, 89, 112	0
3	F	213/215 (99%)	-0.06	0 100 100	38, 61, 85, 130	0
4	H	218/222 (98%)	-0.03	2 (0%) 84 84	38, 54, 91, 141	0
4	X	217/222 (97%)	-0.01	1 (0%) 91 90	32, 56, 96, 145	0
5	L	221/221 (100%)	-0.15	2 (0%) 84 84	37, 52, 78, 156	0
5	Y	220/221 (99%)	-0.19	2 (0%) 84 84	34, 54, 82, 147	0
All	All	2118/2218 (95%)	-0.06	21 (0%) 82 81	32, 56, 96, 167	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	215	SER	5.2
4	H	130	SER	5.1
1	B	519	HIS	4.9
5	Y	214	CYS	4.4
5	L	214	CYS	4.1

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

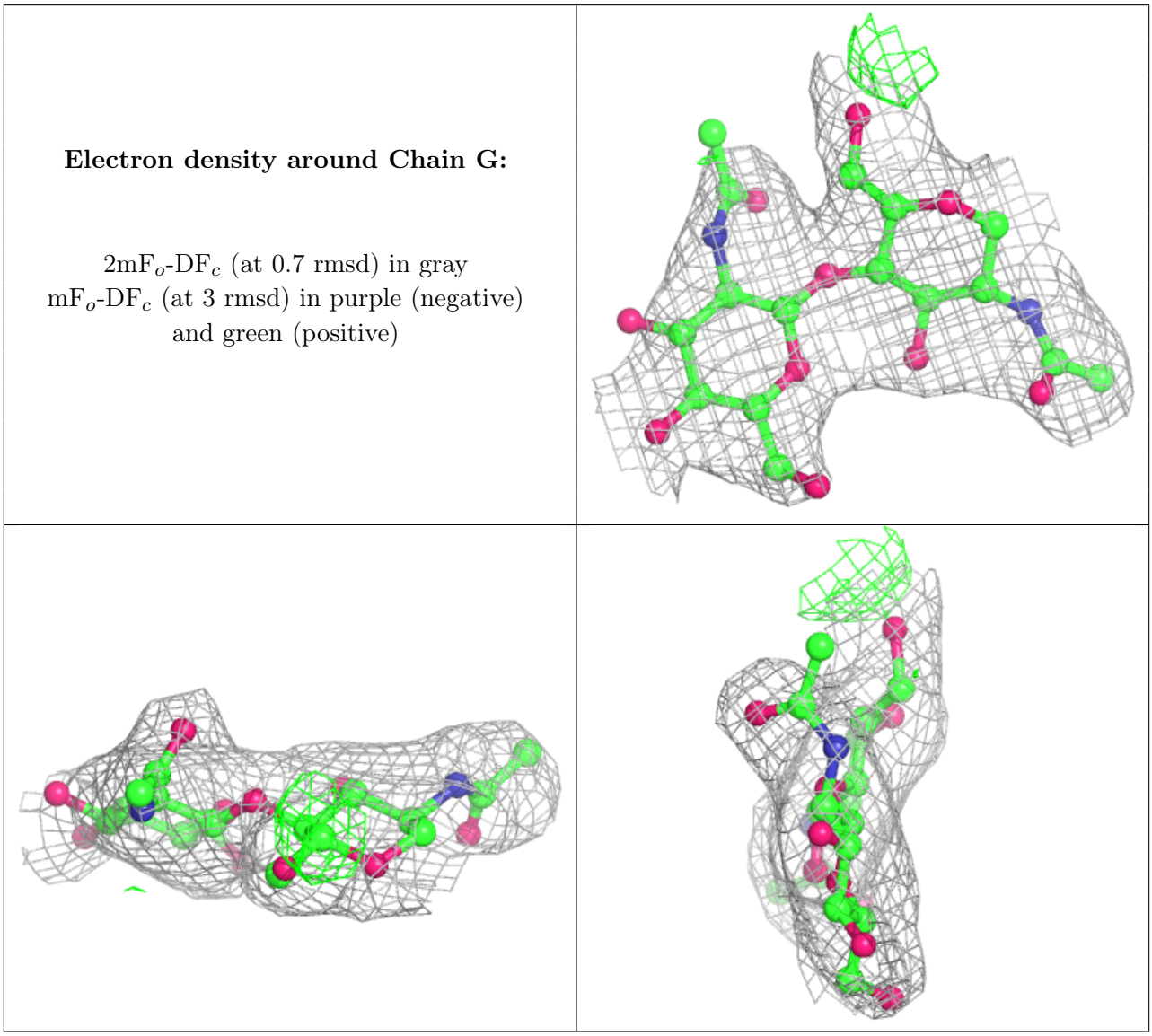
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (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
6	NAG	G	2	14/15	0.90	0.20	58,74,88,93	0
6	NAG	G	1	14/15	0.91	0.16	47,58,67,74	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, 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
7	NAG	A	601	14/15	0.66	0.24	113,118,122,122	0

6.5 Other polymers

There are no such residues in this entry.