W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2023 – 04:24 PM JST

PDB ID	:	7Y3N
Title	:	Crystal structure of SARS-CoV receptor binding domain in complex with human antibody BIOLS56
Authors	:	Rao, X.; Chai, Y.; Wu, Y.; Gao, F.
Deposited on	:	2022-06-11
Resolution	:	2.97 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 ⓘ 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 ⓘ) were used in the production of this report:

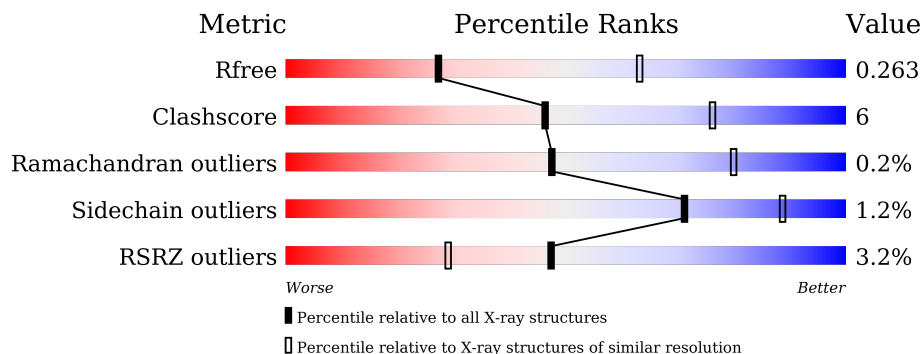|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.97 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		0.263
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		1.2%
RSRZ outliers		3.2%

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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	228	3%; 65% / 20% · 14%
1	B	228	3%; 67% / 18% 14%
1	E	228	5%; 64% / 18% · 17%
2	C	237	2%; 82% / 12% 6%
2	F	237	3%; 81% / 13% 7%
2	H	237	%; 85% / 9% 6%

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WORLDWIDE wwPDB PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
3	D	215	2% ... 88% ... 11%
3	G	215	8% ... 80% ... 18% ...
3	L	215	.% ... 91% ... 9%
4	I	3	33% ... 33% ... 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	I	2	-	-	-	X
5	NAG	B	301	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14620 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	196	Total	C	N	O	S	0	0	0
			1560	1008	254	289	9			
1	B	195	Total	C	N	O	S	0	0	0
			1553	1004	253	287	9			
1	E	190	Total	C	N	O	S	0	0	0
			1516	983	246	278	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	HIS	-	expression tag	UNP P59594
A	224	HIS	-	expression tag	UNP P59594
A	225	HIS	-	expression tag	UNP P59594
A	226	HIS	-	expression tag	UNP P59594
A	227	HIS	-	expression tag	UNP P59594
A	228	HIS	-	expression tag	UNP P59594
B	223	HIS	-	expression tag	UNP P59594
B	224	HIS	-	expression tag	UNP P59594
B	225	HIS	-	expression tag	UNP P59594
B	226	HIS	-	expression tag	UNP P59594
B	227	HIS	-	expression tag	UNP P59594
B	228	HIS	-	expression tag	UNP P59594
E	223	HIS	-	expression tag	UNP P59594
E	224	HIS	-	expression tag	UNP P59594
E	225	HIS	-	expression tag	UNP P59594
E	226	HIS	-	expression tag	UNP P59594
E	227	HIS	-	expression tag	UNP P59594
E	228	HIS	-	expression tag	UNP P59594

- Molecule 2 is a protein called Heavy chain of BIOLS56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total 1677	C 1061	N 278	O 330	S 8	0	0	0
2	C	223	Total 1677	C 1061	N 278	O 330	S 8	0	0	0
2	F	221	Total 1665	C 1055	N 276	O 327	S 7	0	0	0

- Molecule 3 is a protein called Light chain of BIOLS56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total 1646	C 1029	N 274	O 337	S 6	0	0	0
3	D	214	Total 1640	C 1026	N 273	O 335	S 6	0	0	0
3	G	213	Total 1634	C 1023	N 272	O 334	S 5	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
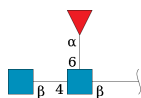
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O5
O1
HO O
C6
C1(R) C5(R)
C2(R) C4(S)
N2 C3(R)
HN OH
O4
C7
OH
C8 O O3
O7

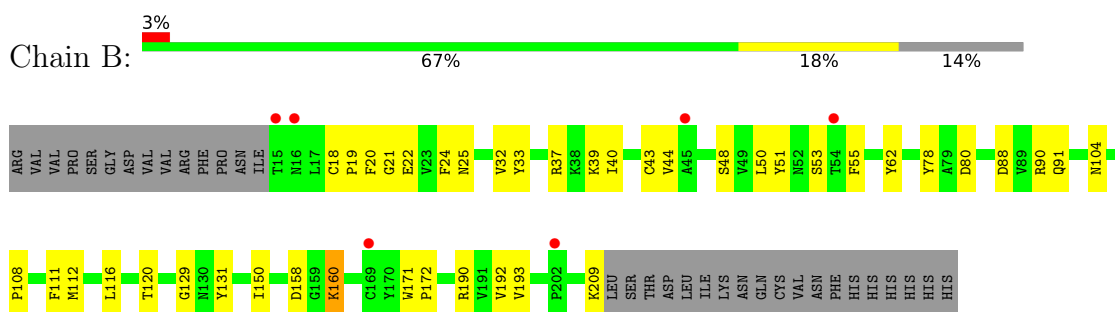| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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.
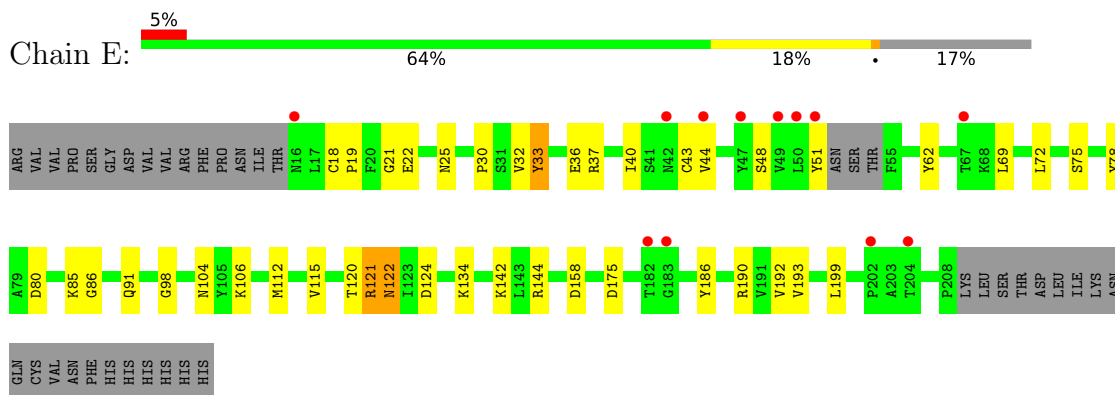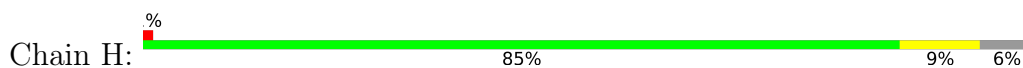
• Molecule 1: Spike protein S1

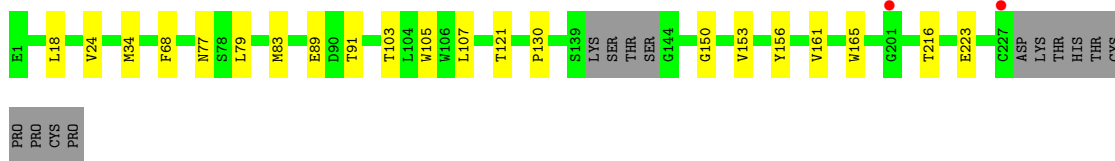Chain A:

• Molecule 1: Spike protein S1

Chain B:

• Molecule 1: Spike protein S1

Chain E:

• Molecule 2: Heavy chain of BIOLS56

Chain H:

E1 L18 V24 M34 F68 N77 S78 L79 M83 E89 D90 T91 T103 L104 W105 W106 L107 T121 P130 S139 LYS SER THR SER G144 G150 V153 Y156 V161 W165 G201 T216 E223 C227 ASP LYS THR HIS THR CYS
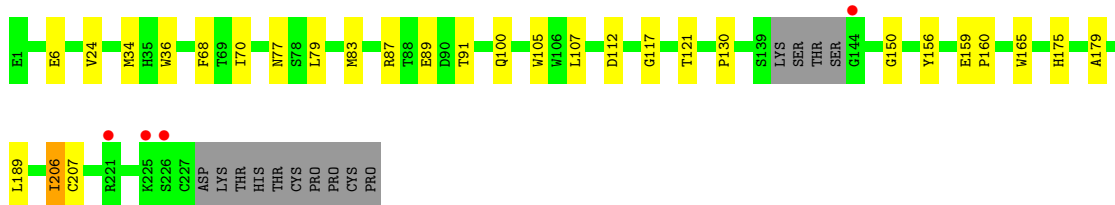
PRO PRO CYS PRO

● Molecule 2: Heavy chain of BIOLS56

Chain C:

E1 E6 V24 M34 H35 W36 F68 T69 I70 N77 S78 L79 M83 R87 T88 E89 D90 T91 Q100 W105 W106 L107 D112 G117 T121 P130 S139 LYS SER THR SER G144 G150 Y156 E159 P160 W165 H175 A179
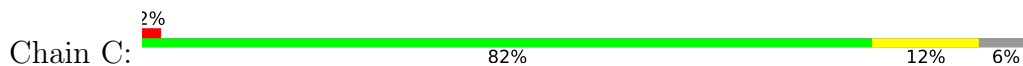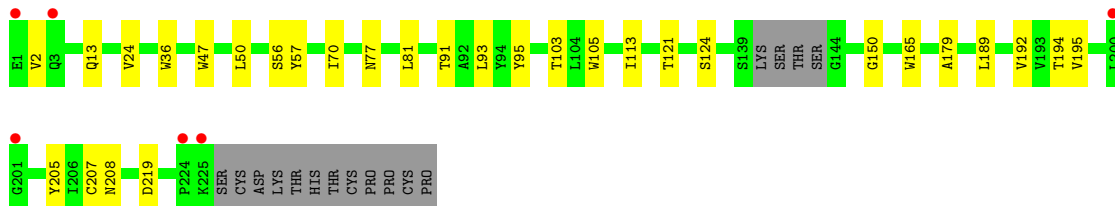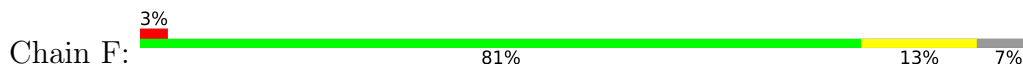
L189 I206 C207 R221 K225 S226 C227 ASP LYS THR HIS THR CYS PRO PRO PRO

● Molecule 2: Heavy chain of BIOLS56

Chain F:

E1 V2 Q3 Q13 V24 W36 W47 L50 S56 Y57 I70 N77 L81 T91 A92 L93 Y94 Y95 T103 L104 W105 I113 T121 S124 S139 LYS SER THR SER G144 G150 W165 A179 L189 V192 V193 T194 V195 L200

G201 Y205 I206 C207 N208 D219 P224 K225 SER CYS ASP LYS THR HIS THR CYS PRO PRO PRO CYS PRO

● Molecule 3: Light chain of BIOLS56

Chain L:

D1 N31 Q37 L47 V50 R108 R142 Q147 A153 L154 Q155 V163 T180 L181 S182 K183 E187 V191 E195 N210 C214 S215

● Molecule 3: Light chain of BIOLS56

Chain D:

D1 L11 V19 N31 N34 Q37 L47 V50 V58 S77 L78 Q89 Y92 F98 D105 R108 T109 E123 K126 R142 V163 Q166 S174 L181 A184 K188 H189 R211 C214 SER

● Molecule 3: Light chain of BIOLS56

Chain G:

D1 G16 D17 R18 V19 T20 R24 L33 N34 W35 Y36 Q37 Q38 K39 K42 L47 I48 Y49 V50 R61 D70 F71 S77 L78 E81 D82 F83 A84 D105 I106 K107 R108 A111 V115 L135 L136 N137 Q147 W148 K149 V150 A153 L154 G157

N158 S159 Q160 E161 Q166 L175 L179 K183 E187 Y192 A193 C194 T197 H198 Q199 G200 L201 K207 N210 R211 G212 E213 CYS SER

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

Chain I:

33%　　　33%　　　33%

NAG1 NAG2 FUC3

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.48Å 159.02Å 175.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.39 – 2.97 47.39 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.39-2.97) 97.4 (47.39-2.97)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.220 , 0.263 0.220 , 0.263	Depositor DCC
R_{free} test set	3179 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.3	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14620	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 2.30% 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, FUC

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	0.32	0/1609	0.59	0/2198
1	B	0.33	0/1602	0.59	0/2187
1	E	0.33	0/1564	0.59	0/2134
2	C	0.31	0/1719	0.57	0/2344
2	F	0.28	0/1707	0.55	0/2328
2	H	0.29	0/1719	0.53	0/2344
3	D	0.43	0/1676	0.59	0/2277
3	G	0.35	0/1670	0.62	0/2269
3	L	0.33	0/1682	0.53	0/2285
All	All	0.33	0/14948	0.57	0/20366

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	1560	0	1482	28	0
1	B	1553	0	1478	27	0
1	E	1516	0	1440	35	0
2	C	1677	0	1626	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1665	0	1617	21	0
2	H	1677	0	1626	12	0
3	D	1640	0	1591	12	0
3	G	1634	0	1587	25	0
3	L	1646	0	1596	10	0
4	I	38	0	34	2	0
5	B	14	0	13	0	0
All	All	14620	0	14090	181	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 181 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:F:103:THR:HG22	2:F:105:TRP:H	1.40	0.86
2:H:103:THR:HG22	2:H:105:TRP:H	1.46	0.81
1:E:30:PRO:HG3	1:E:36:GLU:HG3	1.67	0.75
3:G:161:GLU:HG2	3:G:175:LEU:HD21	1.73	0.71
3:D:47:LEU:HA	3:D:58:VAL:HG21	1.74	0.70

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	194/228 (85%)	178 (92%)	15 (8%)	1 (0%)	29	66
1	B	193/228 (85%)	180 (93%)	12 (6%)	1 (0%)	29	66
1	E	186/228 (82%)	168 (90%)	17 (9%)	1 (0%)	29	66
2	C	219/237 (92%)	213 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	217/237 (92%)	211 (97%)	6 (3%)	0	100	100
2	H	219/237 (92%)	214 (98%)	5 (2%)	0	100	100
3	D	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	29	66
3	G	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
3	L	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
All	All	1864/2040 (91%)	1774 (95%)	86 (5%)	4 (0%)	47	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	122	ASN
1	B	160	LYS
3	D	50	VAL
1	A	159	GLY

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	171/202 (85%)	169 (99%)	2 (1%)	71	89
1	B	170/202 (84%)	168 (99%)	2 (1%)	71	89
1	E	165/202 (82%)	163 (99%)	2 (1%)	71	89
2	C	188/202 (93%)	187 (100%)	1 (0%)	88	95
2	F	186/202 (92%)	186 (100%)	0	100	100
2	H	188/202 (93%)	186 (99%)	2 (1%)	73	90
3	D	190/191 (100%)	187 (98%)	3 (2%)	62	85
3	G	189/191 (99%)	184 (97%)	5 (3%)	46	76
3	L	191/191 (100%)	188 (98%)	3 (2%)	62	85
All	All	1638/1785 (92%)	1618 (99%)	20 (1%)	71	89

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	121	ARG
3	G	42	LYS
3	G	147	GLN
3	G	50	VAL
3	L	108	ARG

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

Mol	Chain	Res	Type
1	A	91	GLN
2	C	175	HIS
3	D	210	ASN
1	E	76	ASN
3	G	198	HIS

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 ⓘ

3 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	I	1	1,4	14,14,15	0.43	0	17,19,21	0.61	0
4	NAG	I	2	4	14,14,15	0.71	0	17,19,21	0.80	1 (5%)
4	FUC	I	3	4	10,10,11	0.94	0	14,14,16	0.63	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
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	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	I	2	NAG	O5-C1-C2	-2.27	107.71	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings
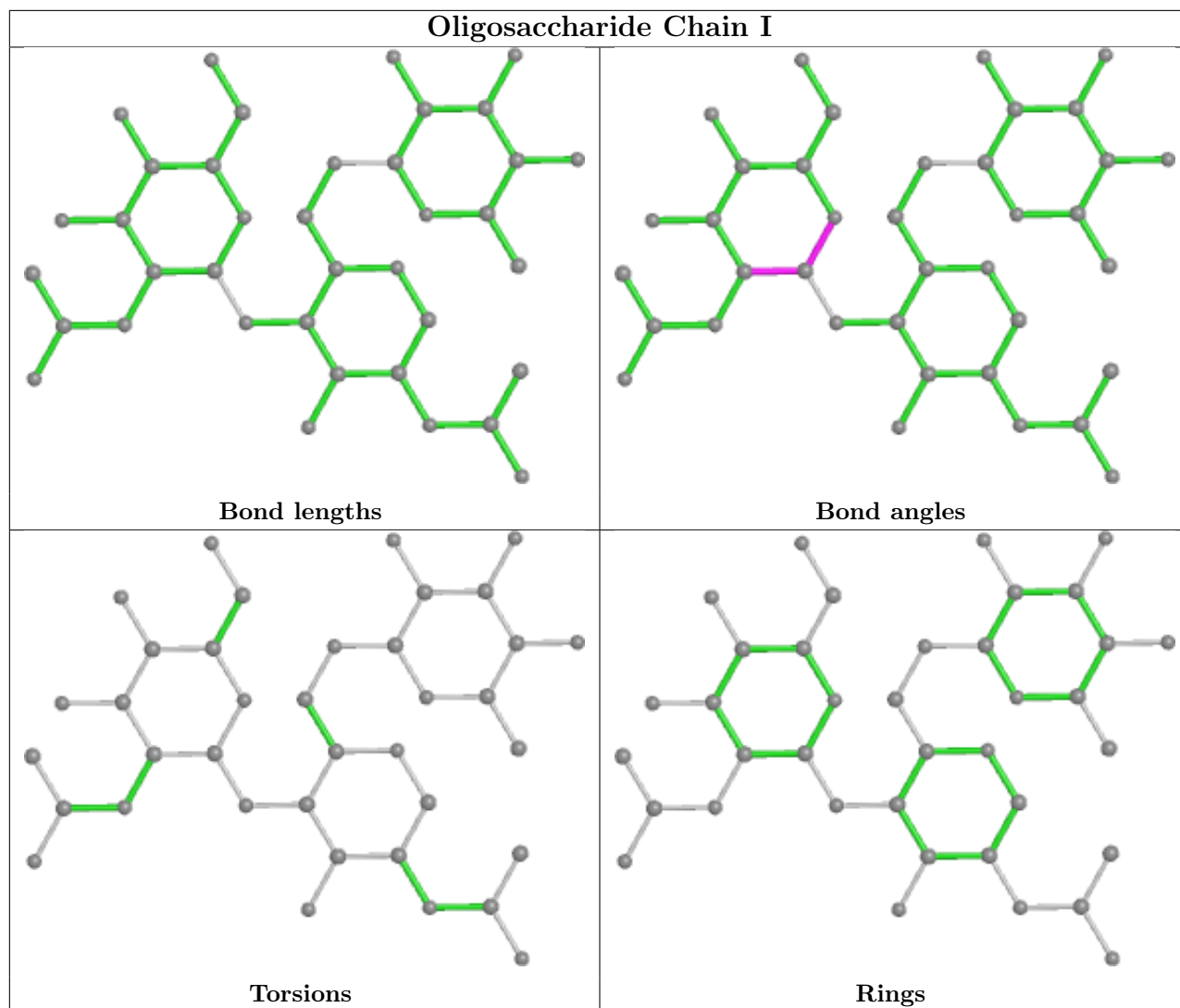
5.6   Ligand geometry ⓘ

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	#$|Z| > 2$
5	NAG	B	301	1	14,14,15	0.38	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
5	NAG	B	301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	NAG	C4-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	196/228 (85%)	0.13	6 (3%)	49	30	32, 51, 79, 96	0
1	B	195/228 (85%)	0.13	6 (3%)	49	30	30, 42, 79, 102	0
1	E	190/228 (83%)	0.38	12 (6%)	20	10	31, 50, 95, 108	0
2	C	223/237 (94%)	-0.02	4 (1%)	68	48	28, 44, 76, 118	0
2	F	221/237 (93%)	0.22	6 (2%)	54	35	38, 53, 93, 106	0
2	H	223/237 (94%)	-0.05	2 (0%)	84	69	29, 40, 71, 100	0
3	D	214/215 (99%)	0.16	4 (1%)	66	46	32, 50, 71, 102	0
3	G	213/215 (99%)	0.55	18 (8%)	10	5	42, 71, 102, 108	0
3	L	215/215 (100%)	-0.10	2 (0%)	84	69	29, 48, 62, 106	0
All	All	1890/2040 (92%)	0.15	60 (3%)	47	29	28, 48, 90, 118	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	THR	4.9
2	F	201	GLY	4.3
2	F	225	LYS	4.1
3	G	154	LEU	3.6
1	E	49	VAL	3.6

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

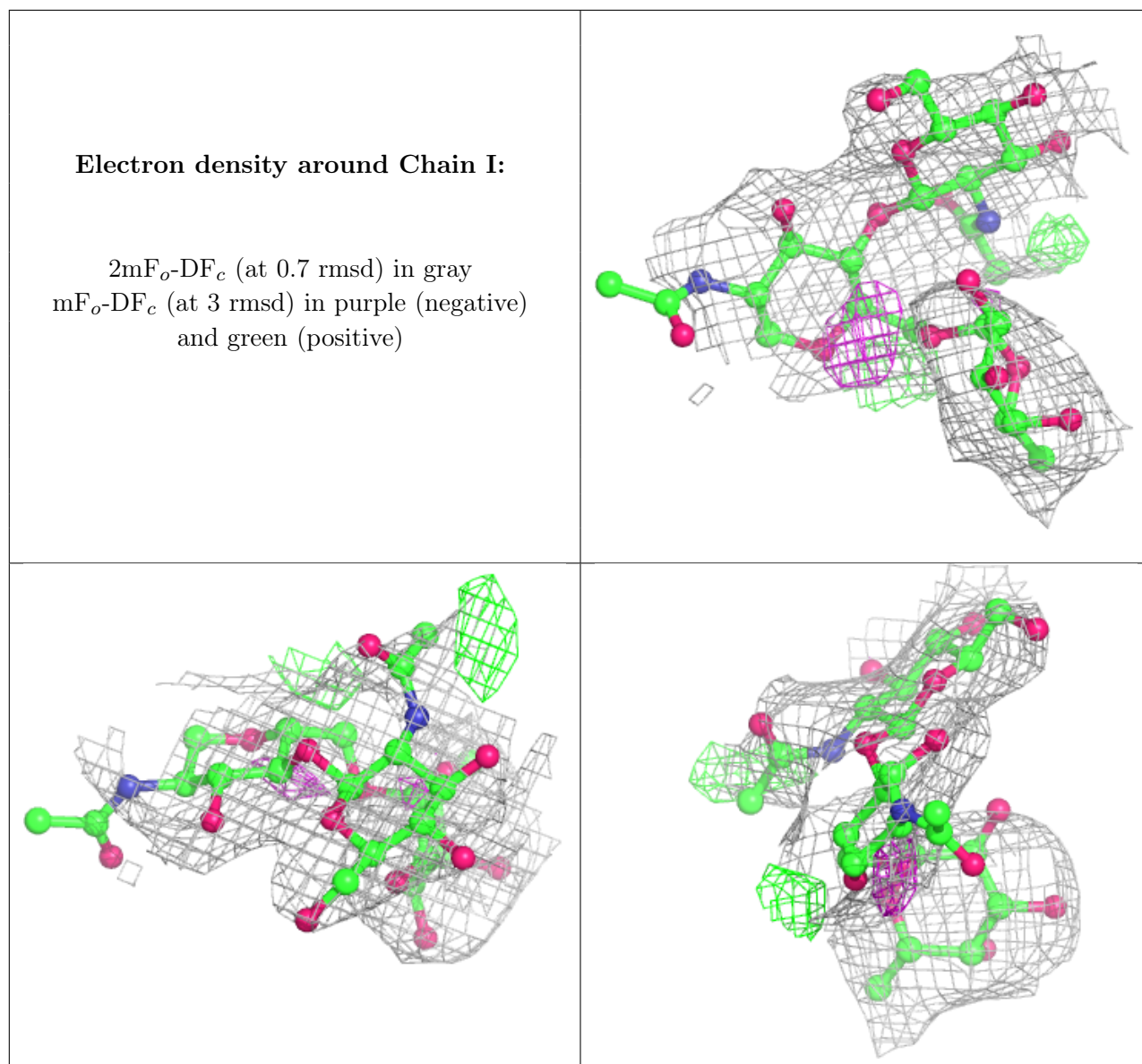There are no non-standard protein/DNA/RNA residues in this entry.

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	NAG	I	2	14/15	0.70	0.43	77,95,99,103	0
4	NAG	I	1	14/15	0.76	0.34	80,93,102,106	0
4	FUC	I	3	10/11	0.80	0.29	70,78,87,91	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 I:

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

6.4 Ligands (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, 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
5	NAG	B	301	14/15	0.73	0.40	85,99,103,105	0

6.5 Other polymers (i)

There are no such residues in this entry.