Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2022 – 12:22 pm GMT

PDB ID	:	7QNX
Title	:	The receptor binding domain of SARS-CoV-2 spike glycoprotein in complex with Beta-55 and EY6A Fabs
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-12-23
Resolution	:	2.92 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:

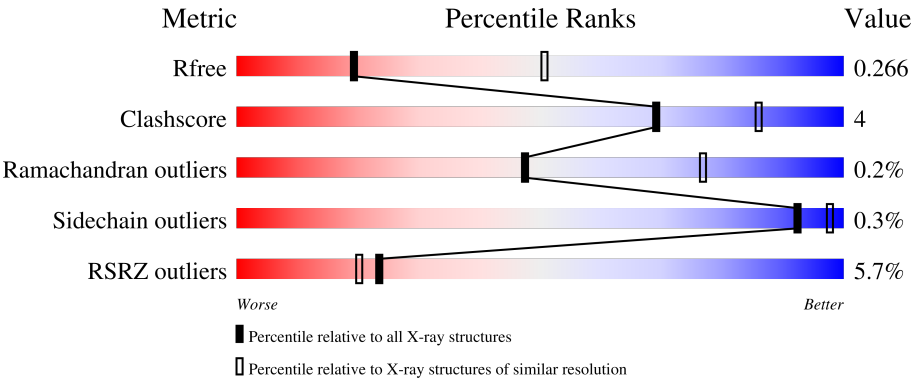
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.92 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))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	226	5% 81% 13% 5%
2	L	215	2% 92% 7%
3	A	232	6% 87% 11%
4	B	215	2% 93% 6%
5	E	202	13% 81% 10% 8%

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Mol	Chain	Length	Quality of chain
6	C	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8125 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 EY6A heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	215	1637	1041	273	317	6	0	0	0

- Molecule 2 is a protein called EY6A light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1618	1012	270	331	5	0	0	0

- Molecule 3 is a protein called Beta-55 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	228	1720	1097	279	339	5	0	0	0

- Molecule 4 is a protein called Beta-55 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	214	1645	1033	277	330	5	0	0	0

- Molecule 5 is a protein called Surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	185	1477	947	245	278	7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP A0A894R379
E	328	HIS	-	expression tag	UNP A0A894R379

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Chain	Residue	Modelled	Actual	Comment	Reference
E	329	HIS	-	expression tag	UNP A0A894R379
E	330	HIS	-	expression tag	UNP A0A894R379
E	331	HIS	-	expression tag	UNP A0A894R379
E	332	HIS	-	expression tag	UNP A0A894R379
E	527	LYS	PRO	variant	UNP A0A894R379

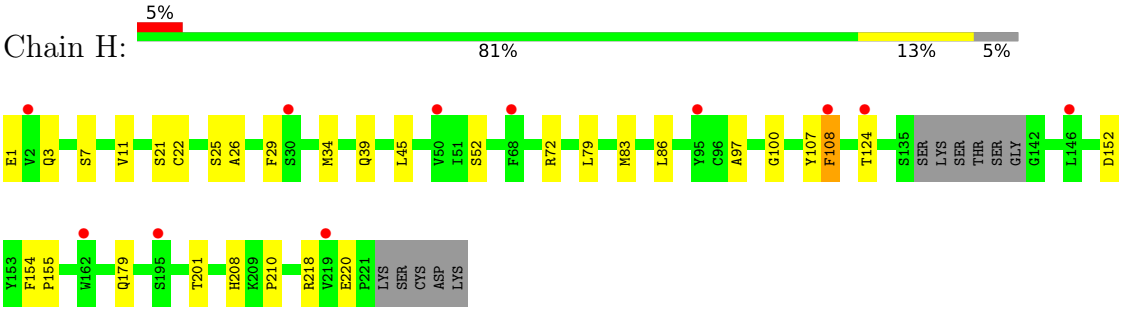
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

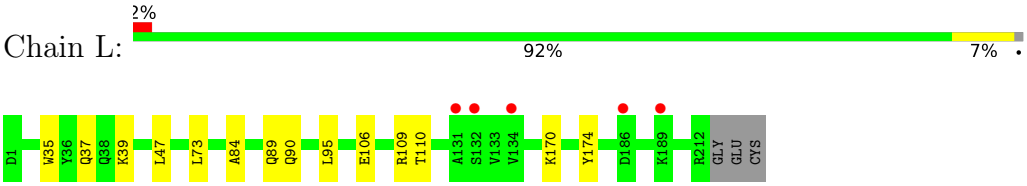
3 Residue-property plots (i)

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.

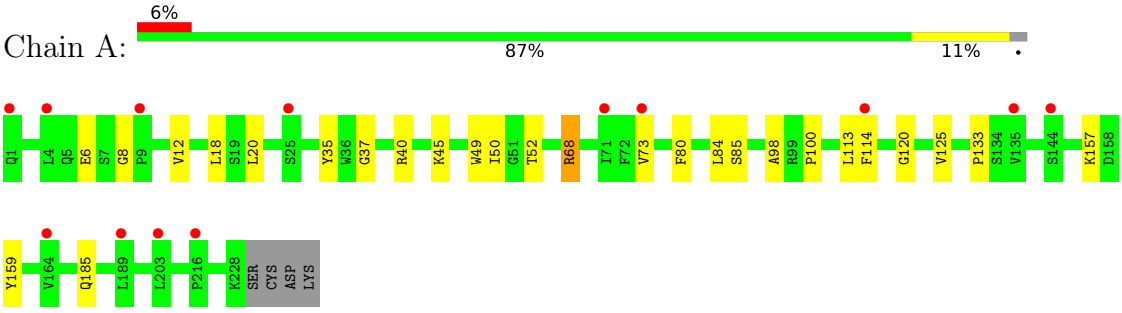
• Molecule 1: EY6A heavy chain



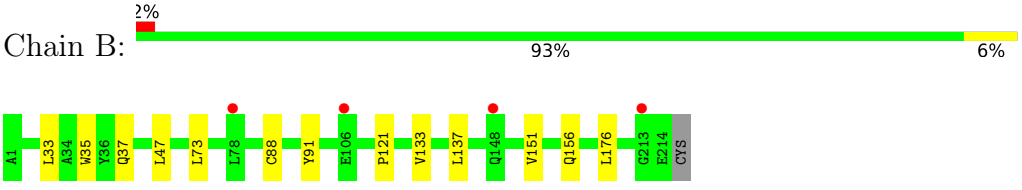
• Molecule 2: EY6A light chain



• Molecule 3: Beta-55 heavy chain

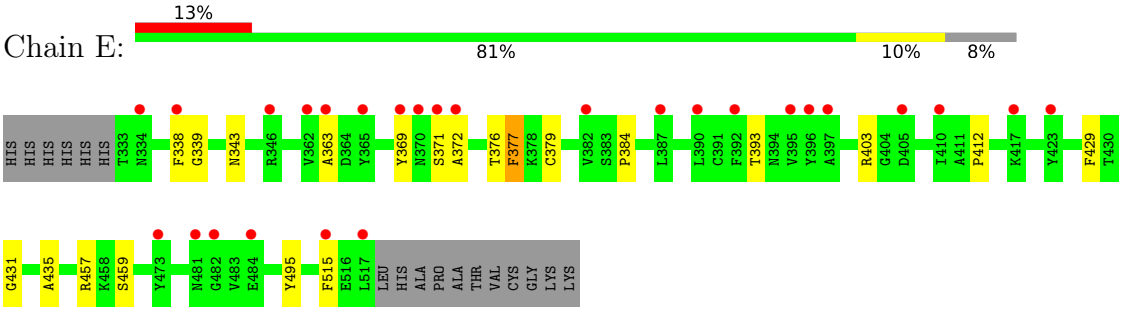


• Molecule 4: Beta-55 light chain



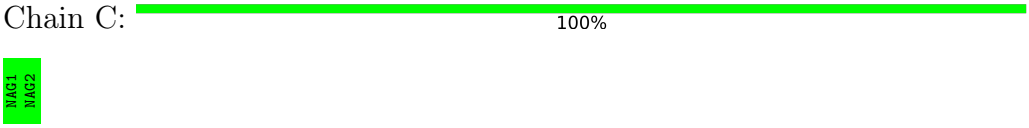
• Molecule 5: Surface glycoprotein

Chain E:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.77Å 131.77Å 116.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.64 – 2.92 81.64 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.64-2.92) 99.6 (81.64-2.92)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.229 , 0.266 0.230 , 0.266	Depositor DCC
R_{free} test set	1236 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	H	0.24	0/1679	0.48	0/2288
2	L	0.25	0/1651	0.47	0/2241
3	A	0.25	0/1768	0.48	0/2419
4	B	0.25	0/1682	0.48	0/2284
5	E	0.26	0/1518	0.47	0/2064
All	All	0.25	0/8298	0.48	0/11296

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	H	1637	0	1591	18	0
2	L	1618	0	1582	8	0
3	A	1720	0	1684	17	0
4	B	1645	0	1608	8	0
5	E	1477	0	1395	11	0
6	C	28	0	25	0	0
All	All	8125	0	7885	59	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 4.

All (59) 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:A:49:TRP:HE1	3:A:52:THR:HG23	1.56	0.71
1:H:29:PHE:O	1:H:72:ARG:NH2	2.34	0.61
3:A:35:TYR:HB2	3:A:100:PRO:HG2	1.82	0.61
3:A:133:PRO:HB3	3:A:159:TYR:HB3	1.86	0.57
1:H:97:ALA:HB1	1:H:108:PHE:HB3	1.86	0.57
5:E:431:GLY:HA2	5:E:515:PHE:HD2	1.69	0.57
5:E:363:ALA:HB2	5:E:393:THR:HG21	1.89	0.55
4:B:121:PRO:HD3	4:B:133:VAL:HG22	1.87	0.55
4:B:37:GLN:HB2	4:B:47:LEU:HD11	1.90	0.54
3:A:37:GLY:HA3	3:A:52:THR:HG22	1.89	0.54
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.89	0.53
1:H:100:GLY:HA3	1:H:107:TYR:CZ	2.43	0.53
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.90	0.52
3:A:8:GLY:HA3	3:A:20:LEU:HD23	1.91	0.52
1:H:124:THR:HG22	1:H:155:PRO:HD3	1.91	0.52
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.93	0.51
3:A:68:ARG:NH1	3:A:85:SER:O	2.42	0.51
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.93	0.51
3:A:113:LEU:HD23	4:B:91:TYR:CE1	2.46	0.51
2:L:39:LYS:HD3	2:L:84:ALA:HB2	1.92	0.50
3:A:157:LYS:NZ	3:A:185:GLN:OE1	2.45	0.50
3:A:40:ARG:HB3	3:A:50:ILE:HD11	1.93	0.49
2:L:109:ARG:NH1	2:L:110:THR:O	2.45	0.49
3:A:73:VAL:HG22	3:A:80:PHE:HB3	1.95	0.49
5:E:379:CYS:SG	5:E:384:PRO:HG3	2.52	0.49
1:H:11:VAL:HG21	1:H:155:PRO:HG3	1.95	0.48
1:H:152:ASP:OD1	1:H:179:GLN:NE2	2.46	0.48
5:E:403:ARG:HG3	5:E:495:TYR:CE1	2.49	0.48
5:E:376:THR:HB	5:E:435:ALA:HB3	1.97	0.47
1:H:1:GLU:HG3	1:H:26:ALA:HB1	1.96	0.47
3:A:113:LEU:HD23	4:B:91:TYR:CZ	2.50	0.47
3:A:18:LEU:HB3	3:A:84:LEU:HB3	1.97	0.47
1:H:208:HIS:CD2	1:H:210:PRO:HD2	2.50	0.46
3:A:98:ALA:HB1	3:A:114:PHE:HB3	1.97	0.46
5:E:338:PHE:HE2	5:E:363:ALA:HB1	1.80	0.46
1:H:201:THR:HG23	1:H:218:ARG:HE	1.80	0.46
1:H:3:GLN:HB2	1:H:25:SER:HB2	1.97	0.46
5:E:339:GLY:O	5:E:343:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:137:LEU:HB2	4:B:176:LEU:HB3	1.96	0.46
4:B:35:TRP:CE2	4:B:73:LEU:HB2	2.51	0.46
2:L:106:GLU:OE1	2:L:174:TYR:OH	2.28	0.45
5:E:457:ARG:NH1	5:E:459:SER:O	2.43	0.45
5:E:369:TYR:HB2	5:E:377:PHE:CE2	2.52	0.45
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.52	0.44
4:B:151:VAL:HB	4:B:156:GLN:HE21	1.83	0.44
3:A:6:GLU:OE1	3:A:120:GLY:N	2.48	0.44
3:A:49:TRP:NE1	3:A:52:THR:HG23	2.27	0.44
3:A:12:VAL:O	3:A:125:VAL:HA	2.19	0.43
4:B:33:LEU:HD11	4:B:88:CYS:HB2	2.01	0.43
1:H:22:CYS:HB3	1:H:79:LEU:HB3	2.01	0.43
1:H:218:ARG:NH1	1:H:220:GLU:OE1	2.52	0.42
2:L:89:GLN:NE2	2:L:90:GLN:O	2.52	0.42
1:H:52:SER:O	1:H:72:ARG:NH1	2.52	0.42
5:E:412:PRO:HG3	5:E:429:PHE:HB3	2.02	0.42
1:H:11:VAL:HG11	1:H:154:PHE:HE1	1.86	0.41
2:L:170:LYS:HE3	2:L:170:LYS:HB2	1.74	0.41
3:A:45:LYS:HA	3:A:45:LYS:HD3	1.72	0.41
2:L:95:LEU:HD11	5:E:384:PRO:HG2	2.02	0.41
1:H:7:SER:OG	1:H:21:SER:OG	2.39	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	H	211/226 (93%)	202 (96%)	9 (4%)	0	100	100
2	L	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
3	A	226/232 (97%)	215 (95%)	11 (5%)	0	100	100
4	B	212/215 (99%)	204 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	183/202 (91%)	171 (93%)	10 (6%)	2 (1%)	14 41
All	All	1042/1090 (96%)	995 (96%)	45 (4%)	2 (0%)	47 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	372	ALA
5	E	371	SER

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	H	181/191 (95%)	180 (99%)	1 (1%)	86 95
2	L	186/188 (99%)	186 (100%)	0	100 100
3	A	197/202 (98%)	196 (100%)	1 (0%)	88 96
4	B	186/187 (100%)	186 (100%)	0	100 100
5	E	161/175 (92%)	160 (99%)	1 (1%)	86 95
All	All	911/943 (97%)	908 (100%)	3 (0%)	92 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	108	PHE
3	A	68	ARG
5	E	377	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	C	1	6,5	14,14,15	0.39	0	17,19,21	0.48	0
6	NAG	C	2	6	14,14,15	0.25	0	17,19,21	0.46	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	C	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	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.

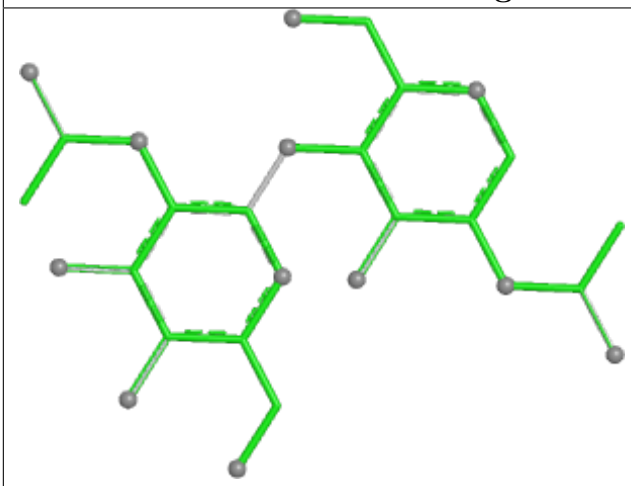
There are no torsion outliers.

There are no ring outliers.

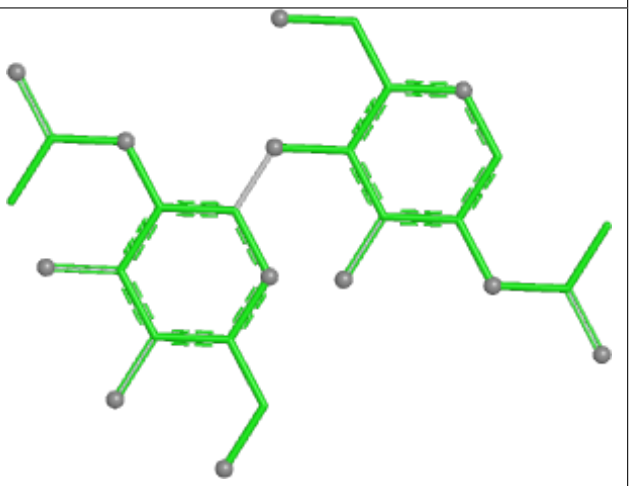
No monomer is involved in short contacts.

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

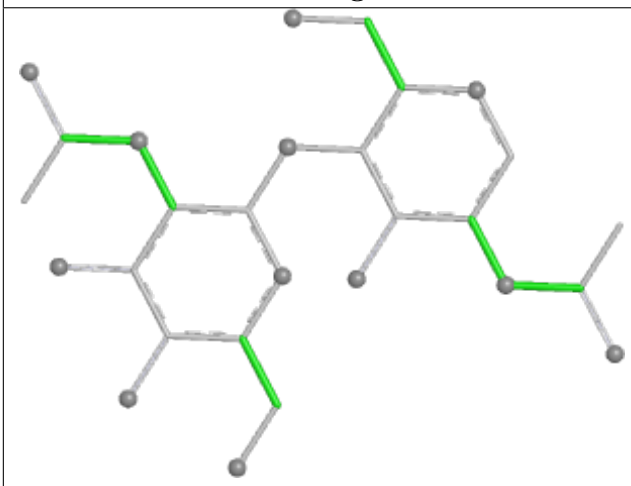
Oligosaccharide Chain C



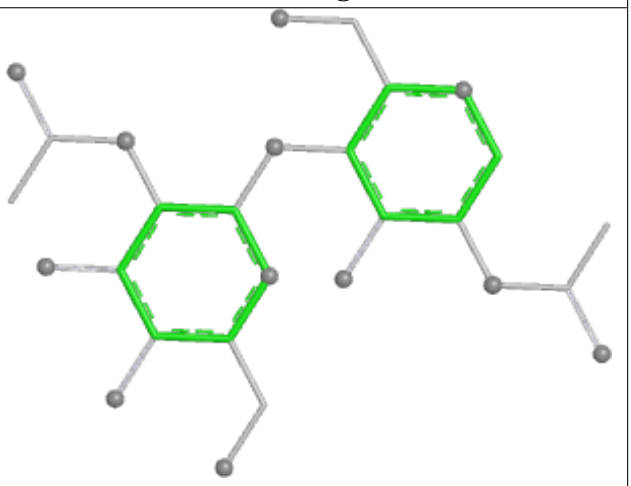
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	H	215/226 (95%)	0.48	11 (5%) 28 24	60, 78, 105, 132	0
2	L	212/215 (98%)	0.42	5 (2%) 59 57	55, 70, 99, 149	0
3	A	228/232 (98%)	0.42	13 (5%) 23 20	51, 67, 107, 139	0
4	B	214/215 (99%)	0.39	4 (1%) 66 65	54, 71, 93, 122	0
5	E	185/202 (91%)	0.98	27 (14%) 2 1	56, 71, 115, 155	0
All	All	1054/1090 (96%)	0.53	60 (5%) 23 20	51, 71, 105, 155	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	517	LEU	5.6
5	E	482	GLY	5.4
3	A	1	GLN	5.0
2	L	189	LYS	4.9
5	E	371	SER	4.7
5	E	370	ASN	4.2
5	E	372	ALA	3.7
5	E	392	PHE	3.5
5	E	481	ASN	3.2
5	E	395	VAL	3.2
2	L	186	ASP	3.1
5	E	365	TYR	3.0
1	H	30	SER	3.0
3	A	144	SER	2.9
5	E	338	PHE	2.9
5	E	423	TYR	2.8
5	E	334	ASN	2.8
5	E	390	LEU	2.8
3	A	216	PRO	2.8
3	A	73	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	382	VAL	2.7
1	H	124	THR	2.6
4	B	78	LEU	2.6
5	E	397	ALA	2.6
5	E	369	TYR	2.6
5	E	515	PHE	2.6
2	L	131	ALA	2.6
1	H	219	VAL	2.5
1	H	2	VAL	2.5
5	E	363	ALA	2.5
5	E	417	LYS	2.5
4	B	106	GLU	2.5
3	A	203	LEU	2.4
1	H	108	PHE	2.4
5	E	362	VAL	2.4
5	E	484	GLU	2.4
5	E	396	TYR	2.3
1	H	95	TYR	2.3
5	E	346	ARG	2.3
1	H	68	PHE	2.2
2	L	132	SER	2.2
3	A	189	LEU	2.2
1	H	146	LEU	2.2
3	A	71	ILE	2.2
5	E	387	LEU	2.1
1	H	162	TRP	2.1
3	A	9	PRO	2.1
2	L	134	VAL	2.1
5	E	410	ILE	2.1
3	A	114	PHE	2.1
5	E	473	TYR	2.1
5	E	405	ASP	2.1
3	A	164	VAL	2.1
4	B	213	GLY	2.1
1	H	50	VAL	2.1
3	A	25	SER	2.0
3	A	4	LEU	2.0
1	H	195	SER	2.0
3	A	135	VAL	2.0
4	B	148	GLN	2.0

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

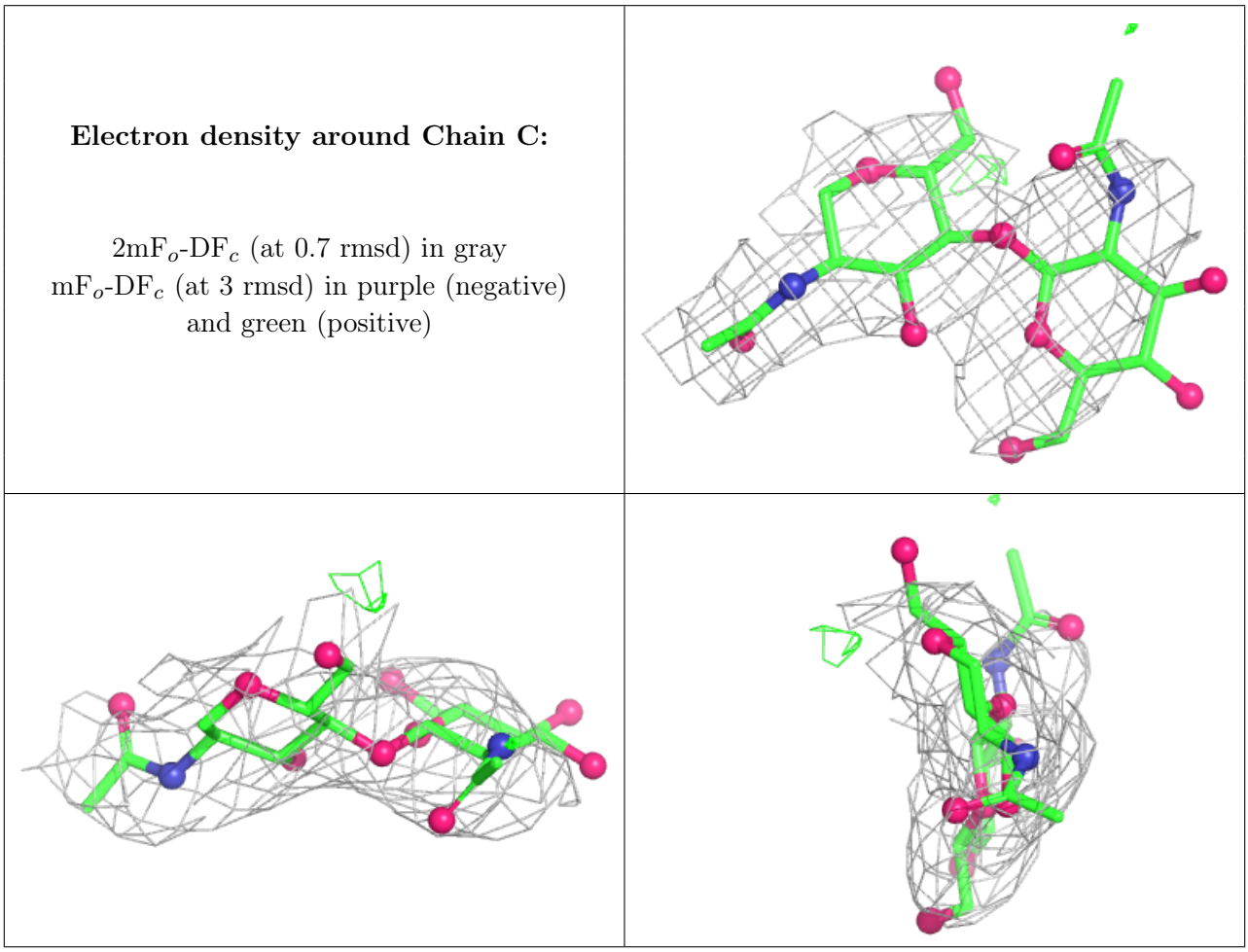
There are no non-standard protein/DNA/RNA residues in this entry.

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
6	NAG	C	2	14/15	0.79	0.29	121,127,133,133	0
6	NAG	C	1	14/15	0.86	0.20	90,111,117,123	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.