Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2022 – 06:11 pm GMT

PDB ID	:	7PQZ
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with FI-3A and FD-11A Fabs
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-09-20
Resolution	:	3.20 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 (i) symbol.

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

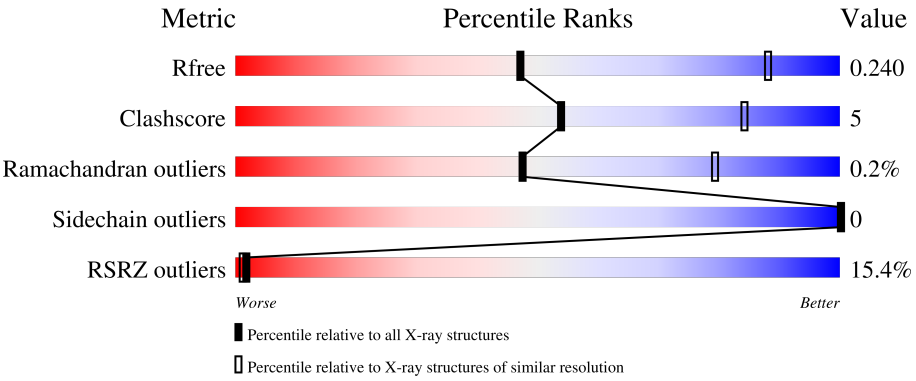
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	E	205	18% 83% 9% 8%
2	H	222	12% 82% 16% .
3	L	214	11% 89% 10%
4	A	232	17% 81% 16% .
5	B	219	16% 88% 11% .

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Mol	Chain	Length	Quality of chain
6	C	2	100%

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
7	PO4	E	601	-	-	-	X
7	PO4	E	602	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8083 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	E	189	Total	C	N	O	S	0	0	0
			1498	959	249	282	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1611	1011	274	317	9			

- Molecule 3 is a protein called FI-3A Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1635	1021	273	336	5			

- Molecule 4 is a protein called FD-11A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	225	Total	C	N	O	S	0	0	0
			1712	1088	284	332	8			

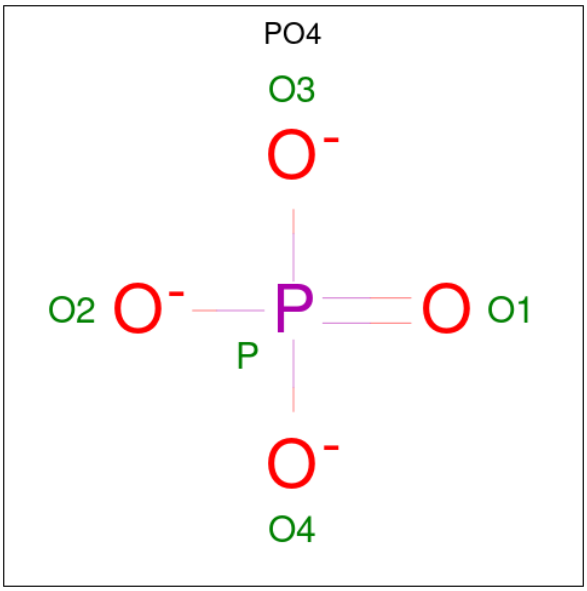
- Molecule 5 is a protein called FD-11A Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	215	Total	C	N	O	S	0	0	0
			1589	996	264	325	4			

- 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			

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

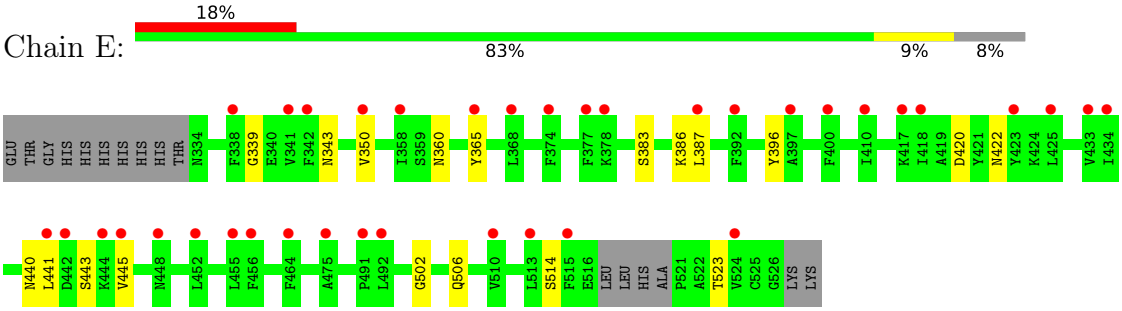


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		

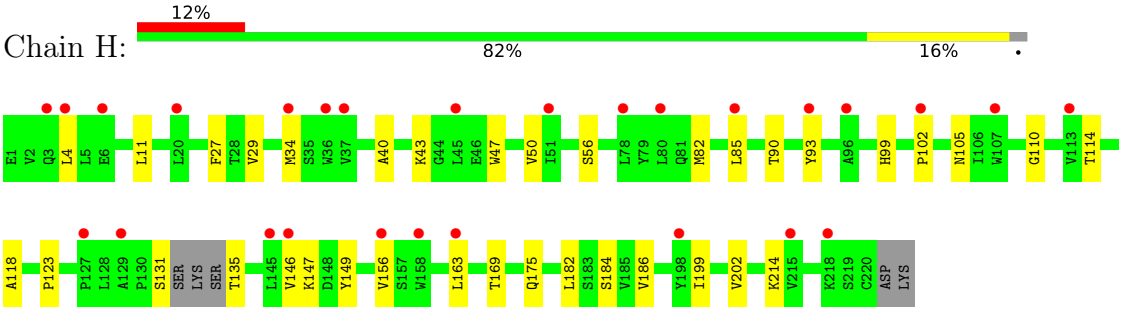
3 Residue-property plots (i)

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.

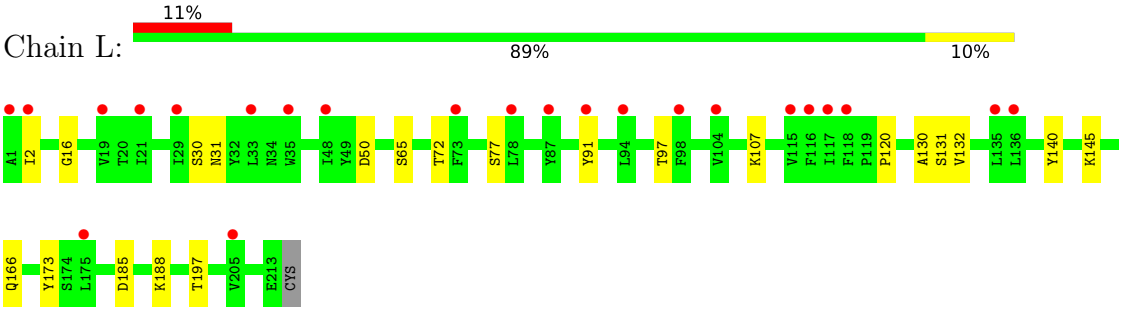
- Molecule 1: Spike protein S1



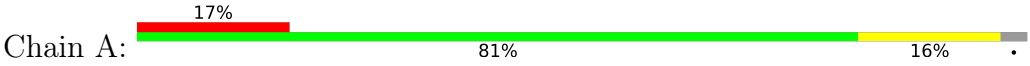
- Molecule 2: FI-3A Fab heavy chain

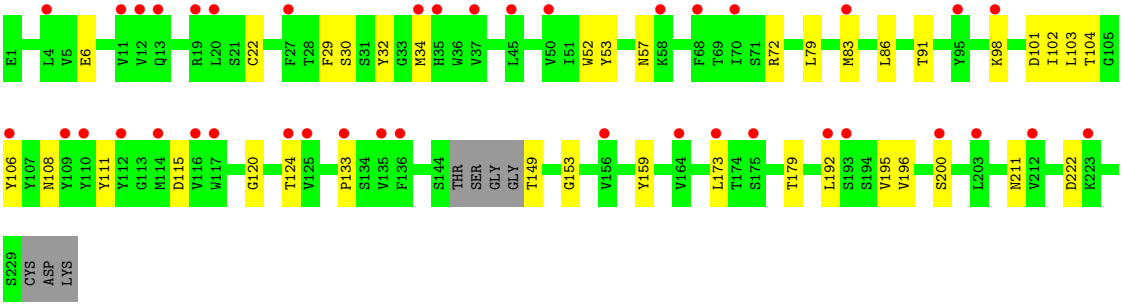


- Molecule 3: FI-3A Fab light chain

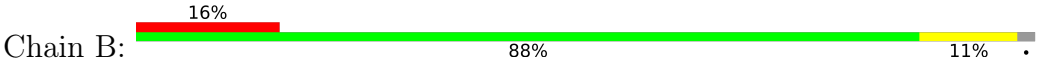


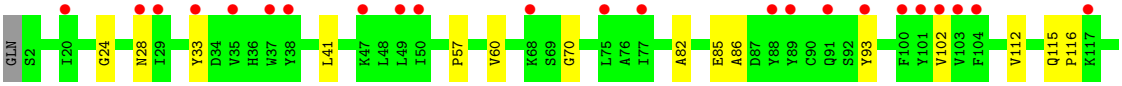
- Molecule 4: FD-11A Fab heavy chain

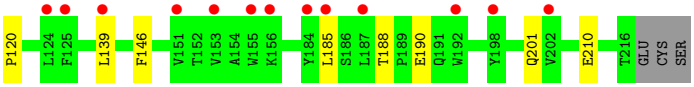




• Molecule 5: FD-11A Fab light chain







• 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	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.81Å 115.81Å 237.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.66 – 3.20 100.30 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (76.66-3.20) 99.7 (100.30-3.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.201 , 0.240 0.202 , 0.240	Depositor DCC
R_{free} test set	1686 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	145.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8083	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, PO4

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	E	0.25	0/1539	0.46	0/2091
2	H	0.26	0/1647	0.49	0/2241
3	L	0.25	0/1669	0.47	0/2268
4	A	0.25	0/1757	0.47	0/2394
5	B	0.26	0/1629	0.48	0/2226
All	All	0.25	0/8241	0.47	0/11220

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	E	1498	0	1411	13	0
2	H	1611	0	1584	19	0
3	L	1635	0	1583	12	0
4	A	1712	0	1656	29	0
5	B	1589	0	1535	15	0
6	C	28	0	25	1	0
7	E	10	0	0	0	0
All	All	8083	0	7794	84	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 5.

All (84) 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)
5:B:82:ALA:HA	5:B:112:VAL:HG21	1.71	0.71
4:A:83:MET:HB3	4:A:86:LEU:HD21	1.71	0.71
2:H:131:SER:HG	2:H:135:THR:N	1.91	0.68
5:B:24:GLY:HA3	5:B:28:ASN:HD21	1.59	0.68
4:A:6:GLU:OE2	4:A:120:GLY:N	2.22	0.66
2:H:47:TRP:HE1	2:H:50:VAL:HG23	1.60	0.66
5:B:120:PRO:HB3	5:B:146:PHE:HB3	1.77	0.65
4:A:52:TRP:O	4:A:72:ARG:NH1	2.29	0.65
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.81	0.62
4:A:22:CYS:HB3	4:A:79:LEU:HB3	1.81	0.62
1:E:360:ASN:H	1:E:523:THR:HB	1.66	0.59
4:A:153:GLY:HA3	4:A:195:VAL:HG12	1.83	0.59
2:H:99:HIS:HB2	2:H:105:ASN:HB2	1.85	0.56
1:E:443:SER:O	4:A:108:ASN:ND2	2.32	0.56
5:B:139:LEU:HD12	5:B:185:LEU:HD23	1.86	0.56
5:B:188:THR:HG22	5:B:190:GLU:H	1.70	0.55
4:A:103:LEU:HG	4:A:104:THR:HG23	1.88	0.55
4:A:173:LEU:HD21	4:A:196:VAL:HG21	1.87	0.54
1:E:440:ASN:HB2	4:A:111:TYR:CE1	2.44	0.53
5:B:85:GLU:HB2	5:B:112:VAL:HG22	1.91	0.53
4:A:133:PRO:HB3	4:A:159:TYR:HB3	1.90	0.52
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.90	0.52
4:A:34:MET:HB3	4:A:79:LEU:HD22	1.92	0.51
4:A:98:LYS:NZ	4:A:115:ASP:OD2	2.40	0.50
5:B:93:TYR:HA	5:B:102:VAL:HA	1.92	0.50
1:E:365:TYR:CD2	1:E:387:LEU:HB3	2.46	0.49
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.94	0.49
4:A:32:TYR:CE1	4:A:101:ASP:HB2	2.46	0.49
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.94	0.49
3:L:65:SER:OG	3:L:72:THR:OG1	2.28	0.49
5:B:115:GLN:HB2	5:B:116:PRO:HD2	1.93	0.49
4:A:30:SER:O	4:A:53:TYR:HB2	2.13	0.48
1:E:365:TYR:HD2	1:E:387:LEU:HB3	1.78	0.48
2:H:169:THR:HG23	2:H:184:SER:HB2	1.96	0.48
2:H:156:VAL:HG22	2:H:202:VAL:HG22	1.96	0.48
5:B:41:LEU:HD23	5:B:86:ALA:HB2	1.96	0.48
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:GLY:O	1:E:343:ASN:HB2	2.14	0.47
4:A:6:GLU:HA	4:A:22:CYS:HA	1.96	0.47
2:H:29:VAL:HG13	2:H:34:MET:HG3	1.96	0.47
2:H:147:LYS:NZ	2:H:175:GLN:OE1	2.47	0.47
6:C:1:NAG:H62	6:C:2:NAG:C7	2.45	0.47
5:B:33:TYR:CD1	5:B:93:TYR:HB2	2.50	0.47
5:B:24:GLY:CA	5:B:28:ASN:HD21	2.25	0.47
4:A:115:ASP:N	4:A:115:ASP:OD1	2.42	0.47
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.96	0.46
3:L:16:GLY:HA2	3:L:77:SER:HB2	1.97	0.46
1:E:396:TYR:HB2	1:E:514:SER:HB2	1.96	0.46
4:A:149:THR:N	4:A:200:SER:HG	2.13	0.46
2:H:90:THR:HG23	2:H:114:THR:HA	1.96	0.46
4:A:52:TRP:NE1	4:A:57:ASN:HB2	2.31	0.46
2:H:93:TYR:O	2:H:110:GLY:HA2	2.16	0.45
2:H:163:LEU:HD21	2:H:186:VAL:HG21	1.97	0.45
1:E:383:SER:HB3	1:E:386:LYS:HB2	1.97	0.45
1:E:502:GLY:O	1:E:506:GLN:HG3	2.16	0.45
4:A:52:TRP:CZ3	4:A:102:ILE:HG12	2.52	0.45
2:H:47:TRP:NE1	2:H:50:VAL:HG23	2.29	0.44
2:H:4:LEU:HD21	2:H:27:PHE:CZ	2.53	0.44
3:L:185:ASP:OD1	3:L:188:LYS:NZ	2.48	0.43
4:A:52:TRP:HZ3	4:A:102:ILE:HG12	1.83	0.43
4:A:91:THR:HG23	4:A:124:THR:HA	2.00	0.43
4:A:211:ASN:ND2	4:A:222:ASP:OD2	2.49	0.43
1:E:445:VAL:HG21	5:B:33:TYR:CD1	2.54	0.43
4:A:52:TRP:HZ3	4:A:102:ILE:HG21	1.84	0.43
2:H:199:ILE:HG12	2:H:214:LYS:HG2	1.99	0.43
3:L:120:PRO:HB3	3:L:131:SER:H	1.84	0.43
2:H:146:VAL:O	2:H:182:LEU:N	2.49	0.42
5:B:57:PRO:HD2	5:B:60:VAL:HG21	2.00	0.42
3:L:2:ILE:O	3:L:97:THR:HG21	2.18	0.42
3:L:120:PRO:HG3	3:L:130:ALA:HB1	2.02	0.42
1:E:441:LEU:HD22	4:A:106:TYR:CD2	2.55	0.42
2:H:11:LEU:HD21	2:H:118:ALA:O	2.18	0.42
4:A:52:TRP:HE1	4:A:57:ASN:HB2	1.85	0.42
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.20	0.42
4:A:52:TRP:CD1	4:A:57:ASN:HB2	2.54	0.42
4:A:29:PHE:O	4:A:72:ARG:NH2	2.52	0.42
3:L:50:ASP:OD1	3:L:91:TYR:OH	2.38	0.41
4:A:52:TRP:HD1	4:A:57:ASN:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:93:TYR:CD2	5:B:102:VAL:HG12	2.56	0.41
5:B:201:GLN:HG2	5:B:210:GLU:HG3	2.02	0.41
3:L:107:LYS:HA	3:L:140:TYR:OH	2.21	0.41
4:A:179:THR:HG23	4:A:192:LEU:HD21	2.02	0.41
1:E:420:ASP:OD2	2:H:56:SER:OG	2.25	0.41
3:L:30:SER:OG	3:L:31:ASN:N	2.52	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	E	185/205 (90%)	172 (93%)	13 (7%)	0	100	100
2	H	213/222 (96%)	204 (96%)	8 (4%)	1 (0%)	29	67
3	L	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
4	A	221/232 (95%)	210 (95%)	11 (5%)	0	100	100
5	B	213/219 (97%)	193 (91%)	19 (9%)	1 (0%)	29	67
All	All	1043/1092 (96%)	983 (94%)	58 (6%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	102	PRO
5	B	70	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	E	163/177 (92%)	163 (100%)	0	100	100
2	H	182/187 (97%)	182 (100%)	0	100	100
3	L	187/188 (100%)	187 (100%)	0	100	100
4	A	189/195 (97%)	189 (100%)	0	100	100
5	B	178/182 (98%)	178 (100%)	0	100	100
All	All	899/929 (97%)	899 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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	C	1	1,6	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	C	2	6	14,14,15	0.29	0	17,19,21	0.55	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	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	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	C	2	NAG	O5-C5-C6-O6

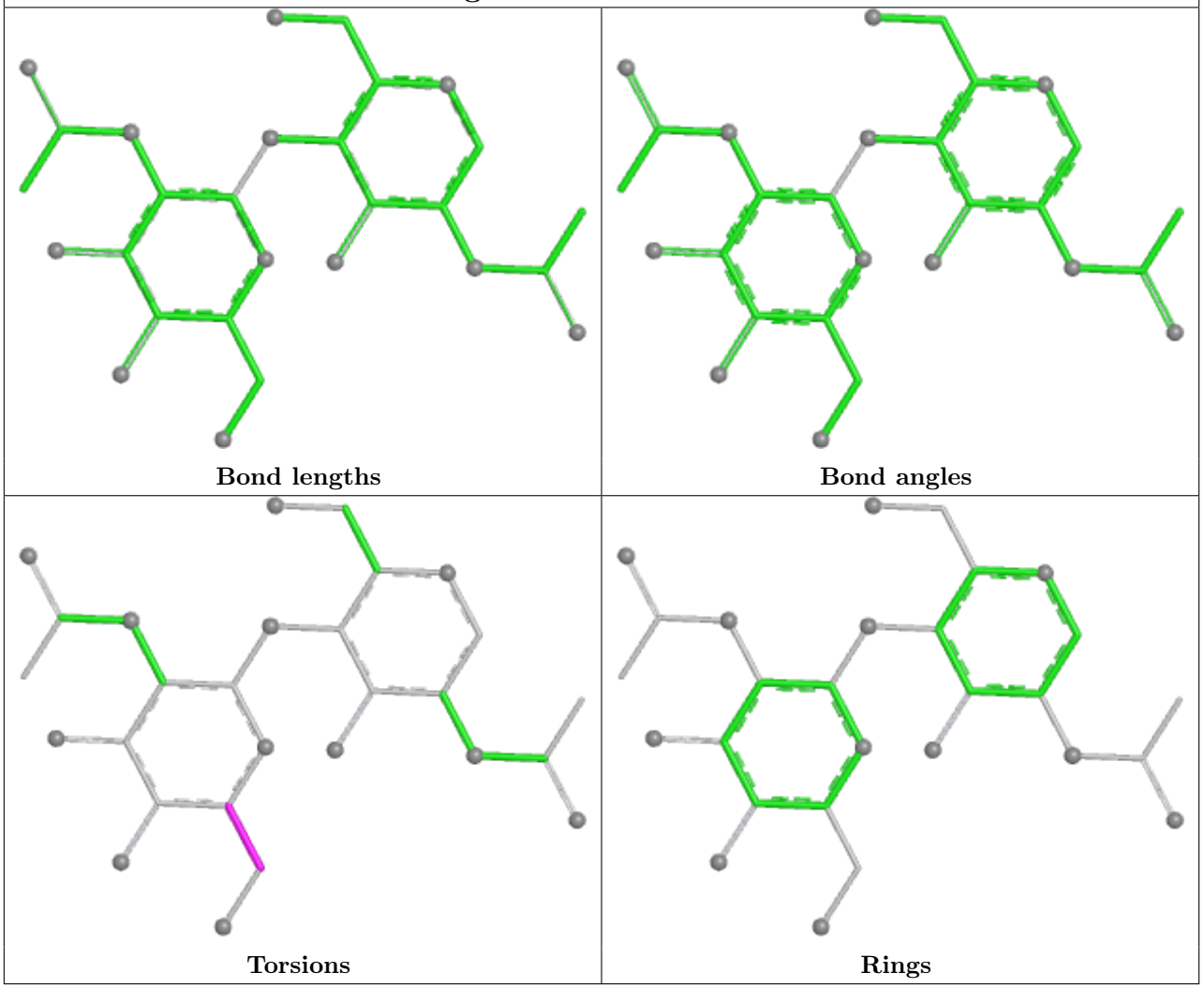
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	1	0
6	C	2	NAG	1	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 C



5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
7	PO4	E	602	-	4,4,4	0.77	0	6,6,6	0.43	0
7	PO4	E	601	-	4,4,4	0.77	0	6,6,6	0.43	0

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	E	189/205 (92%)	0.96	37 (19%)	1	1	124, 156, 231, 285	0
2	H	217/222 (97%)	0.83	27 (12%)	4	2	124, 162, 197, 242	0
3	L	213/214 (99%)	0.87	23 (10%)	5	3	128, 158, 187, 230	0
4	A	225/232 (96%)	0.93	40 (17%)	1	1	140, 178, 213, 253	0
5	B	215/219 (98%)	0.88	36 (16%)	1	1	128, 161, 203, 245	0
All	All	1059/1092 (96%)	0.89	163 (15%)	2	1	124, 163, 215, 285	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	338	PHE	4.6
5	B	155	TRP	4.6
4	A	58	LYS	4.5
5	B	100	PHE	4.2
4	A	203	LEU	4.1
5	B	29	ILE	3.9
1	E	342	PHE	3.8
1	E	433	VAL	3.7
5	B	49	LEU	3.7
1	E	392	PHE	3.7
4	A	68	PHE	3.6
1	E	365	TYR	3.6
2	H	218	LYS	3.6
3	L	2	ILE	3.6
3	L	1	ALA	3.5
3	L	35	TRP	3.5
4	A	37	VAL	3.4
4	A	27	PHE	3.4
1	E	368	LEU	3.4
2	H	45	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
4	A	135	VAL	3.3
5	B	156	LYS	3.3
1	E	513	LEU	3.2
3	L	91	TYR	3.2
2	H	113	VAL	3.2
5	B	124	LEU	3.2
1	E	442	ASP	3.1
4	A	50	VAL	3.1
5	B	101	TYR	3.1
2	H	198	TYR	3.0
1	E	434	ILE	3.0
2	H	215	VAL	2.9
5	B	117	LYS	2.9
4	A	20	LEU	2.9
3	L	118	PHE	2.9
1	E	410	ILE	2.9
4	A	4	LEU	2.9
2	H	145	LEU	2.9
5	B	139	LEU	2.9
5	B	184	TYR	2.9
4	A	34	MET	2.8
4	A	13	GLN	2.8
1	E	464	PHE	2.8
1	E	378	LYS	2.8
4	A	193	SER	2.8
4	A	133	PRO	2.8
5	B	102	VAL	2.8
1	E	444	LYS	2.8
1	E	445	VAL	2.8
1	E	515	PHE	2.8
5	B	125	PHE	2.8
4	A	175	SER	2.7
2	H	93	TYR	2.7
5	B	35	VAL	2.7
4	A	114	MET	2.7
1	E	423	TYR	2.7
3	L	117	ILE	2.7
2	H	3	GLN	2.7
1	E	417	LYS	2.6
5	B	75	LEU	2.6
4	A	125	VAL	2.6
3	L	21	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	124	THR	2.6
3	L	19	VAL	2.6
1	E	455	LEU	2.6
4	A	116	VAL	2.6
2	H	6	GLU	2.6
5	B	198	TYR	2.6
1	E	341	VAL	2.6
5	B	20	ILE	2.6
5	B	77	ILE	2.6
4	A	112	TYR	2.5
5	B	104	PHE	2.5
2	H	80	LEU	2.5
4	A	223	LYS	2.5
4	A	117	TRP	2.5
1	E	425	LEU	2.5
4	A	45	LEU	2.5
4	A	173	LEU	2.5
3	L	48	ILE	2.5
1	E	524	VAL	2.5
5	B	37	TRP	2.5
3	L	104	VAL	2.5
4	A	192	LEU	2.5
3	L	205	VAL	2.5
5	B	151	VAL	2.5
2	H	163	LEU	2.4
2	H	158	TRP	2.4
3	L	98	PHE	2.4
2	H	146	VAL	2.4
4	A	12	VAL	2.4
5	B	185	LEU	2.4
3	L	29	ILE	2.4
4	A	70	ILE	2.4
3	L	115	VAL	2.4
2	H	36	TRP	2.4
4	A	110	TYR	2.3
1	E	400	PHE	2.3
2	H	156	VAL	2.3
4	A	200	SER	2.3
1	E	510	VAL	2.3
1	E	456	PHE	2.3
2	H	51	ILE	2.3
2	H	4	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	85	LEU	2.3
1	E	387	LEU	2.3
2	H	102	PRO	2.3
1	E	374	PHE	2.3
1	E	358	ILE	2.3
4	A	136	PHE	2.3
4	A	212	VAL	2.3
5	B	153	VAL	2.3
3	L	33	LEU	2.2
5	B	33	TYR	2.2
4	A	35	HIS	2.2
4	A	19	ARG	2.2
5	B	68	LYS	2.2
3	L	73	PHE	2.2
4	A	156	VAL	2.2
3	L	135	LEU	2.2
5	B	89	TYR	2.2
1	E	377	PHE	2.2
4	A	164	VAL	2.2
5	B	50	ILE	2.2
2	H	127	PRO	2.2
3	L	94	LEU	2.2
2	H	107	TRP	2.2
2	H	78	LEU	2.2
3	L	136	LEU	2.2
5	B	93	TYR	2.2
1	E	418	ILE	2.2
3	L	78	LEU	2.2
5	B	47	LYS	2.2
5	B	88	TYR	2.2
5	B	192	TRP	2.1
4	A	109	TYR	2.1
5	B	38	TYR	2.1
4	A	106	TYR	2.1
5	B	103	VAL	2.1
4	A	83	MET	2.1
1	E	397	ALA	2.1
5	B	28	ASN	2.1
4	A	11	VAL	2.1
1	E	452	LEU	2.1
2	H	96	ALA	2.1
1	E	492	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	441	LEU	2.1
1	E	475	ALA	2.1
3	L	87	TYR	2.1
5	B	202	VAL	2.1
3	L	116	PHE	2.1
1	E	491	PRO	2.1
4	A	98	LYS	2.1
5	B	91	GLN	2.1
4	A	95	TYR	2.0
2	H	34	MET	2.0
1	E	350	VAL	2.0
2	H	129	ALA	2.0
5	B	187	LEU	2.0
1	E	448	ASN	2.0
2	H	37	VAL	2.0
2	H	20	LEU	2.0
3	L	175	LEU	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)

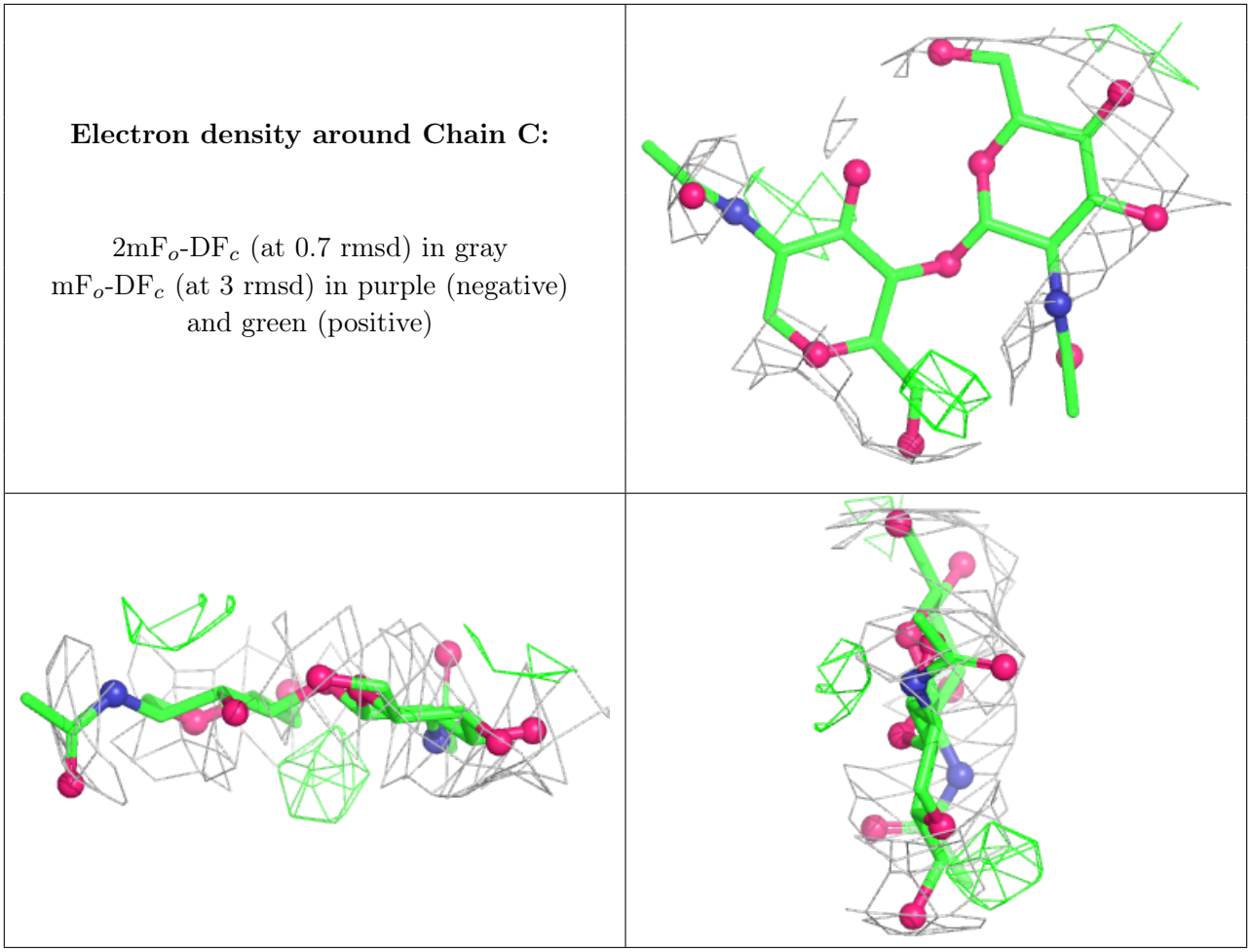
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	1	14/15	0.72	0.24	179,222,245,253	0
6	NAG	C	2	14/15	0.74	0.21	223,245,249,252	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 C:

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



6.4 Ligands

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	PO4	E	602	5/5	0.55	1.18	200,217,247,384	0
7	PO4	E	601	5/5	0.60	1.21	182,193,231,344	0

6.5 Other polymers

There are no such residues in this entry.