



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2022 – 12:16 pm GMT

PDB ID : 7QNW
Title : The receptor binding domain of SARS-CoV-2 Omicron variant spike glycoprotein in complex with Beta-55 and EY6A Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-12-23
Resolution : 2.40 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

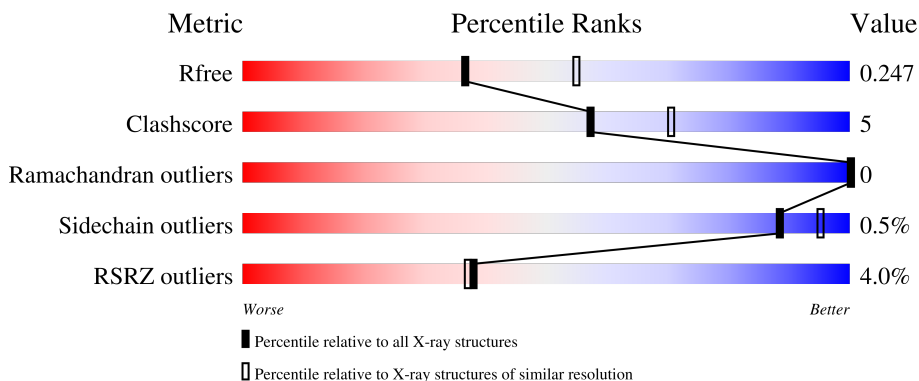
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



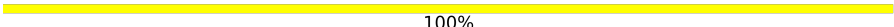
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	L	215	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
3	E	202	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
4	A	232	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>
5	B	215	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
6	C	2	 100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 8326 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 Surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	188	1513	974	255	276	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP A0A7U3CI26
E	328	HIS	-	expression tag	UNP A0A7U3CI26
E	329	HIS	-	expression tag	UNP A0A7U3CI26
E	330	HIS	-	expression tag	UNP A0A7U3CI26
E	331	HIS	-	expression tag	UNP A0A7U3CI26
E	332	HIS	-	expression tag	UNP A0A7U3CI26
E	339	ASP	GLY	variant	UNP A0A7U3CI26
E	371	LEU	SER	variant	UNP A0A7U3CI26
E	373	PRO	SER	variant	UNP A0A7U3CI26
E	375	PHE	SER	variant	UNP A0A7U3CI26
E	440	LYS	ASN	conflict	UNP A0A7U3CI26
E	446	SER	GLY	variant	UNP A0A7U3CI26
E	477	ASN	SER	conflict	UNP A0A7U3CI26
E	478	LYS	THR	variant	UNP A0A7U3CI26

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Chain	Residue	Modelled	Actual	Comment	Reference
E	484	ALA	LYS	conflict	UNP A0A7U3CI26
E	493	ARG	GLN	conflict	UNP A0A7U3CI26
E	496	SER	GLY	conflict	UNP A0A7U3CI26
E	498	ARG	GLN	variant	UNP A0A7U3CI26
E	505	HIS	TYR	conflict	UNP A0A7U3CI26
E	527	LYS	PRO	variant	UNP A0A7U3CI26

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

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

- Molecule 5 is a protein called Beta-55 light chain.

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0

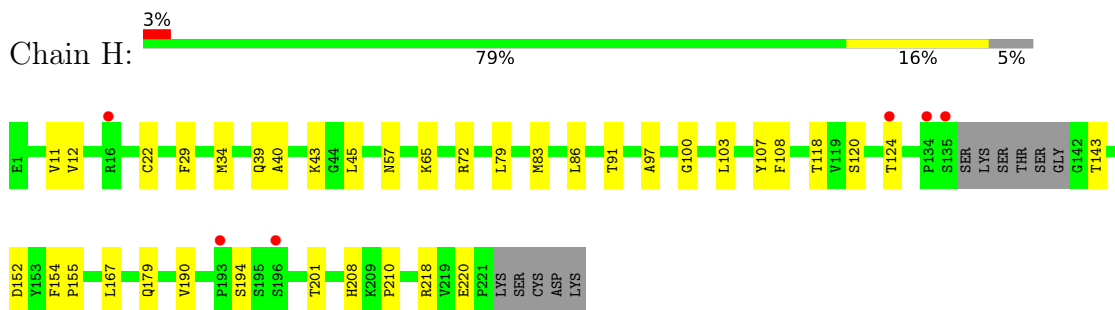
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	11	Total O 11 11	0	0
10	L	13	Total O 13 13	0	0
10	E	26	Total O 26 26	0	0
10	A	29	Total O 29 29	0	0
10	B	23	Total O 23 23	0	0

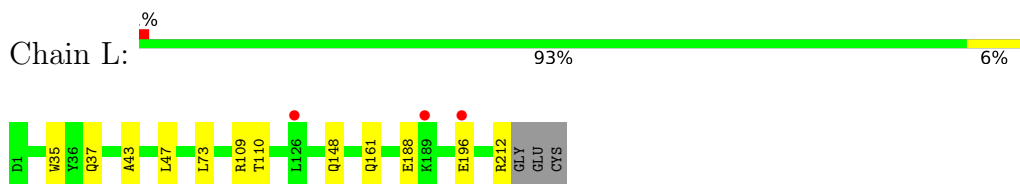
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

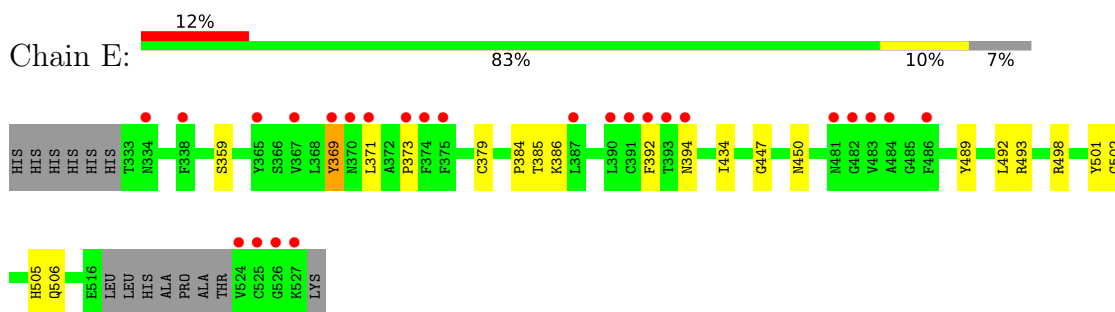
- Molecule 1: EY6A heavy chain



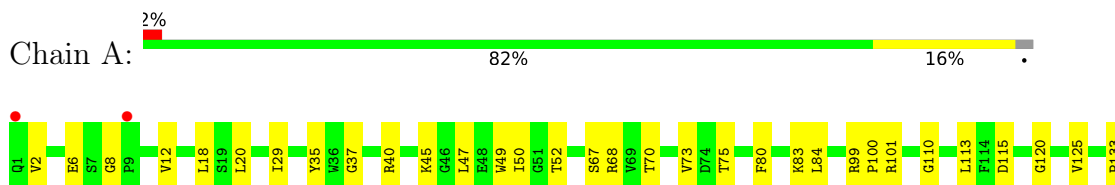
- Molecule 2: EY6A light chain



- Molecule 3: Surface glycoprotein

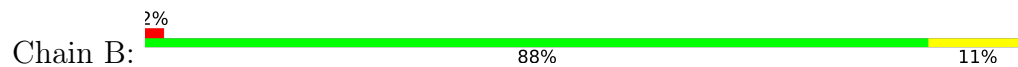


- Molecule 4: Beta-55 heavy chain





- Molecule 5: Beta-55 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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.97Å 131.97Å 117.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.29 – 2.40 114.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (114.29-2.40) 99.9 (114.29-2.40)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.40Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.206 , 0.247 0.205 , 0.247	Depositor DCC
R_{free} test set	2278 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtrriage
Anisotropy	0.168	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8326	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, ACT, 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	0.25	0/1679	0.49	0/2288
2	L	0.25	0/1651	0.48	0/2241
3	E	0.25	0/1556	0.48	0/2114
4	A	0.25	0/1768	0.49	0/2419
5	B	0.25	0/1682	0.49	0/2284
All	All	0.25	0/8336	0.49	0/11346

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 [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	H	1637	0	1591	23	0
2	L	1618	0	1582	6	0
3	E	1513	0	1434	13	0
4	A	1720	0	1684	27	0
5	B	1645	0	1608	17	0
6	C	28	0	25	1	0
7	A	24	0	32	2	0
7	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	6	0	8	0	0
7	L	18	0	24	1	0
8	A	4	0	3	0	0
8	E	4	0	3	1	0
9	A	1	0	0	1	0
10	A	29	0	0	3	0
10	B	23	0	0	5	0
10	E	26	0	0	1	0
10	H	11	0	0	0	0
10	L	13	0	0	0	0
All	All	8326	0	8002	80	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 (80) 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:E:450:ASN:OD1	10:E:901:HOH:O	1.94	0.83
5:B:2:ILE:O	10:B:501:HOH:O	2.01	0.78
4:A:49:TRP:HE1	4:A:52:THR:HG23	1.54	0.72
5:B:97:TRP:O	10:B:501:HOH:O	2.10	0.68
4:A:206:GLN:OE1	10:A:401:HOH:O	2.11	0.68
2:L:43:ALA:O	7:L:302:GOL:O3	2.15	0.65
4:A:35:TYR:HB2	4:A:100:PRO:HG2	1.77	0.65
5:B:67:SER:O	10:B:503:HOH:O	2.14	0.65
5:B:74:THR:OG1	10:B:502:HOH:O	2.13	0.65
2:L:109:ARG:NH1	2:L:110:THR:O	2.32	0.62
9:A:306:CL:CL	5:B:98:THR:HG22	2.40	0.58
1:H:103:LEU:O	3:E:386:LYS:NZ	2.37	0.56
3:E:492:LEU:O	3:E:493:ARG:NH1	2.34	0.56
4:A:113:LEU:HD23	5:B:91:TYR:CE1	2.40	0.56
4:A:182:ALA:H	7:A:302:GOL:H32	1.72	0.55
1:H:11:VAL:HG21	1:H:155:PRO:HG3	1.88	0.55
1:H:29:PHE:O	1:H:72:ARG:NH2	2.41	0.54
1:H:124:THR:HG22	1:H:155:PRO:HD3	1.90	0.54
1:H:100:GLY:HA3	1:H:107:TYR:CZ	2.43	0.53
4:A:47:LEU:O	10:A:403:HOH:O	2.19	0.53
1:H:218:ARG:NH1	1:H:220:GLU:OE1	2.43	0.52
4:A:73:VAL:HG22	4:A:80:PHE:HB3	1.93	0.51
4:A:67:SER:HA	10:A:404:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:LEU:HD21	1:H:190:VAL:HG21	1.95	0.48
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.95	0.48
4:A:40:ARG:HB3	4:A:50:ILE:HD11	1.95	0.48
4:A:70:THR:HB	4:A:83:LYS:HB2	1.95	0.48
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.94	0.48
1:H:201:THR:HG23	1:H:218:ARG:HE	1.78	0.48
4:A:101:ARG:HB2	4:A:115:ASP:HB3	1.95	0.47
1:H:97:ALA:HB1	1:H:108:PHE:HB3	1.96	0.47
5:B:40:PRO:HB3	5:B:166:GLU:HG3	1.95	0.47
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.97	0.47
1:H:91:THR:HG23	1:H:118:THR:HA	1.96	0.46
4:A:8:GLY:HA3	4:A:20:LEU:HD23	1.96	0.46
4:A:49:TRP:NE1	4:A:52:THR:HG23	2.27	0.46
4:A:133:PRO:HB3	4:A:159:TYR:HB3	1.96	0.46
1:H:152:ASP:OD1	1:H:179:GLN:NE2	2.48	0.46
4:A:157:LYS:NZ	4:A:185:GLN:OE1	2.48	0.46
3:E:489:TYR:HD1	8:E:802:ACT:H1	1.81	0.46
5:B:121:PRO:HD3	5:B:133:VAL:HG22	1.96	0.46
5:B:37:GLN:HB2	5:B:47:LEU:HD11	1.97	0.46
4:A:113:LEU:HD21	5:B:49:TYR:HB2	1.98	0.45
3:E:369:TYR:CE1	3:E:434:ILE:HD11	2.52	0.45
3:E:379:CYS:SG	3:E:384:PRO:HG3	2.56	0.45
4:A:37:GLY:HA3	4:A:52:THR:HG22	1.98	0.45
1:H:65:LYS:HE2	3:E:373:PRO:HA	1.99	0.45
2:L:148:GLN:HB3	2:L:196:GLU:HB3	1.99	0.45
4:A:113:LEU:HD23	5:B:91:TYR:CZ	2.51	0.44
6:C:1:NAG:H62	6:C:2:NAG:C7	2.48	0.44
4:A:75:THR:OG1	7:A:304:GOL:O2	2.35	0.43
1:H:208:HIS:CD2	1:H:210:PRO:HD2	2.53	0.43
1:H:143:THR:HA	1:H:194:SER:HB2	2.01	0.43
3:E:498:ARG:HD2	4:A:110:GLY:HA2	2.00	0.43
3:E:502:GLY:O	3:E:506:GLN:HG3	2.18	0.43
4:A:6:GLU:CD	4:A:120:GLY:H	2.22	0.43
4:A:18:LEU:HB3	4:A:84:LEU:HB3	2.00	0.43
1:H:39:GLN:HB2	1:H:45:LEU:HD23	2.01	0.43
1:H:40:ALA:HB3	1:H:43:LYS:HB2	2.01	0.43
4:A:99:ARG:NH1	4:A:115:ASP:OD2	2.51	0.43
5:B:108:LYS:NZ	10:B:506:HOH:O	2.49	0.42
1:H:120:SER:HB3	1:H:154:PHE:CZ	2.54	0.42
1:H:154:PHE:HA	1:H:155:PRO:HA	1.86	0.42
4:A:12:VAL:O	4:A:125:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:359:SER:HB3	3:E:394:ASN:OD1	2.20	0.42
4:A:101:ARG:HD3	4:A:113:LEU:HD11	2.02	0.42
4:A:45:LYS:HD3	4:A:45:LYS:HA	1.73	0.41
1:H:57:ASN:HB2	3:E:385:THR:HG22	2.03	0.41
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.55	0.41
3:E:501:TYR:HB3	3:E:505:HIS:HB2	2.02	0.41
5:B:187:TYR:CE2	5:B:212:ARG:HD3	2.56	0.41
5:B:20:THR:HG23	5:B:72:THR:HG23	2.03	0.41
5:B:35:TRP:CE2	5:B:73:LEU:HB2	2.56	0.40
5:B:185:ALA:O	5:B:189:LYS:HG3	2.21	0.40
2:L:188:GLU:HG3	2:L:212:ARG:NH1	2.36	0.40
3:E:447:GLY:HA2	3:E:498:ARG:HG3	2.04	0.40
5:B:1:ALA:HB2	5:B:96:PRO:HG2	2.03	0.40
1:H:12:VAL:HG11	1:H:86:LEU:HD13	2.04	0.40
1:H:34:MET:HB3	1:H:79:LEU:HD22	2.02	0.40
4:A:2:VAL:HG22	4:A:29:ILE:HD13	2.04	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%)	201 (95%)	10 (5%)	0	100	100
2	L	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
3	E	184/202 (91%)	175 (95%)	9 (5%)	0	100	100
4	A	226/232 (97%)	220 (97%)	6 (3%)	0	100	100
5	B	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	1043/1090 (96%)	1003 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	H	181/191 (95%)	181 (100%)	0	100	100
2	L	186/188 (99%)	185 (100%)	1 (0%)	88	95
3	E	164/177 (93%)	161 (98%)	3 (2%)	59	76
4	A	197/202 (98%)	196 (100%)	1 (0%)	88	95
5	B	186/187 (100%)	186 (100%)	0	100	100
All	All	914/945 (97%)	909 (100%)	5 (0%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	161	GLN
3	E	369	TYR
3	E	371	LEU
3	E	392	PHE
4	A	68	ARG

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	6,3	14,14,15	0.49	0	17,19,21	0.46	0
6	NAG	C	2	6	14,14,15	0.25	0	17,19,21	0.56	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	6,3	-	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.

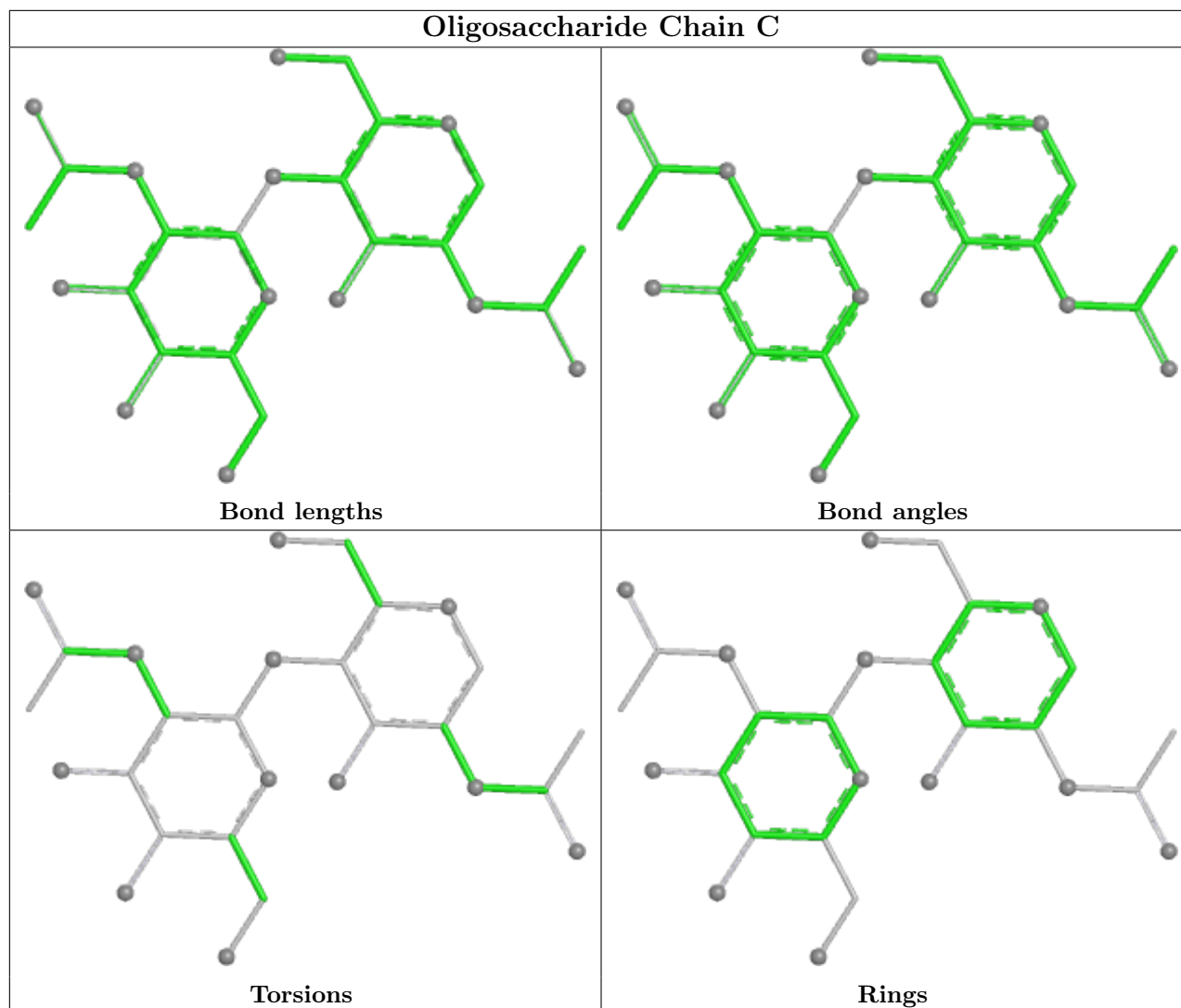
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

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



5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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	GOL	E	801	-	5,5,5	0.89	0	5,5,5	1.03	0
7	GOL	A	302	-	5,5,5	0.83	0	5,5,5	1.10	0
7	GOL	B	401	-	5,5,5	0.86	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACT	E	802	-	1,3,3	6.15	1 (100%)	0,3,3	-	-
7	GOL	L	301	-	5,5,5	0.89	0	5,5,5	1.01	0
7	GOL	L	303	-	5,5,5	0.87	0	5,5,5	1.11	0
7	GOL	A	301	-	5,5,5	0.91	0	5,5,5	1.03	0
7	GOL	A	304	-	5,5,5	0.92	0	5,5,5	1.15	0
8	ACT	A	305	-	1,3,3	6.39	1 (100%)	0,3,3	-	-
7	GOL	A	303	-	5,5,5	0.97	0	5,5,5	1.07	0
7	GOL	L	302	-	5,5,5	0.93	0	5,5,5	1.02	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	GOL	E	801	-	-	3/4/4/4	-
7	GOL	A	302	-	-	2/4/4/4	-
7	GOL	B	401	-	-	2/4/4/4	-
7	GOL	L	301	-	-	0/4/4/4	-
7	GOL	L	303	-	-	1/4/4/4	-
7	GOL	A	301	-	-	2/4/4/4	-
7	GOL	A	304	-	-	2/4/4/4	-
7	GOL	A	303	-	-	0/4/4/4	-
7	GOL	L	302	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	305	ACT	CH3-C	6.39	1.56	1.48
8	E	802	ACT	CH3-C	6.15	1.56	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	801	GOL	C1-C2-C3-O3
7	A	302	GOL	C1-C2-C3-O3
7	A	304	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	B	401	GOL	O1-C1-C2-C3
7	E	801	GOL	O2-C2-C3-O3
7	A	301	GOL	C1-C2-C3-O3
7	A	302	GOL	O2-C2-C3-O3
7	A	304	GOL	O1-C1-C2-O2
7	B	401	GOL	O1-C1-C2-O2
7	A	301	GOL	O2-C2-C3-O3
7	E	801	GOL	O1-C1-C2-C3
7	L	303	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	302	GOL	1	0
8	E	802	ACT	1	0
7	A	304	GOL	1	0
7	L	302	GOL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	H	215/226 (95%)	0.27	6 (2%) 53 51	49, 70, 98, 110	0
2	L	212/215 (98%)	0.12	3 (1%) 75 73	44, 58, 86, 101	0
3	E	188/202 (93%)	0.84	25 (13%) 3 3	43, 62, 117, 142	0
4	A	228/232 (98%)	0.11	4 (1%) 68 66	43, 57, 85, 112	0
5	B	214/215 (99%)	0.14	4 (1%) 66 64	41, 60, 91, 104	0
All	All	1057/1090 (96%)	0.28	42 (3%) 38 37	41, 61, 99, 142	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	482	GLY	10.4
3	E	393	THR	9.3
3	E	486	PHE	8.5
3	E	392	PHE	8.1
3	E	525	CYS	7.8
3	E	481	ASN	7.6
3	E	369	TYR	7.5
3	E	391	CYS	7.5
3	E	484	ALA	5.2
3	E	374	PHE	4.5
3	E	365	TYR	4.4
3	E	390	LEU	4.1
3	E	526	GLY	4.0
3	E	394	ASN	4.0
1	H	193	PRO	3.6
5	B	191	LYS	3.2
4	A	228	LYS	2.9
1	H	16	ARG	2.9
3	E	367	VAL	2.8
3	E	334	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	373	PRO	2.8
3	E	371	LEU	2.8
4	A	1	GLN	2.7
1	H	124	THR	2.6
3	E	338	PHE	2.6
2	L	189	LYS	2.6
1	H	134	PRO	2.5
5	B	204	SER	2.5
4	A	145	THR	2.4
1	H	135	SER	2.4
5	B	77	SER	2.3
3	E	524	VAL	2.2
5	B	3	ARG	2.2
4	A	9	PRO	2.1
3	E	387	LEU	2.1
3	E	370	ASN	2.1
3	E	375	PHE	2.1
2	L	126	LEU	2.1
3	E	483	VAL	2.1
3	E	527	LYS	2.1
2	L	196	GLU	2.0
1	H	196	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

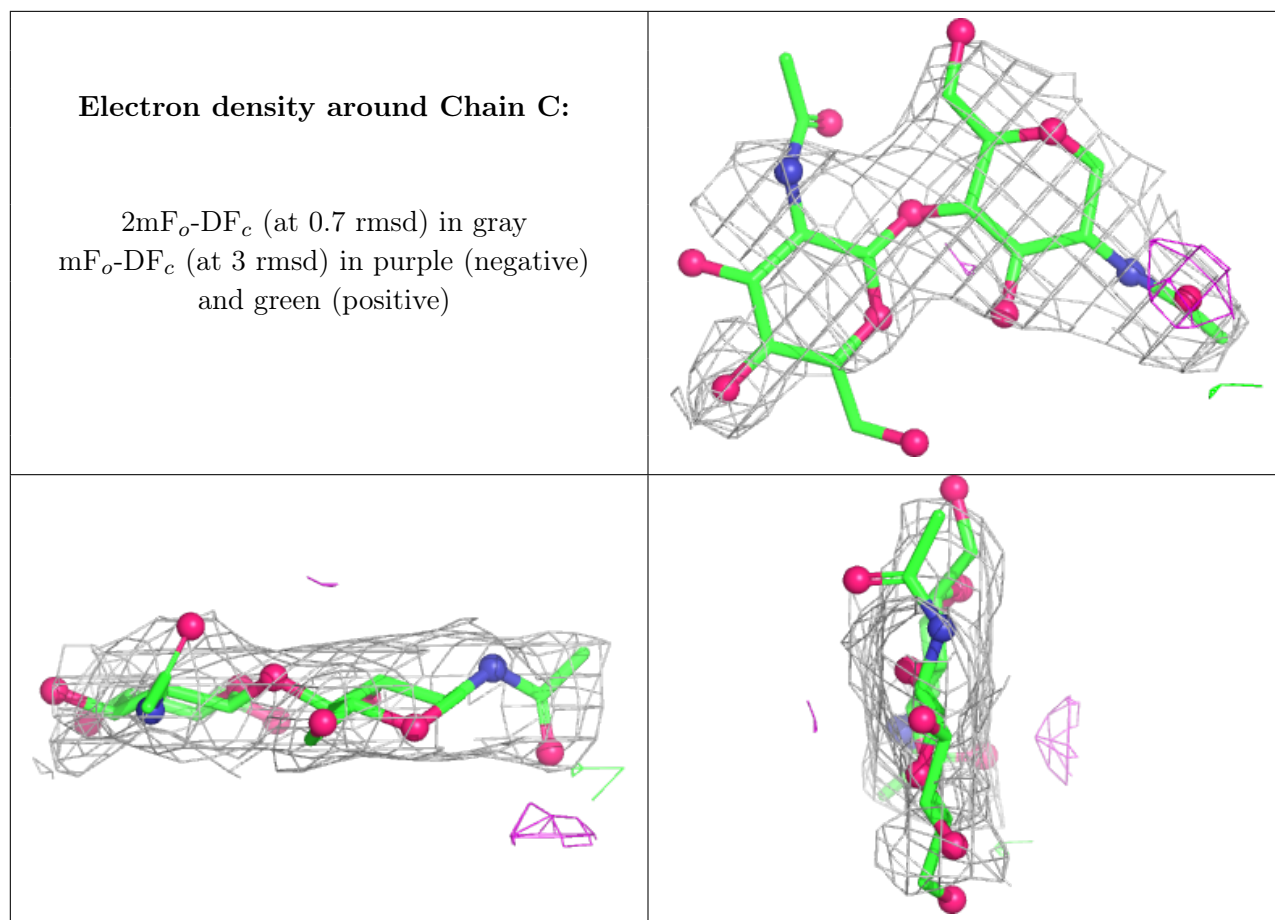
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
6	NAG	C	2	14/15	0.80	0.41	118,126,132,137	0
6	NAG	C	1	14/15	0.89	0.12	82,99,113,120	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 [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
7	GOL	A	303	6/6	0.75	0.16	65,71,74,77	0
9	CL	A	306	1/1	0.79	0.14	75,75,75,75	0
7	GOL	A	301	6/6	0.83	0.16	57,68,73,76	0
7	GOL	A	302	6/6	0.85	0.24	60,66,77,78	0
7	GOL	L	302	6/6	0.86	0.22	56,77,79,95	0
7	GOL	L	301	6/6	0.87	0.13	62,67,71,74	0
7	GOL	E	801	6/6	0.88	0.23	56,63,67,71	0
7	GOL	A	304	6/6	0.90	0.23	77,78,85,91	0
7	GOL	L	303	6/6	0.90	0.28	59,74,78,84	0
8	ACT	A	305	4/4	0.92	0.12	72,76,78,79	0
7	GOL	B	401	6/6	0.93	0.20	56,61,68,70	0
8	ACT	E	802	4/4	0.93	0.47	87,96,108,108	4

6.5 Other polymers [i](#)

There are no such residues in this entry.