



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:24 AM UTC

PDB ID : 7ZFC / pdb_00007zfc
Title : SARS-CoV-2 Beta RBD in complex with nanobody C1, Omi-18 and Omi-31 Fabs
Authors : Zhou, D.; Huo, J.; Ren, J.; Stuart, D.I.
Deposited on : 2022-04-01
Resolution : 3.24 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

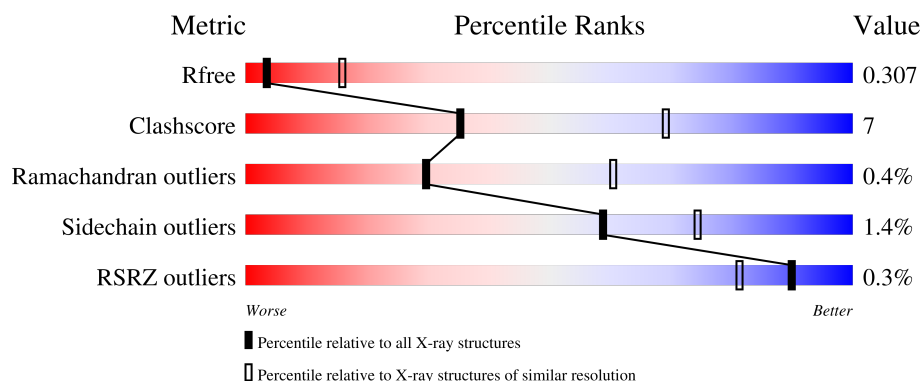
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 $\leq 5\%$. 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	233	
2	L	216	
3	M	131	
4	A	222	
5	B	213	

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Mol	Chain	Length	Quality of chain
6	E	202	 72% 23% .
7	C	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8954 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 Omi-31 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	228	Total	C	N	O	S	0	0	0
			1704	1075	288	334	7			

- Molecule 2 is a protein called Omi-31 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	1	0
			1578	981	267	326	4			

- Molecule 3 is a protein called Nanobody C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	124	Total	C	N	O	S	0	2	0
			973	612	167	190	4			

- Molecule 4 is a protein called Omi-18 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	215	Total	C	N	O	S	0	0	0
			1586	1000	268	311	7			

- Molecule 5 is a protein called Omi-18 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	207	Total	C	N	O	S	0	0	0
			1557	968	267	318	4			

- Molecule 6 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	193	Total	C	N	O	S	0	0	0
			1532	984	255	286	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

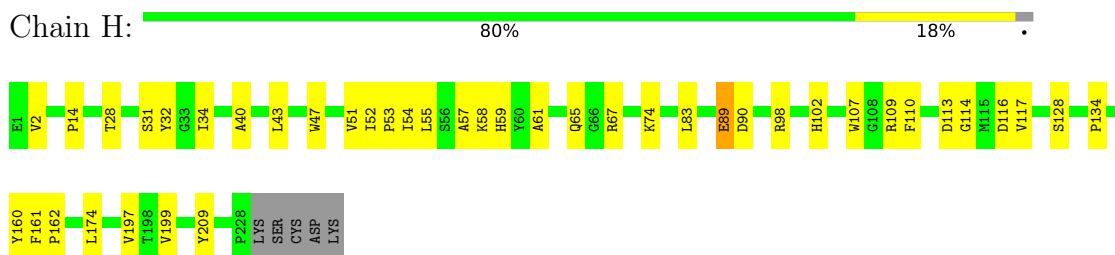


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

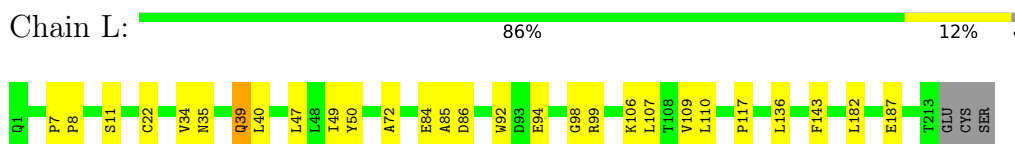
3 Residue-property plots

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.

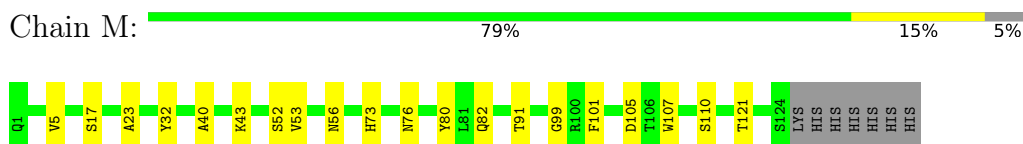
- Molecule 1: Omi-31 heavy chain



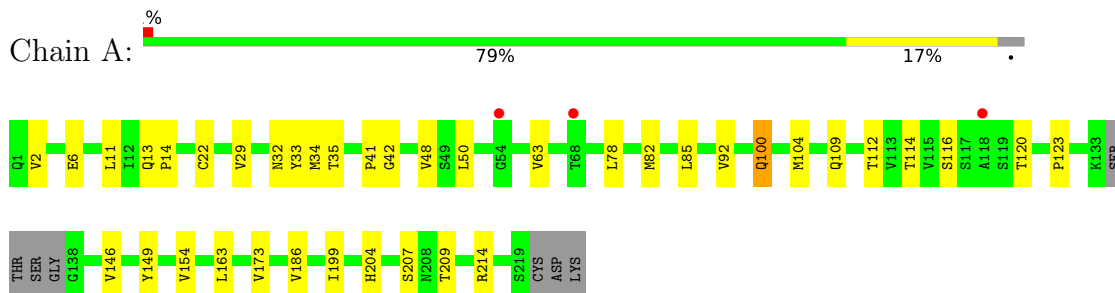
- Molecule 2: Omi-31 light chain



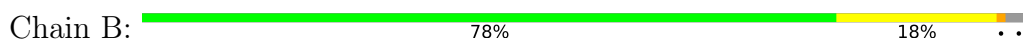
- Molecule 3: Nanobody C1

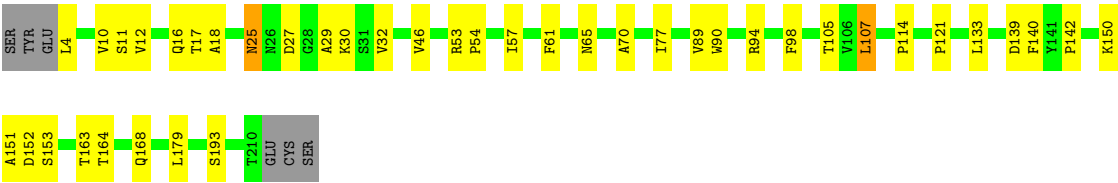


- Molecule 4: Omi-18 heavy chain

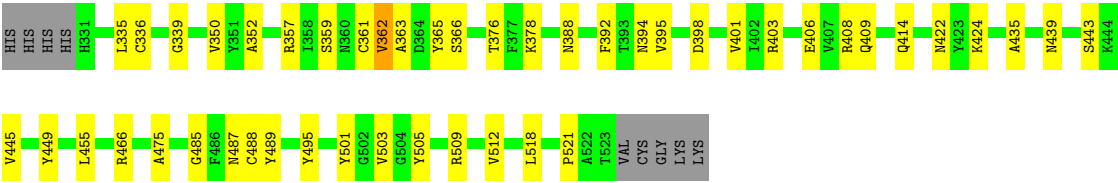


- Molecule 5: Omi-18 light chain





• Molecule 6: Spike protein S1



• Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.00Å 105.00Å 234.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.78 – 3.24 84.78 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.6 (84.78-3.24) 99.9 (84.78-3.24)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.244 , 0.299 0.252 , 0.307	Depositor DCC
R_{free} test set	1206 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	125.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 117.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8954	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	0.10	0/1746	0.26	0/2378
2	L	0.09	0/1618	0.33	0/2212
3	M	0.08	0/1004	0.24	0/1366
4	A	0.08	0/1620	0.26	0/2209
5	B	0.13	0/1596	0.31	0/2185
6	E	0.10	0/1576	0.26	0/2146
All	All	0.10	0/9160	0.28	0/12496

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	1704	0	1671	27	0
2	L	1578	0	1529	18	0
3	M	973	0	922	13	0
4	A	1586	0	1563	23	0
5	B	1557	0	1494	32	0
6	E	1532	0	1444	34	0
7	C	24	0	22	2	0
All	All	8954	0	8645	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (130) 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:L:35:ASN:HD21	2:L:99:ARG:HH12	1.23	0.83
1:H:109:ARG:NH1	2:L:94:GLU:OE2	2.15	0.78
6:E:365:TYR:H	6:E:388:ASN:HD21	1.32	0.76
4:A:199:ILE:HG12	4:A:214:ARG:HG2	1.72	0.71
4:A:29:VAL:HG13	4:A:34:MET:HG3	1.72	0.71
5:B:90:TRP:HA	5:B:90:TRP:CE3	2.25	0.71
5:B:25:ASN:N	5:B:25:ASN:OD1	2.20	0.70
6:E:475:ALA:HB3	6:E:487:ASN:HB3	1.74	0.69
5:B:4:LEU:HD11	5:B:89:VAL:HG13	1.73	0.69
2:L:35:ASN:HD21	2:L:99:ARG:NH1	1.92	0.67
4:A:173:VAL:HG12	5:B:163:THR:HG23	1.77	0.66
4:A:82:MET:HB3	4:A:85:LEU:HD21	1.80	0.64
4:A:123:PRO:HB3	4:A:149:TYR:HB3	1.80	0.63
4:A:92:VAL:HG22	4:A:112:THR:HG22	1.80	0.62
2:L:11:SER:HB2	2:L:110:LEU:HD11	1.81	0.62
2:L:84:GLU:HB2	2:L:109:VAL:HG23	1.82	0.61
5:B:94:ARG:HH21	6:E:409:GLN:HG3	1.65	0.61
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.83	0.61
5:B:90:TRP:HA	5:B:90:TRP:HE3	1.65	0.60
4:A:163:LEU:HD21	4:A:186:VAL:HG21	1.83	0.60
1:H:2:VAL:HG23	1:H:117:VAL:HG11	1.84	0.59
3:M:110:SER:HB3	6:E:378:LYS:NZ	2.17	0.59
1:H:57:ALA:HB1	6:E:449:TYR:HB3	1.83	0.59
5:B:139:ASP:OD1	5:B:168:GLN:NE2	2.37	0.58
5:B:133:LEU:HD12	5:B:179:LEU:HD23	1.86	0.57
5:B:11:SER:HB3	5:B:107:LEU:HD21	1.86	0.57
5:B:94:ARG:NH2	6:E:409:GLN:HG3	2.18	0.57
6:E:406:GLU:OE1	6:E:495:TYR:OH	2.19	0.57
7:C:1:NAG:H4	7:C:2:FUC:H5	1.85	0.56
3:M:110:SER:HB3	6:E:378:LYS:HZ2	1.69	0.56
4:A:48:VAL:HG13	4:A:63:VAL:HG21	1.86	0.56
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.35	0.56
3:M:105:ASP:HB2	6:E:378:LYS:HE3	1.87	0.56
5:B:12:VAL:HG21	5:B:18:ALA:HB2	1.87	0.55
6:E:365:TYR:H	6:E:388:ASN:ND2	2.02	0.55
4:A:22:CYS:HB3	4:A:78:LEU:HB3	1.89	0.55
6:E:485:GLY:H	6:E:488:CYS:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:54:PRO:HG2	5:B:57:ILE:HD12	1.89	0.54
3:M:17[B]:SER:OG	3:M:82:GLN:NE2	2.40	0.54
6:E:339:GLY:HA2	7:C:1:NAG:O7	2.06	0.54
2:L:40:LEU:HD23	2:L:85:ALA:HB2	1.90	0.53
4:A:6:GLU:H	4:A:109:GLN:HE22	1.57	0.53
6:E:350:VAL:HG22	6:E:422:ASN:HB3	1.90	0.52
5:B:16:GLN:HG2	5:B:17:THR:H	1.75	0.52
2:L:86:ASP:OD1	2:L:106:LYS:HG2	2.10	0.51
4:A:35:THR:HG22	4:A:50:LEU:HB3	1.93	0.51
6:E:336:CYS:HB2	6:E:363:ALA:HB2	1.93	0.51
5:B:53:ARG:HD3	5:B:61:PHE:O	2.10	0.51
1:H:174:LEU:HD21	1:H:197:VAL:HG21	1.91	0.51
6:E:357:ARG:NH2	6:E:394:ASN:OD1	2.44	0.50
4:A:34:MET:HB3	4:A:78:LEU:HD22	1.92	0.50
5:B:105:THR:HG21	5:B:142:PRO:HB3	1.93	0.50
1:H:31:SER:H	1:H:54:ILE:HG21	1.76	0.50
1:H:28:THR:O	1:H:32:TYR:HB2	2.11	0.50
4:A:32:ASN:HD21	6:E:475:ALA:HB1	1.77	0.50
6:E:366:SER:OG	6:E:388:ASN:OD1	2.27	0.50
1:H:102:HIS:HB2	1:H:113:ASP:HB2	1.92	0.49
3:M:91:THR:HG23	3:M:121:THR:HA	1.95	0.49
4:A:104:MET:HE1	5:B:98:PHE:HZ	1.78	0.48
1:H:47:TRP:HE3	1:H:61:ALA:HB2	1.78	0.48
1:H:53:PRO:HB3	1:H:74:LYS:HE2	1.95	0.48
2:L:47:LEU:HD21	2:L:50:TYR:HB3	1.95	0.48
5:B:114:PRO:HB3	5:B:140:PHE:HB3	1.95	0.48
4:A:100:GLN:HB3	5:B:90:TRP:CZ2	2.50	0.47
3:M:5:VAL:HB	3:M:23:ALA:HB3	1.96	0.47
5:B:12:VAL:HG12	5:B:16:GLN:HB3	1.96	0.47
2:L:117:PRO:HB3	2:L:143:PHE:HB3	1.97	0.47
2:L:136:LEU:HD12	2:L:182:LEU:HD23	1.97	0.47
1:H:47:TRP:CE3	1:H:61:ALA:HB2	2.51	0.46
1:H:114:GLY:H	2:L:99:ARG:HH22	1.63	0.46
3:M:73:HIS:HB3	3:M:76:ASN:OD1	2.15	0.46
4:A:204:HIS:HB3	4:A:209:THR:HB	1.97	0.46
6:E:403:ARG:HG2	6:E:505:TYR:HA	1.96	0.46
1:H:89:GLU:OE1	1:H:89:GLU:N	2.48	0.46
4:A:42:GLY:HA3	5:B:164:THR:HG21	1.96	0.46
4:A:146:VAL:HG11	4:A:154:VAL:HG21	1.97	0.46
6:E:365:TYR:N	6:E:388:ASN:HD21	2.08	0.46
6:E:439:ASN:O	6:E:443:SER:OG	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:120:THR:HG22	4:A:207:SER:HB3	1.98	0.46
5:B:29:ALA:HB2	6:E:501:TYR:CE2	2.50	0.46
5:B:133:LEU:HB2	5:B:179:LEU:HB3	1.98	0.45
5:B:32:VAL:HG21	5:B:70:ALA:HB2	1.98	0.45
5:B:18:ALA:HB2	5:B:77:ILE:HD11	1.97	0.45
2:L:92:TRP:CZ3	2:L:98:GLY:HA2	2.52	0.45
6:E:359:SER:O	6:E:361:CYS:N	2.42	0.45
6:E:376:THR:HB	6:E:435:ALA:HB3	1.98	0.45
1:H:14:PRO:HD2	1:H:128:SER:HA	1.97	0.45
1:H:51:VAL:HG23	1:H:58:LYS:HB3	1.99	0.45
4:A:11:LEU:HA	4:A:114:THR:O	2.17	0.45
2:L:22:CYS:HB3	2:L:72:ALA:HB3	1.98	0.45
3:M:52:SER:O	3:M:56:ASN:N	2.49	0.45
5:B:46:VAL:HA	5:B:57:ILE:HD13	1.99	0.45
5:B:27:ASP:OD1	5:B:65:ASN:ND2	2.46	0.45
6:E:518:LEU:HD21	6:E:521:PRO:HB3	1.97	0.45
4:A:33:TYR:OH	6:E:455:LEU:O	2.27	0.45
6:E:352:ALA:HB1	6:E:466:ARG:HH21	1.82	0.45
6:E:398:ASP:HB2	6:E:512:VAL:HB	1.98	0.44
6:E:392:PHE:CE1	6:E:395:VAL:HG23	2.53	0.44
2:L:187:GLU:OE1	2:L:187:GLU:N	2.51	0.43
3:M:107:TRP:CH2	6:E:503:VAL:HG12	2.54	0.43
3:M:76:ASN:ND2	3:M:80:TYR:OH	2.52	0.43
5:B:151:ALA:O	5:B:153:SER:N	2.52	0.43
5:B:27:ASP:CG	5:B:30:LYS:HZ1	2.26	0.43
1:H:52:ILE:HG22	1:H:55:LEU:H	1.83	0.43
4:A:13:GLN:H	4:A:13:GLN:CD	2.26	0.42
4:A:14:PRO:HD3	4:A:116:SER:O	2.19	0.42
2:L:35:ASN:HB2	2:L:49:ILE:O	2.19	0.42
2:L:39:GLN:O	2:L:85:ALA:HB1	2.19	0.42
1:H:98:ARG:HG2	1:H:117:VAL:HB	2.01	0.42
6:E:401:VAL:HG22	6:E:509:ARG:HG2	2.00	0.42
1:H:161:PHE:HA	1:H:162:PRO:HA	1.85	0.42
3:M:99:GLY:HA3	3:M:101:PHE:CE2	2.54	0.42
1:H:116:ASP:OD1	1:H:116:ASP:N	2.51	0.42
1:H:40:ALA:HB3	1:H:43:LEU:HD12	2.02	0.41
5:B:46:VAL:HA	5:B:57:ILE:CD1	2.50	0.41
1:H:67:ARG:O	1:H:83:LEU:HD12	2.21	0.41
6:E:414:GLN:O	6:E:424:LYS:NZ	2.53	0.41
5:B:150:LYS:HB2	5:B:193:SER:HB2	2.02	0.41
5:B:121:PRO:HD3	5:B:133:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:84:GLU:HG3	2:L:107:LEU:O	2.21	0.41
1:H:31:SER:HA	1:H:54:ILE:HD13	2.03	0.41
1:H:67:ARG:HH22	1:H:90:ASP:CG	2.27	0.41
1:H:57:ALA:HA	6:E:449:TYR:CD2	2.56	0.41
3:M:32:TYR:CE2	3:M:53:VAL:HG21	2.56	0.41
1:H:102:HIS:HB2	1:H:113:ASP:CB	2.51	0.41
5:B:94:ARG:HH22	6:E:408:ARG:CG	2.33	0.40
1:H:199:VAL:HG11	1:H:209:TYR:CE1	2.57	0.40
6:E:335:LEU:HD23	6:E:335:LEU:HA	1.90	0.40
2:L:7:PRO:HA	2:L:8:PRO:HD3	1.97	0.40
3:M:40:ALA:HB3	3:M:43:LYS:HB2	2.03	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	226/233 (97%)	217 (96%)	9 (4%)	0	100	100
2	L	212/216 (98%)	199 (94%)	13 (6%)	0	100	100
3	M	124/131 (95%)	121 (98%)	3 (2%)	0	100	100
4	A	211/222 (95%)	201 (95%)	7 (3%)	3 (1%)	9	35
5	B	205/213 (96%)	190 (93%)	14 (7%)	1 (0%)	24	56
6	E	191/202 (95%)	172 (90%)	18 (9%)	1 (0%)	24	56
All	All	1169/1217 (96%)	1100 (94%)	64 (6%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	152	ASP

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Mol	Chain	Res	Type
4	A	100	GLN
4	A	2	VAL
4	A	41	PRO
6	E	362	VAL

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	190/195 (97%)	184 (97%)	6 (3%)	34	62
2	L	179/182 (98%)	177 (99%)	2 (1%)	65	77
3	M	105/110 (96%)	105 (100%)	0	100	100
4	A	177/185 (96%)	177 (100%)	0	100	100
5	B	175/181 (97%)	172 (98%)	3 (2%)	53	72
6	E	165/175 (94%)	162 (98%)	3 (2%)	51	71
All	All	991/1028 (96%)	977 (99%)	14 (1%)	59	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	34	ILE
1	H	59	HIS
1	H	65	GLN
1	H	89	GLU
1	H	107	TRP
1	H	110	PHE
2	L	34	VAL
2	L	39	GLN
5	B	10	VAL
5	B	25	ASN
5	B	107	LEU
6	E	362	VAL
6	E	445	VAL
6	E	489	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	103	HIS
2	L	35	ASN
2	L	52	ASN
2	L	132	ASN
2	L	198	GLN
3	M	82	GLN
6	E	388	ASN
6	E	448	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	1	6,7	14,14,15	0.45	0	17,19,21	1.10	1 (5%)
7	FUC	C	2	7	10,10,11	0.90	0	14,14,16	1.05	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1	6,7	-	2/6/23/26	0/1/1/1
7	FUC	C	2	7	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1	NAG	C1-O5-C5	4.19	117.80	112.19
7	C	2	FUC	O5-C5-C4	2.52	114.09	109.55

There are no chirality outliers.

All (2) torsion outliers are listed below:

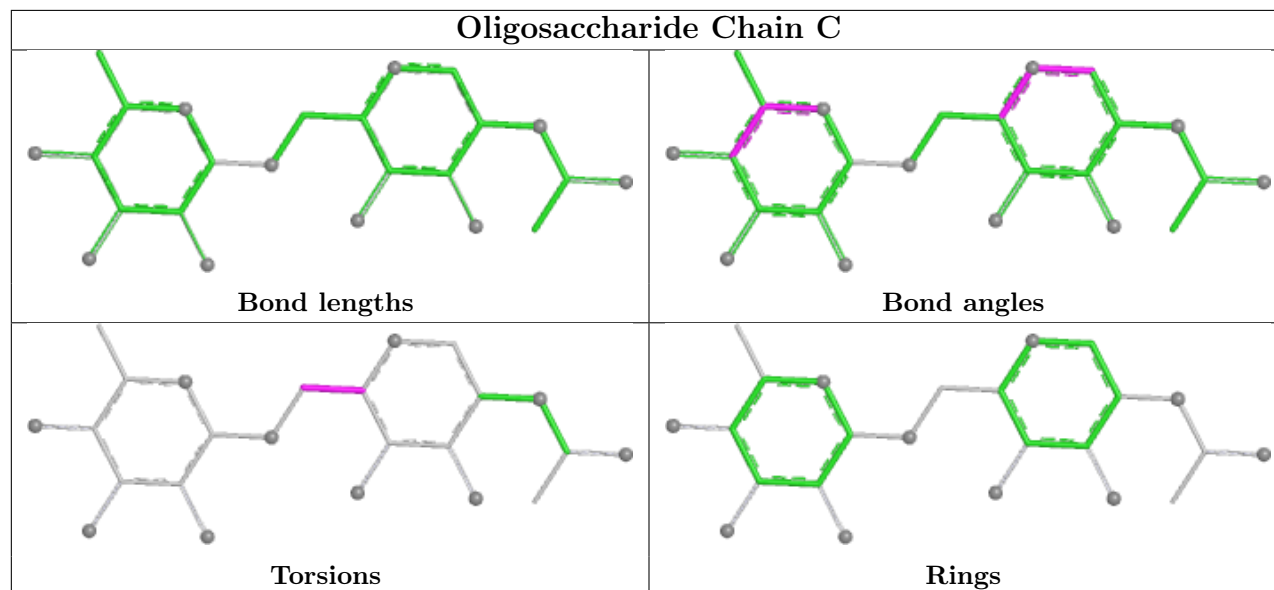
Mol	Chain	Res	Type	Atoms
7	C	1	NAG	C4-C5-C6-O6
7	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	2	FUC	1	0
7	C	1	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.



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 [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	228/233 (97%)	0.00	0	100 100	88, 148, 285, 377	0
2	L	213/216 (98%)	-0.03	0	100 100	89, 147, 266, 321	1 (0%)
3	M	124/131 (94%)	-0.17	0	100 100	102, 132, 176, 201	2 (1%)
4	A	215/222 (96%)	-0.13	3 (1%)	73 54	96, 130, 180, 292	0
5	B	207/213 (97%)	-0.14	0	100 100	98, 137, 187, 262	0
6	E	193/202 (95%)	-0.07	0	100 100	90, 117, 179, 221	0
All	All	1180/1217 (96%)	-0.08	3 (0%)	90 81	88, 134, 250, 377	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	54	GLY	2.7
4	A	68	THR	2.4
4	A	118	ALA	2.2

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.

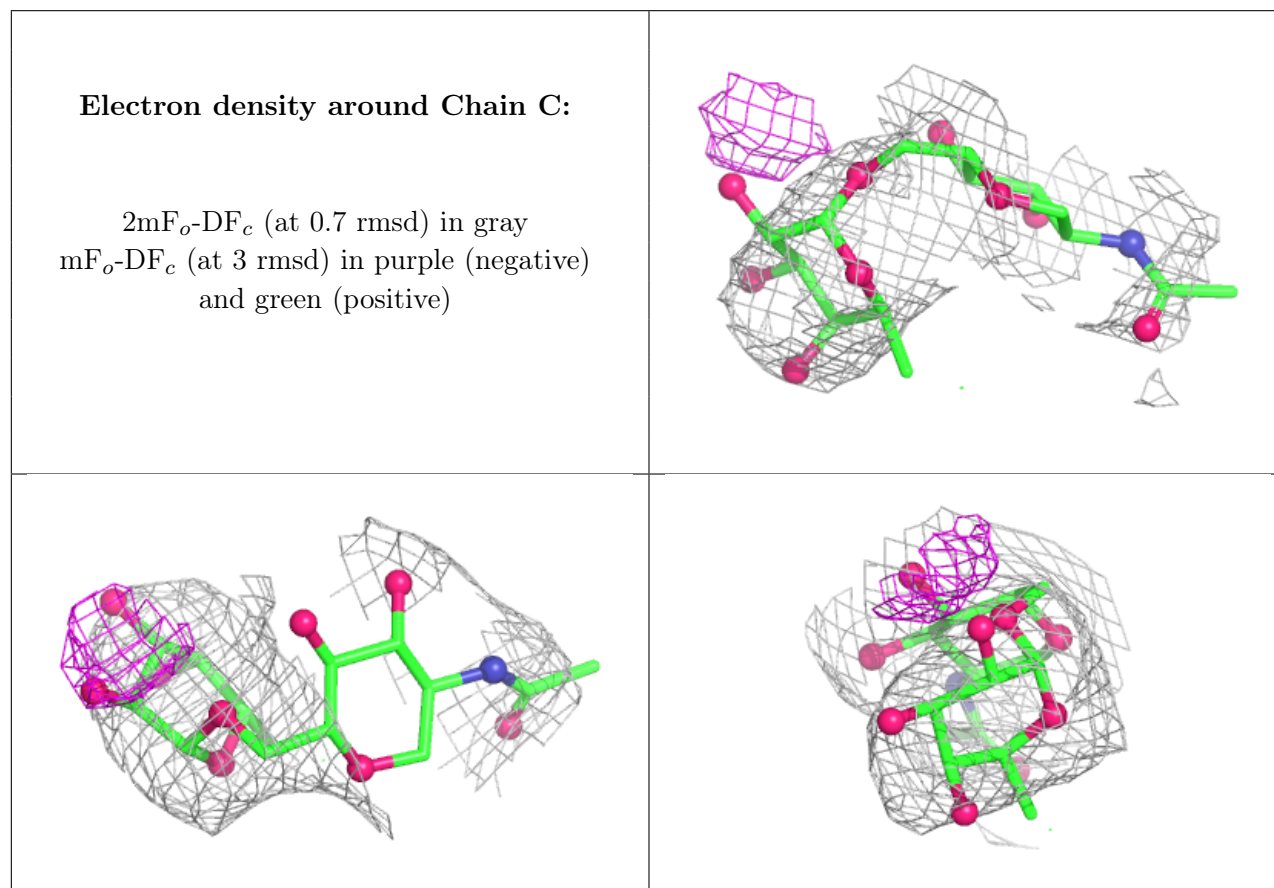
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	1	14/15	-	-	156,191,221,229	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	FUC	C	2	10/11	-	-	215,248,267,293	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.