



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:02 AM UTC

PDB ID : 7MWX / pdb_00007mwx
Title : Structure of the core ectodomain of the hepatitis C virus envelope glycoprotein 2 with tamarin CD81
Authors : Kumar, A.; Hossain, R.A.; Yost, S.A.; Bu, W.; Wang, Y.; Dearborn, A.D.; Grakoui, A.; Cohen, J.I.; Marcotrigiano, J.
Deposited on : 2021-05-17
Resolution : 3.32 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

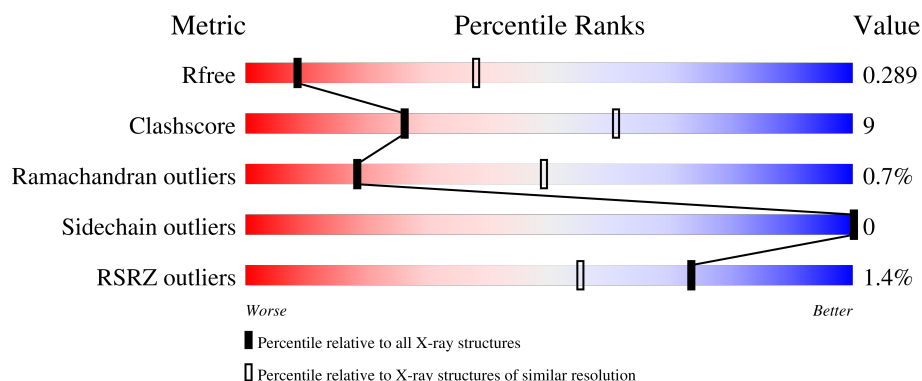
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	C	259	4% 46% 20% • 34%
1	G	259	2% 47% 22% • 31%
2	A	218	91% 9%
2	E	218	82% 17%
3	B	218	90% 10%

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Mol	Chain	Length	Quality of chain
3	F	218	% 88% 12%
4	D	93	60% 27% 13%
4	H	93	% 67% 24% 10%
5	I	3	67% 33%
6	J	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10459 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 Core protein precursor eE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	172	Total	C	N	O	S	0	0	0
			1289	828	214	233	14			
1	G	180	Total	C	N	O	S	0	0	0
			1328	845	222	247	14			

- Molecule 2 is a protein called 2A12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1607	1009	264	329	5			
2	E	218	Total	C	N	O	S	0	0	0
			1628	1020	266	337	5			

- Molecule 3 is a protein called 2A12 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	218	Total	C	N	O	S	0	0	0
			1659	1030	277	344	8			
3	F	218	Total	C	N	O	S	0	0	0
			1676	1040	282	346	8			

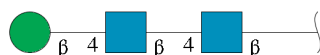
- Molecule 4 is a protein called CD81 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	81	Total	C	N	O	S	0	0	0
			555	338	94	118	5			
4	H	84	Total	C	N	O	S	0	0	0
			608	374	102	127	5			

There are 6 discrepancies between the modelled and reference sequences:

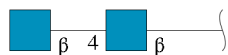
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	THR	-	cloning artifact	UNP Q9N0J9
D	8	GLY	-	cloning artifact	UNP Q9N0J9
D	9	SER	-	cloning artifact	UNP Q9N0J9
H	7	THR	-	cloning artifact	UNP Q9N0J9
H	8	GLY	-	cloning artifact	UNP Q9N0J9
H	9	SER	-	cloning artifact	UNP Q9N0J9

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



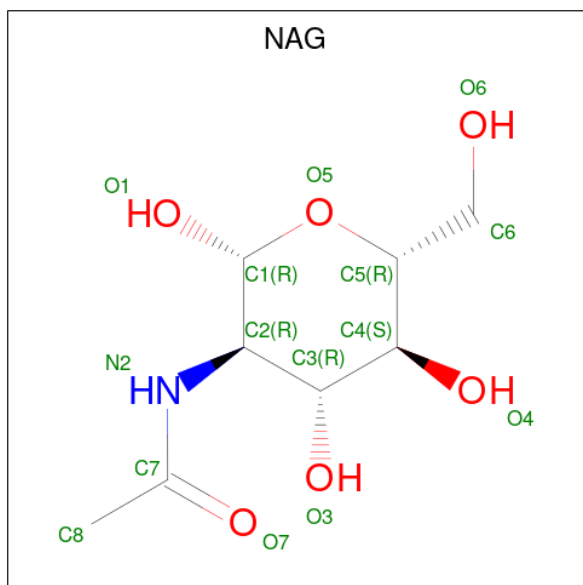
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

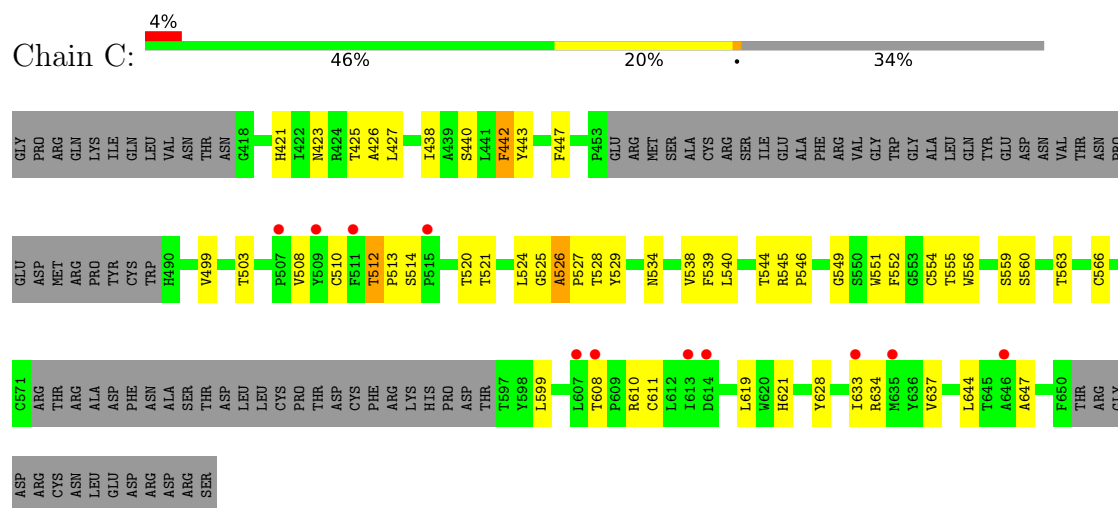


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

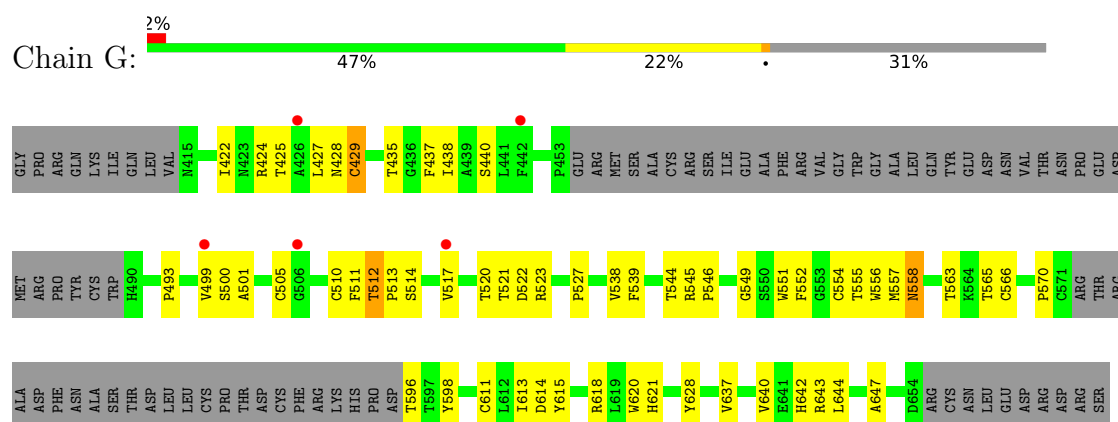
3 Residue-property plots

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

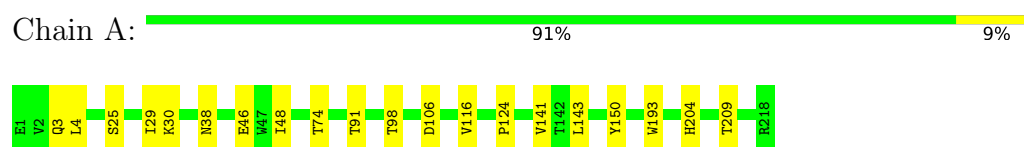
• Molecule 1: Core protein precursor eE2



• Molecule 1: Core protein precursor eE2



• Molecule 2: 2A12 Fab Heavy Chain



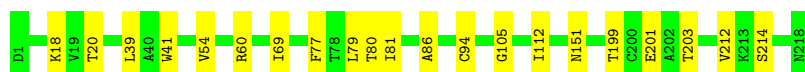
• Molecule 2: 2A12 Fab Heavy Chain

Chain E:  82% 17%



- Molecule 3: 2A12 Fab Light Chain

Chain B:  90% 10%



- Molecule 3: 2A12 Fab Light Chain

Chain F:  88% 12%



- Molecule 4: CD81 protein

Chain D:  60% 27% 13%



- Molecule 4: CD81 protein

Chain H:  67% 24% 10%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  67% 33%



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

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.95Å 127.77Å 212.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.09 – 3.32 53.09 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (53.09-3.32) 99.4 (53.09-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.239 , 0.283 0.244 , 0.289	Depositor DCC
R_{free} test set	1593 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	124.4	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 247.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10459	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: NAG, BMA

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	C	0.19	0/1335	0.54	1/1837 (0.1%)
1	G	0.16	0/1372	0.52	0/1889
2	A	0.09	0/1647	0.29	0/2263
2	E	0.10	0/1668	0.33	0/2288
3	B	0.09	0/1696	0.28	0/2310
3	F	0.09	0/1713	0.29	0/2329
4	D	0.15	0/559	0.46	0/764
4	H	0.14	0/614	0.37	0/834
All	All	0.13	0/10604	0.38	1/14514 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ALA	CB-CA-C	-6.32	107.23	116.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	558	ASN	Peptide

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	C	1289	0	1167	42	0
1	G	1328	0	1189	52	0
2	A	1607	0	1532	12	0
2	E	1628	0	1564	31	0
3	B	1659	0	1543	11	0
3	F	1676	0	1578	15	0
4	D	555	0	495	21	0
4	H	608	0	561	18	0
5	I	39	0	34	2	0
6	J	28	0	25	0	0
7	C	28	0	26	0	0
7	G	14	0	13	0	0
All	All	10459	0	9727	189	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 9.

All (189) 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:E:29:ILE:HD13	2:E:53:PRO:CB	1.93	0.98
1:C:421:HIS:HB3	4:D:80:SER:H	1.31	0.95
1:G:501:ALA:H	1:G:538:VAL:HG22	1.34	0.92
2:A:91:THR:HG22	2:A:116:VAL:H	1.38	0.89
1:G:538:VAL:HG12	1:G:539:PHE:H	1.37	0.88
2:E:29:ILE:HD13	2:E:53:PRO:HB2	1.56	0.84
4:D:29:GLN:HA	4:D:32:VAL:HG22	1.62	0.81
1:C:513:PRO:HG3	1:C:637:VAL:HG21	1.64	0.79
2:E:29:ILE:HD13	2:E:53:PRO:HB3	1.67	0.76
1:G:427:LEU:HD23	1:G:428:ASN:H	1.52	0.75
2:E:11:LEU:HD13	2:E:152:PRO:HG3	1.70	0.74
1:G:521:THR:HG22	1:G:539:PHE:HD2	1.54	0.73
1:C:521:THR:H	1:C:539:PHE:HA	1.52	0.73
1:G:513:PRO:HG2	1:G:637:VAL:HG21	1.73	0.71
1:C:544:THR:HG23	1:C:549:GLY:HA3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:538:VAL:HG12	1:G:539:PHE:N	2.06	0.70
1:C:634:ARG:NH1	2:A:106:ASP:OD2	2.25	0.69
3:F:217:ARG:HH11	3:F:217:ARG:HA	1.57	0.69
1:G:544:THR:HG23	1:G:549:GLY:HA3	1.75	0.69
2:E:91:THR:HG23	2:E:115:THR:HA	1.75	0.69
1:C:438:ILE:HD13	4:D:60:SER:HB2	1.75	0.68
2:E:29:ILE:HD12	2:E:30:LYS:N	2.09	0.68
1:G:440:SER:HB2	1:G:620:TRP:HZ3	1.59	0.67
1:G:501:ALA:HB2	1:G:538:VAL:HA	1.79	0.65
1:G:521:THR:OG1	1:G:522:ASP:N	2.27	0.64
2:A:38:ASN:HB3	2:A:48:ILE:HD11	1.78	0.64
1:G:538:VAL:CG1	1:G:539:PHE:H	2.11	0.64
3:B:201:GLU:HG2	3:B:212:VAL:HG12	1.80	0.63
1:G:521:THR:HA	1:G:539:PHE:HB3	1.78	0.63
2:E:149:GLY:HA2	2:E:179:LEU:HG	1.82	0.62
1:C:512:THR:OG1	1:C:513:PRO:HD2	2.00	0.61
1:C:526:ALA:H	1:C:527:PRO:CD	2.13	0.61
1:G:501:ALA:N	1:G:538:VAL:HG22	2.12	0.61
1:C:520:THR:HA	1:C:539:PHE:HB3	1.83	0.59
1:C:442:PHE:H	4:D:83:PHE:HB2	1.66	0.59
2:E:29:ILE:HD11	2:E:74:THR:HG22	1.85	0.58
1:C:628:TYR:HB3	1:C:647:ALA:HB1	1.87	0.57
4:H:28:LEU:HD21	4:H:66:MET:HE1	1.85	0.57
1:G:551:TRP:NE1	1:G:554:CYS:SG	2.77	0.57
1:C:423:ASN:HB3	4:D:78:ILE:O	2.05	0.57
1:C:608:THR:HG23	1:C:610:ARG:H	1.67	0.57
1:G:555:THR:HG22	1:G:621:HIS:HD2	1.68	0.57
4:D:35:ASP:HB3	4:D:65:SER:OG	2.04	0.57
1:G:425:THR:HG21	1:G:520:THR:HA	1.87	0.57
1:G:521:THR:HG22	1:G:539:PHE:CD2	2.38	0.57
4:H:28:LEU:HD12	4:H:62:LEU:HD13	1.87	0.56
1:G:422:ILE:HB	1:G:517:VAL:HG11	1.86	0.56
1:C:510:CYS:HA	1:C:554:CYS:HA	1.87	0.56
4:H:49:GLU:HG2	4:H:73:PRO:HB3	1.88	0.56
2:E:38:ASN:HB3	2:E:48:ILE:HD11	1.88	0.55
1:C:556:TRP:HZ3	1:C:566:CYS:HB2	1.71	0.55
4:D:63:THR:HA	4:D:66:MET:SD	2.46	0.55
1:G:493:PRO:HB3	1:G:565:THR:HG23	1.89	0.55
2:A:143:LEU:HD11	2:A:193:TRP:CD1	2.42	0.55
1:C:514:SER:HA	1:C:644:LEU:HD21	1.89	0.54
2:A:4:LEU:HD11	2:A:98:THR:HG23	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:546:PRO:HG3	1:G:551:TRP:HA	1.88	0.54
3:F:126:PRO:HD3	3:F:138:VAL:HG22	1.88	0.54
1:G:500:SER:HA	1:G:538:VAL:HG21	1.90	0.54
4:D:66:MET:SD	4:D:66:MET:N	2.64	0.54
5:I:1:NAG:H3	5:I:1:NAG:H83	1.89	0.53
2:A:29:ILE:HD11	2:A:74:THR:HA	1.90	0.53
2:E:29:ILE:CD1	2:E:53:PRO:HB2	2.34	0.52
3:F:116:ASP:OD1	3:F:116:ASP:N	2.43	0.52
1:C:546:PRO:HG3	1:C:551:TRP:HA	1.91	0.52
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.45	0.52
1:G:628:TYR:HB3	1:G:647:ALA:HB1	1.92	0.52
1:G:499:VAL:O	1:G:538:VAL:HG11	2.11	0.51
3:B:54:VAL:HG22	3:B:60:ARG:HA	1.92	0.51
1:G:422:ILE:HD13	1:G:517:VAL:HG11	1.93	0.51
1:G:614:ASP:HA	1:G:618:ARG:HD3	1.92	0.51
1:G:523:ARG:HH22	4:H:68:LYS:NZ	2.10	0.50
1:G:563:THR:HG21	1:G:621:HIS:O	2.11	0.50
4:D:28:LEU:O	4:D:32:VAL:HG13	2.12	0.50
2:E:141:VAL:O	2:E:189:THR:OG1	2.24	0.50
1:C:545:ARG:O	1:C:549:GLY:N	2.44	0.50
1:C:633:ILE:HG22	1:C:634:ARG:H	1.76	0.50
1:G:555:THR:HG22	1:G:621:HIS:CD2	2.46	0.50
1:G:556:TRP:CH2	1:G:566:CYS:HB2	2.47	0.50
3:B:20:THR:HG22	3:B:80:THR:HB	1.94	0.50
1:C:421:HIS:HB3	4:D:80:SER:N	2.13	0.50
4:D:94:LEU:HD12	4:H:46:THR:HG22	1.94	0.50
4:H:32:VAL:HA	4:H:41:LYS:HD2	1.94	0.49
1:C:554:CYS:H	1:C:566:CYS:HB3	1.78	0.49
3:F:151:ASN:HB3	3:F:203:THR:HB	1.94	0.49
1:C:508:VAL:HG13	1:C:556:TRP:HB3	1.94	0.49
1:C:521:THR:N	1:C:538:VAL:O	2.45	0.49
1:C:503:THR:O	1:C:559:SER:HB2	2.12	0.49
2:E:29:ILE:HD12	2:E:29:ILE:C	2.36	0.49
3:B:151:ASN:HB3	3:B:203:THR:HB	1.95	0.49
4:D:34:ASP:CG	4:D:35:ASP:H	2.21	0.48
3:F:54:VAL:HG22	3:F:60:ARG:HA	1.95	0.48
1:G:513:PRO:HB2	1:G:642:HIS:CG	2.49	0.48
4:H:33:VAL:HG22	4:H:41:LYS:HD3	1.95	0.48
2:E:204:HIS:HB3	2:E:209:THR:HB	1.95	0.48
2:A:204:HIS:HB3	2:A:209:THR:HB	1.95	0.48
4:H:26:GLN:O	4:H:30:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:499:VAL:HG12	1:G:500:SER:H	1.79	0.48
3:F:198:TYR:HB2	3:F:215:PHE:CE1	2.49	0.48
3:B:41:TRP:CE2	3:B:79:LEU:HB2	2.50	0.47
4:H:25:ASP:O	4:H:29:GLN:HG2	2.14	0.47
2:A:124:PRO:HB3	2:A:150:TYR:HB3	1.97	0.47
1:G:510:CYS:HA	1:G:554:CYS:HA	1.96	0.47
2:E:143:LEU:HG	2:E:198:ILE:HD11	1.97	0.47
4:D:38:ASN:C	4:D:40:ALA:H	2.23	0.47
4:D:48:HIS:O	4:D:52:ASN:N	2.47	0.47
2:E:176:GLN:OE1	2:E:181:THR:OG1	2.30	0.47
1:G:513:PRO:CG	1:G:637:VAL:HG21	2.44	0.46
1:G:596:THR:HG22	1:G:598:TYR:H	1.80	0.46
3:B:69:ILE:HB	3:B:80:THR:HG23	1.98	0.46
2:A:141:VAL:HG21	2:A:193:TRP:CE3	2.51	0.46
3:F:94:CYS:O	3:F:105:GLY:N	2.49	0.46
1:G:546:PRO:HG2	1:G:552:PHE:CE2	2.51	0.46
1:C:427:LEU:HD11	4:D:64:THR:HB	1.98	0.45
1:G:643:ARG:NH2	2:E:106:ASP:OD1	2.48	0.45
4:H:33:VAL:HG13	4:H:41:LYS:HD3	1.98	0.45
4:H:65:SER:O	4:H:69:ASN:ND2	2.46	0.45
2:A:38:ASN:OD1	2:A:46:GLU:HB3	2.16	0.45
2:E:38:ASN:OD1	2:E:46:GLU:HB3	2.17	0.45
1:C:440:SER:HA	1:C:443:TYR:HB3	1.98	0.45
1:C:524:LEU:HD12	1:C:525:GLY:H	1.81	0.45
4:H:21:LYS:HG3	4:H:88:HIS:NE2	2.32	0.45
4:H:68:LYS:HA	4:H:68:LYS:HD2	1.74	0.45
1:C:528:THR:OG1	1:C:529:TYR:N	2.50	0.45
1:G:511:PHE:C	1:G:551:TRP:HB2	2.41	0.45
1:G:438:ILE:HD11	4:H:61:ALA:HA	1.98	0.45
3:B:199:THR:HG23	3:B:214:SER:HB3	1.99	0.45
2:A:3:GLN:HB3	2:A:25:SER:HB2	1.97	0.45
3:B:86:ALA:HA	3:B:112:ILE:HD13	1.99	0.45
1:G:557:MET:HG3	1:G:558:ASN:N	2.32	0.44
2:E:143:LEU:HD23	2:E:189:THR:HG21	1.98	0.44
2:E:60:TYR:HE1	2:E:70:ILE:HG13	1.81	0.44
3:F:41:TRP:CE2	3:F:79:LEU:HB2	2.52	0.44
4:H:66:MET:HA	4:H:69:ASN:HD21	1.83	0.44
1:C:608:THR:HG22	1:C:611:CYS:HB2	1.99	0.44
1:C:447:PHE:CZ	1:C:619:LEU:HB3	2.54	0.43
1:G:545:ARG:O	1:G:549:GLY:N	2.52	0.43
1:G:437:PHE:CD2	1:G:438:ILE:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:18:LYS:HA	3:B:81:ILE:O	2.19	0.43
3:F:197:SER:HB2	3:F:216:ASN:OD1	2.19	0.43
1:C:560:SER:HB3	5:I:1:NAG:H82	2.01	0.43
1:G:611:CYS:HA	1:G:647:ALA:O	2.19	0.43
2:E:37:VAL:HG22	2:E:47:TRP:HA	2.01	0.43
1:C:545:ARG:HD3	1:C:599:LEU:O	2.19	0.42
1:G:557:MET:SD	1:G:563:THR:HG22	2.59	0.42
2:E:193:TRP:CH2	2:E:215:ILE:HB	2.54	0.42
3:F:125:PRO:HB3	3:F:215:PHE:CE2	2.54	0.42
1:G:613:ILE:HG12	1:G:644:LEU:HD23	2.01	0.42
1:G:429:CYS:HB3	1:G:505:CYS:HB2	1.74	0.42
3:B:94:CYS:O	3:B:105:GLY:N	2.52	0.42
4:D:36:ASP:HB3	4:D:71:LEU:HD13	2.02	0.42
4:D:20:VAL:HG11	4:D:95:PHE:CZ	2.55	0.42
3:F:39:LEU:HD13	3:F:77:PHE:CD1	2.54	0.42
2:E:176:GLN:HB3	3:F:166:LEU:HD11	2.02	0.42
2:E:179:LEU:HD12	2:E:179:LEU:HA	1.85	0.42
2:E:215:ILE:H	2:E:215:ILE:HG12	1.68	0.42
1:G:523:ARG:HH22	4:H:68:LYS:HZ1	1.67	0.42
1:G:637:VAL:HG23	1:G:640:VAL:HG13	2.01	0.42
1:C:512:THR:HG23	1:C:514:SER:H	1.84	0.42
1:C:563:THR:HG21	1:C:621:HIS:O	2.19	0.42
3:B:39:LEU:HD13	3:B:77:PHE:CD1	2.54	0.42
2:E:2:VAL:O	2:E:3:GLN:HB3	2.20	0.42
1:G:512:THR:HG22	1:G:514:SER:O	2.20	0.42
1:C:425:THR:HB	1:C:520:THR:HG23	2.02	0.42
2:E:2:VAL:HG12	2:E:107:SER:CB	2.50	0.42
1:C:540:LEU:H	1:C:540:LEU:HD23	1.85	0.41
1:C:556:TRP:CZ3	1:C:566:CYS:HB2	2.53	0.41
2:E:61:ASP:OD1	2:E:63:LYS:HG2	2.20	0.41
4:H:66:MET:O	4:H:71:LEU:N	2.52	0.41
1:C:552:PHE:HE2	1:C:599:LEU:HA	1.86	0.41
3:F:31:ASN:ND2	3:F:34:ASN:OD1	2.53	0.41
1:C:438:ILE:HG21	4:D:61:ALA:HA	2.03	0.41
3:F:157:ASP:OD2	3:F:195:HIS:ND1	2.54	0.41
1:G:435:THR:HG23	1:G:437:PHE:HB2	2.03	0.41
2:E:204:HIS:CE1	2:E:206:ALA:HB3	2.55	0.41
2:E:121:THR:HG22	2:E:207:SER:HB3	2.02	0.41
1:G:424:ARG:NE	1:G:424:ARG:HA	2.36	0.41
1:G:511:PHE:HZ	1:G:615:TYR:CD1	2.39	0.41
3:F:69:ILE:HB	3:F:80:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:VAL:HG11	1:C:539:PHE:HE1	1.86	0.40
2:A:30:LYS:HE3	2:A:30:LYS:HB3	1.88	0.40
4:D:82:LEU:HD12	4:D:82:LEU:HA	1.86	0.40
4:H:48:HIS:O	4:H:52:ASN:N	2.54	0.40
1:C:555:THR:HG22	1:C:621:HIS:HD2	1.87	0.40
4:D:71:LEU:H	4:D:71:LEU:HG	1.66	0.40
4:D:55:GLY:HA3	4:D:63:THR:CG2	2.51	0.40
2:E:193:TRP:HH2	2:E:215:ILE:O	2.05	0.40
1:G:435:THR:O	1:G:435:THR:OG1	2.38	0.40
1:C:520:THR:OG1	1:C:524:LEU:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	166/259 (64%)	142 (86%)	20 (12%)	4 (2%)	4	25
1	G	174/259 (67%)	146 (84%)	24 (14%)	4 (2%)	5	26
2	A	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
2	E	216/218 (99%)	201 (93%)	13 (6%)	2 (1%)	14	43
3	B	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	F	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
4	D	79/93 (85%)	69 (87%)	10 (13%)	0	100	100
4	H	82/93 (88%)	75 (92%)	7 (8%)	0	100	100
All	All	1365/1576 (87%)	1254 (92%)	101 (7%)	10 (1%)	18	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	512	THR
1	C	526	ALA
1	G	512	THR
1	G	570	PRO
2	E	138	GLY
1	C	442	PHE
1	G	429	CYS
1	G	527	PRO
1	C	534	ASN
2	E	3	GLN

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	C	137/227 (60%)	137 (100%)	0	100	100
1	G	140/227 (62%)	140 (100%)	0	100	100
2	A	180/187 (96%)	180 (100%)	0	100	100
2	E	186/187 (100%)	186 (100%)	0	100	100
3	B	187/195 (96%)	187 (100%)	0	100	100
3	F	191/195 (98%)	191 (100%)	0	100	100
4	D	58/82 (71%)	58 (100%)	0	100	100
4	H	66/82 (80%)	66 (100%)	0	100	100
All	All	1145/1382 (83%)	1145 (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. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	534	ASN
2	A	57	HIS
2	A	65	GLN
3	B	17	GLN

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Mol	Chain	Res	Type
3	B	167	ASN
2	E	82	GLN
3	F	31	ASN
3	F	143	ASN
3	F	167	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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	$\# Z > 2$
5	NAG	I	1	1,5	14,14,15	0.54	0	17,19,21	1.38	2 (11%)
5	NAG	I	2	5	14,14,15	0.31	0	17,19,21	0.45	0
5	BMA	I	3	5	11,11,12	0.60	0	15,15,17	0.73	0
6	NAG	J	1	6,1	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	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(°)
5	I	1	NAG	C2-N2-C7	4.61	129.07	122.90
5	I	1	NAG	C1-C2-N2	2.24	113.96	110.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

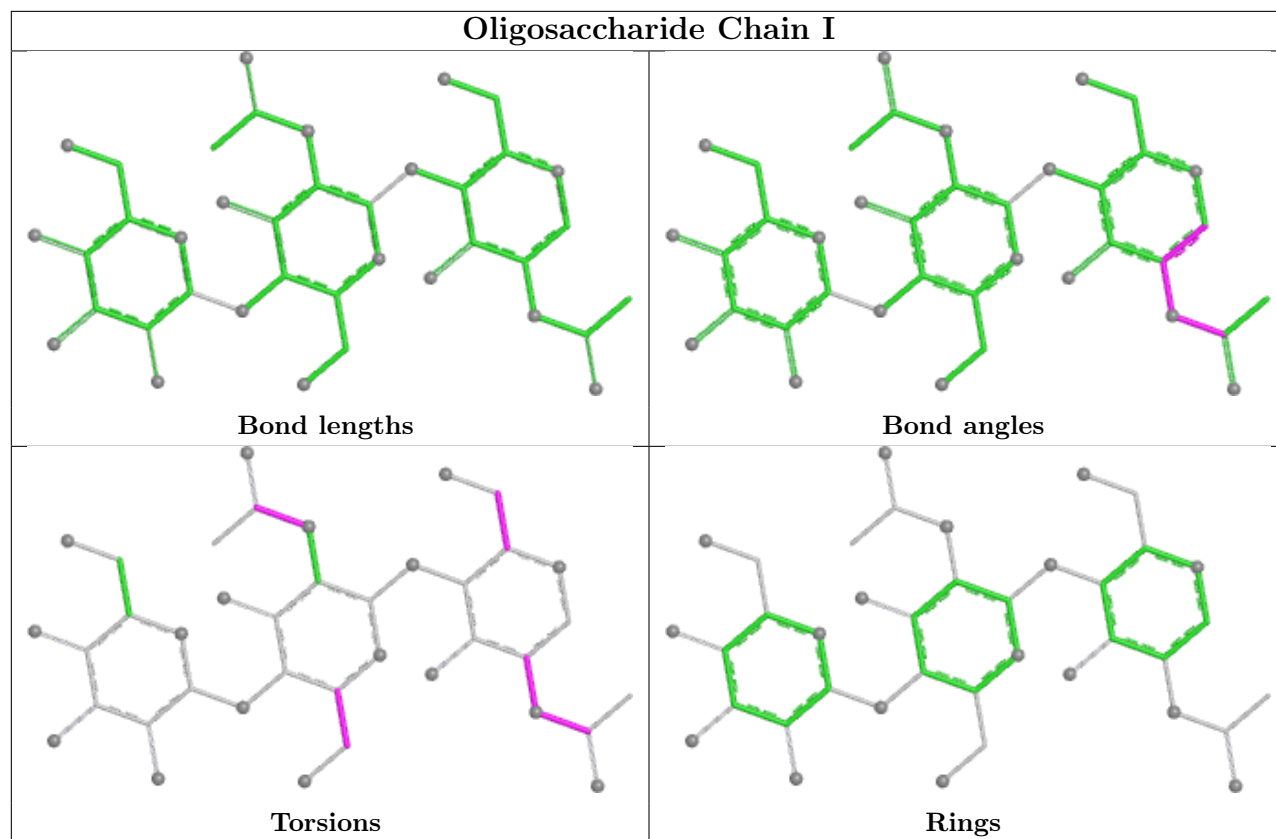
Mol	Chain	Res	Type	Atoms
5	I	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C1-C2-N2-C7
5	I	1	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C3-C2-N2-C7
5	I	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C3-C2-N2-C7

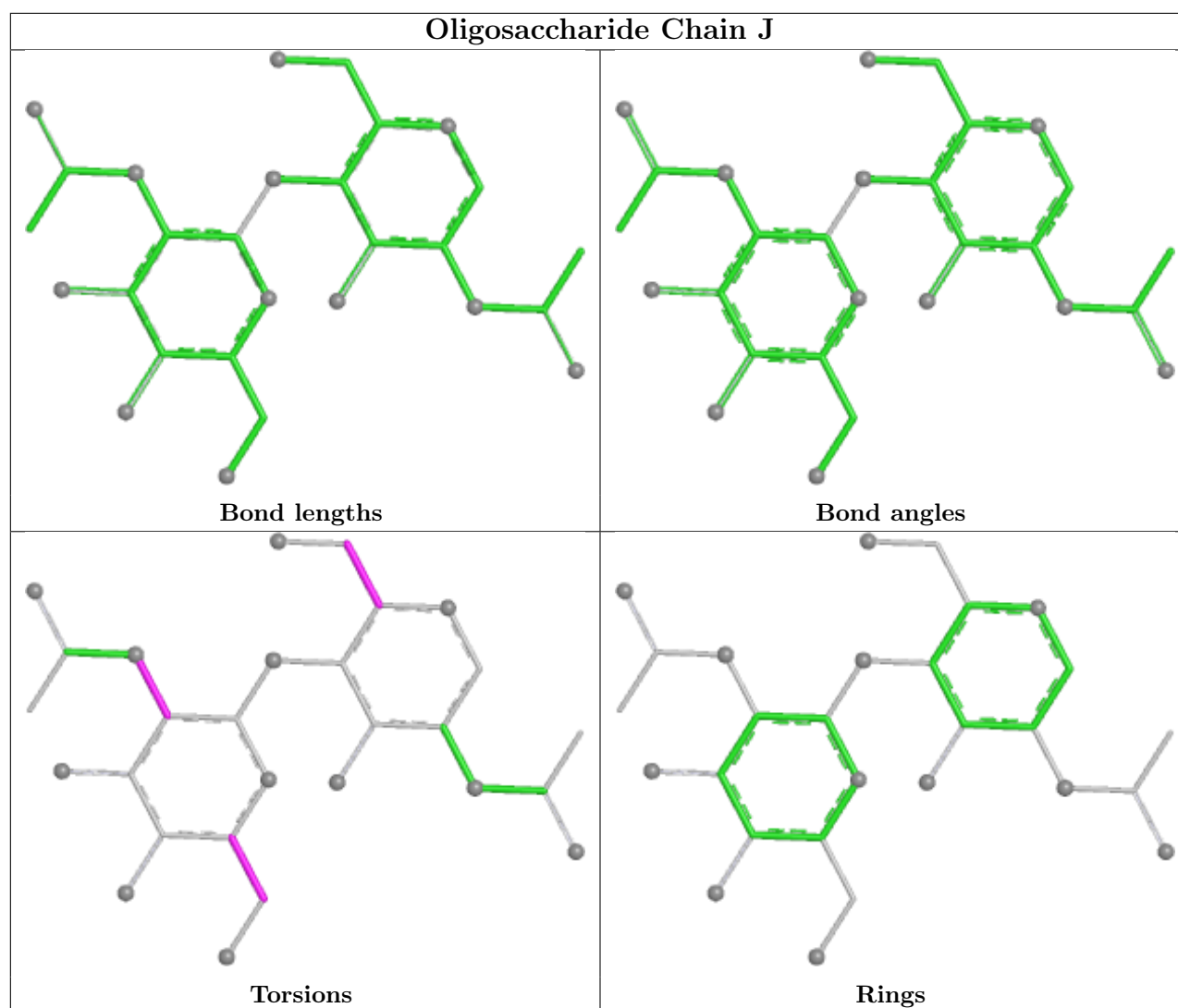
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	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 [i](#)

3 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	NAG	C	701	1	14,14,15	0.43	0	17,19,21	0.54	0
7	NAG	G	701	1	14,14,15	0.26	0	17,19,21	0.46	0
7	NAG	C	702	1	14,14,15	0.29	0	17,19,21	0.52	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	NAG	C	701	1	-	2/6/23/26	0/1/1/1
7	NAG	G	701	1	-	2/6/23/26	0/1/1/1
7	NAG	C	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	702	NAG	O5-C5-C6-O6
7	C	702	NAG	C4-C5-C6-O6
7	G	701	NAG	C4-C5-C6-O6
7	C	701	NAG	C4-C5-C6-O6
7	C	701	NAG	O5-C5-C6-O6
7	G	701	NAG	O5-C5-C6-O6

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, 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	C	172/259 (66%)	0.00	11 (6%) 25 17	121, 209, 273, 347	0
1	G	180/259 (69%)	-0.19	5 (2%) 55 36	119, 214, 290, 351	0
2	A	218/218 (100%)	-0.51	0 100 100	90, 121, 164, 222	0
2	E	218/218 (100%)	-0.42	1 (0%) 87 76	80, 136, 205, 257	0
3	B	218/218 (100%)	-0.42	0 100 100	94, 139, 204, 301	0
3	F	218/218 (100%)	-0.55	2 (0%) 81 66	108, 143, 202, 226	0
4	D	81/93 (87%)	-0.52	0 100 100	163, 228, 294, 355	0
4	H	84/93 (90%)	-0.21	1 (1%) 76 58	169, 219, 288, 328	0
All	All	1389/1576 (88%)	-0.37	20 (1%) 73 55	80, 155, 264, 355	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	509	TYR	4.4
1	C	607	LEU	4.1
1	C	515	PRO	4.0
1	C	511	PHE	4.0
1	C	613	ILE	3.8
4	H	67	LEU	3.4
1	C	633	ILE	3.4
1	C	635	MET	3.3
1	C	507	PRO	2.9
1	C	646	ALA	2.9
1	C	614	ASP	2.7
3	F	1	ASP	2.5
1	C	608	THR	2.5
1	G	517	VAL	2.4
2	E	164	LEU	2.3
3	F	125	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	499	VAL	2.3
1	G	426	ALA	2.2
1	G	442	PHE	2.2
1	G	506	GLY	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](#)

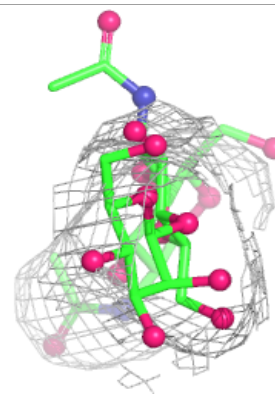
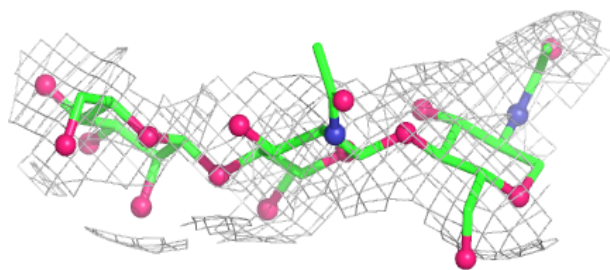
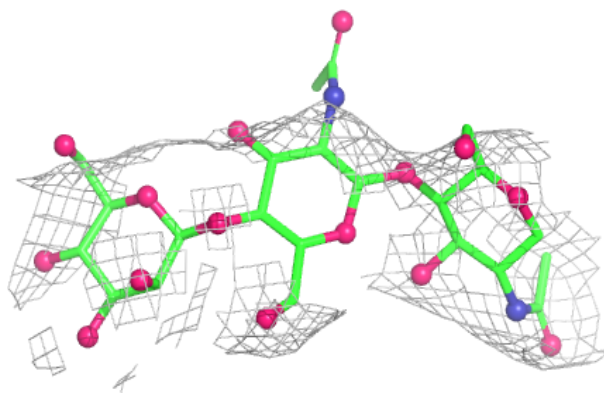
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

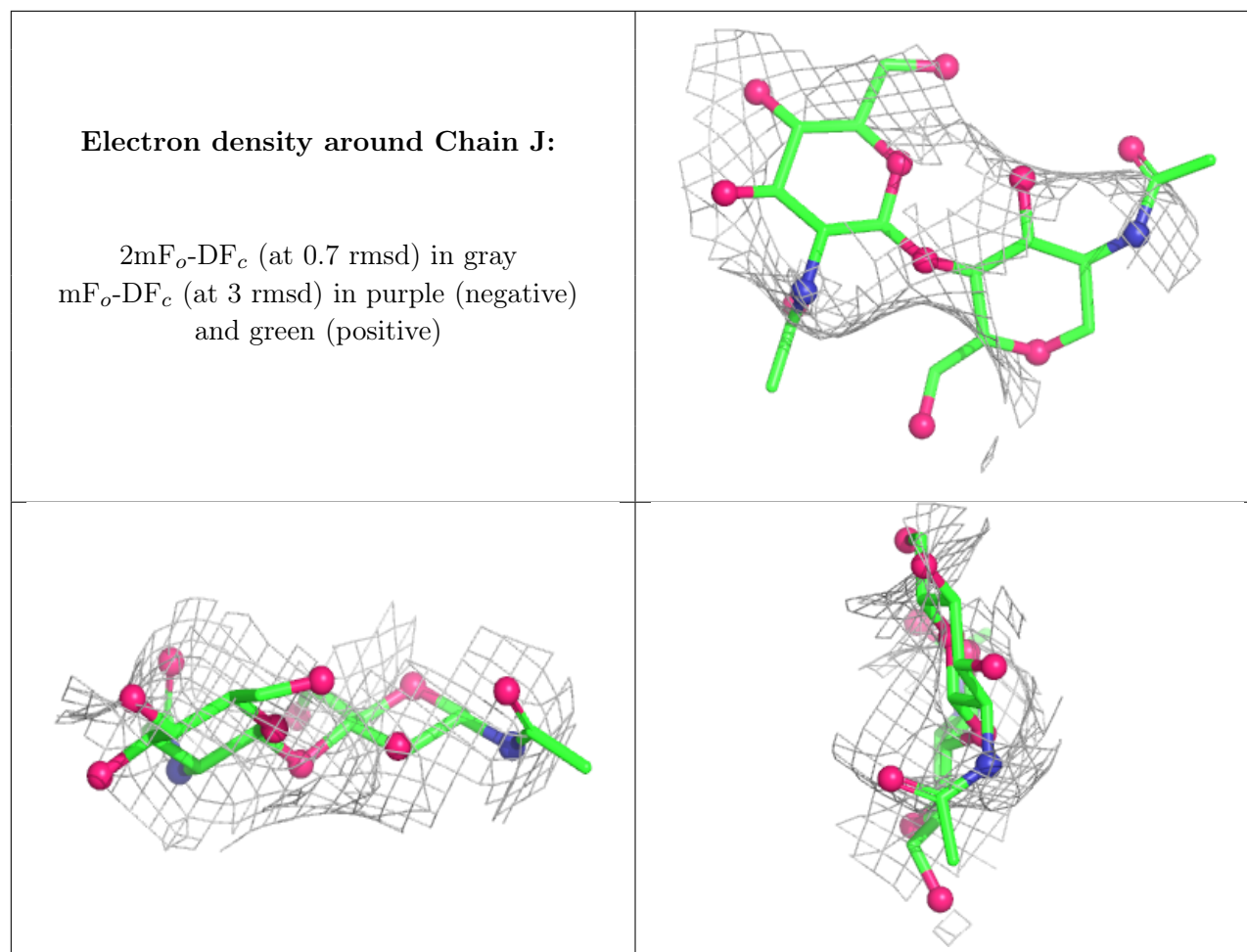
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	I	3	11/12	0.31	0.08	207,250,262,265	0
6	NAG	J	2	14/15	0.38	0.09	272,316,333,333	0
5	NAG	I	2	14/15	0.56	0.07	232,276,302,307	0
5	NAG	I	1	14/15	0.64	0.06	190,227,241,265	0
6	NAG	J	1	14/15	0.73	0.07	246,278,321,325	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	701	14/15	0.39	0.07	218,249,259,260	0
7	NAG	G	701	14/15	0.72	0.06	150,226,238,249	0
7	NAG	C	702	14/15	0.73	0.07	156,207,230,240	0

6.5 Other polymers [i](#)

There are no such residues in this entry.