



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 11:52 PM UTC

PDB ID : 7QO9 / pdb_00007qo9
EMDB ID : EMD-14087
Title : SARS-CoV-2 S Omicron Spike B.1.1.529 - RBD and NTD (Local)
Authors : Ni, D.; Lau, K.; Turelli, P.; Beckert, B.; Nazarov, S.; Pojer, F.; Myasnikov, A.; Stahlberg, H.; Trono, D.
Deposited on : 2021-12-23
Resolution : 3.88 Å(reported)
Based on initial model : 6XM3

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

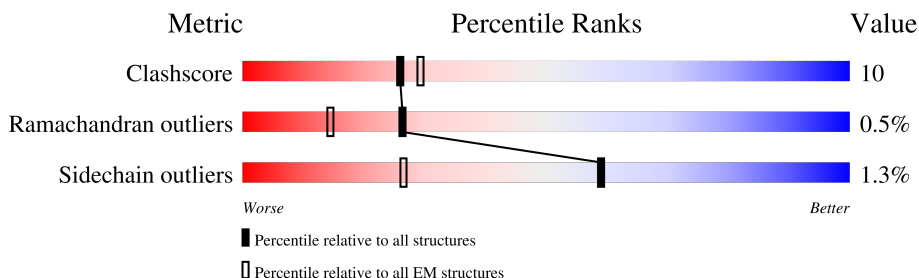
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.88 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1285	35% 10% 54%
1	B	1285	34% 10% 55%
2	D	3	33% 33% 33%
3	C	2	50% 50%
3	E	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9180 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 glycoprotein,SARS-CoV-2 S Omicron Spike B.1.1.529.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	588	Total	C	N	O	S	0	0
			4568	2911	761	875	21		
1	B	578	Total	C	N	O	S	0	0
			4486	2849	754	859	24		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	conflict	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	conflict	UNP P0DTC2
A	209	GLU	LEU	conflict	UNP P0DTC2
A	210	PRO	VAL	conflict	UNP P0DTC2
A	211	GLU	ARG	conflict	UNP P0DTC2
A	336	ASP	GLY	conflict	UNP P0DTC2
A	368	LEU	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2
A	474	ASN	SER	conflict	UNP P0DTC2
A	475	LYS	THR	conflict	UNP P0DTC2
A	481	ALA	GLU	conflict	UNP P0DTC2
A	490	ARG	GLN	conflict	UNP P0DTC2
A	493	SER	GLY	conflict	UNP P0DTC2

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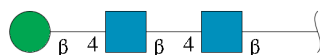
Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	GLN	conflict	UNP P0DTC2
A	498	TYR	ASN	conflict	UNP P0DTC2
A	502	HIS	TYR	conflict	UNP P0DTC2
A	544	LYS	THR	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	652	TYR	HIS	conflict	UNP P0DTC2
A	676	LYS	ASN	conflict	UNP P0DTC2
A	678	HIS	PRO	conflict	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	761	LYS	ASN	conflict	UNP P0DTC2
A	793	TYR	ASP	conflict	UNP P0DTC2
A	853	LYS	ASN	conflict	UNP P0DTC2
A	951	HIS	GLN	conflict	UNP P0DTC2
A	966	LYS	ASN	conflict	UNP P0DTC2
A	978	PHE	LEU	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	140	ASP	TYR	conflict	UNP P0DTC2
B	206	ILE	-	insertion	UNP P0DTC2
B	207	VAL	-	insertion	UNP P0DTC2
B	208	ARG	ASN	conflict	UNP P0DTC2
B	209	GLU	LEU	conflict	UNP P0DTC2
B	210	PRO	VAL	conflict	UNP P0DTC2
B	211	GLU	ARG	conflict	UNP P0DTC2
B	336	ASP	GLY	conflict	UNP P0DTC2
B	368	LEU	SER	conflict	UNP P0DTC2
B	370	PRO	SER	conflict	UNP P0DTC2
B	372	PHE	SER	conflict	UNP P0DTC2
B	414	ASN	LYS	conflict	UNP P0DTC2
B	437	LYS	ASN	conflict	UNP P0DTC2
B	443	SER	GLY	conflict	UNP P0DTC2
B	474	ASN	SER	conflict	UNP P0DTC2
B	475	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	ALA	GLU	conflict	UNP P0DTC2
B	490	ARG	GLN	conflict	UNP P0DTC2
B	493	SER	GLY	conflict	UNP P0DTC2
B	495	ARG	GLN	conflict	UNP P0DTC2
B	498	TYR	ASN	conflict	UNP P0DTC2
B	502	HIS	TYR	conflict	UNP P0DTC2
B	544	LYS	THR	conflict	UNP P0DTC2
B	611	GLY	ASP	conflict	UNP P0DTC2
B	652	TYR	HIS	conflict	UNP P0DTC2
B	676	LYS	ASN	conflict	UNP P0DTC2
B	678	HIS	PRO	conflict	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	761	LYS	ASN	conflict	UNP P0DTC2
B	793	TYR	ASP	conflict	UNP P0DTC2
B	853	LYS	ASN	conflict	UNP P0DTC2
B	951	HIS	GLN	conflict	UNP P0DTC2
B	966	LYS	ASN	conflict	UNP P0DTC2
B	978	PHE	LEU	conflict	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 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				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

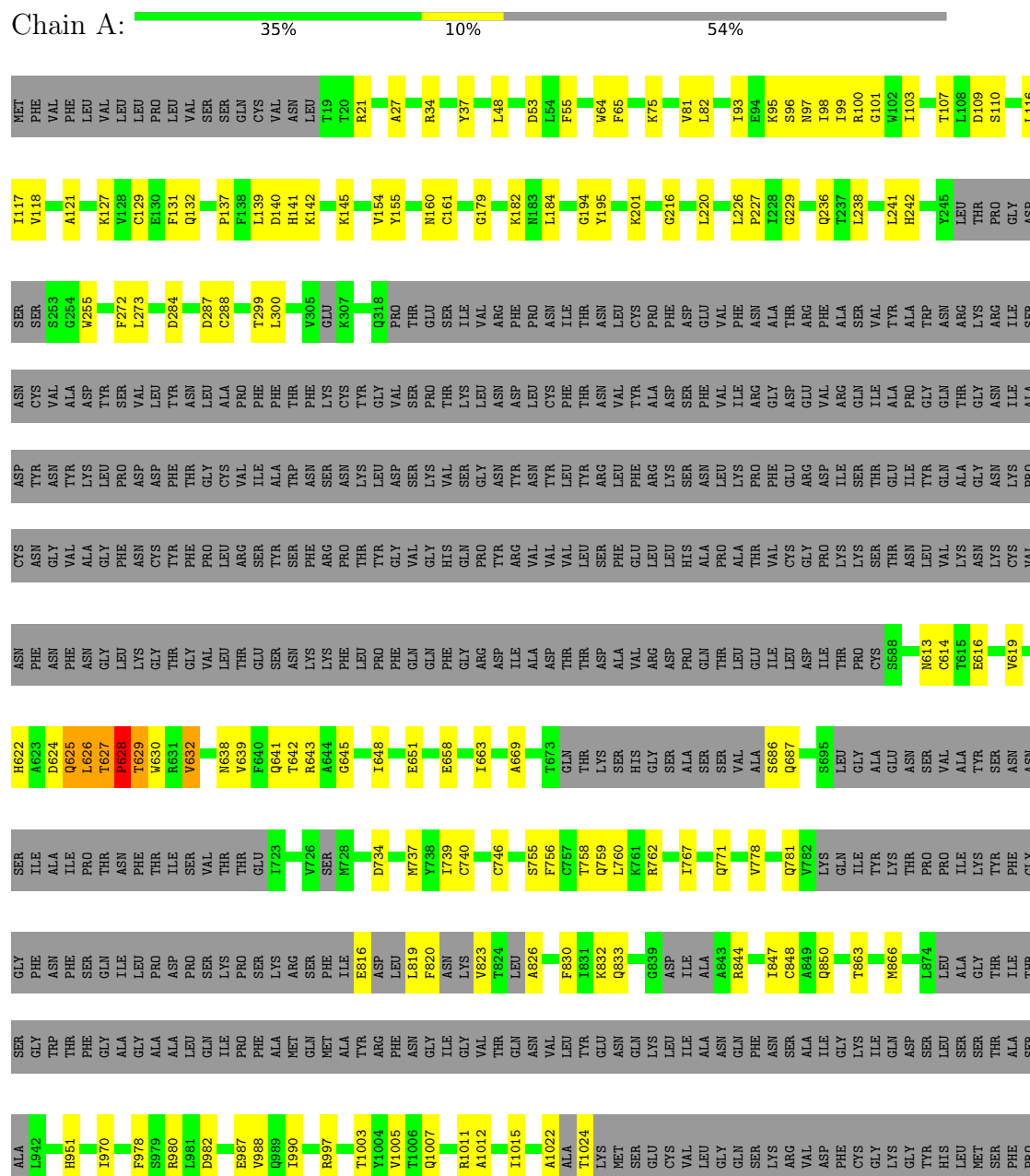
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	O	0
			3	3	

3 Residue-property plots

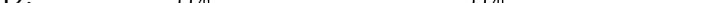
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 glycoprotein,SARS-CoV-2 S Omicron Spike B.1.1.529



[illegible]

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

Chain D:  33% 33% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	76450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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: 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	A	0.18	0/4653	0.41	1/6312 (0.0%)
1	B	0.24	0/4573	0.48	3/6211 (0.0%)
All	All	0.21	0/9226	0.45	4/12523 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	628	PRO	N-CA-CB	-10.00	92.75	103.25
1	B	448	TYR	CB-CA-C	-6.95	99.97	110.88
1	B	486	TYR	CB-CA-C	-6.76	97.99	109.83
1	B	446	TYR	CB-CA-C	-6.61	104.90	114.87

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	A	4568	0	4459	99	0
1	B	4486	0	4418	88	0
2	D	39	0	34	1	0
3	C	28	0	25	1	0
3	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	26	0	0
5	A	3	0	0	0	0
All	All	9180	0	8987	185	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 10.

All (185) 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)
1:A:628:PRO:C	1:A:630:TRP:H	1.86	0.82
1:A:626:LEU:C	1:A:628:PRO:HD3	2.07	0.79
1:B:863:THR:O	1:B:866:MET:N	2.20	0.73
1:A:127:LYS:NZ	1:A:129:CYS:SG	2.61	0.73
1:A:863:THR:HG22	1:A:866:MET:HE2	1.69	0.73
1:A:622:HIS:O	1:A:628:PRO:HB2	1.90	0.72
1:A:628:PRO:C	1:A:630:TRP:N	2.40	0.71
1:B:470:TYR:O	1:B:485:CYS:HB3	1.91	0.70
1:A:619:VAL:O	1:A:622:HIS:ND1	2.23	0.67
1:A:760:LEU:HG	1:A:1005:VAL:HG21	1.77	0.66
1:A:195:TYR:OH	1:B:391:ASN:ND2	2.29	0.66
1:B:447:ASN:HB3	1:B:492:TYR:HD2	1.61	0.65
1:B:617:VAL:HG13	1:B:621:ILE:HD11	1.78	0.64
1:A:816:GLU:O	1:A:819:LEU:N	2.31	0.64
1:B:759:GLN:HG2	1:B:760:LEU:HD12	1.78	0.64
1:A:663:ILE:HD11	1:A:669:ALA:HB2	1.79	0.63
1:B:348:TYR:HB2	1:B:464:ASP:HB3	1.80	0.63
1:A:628:PRO:HD2	1:A:629:THR:H	1.63	0.63
1:B:354:ARG:NH1	1:B:355:ILE:O	2.31	0.63
1:B:355:ILE:HB	1:B:392:VAL:HG23	1.80	0.63
1:A:1022:ALA:O	1:A:1024:THR:N	2.32	0.63
1:A:641:GLN:NE2	1:A:642:THR:O	2.30	0.62
1:B:447:ASN:HB3	1:B:492:TYR:CD2	2.34	0.61
1:B:641:GLN:NE2	1:B:645:GLY:O	2.34	0.61
1:B:309:ILE:HG22	1:B:661:ILE:HD11	1.83	0.61
1:A:739:ILE:O	1:A:997:ARG:NH1	2.34	0.60
1:B:639:VAL:HG12	1:B:648:ILE:HG22	1.83	0.60
1:A:627:THR:N	1:A:628:PRO:HD3	2.15	0.60
1:B:858:LEU:HD12	1:B:859:PRO:HD2	1.81	0.60
1:B:967:PHE:O	1:B:992:ARG:NH1	2.35	0.60
1:B:399:ILE:HD11	1:B:415:ILE:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:HB3	1:A:242:HIS:HD1	1.66	0.60
1:B:389:PHE:N	1:B:521:VAL:O	2.34	0.60
1:A:116:LEU:HD21	1:A:118:VAL:HG13	1.82	0.59
1:A:638:ASN:N	1:A:651:GLU:OE2	2.36	0.58
1:B:990:ILE:O	1:B:994:ILE:HG12	2.04	0.58
1:B:348:TYR:O	1:B:464:ASP:N	2.30	0.58
1:B:480:VAL:HG23	1:B:485:CYS:H	1.69	0.58
1:A:34:ARG:NH1	1:A:216:GLY:O	2.38	0.56
1:A:65:PHE:HE2	1:A:82:LEU:HD11	1.70	0.56
1:A:75:LYS:HD2	1:A:255:TRP:HD1	1.70	0.56
1:A:129:CYS:HB2	1:A:131:PHE:CE1	2.41	0.56
1:A:160:ASN:OD1	3:C:1:NAG:N2	2.39	0.56
1:A:639:VAL:HG12	1:A:648:ILE:HG22	1.88	0.56
1:B:620:ALA:HA	1:B:631:ARG:HH21	1.71	0.56
1:A:1012:ALA:HA	1:A:1015:ILE:HG22	1.88	0.56
1:A:641:GLN:NE2	1:A:645:GLY:O	2.39	0.55
1:B:756:PHE:HA	1:B:759:GLN:HE22	1.71	0.55
1:A:95:LYS:HD3	1:A:182:LYS:HG2	1.89	0.55
1:A:100:ARG:HD3	1:A:139:LEU:HD23	1.89	0.55
1:A:819:LEU:O	1:A:823:VAL:N	2.39	0.55
1:A:1003:THR:O	1:A:1007:GLN:HG2	2.07	0.55
1:A:755:SER:OG	1:A:758:THR:OG1	2.25	0.55
1:B:487:PHE:CD2	1:B:488:PRO:HD2	2.42	0.54
2:D:1:NAG:H83	2:D:1:NAG:H3	1.89	0.54
1:A:103:ILE:HG13	1:A:236:GLN:HB2	1.88	0.54
1:B:397:PHE:HB3	1:B:507:VAL:H	1.73	0.54
1:A:154:VAL:HG23	1:A:155:TYR:HD1	1.73	0.54
1:B:969:ALA:HA	1:B:992:ARG:HH22	1.73	0.54
1:A:823:VAL:O	1:A:826:ALA:N	2.42	0.53
1:A:139:LEU:O	1:A:241:LEU:N	2.40	0.53
1:B:619:VAL:O	1:B:631:ARG:NE	2.42	0.53
1:B:831:ILE:O	1:B:832:LYS:HG2	2.09	0.53
1:B:554:LYS:NZ	1:B:583:ASP:OD1	2.36	0.53
1:B:983:PRO:O	1:B:986:ALA:N	2.43	0.52
1:A:81:VAL:HA	1:A:236:GLN:HE22	1.75	0.52
1:A:613:ASN:N	1:A:616:GLU:OE2	2.43	0.52
1:B:851:LYS:HG3	1:B:852:PHE:H	1.75	0.51
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.45	0.51
1:A:737:MET:HE1	1:B:589:PHE:CZ	2.44	0.51
1:B:459:LYS:HE2	1:B:462:GLU:HG3	1.92	0.51
1:B:767:ILE:O	1:B:771:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASP:O	1:B:525:LYS:NZ	2.42	0.51
1:A:628:PRO:HD2	1:A:629:THR:N	2.25	0.51
1:A:863:THR:H	1:A:866:MET:HE2	1.76	0.51
1:A:137:PRO:HB2	1:A:154:VAL:HG12	1.93	0.50
1:A:987:GLU:OE2	1:A:988:VAL:HG13	2.11	0.50
1:A:194:GLY:HA2	1:A:229:GLY:HA2	1.93	0.50
1:B:441:LYS:HE2	1:B:446:TYR:HB2	1.94	0.50
1:B:315:PHE:HZ	1:B:612:VAL:HG11	1.75	0.50
1:B:616:GLU:N	1:B:616:GLU:OE1	2.45	0.50
1:A:100:ARG:O	1:A:238:LEU:HB2	2.13	0.49
1:A:632:VAL:HG13	1:A:648:ILE:HD12	1.93	0.49
1:B:339:PHE:CE1	1:B:508:VAL:HB	2.47	0.49
1:B:817:ASP:OD1	1:B:818:LEU:N	2.45	0.49
1:B:492:TYR:O	1:B:493:SER:C	2.55	0.49
1:A:127:LYS:NZ	1:A:161:CYS:SG	2.85	0.49
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.95	0.49
1:A:299:THR:HG23	1:A:300:LEU:HD12	1.94	0.49
1:A:287:ASP:OD1	1:A:288:CYS:N	2.46	0.49
1:B:565:ASP:OD1	1:B:569:THR:N	2.46	0.48
1:A:110:SER:OG	1:A:132:GLN:OE1	2.24	0.48
1:A:816:GLU:O	1:A:820:PHE:N	2.43	0.48
1:A:284:ASP:N	1:A:284:ASP:OD1	2.46	0.48
1:A:658:GLU:H	1:A:658:GLU:CD	2.22	0.48
1:A:982:ASP:OD1	1:A:982:ASP:N	2.42	0.47
1:A:21:ARG:HD3	1:A:21:ARG:H	1.79	0.47
1:A:686:SER:OG	1:A:687:GLN:N	2.47	0.47
1:A:96:SER:O	1:A:98:ILE:HG13	2.15	0.47
1:A:99:ILE:O	1:A:100:ARG:HG3	2.14	0.47
1:B:969:ALA:N	1:B:992:ARG:HH12	2.13	0.47
1:A:272:PHE:CD1	1:A:287:ASP:HA	2.50	0.47
1:A:759:GLN:HA	1:A:762:ARG:HH11	1.79	0.47
1:A:778:VAL:C	1:A:781:GLN:HE22	2.23	0.46
1:B:492:TYR:HD1	1:B:492:TYR:HA	1.63	0.46
1:A:628:PRO:O	1:A:630:TRP:N	2.48	0.46
1:B:349:ALA:HB1	1:B:463:ARG:HH21	1.80	0.46
1:B:613:ASN:HB3	1:B:616:GLU:OE1	2.15	0.46
1:A:643:ARG:HD3	1:A:643:ARG:HA	1.78	0.46
1:B:306:GLU:O	1:B:310:TYR:OH	2.25	0.46
1:B:400:ARG:O	1:B:502:HIS:ND1	2.49	0.46
1:A:75:LYS:HD2	1:A:255:TRP:CD1	2.50	0.45
1:B:756:PHE:HA	1:B:759:GLN:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ASP:N	1:B:836:ASP:OD1	2.48	0.45
1:A:734:ASP:OD2	1:B:314:ASN:ND2	2.50	0.45
1:B:428:GLY:HA2	1:B:512:PHE:CE1	2.52	0.45
1:B:829:GLY:O	1:B:833:GLN:NE2	2.49	0.45
1:B:1016:ARG:HB2	1:B:1016:ARG:NH1	2.32	0.45
1:A:141:HIS:CD2	1:A:142:LYS:HG2	2.52	0.45
1:B:369:ALA:HB3	1:B:371:PHE:CE2	2.51	0.45
1:A:137:PRO:HB3	1:A:154:VAL:HA	2.00	0.44
1:B:369:ALA:HB3	1:B:371:PHE:CZ	2.52	0.44
1:A:145:LYS:HD2	1:A:145:LYS:H	1.82	0.44
1:B:977:ILE:HG23	1:B:981:LEU:HD12	1.98	0.44
1:B:991:ASP:O	1:B:995:THR:HG23	2.17	0.44
1:A:184:LEU:HD23	1:A:184:LEU:O	2.18	0.44
1:A:65:PHE:CE2	1:A:82:LEU:HD11	2.50	0.44
1:B:755:SER:O	1:B:759:GLN:NE2	2.50	0.44
1:A:107:THR:OG1	1:A:109:ASP:OD1	2.30	0.44
1:A:613:ASN:OD1	1:A:614:CYS:N	2.51	0.44
1:B:352:ARG:HE	1:B:395:ASP:HB3	1.83	0.43
1:A:630:TRP:HB3	1:A:632:VAL:HG23	1.99	0.43
1:B:615:THR:OG1	1:B:616:GLU:OE1	2.34	0.43
1:A:55:PHE:HB2	1:A:272:PHE:HE2	1.83	0.43
1:B:958:THR:O	1:B:962:GLN:HG2	2.18	0.43
1:B:389:PHE:HB2	1:B:521:VAL:HB	2.00	0.43
1:B:656:SER:HB3	1:B:695:SER:HB3	2.01	0.43
1:A:866:MET:HE3	1:A:866:MET:HB2	1.94	0.43
1:A:970:ILE:HD12	1:A:980:ARG:HH22	1.82	0.43
1:B:770:GLU:HA	1:B:773:LYS:NZ	2.33	0.43
1:B:821:ASN:O	1:B:824:THR:HG22	2.18	0.43
1:A:627:THR:N	1:A:628:PRO:CD	2.81	0.42
1:B:329:ILE:HB	1:B:359:VAL:HG23	2.01	0.42
1:B:418:TYR:O	1:B:454:ARG:HG2	2.18	0.42
1:B:966:LYS:HE3	1:B:971:SER:HA	2.01	0.42
1:B:505:TYR:O	1:B:507:VAL:HG23	2.19	0.42
1:A:767:ILE:O	1:A:771:GLN:OE1	2.37	0.42
1:A:48:LEU:HD12	1:A:273:LEU:HD21	2.01	0.42
1:A:226:LEU:HA	1:A:227:PRO:HD3	1.85	0.42
1:A:830:PHE:HD2	1:A:832:LYS:H	1.68	0.42
1:A:97:ASN:HB3	1:A:100:ARG:HH22	1.85	0.42
1:A:951:HIS:HB3	1:A:1011:ARG:NH2	2.35	0.42
1:B:600:ASN:OD1	1:B:601:THR:N	2.53	0.42
1:B:415:ILE:H	1:B:415:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:CYS:HB3	1:A:746:CYS:HB3	1.89	0.41
1:A:978:PHE:CE1	1:A:990:ILE:HD11	2.55	0.41
1:A:756:PHE:HA	1:A:759:GLN:HE22	1.85	0.41
1:A:833:GLN:NE2	1:A:848:CYS:HB2	2.36	0.41
1:B:535:CYS:HB2	1:B:587:CYS:HB3	1.82	0.41
1:A:844:ARG:O	1:A:848:CYS:HB3	2.19	0.41
1:B:374:PHE:HD1	1:B:431:ILE:HG13	1.86	0.41
1:B:400:ARG:NH2	1:B:491:SER:O	2.53	0.41
1:B:450:TYR:HB3	1:B:491:SER:H	1.86	0.41
1:B:759:GLN:OE1	1:B:759:GLN:N	2.50	0.41
1:B:749:LEU:HG	1:B:990:ILE:HD11	2.01	0.41
1:A:101:GLY:HA2	1:A:117:ILE:O	2.20	0.41
1:B:405:ARG:NE	1:B:405:ARG:O	2.54	0.41
1:B:753:TYR:OH	1:B:991:ASP:OD1	2.30	0.41
1:B:495:ARG:HD3	1:B:498:TYR:HB2	2.03	0.41
1:B:1000:SER:O	1:B:1003:THR:OG1	2.30	0.41
1:A:37:TYR:HB3	1:A:220:LEU:HB2	2.02	0.41
1:A:93:ILE:HG22	1:A:93:ILE:O	2.20	0.41
1:A:95:LYS:HE3	1:A:179:GLY:HA2	2.03	0.41
1:B:344:PHE:CD1	1:B:506:ARG:HG2	2.56	0.41
1:B:388:CYS:SG	1:B:523:GLY:N	2.83	0.41
1:B:392:VAL:HG12	1:B:512:PHE:HB3	2.03	0.41
1:B:428:GLY:HA2	1:B:512:PHE:HE1	1.85	0.41
1:A:127:LYS:HG2	1:A:129:CYS:SG	2.61	0.41
1:A:628:PRO:CD	1:A:629:THR:N	2.83	0.41
1:A:632:VAL:O	1:A:632:VAL:HG12	2.20	0.41
1:B:489:LEU:O	1:B:490:ARG:HB2	2.21	0.41
1:A:201:LYS:HB3	1:A:220:LEU:HD22	2.01	0.40
1:A:847:ILE:O	1:A:850:GLN:HG2	2.20	0.40
1:B:866:MET:N	1:B:866:MET:SD	2.95	0.40
1:B:452:LEU:HD13	1:B:491:SER:OG	2.22	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 PDB entries followed by that with respect to all EM entries.

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	A	560/1285 (44%)	513 (92%)	43 (8%)	4 (1%)	18	52
1	B	564/1285 (44%)	502 (89%)	60 (11%)	2 (0%)	30	64
All	All	1124/2570 (44%)	1015 (90%)	103 (9%)	6 (0%)	26	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	PRO
1	A	121	ALA
1	A	625	GLN
1	B	493	SER
1	A	632	VAL
1	B	830	PHE

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 PDB entries followed by that with respect to all EM entries.

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	A	507/1113 (46%)	501 (99%)	6 (1%)	63	72
1	B	502/1113 (45%)	495 (99%)	7 (1%)	59	70
All	All	1009/2226 (45%)	996 (99%)	13 (1%)	59	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	624	ASP
1	A	625	GLN
1	A	626	LEU
1	A	627	THR
1	A	628	PRO
1	A	629	THR
1	B	446	TYR

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Mol	Chain	Res	Type
1	B	449	LEU
1	B	469	ILE
1	B	485	CYS
1	B	489	LEU
1	B	491	SER
1	B	492	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	183	ASN
1	A	191	ASN
1	A	655	ASN
1	A	781	GLN
1	A	999	GLN
1	B	331	ASN
1	B	391	ASN
1	B	654	ASN
1	B	962	GLN
1	B	1008	GLN

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 ⓘ

7 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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.40	0	17,19,21	0.56	0
3	NAG	C	2	3	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	D	1	2,1	14,14,15	0.41	0	17,19,21	1.42	2 (11%)
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.55	0
2	BMA	D	3	2	11,11,12	0.97	1 (9%)	15,15,17	1.43	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.53	0	17,19,21	1.60	5 (29%)
3	NAG	E	2	3	14,14,15	0.21	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	O5-C5	2.07	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	4.57	118.31	112.19
2	D	1	NAG	C2-N2-C7	4.54	128.98	122.90
2	D	3	BMA	C1-O5-C5	4.54	118.27	112.19
3	E	1	NAG	C2-N2-C7	2.63	126.43	122.90
2	D	1	NAG	C1-C2-N2	2.38	114.19	110.43
3	E	1	NAG	C1-C2-N2	2.31	114.08	110.43
3	E	1	NAG	C3-C4-C5	2.18	114.18	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C4-C3-C2	2.10	114.09	111.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

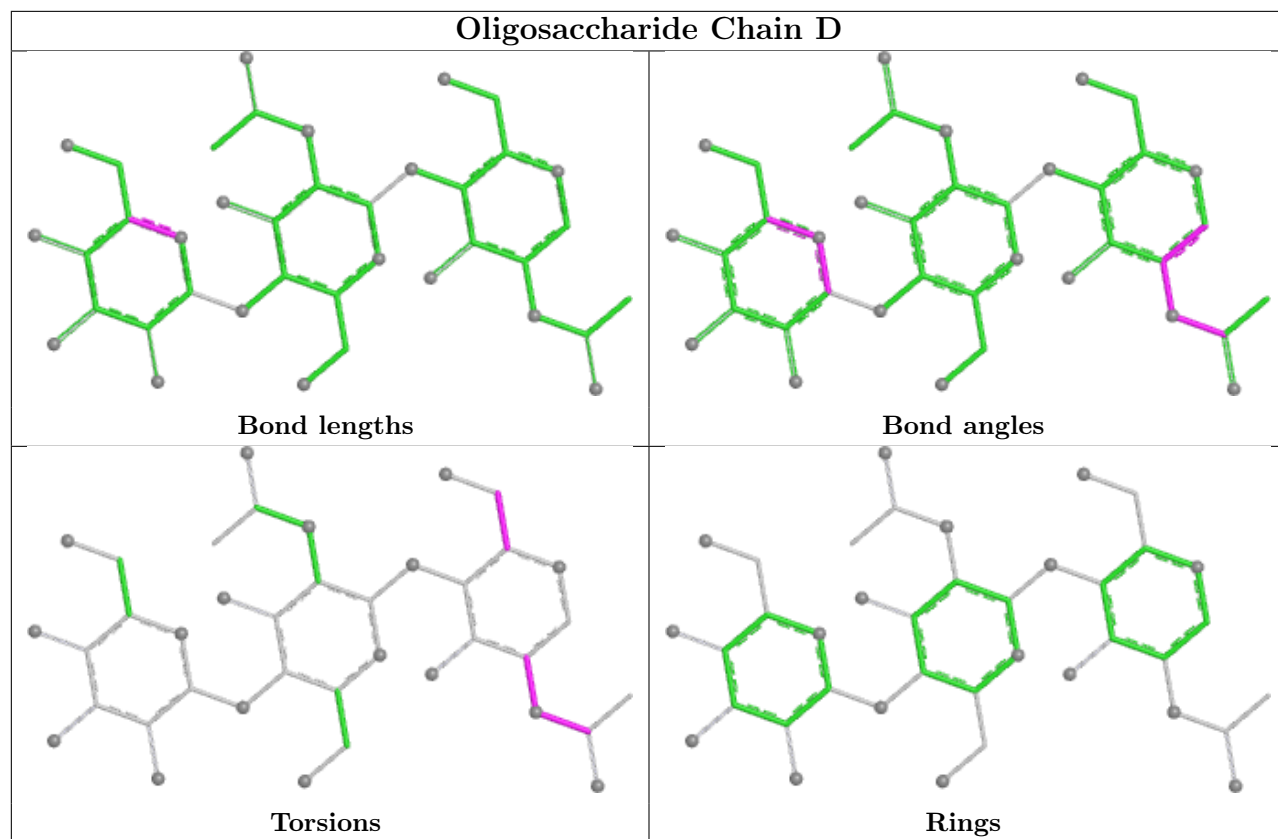
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	C	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

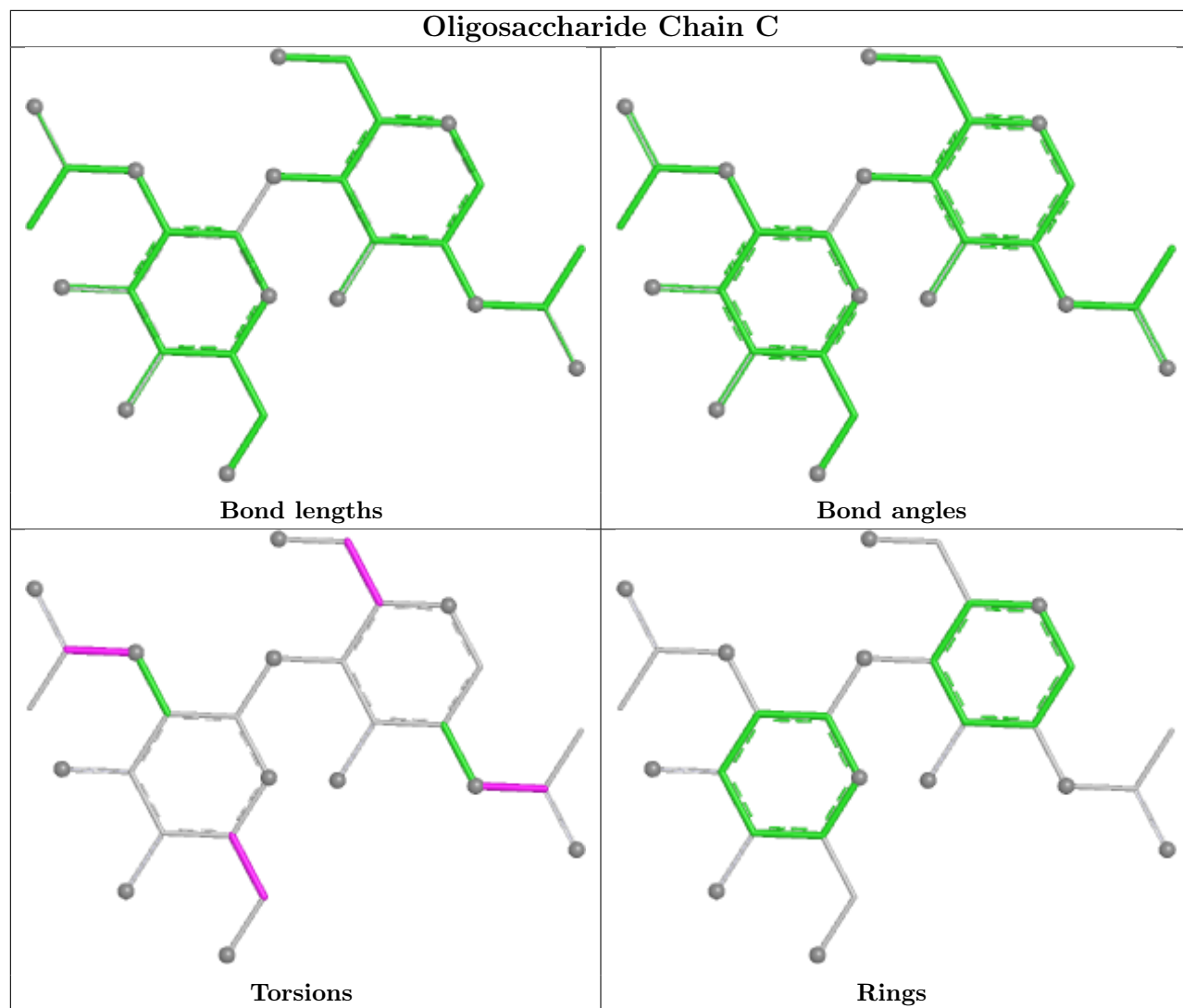
There are no ring outliers.

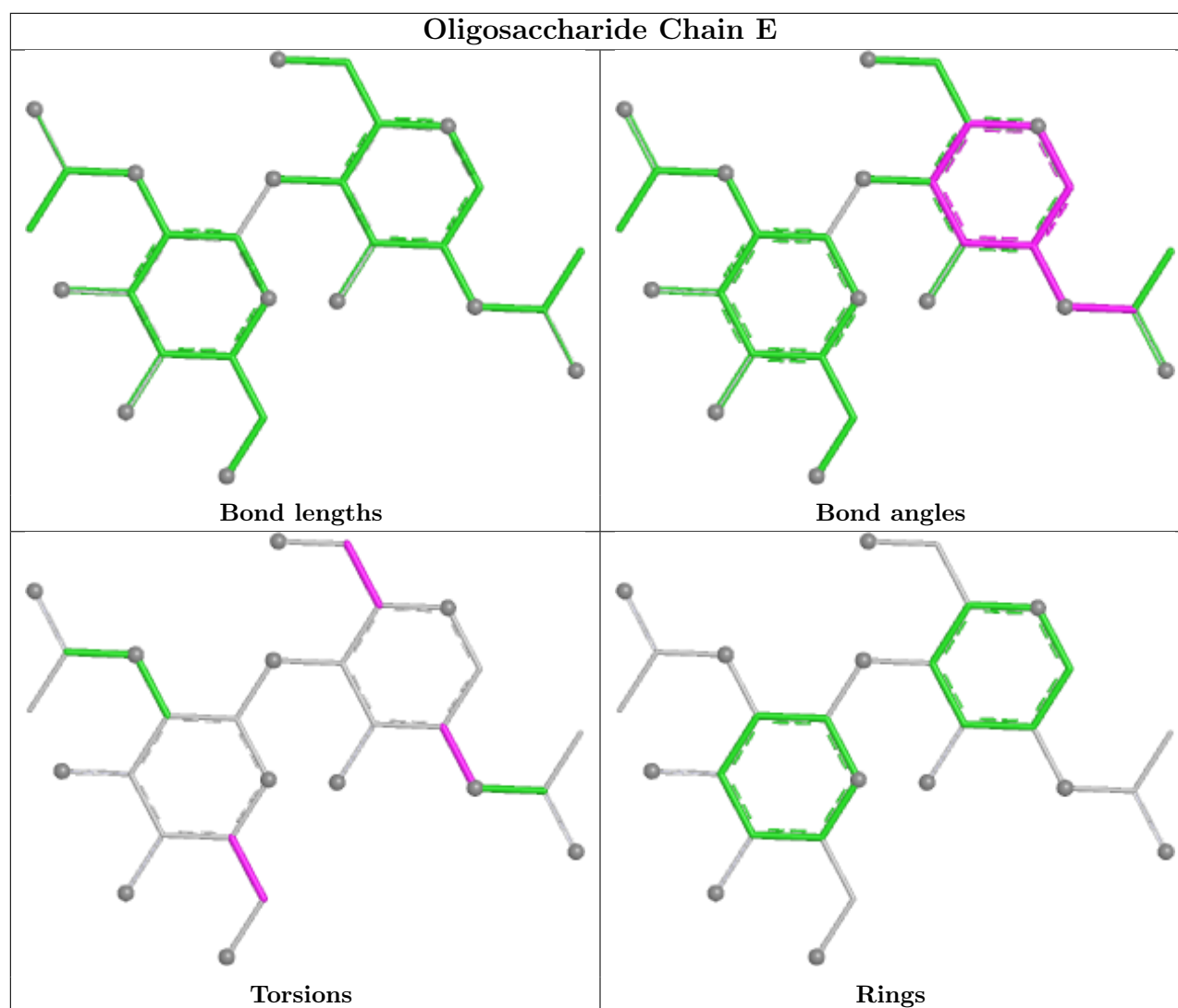
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
3	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](#)

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	$\# Z > 2$
4	NAG	A	1301	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.54	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
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1302	NAG	C1-C2-N2-C7
4	A	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C1-C2-N2-C7
4	A	1302	NAG	C3-C2-N2-C7

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-14087. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.