



# wwPDB EM Validation Summary Report ⓘ

Oct 22, 2024 – 12:19 AM JST

PDB ID : 8IFN  
EMDB ID : EMD-35422  
Title : MERS-CoV spike trimer in complex with nanobody VHH-T148  
Authors : Wang, X.; Tian, L.  
Deposited on : 2023-02-19  
Resolution : 2.81 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

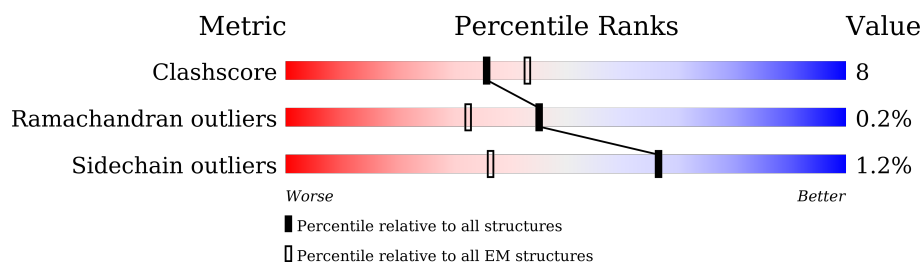
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.81 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	B	1347	
1	C	1347	
1	E	1347	
2	A	135	
2	D	135	
2	F	135	
3	G	4	
3	H	4	
3	I	4	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30441 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1180	Total	C	N	O	S	0	0
			9124	5793	1513	1767	51		
1	C	1180	Total	C	N	O	S	0	0
			9124	5793	1513	1767	51		
1	E	1180	Total	C	N	O	S	0	0
			9124	5793	1513	1767	51		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	748	SER	ARG	conflict	UNP R9UQ53
B	751	GLY	ARG	conflict	UNP R9UQ53
B	1020	GLN	ARG	conflict	UNP R9UQ53
B	1060	PRO	VAL	conflict	UNP R9UQ53
B	1061	PRO	LEU	conflict	UNP R9UQ53
B	1208	GLN	HIS	conflict	UNP R9UQ53
B	1291	SER	-	insertion	UNP R9UQ53
B	1292	ARG	-	insertion	UNP R9UQ53
B	1293	GLU	-	insertion	UNP R9UQ53
B	1294	ASN	-	insertion	UNP R9UQ53
B	1295	LEU	-	insertion	UNP R9UQ53
B	1297	PHE	-	insertion	UNP R9UQ53
B	1298	GLN	-	insertion	UNP R9UQ53
B	1299	GLY	-	insertion	UNP R9UQ53
B	1300	GLY	-	insertion	UNP R9UQ53
B	1301	GLY	TYR	conflict	UNP R9UQ53
B	1302	SER	ASN	conflict	UNP R9UQ53
B	1303	ALA	LYS	conflict	UNP R9UQ53
B	1304	GLY	TRP	conflict	UNP R9UQ53
B	1305	SER	PRO	conflict	UNP R9UQ53
B	1306	GLY	TRP	conflict	UNP R9UQ53
B	1309	PRO	TRP	conflict	UNP R9UQ53
B	1310	GLU	LEU	conflict	UNP R9UQ53
B	1311	ALA	GLY	conflict	UNP R9UQ53

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1312	PRO	PHE	conflict	UNP R9UQ53
B	1313	ARG	ILE	conflict	UNP R9UQ53
B	1314	ASP	ALA	conflict	UNP R9UQ53
B	1316	GLN	LEU	conflict	UNP R9UQ53
B	1317	ALA	VAL	conflict	UNP R9UQ53
B	1318	TYR	ALA	conflict	UNP R9UQ53
B	1319	VAL	LEU	conflict	UNP R9UQ53
B	1320	ARG	ALA	conflict	UNP R9UQ53
B	1321	LYS	LEU	conflict	UNP R9UQ53
B	1322	ASP	CYS	conflict	UNP R9UQ53
B	1323	GLY	VAL	conflict	UNP R9UQ53
B	1324	GLU	PHE	conflict	UNP R9UQ53
B	1325	TRP	PHE	conflict	UNP R9UQ53
B	1326	VAL	ILE	conflict	UNP R9UQ53
B	1328	LEU	CYS	conflict	UNP R9UQ53
B	1329	SER	CYS	conflict	UNP R9UQ53
B	1331	PHE	GLY	conflict	UNP R9UQ53
B	1332	LEU	CYS	conflict	UNP R9UQ53
B	1334	HIS	-	expression tag	UNP R9UQ53
B	1335	HIS	-	expression tag	UNP R9UQ53
B	1336	HIS	-	expression tag	UNP R9UQ53
B	1337	HIS	-	expression tag	UNP R9UQ53
B	1338	HIS	-	expression tag	UNP R9UQ53
B	1339	HIS	-	expression tag	UNP R9UQ53
B	1340	TRP	-	expression tag	UNP R9UQ53
B	1341	SER	-	expression tag	UNP R9UQ53
B	1342	HIS	-	expression tag	UNP R9UQ53
B	1343	PRO	-	expression tag	UNP R9UQ53
B	1344	GLN	-	expression tag	UNP R9UQ53
B	1345	PHE	-	expression tag	UNP R9UQ53
B	1346	GLU	-	expression tag	UNP R9UQ53
B	1347	LYS	-	expression tag	UNP R9UQ53
C	748	SER	ARG	conflict	UNP R9UQ53
C	751	GLY	ARG	conflict	UNP R9UQ53
C	1020	GLN	ARG	conflict	UNP R9UQ53
C	1060	PRO	VAL	conflict	UNP R9UQ53
C	1061	PRO	LEU	conflict	UNP R9UQ53
C	1208	GLN	HIS	conflict	UNP R9UQ53
C	1291	SER	-	insertion	UNP R9UQ53
C	1292	ARG	-	insertion	UNP R9UQ53
C	1293	GLU	-	insertion	UNP R9UQ53
C	1294	ASN	-	insertion	UNP R9UQ53

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1295	LEU	-	insertion	UNP R9UQ53
C	1297	PHE	-	insertion	UNP R9UQ53
C	1298	GLN	-	insertion	UNP R9UQ53
C	1299	GLY	-	insertion	UNP R9UQ53
C	1300	GLY	-	insertion	UNP R9UQ53
C	1301	GLY	TYR	conflict	UNP R9UQ53
C	1302	SER	ASN	conflict	UNP R9UQ53
C	1303	ALA	LYS	conflict	UNP R9UQ53
C	1304	GLY	TRP	conflict	UNP R9UQ53
C	1305	SER	PRO	conflict	UNP R9UQ53
C	1306	GLY	TRP	conflict	UNP R9UQ53
C	1309	PRO	TRP	conflict	UNP R9UQ53
C	1310	GLU	LEU	conflict	UNP R9UQ53
C	1311	ALA	GLY	conflict	UNP R9UQ53
C	1312	PRO	PHE	conflict	UNP R9UQ53
C	1313	ARG	ILE	conflict	UNP R9UQ53
C	1314	ASP	ALA	conflict	UNP R9UQ53
C	1316	GLN	LEU	conflict	UNP R9UQ53
C	1317	ALA	VAL	conflict	UNP R9UQ53
C	1318	TYR	ALA	conflict	UNP R9UQ53
C	1319	VAL	LEU	conflict	UNP R9UQ53
C	1320	ARG	ALA	conflict	UNP R9UQ53
C	1321	LYS	LEU	conflict	UNP R9UQ53
C	1322	ASP	CYS	conflict	UNP R9UQ53
C	1323	GLY	VAL	conflict	UNP R9UQ53
C	1324	GLU	PHE	conflict	UNP R9UQ53
C	1325	TRP	PHE	conflict	UNP R9UQ53
C	1326	VAL	ILE	conflict	UNP R9UQ53
C	1328	LEU	CYS	conflict	UNP R9UQ53
C	1329	SER	CYS	conflict	UNP R9UQ53
C	1331	PHE	GLY	conflict	UNP R9UQ53
C	1332	LEU	CYS	conflict	UNP R9UQ53
C	1334	HIS	-	expression tag	UNP R9UQ53
C	1335	HIS	-	expression tag	UNP R9UQ53
C	1336	HIS	-	expression tag	UNP R9UQ53
C	1337	HIS	-	expression tag	UNP R9UQ53
C	1338	HIS	-	expression tag	UNP R9UQ53
C	1339	HIS	-	expression tag	UNP R9UQ53
C	1340	TRP	-	expression tag	UNP R9UQ53
C	1341	SER	-	expression tag	UNP R9UQ53
C	1342	HIS	-	expression tag	UNP R9UQ53
C	1343	PRO	-	expression tag	UNP R9UQ53

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1344	GLN	-	expression tag	UNP R9UQ53
C	1345	PHE	-	expression tag	UNP R9UQ53
C	1346	GLU	-	expression tag	UNP R9UQ53
C	1347	LYS	-	expression tag	UNP R9UQ53
E	748	SER	ARG	conflict	UNP R9UQ53
E	751	GLY	ARG	conflict	UNP R9UQ53
E	1020	GLN	ARG	conflict	UNP R9UQ53
E	1060	PRO	VAL	conflict	UNP R9UQ53
E	1061	PRO	LEU	conflict	UNP R9UQ53
E	1208	GLN	HIS	conflict	UNP R9UQ53
E	1291	SER	-	insertion	UNP R9UQ53
E	1292	ARG	-	insertion	UNP R9UQ53
E	1293	GLU	-	insertion	UNP R9UQ53
E	1294	ASN	-	insertion	UNP R9UQ53
E	1295	LEU	-	insertion	UNP R9UQ53
E	1297	PHE	-	insertion	UNP R9UQ53
E	1298	GLN	-	insertion	UNP R9UQ53
E	1299	GLY	-	insertion	UNP R9UQ53
E	1300	GLY	-	insertion	UNP R9UQ53
E	1301	GLY	TYR	conflict	UNP R9UQ53
E	1302	SER	ASN	conflict	UNP R9UQ53
E	1303	ALA	LYS	conflict	UNP R9UQ53
E	1304	GLY	TRP	conflict	UNP R9UQ53
E	1305	SER	PRO	conflict	UNP R9UQ53
E	1306	GLY	TRP	conflict	UNP R9UQ53
E	1309	PRO	TRP	conflict	UNP R9UQ53
E	1310	GLU	LEU	conflict	UNP R9UQ53
E	1311	ALA	GLY	conflict	UNP R9UQ53
E	1312	PRO	PHE	conflict	UNP R9UQ53
E	1313	ARG	ILE	conflict	UNP R9UQ53
E	1314	ASP	ALA	conflict	UNP R9UQ53
E	1316	GLN	LEU	conflict	UNP R9UQ53
E	1317	ALA	VAL	conflict	UNP R9UQ53
E	1318	TYR	ALA	conflict	UNP R9UQ53
E	1319	VAL	LEU	conflict	UNP R9UQ53
E	1320	ARG	ALA	conflict	UNP R9UQ53
E	1321	LYS	LEU	conflict	UNP R9UQ53
E	1322	ASP	CYS	conflict	UNP R9UQ53
E	1323	GLY	VAL	conflict	UNP R9UQ53
E	1324	GLU	PHE	conflict	UNP R9UQ53
E	1325	TRP	PHE	conflict	UNP R9UQ53
E	1326	VAL	ILE	conflict	UNP R9UQ53

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1328	LEU	CYS	conflict	UNP R9UQ53
E	1329	SER	CYS	conflict	UNP R9UQ53
E	1331	PHE	GLY	conflict	UNP R9UQ53
E	1332	LEU	CYS	conflict	UNP R9UQ53
E	1334	HIS	-	expression tag	UNP R9UQ53
E	1335	HIS	-	expression tag	UNP R9UQ53
E	1336	HIS	-	expression tag	UNP R9UQ53
E	1337	HIS	-	expression tag	UNP R9UQ53
E	1338	HIS	-	expression tag	UNP R9UQ53
E	1339	HIS	-	expression tag	UNP R9UQ53
E	1340	TRP	-	expression tag	UNP R9UQ53
E	1341	SER	-	expression tag	UNP R9UQ53
E	1342	HIS	-	expression tag	UNP R9UQ53
E	1343	PRO	-	expression tag	UNP R9UQ53
E	1344	GLN	-	expression tag	UNP R9UQ53
E	1345	PHE	-	expression tag	UNP R9UQ53
E	1346	GLU	-	expression tag	UNP R9UQ53
E	1347	LYS	-	expression tag	UNP R9UQ53

- Molecule 2 is a protein called VHH-T148.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	128	Total	C	N	O	S	0	0
			973	609	160	197	7		
2	D	128	Total	C	N	O	S	0	0
			973	609	160	197	7		
2	F	128	Total	C	N	O	S	0	0
			973	609	160	197	7		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
3	G	4	Total	C	N	O	0	0
			50	28	2	20		
3	H	4	Total	C	N	O	0	0
			50	28	2	20		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	I	4	50	28	2	20	0	0



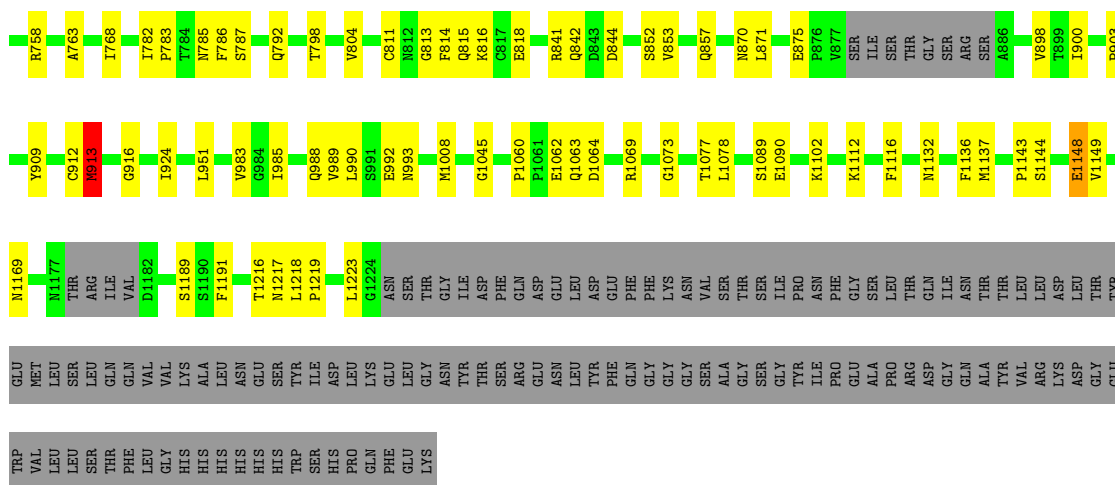


PRO	GLN	PHE	GLU	LYS	LEU	LYS	ASN	GLN	GLY	ASP	GLU	LEU	LEU	THR	PHE	GLN	GLY	GLY	GLY	ASN	GLY	GLY	ASN	VAL	ALA	SER	THR	GLY	ILE	PRO	GLU	ALA	SER	PRO	ARG	THR	ASN	GLN	GLY	ALA	THR	TYR	VAL	LEU	LEU	LYS	ASP	GLY	GLU	TRP	VAL	VAL	LEU	LEU	SER	THR	PHE	LEU	GLY	HIS	HIS	HIS	TRP	SER	HIS
L1223	G1224	ASN	SER	THR	GLY	ILE	ASP	PHE	GLN	ASP	GLU	LEU	P1061	E1062	Q1063	D1064	R1069	G1073	T1077	L1078	S1089	E1090	K1102	K1112	F1116	N1132	F1136	M1137	P1143	S1144	E1148	V1149	N1169	N1177	THR	ARG	ILE	VAL	D1182	S1189	T1216	N1217	L1218	P1219	ASN	GLU	THR	ILE	ASP	GLN	GLY	VAL	LYS	ALA	LEU	ASN	GLU	HIS	TRP	SER	HIS				
Q988	Y989	E992	N993	M1008	G1045	P1060	F1061	E1062	Q1063	D1064	R1069	G1073	T1077	L1078	S1089	E1090	K1102	K1112	F1116	N1132	F1136	M1137	P1143	S1144	E1148	V1149	N1169	N1177	THR	ARG	ILE	VAL	D1182	S1189	T1216	N1217	L1218	P1219	ASN	GLU	THR	ILE	ASP	GLN	GLY	VAL	LYS	ALA	LEU	ASN	GLU	HIS	TRP	SER	HIS										
Q792	T798	V804	C811	H812	G813	F814	Q815	K816	R841	Q842	D843	D844	S852	V853	Q857	N870	L871	E875	P876	R877	SER	ILE	SER	THR	GLY	THR	ARG	SER	A886	V898	T899	I900	P903	Y909	C912	M913	G916	I924	L951	N951	V983	G984	I985	ASN	GLU	THR	ILE	ASP	GLN	GLY	VAL	LYS	ALA	LEU	ASN	GLU	HIS	TRP	SER	HIS					
Q636	V655	S656	V657	I662	K665	H670	F674	V677	Q688	D843	D844	R691	K698	R699	R700	ASP	SER	THR	TYR	G705	F723	D726	P739	D740	T741	PRO	SER	SER	A886	V898	T899	I900	P903	Y909	C912	M913	G916	I924	L951	N951	V983	G984	I985	ASN	GLU	THR	ILE	ASP	GLN	GLY	VAL	LYS	ALA	LEU	ASN	GLU	HIS	TRP	SER	HIS					
H486	K496	S497	S498	Y499	I500	N501	K502	L506	L507	S508	D509	I529	V530	V534	W535	E536	D539	R542	W553	L554	S557	G558	S559	T560	V561	A562	M563	Q566	L567	Q568	F571	C585	P586	K587	I596	E605	R614	C620	V623	N785	Q627	ASN	GLU	THR	ILE	ASP	GLN	GLY	VAL	LYS	ALA	LEU	ASN	GLU	HIS	TRP	SER	HIS							
I131	R141	N155	M161	G162	R163	F165	D174	L179	Y351	C185	I186	L187	E188	P189	R190	N193	A197	S203	A223	S224	E230	Y231	F232	C237	M240	Y241	T242	W253	T259	A260	Q261	H264	L273	Y274	M278	I295	I300	I303	ASN	GLU	THR	ILE	ASP	GLN	GLY	VAL	LYS	ALA	LEU	ASN	GLU	HIS	TRP	SER	HIS										
MET	ILE	HIS	SER	VAL	PHE	LEU	LEU	MET	PHE	LEU	LEU	THR	PRO	THR	GLU	SER	Y18	A29	V33	D34	I35	F40	V50	R62	S65	R66	I67	T68	I69	T70	Q78	M84	Y85	V86	A92	T93	G94	T95	Q98	R99	L100	F112	G115	F116	V117	V130																			

● Molecule 1: Spike glycoprotein

Chain E:  71% 16% 12%

MET	ILE	HIS	SER	VAL	PHE	LEU	LEU	MET	PHE	LEU	LEU	THR	PRO	THR	GLU	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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- Molecule 2: VHH-T148

Chain A: 75% 20% 5%



- Molecule 2: VHH-T148

Chain D: 74% 21% 5%



HIS

- Molecule 2: VHH-T148

Chain F: 75% 20% 5%



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

Chain G: 100%

MAG1  
MAG2  
BWA3  
MAN4

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

Chain H: 100%

NAG1  
NAG2  
BMA3  
MAN4

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

Chain I:

100%

NAG1  
NAG2  
BMA3  
MAN4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	B	0.47	0/9336	0.57	6/12701 (0.0%)
1	C	0.47	0/9336	0.57	6/12701 (0.0%)
1	E	0.47	0/9336	0.57	6/12701 (0.0%)
2	A	0.35	0/994	0.50	0/1346
2	D	0.35	0/994	0.50	0/1346
2	F	0.34	0/994	0.50	0/1346
All	All	0.46	0/30990	0.56	18/42141 (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	B	0	3
1	C	0	3
1	E	0	3
All	All	0	9

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	913	MET	CA-CB-CG	9.47	129.40	113.30
1	C	913	MET	CA-CB-CG	9.44	129.35	113.30
1	B	913	MET	CA-CB-CG	9.44	129.34	113.30
1	C	237	CYS	CA-CB-SG	9.00	130.21	114.00
1	B	237	CYS	CA-CB-SG	8.99	130.19	114.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1148	GLU	Peptide
1	B	237	CYS	Peptide
1	B	361	TYR	Peptide
1	C	237	CYS	Peptide
1	C	361	TYR	Peptide

## 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	B	9124	0	8818	137	0
1	C	9124	0	8818	138	0
1	E	9124	0	8818	141	0
2	A	973	0	916	17	0
2	D	973	0	916	17	0
2	F	973	0	916	17	0
3	G	50	0	43	3	0
3	H	50	0	43	2	0
3	I	50	0	43	3	0
All	All	30441	0	29331	451	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 8.

The worst 5 of 451 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:C:483:THR:HG22	1:C:568:GLN:HG2	1.65	0.79
1:B:483:THR:HG22	1:B:568:GLN:HG2	1.65	0.78
1:C:506:LEU:HB2	1:C:553:TRP:HB2	1.66	0.78
1:E:483:THR:HG22	1:E:568:GLN:HG2	1.65	0.78
1:E:95:THR:HA	1:E:303:ILE:HD12	1.66	0.77

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 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	B	1170/1347 (87%)	1091 (93%)	77 (7%)	2 (0%)	44	71
1	C	1170/1347 (87%)	1091 (93%)	77 (7%)	2 (0%)	44	71
1	E	1170/1347 (87%)	1090 (93%)	78 (7%)	2 (0%)	44	71
2	A	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
2	D	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
2	F	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
All	All	3888/4446 (87%)	3643 (94%)	239 (6%)	6 (0%)	45	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1149	VAL
1	C	1149	VAL
1	E	1149	VAL
1	B	1148	GLU
1	C	1148	GLU

### 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	B	1013/1163 (87%)	999 (99%)	14 (1%)	62	86
1	C	1013/1163 (87%)	1000 (99%)	13 (1%)	65	88
1	E	1013/1163 (87%)	1000 (99%)	13 (1%)	65	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	105/112 (94%)	105 (100%)	0	100	100
2	D	105/112 (94%)	105 (100%)	0	100	100
2	F	105/112 (94%)	105 (100%)	0	100	100
All	All	3354/3825 (88%)	3314 (99%)	40 (1%)	66	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	240	MET
1	E	698	LYS
1	E	352	GLU
1	E	502	LYS
1	E	852	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1146	HIS
1	C	1146	HIS
1	E	1146	HIS

### 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 ⓘ

12 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	G	1	3,1	14,14,15	0.34	0	17,19,21	0.43	0
3	NAG	G	2	3	14,14,15	0.52	0	17,19,21	0.36	0
3	BMA	G	3	3	11,11,12	0.84	0	15,15,17	1.51	2 (13%)
3	MAN	G	4	3	11,11,12	0.63	0	15,15,17	1.39	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.34	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.54	0	17,19,21	0.38	0
3	BMA	H	3	3	11,11,12	0.85	0	15,15,17	1.50	2 (13%)
3	MAN	H	4	3	11,11,12	0.62	0	15,15,17	1.40	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.32	0	17,19,21	0.43	0
3	NAG	I	2	3	14,14,15	0.53	0	17,19,21	0.38	0
3	BMA	I	3	3	11,11,12	0.84	0	15,15,17	1.51	2 (13%)
3	MAN	I	4	3	11,11,12	0.61	0	15,15,17	1.39	2 (13%)

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	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-C2-C3	4.07	114.66	109.67
3	I	3	BMA	C1-C2-C3	4.06	114.66	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-C2-C3	4.02	114.61	109.67
3	H	4	MAN	C1-O5-C5	3.66	117.15	112.19
3	G	4	MAN	C1-O5-C5	3.61	117.08	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

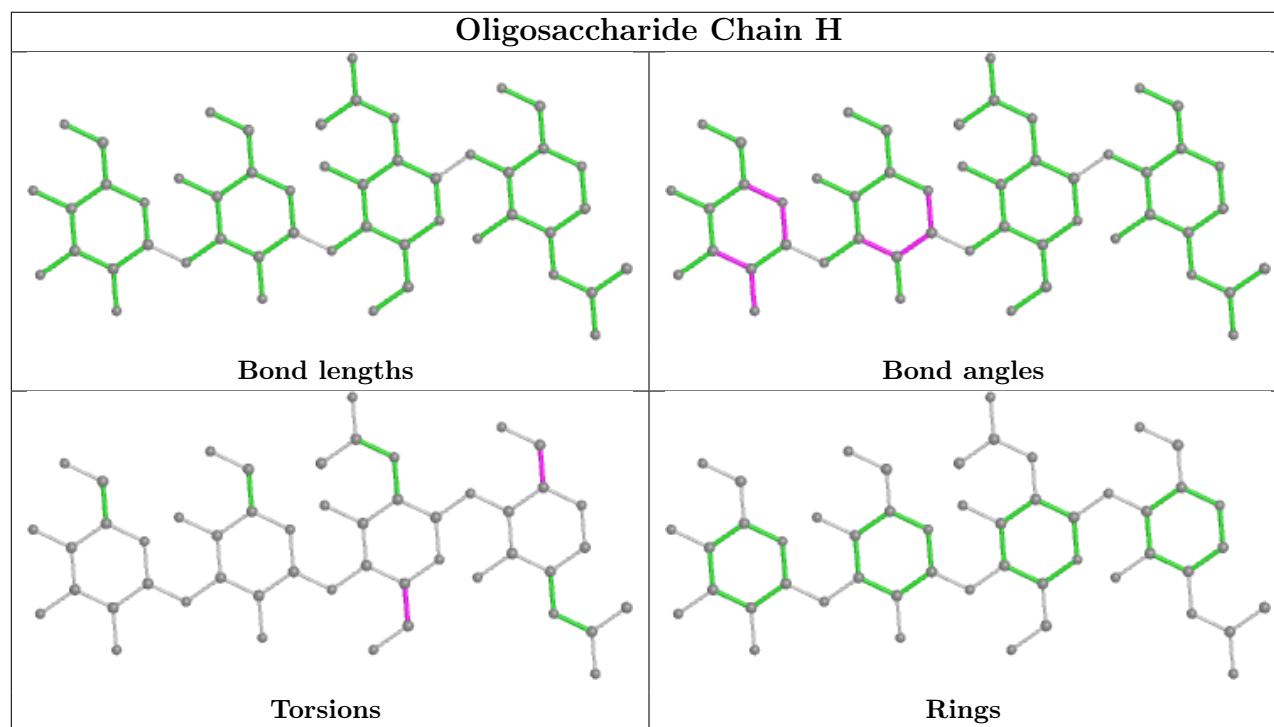
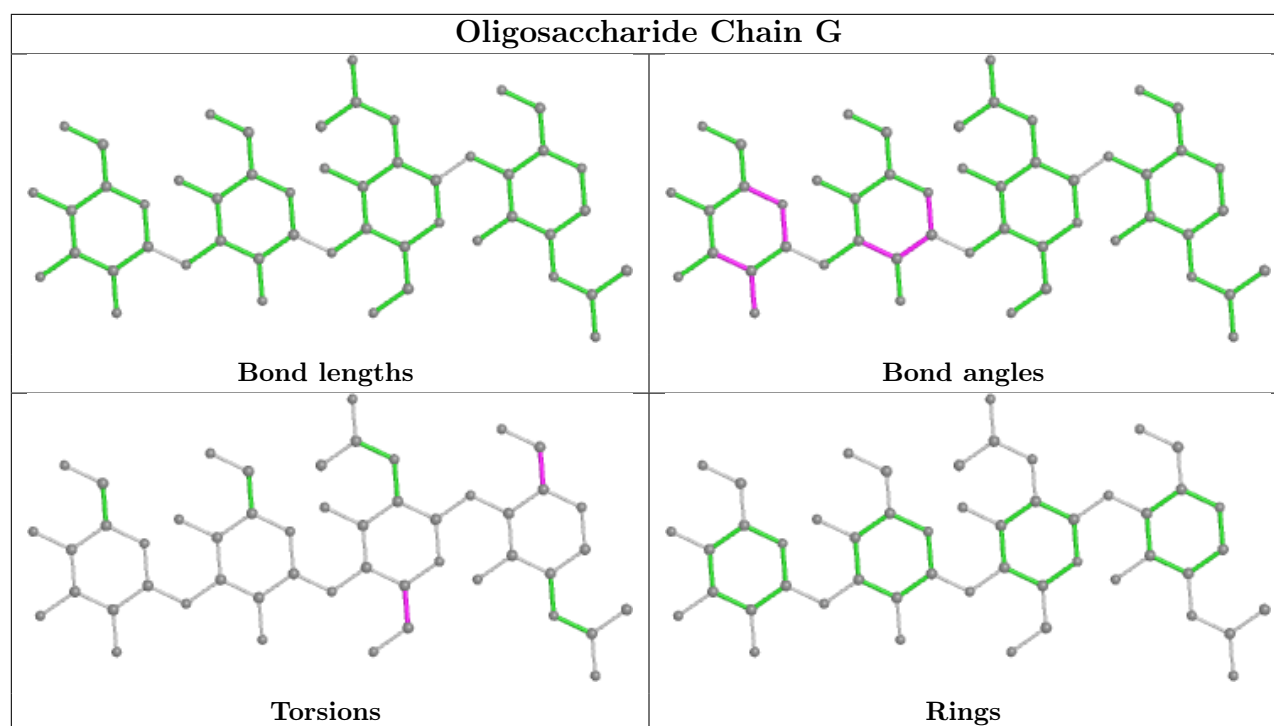
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

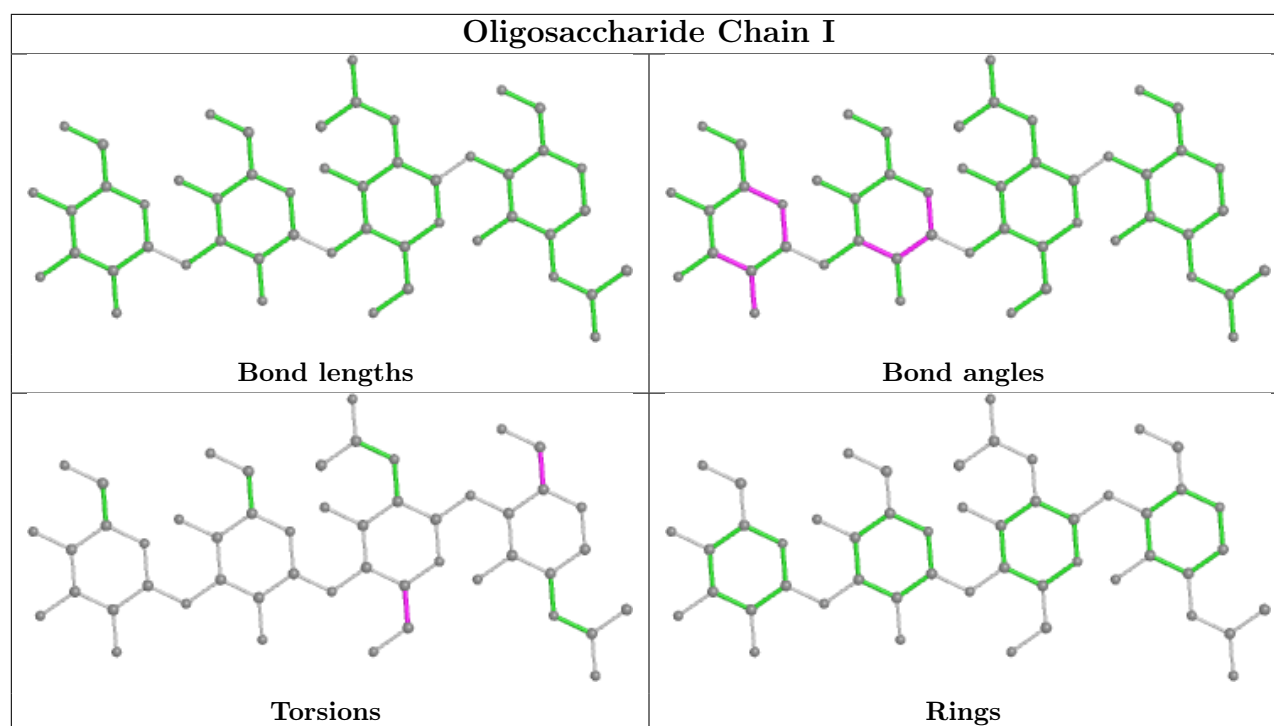
There are no ring outliers.

6 monomers are involved in 8 short contacts:

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

There are no ligands in this entry.

## 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.