



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 1, 2017 – 06:49 PM EDT

PDB ID : 5W9H  
EMDB ID: : EMD-8783  
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4  
Authors : Pallesen, J.; Ward, A.B.  
Deposited on : unknown  
Resolution : 4.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

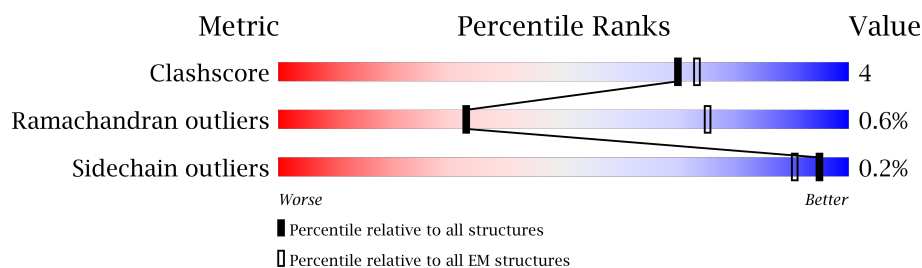
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1329	
1	D	1329	
1	G	1329	
1	p	1329	
1	q	1329	
1	r	1329	
2	B	233	
2	E	233	
2	H	233	

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Mol	Chain	Length	Quality of chain
3	C	218	<div><div></div><div>50%</div><div></div><div>49%</div></div>
3	F	218	<div><div></div><div>50%</div><div></div><div>49%</div></div>
3	I	218	<div><div></div><div>50%</div><div></div><div>49%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33840 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 MERS S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	D	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	G	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	p	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	q	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	r	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
D	506	PHE	LEU	conflict	UNP W5ZZF5
D	748	ALA	ARG	conflict	UNP W5ZZF5
D	751	GLY	ARG	conflict	UNP W5ZZF5
D	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
D	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
D	1292	GLY	-	expression tag	UNP W5ZZF5
D	1293	SER	-	expression tag	UNP W5ZZF5
D	1294	GLY	-	expression tag	UNP W5ZZF5
D	1295	TYR	-	expression tag	UNP W5ZZF5
D	1296	ILE	-	expression tag	UNP W5ZZF5
D	1297	PRO	-	expression tag	UNP W5ZZF5
D	1298	GLU	-	expression tag	UNP W5ZZF5
D	1299	ALA	-	expression tag	UNP W5ZZF5
D	1300	PRO	-	expression tag	UNP W5ZZF5
D	1301	ARG	-	expression tag	UNP W5ZZF5
D	1302	ASP	-	expression tag	UNP W5ZZF5
D	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1304	GLN	-	expression tag	UNP W5ZZF5
D	1305	ALA	-	expression tag	UNP W5ZZF5
D	1306	TYR	-	expression tag	UNP W5ZZF5
D	1307	VAL	-	expression tag	UNP W5ZZF5
D	1308	ARG	-	expression tag	UNP W5ZZF5
D	1309	LYS	-	expression tag	UNP W5ZZF5
D	1310	ASP	-	expression tag	UNP W5ZZF5
D	1311	GLY	-	expression tag	UNP W5ZZF5
D	1312	GLU	-	expression tag	UNP W5ZZF5
D	1313	TRP	-	expression tag	UNP W5ZZF5
D	1314	VAL	-	expression tag	UNP W5ZZF5
D	1315	LEU	-	expression tag	UNP W5ZZF5
D	1316	LEU	-	expression tag	UNP W5ZZF5
D	1317	SER	-	expression tag	UNP W5ZZF5
D	1318	THR	-	expression tag	UNP W5ZZF5
D	1319	PHE	-	expression tag	UNP W5ZZF5
D	1320	LEU	-	expression tag	UNP W5ZZF5
D	1321	GLY	-	expression tag	UNP W5ZZF5
D	1322	ARG	-	expression tag	UNP W5ZZF5
D	1323	SER	-	expression tag	UNP W5ZZF5
D	1324	LEU	-	expression tag	UNP W5ZZF5
D	1325	GLU	-	expression tag	UNP W5ZZF5
D	1326	VAL	-	expression tag	UNP W5ZZF5
D	1327	LEU	-	expression tag	UNP W5ZZF5
D	1328	PHE	-	expression tag	UNP W5ZZF5
D	1329	GLN	-	expression tag	UNP W5ZZF5
G	506	PHE	LEU	conflict	UNP W5ZZF5
G	748	ALA	ARG	conflict	UNP W5ZZF5
G	751	GLY	ARG	conflict	UNP W5ZZF5
G	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
G	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
G	1292	GLY	-	expression tag	UNP W5ZZF5
G	1293	SER	-	expression tag	UNP W5ZZF5
G	1294	GLY	-	expression tag	UNP W5ZZF5
G	1295	TYR	-	expression tag	UNP W5ZZF5
G	1296	ILE	-	expression tag	UNP W5ZZF5
G	1297	PRO	-	expression tag	UNP W5ZZF5
G	1298	GLU	-	expression tag	UNP W5ZZF5
G	1299	ALA	-	expression tag	UNP W5ZZF5
G	1300	PRO	-	expression tag	UNP W5ZZF5
G	1301	ARG	-	expression tag	UNP W5ZZF5
G	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1303	GLY	-	expression tag	UNP W5ZZF5
G	1304	GLN	-	expression tag	UNP W5ZZF5
G	1305	ALA	-	expression tag	UNP W5ZZF5
G	1306	TYR	-	expression tag	UNP W5ZZF5
G	1307	VAL	-	expression tag	UNP W5ZZF5
G	1308	ARG	-	expression tag	UNP W5ZZF5
G	1309	LYS	-	expression tag	UNP W5ZZF5
G	1310	ASP	-	expression tag	UNP W5ZZF5
G	1311	GLY	-	expression tag	UNP W5ZZF5
G	1312	GLU	-	expression tag	UNP W5ZZF5
G	1313	TRP	-	expression tag	UNP W5ZZF5
G	1314	VAL	-	expression tag	UNP W5ZZF5
G	1315	LEU	-	expression tag	UNP W5ZZF5
G	1316	LEU	-	expression tag	UNP W5ZZF5
G	1317	SER	-	expression tag	UNP W5ZZF5
G	1318	THR	-	expression tag	UNP W5ZZF5
G	1319	PHE	-	expression tag	UNP W5ZZF5
G	1320	LEU	-	expression tag	UNP W5ZZF5
G	1321	GLY	-	expression tag	UNP W5ZZF5
G	1322	ARG	-	expression tag	UNP W5ZZF5
G	1323	SER	-	expression tag	UNP W5ZZF5
G	1324	LEU	-	expression tag	UNP W5ZZF5
G	1325	GLU	-	expression tag	UNP W5ZZF5
G	1326	VAL	-	expression tag	UNP W5ZZF5
G	1327	LEU	-	expression tag	UNP W5ZZF5
G	1328	PHE	-	expression tag	UNP W5ZZF5
G	1329	GLN	-	expression tag	UNP W5ZZF5
p	506	PHE	LEU	conflict	UNP W5ZZF5
p	748	ALA	ARG	conflict	UNP W5ZZF5
p	751	GLY	ARG	conflict	UNP W5ZZF5
p	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
p	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
p	1292	GLY	-	expression tag	UNP W5ZZF5
p	1293	SER	-	expression tag	UNP W5ZZF5
p	1294	GLY	-	expression tag	UNP W5ZZF5
p	1295	TYR	-	expression tag	UNP W5ZZF5
p	1296	ILE	-	expression tag	UNP W5ZZF5
p	1297	PRO	-	expression tag	UNP W5ZZF5
p	1298	GLU	-	expression tag	UNP W5ZZF5
p	1299	ALA	-	expression tag	UNP W5ZZF5
p	1300	PRO	-	expression tag	UNP W5ZZF5
p	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
p	1302	ASP	-	expression tag	UNP W5ZZF5
p	1303	GLY	-	expression tag	UNP W5ZZF5
p	1304	GLN	-	expression tag	UNP W5ZZF5
p	1305	ALA	-	expression tag	UNP W5ZZF5
p	1306	TYR	-	expression tag	UNP W5ZZF5
p	1307	VAL	-	expression tag	UNP W5ZZF5
p	1308	ARG	-	expression tag	UNP W5ZZF5
p	1309	LYS	-	expression tag	UNP W5ZZF5
p	1310	ASP	-	expression tag	UNP W5ZZF5
p	1311	GLY	-	expression tag	UNP W5ZZF5
p	1312	GLU	-	expression tag	UNP W5ZZF5
p	1313	TRP	-	expression tag	UNP W5ZZF5
p	1314	VAL	-	expression tag	UNP W5ZZF5
p	1315	LEU	-	expression tag	UNP W5ZZF5
p	1316	LEU	-	expression tag	UNP W5ZZF5
p	1317	SER	-	expression tag	UNP W5ZZF5
p	1318	THR	-	expression tag	UNP W5ZZF5
p	1319	PHE	-	expression tag	UNP W5ZZF5
p	1320	LEU	-	expression tag	UNP W5ZZF5
p	1321	GLY	-	expression tag	UNP W5ZZF5
p	1322	ARG	-	expression tag	UNP W5ZZF5
p	1323	SER	-	expression tag	UNP W5ZZF5
p	1324	LEU	-	expression tag	UNP W5ZZF5
p	1325	GLU	-	expression tag	UNP W5ZZF5
p	1326	VAL	-	expression tag	UNP W5ZZF5
p	1327	LEU	-	expression tag	UNP W5ZZF5
p	1328	PHE	-	expression tag	UNP W5ZZF5
p	1329	GLN	-	expression tag	UNP W5ZZF5
q	506	PHE	LEU	conflict	UNP W5ZZF5
q	748	ALA	ARG	conflict	UNP W5ZZF5
q	751	GLY	ARG	conflict	UNP W5ZZF5
q	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
q	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
q	1292	GLY	-	expression tag	UNP W5ZZF5
q	1293	SER	-	expression tag	UNP W5ZZF5
q	1294	GLY	-	expression tag	UNP W5ZZF5
q	1295	TYR	-	expression tag	UNP W5ZZF5
q	1296	ILE	-	expression tag	UNP W5ZZF5
q	1297	PRO	-	expression tag	UNP W5ZZF5
q	1298	GLU	-	expression tag	UNP W5ZZF5
q	1299	ALA	-	expression tag	UNP W5ZZF5
q	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
q	1301	ARG	-	expression tag	UNP W5ZZF5
q	1302	ASP	-	expression tag	UNP W5ZZF5
q	1303	GLY	-	expression tag	UNP W5ZZF5
q	1304	GLN	-	expression tag	UNP W5ZZF5
q	1305	ALA	-	expression tag	UNP W5ZZF5
q	1306	TYR	-	expression tag	UNP W5ZZF5
q	1307	VAL	-	expression tag	UNP W5ZZF5
q	1308	ARG	-	expression tag	UNP W5ZZF5
q	1309	LYS	-	expression tag	UNP W5ZZF5
q	1310	ASP	-	expression tag	UNP W5ZZF5
q	1311	GLY	-	expression tag	UNP W5ZZF5
q	1312	GLU	-	expression tag	UNP W5ZZF5
q	1313	TRP	-	expression tag	UNP W5ZZF5
q	1314	VAL	-	expression tag	UNP W5ZZF5
q	1315	LEU	-	expression tag	UNP W5ZZF5
q	1316	LEU	-	expression tag	UNP W5ZZF5
q	1317	SER	-	expression tag	UNP W5ZZF5
q	1318	THR	-	expression tag	UNP W5ZZF5
q	1319	PHE	-	expression tag	UNP W5ZZF5
q	1320	LEU	-	expression tag	UNP W5ZZF5
q	1321	GLY	-	expression tag	UNP W5ZZF5
q	1322	ARG	-	expression tag	UNP W5ZZF5
q	1323	SER	-	expression tag	UNP W5ZZF5
q	1324	LEU	-	expression tag	UNP W5ZZF5
q	1325	GLU	-	expression tag	UNP W5ZZF5
q	1326	VAL	-	expression tag	UNP W5ZZF5
q	1327	LEU	-	expression tag	UNP W5ZZF5
q	1328	PHE	-	expression tag	UNP W5ZZF5
q	1329	GLN	-	expression tag	UNP W5ZZF5
r	506	PHE	LEU	conflict	UNP W5ZZF5
r	748	ALA	ARG	conflict	UNP W5ZZF5
r	751	GLY	ARG	conflict	UNP W5ZZF5
r	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
r	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
r	1292	GLY	-	expression tag	UNP W5ZZF5
r	1293	SER	-	expression tag	UNP W5ZZF5
r	1294	GLY	-	expression tag	UNP W5ZZF5
r	1295	TYR	-	expression tag	UNP W5ZZF5
r	1296	ILE	-	expression tag	UNP W5ZZF5
r	1297	PRO	-	expression tag	UNP W5ZZF5
r	1298	GLU	-	expression tag	UNP W5ZZF5
r	1299	ALA	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
r	1300	PRO	-	expression tag	UNP W5ZZF5
r	1301	ARG	-	expression tag	UNP W5ZZF5
r	1302	ASP	-	expression tag	UNP W5ZZF5
r	1303	GLY	-	expression tag	UNP W5ZZF5
r	1304	GLN	-	expression tag	UNP W5ZZF5
r	1305	ALA	-	expression tag	UNP W5ZZF5
r	1306	TYR	-	expression tag	UNP W5ZZF5
r	1307	VAL	-	expression tag	UNP W5ZZF5
r	1308	ARG	-	expression tag	UNP W5ZZF5
r	1309	LYS	-	expression tag	UNP W5ZZF5
r	1310	ASP	-	expression tag	UNP W5ZZF5
r	1311	GLY	-	expression tag	UNP W5ZZF5
r	1312	GLU	-	expression tag	UNP W5ZZF5
r	1313	TRP	-	expression tag	UNP W5ZZF5
r	1314	VAL	-	expression tag	UNP W5ZZF5
r	1315	LEU	-	expression tag	UNP W5ZZF5
r	1316	LEU	-	expression tag	UNP W5ZZF5
r	1317	SER	-	expression tag	UNP W5ZZF5
r	1318	THR	-	expression tag	UNP W5ZZF5
r	1319	PHE	-	expression tag	UNP W5ZZF5
r	1320	LEU	-	expression tag	UNP W5ZZF5
r	1321	GLY	-	expression tag	UNP W5ZZF5
r	1322	ARG	-	expression tag	UNP W5ZZF5
r	1323	SER	-	expression tag	UNP W5ZZF5
r	1324	LEU	-	expression tag	UNP W5ZZF5
r	1325	GLU	-	expression tag	UNP W5ZZF5
r	1326	VAL	-	expression tag	UNP W5ZZF5
r	1327	LEU	-	expression tag	UNP W5ZZF5
r	1328	PHE	-	expression tag	UNP W5ZZF5
r	1329	GLN	-	expression tag	UNP W5ZZF5

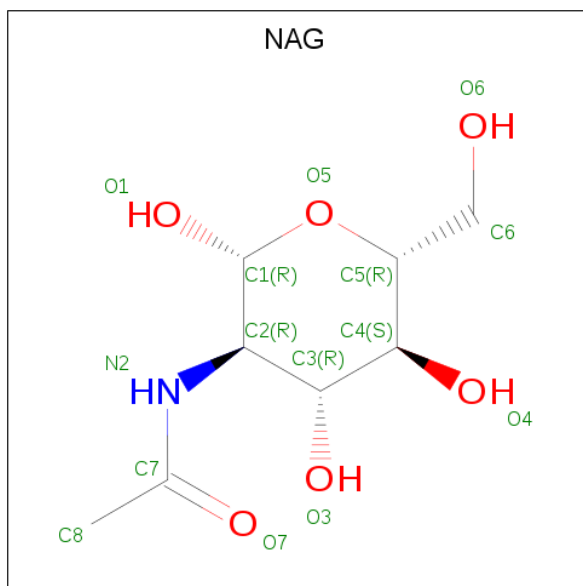
- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	F	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	I	111	Total	C	N	O	S	0	0
			835	522	143	166	4		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	D	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	G	1	Total 126	72	9	45	0
4	p	1	Total 168	96	12	60	0
4	p	1	Total 168	96	12	60	0
4	p	1	Total 168	96	12	60	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	p	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0
4	q	1	168	96	12	60	0

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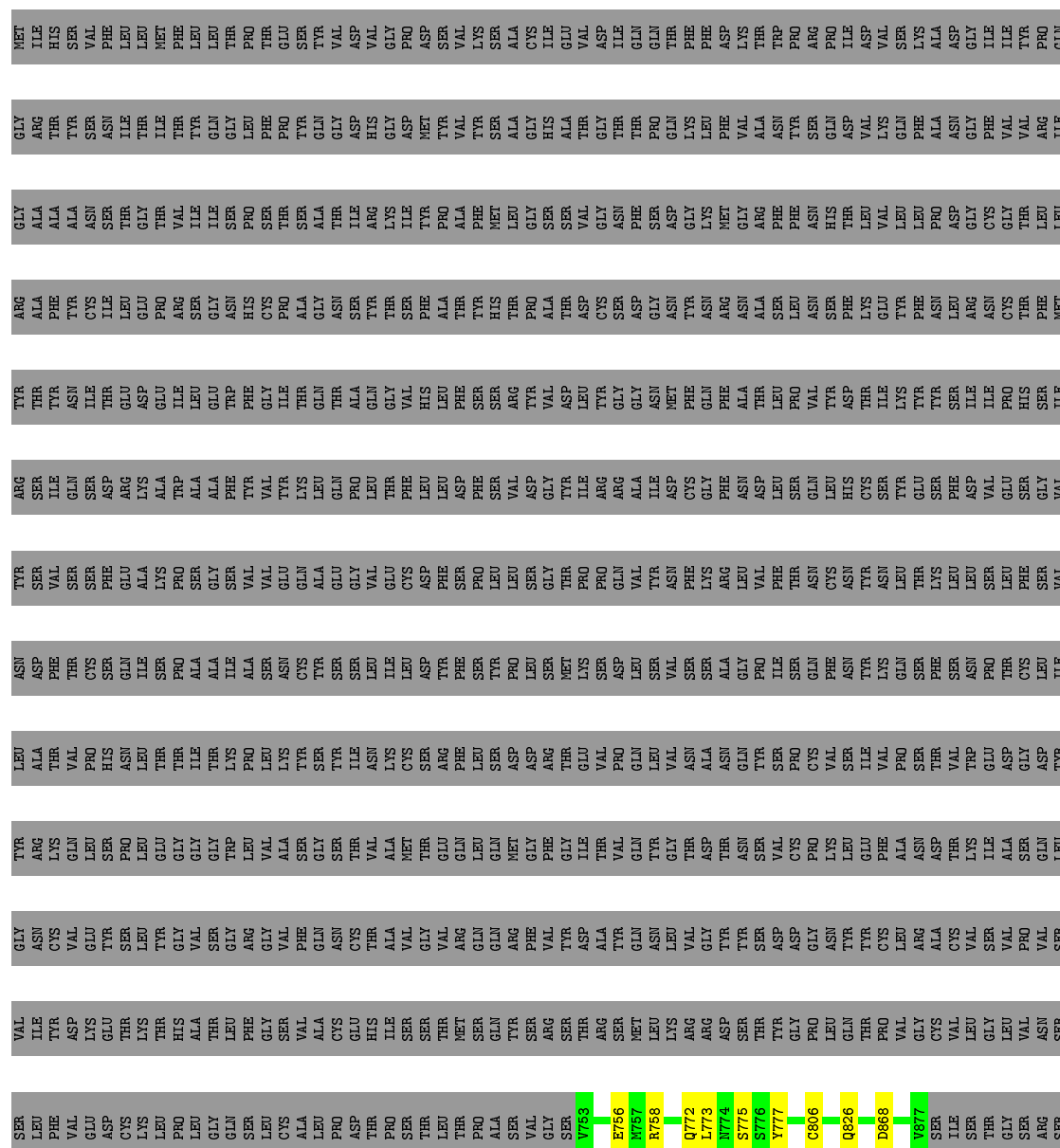
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Mol	Chain	Residues	Atoms				AltConf
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0
4	r	1	Total 168	C 96	N 12	O 60	0





Chain D:  32% . 65%





ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER SER THR PHE LEU GLY ARG SER SER LEU GLU VAL LEU PHE GLN

- Molecule 1: MERS S

Chain G:  33% 1% 65%

GLY	ARG	THR	THR	TYR	SER	ASN	ILE	THR	THR	THR	TYR	GLN	GLY	GLY	ASP	HIS	GLY	ASP	MET	TYR	VAL	TYR	SER	ALA	ALA	GLY	HIS	ALA	HIS	THR	THR	GLN	GLN	LYS	LEU	PHE	VAL	VAL	VAL	VAL	ARG
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GLY	ALA	ALA	ALA	ASN	SER	THR	THR	VAL	ILE	ILE	ILE	SER	PRO	SER	SER	SER	SER	ALA	THR	THR	ILE	ILE	LYS	ARG	LYS	ILE	TYR	PRO	PRO	ALA	ALA	PHE	MET	LEU	GLY	SER	SER	SER	VAL	GLY	ASN	PHE	SER	SER	ASP	GLY	GLY	LYS	MET	GLY	ARG	PHE	ASN	PHE	THR	LEU	VAL	LEU	LEU	PRO	ASP	GLY	CYS	GLY	THR	LEU
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ARG	PHE	TYR	CYS	ILE	LEU	GLU	PRO	ARG	SER	GLY	ASN	CYS	HIS	TYR	THR	THR	SER	PHE	ALA	ALA	THR	THR	TYR	HIS	HIS	THR	PRO	ALA	ALA	THR	THR	ASP	CYS	SER	ASP	GLY	ASN	TYR	TYR	ASN	ASN	ARG	ASN	ALA	ALA	SER	SER	LEU	SER	ASN	PHE	LYS	GLY	TYR	PHE	ASN	LEU	ARG	ASN	CYS	THR	PHE
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TYR	THR	TYR	ASN	ILE	THR	GLU	ASP	GLU	ILE	LEU	GLU	TRP	THR	GLY	ILE	THR	GLN	THR	ALA	ALA	GLY	VAL	HIS	LEU	LEU	PHE	THR	SER	SER	ARG	TYR	VAL	ASP	LEU	LEU	TYR	GLY	GLY	ASN	MET	PHE	PHE	GLN	PHE	ALA	THR	LEU	THR	PRO	VAL	VAL	TYR	ASP	THR	ILE	LYS	TYR	TYR	SER	ILE	ILE	PRO	HIS	SER
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ARG	SER	ILE	GLN	SER	ASP	ARG	LYS	ALA	TRP	ALA	ALA	PHE	TYR	VAL	VAL	TYR	LYS	GLN	PRO	LEU	THR	PHE	LEU	LEU	ASP	PHE	SER	VAL	ASP	GLY	TYR	ILE	ARG	ARG	ALA	ILE	ASP	CYS	GLY	PHE	ASN	ASP	LEU	SER	SER	GLN	LEU	HIS	CYS	SER	TYR	GLU	GLU	SER	PHE	ASP	VAL	ASP	GLU	SER	GLY
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[illegible]

ASN	ASP	THR	CYS	GLN	PRO	ALA	ALA	ILE	ALA	ASN	CYS	TYR	LEU	LEU	ASP	TYR	PHE	SER	SER	TVR	PRO	LEU	SER	SER	LYS	ASP	LEU	VAL	SER	SER	SER	GLN	PHE	ASN	TYR	GLN	LYS	SER	PHE	ASN	PRO	THR	CYS	LEU
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[illegible]

TYR	ARG	LYS	GLN	LEU	SER	PRO	GLU	GLY	GLY	GLY	TRP	LEU	VAL	ALA	SER	GLY	SER	THR	VAL	VAL	MET	THR	GLU	GLN	LEU	LEU	GLN	GLN	GLY	PHE	GLY	ILE	THR	THR	ASP	THR	ASN	ASN	VAL	VAL	CYS	PRO	LYS	LEU	GLU	PHE	ALA	ALA	ASN	ASP	THR	THR	LYS	ILE	ALA	SER	SER	GLN
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GLY	ASN	CYS	VAL	GILU	TYR	SER	LEU	GLY	TYR	PHE	GLN	CYS	THR	ALA	VAL	GLY	VAL	ARG	GLN	GLN	ARG	ASP	TYR	ALA	TYR	GLN	ASN	LEU	VAL	GLY	TYR	TYR	SER	ASP	ASP	GLY	ASN	TYR	CYS	THR	ALA	ARG	VAL	PRO	VAL
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VAL	ILE	TYR	ASP	LYS	GLU	THR	THR	HIS	ALA	LEU	THR	PHE	GLY	VAL	ALA	CYS	GLU	HIS	ILE	SER	SER	THR	THR	MET	SER	SER	SER	GLN	TYR	SER	ARG	ARG	THR	THR	ARG	SER	SER	MET	LYS	ARG	ARG	ASP	SER	THR	TYR	GLY	PRO	LEU	GLN	LEU	THR	THR	PRO	VAL	VAL	GLY	CYS	VAL	LEU	LEU	LEU	VAL	ASN
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SER	LEU	PHE	VAL	GLU	ASP	CYS	LYS	LEU	PRO	LEU	GLY	GLN	SER	SER	LEU	CYS	ALA	LEU	ASP	ASP	THR	PRO	SER	THR	THR	THR	PRO	THR	ALA	SER	VAL	GLY	GLY	<b>V753</b>	<b>M774</b>	<b>C806</b>	<b>Q826</b>	<b>R841</b>	<b>D868</b>	<b>T872</b>	<b>V877</b>	SER	ILE	SER	THR	GLY	SER	ARG	SER	<b>A886</b>	<b>R887</b>	<b>Y905</b>
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C912	Y932	P936	T961	F1001	G1120 T1121	N1145	M1160 P1161 T1162	V1209	P1220	L1223	GLY	ASN	SER	THR	GLY	ILE	ASP	PHE	GLN	ASP	GLU	LEU	GLU	ASP	GLU	PHE	PHE	LYS	VAL	ASN	SER	THR	SER	ILE	PRO	ASN	PHE	PHE	GLY	GLY	LEU	THR	GLN	ILE	ASN	THR
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LEU	LEU	ASP	THR	TYR	GLU	LEU	SER	LEU	GLN	GLN	VAL	VAL	LYS	ALA	LEU	ASN	GLU	SER	TYR	ILE	ASP	LYS	GLU	LEU	GLY	SER	GLY	TYR	ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	SER
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- Molecule 1: MERS S

Chain r:

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TRP	THR	ASP	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	SER	MET	SER	SER	THR	LEU	THR	LEU	THR	LYS	ASP	GLU	TYR	GLU	ARG	HIS	ASN	SER	TYR	THR	CYS	GLU	ALA	THR	HIS	LYS	THR	SER	THR	SER	PRO	ILE	VAL	LYS	SER	PHE	ASN	ARG	ASN	GLU	CYS
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● Molecule 3: G4 VL



B1	P77	R96	K107	ARG	THR	ASP	ALA	ALA	PRO	THR	THR	VAL	ILE	PHE	PRO	PRO	SER	SER	GLU	GLN	LEU	THR	SER	GLY	GLY	ALA	SER	VAL	VAL	CYS	PHE	LEU	ASN	ASN	PHE	TYR	PRO	LYS	ASP	ILE	ASN	VAL	LYS	TRP	PHE	ASN	ARG	ILE	ASP	GLY	SER	GLU	ARG	GLN	ASN	GLY	VAL	LEU
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ASN	SER	TRP	THR	ASP	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	SER	MET	SER	THR	LEU	THR	LEU	THR	LYS	ASP	GLU	TYR	GLU	ARG	HIS	ASN	SER	TYR	THR	CYS	GLU	ALA	THR	HIS	LYS	THR	SER	THR	SER	PRO	ILE	VAL	LYS	SER	PHE	ASN	ARG	ASN	GLU	CYS
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.78	0/3618	0.80	2/4921 (0.0%)
1	D	0.78	0/3618	0.80	6/4921 (0.1%)
1	G	0.79	0/3618	0.82	4/4921 (0.1%)
1	p	0.69	0/5803	0.85	6/7901 (0.1%)
1	q	0.71	0/5803	0.86	4/7901 (0.1%)
1	r	0.72	0/5803	0.88	10/7901 (0.1%)
2	B	0.69	0/972	0.80	1/1317 (0.1%)
2	E	0.69	0/972	0.80	0/1317
2	H	0.70	0/972	0.81	0/1317
3	C	0.72	0/852	0.79	0/1153
3	F	0.75	0/852	0.82	0/1153
3	I	0.72	0/852	0.84	1/1153 (0.1%)
All	All	0.73	0/33735	0.84	34/45876 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	965	SER	CB-CA-C	-8.38	94.17	110.10
1	q	642	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	p	694	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	G	961	THR	C-N-CA	7.68	140.90	121.70
1	r	641	TYR	CB-CG-CD2	-7.49	116.51	121.00
1	r	399	PHE	CB-CG-CD1	-6.71	116.10	120.80
1	p	642	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	r	642	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	G	932	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	932	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	D	932	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	p	307	ARG	NE-CZ-NH1	-6.37	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	q	629	ARG	CB-CA-C	-6.34	97.72	110.40
1	q	184	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	r	437	CYS	O-C-N	-6.27	112.67	122.70
1	r	691	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	r	293	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	r	184	TYR	CB-CG-CD1	-5.93	117.44	121.00
3	I	96	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	D	909	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	p	384	ASP	C-N-CA	5.43	135.27	121.70
1	r	609	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	q	652	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	r	307	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	D	868	ASP	CB-CG-OD2	5.22	122.99	118.30
1	r	688	GLN	C-N-CA	5.20	134.71	121.70
1	G	868	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	758	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	868	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	1186	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	p	293	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	p	369	LYS	C-N-CD	5.06	139.03	128.40
2	B	97	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	G	912	CYS	C-N-CA	5.00	134.21	121.70

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	A	3545	0	3464	48	0
1	D	3545	0	3465	40	0
1	G	3545	0	3463	13	0
1	p	5658	0	5413	0	0
1	q	5658	0	5417	0	0
1	r	5658	0	5414	0	0
2	B	948	0	904	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	948	0	904	0	0
2	H	948	0	904	0	0
3	C	835	0	816	2	0
3	F	835	0	816	0	0
3	I	835	0	816	0	0
4	A	126	0	113	1	0
4	D	126	0	113	0	0
4	G	126	0	113	5	0
4	p	168	0	153	0	0
4	q	168	0	153	0	0
4	r	168	0	153	0	0
All	All	33840	0	32594	91	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 4.

All (91) 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:D:905:TYR:CE1	1:D:936:PRO:HB3	1.53	1.18
1:A:1121:THR:HA	1:D:964:LEU:HD13	1.44	0.99
1:D:905:TYR:HE1	1:D:936:PRO:HB3	1.28	0.99
1:D:905:TYR:CE1	1:D:936:PRO:CB	2.45	0.98
1:A:958:VAL:HG11	1:A:1108:LYS:O	1.65	0.96
1:A:961:THR:HG22	1:A:962:ALA:H	1.32	0.91
1:A:1121:THR:HA	1:D:964:LEU:CD1	2.01	0.90
1:A:1121:THR:HG22	1:D:964:LEU:HB3	1.56	0.87
1:A:958:VAL:CG1	1:A:1108:LYS:O	2.25	0.85
1:D:964:LEU:O	1:D:965:SER:OG	1.97	0.82
1:A:1121:THR:HG22	1:D:964:LEU:CD1	2.10	0.81
1:G:1160:ASN:OD1	1:G:1162:THR:OG1	1.97	0.81
1:D:957:GLY:CA	1:D:968:ALA:HB3	2.15	0.77
1:A:961:THR:HG22	1:A:962:ALA:N	2.01	0.76
1:D:957:GLY:HA3	1:D:968:ALA:HB3	1.68	0.75
1:D:775:SER:HB3	1:D:777:TYR:CE1	2.24	0.72
1:A:1121:THR:HG22	1:D:964:LEU:CB	2.21	0.70
1:D:960:TRP:O	1:D:961:THR:OG1	2.07	0.69
1:A:1121:THR:CA	1:D:964:LEU:HD13	2.22	0.67
1:A:1121:THR:HG22	1:D:964:LEU:HD13	1.77	0.66
1:A:804:VAL:HG12	1:A:805:ASP:N	2.12	0.64
1:A:811:CYS:SG	1:A:1051:ILE:HD13	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:GLY:HA3	1:D:968:ALA:CB	2.30	0.62
2:B:85:GLU:N	2:B:85:GLU:OE1	2.32	0.61
1:G:905:TYR:CE1	1:G:936:PRO:HG3	2.37	0.60
1:A:1121:THR:HB	1:D:964:LEU:HD12	1.83	0.60
1:A:961:THR:CG2	1:A:962:ALA:H	2.04	0.60
1:D:775:SER:HB3	1:D:777:TYR:CD1	2.37	0.60
1:A:1121:THR:CB	1:D:964:LEU:HD12	2.33	0.59
1:A:811:CYS:SG	1:A:1051:ILE:CD1	2.92	0.58
1:D:905:TYR:HE1	1:D:936:PRO:CB	2.02	0.57
1:A:1121:THR:CG2	1:D:964:LEU:CD1	2.83	0.57
1:A:1121:THR:CB	1:D:964:LEU:CD1	2.84	0.56
1:A:805:ASP:OD1	1:A:807:LYS:HB3	2.07	0.55
1:D:826:GLN:N	1:D:826:GLN:OE1	2.25	0.54
1:D:964:LEU:O	1:D:965:SER:CB	2.55	0.54
1:G:906:MET:HG2	1:G:906:MET:O	2.08	0.54
1:D:905:TYR:O	1:D:908:GLY:HA3	2.08	0.53
1:A:1209:VAL:HG12	4:A:1405:NAG:H2	1.90	0.53
1:G:1145:ASN:ND2	4:G:1402:NAG:O7	2.42	0.52
1:A:958:VAL:HG11	1:A:1109:ALA:HA	1.92	0.51
1:A:958:VAL:HG12	1:A:1108:LYS:O	2.09	0.51
1:A:805:ASP:C	1:A:807:LYS:H	2.14	0.51
1:A:804:VAL:HG12	1:A:805:ASP:H	1.76	0.50
1:D:1175:THR:HG23	1:D:1175:THR:O	2.12	0.49
1:G:872:THR:HA	4:G:1406:NAG:H82	1.94	0.49
1:A:1175:THR:O	1:A:1175:THR:HG23	2.13	0.49
1:D:772:GLN:HG2	1:D:773:LEU:H	1.78	0.49
1:D:756:GLU:OE1	1:D:756:GLU:N	2.35	0.48
3:C:1:ASP:C	3:C:1:ASP:OD1	2.50	0.48
1:A:804:VAL:CG1	1:A:805:ASP:N	2.76	0.47
1:A:826:GLN:OE1	1:A:826:GLN:N	2.28	0.47
1:A:1121:THR:CG2	1:D:964:LEU:HD12	2.44	0.47
1:D:957:GLY:N	1:D:968:ALA:HB3	2.29	0.47
1:A:810:VAL:HG12	1:A:811:CYS:SG	2.55	0.47
1:A:817:CYS:SG	1:A:1071:ILE:HD11	2.54	0.47
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.14	0.47
1:A:1219:PRO:HB2	1:A:1220:PRO:HD3	1.96	0.46
1:D:806:CYS:SG	1:D:806:CYS:O	2.73	0.46
1:D:775:SER:CB	1:D:777:TYR:CE1	2.96	0.46
1:G:1161:PRO:HG3	4:G:1408:NAG:H81	1.97	0.46
1:A:956:ALA:N	1:A:957:GLY:HA2	2.31	0.45
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:959:GLY:HA3	1:D:978:TYR:CE1	2.51	0.45
1:A:805:ASP:HB3	1:A:808:GLN:HB2	1.98	0.45
1:A:1121:THR:CG2	1:D:964:LEU:HD13	2.44	0.45
1:G:826:GLN:N	1:G:826:GLN:OE1	2.37	0.45
1:G:1120:GLY:O	1:G:1121:THR:OG1	2.24	0.44
1:G:1209:VAL:HG12	4:G:1409:NAG:H2	1.98	0.44
1:A:1121:THR:CA	1:D:964:LEU:CD1	2.82	0.44
1:D:1060:PRO:HA	1:D:1063:GLN:HB3	2.00	0.44
1:A:872:THR:HG22	1:A:872:THR:O	2.18	0.43
1:G:806:CYS:SG	1:G:806:CYS:O	2.75	0.43
1:D:777:TYR:N	1:D:777:TYR:CD1	2.86	0.43
1:A:1001:PHE:C	1:A:1001:PHE:CD1	2.92	0.43
2:B:6:GLN:HG2	2:B:22:CYS:SG	2.57	0.43
1:A:875:GLU:N	1:A:875:GLU:OE1	2.35	0.42
1:A:959:GLY:O	1:A:960:TRP:HB2	2.19	0.42
1:A:1116:PHE:O	1:A:1117:CYS:HB2	2.19	0.42
1:A:965:SER:OG	1:A:966:SER:N	2.51	0.42
1:D:1120:GLY:O	1:D:1121:THR:OG1	2.26	0.42
1:A:805:ASP:C	1:A:807:LYS:N	2.73	0.42
1:D:773:LEU:HA	1:D:773:LEU:HD23	1.79	0.42
1:A:960:TRP:O	1:A:961:THR:HB	2.20	0.41
3:C:92:LYS:C	3:C:92:LYS:HD3	2.40	0.41
1:G:1001:PHE:C	1:G:1001:PHE:CD1	2.94	0.41
1:A:971:PRO:HB3	4:G:1401:NAG:H81	2.03	0.41
1:A:804:VAL:CG1	1:A:805:ASP:H	2.33	0.41
1:G:841:ARG:NE	1:G:841:ARG:HA	2.35	0.41
1:A:944:GLU:OE1	1:A:944:GLU:HA	2.21	0.40
1:G:1160:ASN:OD1	1:G:1160:ASN:C	2.58	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	459/1329 (34%)	440 (96%)	15 (3%)	4 (1%)	20	63
1	D	459/1329 (34%)	440 (96%)	16 (4%)	3 (1%)	25	68
1	G	459/1329 (34%)	440 (96%)	17 (4%)	2 (0%)	38	77
1	p	724/1329 (54%)	688 (95%)	32 (4%)	4 (1%)	28	70
1	q	724/1329 (54%)	691 (95%)	29 (4%)	4 (1%)	28	70
1	r	724/1329 (54%)	693 (96%)	25 (4%)	6 (1%)	22	66
2	B	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	E	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	H	117/233 (50%)	113 (97%)	4 (3%)	0	100	100
3	C	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	20	63
3	F	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	20	63
3	I	109/218 (50%)	105 (96%)	3 (3%)	1 (1%)	20	63
All	All	4227/9327 (45%)	4048 (96%)	153 (4%)	26 (1%)	33	70

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	q	622	ALA
1	r	621	THR
1	A	940	ASP
1	A	961	THR
1	p	718	VAL
1	q	621	THR
1	q	718	VAL
1	r	377	GLN
1	A	1220	PRO
1	D	1220	PRO
1	G	887	ARG
1	G	1220	PRO
1	p	382	GLU
1	q	623	VAL
1	r	629	ARG
1	D	956	ALA
1	p	621	THR
1	r	718	VAL
1	D	905	TYR
1	A	960	TRP
1	r	596	ILE
3	C	77	PRO

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Mol	Chain	Res	Type
3	I	77	PRO
1	r	623	VAL
3	F	77	PRO
1	p	381	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 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	388/1148 (34%)	388 (100%)	0	100	100
1	D	388/1148 (34%)	388 (100%)	0	100	100
1	G	388/1148 (34%)	387 (100%)	1 (0%)	94	97
1	p	635/1148 (55%)	634 (100%)	1 (0%)	94	97
1	q	635/1148 (55%)	633 (100%)	2 (0%)	94	97
1	r	635/1148 (55%)	632 (100%)	3 (0%)	91	96
2	B	102/202 (50%)	102 (100%)	0	100	100
2	E	102/202 (50%)	102 (100%)	0	100	100
2	H	102/202 (50%)	102 (100%)	0	100	100
3	C	93/192 (48%)	93 (100%)	0	100	100
3	F	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3654/8070 (45%)	3647 (100%)	7 (0%)	95	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	774	ASN
1	p	104	ASN
1	q	619	ASN
1	q	670	HIS
1	r	423	PHE
1	r	629	ARG

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Mol	Chain	Res	Type
1	r	630	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1163	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

63 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	1401	1	14,14,15	0.54	0	15,19,21	0.94	1 (6%)
4	NAG	A	1402	1,4	14,14,15	1.24	1 (7%)	15,19,21	1.28	3 (20%)
4	NAG	A	1403	4	14,14,15	0.46	0	15,19,21	0.39	0
4	NAG	A	1404	1,4	14,14,15	0.85	1 (7%)	15,19,21	1.00	1 (6%)
4	NAG	A	1405	4	14,14,15	0.31	0	15,19,21	0.97	1 (6%)
4	NAG	A	1406	1,4	14,14,15	0.26	0	15,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1407	4	14,14,15	0.81	1 (7%)	15,19,21	0.91	1 (6%)
4	NAG	A	1408	1,4	14,14,15	0.71	1 (7%)	15,19,21	1.07	1 (6%)
4	NAG	A	1409	4	14,14,15	0.29	0	15,19,21	0.56	0
4	NAG	D	1401	1	14,14,15	1.52	2 (14%)	15,19,21	1.59	2 (13%)
4	NAG	D	1402	1,4	14,14,15	0.53	0	15,19,21	0.69	0
4	NAG	D	1403	4	14,14,15	0.39	0	15,19,21	0.65	0
4	NAG	D	1404	1,4	14,14,15	1.12	2 (14%)	15,19,21	2.61	3 (20%)
4	NAG	D	1405	4	14,14,15	0.47	0	15,19,21	0.46	0
4	NAG	D	1406	1,4	14,14,15	0.49	0	15,19,21	0.58	0
4	NAG	D	1407	4	14,14,15	0.45	0	15,19,21	0.39	0
4	NAG	D	1408	1,4	14,14,15	0.21	0	15,19,21	0.61	0
4	NAG	D	1409	4	14,14,15	0.91	1 (7%)	15,19,21	2.25	3 (20%)
4	NAG	G	1401	1	14,14,15	0.74	1 (7%)	15,19,21	0.85	1 (6%)
4	NAG	G	1402	1,4	14,14,15	0.38	0	15,19,21	0.74	1 (6%)
4	NAG	G	1403	4	14,14,15	0.37	0	15,19,21	0.43	0
4	NAG	G	1404	1,4	14,14,15	1.25	1 (7%)	15,19,21	1.33	3 (20%)
4	NAG	G	1405	4	14,14,15	0.51	0	15,19,21	0.52	0
4	NAG	G	1406	1,4	14,14,15	0.73	1 (7%)	15,19,21	0.70	0
4	NAG	G	1407	4	14,14,15	0.34	0	15,19,21	0.51	0
4	NAG	G	1408	1,4	14,14,15	0.79	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	G	1409	4	14,14,15	0.39	0	15,19,21	0.77	1 (6%)
4	NAG	p	1401	1	14,14,15	0.89	1 (7%)	15,19,21	2.35	3 (20%)
4	NAG	p	1402	1	14,14,15	0.56	0	15,19,21	1.14	2 (13%)
4	NAG	p	1403	1	14,14,15	0.45	0	15,19,21	0.57	0
4	NAG	p	1404	1	14,14,15	0.36	0	15,19,21	2.07	2 (13%)
4	NAG	p	1405	1	14,14,15	0.50	0	15,19,21	0.82	1 (6%)
4	NAG	p	1406	1	14,14,15	0.78	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	p	1407	1,4	14,14,15	0.55	0	15,19,21	1.00	1 (6%)
4	NAG	p	1408	4	14,14,15	0.43	0	15,19,21	0.58	0
4	NAG	p	1409	1,4	14,14,15	1.13	1 (7%)	15,19,21	1.31	2 (13%)
4	NAG	p	1410	4	14,14,15	0.23	0	15,19,21	0.50	0
4	NAG	p	1411	1,4	14,14,15	1.25	1 (7%)	15,19,21	1.61	1 (6%)
4	NAG	p	1412	4	14,14,15	0.88	1 (7%)	15,19,21	2.33	3 (20%)
4	NAG	q	1401	1	14,14,15	0.69	0	15,19,21	0.82	1 (6%)
4	NAG	q	1402	1	14,14,15	1.25	2 (14%)	15,19,21	2.71	4 (26%)
4	NAG	q	1403	1	14,14,15	0.60	0	15,19,21	0.51	0
4	NAG	q	1404	1	14,14,15	0.24	0	15,19,21	0.48	0
4	NAG	q	1405	1	14,14,15	0.65	1 (7%)	15,19,21	1.25	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	q	1406	1	14,14,15	0.44	0	15,19,21	0.59	0
4	NAG	q	1407	1,4	14,14,15	0.85	1 (7%)	15,19,21	0.91	0
4	NAG	q	1408	4	14,14,15	0.26	0	15,19,21	0.60	0
4	NAG	q	1409	1,4	14,14,15	0.23	0	15,19,21	1.08	1 (6%)
4	NAG	q	1410	4	14,14,15	0.33	0	15,19,21	0.59	0
4	NAG	q	1411	1,4	14,14,15	1.06	1 (7%)	15,19,21	0.82	0
4	NAG	q	1412	4	14,14,15	0.72	1 (7%)	15,19,21	0.65	0
4	NAG	r	1401	1	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
4	NAG	r	1402	1	14,14,15	1.31	1 (7%)	15,19,21	2.38	4 (26%)
4	NAG	r	1403	1	14,14,15	0.39	0	15,19,21	0.76	1 (6%)
4	NAG	r	1404	1	14,14,15	0.85	1 (7%)	15,19,21	0.89	1 (6%)
4	NAG	r	1405	1	14,14,15	0.24	0	15,19,21	0.44	0
4	NAG	r	1406	1	14,14,15	0.25	0	15,19,21	0.57	0
4	NAG	r	1407	1,4	14,14,15	0.94	1 (7%)	15,19,21	0.93	1 (6%)
4	NAG	r	1408	4	14,14,15	1.38	1 (7%)	15,19,21	2.33	4 (26%)
4	NAG	r	1409	1,4	14,14,15	0.65	0	15,19,21	0.73	1 (6%)
4	NAG	r	1410	4	14,14,15	0.41	0	15,19,21	0.67	0
4	NAG	r	1411	1,4	14,14,15	0.79	1 (7%)	15,19,21	2.36	3 (20%)
4	NAG	r	1412	4	14,14,15	0.43	0	15,19,21	0.60	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	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1408	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1409	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1403	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1405	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1408	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1409	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	G	1402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1403	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1405	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1408	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	1409	4	-	0/6/23/26	0/1/1/1
4	NAG	p	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	p	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	p	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	p	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	p	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	p	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	p	1407	1,4	-	0/6/23/26	0/1/1/1
4	NAG	p	1408	4	-	0/6/23/26	0/1/1/1
4	NAG	p	1409	1,4	-	0/6/23/26	0/1/1/1
4	NAG	p	1410	4	-	0/6/23/26	0/1/1/1
4	NAG	p	1411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	p	1412	4	-	0/6/23/26	0/1/1/1
4	NAG	q	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	q	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	q	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	q	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	q	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	q	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	q	1407	1,4	-	0/6/23/26	0/1/1/1
4	NAG	q	1408	4	-	0/6/23/26	0/1/1/1
4	NAG	q	1409	1,4	-	0/6/23/26	0/1/1/1
4	NAG	q	1410	4	-	0/6/23/26	0/1/1/1
4	NAG	q	1411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	q	1412	4	-	0/6/23/26	0/1/1/1
4	NAG	r	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	r	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	r	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	r	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	r	1405	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	r	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	r	1407	1,4	-	0/6/23/26	0/1/1/1
4	NAG	r	1408	4	-	0/6/23/26	0/1/1/1
4	NAG	r	1409	1,4	-	0/6/23/26	0/1/1/1
4	NAG	r	1410	4	-	0/6/23/26	0/1/1/1
4	NAG	r	1411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	r	1412	4	-	0/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1402	NAG	O5-C1	-4.24	1.36	1.43
4	G	1404	NAG	O5-C1	-4.19	1.36	1.43
4	p	1409	NAG	O5-C1	-3.99	1.37	1.43
4	r	1407	NAG	O5-C1	-3.04	1.38	1.43
4	q	1407	NAG	O5-C1	-2.93	1.38	1.43
4	A	1408	NAG	O5-C1	-2.52	1.39	1.43
4	G	1406	NAG	O5-C1	-2.49	1.39	1.43
4	q	1405	NAG	C1-C2	2.07	1.55	1.52
4	q	1412	NAG	O5-C1	2.21	1.47	1.43
4	p	1406	NAG	O5-C1	2.32	1.47	1.43
4	r	1411	NAG	C1-C2	2.39	1.55	1.52
4	D	1404	NAG	O5-C1	2.52	1.47	1.43
4	q	1402	NAG	C1-C2	2.54	1.55	1.52
4	D	1401	NAG	C1-C2	2.57	1.56	1.52
4	p	1401	NAG	C1-C2	2.61	1.56	1.52
4	G	1408	NAG	C1-C2	2.65	1.56	1.52
4	G	1401	NAG	O5-C1	2.66	1.48	1.43
4	p	1412	NAG	C1-C2	2.71	1.56	1.52
4	A	1407	NAG	C1-C2	2.86	1.56	1.52
4	D	1409	NAG	C1-C2	2.86	1.56	1.52
4	r	1404	NAG	C1-C2	2.97	1.56	1.52
4	D	1404	NAG	C1-C2	2.97	1.56	1.52
4	A	1404	NAG	C1-C2	3.05	1.56	1.52
4	q	1411	NAG	C1-C2	3.55	1.57	1.52
4	q	1402	NAG	O5-C1	3.56	1.49	1.43
4	r	1402	NAG	C1-C2	4.38	1.58	1.52
4	p	1411	NAG	O5-C1	4.44	1.51	1.43
4	r	1408	NAG	C1-C2	4.54	1.58	1.52
4	D	1401	NAG	O5-C1	5.04	1.52	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	G	1404	NAG	O3-C3-C2	-2.43	104.17	109.39
4	p	1402	NAG	O5-C1-C2	-2.33	108.23	111.47
4	G	1404	NAG	C1-O5-C5	-2.17	109.18	112.17
4	p	1409	NAG	C1-O5-C5	-2.11	109.26	112.17
4	A	1402	NAG	O3-C3-C2	-2.10	104.90	109.39
4	r	1411	NAG	C8-C7-N2	2.00	119.72	116.11
4	r	1402	NAG	C8-C7-N2	2.03	119.78	116.11
4	A	1402	NAG	C2-N2-C7	2.04	125.92	122.94
4	r	1409	NAG	C3-C4-C5	2.05	113.83	110.22
4	r	1408	NAG	C8-C7-N2	2.05	119.82	116.11
4	D	1409	NAG	C8-C7-N2	2.06	119.82	116.11
4	q	1402	NAG	C8-C7-N2	2.06	119.83	116.11
4	G	1408	NAG	O4-C4-C5	2.13	114.66	109.28
4	A	1402	NAG	C4-C3-C2	2.16	114.18	111.02
4	A	1404	NAG	O4-C4-C5	2.18	114.79	109.28
4	p	1412	NAG	C1-O5-C5	2.19	115.19	112.17
4	p	1401	NAG	C1-O5-C5	2.20	115.20	112.17
4	G	1402	NAG	C1-O5-C5	2.25	115.27	112.17
4	r	1407	NAG	C1-O5-C5	2.25	115.27	112.17
4	r	1403	NAG	C1-O5-C5	2.33	115.38	112.17
4	G	1401	NAG	C1-O5-C5	2.37	115.43	112.17
4	q	1401	NAG	C1-O5-C5	2.48	115.59	112.17
4	G	1409	NAG	C1-O5-C5	2.50	115.62	112.17
4	r	1402	NAG	C1-O5-C5	2.51	115.63	112.17
4	G	1404	NAG	C4-C3-C2	2.58	114.80	111.02
4	r	1404	NAG	C2-N2-C7	2.66	126.83	122.94
4	p	1405	NAG	C1-O5-C5	2.79	116.02	112.17
4	p	1407	NAG	C2-N2-C7	2.80	127.03	122.94
4	D	1401	NAG	C2-N2-C7	2.81	127.04	122.94
4	r	1408	NAG	C1-O5-C5	2.81	116.04	112.17
4	r	1401	NAG	C2-N2-C7	2.91	127.19	122.94
4	q	1405	NAG	C2-N2-C7	2.95	127.25	122.94
4	q	1409	NAG	C2-N2-C7	2.99	127.30	122.94
4	A	1401	NAG	C2-N2-C7	3.02	127.35	122.94
4	p	1409	NAG	C2-N2-C7	3.04	127.38	122.94
4	q	1405	NAG	C1-O5-C5	3.05	116.37	112.17
4	A	1407	NAG	C1-O5-C5	3.07	116.40	112.17
4	A	1408	NAG	C2-N2-C7	3.11	127.48	122.94
4	p	1406	NAG	C1-O5-C5	3.12	116.46	112.17
4	D	1409	NAG	C1-C2-N2	3.22	116.00	110.49
4	r	1408	NAG	C1-C2-N2	3.26	116.06	110.49
4	A	1405	NAG	C1-O5-C5	3.28	116.69	112.17
4	p	1402	NAG	C1-C2-N2	3.29	116.11	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	q	1402	NAG	C1-C2-N2	3.42	116.33	110.49
4	p	1412	NAG	C1-C2-N2	3.44	116.37	110.49
4	p	1401	NAG	C1-C2-N2	3.57	116.58	110.49
4	r	1411	NAG	C1-C2-N2	3.69	116.78	110.49
4	r	1402	NAG	C1-C2-N2	3.77	116.93	110.49
4	D	1404	NAG	C1-C2-N2	3.83	117.02	110.49
4	p	1404	NAG	C3-C4-C5	4.04	117.33	110.22
4	D	1404	NAG	C1-O5-C5	4.19	117.95	112.17
4	D	1401	NAG	C1-O5-C5	4.91	118.93	112.17
4	q	1402	NAG	C1-O5-C5	5.63	119.93	112.17
4	p	1411	NAG	C1-O5-C5	5.90	120.29	112.17
4	p	1404	NAG	C1-O5-C5	6.44	121.04	112.17
4	r	1408	NAG	C2-N2-C7	7.31	133.60	122.94
4	r	1402	NAG	C2-N2-C7	7.46	133.83	122.94
4	D	1404	NAG	C2-N2-C7	7.53	133.93	122.94
4	D	1409	NAG	C2-N2-C7	7.54	133.95	122.94
4	p	1412	NAG	C2-N2-C7	7.57	133.98	122.94
4	p	1401	NAG	C2-N2-C7	7.59	134.01	122.94
4	r	1411	NAG	C2-N2-C7	7.59	134.02	122.94
4	q	1402	NAG	C2-N2-C7	7.62	134.07	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1405	NAG	1	0
4	G	1401	NAG	1	0
4	G	1402	NAG	1	0
4	G	1406	NAG	1	0
4	G	1408	NAG	1	0
4	G	1409	NAG	1	0

## 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.