



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

Jan 30, 2020 – 02:09 PM EST

PDB ID : 6V8X  
EMDB ID: : EMD-21111  
Title : VRC01 Bound BG505 F14 HIV-1 SOSIP Envelope Trimer Structure  
Authors : Henderson, R.; Acharya, P.  
Deposited on : 2019-12-12  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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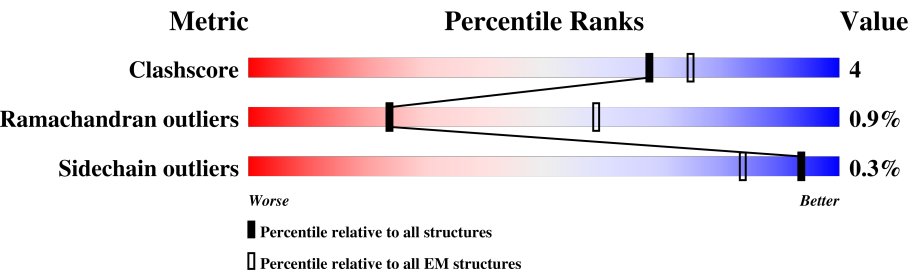
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	471	82% 11% • 7%
1	E	471	83% 10% • 7%
1	I	471	82% 11% • 7%
2	B	145	81% 7% 12%
2	F	145	81% 7% 12%
2	J	145	81% 7% 12%
3	C	224	92% 8% •
3	G	224	91% 8% •
3	K	224	92% 7% •

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Mol	Chain	Length	Quality of chain
4	D	208	<div><div></div><div>91%</div><div>7% •</div></div>
4	H	208	<div><div></div><div>92%</div><div>7% •</div></div>
4	L	208	<div><div></div><div>91%</div><div>7% •</div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 24825 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3453	2172	609	645	27		
1	E	439	Total	C	N	O	S	0	0
			3453	2172	609	645	27		
1	I	439	Total	C	N	O	S	0	0
			3453	2172	609	645	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ILE	VAL	conflict	UNP Q2N0S6
A	148	ALA	ASN	conflict	UNP Q2N0S6
A	204	VAL	ALA	conflict	UNP Q2N0S6
A	208	LEU	VAL	conflict	UNP Q2N0S6
A	255	LEU	VAL	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
E	68	ILE	VAL	conflict	UNP Q2N0S6
E	148	ALA	ASN	conflict	UNP Q2N0S6
E	204	VAL	ALA	conflict	UNP Q2N0S6
E	208	LEU	VAL	conflict	UNP Q2N0S6
E	255	LEU	VAL	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
I	68	ILE	VAL	conflict	UNP Q2N0S6
I	148	ALA	ASN	conflict	UNP Q2N0S6
I	204	VAL	ALA	conflict	UNP Q2N0S6
I	208	LEU	VAL	conflict	UNP Q2N0S6
I	255	LEU	VAL	conflict	UNP Q2N0S6
I	332	ASN	THR	conflict	UNP Q2N0S6
I	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	128	Total	C	N	O	S	0	0
			1025	649	178	192	6		
2	F	128	Total	C	N	O	S	0	0
			1025	649	178	192	6		
2	J	128	Total	C	N	O	S	0	0
			1025	649	178	192	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S9
F	605	CYS	THR	conflict	UNP Q2N0S9
J	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called VRC01 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	224	Total	C	N	O	S	0	0
			1710	1077	297	325	11		
3	G	224	Total	C	N	O	S	0	0
			1710	1077	297	325	11		
3	K	224	Total	C	N	O	S	0	0
			1710	1077	297	325	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	211	ALA	VAL	conflict	UNP Q6N095
G	211	ALA	VAL	conflict	UNP Q6N095
K	211	ALA	VAL	conflict	UNP Q6N095

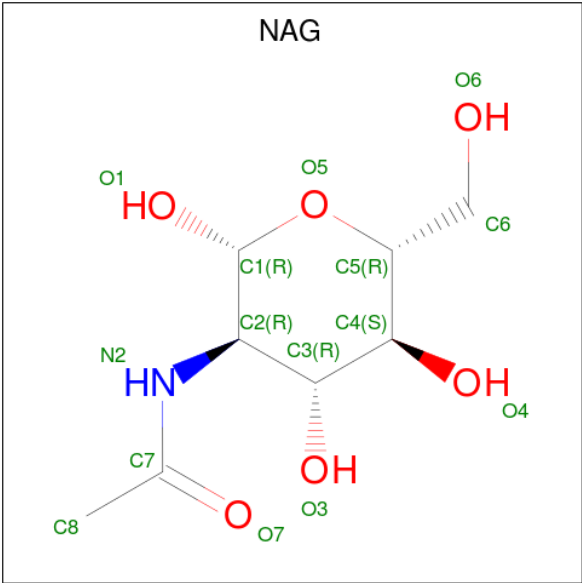
- Molecule 4 is a protein called VRC01 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1615	1011	277	322	5		
4	H	208	Total	C	N	O	S	0	0
			1615	1011	277	322	5		
4	L	208	Total	C	N	O	S	0	0
			1615	1011	277	322	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	204	ARG	SER	conflict	UNP Q6PIL8
H	204	ARG	SER	conflict	UNP Q6PIL8
L	204	ARG	SER	conflict	UNP Q6PIL8

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	A	1	Total 392	C 224	N 28	O 140	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	E	1	Total 392	C 224	N 28	O 140	0
5	E	1	Total 392	C 224	N 28	O 140	0

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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	

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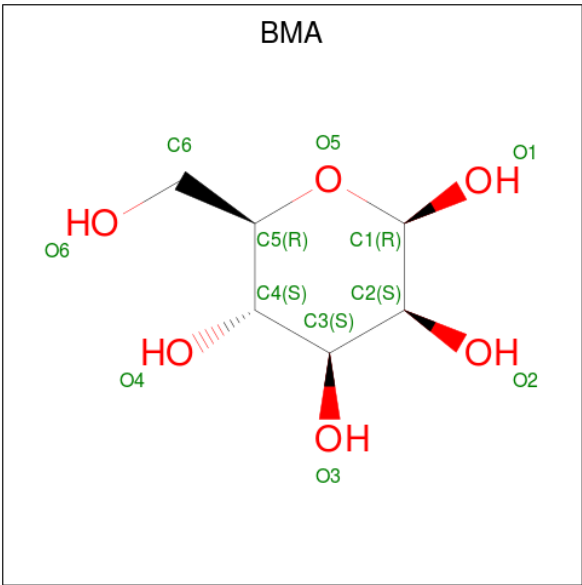
Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	J	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



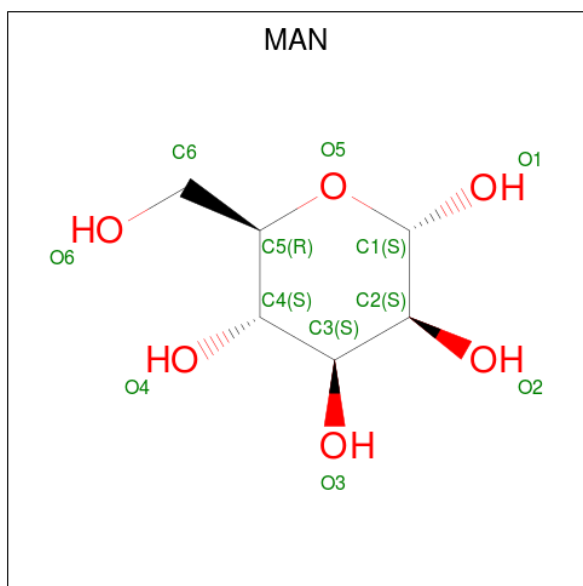
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	

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Mol	Chain	Residues	Atoms			AltConf
6	I	1	Total	C	O	0
			55	30	25	

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

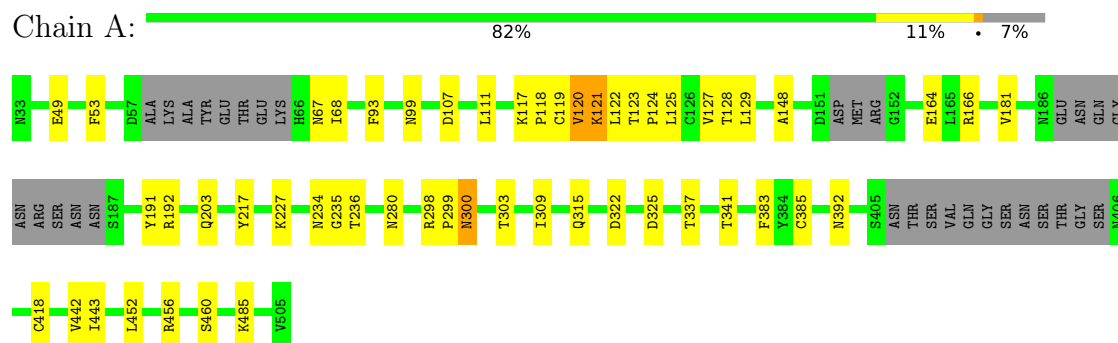


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			11	6	5	
7	E	1	Total	C	O	0
			11	6	5	
7	I	1	Total	C	O	0
			11	6	5	

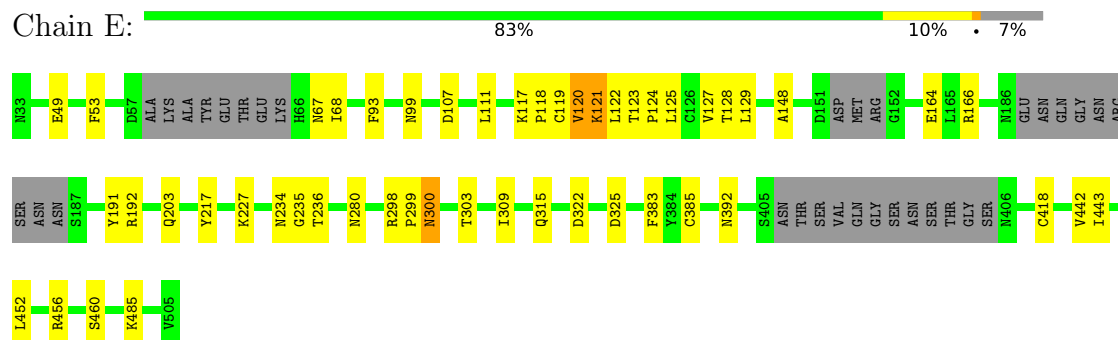
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

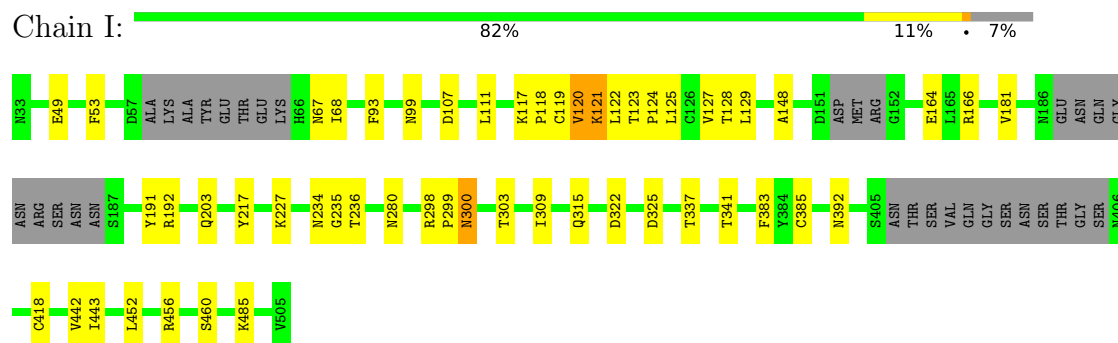
- Molecule 1: Envelope glycoprotein gp120




- Molecule 1: Envelope glycoprotein gp120

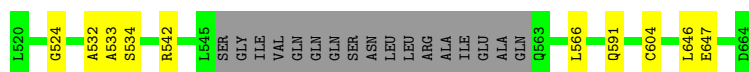


- Molecule 1: Envelope glycoprotein gp120




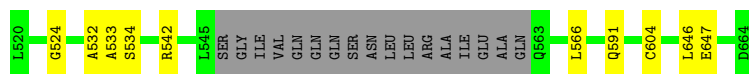
- Molecule 2: Envelope glycoprotein gp41

Chain B:  81% 7% 12%




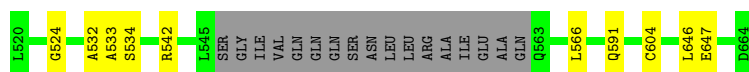
- Molecule 2: Envelope glycoprotein gp41

Chain F:  81% 7% 12%




- Molecule 2: Envelope glycoprotein gp41

Chain J:  81% 7% 12%




- Molecule 3: VRC01 Fab Heavy Chain

Chain C:  92% 8%



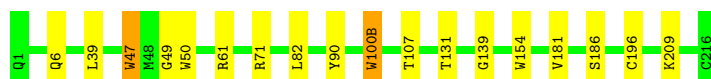
- Molecule 3: VRC01 Fab Heavy Chain

Chain G:  91% 8%



- Molecule 3: VRC01 Fab Heavy Chain

Chain K:  92% 7%



- Molecule 4: VRC01 Fab Light Chain

Chain D:  91% 7%

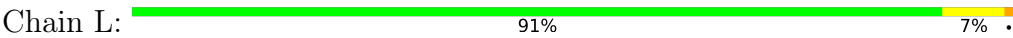


- Molecule 4: VRC01 Fab Light Chain

Chain H:  92% 7%



● Molecule 4: VRC01 Fab Light Chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	77632	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 ( $e^-/\text{\AA}^2$ )	54.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
1	E	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
1	I	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
2	B	0.80	1/1043 (0.1%)	0.81	0/1414
2	F	0.80	1/1043 (0.1%)	0.81	0/1414
2	J	0.81	1/1043 (0.1%)	0.81	0/1414
3	C	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
3	G	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
3	K	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
4	D	0.61	0/1652	0.70	1/2242 (0.0%)
4	H	0.61	0/1652	0.70	1/2242 (0.0%)
4	L	0.61	0/1652	0.70	1/2242 (0.0%)
All	All	0.83	21/23922 (0.1%)	0.78	27/32481 (0.1%)

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
4	D	0	1
4	H	0	1
4	L	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	50	TRP	CB-CG	-11.02	1.30	1.50
3	K	50	TRP	CB-CG	-11.02	1.30	1.50
3	C	50	TRP	CB-CG	-11.01	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	299	PRO	N-CD	7.37	1.58	1.47
1	A	299	PRO	N-CD	7.30	1.58	1.47
1	E	299	PRO	N-CD	7.29	1.58	1.47
3	G	100(B)	TRP	CB-CG	-6.52	1.38	1.50
3	C	100(B)	TRP	CB-CG	-6.52	1.38	1.50
3	K	100(B)	TRP	CB-CG	-6.52	1.38	1.50
3	K	100(B)	TRP	CE3-CZ3	-6.19	1.27	1.38
3	G	100(B)	TRP	CE3-CZ3	-6.17	1.27	1.38
3	C	100(B)	TRP	CE3-CZ3	-6.16	1.27	1.38
3	K	90	TYR	CD1-CE1	-5.57	1.30	1.39
3	G	90	TYR	CD1-CE1	-5.55	1.31	1.39
3	C	90	TYR	CD1-CE1	-5.55	1.31	1.39
3	K	47	TRP	CB-CG	-5.32	1.40	1.50
3	C	47	TRP	CB-CG	-5.29	1.40	1.50
3	G	47	TRP	CB-CG	-5.28	1.40	1.50
2	J	604	CYS	CB-SG	-5.04	1.73	1.81
2	F	604	CYS	CB-SG	-5.04	1.73	1.81
2	B	604	CYS	CB-SG	-5.04	1.73	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	88	CYS	CA-CB-SG	6.31	125.35	114.00
4	L	88	CYS	CA-CB-SG	6.31	125.35	114.00
4	H	88	CYS	CA-CB-SG	6.30	125.35	114.00
1	A	129	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	129	LEU	CA-CB-CG	6.19	129.53	115.30
1	I	129	LEU	CA-CB-CG	6.18	129.50	115.30
3	C	50	TRP	CB-CA-C	-6.13	98.15	110.40
3	K	50	TRP	CB-CA-C	-6.12	98.16	110.40
3	G	50	TRP	CB-CA-C	-6.12	98.17	110.40
1	I	299	PRO	N-CD-CG	-5.95	94.27	103.20
1	A	299	PRO	N-CD-CG	-5.95	94.28	103.20
1	E	299	PRO	N-CD-CG	-5.94	94.29	103.20
1	A	452	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	E	452	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	I	452	LEU	CB-CG-CD2	-5.72	101.28	111.00
3	K	50	TRP	CA-CB-CG	5.69	124.51	113.70
3	G	50	TRP	CA-CB-CG	5.69	124.50	113.70
3	C	50	TRP	CA-CB-CG	5.68	124.49	113.70
3	C	82	LEU	CB-CG-CD2	-5.45	101.74	111.00
3	G	82	LEU	CB-CG-CD2	-5.45	101.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	82	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	I	93	PHE	CB-CG-CD1	5.22	124.45	120.80
1	A	93	PHE	CB-CG-CD1	5.16	124.41	120.80
1	E	93	PHE	CB-CG-CD1	5.12	124.39	120.80
3	C	39	LEU	CB-CG-CD2	-5.03	102.45	111.00
3	G	39	LEU	CB-CG-CD2	-5.01	102.47	111.00
3	K	39	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	90	GLN	Peptide
4	H	90	GLN	Peptide
4	L	90	GLN	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3453	0	3397	48	0
1	E	3453	0	3397	46	0
1	I	3453	0	3397	49	0
2	B	1025	0	1012	4	0
2	F	1025	0	1012	4	0
2	J	1025	0	1012	4	0
3	C	1710	0	1680	8	0
3	G	1710	0	1680	9	0
3	K	1710	0	1680	8	0
4	D	1615	0	1554	12	0
4	H	1615	0	1554	11	0
4	L	1615	0	1554	12	0
5	A	392	0	347	1	0
5	B	14	0	13	0	0
5	E	392	0	347	2	0
5	F	14	0	13	0	0
5	I	392	0	347	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	14	0	13	0	0
6	A	55	0	49	0	0
6	E	55	0	49	0	0
6	I	55	0	49	0	0
7	A	11	0	10	0	0
7	E	11	0	10	0	0
7	I	11	0	10	0	0
All	All	24825	0	24186	201	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 (201) 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:I:120:VAL:CG1	1:I:121:LYS:H	1.56	1.17
1:E:120:VAL:HG12	1:E:121:LYS:N	1.54	1.17
1:A:120:VAL:HG12	1:A:121:LYS:N	1.54	1.15
1:I:120:VAL:HG12	1:I:121:LYS:N	1.54	1.15
1:A:120:VAL:CG1	1:A:121:LYS:H	1.56	1.09
1:E:120:VAL:CG1	1:E:121:LYS:H	1.56	1.08
1:E:124:PRO:HG2	1:E:309:ILE:HD11	1.33	1.08
1:A:124:PRO:HG2	1:A:309:ILE:HD11	1.33	1.07
1:I:124:PRO:HG2	1:I:309:ILE:HD11	1.33	1.04
1:I:124:PRO:CG	1:I:309:ILE:HD11	1.93	0.98
1:E:124:PRO:CG	1:E:309:ILE:HD11	1.93	0.98
1:A:124:PRO:CG	1:A:309:ILE:HD11	1.93	0.97
1:A:120:VAL:HG12	1:A:121:LYS:H	0.72	0.86
1:E:120:VAL:HG12	1:E:121:LYS:H	0.72	0.86
1:I:120:VAL:HG12	1:I:121:LYS:H	0.72	0.85
1:I:120:VAL:CG1	1:I:121:LYS:N	2.28	0.80
1:A:124:PRO:HG2	1:A:309:ILE:CD1	2.13	0.79
1:E:124:PRO:HG2	1:E:309:ILE:CD1	2.13	0.79
1:E:122:LEU:HD13	1:E:125:LEU:HD22	1.65	0.79
1:A:120:VAL:CG1	1:A:121:LYS:N	2.28	0.78
1:I:122:LEU:HD13	1:I:125:LEU:HD22	1.65	0.78
1:I:124:PRO:HG2	1:I:309:ILE:CD1	2.13	0.77
1:A:122:LEU:HD13	1:A:125:LEU:HD22	1.65	0.76
1:I:121:LYS:O	1:I:122:LEU:HD23	1.86	0.76
1:E:120:VAL:CG1	1:E:121:LYS:N	2.28	0.76
1:A:121:LYS:O	1:A:122:LEU:HD23	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:LYS:O	1:E:122:LEU:HD23	1.86	0.75
1:E:303:THR:OG1	1:E:322:ASP:N	2.26	0.69
1:I:303:THR:OG1	1:I:322:ASP:N	2.26	0.69
1:A:303:THR:OG1	1:A:322:ASP:N	2.26	0.68
1:I:123:THR:N	1:I:124:PRO:HD2	2.10	0.67
1:A:123:THR:N	1:A:124:PRO:HD2	2.10	0.67
1:E:123:THR:N	1:E:124:PRO:HD2	2.10	0.65
1:E:123:THR:N	1:E:124:PRO:CD	2.60	0.65
4:H:153:ASP:OD1	4:H:193:VAL:HB	1.97	0.65
4:L:153:ASP:OD1	4:L:193:VAL:HB	1.97	0.64
1:A:123:THR:N	1:A:124:PRO:CD	2.60	0.64
1:I:123:THR:N	1:I:124:PRO:CD	2.60	0.64
1:A:121:LYS:O	1:A:122:LEU:CD2	2.46	0.64
1:I:121:LYS:O	1:I:122:LEU:CD2	2.46	0.64
4:D:153:ASP:OD1	4:D:193:VAL:HB	1.97	0.63
1:E:121:LYS:O	1:E:122:LEU:CD2	2.46	0.63
1:E:124:PRO:CG	1:E:309:ILE:CD1	2.76	0.61
1:I:234:ASN:O	1:I:236:THR:N	2.34	0.61
1:E:234:ASN:O	1:E:236:THR:N	2.34	0.61
1:A:234:ASN:O	1:A:236:THR:N	2.34	0.60
1:A:120:VAL:HG12	1:A:121:LYS:O	2.01	0.60
2:B:532:ALA:O	2:B:534:SER:N	2.30	0.60
1:E:120:VAL:HG12	1:E:121:LYS:O	2.01	0.59
2:J:532:ALA:O	2:J:534:SER:N	2.30	0.59
1:I:120:VAL:HG12	1:I:121:LYS:O	2.01	0.59
1:E:303:THR:HG1	1:E:322:ASP:N	2.00	0.58
2:F:542:ARG:HA	2:J:591:GLN:HE22	1.67	0.58
2:B:591:GLN:HE22	2:J:542:ARG:HA	1.67	0.58
2:B:542:ARG:HA	2:F:591:GLN:HE22	1.67	0.58
1:I:303:THR:HG1	1:I:322:ASP:N	2.01	0.58
3:K:6:GLN:OE1	3:K:107:THR:OG1	2.18	0.57
3:G:6:GLN:OE1	3:G:107:THR:OG1	2.18	0.57
1:E:164:GLU:OE1	1:I:192:ARG:NH1	2.38	0.56
1:A:124:PRO:CG	1:A:309:ILE:CD1	2.76	0.56
2:F:532:ALA:O	2:F:534:SER:N	2.30	0.56
1:A:164:GLU:OE1	1:E:192:ARG:NH1	2.39	0.56
1:A:192:ARG:NH1	1:I:164:GLU:OE1	2.38	0.56
1:I:117:LYS:HB2	1:I:118:PRO:HD3	1.88	0.56
1:I:124:PRO:CG	1:I:309:ILE:CD1	2.76	0.56
1:A:122:LEU:C	1:A:124:PRO:HD2	2.27	0.55
1:E:300:ASN:OD1	1:E:442:VAL:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LEU:C	1:E:124:PRO:HD2	2.27	0.55
1:I:300:ASN:OD1	1:I:442:VAL:HA	2.06	0.55
1:A:117:LYS:HB2	1:A:118:PRO:HD3	1.88	0.55
1:I:122:LEU:C	1:I:124:PRO:HD2	2.27	0.55
1:A:300:ASN:OD1	1:A:442:VAL:HA	2.06	0.54
1:A:383:PHE:HB3	1:A:418:CYS:SG	2.48	0.54
1:E:117:LYS:HB2	1:E:118:PRO:HD3	1.88	0.54
1:I:383:PHE:HB3	1:I:418:CYS:SG	2.48	0.53
1:E:383:PHE:HB3	1:E:418:CYS:SG	2.48	0.53
3:C:6:GLN:OE1	3:C:107:THR:OG1	2.18	0.53
4:D:6:GLN:HE21	4:D:88:CYS:HB3	1.74	0.53
4:H:6:GLN:HE21	4:H:88:CYS:HB3	1.74	0.53
4:L:6:GLN:HE21	4:L:88:CYS:HB3	1.74	0.53
3:K:100(B):TRP:CD1	4:L:91:TYR:O	2.63	0.52
1:A:303:THR:HG1	1:A:322:ASP:N	2.07	0.52
3:C:100(B):TRP:CD1	4:D:91:TYR:O	2.63	0.52
3:G:100(B):TRP:CD1	4:H:91:TYR:O	2.63	0.52
1:A:49:GLU:HG3	1:A:99:ASN:HD22	1.75	0.51
4:H:13:LEU:CD1	4:H:19:ALA:HB2	2.40	0.51
1:I:49:GLU:HG3	1:I:99:ASN:HD22	1.75	0.51
1:A:122:LEU:HD13	1:A:125:LEU:CD2	2.39	0.51
4:D:13:LEU:CD1	4:D:19:ALA:HB2	2.40	0.51
4:L:13:LEU:CD1	4:L:19:ALA:HB2	2.40	0.50
1:E:49:GLU:HG3	1:E:99:ASN:HD22	1.75	0.50
3:K:154:TRP:CH2	3:K:196:CYS:HB2	2.47	0.49
1:A:121:LYS:C	1:A:122:LEU:HG	2.33	0.48
3:G:154:TRP:CH2	3:G:196:CYS:HB2	2.47	0.48
3:C:154:TRP:CH2	3:C:196:CYS:HB2	2.47	0.48
1:I:121:LYS:C	1:I:122:LEU:HG	2.33	0.48
1:E:122:LEU:HD13	1:E:125:LEU:CD2	2.39	0.48
1:I:122:LEU:HD13	1:I:125:LEU:CD2	2.39	0.48
1:A:120:VAL:HG22	1:A:315:GLN:OE1	2.14	0.48
1:I:280:ASN:OD1	1:I:456:ARG:NH2	2.47	0.47
1:E:121:LYS:C	1:E:122:LEU:HG	2.33	0.47
1:E:120:VAL:HG22	1:E:315:GLN:OE1	2.14	0.47
4:H:11:LEU:HB2	4:H:104:VAL:HA	1.97	0.47
1:A:280:ASN:OD1	1:A:456:ARG:NH2	2.47	0.47
1:E:280:ASN:OD1	1:E:456:ARG:NH2	2.47	0.47
1:E:67:ASN:OD1	1:E:68:ILE:N	2.48	0.47
1:I:67:ASN:OD1	1:I:68:ILE:N	2.48	0.47
1:E:122:LEU:HB3	1:E:125:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:6:GLN:HE21	4:L:88:CYS:CB	2.27	0.47
4:D:6:GLN:HE21	4:D:88:CYS:CB	2.27	0.47
1:I:120:VAL:HG22	1:I:315:GLN:OE1	2.14	0.47
4:L:11:LEU:HB2	4:L:104:VAL:HA	1.96	0.47
1:I:117:LYS:N	1:I:118:PRO:CD	2.78	0.46
1:E:117:LYS:N	1:E:118:PRO:CD	2.78	0.46
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.51	0.46
3:K:196:CYS:N	3:K:209:LYS:O	2.46	0.46
1:A:122:LEU:HB3	1:A:125:LEU:HB2	1.97	0.46
1:A:67:ASN:OD1	1:A:68:ILE:N	2.48	0.46
4:D:11:LEU:HB2	4:D:104:VAL:HA	1.97	0.46
3:G:196:CYS:N	3:G:209:LYS:O	2.46	0.46
4:H:6:GLN:HE21	4:H:88:CYS:CB	2.27	0.46
1:A:117:LYS:N	1:A:118:PRO:CD	2.78	0.46
1:I:122:LEU:HB3	1:I:125:LEU:HB2	1.97	0.46
3:G:47:TRP:CZ2	3:G:49:GLY:HA2	2.51	0.46
1:E:117:LYS:HG3	2:F:566:LEU:HD21	1.98	0.46
4:H:141:PHE:CE2	4:H:198:VAL:HG11	2.51	0.46
1:I:117:LYS:HG3	2:J:566:LEU:HD21	1.98	0.46
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.51	0.46
4:L:141:PHE:CE2	4:L:198:VAL:HG11	2.51	0.46
1:A:117:LYS:HG3	2:B:566:LEU:HD21	1.98	0.45
4:D:141:PHE:CE2	4:D:198:VAL:HG11	2.51	0.45
1:E:385:CYS:HA	1:E:418:CYS:HA	1.99	0.44
4:L:197:GLU:HA	4:L:207:VAL:O	2.17	0.44
4:D:197:GLU:HA	4:D:207:VAL:O	2.17	0.44
1:I:119:CYS:HB3	1:I:203:GLN:O	2.18	0.44
1:A:121:LYS:O	1:A:122:LEU:HG	2.17	0.44
1:A:121:LYS:O	1:A:122:LEU:CG	2.66	0.44
1:A:128:THR:O	1:A:191:TYR:O	2.35	0.44
1:E:121:LYS:O	1:E:122:LEU:CG	2.66	0.44
1:E:128:THR:O	1:E:191:TYR:O	2.35	0.44
1:I:128:THR:O	1:I:191:TYR:O	2.35	0.44
1:A:119:CYS:HB3	1:A:203:GLN:O	2.18	0.44
1:A:385:CYS:HA	1:A:418:CYS:HA	1.99	0.44
4:D:197:GLU:HB3	4:D:206:PRO:HB2	2.00	0.44
1:E:119:CYS:HB3	1:E:203:GLN:O	2.18	0.44
1:I:385:CYS:HA	1:I:418:CYS:HA	1.99	0.44
1:E:121:LYS:O	1:E:122:LEU:HG	2.17	0.44
4:H:197:GLU:HA	4:H:207:VAL:O	2.17	0.44
4:L:197:GLU:HB3	4:L:206:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:LYS:O	1:I:122:LEU:CG	2.66	0.43
1:E:298:ARG:CZ	1:E:300:ASN:HB3	2.48	0.43
5:E:633:NAG:H83	5:E:633:NAG:H2	1.88	0.43
1:I:303:THR:HG23	1:I:322:ASP:O	2.19	0.43
1:E:303:THR:HG23	1:E:322:ASP:O	2.19	0.43
3:G:131:THR:O	3:G:186:SER:HB3	2.19	0.43
1:A:303:THR:HG23	1:A:322:ASP:O	2.19	0.43
3:C:139:GLY:HA3	3:C:181:VAL:HA	2.01	0.43
3:C:131:THR:O	3:C:186:SER:HB3	2.19	0.43
1:A:53:PHE:O	1:A:217:TYR:CD1	2.72	0.43
1:I:121:LYS:O	1:I:122:LEU:HG	2.17	0.43
3:K:131:THR:O	3:K:186:SER:HB3	2.19	0.43
4:L:115:PRO:HB2	4:L:207:VAL:HG11	2.01	0.43
1:A:298:ARG:CZ	1:A:300:ASN:HB3	2.48	0.43
3:G:139:GLY:HA3	3:G:181:VAL:HA	2.01	0.42
1:A:148:ALA:HB3	1:A:325:ASP:OD1	2.19	0.42
1:A:392:ASN:HD22	5:A:605:NAG:C7	2.32	0.42
4:D:115:PRO:HB2	4:D:207:VAL:HG11	2.01	0.42
1:E:148:ALA:HB3	1:E:325:ASP:OD1	2.19	0.42
1:I:298:ARG:CZ	1:I:300:ASN:HB3	2.48	0.42
1:I:53:PHE:O	1:I:217:TYR:CD1	2.72	0.42
1:I:392:ASN:HD22	5:I:605:NAG:C7	2.32	0.42
1:I:148:ALA:HB3	1:I:325:ASP:OD1	2.19	0.42
3:K:139:GLY:HA3	3:K:181:VAL:HA	2.00	0.42
1:E:53:PHE:O	1:E:217:TYR:CD1	2.72	0.42
4:H:197:GLU:HB3	4:H:206:PRO:HB2	2.00	0.42
1:I:125:LEU:HD12	1:I:125:LEU:HA	1.81	0.42
4:H:115:PRO:HB2	4:H:207:VAL:HG11	2.01	0.41
1:E:443:ILE:CD1	1:E:443:ILE:N	2.83	0.41
1:I:227:LYS:HA	1:I:485:LYS:O	2.21	0.41
1:A:227:LYS:HA	1:A:485:LYS:O	2.20	0.41
1:E:460:SER:O	3:G:61:ARG:NH2	2.54	0.41
1:E:227:LYS:HA	1:E:485:LYS:O	2.20	0.41
1:A:460:SER:O	3:C:61:ARG:NH2	2.54	0.41
4:D:90:GLN:O	4:D:96:GLU:N	2.54	0.41
1:E:392:ASN:HD22	5:E:605:NAG:C7	2.32	0.41
4:L:138:LEU:HB3	4:L:141:PHE:CZ	2.56	0.41
1:I:107:ASP:O	1:I:111:LEU:HG	2.21	0.41
3:G:124:LEU:O	3:G:211:ALA:HB1	2.21	0.41
1:I:181:VAL:CG1	1:I:191:TYR:CD2	3.04	0.41
1:I:443:ILE:CD1	1:I:443:ILE:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:LEU:O	3:C:211:ALA:HB1	2.21	0.41
1:A:107:ASP:O	1:A:111:LEU:HG	2.21	0.41
4:H:138:LEU:HB3	4:H:141:PHE:CZ	2.56	0.40
1:I:337:THR:O	1:I:341:THR:OG1	2.30	0.40
1:A:181:VAL:CG1	1:A:191:TYR:CD2	3.04	0.40
1:A:337:THR:O	1:A:341:THR:OG1	2.30	0.40
1:A:443:ILE:CD1	1:A:443:ILE:N	2.83	0.40
1:E:107:ASP:O	1:E:111:LEU:HG	2.21	0.40
4:D:138:LEU:HB3	4:D:141:PHE:CZ	2.56	0.40
4:L:90:GLN:O	4:L:96:GLU:N	2.54	0.40
1:I:460:SER:O	3:K:61:ARG:NH2	2.54	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	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	19 59
1	E	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	19 59
1	I	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	19 59
2	B	124/145 (86%)	114 (92%)	6 (5%)	4 (3%)	4 24
2	F	124/145 (86%)	113 (91%)	7 (6%)	4 (3%)	4 24
2	J	124/145 (86%)	114 (92%)	6 (5%)	4 (3%)	4 24
3	C	222/224 (99%)	195 (88%)	27 (12%)	0	100 100
3	G	222/224 (99%)	195 (88%)	27 (12%)	0	100 100
3	K	222/224 (99%)	195 (88%)	27 (12%)	0	100 100
4	D	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	31 71
4	H	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	31 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	31	71
All	All	2943/3144 (94%)	2666 (91%)	250 (8%)	27 (1%)	24	59

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	533	ALA
2	B	646	LEU
2	F	533	ALA
2	F	646	LEU
2	J	533	ALA
2	J	646	LEU
1	A	235	GLY
2	B	647	GLU
4	D	91	TYR
1	E	235	GLY
2	F	647	GLU
4	H	91	TYR
1	I	235	GLY
2	J	647	GLU
4	L	91	TYR
1	A	121	LYS
1	E	121	LYS
1	I	121	LYS
1	A	120	VAL
2	B	524	GLY
1	E	120	VAL
2	F	524	GLY
1	I	120	VAL
2	J	524	GLY
1	A	300	ASN
1	E	300	ASN
1	I	300	ASN

### 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	393/420 (94%)	391 (100%)	2 (0%)	90	96
1	E	393/420 (94%)	391 (100%)	2 (0%)	90	96
1	I	393/420 (94%)	391 (100%)	2 (0%)	90	96
2	B	111/125 (89%)	111 (100%)	0	100	100
2	F	111/125 (89%)	111 (100%)	0	100	100
2	J	111/125 (89%)	111 (100%)	0	100	100
3	C	192/192 (100%)	191 (100%)	1 (0%)	90	96
3	G	192/192 (100%)	191 (100%)	1 (0%)	90	96
3	K	192/192 (100%)	191 (100%)	1 (0%)	90	96
4	D	180/180 (100%)	180 (100%)	0	100	100
4	H	180/180 (100%)	180 (100%)	0	100	100
4	L	180/180 (100%)	180 (100%)	0	100	100
All	All	2628/2751 (96%)	2619 (100%)	9 (0%)	93	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	166	ARG
3	C	71	ARG
1	E	127	VAL
1	E	166	ARG
3	G	71	ARG
1	I	127	VAL
1	I	166	ARG
3	K	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	130	GLN
1	A	234	ASN
2	B	591	GLN
4	D	6	GLN
1	E	99	ASN
1	E	130	GLN
1	E	234	ASN

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Mol	Chain	Res	Type
2	F	591	GLN
4	H	6	GLN
1	I	99	ASN
1	I	130	GLN
1	I	234	ASN
2	J	591	GLN
4	L	6	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

105 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	$\# Z  > 2$
5	NAG	A	601	1,5	14,14,15	0.68	0	17,19,21	0.50	0
5	NAG	A	602	5,6	14,14,15	0.75	1 (7%)	17,19,21	1.12	1 (5%)
6	BMA	A	603	5,7	11,11,12	1.06	0	15,15,17	1.19	2 (13%)
7	MAN	A	604	6	11,11,12	0.90	0	15,15,17	1.15	2 (13%)
5	NAG	A	605	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	A	606	5	14,14,15	0.46	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	607	1,5	14,14,15	0.78	0	17,19,21	0.82	1 (5%)
5	NAG	A	608	5,6	14,14,15	0.43	0	17,19,21	2.41	3 (17%)
6	BMA	A	609	5	11,11,12	0.66	0	15,15,17	1.10	1 (6%)
5	NAG	A	610	1,5	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
5	NAG	A	611	5,6	14,14,15	0.68	0	17,19,21	2.24	3 (17%)
6	BMA	A	612	5	11,11,12	0.73	0	15,15,17	0.89	0
5	NAG	A	613	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	4 (23%)
5	NAG	A	614	1,5	14,14,15	0.30	0	17,19,21	0.65	0
5	NAG	A	615	5,6	14,14,15	0.68	1 (7%)	17,19,21	0.73	0
6	BMA	A	616	5	11,11,12	0.92	0	15,15,17	1.30	3 (20%)
5	NAG	A	617	1	14,14,15	0.41	0	17,19,21	0.51	0
5	NAG	A	618	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.65	0
5	NAG	A	619	5	14,14,15	0.30	0	17,19,21	0.95	1 (5%)
5	NAG	A	620	1,5	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
5	NAG	A	621	5	14,14,15	0.22	0	17,19,21	0.54	0
5	NAG	A	622	1,5	14,14,15	0.52	0	17,19,21	0.60	0
5	NAG	A	623	5,6	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
6	BMA	A	624	5	11,11,12	0.50	0	15,15,17	1.35	1 (6%)
5	NAG	A	625	1,5	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
5	NAG	A	626	5	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
5	NAG	A	627	1	14,14,15	0.30	0	17,19,21	0.52	0
5	NAG	A	628	1,5	14,14,15	0.71	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	A	629	5	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	NAG	A	630	1,5	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
5	NAG	A	631	5	14,14,15	0.74	1 (7%)	17,19,21	0.56	0
5	NAG	A	632	1	14,14,15	0.27	0	17,19,21	1.41	1 (5%)
5	NAG	A	633	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	A	634	5	14,14,15	0.29	0	17,19,21	0.72	0
5	NAG	B	701	2	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
5	NAG	E	601	1,5	14,14,15	0.69	0	17,19,21	0.50	0
5	NAG	E	602	5,6	14,14,15	0.75	1 (7%)	17,19,21	1.12	1 (5%)
6	BMA	E	603	5,7	11,11,12	1.05	0	15,15,17	1.19	2 (13%)
7	MAN	E	604	6	11,11,12	0.91	0	15,15,17	1.15	2 (13%)
5	NAG	E	605	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	E	606	5	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
5	NAG	E	607	1,5	14,14,15	0.79	0	17,19,21	0.82	1 (5%)
5	NAG	E	608	5,6	14,14,15	0.43	0	17,19,21	2.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	E	609	5	11,11,12	0.66	0	15,15,17	1.11	1 (6%)
5	NAG	E	610	1,5	14,14,15	0.62	0	17,19,21	1.06	1 (5%)
5	NAG	E	611	5,6	14,14,15	0.68	0	17,19,21	2.25	3 (17%)
6	BMA	E	612	5	11,11,12	0.73	0	15,15,17	0.89	0
5	NAG	E	613	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	4 (23%)
5	NAG	E	614	1,5	14,14,15	0.31	0	17,19,21	0.65	0
5	NAG	E	615	5,6	14,14,15	0.68	1 (7%)	17,19,21	0.73	0
6	BMA	E	616	5	11,11,12	0.92	0	15,15,17	1.30	3 (20%)
5	NAG	E	617	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	E	618	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.64	0
5	NAG	E	619	5	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
5	NAG	E	620	1,5	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
5	NAG	E	621	5	14,14,15	0.23	0	17,19,21	0.54	0
5	NAG	E	622	1,5	14,14,15	0.53	0	17,19,21	0.60	0
5	NAG	E	623	5,6	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
6	BMA	E	624	5	11,11,12	0.49	0	15,15,17	1.35	1 (6%)
5	NAG	E	625	1,5	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
5	NAG	E	626	5	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
5	NAG	E	627	1	14,14,15	0.30	0	17,19,21	0.52	0
5	NAG	E	628	1,5	14,14,15	0.71	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	E	629	5	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
5	NAG	E	630	1,5	14,14,15	0.58	0	17,19,21	1.18	1 (5%)
5	NAG	E	631	5	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
5	NAG	E	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
5	NAG	E	633	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	E	634	5	14,14,15	0.29	0	17,19,21	0.73	0
5	NAG	F	701	2	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
5	NAG	I	601	1,5	14,14,15	0.68	0	17,19,21	0.50	0
5	NAG	I	602	5,6	14,14,15	0.76	1 (7%)	17,19,21	1.12	1 (5%)
6	BMA	I	603	5,7	11,11,12	1.07	0	15,15,17	1.19	2 (13%)
7	MAN	I	604	6	11,11,12	0.89	0	15,15,17	1.15	2 (13%)
5	NAG	I	605	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	I	606	5	14,14,15	0.45	0	17,19,21	0.83	1 (5%)
5	NAG	I	607	1,5	14,14,15	0.78	0	17,19,21	0.82	1 (5%)
5	NAG	I	608	5,6	14,14,15	0.43	0	17,19,21	2.41	3 (17%)
6	BMA	I	609	5	11,11,12	0.66	0	15,15,17	1.10	1 (6%)
5	NAG	I	610	1,5	14,14,15	0.63	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	I	611	5,6	14,14,15	0.67	0	17,19,21	2.25	3 (17%)
6	BMA	I	612	5	11,11,12	0.73	0	15,15,17	0.89	0
5	NAG	I	613	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	4 (23%)
5	NAG	I	614	1,5	14,14,15	0.30	0	17,19,21	0.65	0
5	NAG	I	615	5,6	14,14,15	0.67	1 (7%)	17,19,21	0.73	0
6	BMA	I	616	5	11,11,12	0.91	0	15,15,17	1.30	3 (20%)
5	NAG	I	617	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	I	618	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.64	0
5	NAG	I	619	5	14,14,15	0.31	0	17,19,21	0.96	1 (5%)
5	NAG	I	620	1,5	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
5	NAG	I	621	5	14,14,15	0.22	0	17,19,21	0.54	0
5	NAG	I	622	1,5	14,14,15	0.52	0	17,19,21	0.60	0
5	NAG	I	623	5,6	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
6	BMA	I	624	5	11,11,12	0.50	0	15,15,17	1.35	1 (6%)
5	NAG	I	625	1,5	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
5	NAG	I	626	5	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
5	NAG	I	627	1	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	I	628	1,5	14,14,15	0.70	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	I	629	5	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	NAG	I	630	1,5	14,14,15	0.58	0	17,19,21	1.19	1 (5%)
5	NAG	I	631	5	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
5	NAG	I	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
5	NAG	I	633	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	I	634	5	14,14,15	0.29	0	17,19,21	0.72	0
5	NAG	J	701	2	14,14,15	0.25	0	17,19,21	0.68	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5,6	-	2/6/23/26	0/1/1/1
6	BMA	A	603	5,7	-	2/2/19/22	0/1/1/1
7	MAN	A	604	6	-	0/2/19/22	0/1/1/1
5	NAG	A	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	606	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	608	5,6	-	5/6/23/26	0/1/1/1
6	BMA	A	609	5	-	1/2/19/22	0/1/1/1
5	NAG	A	610	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	611	5,6	-	4/6/23/26	0/1/1/1
6	BMA	A	612	5	-	2/2/19/22	0/1/1/1
5	NAG	A	613	1	-	5/6/23/26	0/1/1/1
5	NAG	A	614	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	615	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	616	5	-	1/2/19/22	0/1/1/1
5	NAG	A	617	1	-	1/6/23/26	0/1/1/1
5	NAG	A	618	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	619	5	-	3/6/23/26	0/1/1/1
5	NAG	A	620	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	621	5	-	2/6/23/26	0/1/1/1
5	NAG	A	622	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	623	5,6	-	3/6/23/26	0/1/1/1
6	BMA	A	624	5	-	2/2/19/22	0/1/1/1
5	NAG	A	625	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	626	5	-	1/6/23/26	0/1/1/1
5	NAG	A	627	1	-	2/6/23/26	0/1/1/1
5	NAG	A	628	1,5	-	3/6/23/26	0/1/1/1
5	NAG	A	629	5	-	3/6/23/26	0/1/1/1
5	NAG	A	630	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	631	5	-	0/6/23/26	0/1/1/1
5	NAG	A	632	1	-	0/6/23/26	0/1/1/1
5	NAG	A	633	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	634	5	-	0/6/23/26	0/1/1/1
5	NAG	B	701	2	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	602	5,6	-	2/6/23/26	0/1/1/1
6	BMA	E	603	5,7	-	2/2/19/22	0/1/1/1
7	MAN	E	604	6	-	0/2/19/22	0/1/1/1
5	NAG	E	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	606	5	-	2/6/23/26	0/1/1/1
5	NAG	E	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	608	5,6	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	E	609	5	-	1/2/19/22	0/1/1/1
5	NAG	E	610	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	611	5,6	-	4/6/23/26	0/1/1/1
6	BMA	E	612	5	-	2/2/19/22	0/1/1/1
5	NAG	E	613	1	-	5/6/23/26	0/1/1/1
5	NAG	E	614	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	615	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	616	5	-	1/2/19/22	0/1/1/1
5	NAG	E	617	1	-	1/6/23/26	0/1/1/1
5	NAG	E	618	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	619	5	-	3/6/23/26	0/1/1/1
5	NAG	E	620	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	621	5	-	2/6/23/26	0/1/1/1
5	NAG	E	622	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	623	5,6	-	3/6/23/26	0/1/1/1
6	BMA	E	624	5	-	2/2/19/22	0/1/1/1
5	NAG	E	625	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	626	5	-	1/6/23/26	0/1/1/1
5	NAG	E	627	1	-	2/6/23/26	0/1/1/1
5	NAG	E	628	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	629	5	-	3/6/23/26	0/1/1/1
5	NAG	E	630	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	631	5	-	0/6/23/26	0/1/1/1
5	NAG	E	632	1	-	0/6/23/26	0/1/1/1
5	NAG	E	633	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	634	5	-	0/6/23/26	0/1/1/1
5	NAG	F	701	2	-	2/6/23/26	0/1/1/1
5	NAG	I	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	602	5,6	-	2/6/23/26	0/1/1/1
6	BMA	I	603	5,7	-	2/2/19/22	0/1/1/1
7	MAN	I	604	6	-	0/2/19/22	0/1/1/1
5	NAG	I	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	606	5	-	2/6/23/26	0/1/1/1
5	NAG	I	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	608	5,6	-	5/6/23/26	0/1/1/1
6	BMA	I	609	5	-	1/2/19/22	0/1/1/1
5	NAG	I	610	1,5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	611	5,6	-	4/6/23/26	0/1/1/1
6	BMA	I	612	5	-	2/2/19/22	0/1/1/1
5	NAG	I	613	1	-	5/6/23/26	0/1/1/1
5	NAG	I	614	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	615	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	616	5	-	1/2/19/22	0/1/1/1
5	NAG	I	617	1	-	1/6/23/26	0/1/1/1
5	NAG	I	618	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	619	5	-	3/6/23/26	0/1/1/1
5	NAG	I	620	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	621	5	-	2/6/23/26	0/1/1/1
5	NAG	I	622	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	623	5,6	-	3/6/23/26	0/1/1/1
6	BMA	I	624	5	-	2/2/19/22	0/1/1/1
5	NAG	I	625	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	626	5	-	1/6/23/26	0/1/1/1
5	NAG	I	627	1	-	2/6/23/26	0/1/1/1
5	NAG	I	628	1,5	-	3/6/23/26	0/1/1/1
5	NAG	I	629	5	-	3/6/23/26	0/1/1/1
5	NAG	I	630	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	631	5	-	0/6/23/26	0/1/1/1
5	NAG	I	632	1	-	0/6/23/26	0/1/1/1
5	NAG	I	633	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	634	5	-	0/6/23/26	0/1/1/1
5	NAG	J	701	2	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	602	NAG	O5-C1	-2.74	1.39	1.43
5	E	602	NAG	O5-C1	-2.72	1.39	1.43
5	A	602	NAG	O5-C1	-2.72	1.39	1.43
5	E	613	NAG	C1-C2	2.48	1.56	1.52
5	A	613	NAG	C1-C2	2.46	1.56	1.52
5	A	628	NAG	O5-C1	-2.45	1.39	1.43
5	I	613	NAG	C1-C2	2.44	1.56	1.52
5	E	628	NAG	O5-C1	-2.44	1.39	1.43
5	I	628	NAG	O5-C1	-2.42	1.39	1.43
5	E	631	NAG	O5-C1	2.34	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	631	NAG	O5-C1	2.34	1.47	1.43
5	A	615	NAG	O5-C1	-2.32	1.40	1.43
5	I	631	NAG	O5-C1	2.31	1.47	1.43
5	E	615	NAG	O5-C1	-2.30	1.40	1.43
5	I	615	NAG	O5-C1	-2.28	1.40	1.43
5	I	618	NAG	O5-C1	-2.14	1.40	1.43
5	A	618	NAG	O5-C1	-2.11	1.40	1.43
5	E	618	NAG	O5-C1	-2.11	1.40	1.43

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	611	NAG	C2-N2-C7	7.87	134.20	122.92
5	I	611	NAG	C2-N2-C7	7.86	134.19	122.92
5	A	611	NAG	C2-N2-C7	7.85	134.17	122.92
5	E	613	NAG	C2-N2-C7	7.76	134.04	122.92
5	I	613	NAG	C2-N2-C7	7.74	134.00	122.92
5	A	613	NAG	C2-N2-C7	7.73	133.99	122.92
5	E	608	NAG	C2-N2-C7	7.71	133.97	122.92
5	A	608	NAG	C2-N2-C7	7.70	133.96	122.92
5	I	608	NAG	C2-N2-C7	7.70	133.96	122.92
5	E	632	NAG	C1-O5-C5	5.49	119.66	112.20
5	I	632	NAG	C1-O5-C5	5.48	119.65	112.20
5	A	632	NAG	C1-O5-C5	5.46	119.63	112.20
5	I	608	NAG	C1-C2-N2	4.77	118.63	110.49
5	E	608	NAG	C1-C2-N2	4.76	118.62	110.49
5	A	608	NAG	C1-C2-N2	4.76	118.62	110.49
6	I	624	BMA	C1-O5-C5	4.40	118.18	112.20
6	A	624	BMA	C1-O5-C5	4.38	118.16	112.20
6	E	624	BMA	C1-O5-C5	4.37	118.14	112.20
5	I	611	NAG	C1-C2-N2	3.69	116.79	110.49
5	A	611	NAG	C1-C2-N2	3.68	116.78	110.49
5	E	613	NAG	C1-C2-N2	3.68	116.77	110.49
5	A	613	NAG	C1-C2-N2	3.67	116.76	110.49
5	E	611	NAG	C1-C2-N2	3.67	116.76	110.49
5	I	613	NAG	C1-C2-N2	3.66	116.74	110.49
5	E	610	NAG	C1-O5-C5	3.52	116.98	112.20
5	A	610	NAG	C1-O5-C5	3.52	116.98	112.20
5	I	610	NAG	C1-O5-C5	3.48	116.94	112.20
5	A	620	NAG	C2-N2-C7	3.33	127.69	122.92
5	E	620	NAG	C2-N2-C7	3.32	127.68	122.92
5	I	620	NAG	C2-N2-C7	3.32	127.67	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	619	NAG	C2-N2-C7	3.09	127.34	122.92
5	I	619	NAG	C2-N2-C7	3.08	127.34	122.92
5	E	613	NAG	C1-O5-C5	3.08	116.38	112.20
5	I	613	NAG	C1-O5-C5	3.07	116.38	112.20
5	A	613	NAG	C1-O5-C5	3.07	116.37	112.20
5	A	619	NAG	C2-N2-C7	3.06	127.31	122.92
5	E	623	NAG	C2-N2-C7	3.04	127.28	122.92
5	A	623	NAG	C2-N2-C7	3.04	127.28	122.92
5	I	623	NAG	C2-N2-C7	3.03	127.27	122.92
5	E	629	NAG	C2-N2-C7	2.96	127.17	122.92
5	A	629	NAG	C2-N2-C7	2.96	127.16	122.92
5	I	606	NAG	C1-O5-C5	2.95	116.21	112.20
5	A	630	NAG	O4-C4-C5	-2.94	101.94	109.29
5	I	628	NAG	C2-N2-C7	2.94	127.14	122.92
7	E	604	MAN	C1-O5-C5	2.94	116.20	112.20
7	A	604	MAN	C1-O5-C5	2.94	116.20	112.20
7	I	604	MAN	C1-O5-C5	2.94	116.19	112.20
5	E	628	NAG	C2-N2-C7	2.94	127.13	122.92
5	I	629	NAG	C2-N2-C7	2.94	127.13	122.92
5	E	630	NAG	O4-C4-C5	-2.93	101.95	109.29
5	A	628	NAG	C2-N2-C7	2.93	127.13	122.92
5	I	630	NAG	O4-C4-C5	-2.93	101.95	109.29
5	A	606	NAG	C1-O5-C5	2.92	116.17	112.20
5	E	626	NAG	C2-N2-C7	2.92	127.10	122.92
5	E	606	NAG	C1-O5-C5	2.92	116.17	112.20
5	A	626	NAG	C2-N2-C7	2.91	127.09	122.92
5	I	626	NAG	C2-N2-C7	2.90	127.08	122.92
5	I	602	NAG	C2-N2-C7	2.89	127.06	122.92
5	A	602	NAG	C2-N2-C7	2.88	127.05	122.92
5	E	602	NAG	C2-N2-C7	2.87	127.03	122.92
6	A	609	BMA	C1-O5-C5	2.85	116.08	112.20
6	E	609	BMA	C1-O5-C5	2.84	116.06	112.20
6	I	609	BMA	C1-O5-C5	2.84	116.06	112.20
5	E	620	NAG	C1-O5-C5	2.74	115.92	112.20
5	I	620	NAG	C1-O5-C5	2.73	115.91	112.20
5	A	620	NAG	C1-O5-C5	2.73	115.91	112.20
6	E	616	BMA	O5-C1-C2	-2.59	106.79	110.79
6	A	616	BMA	O5-C1-C2	-2.59	106.80	110.79
6	I	616	BMA	O5-C1-C2	-2.57	106.82	110.79
6	I	603	BMA	C3-C4-C5	-2.41	105.90	110.23
6	A	603	BMA	C3-C4-C5	-2.41	105.90	110.23
6	E	603	BMA	C3-C4-C5	-2.41	105.90	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	625	NAG	C1-O5-C5	2.31	115.35	112.20
5	F	701	NAG	C1-O5-C5	2.31	115.34	112.20
5	A	625	NAG	C1-O5-C5	2.30	115.33	112.20
5	B	701	NAG	C1-O5-C5	2.29	115.32	112.20
5	J	701	NAG	C1-O5-C5	2.29	115.31	112.20
7	A	604	MAN	O2-C2-C3	-2.29	105.70	110.16
7	I	604	MAN	O2-C2-C3	-2.28	105.70	110.16
5	I	625	NAG	C1-O5-C5	2.27	115.29	112.20
7	E	604	MAN	O2-C2-C3	-2.27	105.73	110.16
6	E	603	BMA	O5-C5-C4	-2.27	105.31	110.83
6	A	603	BMA	O5-C5-C4	-2.25	105.34	110.83
6	I	603	BMA	O5-C5-C4	-2.24	105.37	110.83
5	I	607	NAG	C3-C4-C5	-2.24	106.21	110.23
5	E	607	NAG	C3-C4-C5	-2.23	106.22	110.23
5	A	607	NAG	C3-C4-C5	-2.23	106.22	110.23
5	I	626	NAG	C1-O5-C5	2.19	115.18	112.20
5	A	626	NAG	C1-O5-C5	2.17	115.15	112.20
5	E	626	NAG	C1-O5-C5	2.16	115.14	112.20
5	A	611	NAG	C8-C7-N2	2.14	119.79	116.10
6	I	616	BMA	C1-C2-C3	-2.13	107.03	109.66
6	E	616	BMA	C1-C2-C3	-2.13	107.03	109.66
5	I	611	NAG	C8-C7-N2	2.13	119.77	116.10
6	I	616	BMA	O2-C2-C3	-2.12	106.01	110.16
5	E	611	NAG	C8-C7-N2	2.12	119.76	116.10
6	A	616	BMA	C1-C2-C3	-2.12	107.05	109.66
6	A	616	BMA	O2-C2-C3	-2.11	106.04	110.16
6	E	616	BMA	O2-C2-C3	-2.10	106.05	110.16
5	A	613	NAG	C8-C7-N2	2.02	119.59	116.10
5	E	613	NAG	C8-C7-N2	2.01	119.56	116.10
5	A	608	NAG	C8-C7-N2	2.01	119.56	116.10
5	I	613	NAG	C8-C7-N2	2.01	119.56	116.10
5	I	608	NAG	C8-C7-N2	2.00	119.56	116.10

There are no chirality outliers.

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	633	NAG	C8-C7-N2-C2
5	E	633	NAG	O7-C7-N2-C2
5	A	633	NAG	C8-C7-N2-C2
5	A	633	NAG	O7-C7-N2-C2
5	I	633	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	I	633	NAG	O7-C7-N2-C2
5	I	630	NAG	C4-C5-C6-O6
5	E	630	NAG	C4-C5-C6-O6
5	A	630	NAG	C4-C5-C6-O6
5	A	627	NAG	O5-C5-C6-O6
5	J	701	NAG	O5-C5-C6-O6
5	B	701	NAG	O5-C5-C6-O6
5	F	701	NAG	O5-C5-C6-O6
5	I	627	NAG	O5-C5-C6-O6
5	E	627	NAG	O5-C5-C6-O6
5	I	630	NAG	O5-C5-C6-O6
5	E	630	NAG	O5-C5-C6-O6
5	A	630	NAG	O5-C5-C6-O6
5	E	606	NAG	O5-C5-C6-O6
5	I	606	NAG	O5-C5-C6-O6
6	I	612	BMA	O5-C5-C6-O6
6	A	612	BMA	O5-C5-C6-O6
5	A	606	NAG	O5-C5-C6-O6
6	E	612	BMA	O5-C5-C6-O6
5	J	701	NAG	C4-C5-C6-O6
5	B	701	NAG	C4-C5-C6-O6
5	F	701	NAG	C4-C5-C6-O6
5	I	622	NAG	O5-C5-C6-O6
5	E	622	NAG	O5-C5-C6-O6
5	A	622	NAG	O5-C5-C6-O6
5	I	619	NAG	O5-C5-C6-O6
5	E	619	NAG	O5-C5-C6-O6
5	A	619	NAG	O5-C5-C6-O6
5	A	621	NAG	C4-C5-C6-O6
5	I	621	NAG	C4-C5-C6-O6
5	E	621	NAG	C4-C5-C6-O6
5	A	621	NAG	O5-C5-C6-O6
5	I	621	NAG	O5-C5-C6-O6
5	E	621	NAG	O5-C5-C6-O6
5	A	623	NAG	O5-C5-C6-O6
5	E	623	NAG	O5-C5-C6-O6
5	I	623	NAG	O5-C5-C6-O6
5	A	614	NAG	C4-C5-C6-O6
5	E	614	NAG	C4-C5-C6-O6
5	I	614	NAG	C4-C5-C6-O6
5	A	627	NAG	C4-C5-C6-O6
5	I	627	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	627	NAG	C4-C5-C6-O6
5	I	628	NAG	O5-C5-C6-O6
5	E	628	NAG	O5-C5-C6-O6
5	E	606	NAG	C4-C5-C6-O6
5	I	622	NAG	C4-C5-C6-O6
5	E	622	NAG	C4-C5-C6-O6
5	I	606	NAG	C4-C5-C6-O6
5	A	622	NAG	C4-C5-C6-O6
5	A	606	NAG	C4-C5-C6-O6
5	I	619	NAG	C4-C5-C6-O6
5	E	619	NAG	C4-C5-C6-O6
5	A	619	NAG	C4-C5-C6-O6
5	A	628	NAG	O5-C5-C6-O6
6	I	612	BMA	C4-C5-C6-O6
6	A	612	BMA	C4-C5-C6-O6
6	E	612	BMA	C4-C5-C6-O6
5	I	613	NAG	C8-C7-N2-C2
5	I	613	NAG	O7-C7-N2-C2
5	I	618	NAG	C8-C7-N2-C2
5	I	618	NAG	O7-C7-N2-C2
5	A	618	NAG	C8-C7-N2-C2
5	A	618	NAG	O7-C7-N2-C2
5	E	618	NAG	C8-C7-N2-C2
5	E	618	NAG	O7-C7-N2-C2
5	E	611	NAG	C8-C7-N2-C2
5	E	611	NAG	O7-C7-N2-C2
5	I	611	NAG	C8-C7-N2-C2
5	I	611	NAG	O7-C7-N2-C2
5	E	608	NAG	C8-C7-N2-C2
5	E	608	NAG	O7-C7-N2-C2
5	A	611	NAG	C8-C7-N2-C2
5	A	611	NAG	O7-C7-N2-C2
5	E	613	NAG	C8-C7-N2-C2
5	E	613	NAG	O7-C7-N2-C2
5	A	613	NAG	C8-C7-N2-C2
5	A	613	NAG	O7-C7-N2-C2
5	I	608	NAG	C8-C7-N2-C2
5	I	608	NAG	O7-C7-N2-C2
5	A	608	NAG	C8-C7-N2-C2
5	A	608	NAG	O7-C7-N2-C2
5	A	623	NAG	C4-C5-C6-O6
5	E	623	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	I	623	NAG	C4-C5-C6-O6
5	A	629	NAG	O5-C5-C6-O6
5	E	629	NAG	O5-C5-C6-O6
5	I	629	NAG	O5-C5-C6-O6
5	E	608	NAG	O5-C5-C6-O6
5	I	608	NAG	O5-C5-C6-O6
5	A	608	NAG	O5-C5-C6-O6
5	E	608	NAG	C4-C5-C6-O6
5	I	608	NAG	C4-C5-C6-O6
5	A	608	NAG	C4-C5-C6-O6
6	I	624	BMA	O5-C5-C6-O6
6	A	624	BMA	O5-C5-C6-O6
6	E	624	BMA	O5-C5-C6-O6
5	A	629	NAG	C4-C5-C6-O6
5	E	629	NAG	C4-C5-C6-O6
5	I	629	NAG	C4-C5-C6-O6
6	A	603	BMA	C4-C5-C6-O6
6	I	603	BMA	C4-C5-C6-O6
6	E	603	BMA	C4-C5-C6-O6
6	A	603	BMA	O5-C5-C6-O6
6	I	603	BMA	O5-C5-C6-O6
6	E	603	BMA	O5-C5-C6-O6
6	I	624	BMA	C4-C5-C6-O6
6	A	624	BMA	C4-C5-C6-O6
6	E	624	BMA	C4-C5-C6-O6
5	I	613	NAG	O5-C5-C6-O6
5	E	613	NAG	O5-C5-C6-O6
5	A	613	NAG	O5-C5-C6-O6
5	E	614	NAG	O5-C5-C6-O6
5	A	614	NAG	O5-C5-C6-O6
5	I	614	NAG	O5-C5-C6-O6
5	I	613	NAG	C4-C5-C6-O6
5	E	613	NAG	C4-C5-C6-O6
5	A	613	NAG	C4-C5-C6-O6
6	I	609	BMA	O5-C5-C6-O6
6	E	609	BMA	O5-C5-C6-O6
6	E	616	BMA	O5-C5-C6-O6
6	A	609	BMA	O5-C5-C6-O6
6	A	616	BMA	O5-C5-C6-O6
6	I	616	BMA	O5-C5-C6-O6
5	I	617	NAG	O5-C5-C6-O6
5	E	617	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	617	NAG	O5-C5-C6-O6
5	E	611	NAG	O5-C5-C6-O6
5	I	611	NAG	O5-C5-C6-O6
5	A	611	NAG	O5-C5-C6-O6
5	A	625	NAG	O5-C5-C6-O6
5	I	625	NAG	O5-C5-C6-O6
5	E	625	NAG	O5-C5-C6-O6
5	I	628	NAG	C4-C5-C6-O6
5	A	628	NAG	C4-C5-C6-O6
5	E	628	NAG	C4-C5-C6-O6
5	I	602	NAG	O5-C5-C6-O6
5	E	602	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	E	610	NAG	C4-C5-C6-O6
5	A	610	NAG	C4-C5-C6-O6
5	I	610	NAG	C4-C5-C6-O6
5	I	613	NAG	C3-C2-N2-C7
5	A	620	NAG	C3-C2-N2-C7
5	I	602	NAG	C3-C2-N2-C7
5	I	620	NAG	C3-C2-N2-C7
5	A	628	NAG	C3-C2-N2-C7
5	I	628	NAG	C3-C2-N2-C7
5	E	620	NAG	C3-C2-N2-C7
5	E	628	NAG	C3-C2-N2-C7
5	E	613	NAG	C3-C2-N2-C7
5	A	613	NAG	C3-C2-N2-C7
5	E	602	NAG	C3-C2-N2-C7
5	A	602	NAG	C3-C2-N2-C7
5	A	623	NAG	C3-C2-N2-C7
5	I	626	NAG	C3-C2-N2-C7
5	E	611	NAG	C3-C2-N2-C7
5	I	611	NAG	C3-C2-N2-C7
5	E	626	NAG	C3-C2-N2-C7
5	E	623	NAG	C3-C2-N2-C7
5	A	626	NAG	C3-C2-N2-C7
5	I	623	NAG	C3-C2-N2-C7
5	E	608	NAG	C3-C2-N2-C7
5	A	611	NAG	C3-C2-N2-C7
5	I	608	NAG	C3-C2-N2-C7
5	A	608	NAG	C3-C2-N2-C7
5	I	619	NAG	C3-C2-N2-C7
5	A	629	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	E	619	NAG	C3-C2-N2-C7
5	E	629	NAG	C3-C2-N2-C7
5	A	619	NAG	C3-C2-N2-C7
5	I	629	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	NAG	1	0
5	E	605	NAG	1	0
5	E	633	NAG	1	0
5	I	605	NAG	1	0

## 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.