



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 07:22 AM EDT

PDB ID : 5KEL  
EMDB ID: : EMD-8240  
Title : EBOV GP in complex with variable Fab domains of IgGs c2G4 and c13C6  
Authors : Pallesen, J.; Murin, C.D.; de Val, N.; Cottrell, C.A.; Hastie, K.M.; Turner, H.L.; Fusco, M.L.; Flyak, A.I.; Zeitlin, L.; Crowe Jr., J.E.; Andersen, K.G.; Saphire, E.O.; Ward, A.B.  
Deposited on : unknown  
Resolution : 4.30 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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.

---

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-20029824

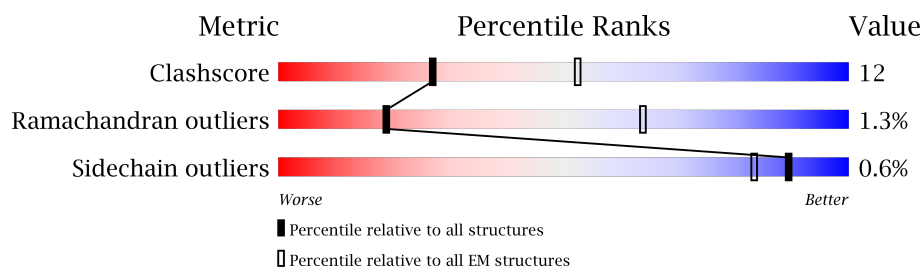
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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	469	
1	E	469	
1	F	469	
2	B	143	
2	G	143	
2	I	143	
3	H	120	
3	P	120	
3	Q	120	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain	
4	L	107		94% 6%
4	T	107		94% 6%
4	U	107		94% 6%
5	C	121		88% 10% •
5	J	121		88% 10% •
5	M	121		88% 10% •
6	D	107		92% 8%
6	N	107		93% 7%
6	O	107		93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	B	701	-	-	X	-
7	NAG	G	701	-	-	X	-
7	NAG	I	701	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19278 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 Ebola surface glycoprotein, GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	235	Total	C	N	O	S	0	0
			1828	1162	316	345	5		
1	E	235	Total	C	N	O	S	0	0
			1828	1162	316	345	5		
1	F	235	Total	C	N	O	S	0	0
			1828	1162	316	345	5		

- Molecule 2 is a protein called Ebola surface glycoprotein, GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	113	Total	C	N	O	S	0	0
			889	567	155	161	6		
2	G	113	Total	C	N	O	S	0	0
			889	567	155	161	6		
2	I	113	Total	C	N	O	S	0	0
			889	567	155	161	6		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	THR	ILE	conflict	UNP Q05320
B	638	LEU	-	expression tag	UNP Q05320
B	639	GLU	-	expression tag	UNP Q05320
B	640	VAL	-	expression tag	UNP Q05320
B	641	ASP	-	expression tag	UNP Q05320
B	642	ASP	-	expression tag	UNP Q05320
B	643	ASP	-	expression tag	UNP Q05320
B	644	ASP	-	expression tag	UNP Q05320
G	544	THR	ILE	conflict	UNP Q05320
G	638	LEU	-	expression tag	UNP Q05320
G	639	GLU	-	expression tag	UNP Q05320
G	640	VAL	-	expression tag	UNP Q05320
G	641	ASP	-	expression tag	UNP Q05320

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	642	ASP	-	expression tag	UNP Q05320
G	643	ASP	-	expression tag	UNP Q05320
G	644	ASP	-	expression tag	UNP Q05320
I	544	THR	ILE	conflict	UNP Q05320
I	638	LEU	-	expression tag	UNP Q05320
I	639	GLU	-	expression tag	UNP Q05320
I	640	VAL	-	expression tag	UNP Q05320
I	641	ASP	-	expression tag	UNP Q05320
I	642	ASP	-	expression tag	UNP Q05320
I	643	ASP	-	expression tag	UNP Q05320
I	644	ASP	-	expression tag	UNP Q05320

- Molecule 3 is a protein called c2G4 variable Fab domain heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	120	Total	C	N	O	S	0	0
			952	592	168	185	7		
3	P	120	Total	C	N	O	S	0	0
			952	592	168	185	7		
3	Q	120	Total	C	N	O	S	0	0
			952	592	168	185	7		

- Molecule 4 is a protein called c2G4 variable Fab domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			820	518	133	166	3		
4	T	107	Total	C	N	O	S	0	0
			820	518	133	166	3		
4	U	107	Total	C	N	O	S	0	0
			820	518	133	166	3		

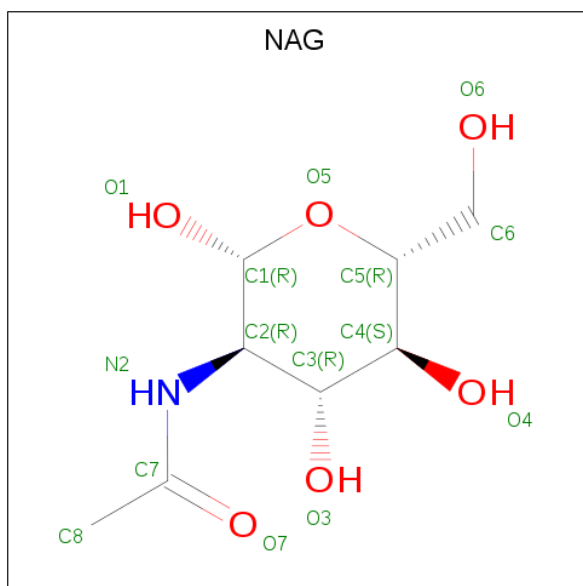
- Molecule 5 is a protein called c13C6 variable Fab domain heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	121	Total	C	N	O	S	0	0
			930	593	154	180	3		
5	J	121	Total	C	N	O	S	0	0
			930	593	154	180	3		
5	M	121	Total	C	N	O	S	0	0
			930	593	154	180	3		

- Molecule 6 is a protein called c13C6 variable Fab domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	107	Total	C	N	O	S	0	0
			815	509	135	167	4		
6	N	107	Total	C	N	O	S	0	0
			815	509	135	167	4		
6	O	107	Total	C	N	O	S	0	0
			815	509	135	167	4		

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



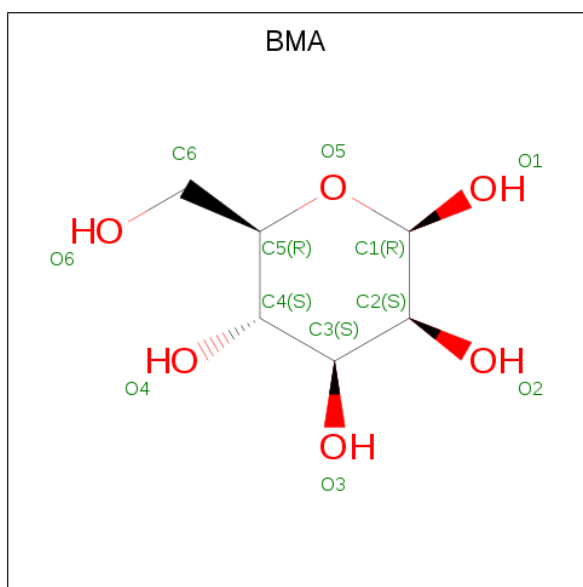
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			98	56	7	35	
7	A	1	Total	C	N	O	0
			98	56	7	35	
7	A	1	Total	C	N	O	0
			98	56	7	35	
7	A	1	Total	C	N	O	0
			98	56	7	35	
7	A	1	Total	C	N	O	0
			98	56	7	35	
7	A	1	Total	C	N	O	0
			98	56	7	35	
7	B	1	Total	C	N	O	0
			28	16	2	10	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			28	16	2	10	
7	E	1	Total	C	N	O	0
			98	56	7	35	
7	E	1	Total	C	N	O	0
			98	56	7	35	
7	E	1	Total	C	N	O	0
			98	56	7	35	
7	E	1	Total	C	N	O	0
			98	56	7	35	
7	E	1	Total	C	N	O	0
			98	56	7	35	
7	E	1	Total	C	N	O	0
			98	56	7	35	
7	G	1	Total	C	N	O	0
			28	16	2	10	
7	G	1	Total	C	N	O	0
			28	16	2	10	
7	F	1	Total	C	N	O	0
			98	56	7	35	
7	F	1	Total	C	N	O	0
			98	56	7	35	
7	F	1	Total	C	N	O	0
			98	56	7	35	
7	F	1	Total	C	N	O	0
			98	56	7	35	
7	F	1	Total	C	N	O	0
			98	56	7	35	
7	F	1	Total	C	N	O	0
			98	56	7	35	
7	I	1	Total	C	N	O	0
			28	16	2	10	
7	I	1	Total	C	N	O	0
			28	16	2	10	

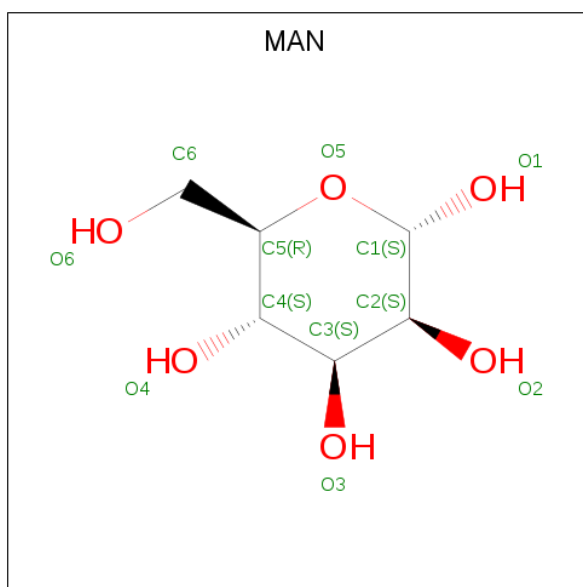
- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			22	12	10	
8	A	1	Total	C	O	0
			22	12	10	
8	B	1	Total	C	O	0
			11	6	5	
8	E	1	Total	C	O	0
			22	12	10	
8	E	1	Total	C	O	0
			22	12	10	
8	G	1	Total	C	O	0
			11	6	5	
8	F	1	Total	C	O	0
			22	12	10	
8	F	1	Total	C	O	0
			22	12	10	
8	I	1	Total	C	O	0
			11	6	5	

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



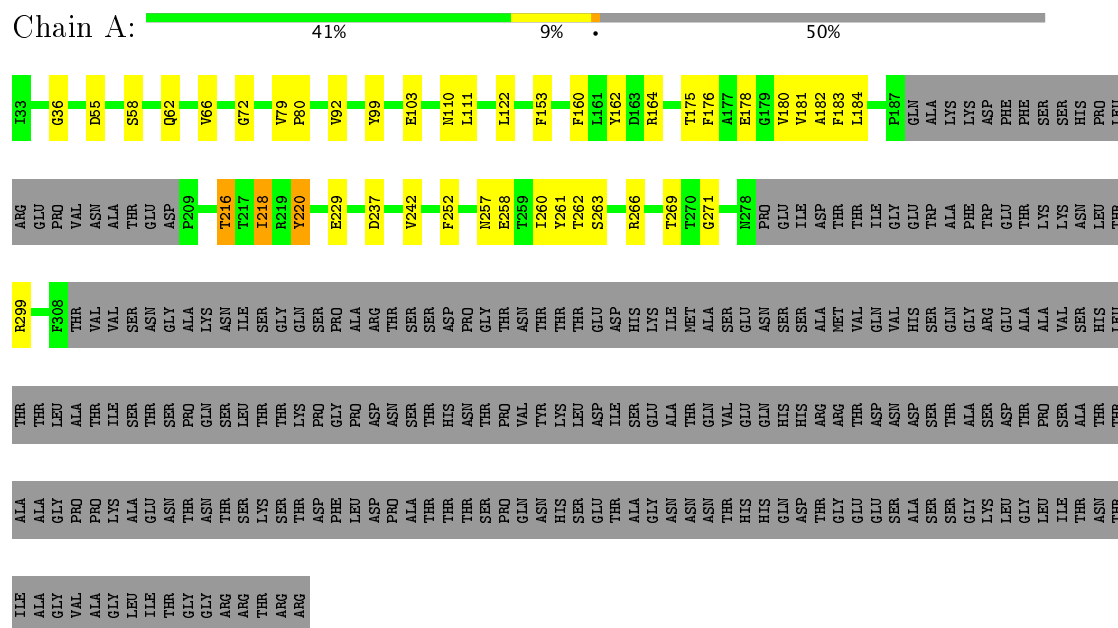


Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			22	12	10	
9	B	1	Total	C	O	0
			22	12	10	
9	E	1	Total	C	O	0
			11	6	5	
9	G	1	Total	C	O	0
			22	12	10	
9	G	1	Total	C	O	0
			22	12	10	
9	F	1	Total	C	O	0
			11	6	5	
9	I	1	Total	C	O	0
			22	12	10	
9	I	1	Total	C	O	0
			22	12	10	

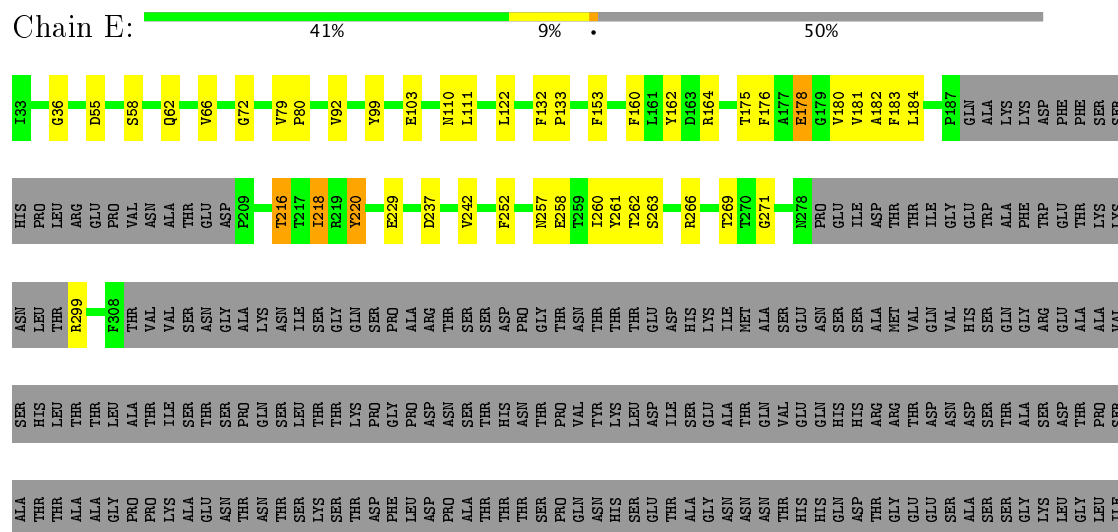
### 3 Residue-property plots

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: Ebola surface glycoprotein, GP1



- Molecule 1: Ebola surface glycoprotein, GP1



GLT	A503		A507	A508	P509	K510		Y517	Y518	T519		R531	I532	I533	Y534		R559	Q560	L561	A562	N563	E564	T565	T566	Q567		Q570		E578		I584		R587		R586	K597		H602	I603		H613	D614	M615		TRX	TRX	TRX	ASU	ASU	ILE	ILE	ILE	ILE	ILE	ILE	ASP	ASP	GLN	GLN	ASP	ASP	ASP	ASP	PRE	PRE	VNI	VNI
-----	------	--	------	------	------	------	--	------	------	------	--	------	------	------	------	--	------	------	------	------	------	------	------	------	------	--	------	--	------	--	------	--	------	--	------	------	--	------	------	--	------	------	------	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP  
LYS  
THR  
LEU  
PRO  
ASP  
LEU  
GLU  
VAL  
ASP  
ASP  
ASP  
ASP

- Molecule 3: c2G4 variable Fab domain heavy chain

Chain H:  90% 9% .


E1 S7 G15 S21 T28 S40 P41 E42 R66 I69 Y91 L82C Y91 R94 M100B S112

- Molecule 3: c2G4 variable Fab domain heavy chain

Chain P:  92% 8% .

E1 S7 S21 T28 S40 P41 E42 R66 I69 Y91 R94 M100B S112

- Molecule 3: c2G4 variable Fab domain heavy chain

Chain Q:  90% 9% .

E1 S7 G15 S21 T28 S40 P41 E42 R66 I69 Y91 L82C Y91 R94 M100B S112

- Molecule 4: c2G4 variable Fab domain light chain

Chain L:  94% 6% .

D1 S43 P44 F62 Y71 Q89 G93 K107

- Molecule 4: c2G4 variable Fab domain light chain

Chain T:  94% 6% .


D1 S43 P44 F62 Y71 Q89 G93 K107

- Molecule 4: c2G4 variable Fab domain light chain

Chain U:  94% 6% .

D1 S43 P44 F62 Y71 Q89 G93 K107

- Molecule 5: c13C6 variable Fab domain heavy chain

Chain C:  88% 10% .



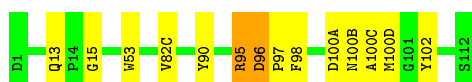
- Molecule 5: c13C6 variable Fab domain heavy chain

Chain J: 88% 10% .



- Molecule 5: c13C6 variable Fab domain heavy chain

Chain M: 88% 10% .



- Molecule 6: c13C6 variable Fab domain light chain

Chain D: 92% 8%



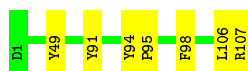
- Molecule 6: c13C6 variable Fab domain light chain

Chain N: 93% 7%



- Molecule 6: c13C6 variable Fab domain light chain

Chain O: 93% 7%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	86000	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 ( $e^-/\text{\AA}^2$ )	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (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	0.87	0/1868	0.93	4/2532 (0.2%)
1	E	0.87	0/1868	0.93	4/2532 (0.2%)
1	F	0.87	0/1868	0.93	4/2532 (0.2%)
2	B	0.84	1/913 (0.1%)	0.87	2/1246 (0.2%)
2	G	0.84	1/913 (0.1%)	0.87	2/1246 (0.2%)
2	I	0.84	2/913 (0.2%)	0.87	2/1246 (0.2%)
3	H	0.87	0/973	0.98	3/1311 (0.2%)
3	P	0.87	0/973	0.98	3/1311 (0.2%)
3	Q	0.87	0/973	0.98	3/1311 (0.2%)
4	L	0.78	0/839	0.88	0/1136
4	T	0.78	0/839	0.88	0/1136
4	U	0.78	0/839	0.88	0/1136
5	C	0.74	0/954	0.93	3/1292 (0.2%)
5	J	0.74	0/954	0.93	3/1292 (0.2%)
5	M	0.74	0/954	0.93	3/1292 (0.2%)
6	D	0.69	0/831	0.84	0/1127
6	N	0.69	0/831	0.84	0/1127
6	O	0.69	0/831	0.84	0/1127
All	All	0.82	4/19134 (0.0%)	0.91	36/25932 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	578	GLU	CG-CD	-5.45	1.43	1.51
2	G	578	GLU	CG-CD	-5.42	1.43	1.51
2	I	578	GLU	CG-CD	-5.39	1.43	1.51
2	I	578	GLU	CD-OE1	-5.01	1.20	1.25

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	164	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	164	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	E	164	ARG	NE-CZ-NH2	-7.01	116.79	120.30
5	M	102	TYR	CB-CG-CD1	-6.60	117.04	121.00
5	J	102	TYR	CB-CG-CD1	-6.59	117.04	121.00

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	1828	0	1783	47	0
1	E	1828	0	1783	49	0
1	F	1828	0	1783	49	0
2	B	889	0	854	100	0
2	G	889	0	854	103	0
2	I	889	0	854	102	0
3	H	952	0	904	8	0
3	P	952	0	904	7	0
3	Q	952	0	904	8	0
4	L	820	0	789	4	0
4	T	820	0	789	4	0
4	U	820	0	789	4	0
5	C	930	0	894	19	0
5	J	930	0	894	18	0
5	M	930	0	894	19	0
6	D	815	0	791	6	0
6	N	815	0	791	5	0
6	O	815	0	791	5	0
7	A	98	0	86	12	0
7	B	28	0	24	11	0
7	E	98	0	86	13	0
7	F	98	0	86	11	0
7	G	28	0	24	10	0
7	I	28	0	24	11	0
8	A	22	0	19	3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	11	0	8	0	0
8	E	22	0	19	3	0
8	F	22	0	19	2	0
8	G	11	0	8	0	0
8	I	11	0	8	0	0
9	A	11	0	10	0	0
9	B	22	0	20	0	0
9	E	11	0	10	0	0
9	F	11	0	10	0	0
9	G	22	0	20	0	0
9	I	22	0	20	0	0
All	All	19278	0	18546	467	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 12.

The worst 5 of 467 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:507:ALA:C	2:G:509:PRO:HD2	1.39	1.42
2:I:507:ALA:C	2:I:509:PRO:HD2	1.39	1.41
2:B:507:ALA:C	2:B:509:PRO:HD2	1.39	1.40
2:B:531:TRP:CE2	2:I:567:GLN:OE1	1.76	1.38
2:B:567:GLN:OE1	2:G:531:TRP:CE2	1.76	1.37

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	229/469 (49%)	216 (94%)	8 (4%)	5 (2%)	<b>8</b> 46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	229/469 (49%)	216 (94%)	8 (4%)	5 (2%)	8	46
1	F	229/469 (49%)	216 (94%)	8 (4%)	5 (2%)	8	46
2	B	111/143 (78%)	103 (93%)	6 (5%)	2 (2%)	10	50
2	G	111/143 (78%)	103 (93%)	6 (5%)	2 (2%)	10	50
2	I	111/143 (78%)	103 (93%)	6 (5%)	2 (2%)	10	50
3	H	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
3	P	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
3	Q	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
4	L	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	18	61
4	T	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	18	61
4	U	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	18	61
5	C	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	11	52
5	J	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	11	52
5	M	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	11	52
6	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
6	N	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
6	O	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
All	All	2361/3201 (74%)	2250 (95%)	81 (3%)	30 (1%)	19	56

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	THR
1	A	242	VAL
1	E	216	THR
1	E	242	VAL
1	F	216	THR

### 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	197/399 (49%)	196 (100%)	1 (0%)	91	95
1	E	197/399 (49%)	196 (100%)	1 (0%)	91	95
1	F	197/399 (49%)	196 (100%)	1 (0%)	91	95
2	B	92/122 (75%)	90 (98%)	2 (2%)	57	80
2	G	92/122 (75%)	90 (98%)	2 (2%)	57	80
2	I	92/122 (75%)	90 (98%)	2 (2%)	57	80
3	H	101/101 (100%)	100 (99%)	1 (1%)	80	90
3	P	101/101 (100%)	100 (99%)	1 (1%)	80	90
3	Q	101/101 (100%)	100 (99%)	1 (1%)	80	90
4	L	91/91 (100%)	91 (100%)	0	100	100
4	T	91/91 (100%)	91 (100%)	0	100	100
4	U	91/91 (100%)	91 (100%)	0	100	100
5	C	99/99 (100%)	99 (100%)	0	100	100
5	J	99/99 (100%)	99 (100%)	0	100	100
5	M	99/99 (100%)	99 (100%)	0	100	100
6	D	92/92 (100%)	92 (100%)	0	100	100
6	N	92/92 (100%)	92 (100%)	0	100	100
6	O	92/92 (100%)	92 (100%)	0	100	100
All	All	2016/2712 (74%)	2004 (99%)	12 (1%)	89	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	564	GLU
2	G	567	GLN
2	I	564	GLU
1	E	178	GLU
1	F	178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	570	GLN
5	M	100(B)	ASN
2	I	567	GLN
2	G	567	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	J	100(B)	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 ⓘ

45 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	A	601	1,7	14,14,15	0.70	1 (7%)	15,19,21	2.56	3 (20%)
7	NAG	A	602	7	14,14,15	0.27	0	15,19,21	0.51	0
7	NAG	A	603	1	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
7	NAG	A	604	1,7	14,14,15	0.51	0	15,19,21	0.82	0
7	NAG	A	605	8,7	14,14,15	0.29	0	15,19,21	0.55	0
8	BMA	A	606	7	11,11,12	0.23	0	13,15,17	0.65	0
7	NAG	A	607	1,7	14,14,15	0.30	0	15,19,21	0.95	1 (6%)
7	NAG	A	608	8,7	14,14,15	0.26	0	15,19,21	0.63	0
8	BMA	A	609	9,7	11,11,12	0.24	0	13,15,17	0.64	0
9	MAN	A	610	8	11,11,12	0.22	0	13,15,17	0.48	0
7	NAG	B	701	2,7	14,14,15	0.29	0	15,19,21	0.94	1 (6%)
7	NAG	B	702	8,7	14,14,15	0.32	0	15,19,21	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	B	703	9,7	11,11,12	0.24	0	13,15,17	0.97	1 (7%)
9	MAN	B	704	8	11,11,12	0.24	0	13,15,17	1.10	1 (7%)
9	MAN	B	705	8	11,11,12	0.26	0	13,15,17	0.96	2 (15%)
7	NAG	E	601	1,7	14,14,15	0.70	1 (7%)	15,19,21	2.56	3 (20%)
7	NAG	E	602	7	14,14,15	0.27	0	15,19,21	0.51	0
7	NAG	E	603	1	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
7	NAG	E	604	1,7	14,14,15	0.51	0	15,19,21	0.83	0
7	NAG	E	605	8,7	14,14,15	0.30	0	15,19,21	0.55	0
8	BMA	E	606	7	11,11,12	0.23	0	13,15,17	0.64	0
7	NAG	E	607	1,7	14,14,15	0.30	0	15,19,21	0.96	2 (13%)
7	NAG	E	608	8,7	14,14,15	0.26	0	15,19,21	0.64	0
8	BMA	E	609	9,7	11,11,12	0.24	0	13,15,17	0.64	0
9	MAN	E	610	8	11,11,12	0.22	0	13,15,17	0.48	0
7	NAG	F	601	1,7	14,14,15	0.70	1 (7%)	15,19,21	2.55	3 (20%)
7	NAG	F	602	7	14,14,15	0.26	0	15,19,21	0.51	0
7	NAG	F	603	1	14,14,15	0.32	0	15,19,21	0.95	1 (6%)
7	NAG	F	604	1,7	14,14,15	0.50	0	15,19,21	0.82	0
7	NAG	F	605	8,7	14,14,15	0.29	0	15,19,21	0.54	0
8	BMA	F	606	7	11,11,12	0.24	0	13,15,17	0.65	0
7	NAG	F	607	1,7	14,14,15	0.29	0	15,19,21	0.95	1 (6%)
7	NAG	F	608	8,7	14,14,15	0.26	0	15,19,21	0.63	0
8	BMA	F	609	9,7	11,11,12	0.24	0	13,15,17	0.64	0
9	MAN	F	610	8	11,11,12	0.22	0	13,15,17	0.48	0
7	NAG	G	701	2,7	14,14,15	0.29	0	15,19,21	0.95	1 (6%)
7	NAG	G	702	8,7	14,14,15	0.31	0	15,19,21	1.00	1 (6%)
8	BMA	G	703	9,7	11,11,12	0.24	0	13,15,17	0.96	1 (7%)
9	MAN	G	704	8	11,11,12	0.25	0	13,15,17	1.10	1 (7%)
9	MAN	G	705	8	11,11,12	0.25	0	13,15,17	0.96	2 (15%)
7	NAG	I	701	2,7	14,14,15	0.29	0	15,19,21	0.94	2 (13%)
7	NAG	I	702	8,7	14,14,15	0.32	0	15,19,21	1.00	1 (6%)
8	BMA	I	703	9,7	11,11,12	0.24	0	13,15,17	0.97	1 (7%)
9	MAN	I	704	8	11,11,12	0.25	0	13,15,17	1.10	1 (7%)
9	MAN	I	705	8	11,11,12	0.25	0	13,15,17	0.96	2 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	602	7	-	0/6/23/26	0/1/1/1
7	NAG	A	603	1	-	0/6/23/26	0/1/1/1
7	NAG	A	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	605	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	606	7	-	0/2/19/22	0/1/1/1
7	NAG	A	607	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	608	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	609	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	610	8	-	0/2/19/22	0/1/1/1
7	NAG	B	701	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	B	703	9,7	-	0/2/19/22	0/1/1/1
9	MAN	B	704	8	-	0/2/19/22	0/1/1/1
9	MAN	B	705	8	-	0/2/19/22	0/1/1/1
7	NAG	E	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	602	7	-	0/6/23/26	0/1/1/1
7	NAG	E	603	1	-	0/6/23/26	0/1/1/1
7	NAG	E	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	605	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	606	7	-	0/2/19/22	0/1/1/1
7	NAG	E	607	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	608	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	609	9,7	-	0/2/19/22	0/1/1/1
9	MAN	E	610	8	-	0/2/19/22	0/1/1/1
7	NAG	F	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	602	7	-	0/6/23/26	0/1/1/1
7	NAG	F	603	1	-	0/6/23/26	0/1/1/1
7	NAG	F	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	605	8,7	-	0/6/23/26	0/1/1/1
8	BMA	F	606	7	-	0/2/19/22	0/1/1/1
7	NAG	F	607	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	608	8,7	-	0/6/23/26	0/1/1/1
8	BMA	F	609	9,7	-	0/2/19/22	0/1/1/1
9	MAN	F	610	8	-	0/2/19/22	0/1/1/1
7	NAG	G	701	2,7	-	0/6/23/26	0/1/1/1
7	NAG	G	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	703	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	704	8	-	0/2/19/22	0/1/1/1
9	MAN	G	705	8	-	0/2/19/22	0/1/1/1
7	NAG	I	701	2,7	-	0/6/23/26	0/1/1/1
7	NAG	I	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	I	703	9,7	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	I	704	8	-	0/2/19/22	0/1/1/1
9	MAN	I	705	8	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	601	NAG	C1-C2	2.05	1.55	1.52
7	E	601	NAG	C1-C2	2.07	1.55	1.52
7	A	601	NAG	C1-C2	2.08	1.55	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	NAG	O5-C1-C2	-5.81	103.39	111.47
7	E	601	NAG	O5-C1-C2	-5.80	103.41	111.47
7	F	601	NAG	O5-C1-C2	-5.78	103.43	111.47
7	I	702	NAG	O5-C1-C2	-3.15	107.09	111.47
7	B	702	NAG	O5-C1-C2	-3.14	107.11	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	NAG	4	0
7	A	602	NAG	5	0
7	A	604	NAG	1	0
7	A	605	NAG	2	0
7	A	607	NAG	1	0
7	A	608	NAG	4	0
8	A	609	BMA	3	0
7	B	701	NAG	9	0
7	B	702	NAG	6	0
7	E	601	NAG	4	0
7	E	602	NAG	5	0
7	E	604	NAG	1	0
7	E	605	NAG	2	0
7	E	607	NAG	2	0
7	E	608	NAG	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	609	BMA	3	0
7	F	601	NAG	4	0
7	F	602	NAG	5	0
7	F	604	NAG	1	0
7	F	605	NAG	2	0
7	F	607	NAG	1	0
7	F	608	NAG	3	0
8	F	609	BMA	2	0
7	G	701	NAG	8	0
7	G	702	NAG	6	0
7	I	701	NAG	9	0
7	I	702	NAG	6	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.