



wwPDB EM Map/Model Validation Report ⓘ

Aug 29, 2016 – 11:02 AM EDT

PDB ID : 5KEN
EMDB ID: : EMD-8242
Title : EBOV GP in complex with variable Fab domains of IgGs c4G7 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 : 2016-06-09
Resolution : 4.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

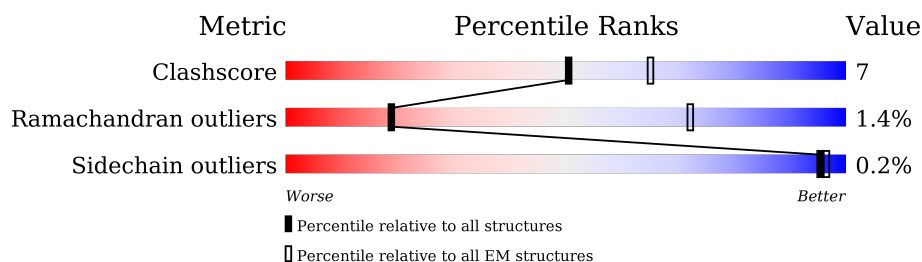
1 Overall quality at a glance

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.



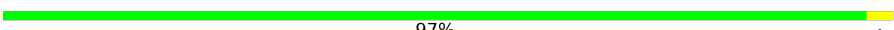

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	276	
1	E	276	
1	K	276	
2	B	113	
2	F	113	
2	M	113	
3	C	118	
3	G	118	
3	N	118	

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Mol	Chain	Length	Quality of chain
4	D	107	 96% .
4	H	107	 96% .
4	O	107	 97% .
5	I	107	 93% 7%
5	P	107	 93% 7%
6	J	121	 94% 6%
6	Q	121	 94% 5% .

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	A	401	-	-	X	-
7	NAG	E	401	X	-	X	-
7	NAG	F	701	X	-	X	-
7	NAG	K	401	-	-	X	-
7	NAG	K	402	-	-	X	-
7	NAG	K	406	X	-	-	-
7	NAG	K	407	-	-	X	-
7	NAG	K	408	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16913 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	207	Total	C	N	O	S	0	0
			1596	1016	272	303	5		
1	E	235	Total	C	N	O	S	0	0
			1829	1162	316	346	5		
1	K	235	Total	C	N	O	S	0	0
			1829	1162	316	346	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
			890	567	155	162	6		
2	F	113	Total	C	N	O	S	0	0
			890	567	155	162	6		
2	M	113	Total	C	N	O	S	0	0
			890	567	155	162	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	THR	ILE	conflict	UNP Q05320
F	544	THR	ILE	conflict	UNP Q05320
M	544	THR	ILE	conflict	UNP Q05320

- Molecule 3 is a protein called c4G7 variable Fab domain heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	118	Total	C	N	O	S	0	0
			903	570	143	185	5		
3	G	118	Total	C	N	O	S	0	0
			903	570	143	185	5		
3	N	118	Total	C	N	O	S	0	0
			903	570	143	185	5		

- Molecule 4 is a protein called c4G7 variable Fab domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total	C	N	O	S	0	0
			827	524	135	165	3		
4	H	107	Total	C	N	O	S	0	0
			827	524	135	165	3		
4	O	107	Total	C	N	O	S	0	0
			827	524	135	165	3		

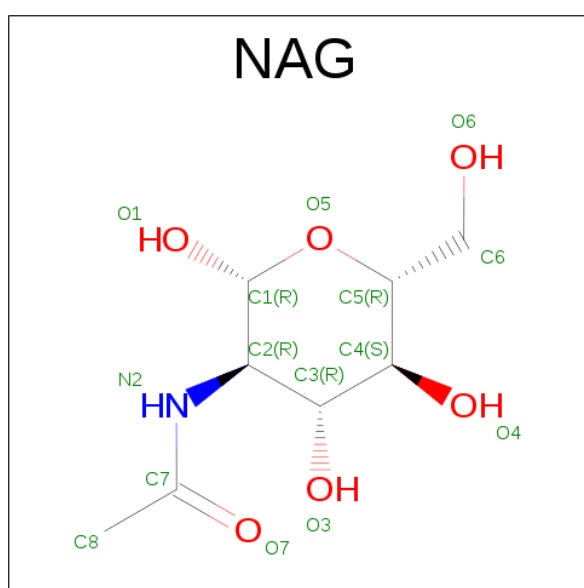
- Molecule 5 is a protein called c13C6 variable Fab domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	107	Total	C	N	O	S	0	0
			815	509	135	167	4		
5	P	107	Total	C	N	O	S	0	0
			815	509	135	167	4		

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

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

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



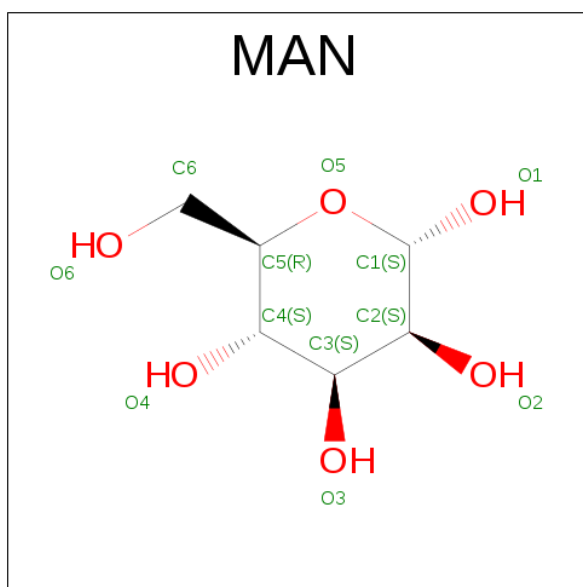
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			28	16	2	10	
7	A	1	Total	C	N	O	0
			28	16	2	10	
7	E	1	Total	C	N	O	0
			42	24	3	15	
7	E	1	Total	C	N	O	0
			42	24	3	15	
7	E	1	Total	C	N	O	0
			42	24	3	15	
7	F	1	Total	C	N	O	0
			28	16	2	10	
7	F	1	Total	C	N	O	0
			28	16	2	10	
7	K	1	Total	C	N	O	0
			112	64	8	40	
7	K	1	Total	C	N	O	0
			112	64	8	40	
7	K	1	Total	C	N	O	0
			112	64	8	40	
7	K	1	Total	C	N	O	0
			112	64	8	40	
7	K	1	Total	C	N	O	0
			112	64	8	40	
7	K	1	Total	C	N	O	0
			112	64	8	40	
7	K	1	Total	C	N	O	0
			112	64	8	40	

- 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
			11	6	5	
8	F	1	Total	C	O	0
			11	6	5	
8	K	1	Total	C	O	0
			11	6	5	

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			22	12	10	

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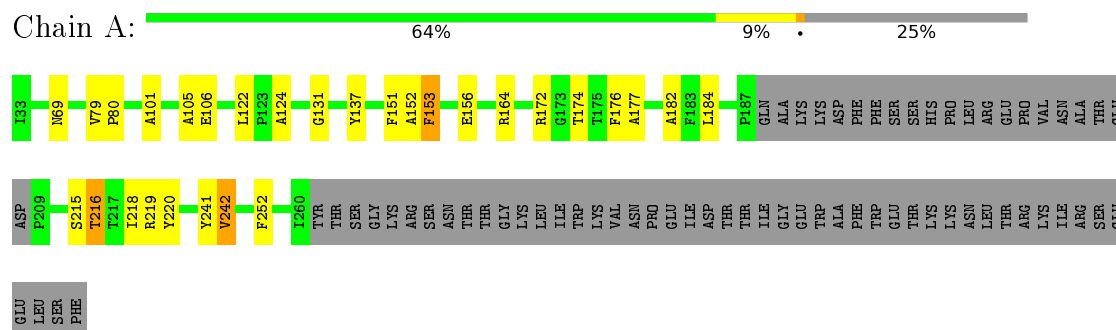
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Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			22	12	10	
9	F	1	Total	C	O	0
			22	12	10	
9	F	1	Total	C	O	0
			22	12	10	
9	K	1	Total	C	O	0
			22	12	10	
9	K	1	Total	C	O	0
			22	12	10	

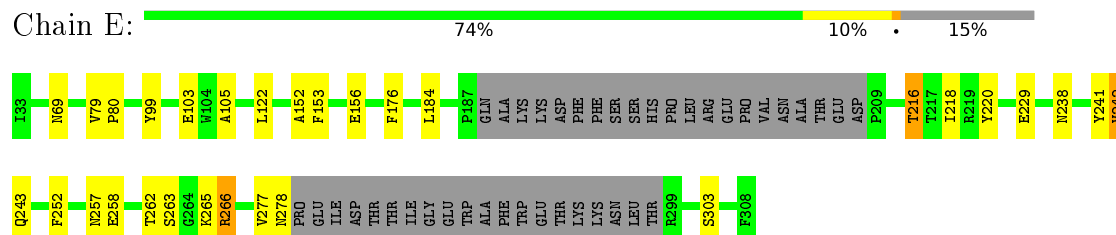
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

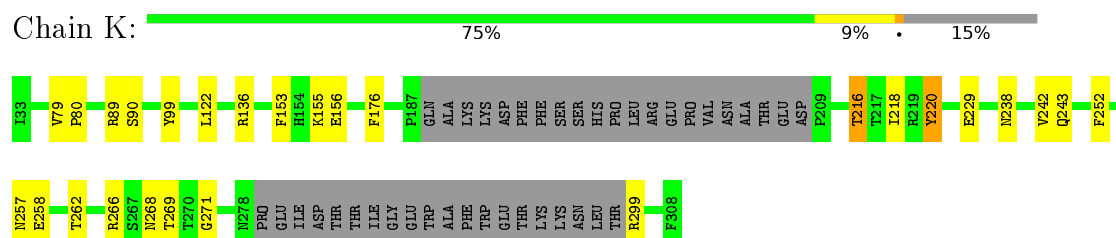
- Molecule 1: Ebola surface glycoprotein, GP1



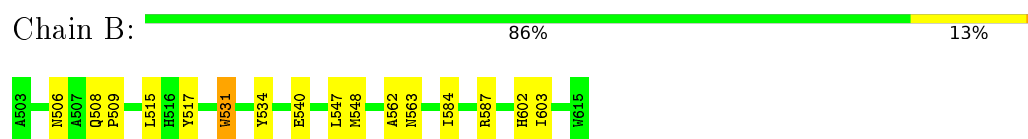
- Molecule 1: Ebola surface glycoprotein, GP1




- Molecule 1: Ebola surface glycoprotein, GP1



- Molecule 2: Ebola surface glycoprotein, GP2




- Molecule 2: Ebola surface glycoprotein, GP2

Chain F:  84% 16%



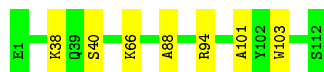
- Molecule 2: Ebola surface glycoprotein, GP2

Chain M:  88% 12%



- Molecule 3: c4G7 variable Fab domain heavy chain

Chain C:  94% 6%



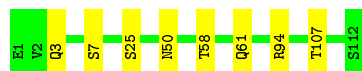
- Molecule 3: c4G7 variable Fab domain heavy chain

Chain G:  94% 6%



- Molecule 3: c4G7 variable Fab domain heavy chain

Chain N:  93% 7%



- Molecule 4: c4G7 variable Fab domain light chain

Chain D:  96%



- Molecule 4: c4G7 variable Fab domain light chain

Chain H:  96%



- Molecule 4: c4G7 variable Fab domain light chain

Chain O:  97%



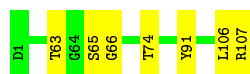
- Molecule 5: c13C6 variable Fab domain light chain

Chain I: 93% 7%



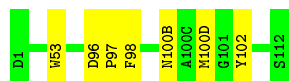
- Molecule 5: c13C6 variable Fab domain light chain

Chain P: 93% 7%



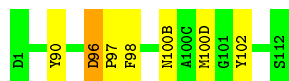
- Molecule 6: c13C6 variable Fab domain heavy chain

Chain J: 94% 6%



- Molecule 6: c13C6 variable Fab domain heavy chain

Chain Q: 94% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	73000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	Not provided	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: 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	0.82	0/1633	0.90	2/2220 (0.1%)
1	E	0.83	0/1869	0.91	2/2532 (0.1%)
1	K	0.83	0/1869	0.94	5/2532 (0.2%)
2	B	0.81	0/914	0.87	2/1246 (0.2%)
2	F	0.81	0/914	0.85	1/1246 (0.1%)
2	M	0.80	0/914	0.84	0/1246
3	C	0.81	0/923	0.89	0/1246
3	G	0.81	0/923	0.95	1/1246 (0.1%)
3	N	0.82	0/923	0.93	1/1246 (0.1%)
4	D	0.77	0/847	0.84	0/1145
4	H	0.79	0/847	0.85	0/1145
4	O	0.78	0/847	0.86	0/1145
5	I	0.70	0/831	0.86	1/1127 (0.1%)
5	P	0.69	0/831	0.85	1/1127 (0.1%)
6	J	0.73	0/954	0.87	1/1292 (0.1%)
6	Q	0.73	0/954	0.93	2/1292 (0.2%)
All	All	0.79	0/16993	0.89	19/23033 (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
6	J	0	2
6	Q	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	TYR	CB-CG-CD2	-7.38	116.57	121.00
3	G	98	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	K	220	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	E	99	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	K	99	TYR	CB-CG-CD1	-6.92	116.85	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	J	100(D)	MET	Mainchain,Peptide
6	Q	100(D)	MET	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1545	22	0
1	E	1829	0	1785	30	0
1	K	1829	0	1787	50	0
2	B	890	0	855	26	0
2	F	890	0	855	29	0
2	M	890	0	855	43	0
3	C	903	0	864	7	0
3	G	903	0	864	4	0
3	N	903	0	864	4	0
4	D	827	0	794	3	0
4	H	827	0	794	3	0
4	O	827	0	794	2	0
5	I	815	0	791	3	0
5	P	815	0	791	5	0
6	J	930	0	894	5	0
6	Q	930	0	894	2	0
7	A	28	0	24	19	0
7	E	42	0	37	13	0
7	F	28	0	24	22	0
7	K	112	0	99	59	0
8	A	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	11	0	8	0	0
8	K	11	0	8	0	0
9	A	22	0	20	1	0
9	F	22	0	20	0	0
9	K	22	0	20	1	0
All	All	16913	0	16294	240	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 7.

The worst 5 of 240 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:E:257:ASN:HB3	7:E:402:NAG:C1	1.21	1.58
1:K:238:ASN:ND2	7:K:407:NAG:C1	1.85	1.40
1:E:238:ASN:HD21	7:E:401:NAG:C2	1.34	1.36
1:E:238:ASN:ND2	7:E:401:NAG:N2	1.69	1.34
7:K:401:NAG:O6	2:M:509:PRO:CG	1.76	1.34

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/276 (74%)	191 (94%)	4 (2%)	8 (4%)	4	37
1	E	229/276 (83%)	217 (95%)	5 (2%)	7 (3%)	5	44
1	K	229/276 (83%)	214 (93%)	10 (4%)	5 (2%)	8	51
2	B	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	21	67
2	F	111/113 (98%)	103 (93%)	7 (6%)	1 (1%)	21	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	111/113 (98%)	103 (93%)	7 (6%)	1 (1%)	21	67
3	C	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
3	G	116/118 (98%)	115 (99%)	0	1 (1%)	21	67
3	N	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
4	D	105/107 (98%)	104 (99%)	0	1 (1%)	19	65
4	H	105/107 (98%)	104 (99%)	0	1 (1%)	19	65
4	O	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	19	65
5	I	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
5	P	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
6	J	119/121 (98%)	111 (93%)	7 (6%)	1 (1%)	24	70
6	Q	119/121 (98%)	112 (94%)	5 (4%)	2 (2%)	11	56
All	All	2105/2298 (92%)	2013 (96%)	62 (3%)	30 (1%)	19	59

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ALA
2	B	584	ILE
2	F	584	ILE
1	K	153	PHE
2	M	584	ILE

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	171/238 (72%)	171 (100%)	0	100	100
1	E	197/238 (83%)	197 (100%)	0	100	100
1	K	197/238 (83%)	197 (100%)	0	100	100
2	B	92/92 (100%)	91 (99%)	1 (1%)	80	90
2	F	92/92 (100%)	91 (99%)	1 (1%)	80	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	92/92 (100%)	91 (99%)	1 (1%)	80	90
3	C	98/98 (100%)	98 (100%)	0	100	100
3	G	98/98 (100%)	98 (100%)	0	100	100
3	N	98/98 (100%)	98 (100%)	0	100	100
4	D	92/92 (100%)	92 (100%)	0	100	100
4	H	92/92 (100%)	92 (100%)	0	100	100
4	O	92/92 (100%)	92 (100%)	0	100	100
5	I	92/92 (100%)	92 (100%)	0	100	100
5	P	92/92 (100%)	92 (100%)	0	100	100
6	J	99/99 (100%)	99 (100%)	0	100	100
6	Q	99/99 (100%)	99 (100%)	0	100	100
All	All	1793/1942 (92%)	1790 (100%)	3 (0%)	95	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	531	TRP
2	F	545	GLU
2	M	531	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	602	HIS
2	M	602	HIS
1	K	238	ASN
1	E	238	ASN
1	K	268	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 ⓘ

24 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	401	7	14,14,15	0.38	0	15,19,21	1.33	2 (13%)
7	NAG	A	402	8,7	14,14,15	0.31	0	15,19,21	0.88	1 (6%)
8	BMA	A	403	9,7	11,11,12	0.25	0	15,15,17	0.67	0
9	MAN	A	404	8	11,11,12	0.28	0	15,15,17	0.65	0
9	MAN	A	405	8	11,11,12	0.26	0	15,15,17	0.52	0
7	NAG	E	401	1	14,14,15	0.27	0	15,19,21	0.74	1 (6%)
7	NAG	E	402	1,7	14,14,15	0.29	0	15,19,21	0.73	1 (6%)
7	NAG	E	403	7	14,14,15	0.27	0	15,19,21	0.70	0
7	NAG	F	701	2,7	14,14,15	0.37	0	15,19,21	1.33	2 (13%)
7	NAG	F	702	8,7	14,14,15	0.28	0	15,19,21	0.90	1 (6%)
8	BMA	F	703	9,7	11,11,12	0.26	0	15,15,17	0.66	0
9	MAN	F	704	8	11,11,12	0.27	0	15,15,17	0.65	0
9	MAN	F	705	8	11,11,12	0.27	0	15,15,17	0.53	0
7	NAG	K	401	7	14,14,15	0.38	0	15,19,21	1.32	2 (13%)
7	NAG	K	402	8,7	14,14,15	0.30	0	15,19,21	0.90	1 (6%)
8	BMA	K	403	9,7	11,11,12	0.27	0	15,15,17	0.66	0
9	MAN	K	404	8	11,11,12	0.28	0	15,15,17	0.66	0
9	MAN	K	405	8	11,11,12	0.27	0	15,15,17	0.53	0
7	NAG	K	406	1	14,14,15	0.67	0	15,19,21	1.96	1 (6%)
7	NAG	K	407	-	14,14,15	0.32	0	15,19,21	0.74	1 (6%)
7	NAG	K	408	7	14,14,15	0.50	0	15,19,21	0.71	0
7	NAG	K	409	7	14,14,15	0.28	0	15,19,21	0.51	0
7	NAG	K	410	7	14,14,15	0.29	0	15,19,21	0.74	1 (6%)
7	NAG	K	411	7	14,14,15	0.25	0	15,19,21	0.69	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
7	NAG	A	401	7	-	0/6/23/26	0/1/1/1
7	NAG	A	402	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	403	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	404	8	-	0/2/19/22	0/1/1/1
9	MAN	A	405	8	-	0/2/19/22	0/1/1/1
7	NAG	E	401	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	E	402	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	403	7	-	0/6/23/26	0/1/1/1
7	NAG	F	701	2,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	F	702	8,7	-	0/6/23/26	0/1/1/1
8	BMA	F	703	9,7	-	0/2/19/22	0/1/1/1
9	MAN	F	704	8	-	0/2/19/22	0/1/1/1
9	MAN	F	705	8	-	0/2/19/22	0/1/1/1
7	NAG	K	401	7	-	0/6/23/26	0/1/1/1
7	NAG	K	402	8,7	-	0/6/23/26	0/1/1/1
8	BMA	K	403	9,7	-	0/2/19/22	0/1/1/1
9	MAN	K	404	8	-	0/2/19/22	0/1/1/1
9	MAN	K	405	8	-	0/2/19/22	0/1/1/1
7	NAG	K	406	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	K	407	-	-	0/6/23/26	0/1/1/1
7	NAG	K	408	7	-	0/6/23/26	0/1/1/1
7	NAG	K	409	7	-	0/6/23/26	0/1/1/1
7	NAG	K	410	7	-	0/6/23/26	0/1/1/1
7	NAG	K	411	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	NAG	O5-C5-C4	-3.39	104.51	110.13
7	K	401	NAG	O5-C5-C4	-3.37	104.55	110.13
7	F	701	NAG	O5-C5-C4	-3.36	104.56	110.13
7	F	701	NAG	C2-N2-C7	-2.80	119.46	123.11
7	A	401	NAG	C2-N2-C7	-2.78	119.49	123.11

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	F	701	NAG	C1
7	E	401	NAG	C1
7	K	406	NAG	C1

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	NAG	18	0
7	A	402	NAG	5	0
9	A	404	MAN	1	0
7	E	401	NAG	9	0
7	E	402	NAG	4	0
7	E	403	NAG	2	0
7	F	701	NAG	20	0
7	F	702	NAG	6	0
7	K	401	NAG	26	0
7	K	402	NAG	7	0
9	K	404	MAN	1	0
7	K	406	NAG	4	0
7	K	407	NAG	7	0
7	K	408	NAG	14	0
7	K	409	NAG	2	0
7	K	410	NAG	4	0
7	K	411	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.