



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 16, 2017 – 02:24 PM EST

PDB ID : 5H37
EMDB ID: : EMD-9575
Title : Cryo-EM structure of zika virus complexed with Fab C10 at pH 8.0
Authors : Zhang, S.; Kostyuchenko, V.; Ng, T.-S.; Lim, X.-N.; Ooi, J.S.G.; Lambert, S.;
Tan, T.Y.; Widman, D.; Shi, J.; Baric, R.S.; Lok, S.-M.
Deposited on : 2016-10-20
Resolution : 4.00 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

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 : 1.7.1 (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-20028442

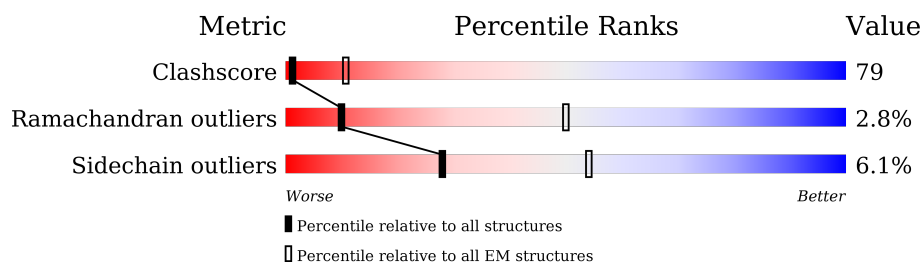
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	504	37% 54% 8% .
1	B	504	43% 49% . . .
1	C	504	31% 59% 7% .
2	D	75	32% 59% 9%
2	E	75	39% 45% 13% .
2	F	75	36% 59% 5%
3	G	127	36% 53% 11%
3	I	127	28% 63% 9%
3	K	127	35% 59% . .

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Mol	Chain	Length	Quality of chain
4	H	109	 41% 51% 5% •
4	L	109	 42% 46% 10% •
4	M	109	 27% 61% 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18517 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 structural protein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3798	2395	660	712	31		
1	C	494	Total	C	N	O	S	0	0
			3731	2350	647	704	30		
1	B	494	Total	C	N	O	S	0	0
			3732	2350	647	705	30		

- Molecule 2 is a protein called strutral protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

- Molecule 3 is a protein called C10 IgG heavy chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		
3	K	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		
3	I	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		

- Molecule 4 is a protein called C10 IgG light chain variable region.

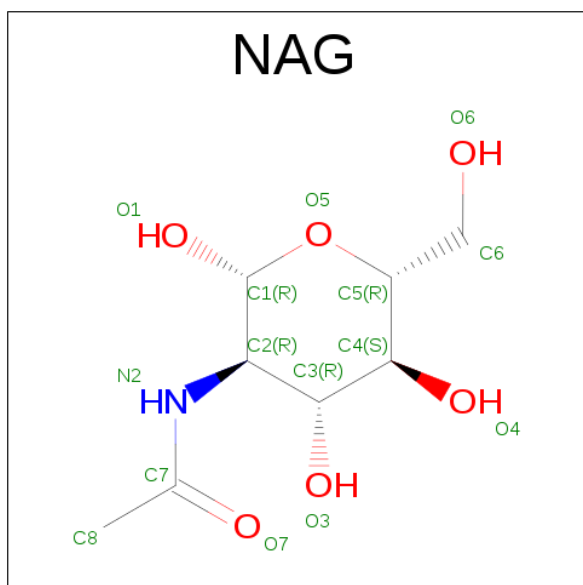
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	109	Total	C	N	O	S	0	0
			793	491	135	164	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	109	Total	C	N	O	S	0	0
			793	491	135	164	3		
4	M	109	Total	C	N	O	S	0	0
			793	491	135	164	3		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



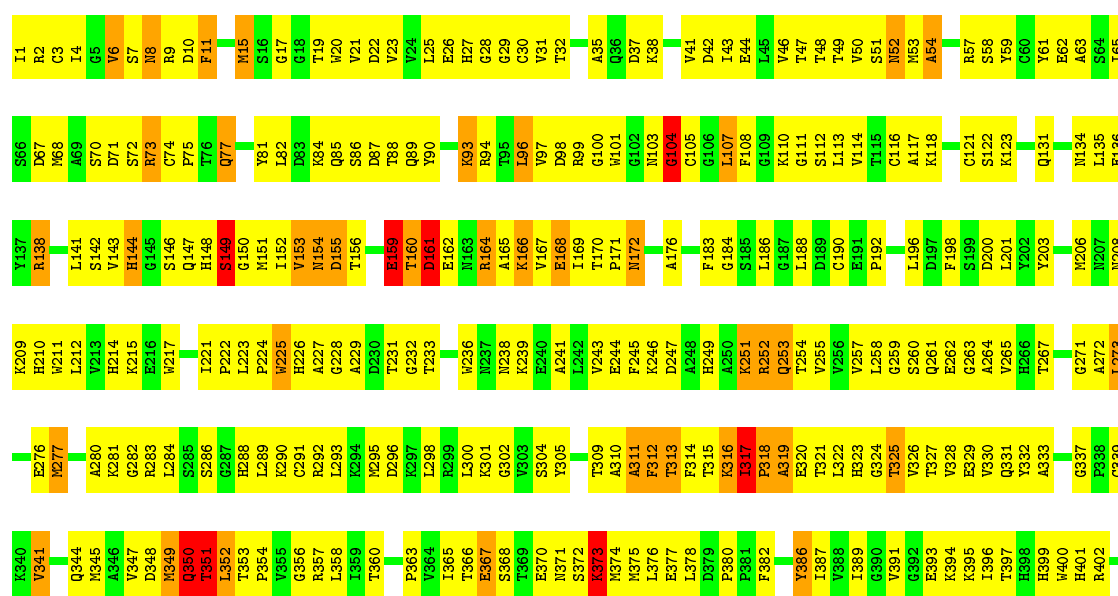
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

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 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.

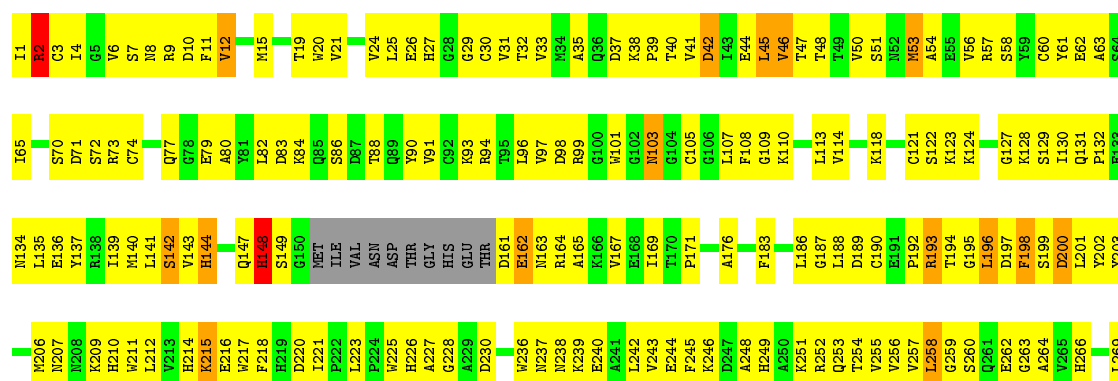
• Molecule 1: structural protein E

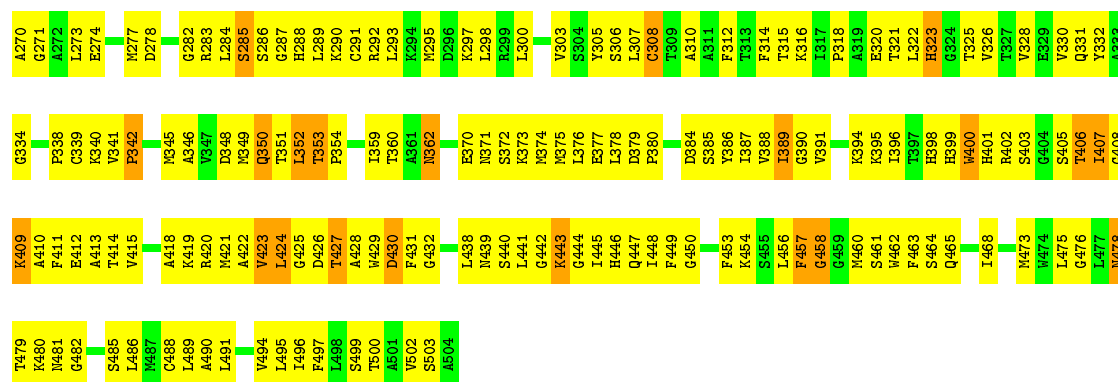
Chain A: 



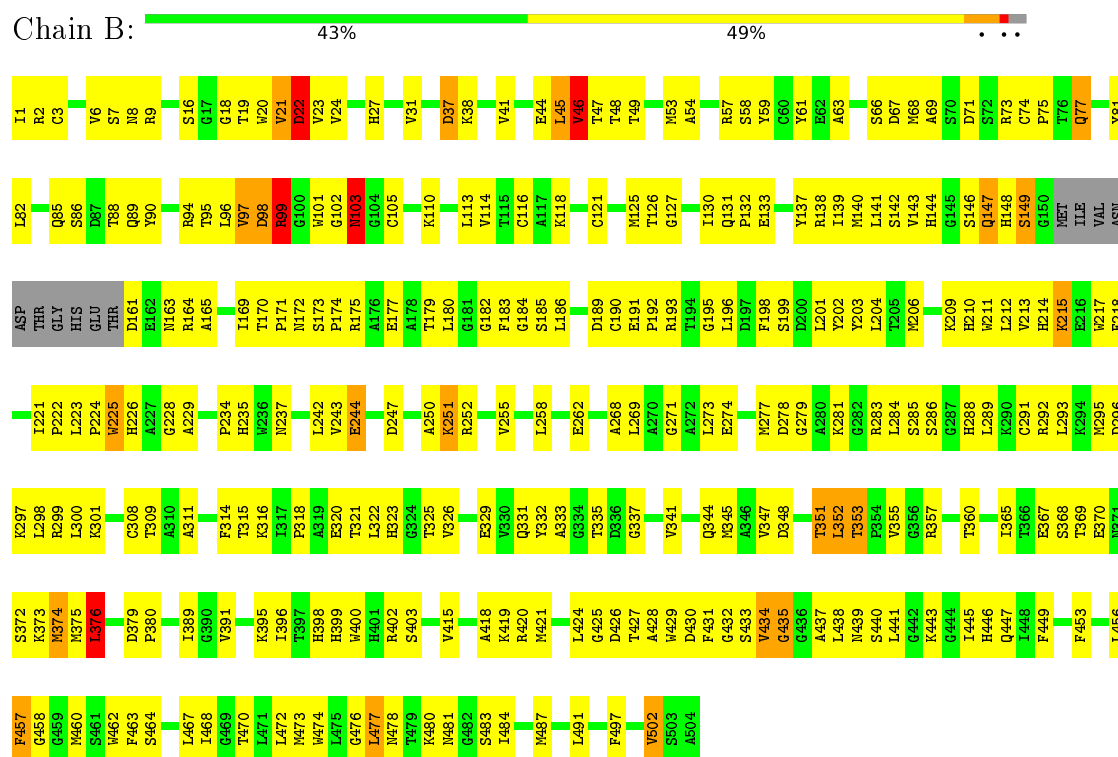
• Molecule 1: structural protein E

Chain C: 





• Molecule 1: structural protein E

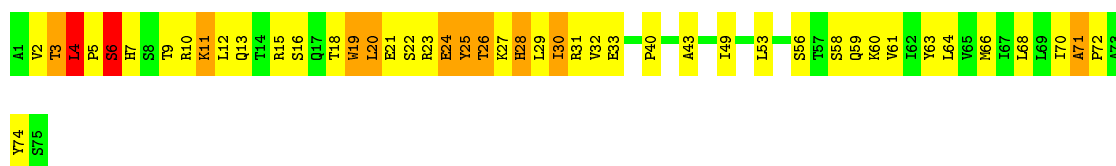


• Molecule 2: strutral protein M



• Molecule 2: strutral protein M





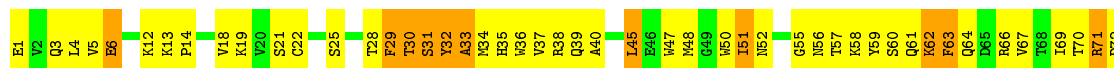
- Molecule 2: strutral protein M

Chain F: 36% 59% 5%



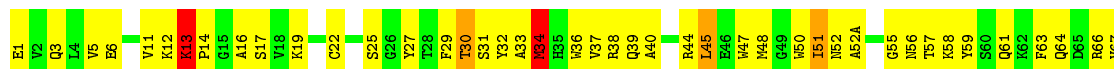
- Molecule 3: C10 IgG heavy chain variable region

Chain G: 36% 53% 11%



- Molecule 3: C10 IgG heavy chain variable region

Chain K: 35% 59% . .



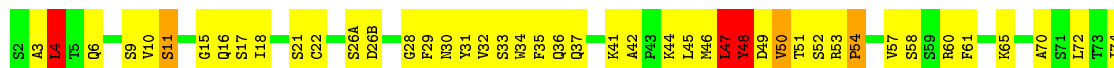
- Molecule 3: C10 IgG heavy chain variable region

Chain I: 28% 63% 9%



- Molecule 4: C10 IgG light chain variable region

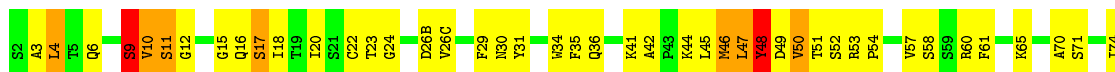
Chain H: 41% 51% 5% .





- Molecule 4: C10 IgG light chain variable region

Chain L: 42% 46% 10%



- Molecule 4: C10 IgG light chain variable region

Chain M: 27% 61% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	49100	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)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.62	2/3877 (0.1%)	0.92	17/5239 (0.3%)
1	B	0.56	2/3809 (0.1%)	0.84	8/5152 (0.2%)
1	C	0.57	2/3808 (0.1%)	0.91	17/5152 (0.3%)
2	D	0.43	0/615	0.85	2/838 (0.2%)
2	E	0.52	0/615	1.09	5/838 (0.6%)
2	F	0.44	0/615	0.95	5/838 (0.6%)
3	G	0.50	0/1050	0.87	5/1427 (0.4%)
3	I	0.59	1/1050 (0.1%)	0.96	4/1427 (0.3%)
3	K	0.47	0/1050	0.88	6/1427 (0.4%)
4	H	0.60	1/811 (0.1%)	0.88	3/1101 (0.3%)
4	L	0.62	0/811	0.95	6/1101 (0.5%)
4	M	0.47	0/811	0.82	2/1101 (0.2%)
All	All	0.56	8/18922 (0.0%)	0.90	80/25641 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	E	0	2
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	PRO	N-CD	-11.89	1.31	1.47
1	A	341	VAL	C-N	11.35	1.55	1.34
3	I	14	PRO	N-CD	-9.73	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLU	C-N	9.39	1.55	1.34
1	C	400	TRP	CB-CG	-5.66	1.40	1.50

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ILE	C-N-CD	-16.95	83.31	120.60
1	C	148	HIS	N-CA-CB	16.02	139.44	110.60
3	K	51	ILE	N-CA-C	12.34	144.32	111.00
3	G	51	ILE	N-CA-C	12.33	144.30	111.00
1	A	325	THR	N-CA-C	9.40	136.38	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	MET	Peptide
1	C	427	THR	Mainchain
2	E	20	LEU	Mainchain
2	E	71	ALA	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	3798	0	3759	615	0
1	B	3732	0	3693	436	0
1	C	3731	0	3690	673	0
2	D	600	0	624	145	0
2	E	600	0	624	115	0
2	F	600	0	624	153	0
3	G	1021	0	960	166	0
3	I	1021	0	960	333	0
3	K	1021	0	960	130	0
4	H	793	0	754	144	0
4	L	793	0	755	122	0
4	M	793	0	753	201	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	13	6	0
All	All	18517	0	18169	2881	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 79.

The worst 5 of 2881 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)
3:I:11:VAL:HG12	3:I:110:THR:CB	1.26	1.63
4:M:4:LEU:HB3	4:M:98:GLY:CA	1.22	1.59
1:A:108:PHE:CZ	1:C:4:ILE:CD1	1.87	1.58
3:I:11:VAL:CG1	3:I:110:THR:HB	1.30	1.58
1:C:320:GLU:HB2	1:C:400:TRP:CH2	1.10	1.58

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	502/504 (100%)	397 (79%)	85 (17%)	20 (4%)	4	37
1	B	490/504 (97%)	402 (82%)	78 (16%)	10 (2%)	9	54
1	C	490/504 (97%)	402 (82%)	79 (16%)	9 (2%)	11	55
2	D	73/75 (97%)	60 (82%)	12 (16%)	1 (1%)	14	59
2	E	73/75 (97%)	60 (82%)	10 (14%)	3 (4%)	3	37
2	F	73/75 (97%)	59 (81%)	13 (18%)	1 (1%)	14	59
3	G	125/127 (98%)	110 (88%)	9 (7%)	6 (5%)	3	32
3	I	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	5	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	7	50
4	H	107/109 (98%)	94 (88%)	9 (8%)	4 (4%)	4	40
4	L	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	10	54
4	M	107/109 (98%)	87 (81%)	16 (15%)	4 (4%)	4	40
All	All	2397/2445 (98%)	1980 (83%)	350 (15%)	67 (3%)	10	47

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	153	VAL
1	A	154	ASN
1	A	155	ASP
1	A	159	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/410 (100%)	383 (93%)	27 (7%)	21	60
1	B	401/410 (98%)	381 (95%)	20 (5%)	30	68
1	C	401/410 (98%)	374 (93%)	27 (7%)	20	60
2	D	64/64 (100%)	60 (94%)	4 (6%)	22	61
2	E	64/64 (100%)	59 (92%)	5 (8%)	16	54
2	F	64/64 (100%)	63 (98%)	1 (2%)	70	88
3	G	107/107 (100%)	101 (94%)	6 (6%)	26	65
3	I	107/107 (100%)	102 (95%)	5 (5%)	32	70
3	K	107/107 (100%)	103 (96%)	4 (4%)	41	75
4	H	89/89 (100%)	85 (96%)	4 (4%)	34	71
4	L	89/89 (100%)	80 (90%)	9 (10%)	9	41
4	M	89/89 (100%)	79 (89%)	10 (11%)	7	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1992/2010 (99%)	1870 (94%)	122 (6%)	28 63

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	25	TYR
1	B	147	GLN
4	M	4	LEU
2	D	26	THR
1	B	77	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	323	HIS
2	F	7	HIS
4	M	36	GLN
1	B	481	ASN
2	F	59	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 ⓘ

1 ligand is 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	14,14,15	0.39	0	15,19,21	1.15	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	601	NAG	C2-N2-C7	-2.36	120.03	123.11
5	A	601	NAG	C8-C7-N2	2.06	120.04	116.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	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.