



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

Feb 26, 2018 – 07:38 PM EST

PDB ID : 5O6V  
EMDB ID: : EMD-3754  
Title : The cryo-EM structure of Tick-borne encephalitis virus complexed with Fab  
fragment of neutralizing antibody 19/1786  
Authors : Fuzik, T.; Plevka, P.  
Deposited on : 2017-06-07  
Resolution : 3.90 Å(reported)

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

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

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

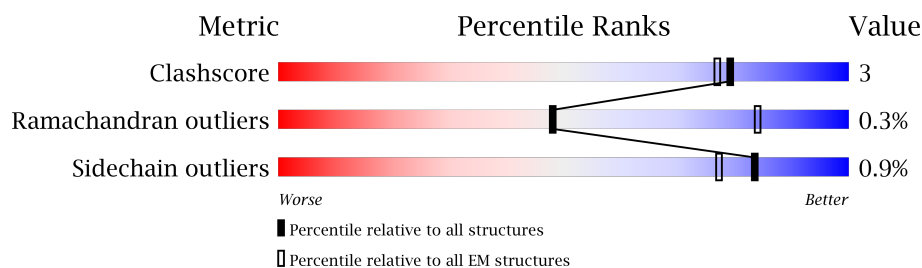
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	496	90% 9% .
1	B	496	87% 12% .
1	C	496	89% 10% .
2	D	75	89% 5% 5%
2	E	75	85% 9% 5%
2	F	75	81% 13% 5%
3	H	212	91% 9%
3	I	212	92% 8%
4	L	208	93% 7%

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Mol	Chain	Length	Quality of chain
4	M	208	 <div>90%10%</div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19346 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	492	Total	C	N	O	S	0	0
			3743	2371	654	693	25		
1	B	492	Total	C	N	O	S	0	0
			3743	2371	654	693	25		
1	C	492	Total	C	N	O	S	0	0
			3743	2371	654	693	25		

- Molecule 2 is a protein called Small envelope protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	71	Total	C	N	O	S	0	0
			557	363	100	92	2		
2	E	71	Total	C	N	O	S	0	0
			557	363	100	92	2		
2	F	71	Total	C	N	O	S	0	0
			557	363	100	92	2		

- Molecule 3 is a protein called Fab 19/1786 - Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	212	Total	C	N	O	S	0	0
			1597	1007	259	323	8		
3	I	212	Total	C	N	O	S	0	0
			1597	1007	259	323	8		

- Molecule 4 is a protein called Fab 19/1786 - Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	208	Total	C	N	O	S	0	0
			1605	998	270	330	7		
4	M	208	Total	C	N	O	S	0	0
			1605	998	270	330	7		

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

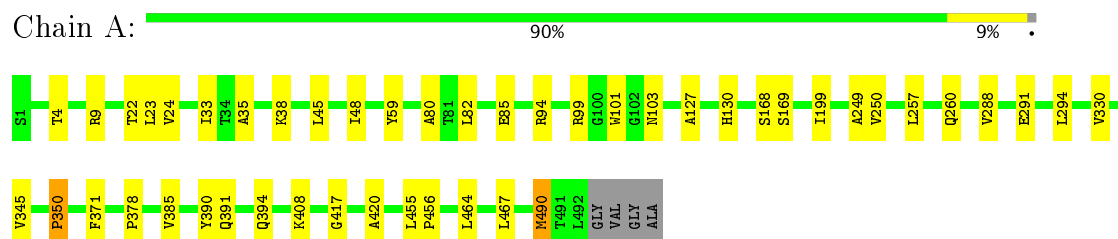


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

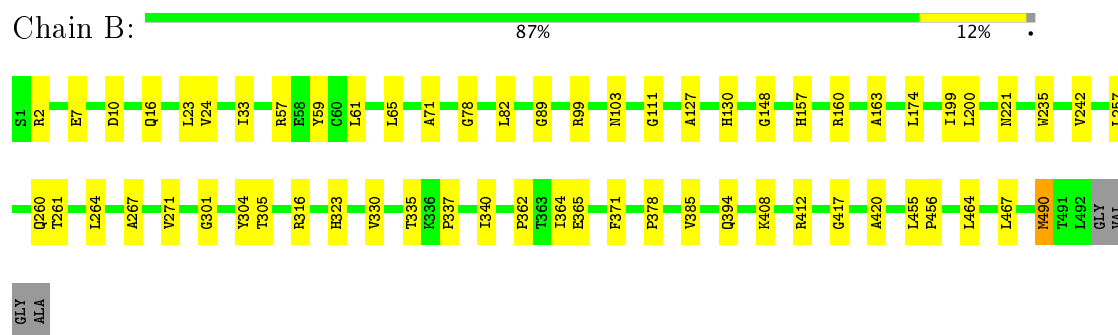
### 3 Residue-property plots

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

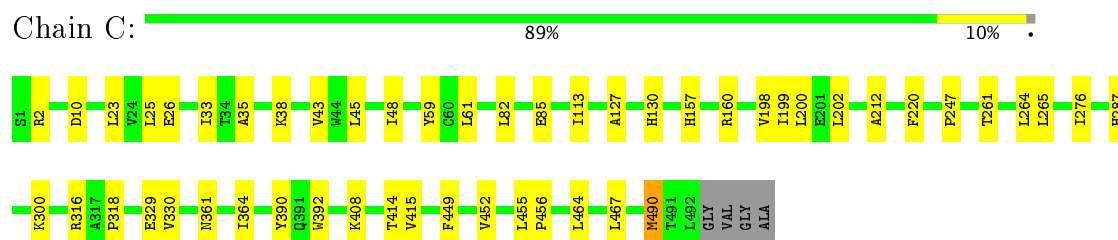
- Molecule 1: Envelope protein



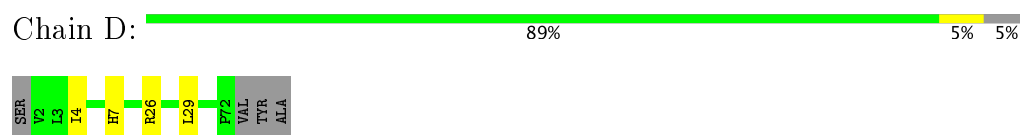
- Molecule 1: Envelope protein




- Molecule 1: Envelope protein



- Molecule 2: Small envelope protein M




- Molecule 2: Small envelope protein M

Chain E:  85% 9% 5%



- Molecule 2: Small envelope protein M

Chain F:  81% 13% 5%



- Molecule 3: Fab 19/1786 - Heavy chain

Chain H:  91% 9%



- Molecule 3: Fab 19/1786 - Heavy chain

Chain I:  92% 8%



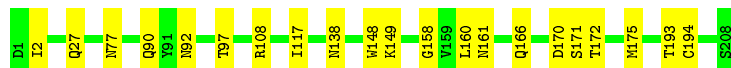
- Molecule 4: Fab 19/1786 - Light chain

Chain L:  93% 7%



- Molecule 4: Fab 19/1786 - Light chain

Chain M:  90% 10%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9797	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 ( $e^-/\text{\AA}^2$ )	22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (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: 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	0.36	0/3826	0.58	0/5190
1	B	0.35	0/3826	0.59	0/5190
1	C	0.40	0/3826	0.63	3/5190 (0.1%)
2	D	0.40	0/569	0.60	0/779
2	E	0.41	0/569	0.58	0/779
2	F	0.42	0/569	0.58	0/779
3	H	0.38	0/1637	0.56	0/2234
3	I	0.37	0/1637	0.56	0/2234
4	L	0.37	0/1640	0.58	0/2225
4	M	0.38	0/1640	0.56	0/2225
All	All	0.38	0/19739	0.59	3/26825 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	LEU	CA-CB-CG	7.62	132.83	115.30
1	C	265	LEU	N-CA-C	5.82	126.71	111.00
1	C	264	LEU	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	SER	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	3743	0	3732	25	0
1	B	3743	0	3732	34	0
1	C	3743	0	3732	27	0
2	D	557	0	591	3	0
2	E	557	0	591	3	0
2	F	557	0	591	3	0
3	H	1597	0	1548	9	0
3	I	1597	0	1548	8	0
4	L	1605	0	1535	7	0
4	M	1605	0	1535	10	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
All	All	19346	0	19174	123	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 3.

All (123) 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:B:23:LEU:HD11	1:B:33:ILE:HD11	1.70	0.73
1:A:45:LEU:HD21	1:A:48:ILE:HD11	1.77	0.66
1:C:390:TYR:HE2	1:C:392:TRP:CE3	2.16	0.63
1:B:490:MET:SD	1:B:490:MET:N	2.75	0.59
1:C:318:PRO:HG2	1:C:390:TYR:CD2	2.38	0.59
3:H:4:LEU:HD11	3:H:98:ARG:HB2	1.85	0.58
1:C:318:PRO:HB2	1:C:390:TYR:CE2	2.38	0.58
1:C:10:ASP:OD1	1:C:408:LYS:NZ	2.36	0.58
2:F:26:ARG:HG2	2:F:29:LEU:HD12	1.86	0.58
1:B:271:VAL:HG22	2:D:7:HIS:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.86	0.57
1:C:59:TYR:HB2	1:C:127:ALA:HB3	1.85	0.57
4:L:2:ILE:HD12	4:L:93:ASN:HB2	1.85	0.57
1:B:163:ALA:HB2	1:B:174:LEU:HD11	1.88	0.56
1:A:345:VAL:HB	1:A:350:PRO:HG2	1.89	0.55
1:C:390:TYR:CE2	1:C:392:TRP:CE3	2.94	0.55
1:A:101:TRP:CH2	1:B:316:ARG:HG3	2.42	0.54
1:B:59:TYR:HB2	1:B:127:ALA:HB3	1.89	0.54
1:C:316:ARG:HB3	1:C:329:GLU:HB3	1.89	0.54
1:A:130:HIS:HB2	1:A:199:ILE:HB	1.90	0.54
4:M:2:ILE:HD11	4:M:27:GLN:HE21	1.73	0.54
1:B:10:ASP:OD1	1:B:408:LYS:NZ	2.40	0.53
2:E:50:VAL:HG13	2:E:60:ARG:HD3	1.89	0.53
1:C:35:ALA:HB3	1:C:38:LYS:HB2	1.91	0.53
1:C:23:LEU:HD11	1:C:33:ILE:HD11	1.89	0.53
1:A:417:GLY:HA2	1:A:420:ALA:HB3	1.91	0.52
1:C:130:HIS:HB2	1:C:199:ILE:HB	1.92	0.52
1:B:257:LEU:O	1:B:260:GLN:NE2	2.43	0.52
1:B:10:ASP:OD2	1:B:412:ARG:NH1	2.43	0.52
1:B:71:ALA:HB2	1:B:82:LEU:HD21	1.91	0.52
2:D:26:ARG:HG2	2:D:29:LEU:HD12	1.92	0.51
1:C:127:ALA:HB1	1:C:200:LEU:HD11	1.92	0.51
1:A:59:TYR:HB2	1:A:127:ALA:HB3	1.92	0.51
1:A:455:LEU:HB2	1:A:456:PRO:HD3	1.93	0.51
1:B:340:ILE:HD12	1:B:362:PRO:HB2	1.91	0.50
1:B:61:LEU:HD13	1:B:261:THR:HA	1.93	0.50
3:I:22:CYS:HB3	3:I:79:LEU:HB3	1.94	0.50
3:H:99:VAL:HG11	3:H:103:TYR:HD1	1.76	0.49
1:A:82:LEU:HB2	1:A:85:GLU:HG3	1.95	0.49
1:C:61:LEU:HD11	1:C:202:LEU:HD22	1.95	0.49
1:B:57:ARG:NH1	1:B:221:ASN:O	2.45	0.49
1:C:45:LEU:HD21	1:C:48:ILE:HD11	1.94	0.49
2:E:23:ASP:O	2:E:27:THR:N	2.46	0.49
1:A:257:LEU:O	1:A:260:GLN:NE2	2.46	0.49
1:A:490:MET:N	1:A:490:MET:SD	2.84	0.48
1:A:103:ASN:ND2	1:A:249:ALA:HB1	2.29	0.48
3:I:162:ASN:HD21	3:I:200:VAL:HA	1.78	0.48
1:A:80:ALA:O	1:A:94:ARG:NH1	2.46	0.48
1:B:417:GLY:HA2	1:B:420:ALA:HB3	1.95	0.48
4:M:117:ILE:HD13	4:M:194:CYS:HB2	1.96	0.48
1:B:455:LEU:HB2	1:B:456:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:HD23	1:B:467:LEU:HD12	1.97	0.47
1:C:449:PHE:HB3	1:C:452:VAL:HB	1.96	0.47
1:C:212:ALA:HB2	1:C:276:ILE:HG13	1.96	0.47
3:H:5:GLU:HB3	3:H:23:ALA:HB3	1.96	0.47
1:A:330:VAL:HG11	1:A:385:VAL:HG11	1.96	0.47
1:B:130:HIS:HB2	1:B:199:ILE:HB	1.97	0.47
3:I:52:ASN:O	3:I:72:ARG:NH2	2.48	0.47
4:L:138:ASN:HD22	4:L:172:THR:HG21	1.79	0.47
4:M:138:ASN:HD22	4:M:172:THR:HG21	1.80	0.47
3:I:90:ASP:HB2	3:I:118:VAL:HG21	1.97	0.46
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.98	0.46
2:F:50:VAL:HG13	2:F:60:ARG:HD3	1.98	0.46
1:C:113:ILE:HG21	1:C:247:PRO:HG3	1.98	0.46
1:C:490:MET:SD	1:C:490:MET:N	2.85	0.45
3:I:20:LEU:HD12	3:I:81:LEU:HD23	1.98	0.45
1:A:23:LEU:HD11	1:A:33:ILE:HD11	1.98	0.45
1:B:378:PRO:HA	1:B:394:GLN:HB3	1.98	0.45
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.82	0.45
1:B:200:LEU:HD21	1:B:264:LEU:HD21	1.98	0.45
1:C:330:VAL:HG23	1:C:364:ILE:HD11	1.98	0.45
2:E:26:ARG:HG2	2:E:29:LEU:HD12	1.99	0.45
1:A:24:VAL:HG11	1:A:420:ALA:HB2	1.99	0.45
1:B:305:THR:HG21	3:H:59:TYR:HB2	1.98	0.45
3:I:52:ASN:HD21	3:I:56:ASP:HB2	1.82	0.45
1:B:330:VAL:HG11	1:B:385:VAL:HG11	1.99	0.44
1:B:89:GLY:HA2	1:B:235:TRP:HB2	1.98	0.44
1:C:82:LEU:HB2	1:C:85:GLU:HG3	1.99	0.44
1:C:198:VAL:HG11	1:C:220:PHE:CD1	2.53	0.44
1:C:26:GLU:HA	1:C:287:HIS:HA	2.00	0.44
1:B:103:ASN:N	1:B:103:ASN:OD1	2.51	0.43
1:B:337:PRO:HB3	1:B:365:GLU:HA	1.99	0.43
4:L:117:ILE:HD13	4:L:194:CYS:HB2	2.00	0.43
4:L:134:CYS:SG	4:L:135:PHE:N	2.91	0.43
1:A:9:ARG:O	1:A:408:LYS:NZ	2.51	0.43
3:H:155:GLU:HB3	3:H:156:PRO:HA	2.00	0.43
3:H:9:GLY:HA2	3:H:116:VAL:HG22	2.01	0.43
4:L:117:ILE:HD11	4:L:132:VAL:HG12	2.01	0.43
1:B:267:ALA:HB2	2:D:4:ILE:HD13	2.00	0.43
1:A:390:TYR:CE2	1:A:391:GLN:O	2.72	0.43
1:A:4:THR:HG21	1:A:371:PHE:HZ	1.84	0.43
1:A:45:LEU:HD22	1:A:288:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:HG2	1:B:111:GLY:HA3	2.01	0.42
4:M:166:GLN:NE2	4:M:171:SER:OG	2.46	0.42
1:C:464:LEU:HD23	1:C:467:LEU:HD12	2.02	0.42
1:B:148:GLY:O	1:B:371:PHE:N	2.44	0.42
3:H:130:PRO:HG3	3:H:201:THR:HG23	2.01	0.42
3:H:128:VAL:HG22	3:H:204:VAL:HB	2.02	0.42
1:A:378:PRO:HA	1:A:394:GLN:HB3	2.02	0.42
4:M:161:ASN:ND2	4:M:175:MET:SD	2.93	0.42
4:M:90:GLN:HE21	4:M:97:THR:H	1.68	0.41
4:M:138:ASN:ND2	4:M:170:ASP:OD2	2.53	0.41
1:A:464:LEU:HD23	1:A:467:LEU:HD12	2.02	0.41
1:B:65:LEU:HD21	1:B:242:VAL:HG22	2.02	0.41
1:B:24:VAL:HG21	1:B:420:ALA:HB1	2.03	0.41
4:M:149:LYS:HB2	4:M:193:THR:HB	2.03	0.41
1:B:301:GLY:HA2	1:B:304:TYR:CD2	2.56	0.41
1:C:300:LYS:O	1:C:361:ASN:ND2	2.54	0.41
4:M:148:TRP:NE1	4:M:158:GLY:O	2.54	0.41
1:B:157:HIS:HB3	1:B:160:ARG:HB2	2.01	0.41
1:B:340:ILE:HD11	1:B:364:ILE:HD11	2.03	0.41
1:C:455:LEU:HB2	1:C:456:PRO:HD3	2.02	0.41
3:I:34:MET:HB3	3:I:79:LEU:HD22	2.03	0.41
1:A:33:ILE:HG21	1:A:294:LEU:HD21	2.02	0.41
1:A:22:THR:HA	1:A:291:GLU:HA	2.02	0.40
3:I:176:VAL:HG11	4:M:160:LEU:HB3	2.02	0.40
1:B:7:GLU:O	1:B:323:HIS:NE2	2.54	0.40
1:C:414:THR:OG1	1:C:415:VAL:N	2.52	0.40
1:C:157:HIS:HB3	1:C:160:ARG:HB2	2.02	0.40
1:C:25:LEU:HD11	1:C:43:VAL:HG12	2.03	0.40
2:F:24:SER:HA	2:F:27:THR:HG23	2.03	0.40
4:L:2:ILE:HD11	4:L:27:GLN:HE21	1.85	0.40
1:B:335:THR:HB	4:L:94:HIS:CE1	2.57	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	490/496 (99%)	440 (90%)	48 (10%)	2 (0%)	38	76
1	B	490/496 (99%)	456 (93%)	33 (7%)	1 (0%)	51	84
1	C	490/496 (99%)	443 (90%)	47 (10%)	0	100	100
2	D	69/75 (92%)	56 (81%)	13 (19%)	0	100	100
2	E	69/75 (92%)	57 (83%)	11 (16%)	1 (1%)	13	55
2	F	69/75 (92%)	57 (83%)	9 (13%)	3 (4%)	3	32
3	H	210/212 (99%)	191 (91%)	19 (9%)	0	100	100
3	I	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	32	73
4	L	206/208 (99%)	186 (90%)	20 (10%)	0	100	100
4	M	206/208 (99%)	183 (89%)	23 (11%)	0	100	100
All	All	2509/2553 (98%)	2267 (90%)	234 (9%)	8 (0%)	48	80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	22	GLY
2	F	11	GLU
1	A	350	PRO
1	A	169	SER
1	B	78	GLY
2	F	16	GLY
3	I	174	PRO
2	E	10	GLY

### 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	400/401 (100%)	398 (100%)	2 (0%)	91	96
1	B	400/401 (100%)	397 (99%)	3 (1%)	85	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	400/401 (100%)	397 (99%)	3 (1%)	85	93
2	D	61/64 (95%)	61 (100%)	0	100	100
2	E	61/64 (95%)	61 (100%)	0	100	100
2	F	61/64 (95%)	60 (98%)	1 (2%)	68	86
3	H	180/180 (100%)	178 (99%)	2 (1%)	78	89
3	I	180/180 (100%)	178 (99%)	2 (1%)	78	89
4	L	183/183 (100%)	179 (98%)	4 (2%)	57	81
4	M	183/183 (100%)	180 (98%)	3 (2%)	68	86
All	All	2109/2121 (99%)	2089 (99%)	20 (1%)	83	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	VAL
1	A	490	MET
1	B	2	ARG
1	B	16	GLN
1	B	490	MET
1	C	2	ARG
1	C	261	THR
1	C	490	MET
2	F	18	LYS
3	H	150	LYS
3	H	184	LEU
3	I	150	LYS
3	I	184	LEU
4	L	77	ASN
4	L	92	ASN
4	L	96	LEU
4	L	108	ARG
4	M	77	ASN
4	M	92	ASN
4	M	108	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN

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Mol	Chain	Res	Type
1	A	208	HIS
1	B	347	HIS
1	C	196	GLN
2	D	7	HIS
2	E	39	ASN
3	H	178	GLN
3	I	162	ASN
4	L	27	GLN
4	L	77	ASN
4	L	92	ASN
4	L	94	HIS
4	L	138	ASN
4	L	161	ASN
4	M	27	GLN
4	M	77	ASN
4	M	137	ASN
4	M	138	ASN
4	M	161	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	500	1	14,14,15	0.67	0	15,19,21	1.76	2 (13%)
5	NAG	B	500	1	14,14,15	0.39	0	15,19,21	1.09	1 (6%)
5	NAG	C	500	1	14,14,15	0.35	0	15,19,21	0.99	1 (6%)

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	500	1	-	0/6/23/26	0/1/1/1
5	NAG	B	500	1	-	0/6/23/26	0/1/1/1
5	NAG	C	500	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	NAG	O5-C1-C2	-2.59	107.87	111.47
5	C	500	NAG	O5-C1-C2	-2.45	108.06	111.47
5	A	500	NAG	O5-C1-C2	2.02	114.29	111.47
5	A	500	NAG	C1-O5-C5	5.98	120.40	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.