



## Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 04:10 PM JST

PDB ID : 7YER  
EMDB ID : EMD-33775  
Title : The structure of EBOV L-VP35 complex  
Authors : Shi, Y.; Yuan, B.; Peng, Q.  
Deposited on : 2022-07-06  
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

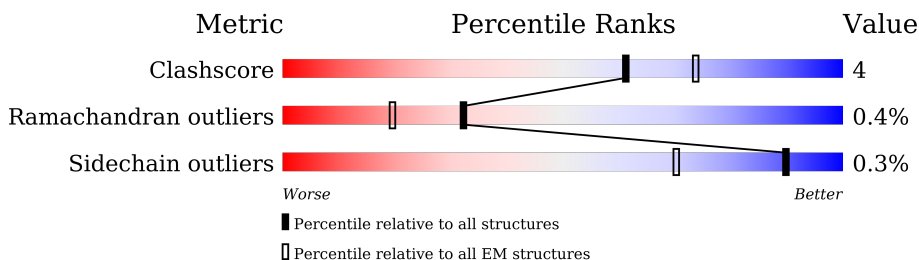
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	2212	
2	B	340	
2	C	340	
2	D	340	
2	E	340	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14313 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1316	Total	C	N	O	S	0	0
			10540	6780	1778	1926	56		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	ASP	GLY	engineered mutation	UNP A0A1C4HDB0

- Molecule 2 is a protein called Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	260	Total	C	N	O	S	4	0
			2011	1259	346	396	10		
2	C	99	Total	C	N	O	S	0	0
			733	458	118	153	4		
2	D	68	Total	C	N	O	S	0	0
			515	323	81	107	4		
2	E	67	Total	C	N	O	S	0	0
			513	320	85	105	3		

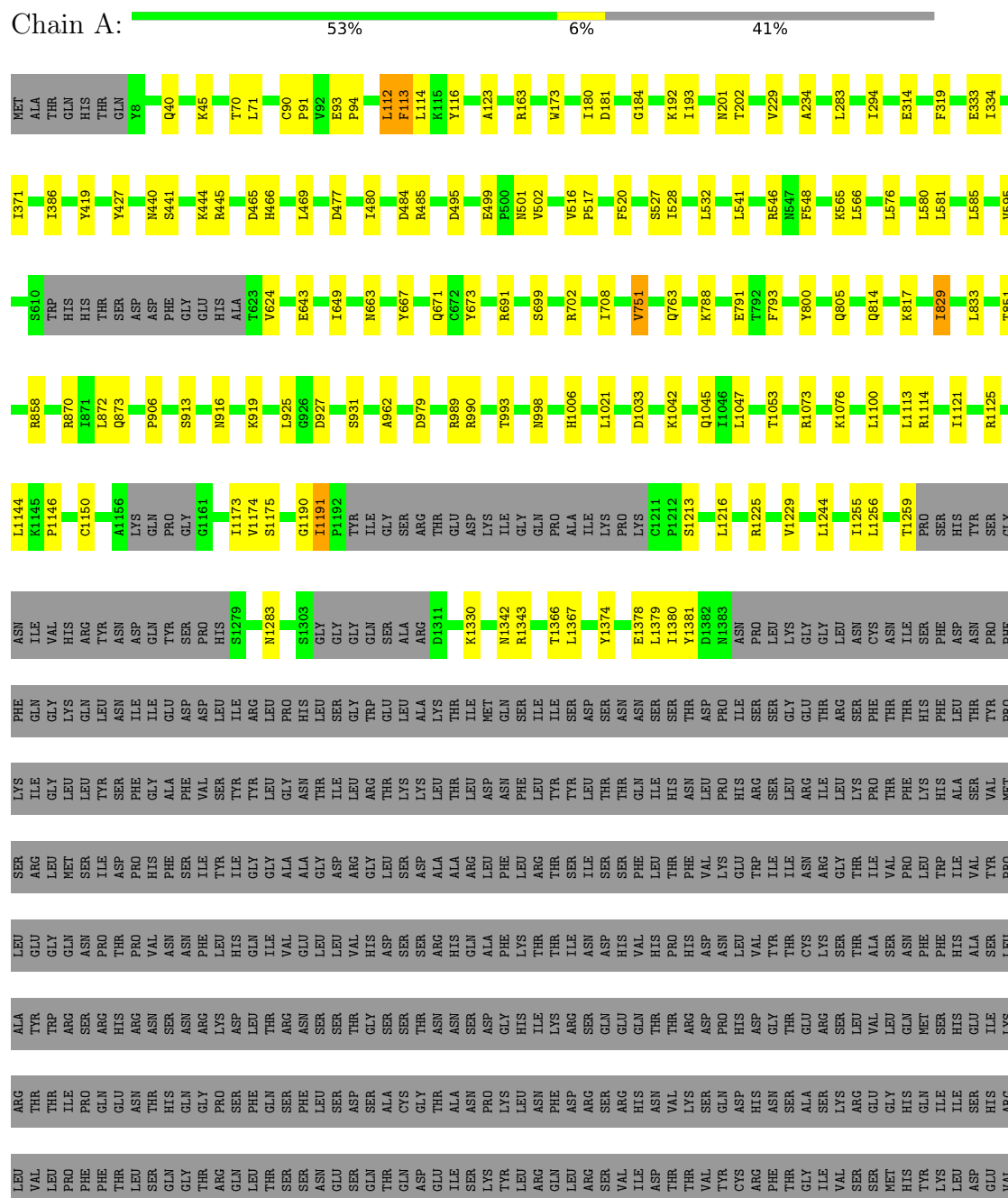
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: RNA-directed RNA polymerase L



[illegible]

- Molecule 2: Polymerase cofactor VP35

Chain B:  67% 9% 24%

[illegible]

- Molecule 2: Polymerase cofactor VP35

Chain C:  26% 1% 71%

[illegible]

- Molecule 2: Polymerase cofactor VP35

Chain D:  18% 80%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1083293	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: ZN

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  >5	RMSZ	# Z  >5
1	A	0.25	0/10795	0.48	0/14657
2	B	0.24	0/2050	0.44	0/2789
2	C	0.24	0/746	0.42	0/1022
2	D	0.23	0/518	0.39	0/703
2	E	0.25	0/517	0.44	0/702
All	All	0.25	0/14626	0.47	0/19873

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	10540	0	10521	89	0
2	B	2011	0	1980	23	0
2	C	733	0	698	9	0
2	D	515	0	525	7	0
2	E	513	0	515	11	0
3	A	1	0	0	0	0
All	All	14313	0	14239	121	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 (121) 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:A:70:THR:HG23	1:A:229:VAL:O	1.59	1.02
1:A:114:LEU:HD22	1:A:858:ARG:HD3	1.59	0.82
1:A:70:THR:HG22	1:A:71:LEU:H	1.45	0.81
1:A:70:THR:HG22	1:A:71:LEU:N	1.97	0.80
2:D:121:VAL:HG22	2:E:121:VAL:HG21	1.72	0.70
1:A:70:THR:CG2	1:A:71:LEU:H	2.08	0.66
1:A:386:ILE:HG21	1:A:699:SER:HA	1.78	0.65
1:A:1006:HIS:HE2	1:A:1374:TYR:HH	1.44	0.65
1:A:649:ILE:HG21	1:A:663:ASN:HB3	1.78	0.65
1:A:112:LEU:O	1:A:114:LEU:N	2.30	0.65
1:A:548:PHE:HA	1:A:565:LYS:O	2.01	0.61
1:A:70:THR:CG2	1:A:71:LEU:N	2.64	0.60
1:A:962:ALA:HB2	1:A:1121:ILE:HD12	1.82	0.59
1:A:427:TYR:CE1	1:A:466:HIS:HB3	2.39	0.58
1:A:201:ASN:OD1	1:A:202:THR:N	2.36	0.58
2:B:194:GLN:O	2:B:198:GLU:HG3	2.03	0.57
1:A:990:ARG:HH22	1:A:1073:ARG:HH12	1.53	0.56
1:A:1033:ASP:OD2	1:A:1225:ARG:NH2	2.38	0.56
1:A:1144:LEU:HD11	1:A:1150:CYS:HB2	1.87	0.56
1:A:485:ARG:HG2	1:A:516:VAL:HG21	1.87	0.56
1:A:477:ASP:OD1	1:A:1045:GLN:NE2	2.39	0.56
1:A:829:ILE:HA	1:A:1053:THR:HB	1.87	0.56
1:A:548:PHE:HZ	1:A:708:ILE:HG21	1.71	0.55
2:C:124:MET:O	2:C:128:ILE:HG12	2.06	0.55
1:A:671:GLN:HG2	2:C:175:LEU:HD22	1.89	0.55
1:A:480:ILE:O	1:A:485:ARG:NH2	2.39	0.55
1:A:180:ILE:HD12	1:A:193:ILE:HG22	1.87	0.55
1:A:319:PHE:HD1	1:A:793:PHE:CD2	2.25	0.55
1:A:541:LEU:O	1:A:546:ARG:NH1	2.40	0.55
1:A:93:GLU:HB2	1:A:94:PRO:HD3	1.88	0.55
1:A:1021:LEU:O	1:A:1125:ARG:NH1	2.40	0.54
1:A:667:TYR:O	1:A:671:GLN:NE2	2.40	0.54
2:B:115:GLU:OE1	2:E:109:GLN:NE2	2.41	0.54
1:A:643:GLU:O	2:B:148:THR:OG1	2.25	0.54
2:D:93:LEU:HA	2:E:93:LEU:HD21	1.90	0.54
1:A:1073:ARG:HA	1:A:1076:LYS:HE3	1.90	0.53
2:B:311:LEU:HD12	2:B:336:LEU:HB3	1.91	0.53
1:A:484:ASP:HA	1:A:517:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:SER:H	1:A:1216:LEU:HD12	1.73	0.53
1:A:1244:LEU:HD11	1:A:1255:ILE:HG13	1.91	0.53
1:A:163:ARG:HH11	1:A:234:ALA:HB3	1.73	0.53
1:A:870:ARG:NH1	1:A:873:GLN:OE1	2.40	0.52
2:B:153:THR:HG23	2:E:145:LEU:HD11	1.92	0.52
2:B:139:VAL:HA	2:E:138:MET:CE	2.40	0.51
2:B:181:ILE:O	2:B:185:ILE:HG12	2.11	0.51
2:B:263:PHE:HB2	2:B:280:ILE:HD11	1.92	0.51
1:A:989:ARG:NH1	1:A:993:THR:OG1	2.43	0.51
1:A:1366:THR:HG22	1:A:1367:LEU:H	1.76	0.51
2:C:131:LEU:HD21	2:D:132:ASN:HA	1.93	0.51
2:B:285:PRO:HA	2:B:288:GLN:HG3	1.93	0.50
1:A:800:TYR:HB2	1:A:805:GLN:HG2	1.94	0.50
1:A:371:ILE:HG13	1:A:371:ILE:O	2.12	0.50
1:A:919:LYS:O	1:A:1283:ASN:ND2	2.41	0.49
1:A:927:ASP:OD1	1:A:1114:ARG:NH2	2.45	0.49
1:A:40:GLN:NE2	1:A:502:VAL:O	2.44	0.49
1:A:979:ASP:N	1:A:979:ASP:OD1	2.44	0.49
1:A:123:ALA:O	1:A:1330:LYS:HD3	2.13	0.49
2:B:114:LEU:HA	2:C:114:LEU:HD13	1.93	0.49
1:A:465:ASP:OD1	1:A:466:HIS:N	2.45	0.49
1:A:1225:ARG:O	1:A:1229:VAL:HG23	2.13	0.48
1:A:499:GLU:OE1	1:A:501:ASN:HB2	2.13	0.48
1:A:440:ASN:HB3	1:A:444:LYS:NZ	2.29	0.48
1:A:1190:GLY:O	1:A:1191:ILE:HB	2.14	0.48
1:A:1173:ILE:O	1:A:1175:SER:N	2.46	0.47
2:D:82:SER:OG	2:D:83:PHE:N	2.47	0.47
1:A:624:VAL:HG22	1:A:751:VAL:HG22	1.96	0.47
1:A:173:TRP:CE2	1:A:184:GLY:HA3	2.49	0.47
1:A:833:LEU:HD13	1:A:872:LEU:HD12	1.97	0.47
1:A:427:TYR:CD1	1:A:466:HIS:HB3	2.50	0.46
1:A:990:ARG:NH2	1:A:1073:ARG:HH12	2.13	0.46
1:A:906:PRO:HA	1:A:913:SER:HB3	1.96	0.46
2:D:107:LEU:HD13	2:E:107:LEU:HB2	1.96	0.46
1:A:113:PHE:HA	1:A:116:TYR:HB3	1.96	0.46
2:B:298:ARG:NH1	2:B:299:SER:OG	2.49	0.46
2:D:134:VAL:HG13	2:E:139:VAL:HG21	1.98	0.45
1:A:1006:HIS:NE2	1:A:1374:TYR:OH	2.35	0.45
2:B:107:LEU:HD11	2:C:103:ALA:HB1	1.98	0.45
2:B:300:ARG:HG2	2:B:308:GLN:HE22	1.82	0.45
1:A:181:ASP:HB2	1:A:192:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1380:ILE:HG22	1:A:1381:TYR:N	2.31	0.45
1:A:817:LYS:HB3	1:A:817:LYS:HE3	1.83	0.44
2:B:192:VAL:O	2:B:197:ARG:NH2	2.46	0.44
1:A:788:LYS:HB2	1:A:791:GLU:HB2	1.99	0.44
1:A:673:TYR:HD1	1:A:702:ARG:HE	1.66	0.44
1:A:419:TYR:CD2	1:A:427:TYR:HB3	2.53	0.44
1:A:1146:PRO:HG3	1:A:1342:ASN:HB2	2.00	0.44
2:B:272:SER:OG	2:B:275[B]:CYS:SG	2.69	0.43
2:B:139:VAL:HA	2:E:138:MET:HE1	2.00	0.43
1:A:528:ILE:HG13	1:A:1378:GLU:OE2	2.18	0.43
1:A:1042:LYS:HD2	1:A:1379:LEU:HD23	2.01	0.43
2:B:169:PRO:O	2:C:151:ARG:NH1	2.37	0.43
1:A:314:GLU:OE2	1:A:763:GLN:NE2	2.51	0.43
2:B:134:VAL:HG12	2:C:135:CYS:HB3	2.00	0.43
1:A:548:PHE:HD1	1:A:566:LEU:HG	1.83	0.42
1:A:45:LYS:HB3	1:A:45:LYS:HE2	1.74	0.42
2:B:188:ARG:HH22	2:B:191:THR:HG22	1.83	0.42
1:A:283:LEU:HD21	1:A:294:ILE:HB	2.01	0.42
1:A:90:CYS:HA	1:A:91:PRO:HD3	1.92	0.42
2:E:130:SER:O	2:E:134:VAL:HG23	2.20	0.42
1:A:581:LEU:HD12	1:A:585:LEU:HB2	2.01	0.42
2:C:166:HIS:O	2:C:168:GLN:N	2.46	0.42
1:A:1256:LEU:O	1:A:1259:THR:OG1	2.36	0.42
1:A:1366:THR:HG22	1:A:1367:LEU:N	2.34	0.42
2:B:151:ARG:HG3	2:C:160:GLU:HG3	2.02	0.42
1:A:466:HIS:HD1	1:A:469:LEU:HG	1.85	0.41
1:A:520:PHE:O	1:A:998:ASN:ND2	2.53	0.41
1:A:1100:LEU:HD11	1:A:1113:LEU:HD21	2.02	0.41
1:A:916:ASN:HB3	1:A:919:LYS:HG2	2.02	0.41
1:A:1380:ILE:CG2	1:A:1381:TYR:N	2.84	0.41
1:A:333:GLU:HG3	1:A:334:ILE:HG23	2.02	0.41
1:A:1047:LEU:HD23	1:A:1047:LEU:HA	1.95	0.41
1:A:576:LEU:O	1:A:580:LEU:HG	2.20	0.41
1:A:495:ASP:OD1	1:A:691:ARG:NH1	2.54	0.40
2:B:249:LEU:HD23	2:B:249:LEU:HA	1.90	0.40
1:A:441:SER:O	1:A:445:ARG:HG3	2.21	0.40
2:B:162:TYR:HE1	2:B:168:GLN:HB3	1.86	0.40
1:A:532:LEU:HD22	1:A:576:LEU:HD21	2.03	0.40
1:A:814:GLN:HG3	1:A:814:GLN:O	2.20	0.40
1:A:925:LEU:HD21	1:A:931:SER:OG	2.21	0.40
2:B:132:ASN:HA	2:E:131:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:PRO:HG2	2:E:122:TYR: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	1304/2212 (59%)	1200 (92%)	96 (7%)	8 (1%)	22	57
2	B	262/340 (77%)	255 (97%)	7 (3%)	0	100	100
2	C	97/340 (28%)	90 (93%)	7 (7%)	0	100	100
2	D	66/340 (19%)	64 (97%)	2 (3%)	0	100	100
2	E	65/340 (19%)	64 (98%)	1 (2%)	0	100	100
All	All	1794/3572 (50%)	1673 (93%)	113 (6%)	8 (0%)	32	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	1191	ILE
1	A	527	SER
1	A	112	LEU
1	A	751	VAL
1	A	851	THR
1	A	829	ILE
1	A	1174	VAL

### 5.3.2 Protein sidechains [i](#)

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	1174/1994 (59%)	1172 (100%)	2 (0%)	92	97
2	B	222/294 (76%)	221 (100%)	1 (0%)	86	94
2	C	78/294 (26%)	77 (99%)	1 (1%)	65	85
2	D	60/294 (20%)	60 (100%)	0	100	100
2	E	59/294 (20%)	59 (100%)	0	100	100
All	All	1593/3170 (50%)	1589 (100%)	4 (0%)	90	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	VAL
1	A	1343	ARG
2	B	298	ARG
2	C	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33775. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.