



Full wwPDB EM Validation Report (i)

Oct 22, 2023 – 12:07 AM JST

PDB ID : 8JSL
EMDB ID : EMD-36622
Title : The structure of EBOV L-VP35-RNA complex
Authors : Qi, P.; Yi, S.
Deposited on : 2023-06-20
Resolution : 2.95 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
A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

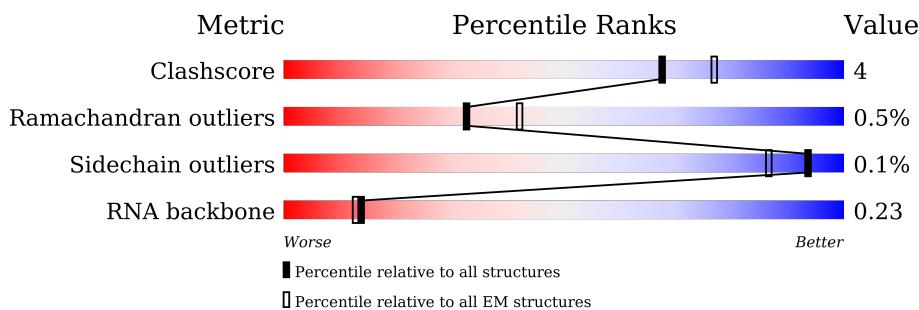
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

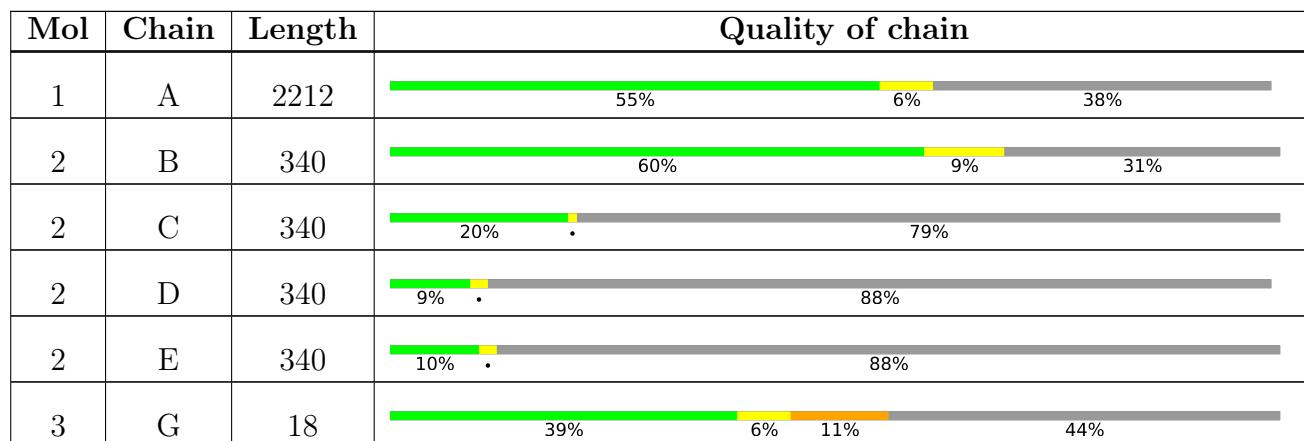
The reported resolution of this entry is 2.95 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 >=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 <=5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14069 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
			Total	C	N	O	S		
1	A	1362	10897	7002	1853	1986	56	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	235	Total	C	N	O	S		
			1799	1129	311	350	9	1	0
2	C	72	Total	C	N	O	S		
			533	333	86	110	4	0	0
2	D	40	Total	C	N	O	S		
			303	192	48	59	4	0	0
2	E	42	Total	C	N	O	S		
			324	203	53	65	3	0	0

- Molecule 3 is a RNA chain called The leader sequence of EBOV.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	10	Total	C	N	O	P	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

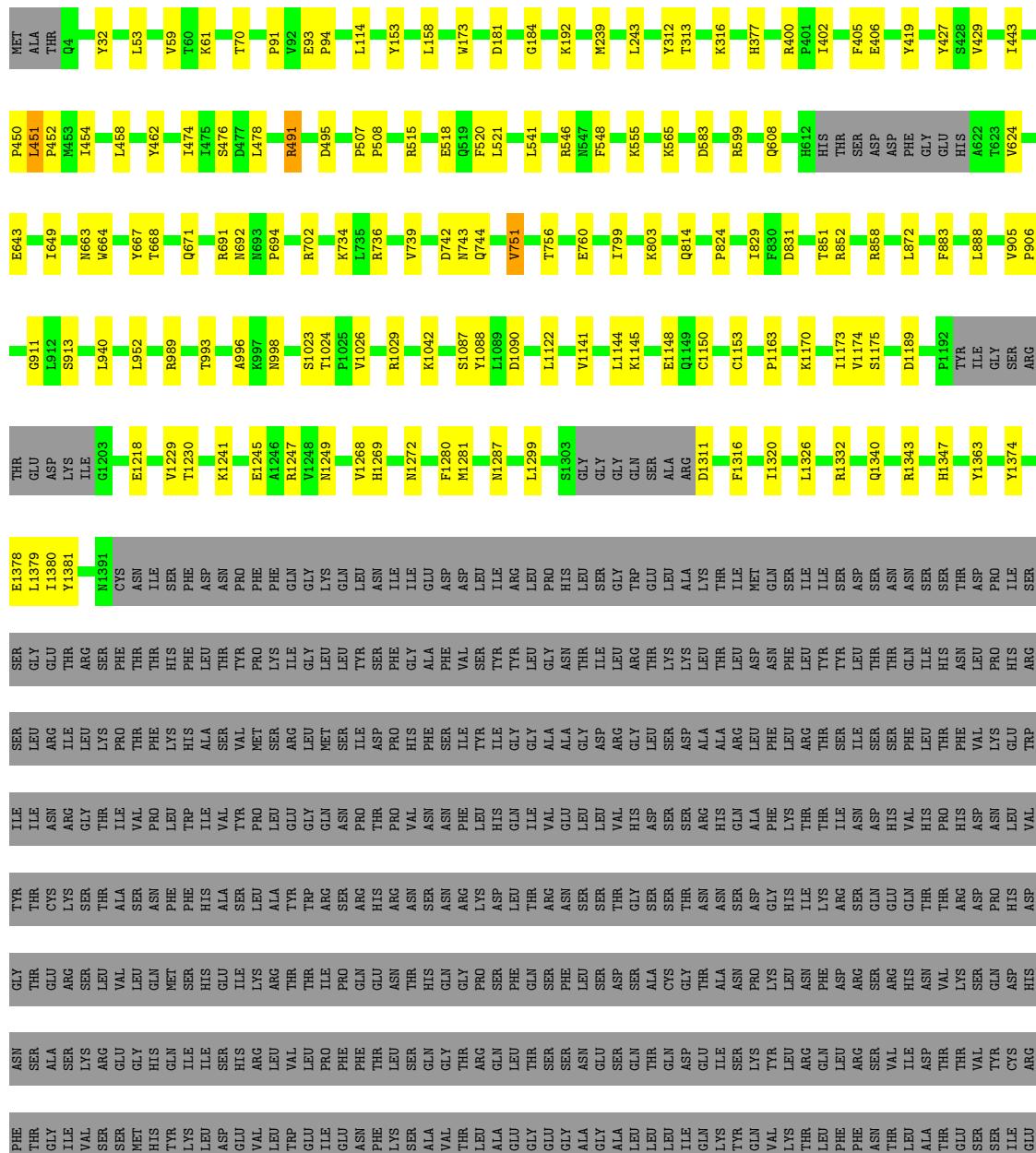
3 Residue-property plots [\(i\)](#)

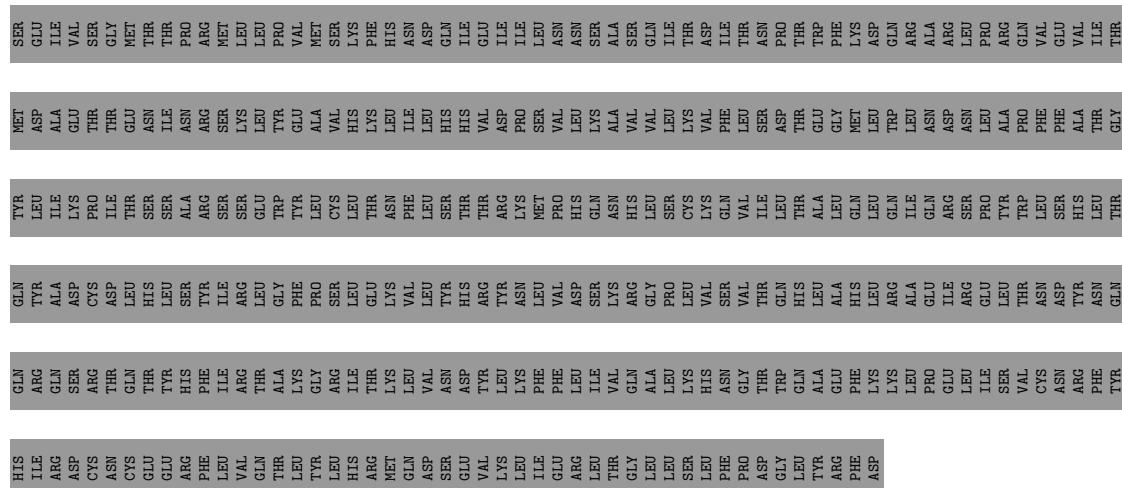
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

Chain A: 55% 6% 38%

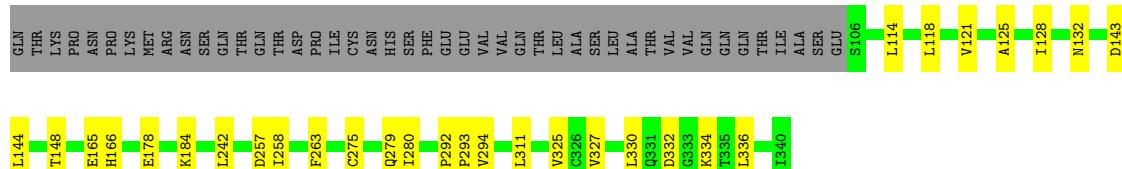
A horizontal progress bar divided into three segments by vertical tick marks. The first segment is green and spans from the start to 55%. The second segment is yellow and spans from 55% to 61%. The third segment is grey and spans from 61% to 99%. The percentage values (55%, 6%, 38%) are displayed as text labels next to their respective colored segments.





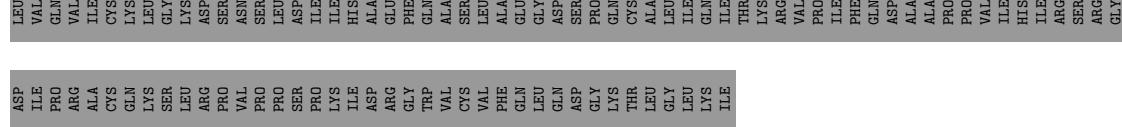
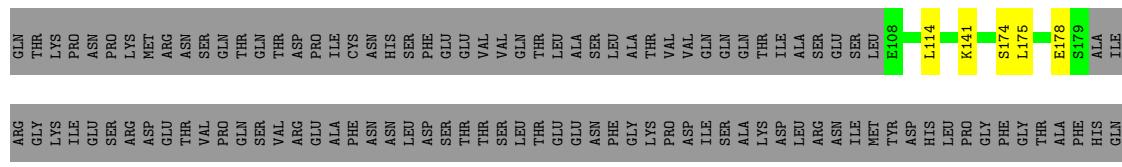
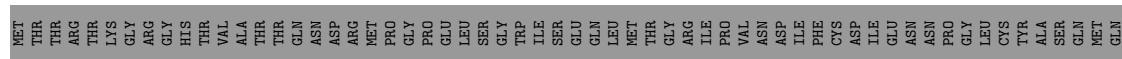
- Molecule 2: Polymerase cofactor VP35

Chain B:



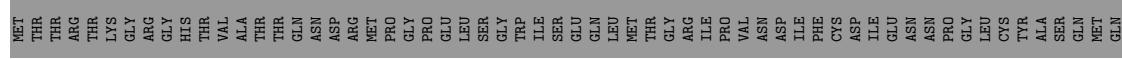
- Molecule 2: Polymerase cofactor VP35

Chain C:



- Molecule 2: Polymerase cofactor VP35

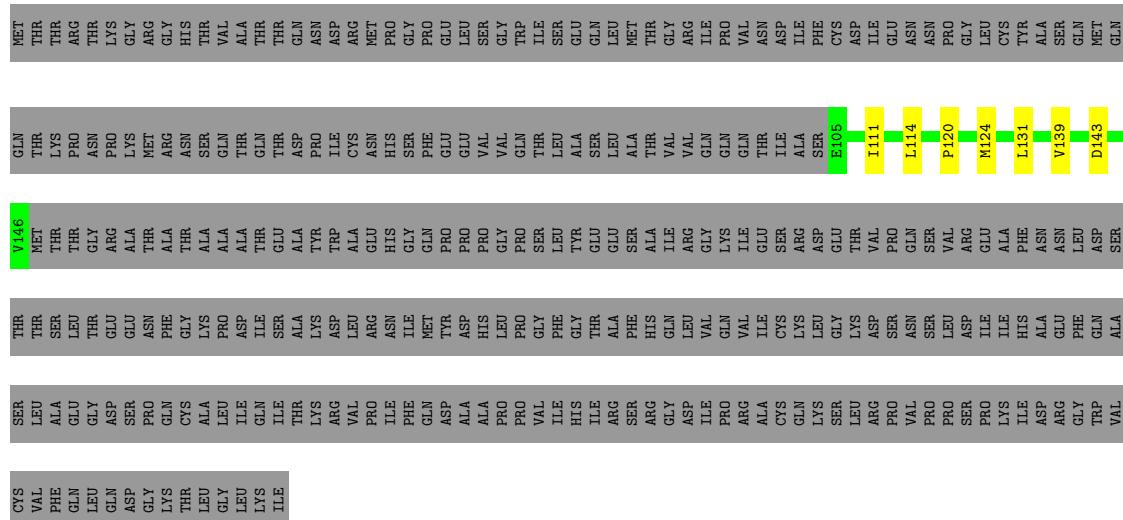
Chain D:



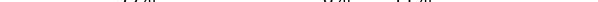


- Molecule 2: Polymerase cofactor VP35

Chain E: 10% : 88%



- Molecule 3: The leader sequence of EBOV

Chain G:  39% 6% 11% 44%



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	642661	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	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	0/11168	0.47	0/15169
2	B	0.25	0/1836	0.48	0/2496
2	C	0.26	0/544	0.45	0/745
2	D	0.25	0/305	0.50	0/412
2	E	0.24	0/326	0.50	0/440
3	G	0.18	0/235	0.78	0/364
All	All	0.25	0/14414	0.48	0/19626

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	10897	0	10861	82	0
2	B	1799	0	1777	21	0
2	C	533	0	502	4	0
2	D	303	0	316	7	0
2	E	324	0	329	6	0
3	G	212	0	107	1	0
4	A	1	0	0	0	0
All	All	14069	0	13892	108	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 (108) 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:B:263:PHE:HB2	2:B:280:ILE:HD11	1.69	0.74
1:A:1153:CYS:SG	1:A:1347:HIS:HE1	2.10	0.73
2:B:275:CYS:O	2:B:279:GLN:NE2	2.27	0.68
1:A:114:LEU:HD22	1:A:858:ARG:HD3	1.77	0.66
1:A:905:VAL:HG23	1:A:911:GLY:HA3	1.77	0.66
2:B:330:LEU:HB2	2:B:334:LYS:HB2	1.77	0.66
1:A:667:TYR:O	1:A:671:GLN:NE2	2.29	0.66
2:D:119:LYS:HG3	2:D:120:PRO:HD3	1.76	0.66
1:A:1029:ARG:NH1	1:A:1272:ASN:OD1	2.28	0.65
2:B:257:ASP:OD1	2:B:258:ILE:HD12	1.98	0.64
1:A:1218:GLU:OE1	1:A:1247:ARG:NH2	2.31	0.64
1:A:608:GLN:OE1	1:A:736:ARG:NH1	2.31	0.63
1:A:313:THR:HG23	1:A:316:LYS:HE2	1.80	0.63
1:A:93:GLU:HB3	1:A:94:PRO:HD3	1.80	0.63
1:A:429:VAL:HG21	1:A:443:ILE:HD13	1.82	0.61
1:A:491:ARG:NH2	1:A:692:ASN:O	2.31	0.61
1:A:906:PRO:HA	1:A:913:SER:HB3	1.83	0.61
2:C:174:SER:HB2	2:C:178:GLU:HG3	1.82	0.60
1:A:649:ILE:HG21	1:A:663:ASN:HB3	1.83	0.60
1:A:1229:VAL:HG13	1:A:1230:THR:HG23	1.84	0.59
1:A:1380:ILE:HG22	1:A:1381:TYR:H	1.67	0.59
1:A:1268:VAL:HG23	1:A:1269:HIS:HD2	1.69	0.58
2:B:294:VAL:HG22	2:B:327:VAL:HB	1.87	0.57
1:A:520:PHE:O	1:A:998:ASN:ND2	2.39	0.56
1:A:883:PHE:CE1	1:A:888:LEU:HD21	2.40	0.56
1:A:803:LYS:O	1:A:814:GLN:NE2	2.39	0.55
1:A:1026:VAL:HG21	1:A:1122:LEU:HD22	1.89	0.55
2:E:120:PRO:O	2:E:124:MET:HG2	2.07	0.55
1:A:1145:LYS:O	1:A:1343:ARG:NH1	2.40	0.55
1:A:1145:LYS:HB2	1:A:1148:GLU:HG3	1.90	0.54
1:A:643:GLU:O	2:B:148:THR:OG1	2.27	0.52
1:A:989:ARG:NH1	1:A:993:THR:OG1	2.43	0.52
1:A:1170:LYS:NZ	1:A:1189:ASP:O	2.35	0.51
1:A:476:SER:HA	1:A:1379:LEU:HD21	1.93	0.51
1:A:1144:LEU:HD11	1:A:1150:CYS:HB2	1.92	0.51
2:B:242:LEU:HD13	2:B:325:VAL:HG12	1.93	0.51
1:A:742:ASP:O	1:A:743:ASN:ND2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:ILE:O	1:A:1175:SER:N	2.44	0.51
1:A:454:ILE:O	1:A:454:ILE:HG13	2.11	0.50
1:A:495:ASP:OD1	1:A:691:ARG:NH1	2.44	0.50
1:A:548:PHE:HA	1:A:565:LYS:O	2.12	0.50
1:A:1141:VAL:HG21	1:A:1326:LEU:HD21	1.92	0.50
1:A:405:PHE:HD1	2:B:144:LEU:HD13	1.77	0.49
2:B:132:ASN:HA	2:E:131:LEU:HD11	1.95	0.49
1:A:694:PRO:O	1:A:702:ARG:NH2	2.46	0.48
1:A:400:ARG:NH1	2:B:178:GLU:OE2	2.46	0.48
1:A:474:ILE:HD12	1:A:583:ASP:HB3	1.95	0.48
1:A:1042:LYS:HD2	1:A:1379:LEU:HD13	1.95	0.47
1:A:1340:GLN:N	1:A:1340:GLN:OE1	2.47	0.47
1:A:521:LEU:HB3	1:A:996:ALA:HA	1.95	0.47
1:A:450:PRO:O	1:A:451:LEU:HB2	2.15	0.47
1:A:599:ARG:NH2	1:A:1287:ASN:OD1	2.46	0.47
1:A:608:GLN:HG2	1:A:734:LYS:HE3	1.97	0.47
1:A:671:GLN:HG2	2:C:175:LEU:HD22	1.97	0.47
2:D:110:ARG:HD3	2:E:111:ILE:HD11	1.96	0.47
1:A:1269:HIS:HE1	1:A:1311:ASP:HB2	1.80	0.47
1:A:515:ARG:HB2	1:A:518:GLU:OE1	2.15	0.47
1:A:173:TRP:CE2	1:A:184:GLY:HA3	2.50	0.47
2:B:118:LEU:O	2:B:121:VAL:HG22	2.15	0.46
1:A:1249:ASN:ND2	1:A:1381:TYR:OH	2.26	0.46
2:D:114:LEU:HD23	2:E:114:LEU:HD13	1.97	0.46
2:B:125:ALA:HA	2:B:128:ILE:HG22	1.97	0.46
1:A:181:ASP:HB2	1:A:192:LYS:HB3	1.97	0.46
1:A:239:MET:O	1:A:243:LEU:HG	2.16	0.45
1:A:852:ARG:NH1	1:A:1332:ARG:O	2.50	0.45
1:A:32:TYR:O	1:A:70:THR:OG1	2.29	0.44
1:A:756:THR:OG1	1:A:760:GLU:OE2	2.35	0.44
1:A:312:TYR:HA	1:A:316:LYS:HD2	1.98	0.44
1:A:507:PRO:HA	1:A:508:PRO:HD3	1.91	0.44
1:A:541:LEU:O	1:A:546:ARG:NH1	2.50	0.44
1:A:624:VAL:HG22	1:A:751:VAL:HG23	2.00	0.44
1:A:462:TYR:OH	2:B:143:ASP:OD2	2.28	0.44
1:A:153:TYR:OH	1:A:824:PRO:HD2	2.18	0.44
1:A:1023:SER:HB2	1:A:1363:TYR:CZ	2.53	0.43
1:A:451:LEU:HB3	1:A:452:PRO:HD3	2.01	0.43
1:A:1023:SER:OG	1:A:1024:THR:N	2.52	0.43
1:A:1241:LYS:O	1:A:1245:GLU:HG2	2.18	0.43
1:A:1087:SER:OG	1:A:1088:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:GLU:HG2	2:B:166:HIS:CE1	2.54	0.43
1:A:664:TRP:O	1:A:668:THR:HG22	2.19	0.42
2:B:311:LEU:HD12	2:B:336:LEU:HD13	2.00	0.42
1:A:940:LEU:HD11	1:A:952:LEU:HD12	2.02	0.42
2:B:292:PRO:HA	2:B:293:PRO:HD3	1.96	0.42
3:G:7:C:HO2'	3:G:8:C:H6	1.68	0.41
1:A:91:PRO:HD2	1:A:158:LEU:HD11	2.02	0.41
1:A:451:LEU:O	1:A:454:ILE:HG12	2.20	0.41
1:A:458:LEU:HD12	1:A:458:LEU:HA	1.94	0.41
1:A:1316:PHE:O	1:A:1320:ILE:HG12	2.20	0.41
1:A:377:HIS:NE2	1:A:555:LYS:HB2	2.35	0.41
1:A:739:VAL:HG22	1:A:744:GLN:HB3	2.01	0.41
2:D:134:VAL:HG22	2:E:139:VAL:HG21	2.02	0.41
2:D:141:LYS:NZ	2:E:143:ASP:HA	2.36	0.41
2:B:184:LYS:HE2	2:B:184:LYS:HB2	1.81	0.41
2:B:257:ASP:OD1	2:B:258:ILE:N	2.53	0.41
2:D:110:ARG:O	2:D:113:SER:OG	2.26	0.41
1:A:799:ILE:HG13	1:A:799:ILE:O	2.20	0.41
2:B:332:ASP:OD1	2:B:332:ASP:N	2.49	0.41
1:A:402:ILE:O	1:A:406:GLU:HG2	2.21	0.41
1:A:1163:PRO:HB3	1:A:1299:LEU:HA	2.02	0.41
1:A:61:LYS:HB3	1:A:61:LYS:HE2	1.79	0.40
1:A:1374:TYR:HB3	1:A:1380:ILE:CG2	2.50	0.40
1:A:419:TYR:CE1	1:A:427:TYR:HB3	2.56	0.40
1:A:53:LEU:HD22	1:A:59:VAL:HG21	2.03	0.40
2:C:141:LYS:HD3	2:D:142:TYR:CE2	2.56	0.40
1:A:478:LEU:HD11	1:A:1378:GLU:HG2	2.02	0.40
1:A:831:ASP:HB3	1:A:872:LEU:HD21	2.03	0.40
2:B:114:LEU:HA	2:C:114:LEU:HD12	2.03	0.40
1:A:405:PHE:CD1	2:B:144:LEU:HD13	2.56	0.40

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	1354/2212 (61%)	1261 (93%)	85 (6%)	8 (1%)	25 60
2	B	234/340 (69%)	220 (94%)	14 (6%)	0	100 100
2	C	70/340 (21%)	65 (93%)	5 (7%)	0	100 100
2	D	38/340 (11%)	37 (97%)	1 (3%)	0	100 100
2	E	40/340 (12%)	38 (95%)	2 (5%)	0	100 100
All	All	1736/3572 (49%)	1621 (93%)	107 (6%)	8 (0%)	32 64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	LEU
1	A	751	VAL
1	A	1174	VAL
1	A	851	THR
1	A	829	ILE
1	A	1281	MET
1	A	1090	ASP
1	A	1280	PHE

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	1210/1994 (61%)	1209 (100%)	1 (0%)	93 98
2	B	197/294 (67%)	197 (100%)	0	100 100
2	C	55/294 (19%)	55 (100%)	0	100 100
2	D	35/294 (12%)	34 (97%)	1 (3%)	42 73
2	E	37/294 (13%)	37 (100%)	0	100 100
All	All	1534/3170 (48%)	1532 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	ARG
2	D	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1269	HIS
2	B	279	GLN

5.3.3 RNA [\(i\)](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	9/18 (50%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	1	G
3	G	7	C
3	G	8	C

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.