



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:48 PM BST

PDB ID : 3J9D
EMDB ID: : EMD-6239
Title : Atomic structure of a non-enveloped virus reveals pH sensors for a coordinated process of cell entry
Authors : Zhang, X.; Patel, A.; Celma, C.; Roy, P.; Zhou, Z.H.
Deposited on : 2015-01-09
Resolution : 3.50 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 : unknown
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) : trunk27241

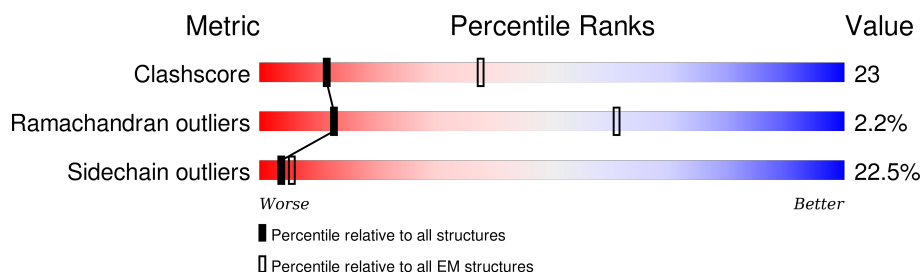
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	961	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6086 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 Outer capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	746	6085	3891	1057	1105	32	0	0

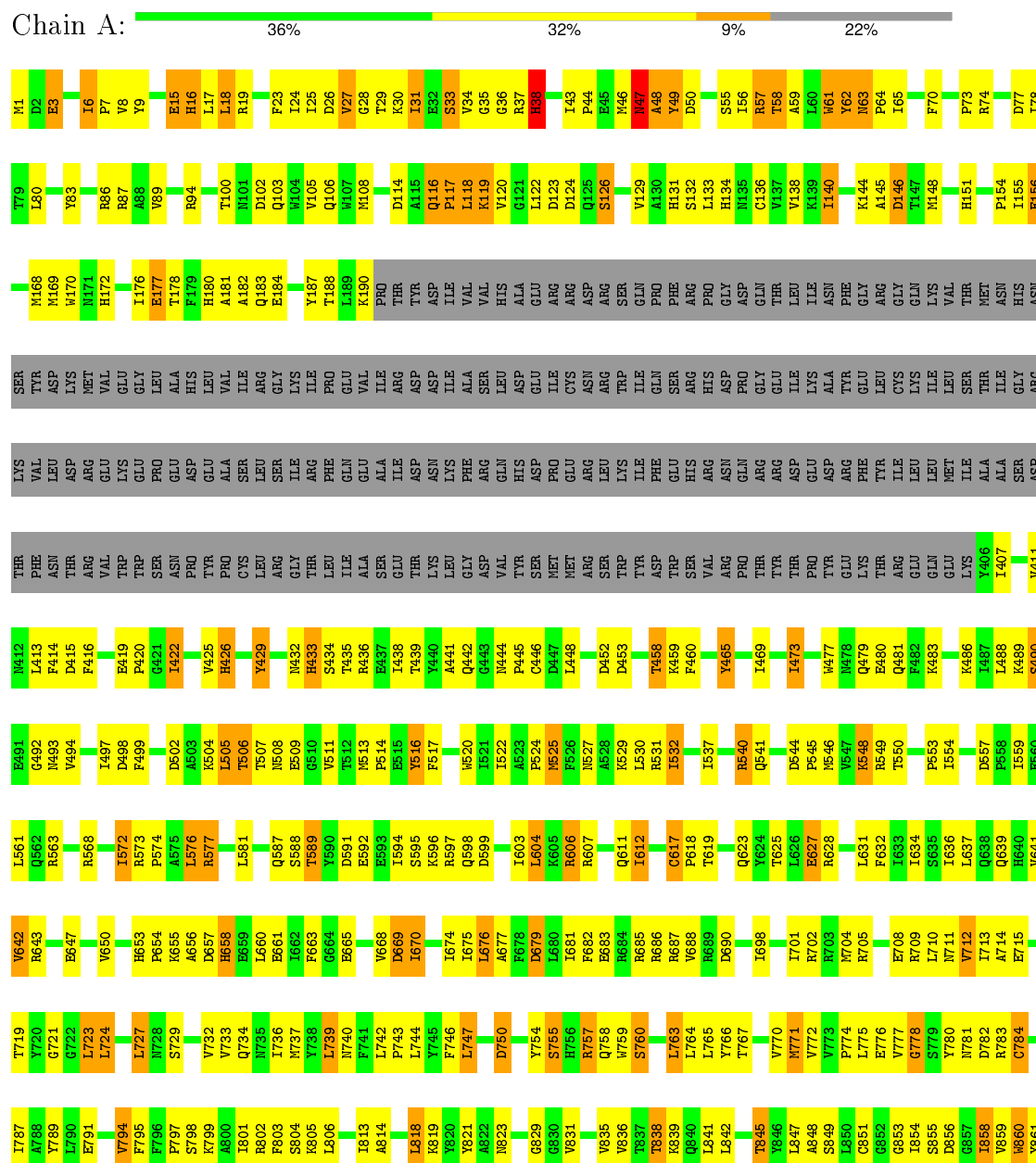
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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: Outer capsid protein VP2





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	5008	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	14000	Depositor
Image detector	GATAN K2 (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: 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.35	9/6221 (0.1%)	0.92	12/8420 (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
1	A	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	TYR	CD2-CE2	45.19	2.07	1.39
1	A	465	TYR	CD1-CE1	44.69	2.06	1.39
1	A	465	TYR	CE1-CZ	33.15	1.81	1.38
1	A	465	TYR	CE2-CZ	32.32	1.80	1.38
1	A	465	TYR	CG-CD2	24.61	1.71	1.39
1	A	465	TYR	CG-CD1	24.48	1.71	1.39
1	A	771	MET	SD-CE	21.19	2.96	1.77
1	A	156	GLU	CG-CD	8.55	1.64	1.51
1	A	156	GLU	CB-CG	8.30	1.68	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	MET	CG-SD-CE	18.30	129.48	100.20
1	A	723	LEU	CA-CB-CG	7.79	133.21	115.30
1	A	63	ASN	C-N-CD	-7.43	104.25	120.60
1	A	778	GLY	N-CA-C	-6.53	96.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	727	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	16	HIS	N-CA-C	-5.75	95.49	111.00
1	A	63	ASN	N-CA-C	5.69	126.36	111.00
1	A	47	ASN	C-N-CA	5.34	135.04	121.70
1	A	63	ASN	C-N-CA	5.34	144.42	122.00
1	A	862	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	922	ILE	CG1-CB-CG2	-5.14	100.09	111.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	VAL	Peptide
1	A	34	VAL	Peptide
1	A	38	HIS	Peptide
1	A	49	TYR	Peptide
1	A	55	SER	Peptide
1	A	62	TYR	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	6085	0	6087	282	0
2	A	1	0	0	0	0
All	All	6086	0	6087	282	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 23.

All (282) 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:465:TYR:CZ	1:A:465:TYR:CE2	1.80	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:CZ	1:A:465:TYR:CE1	1.81	1.60
1:A:465:TYR:CD1	1:A:465:TYR:CE1	2.06	1.43
1:A:465:TYR:CE2	1:A:465:TYR:CD2	2.07	1.39
1:A:465:TYR:CE2	1:A:771:MET:SD	2.35	1.19
1:A:465:TYR:CD2	1:A:771:MET:SD	2.36	1.18
1:A:465:TYR:CZ	1:A:771:MET:SD	2.39	1.16
1:A:465:TYR:CD1	1:A:771:MET:SD	2.39	1.15
1:A:465:TYR:CE1	1:A:771:MET:SD	2.41	1.14
1:A:465:TYR:CZ	1:A:771:MET:CE	2.33	1.12
1:A:465:TYR:CE1	1:A:771:MET:CE	2.32	1.12
1:A:465:TYR:CG	1:A:771:MET:SD	2.44	1.11
1:A:465:TYR:CE2	1:A:771:MET:CE	2.35	1.10
1:A:465:TYR:CD1	1:A:771:MET:CE	2.38	1.07
1:A:465:TYR:CD2	1:A:771:MET:CE	2.39	1.05
1:A:465:TYR:CG	1:A:771:MET:CE	2.46	0.98
1:A:559:ILE:HG12	1:A:628:ARG:HE	1.29	0.96
1:A:465:TYR:CZ	1:A:771:MET:HE3	2.00	0.94
1:A:607:ARG:HE	1:A:627:GLU:HG3	1.33	0.92
1:A:47:ASN:O	1:A:47:ASN:ND2	2.03	0.91
1:A:465:TYR:CD2	1:A:771:MET:HE1	2.06	0.90
1:A:465:TYR:CD1	1:A:771:MET:HE2	2.08	0.88
1:A:47:ASN:HB2	1:A:119:LYS:HG2	1.57	0.86
1:A:435:THR:HA	1:A:654:PRO:HD2	1.55	0.85
1:A:544:ASP:HB3	1:A:577:ARG:HG3	1.62	0.82
1:A:714:ALA:HB2	1:A:721:GLY:HA3	1.62	0.81
1:A:803:PHE:O	1:A:805:LYS:N	2.13	0.81
1:A:74:ARG:NE	1:A:114:ASP:OD2	2.16	0.78
1:A:516:TYR:HE1	1:A:532:ILE:HD11	1.49	0.78
1:A:1:MET:HG2	1:A:948:VAL:HG13	1.68	0.75
1:A:465:TYR:CE1	1:A:771:MET:HE2	2.23	0.73
1:A:177:GLU:HA	1:A:180:HIS:CE1	2.23	0.72
1:A:734:GLN:HA	1:A:737:MET:HE3	1.71	0.72
1:A:465:TYR:CE2	1:A:771:MET:HE3	2.26	0.70
1:A:661:GLU:HB3	1:A:686:ARG:HD3	1.73	0.70
1:A:47:ASN:HA	1:A:48:ALA:CB	2.23	0.69
1:A:483:LYS:HB2	1:A:486:LYS:HD3	1.75	0.68
1:A:772:VAL:HG21	1:A:813:ILE:HG21	1.75	0.68
1:A:73:PRO:HD2	1:A:114:ASP:HB3	1.77	0.67
1:A:611:GLN:HB3	1:A:612:ILE:HB	1.76	0.67
1:A:459:LYS:HB2	1:A:489:LYS:HD3	1.77	0.67
1:A:6:ILE:HG21	1:A:23:PHE:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:THR:OG1	1:A:507:THR:N	2.25	0.67
1:A:617:CYS:SG	1:A:619:THR:OG1	2.50	0.67
1:A:169:MET:HE1	1:A:623:GLN:HG3	1.78	0.66
1:A:458:THR:HG22	1:A:493:ASN:HA	1.76	0.66
1:A:465:TYR:OH	1:A:771:MET:HA	1.96	0.65
1:A:641:VAL:HG21	1:A:681:ILE:HG23	1.77	0.65
1:A:458:THR:CG2	1:A:493:ASN:HA	2.27	0.65
1:A:146:ASP:OD1	1:A:146:ASP:N	2.25	0.65
1:A:83:TYR:HB2	1:A:961:VAL:HG21	1.78	0.64
1:A:559:ILE:HD11	1:A:628:ARG:HH11	1.61	0.64
1:A:607:ARG:HE	1:A:627:GLU:CG	2.07	0.64
1:A:140:ILE:HG13	1:A:148:MET:HE1	1.78	0.64
1:A:47:ASN:HA	1:A:48:ALA:HB2	1.79	0.64
1:A:687:ARG:HB2	1:A:687:ARG:HH11	1.63	0.64
1:A:425:VAL:HG21	1:A:499:PHE:CE1	2.33	0.63
1:A:923:VAL:HG13	1:A:944:PHE:CE1	2.34	0.63
1:A:559:ILE:HG12	1:A:628:ARG:NE	2.08	0.63
1:A:420:PRO:HD3	1:A:540:ARG:HB3	1.81	0.62
1:A:184:GLU:N	1:A:184:GLU:OE1	2.23	0.62
1:A:702:ARG:HA	1:A:709:ARG:HH12	1.65	0.61
1:A:465:TYR:CE1	1:A:771:MET:HG3	2.36	0.61
1:A:493:ASN:O	1:A:497:ILE:HG23	2.01	0.61
1:A:557:ASP:HB3	1:A:597:ARG:CZ	2.31	0.61
1:A:563:ARG:O	1:A:791:GLU:HG3	2.01	0.60
1:A:631:LEU:HD13	1:A:658:HIS:H	1.65	0.60
1:A:465:TYR:CE1	1:A:771:MET:CG	2.85	0.60
1:A:599:ASP:OD2	1:A:628:ARG:NH2	2.34	0.60
1:A:732:VAL:HA	1:A:805:LYS:HA	1.84	0.60
1:A:446:CYS:HB3	1:A:795:PHE:CD1	2.37	0.59
1:A:859:VAL:HB	1:A:875:GLU:HG2	1.85	0.58
1:A:155:ILE:HG12	1:A:853:GLY:O	2.04	0.58
1:A:763:LEU:HD13	1:A:775:LEU:HD21	1.84	0.58
1:A:63:ASN:HA	1:A:835:VAL:HG22	1.86	0.58
1:A:687:ARG:HB2	1:A:687:ARG:NH1	2.19	0.58
1:A:634:ILE:HD11	1:A:676:LEU:HD13	1.86	0.57
1:A:176:ILE:HD13	1:A:670:ILE:HG13	1.86	0.57
1:A:419:GLU:HG3	1:A:420:PRO:HD2	1.85	0.57
1:A:448:LEU:HD11	1:A:767:THR:HG21	1.86	0.57
1:A:116:GLN:HG3	1:A:118:LEU:HD21	1.86	0.57
1:A:863:PRO:HG3	1:A:955:LEU:HD23	1.85	0.57
1:A:86:ARG:HG2	1:A:100:THR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:PHE:O	1:A:687:ARG:HA	2.05	0.56
1:A:64:PRO:HG3	1:A:838:THR:HG21	1.86	0.56
1:A:657:ASP:HB3	1:A:660:LEU:HB2	1.88	0.56
1:A:606:ARG:HB3	1:A:606:ARG:HH11	1.71	0.56
1:A:548:LYS:HG3	1:A:553:PRO:HB2	1.88	0.56
1:A:23:PHE:CD1	1:A:140:ILE:HG12	2.41	0.55
1:A:885:ILE:HG13	1:A:886:ARG:N	2.21	0.55
1:A:49:TYR:CD2	1:A:841:LEU:HD13	2.41	0.55
1:A:757:ARG:O	1:A:758:GLN:HB2	2.07	0.55
1:A:74:ARG:O	1:A:78:ILE:HG12	2.05	0.55
1:A:516:TYR:CE1	1:A:532:ILE:HD11	2.37	0.55
1:A:444:ASN:N	1:A:445:PRO:HD3	2.22	0.55
1:A:477:TRP:CH2	1:A:774:PRO:HB3	2.42	0.55
1:A:415:ASP:HA	1:A:541:GLN:HE21	1.72	0.54
1:A:3:GLU:HB3	1:A:943:LYS:HA	1.89	0.54
1:A:9:TYR:HE1	1:A:24:ILE:HG23	1.73	0.54
1:A:681:ILE:HG22	1:A:682:PHE:CD2	2.42	0.54
1:A:771:MET:SD	1:A:771:MET:CE	2.96	0.53
1:A:73:PRO:HB3	1:A:893:ARG:NH1	2.23	0.53
1:A:27:VAL:HG12	1:A:136:CYS:HB3	1.91	0.53
1:A:841:LEU:O	1:A:845:THR:HG23	2.09	0.53
1:A:172:HIS:HD1	1:A:750:ASP:HB3	1.73	0.53
1:A:798:SER:H	1:A:801:ILE:HD12	1.74	0.53
1:A:598:GLN:O	1:A:599:ASP:HB3	2.09	0.53
1:A:446:CYS:HB3	1:A:795:PHE:CE1	2.43	0.53
1:A:184:GLU:HG3	1:A:426:HIS:ND1	2.24	0.53
1:A:102:ASP:O	1:A:106:GLN:HG2	2.09	0.53
1:A:23:PHE:HD1	1:A:140:ILE:HG12	1.73	0.53
1:A:740:ASN:O	1:A:743:PRO:HD2	2.09	0.53
1:A:527:ASN:HB2	1:A:795:PHE:HZ	1.74	0.52
1:A:62:TYR:CE2	1:A:64:PRO:HB3	2.44	0.52
1:A:683:GLU:HB3	1:A:685:ARG:HG3	1.91	0.52
1:A:737:MET:HG3	1:A:766:TYR:OH	2.09	0.52
1:A:57:ARG:HD2	1:A:57:ARG:H	1.73	0.52
1:A:78:ILE:HD12	1:A:108:MET:CG	2.40	0.52
1:A:520:TRP:HA	1:A:531:ARG:HB3	1.91	0.52
1:A:465:TYR:CG	1:A:771:MET:HE1	2.35	0.52
1:A:938:ASP:N	1:A:938:ASP:OD1	2.42	0.52
1:A:460:PHE:CE2	1:A:525:MET:HG2	2.45	0.52
1:A:490:SER:O	1:A:492:GLY:HA2	2.10	0.51
1:A:750:ASP:OD1	1:A:750:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ILE:CG1	1:A:628:ARG:HE	2.12	0.51
1:A:425:VAL:HG21	1:A:499:PHE:HE1	1.74	0.51
1:A:524:PRO:HD2	1:A:525:MET:HE2	1.91	0.51
1:A:438:ILE:HG12	1:A:444:ASN:H	1.76	0.51
1:A:170:TRP:HZ3	1:A:847:LEU:HB2	1.75	0.50
1:A:639:GLN:HG3	1:A:653:HIS:NE2	2.27	0.50
1:A:23:PHE:CE2	1:A:860:TRP:HZ3	2.29	0.50
1:A:864:ILE:HB	1:A:870:CYS:O	2.11	0.50
1:A:133:LEU:HD23	1:A:134:HIS:N	2.27	0.49
1:A:606:ARG:HD3	1:A:627:GLU:OE1	2.12	0.49
1:A:607:ARG:NE	1:A:627:GLU:HG3	2.14	0.49
1:A:23:PHE:CE1	1:A:138:VAL:HG13	2.47	0.49
1:A:755:SER:HA	1:A:829:GLY:HA3	1.94	0.49
1:A:861:TYR:HB3	1:A:871:ILE:HG23	1.93	0.49
1:A:655:LYS:HG2	1:A:656:ALA:O	2.12	0.49
1:A:544:ASP:OD2	1:A:589:THR:HG23	2.13	0.49
1:A:187:TYR:HB2	1:A:425:VAL:CG2	2.42	0.49
1:A:438:ILE:HG12	1:A:444:ASN:N	2.27	0.49
1:A:907:ILE:HD12	1:A:907:ILE:H	1.78	0.49
1:A:78:ILE:HD12	1:A:108:MET:HG3	1.94	0.49
1:A:746:PHE:N	1:A:746:PHE:CD1	2.80	0.49
1:A:747:LEU:HD21	1:A:777:VAL:HG11	1.95	0.48
1:A:62:TYR:CG	1:A:63:ASN:N	2.80	0.48
1:A:941:LEU:HD13	1:A:941:LEU:HA	1.61	0.48
1:A:572:ILE:HG12	1:A:783:ARG:HH12	1.79	0.48
1:A:923:VAL:HG12	1:A:924:SER:N	2.28	0.48
1:A:676:LEU:HG	1:A:688:VAL:HG22	1.96	0.48
1:A:441:ALA:N	1:A:647:GLU:HB3	2.29	0.48
1:A:433:HIS:CE1	1:A:436:ARG:HD3	2.49	0.48
1:A:411:VAL:HG21	1:A:416:PHE:CD1	2.49	0.48
1:A:777:VAL:O	1:A:777:VAL:HG23	2.14	0.48
1:A:133:LEU:HD23	1:A:134:HIS:H	1.78	0.48
1:A:120:VAL:HG12	1:A:131:HIS:CE1	2.49	0.48
1:A:182:ALA:HB1	1:A:554:ILE:HD11	1.96	0.48
1:A:568:ARG:HD3	1:A:780:TYR:HB3	1.96	0.47
1:A:522:ILE:HG12	1:A:529:LYS:HG3	1.95	0.47
1:A:70:PHE:N	1:A:70:PHE:CD1	2.82	0.47
1:A:711:ASN:O	1:A:715:GLU:HB2	2.14	0.47
1:A:544:ASP:CG	1:A:544:ASP:O	2.53	0.47
1:A:596:LYS:HE3	1:A:596:LYS:HB2	1.42	0.47
1:A:78:ILE:HG23	1:A:108:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PRO:HG2	1:A:24:ILE:HG12	1.96	0.47
1:A:480:GLU:OE2	1:A:759:TRP:NE1	2.48	0.47
1:A:754:TYR:CE2	1:A:784:CYS:HB2	2.50	0.47
1:A:477:TRP:HH2	1:A:774:PRO:HB3	1.80	0.47
1:A:74:ARG:NH1	1:A:78:ILE:HD11	2.30	0.46
1:A:604:LEU:HA	1:A:604:LEU:HD12	1.63	0.46
1:A:25:ILE:HG21	1:A:909:ILE:HD11	1.97	0.46
1:A:181:ALA:HB3	1:A:545:PRO:HB2	1.98	0.46
1:A:743:PRO:HG3	1:A:821:TYR:OH	2.15	0.46
1:A:123:ASP:OD1	1:A:124:ASP:N	2.48	0.46
1:A:498:ASP:O	1:A:502:ASP:HB2	2.16	0.46
1:A:172:HIS:NE2	1:A:669:ASP:HA	2.30	0.46
1:A:916:THR:O	1:A:916:THR:OG1	2.31	0.46
1:A:19:ARG:HD3	1:A:126:SER:HB2	1.98	0.46
1:A:757:ARG:HG2	1:A:782:ASP:OD2	2.16	0.46
1:A:444:ASN:ND2	1:A:794:VAL:O	2.50	0.45
1:A:587:GLN:NE2	1:A:591:ASP:OD2	2.49	0.45
1:A:414:PHE:HB2	1:A:573:ARG:HH11	1.81	0.45
1:A:58:THR:HG22	1:A:61:TRP:NE1	2.32	0.45
1:A:416:PHE:HB3	1:A:549:ARG:NH2	2.31	0.45
1:A:708:GLU:H	1:A:708:GLU:HG3	1.52	0.45
1:A:677:ALA:O	1:A:681:ILE:HB	2.15	0.45
1:A:776:GLU:HG2	1:A:778:GLY:HA2	1.98	0.45
1:A:587:GLN:NE2	1:A:618:PRO:HD3	2.32	0.45
1:A:429:TYR:C	1:A:429:TYR:CD1	2.90	0.45
1:A:714:ALA:HB2	1:A:721:GLY:CA	2.41	0.45
1:A:905:VAL:CG2	1:A:923:VAL:HG11	2.47	0.45
1:A:514:PRO:O	1:A:516:TYR:N	2.47	0.45
1:A:422:ILE:HG13	1:A:422:ILE:O	2.17	0.44
1:A:434:SER:HB2	1:A:563:ARG:HH12	1.82	0.44
1:A:62:TYR:CD1	1:A:63:ASN:N	2.78	0.44
1:A:465:TYR:CZ	1:A:771:MET:CG	3.00	0.44
1:A:755:SER:HA	1:A:829:GLY:CA	2.47	0.44
1:A:181:ALA:HB1	1:A:546:MET:HB3	1.99	0.44
1:A:742:LEU:HD23	1:A:742:LEU:HA	1.65	0.44
1:A:35:GLY:HA2	1:A:36:GLY:HA2	1.66	0.44
1:A:33:SER:HB2	1:A:38:HIS:HB3	2.00	0.44
1:A:151:HIS:O	1:A:151:HIS:CG	2.70	0.44
1:A:956:THR:O	1:A:960:ASN:HB2	2.17	0.44
1:A:44:PRO:HD3	1:A:581:LEU:CD1	2.48	0.44
1:A:43:ILE:HA	1:A:46:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:HIS:HB3	1:A:654:PRO:HD3	2.00	0.44
1:A:606:ARG:NH2	1:A:660:LEU:O	2.50	0.44
1:A:923:VAL:HG12	1:A:924:SER:H	1.83	0.44
1:A:959:LEU:C	1:A:961:VAL:H	2.21	0.44
1:A:26:ASP:C	1:A:28:GLY:HA3	2.38	0.44
1:A:488:LEU:HB2	1:A:493:ASN:HD22	1.83	0.43
1:A:701:ILE:HD13	1:A:713:ILE:HG12	2.00	0.43
1:A:607:ARG:NH1	1:A:623:GLN:HG2	2.33	0.43
1:A:862:LEU:HA	1:A:863:PRO:HD3	1.90	0.43
1:A:757:ARG:HG3	1:A:757:ARG:H	1.47	0.43
1:A:9:TYR:N	1:A:9:TYR:CD1	2.86	0.43
1:A:59:ALA:O	1:A:62:TYR:HB3	2.18	0.43
1:A:9:TYR:OH	1:A:26:ASP:HB2	2.19	0.43
1:A:435:THR:OG1	1:A:435:THR:O	2.31	0.43
1:A:140:ILE:HG21	1:A:145:ALA:HA	2.01	0.43
1:A:502:ASP:HB3	1:A:514:PRO:HG3	2.00	0.43
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.71	0.43
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.56	0.43
1:A:854:ILE:HG12	1:A:855:SER:N	2.34	0.43
1:A:799:LYS:HG2	1:A:803:PHE:CE1	2.53	0.43
1:A:505:LEU:HB2	1:A:506:THR:HA	1.99	0.43
1:A:527:ASN:HB2	1:A:795:PHE:CZ	2.53	0.43
1:A:508:ASN:HA	1:A:509:GLU:HA	1.74	0.43
1:A:432:ASN:HB3	1:A:527:ASN:OD1	2.19	0.43
1:A:890:ILE:HA	1:A:890:ILE:HD13	1.66	0.43
1:A:559:ILE:HG13	1:A:559:ILE:H	1.67	0.42
1:A:642:VAL:HG13	1:A:734:GLN:OE1	2.19	0.42
1:A:637:LEU:HA	1:A:637:LEU:HD23	1.70	0.42
1:A:607:ARG:HD3	1:A:607:ARG:HA	1.42	0.42
1:A:155:ILE:HG22	1:A:156:GLU:O	2.19	0.42
1:A:705:ARG:HD3	1:A:705:ARG:HA	1.87	0.42
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.92	0.42
1:A:479:GLN:HG3	1:A:480:GLU:N	2.35	0.42
1:A:574:PRO:HB2	1:A:576:LEU:HD22	2.01	0.42
1:A:74:ARG:HH12	1:A:78:ILE:HD11	1.85	0.42
1:A:144:LYS:HA	1:A:144:LYS:HD2	1.68	0.42
1:A:473:ILE:HG13	1:A:813:ILE:HD12	2.00	0.42
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.59	0.42
1:A:419:GLU:O	1:A:422:ILE:HG23	2.20	0.42
1:A:592:GLU:O	1:A:595:SER:HB3	2.20	0.42
1:A:116:GLN:HA	1:A:117:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ASP:O	1:A:683:GLU:HB2	2.20	0.41
1:A:917:VAL:HG12	1:A:918:TYR:N	2.35	0.41
1:A:138:VAL:HB	1:A:858:ILE:HD11	2.01	0.41
1:A:665:GLU:HG3	1:A:690:ASP:OD1	2.20	0.41
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.69	0.41
1:A:736:ILE:HG12	1:A:814:ALA:CB	2.51	0.41
1:A:739:LEU:HD11	1:A:818:LEU:HB2	2.01	0.41
1:A:737:MET:HB2	1:A:737:MET:HE2	1.82	0.41
1:A:949:PHE:O	1:A:949:PHE:CD1	2.74	0.41
1:A:187:TYR:HB2	1:A:425:VAL:HG22	2.02	0.41
1:A:758:GLN:HA	1:A:776:GLU:CD	2.41	0.41
1:A:910:ASP:HB2	1:A:914:GLU:O	2.21	0.41
1:A:661:GLU:HB3	1:A:686:ARG:CD	2.47	0.41
1:A:674:ILE:HG12	1:A:744:LEU:HD22	2.02	0.41
1:A:78:ILE:HD12	1:A:108:MET:HG2	2.03	0.41
1:A:70:PHE:CE2	1:A:117:PRO:HB3	2.56	0.41
1:A:760:SER:HB2	1:A:774:PRO:HB2	2.03	0.41
1:A:747:LEU:HA	1:A:747:LEU:HD22	1.85	0.41
1:A:881:VAL:HG23	1:A:882:PRO:HD2	2.02	0.41
1:A:154:PRO:HB3	1:A:848:ALA:CA	2.51	0.41
1:A:154:PRO:HB3	1:A:848:ALA:HA	2.02	0.41
1:A:574:PRO:HB2	1:A:576:LEU:CD2	2.51	0.40
1:A:952:ASP:OD1	1:A:952:ASP:N	2.52	0.40
1:A:802:ARG:HG2	1:A:802:ARG:O	2.19	0.40
1:A:31:ILE:HA	1:A:31:ILE:HD12	1.60	0.40
1:A:169:MET:CE	1:A:623:GLN:HG3	2.50	0.40
1:A:701:ILE:HG12	1:A:712:VAL:HG23	2.03	0.40
1:A:872:VAL:HG13	1:A:903:GLY:O	2.21	0.40
1:A:6:ILE:HG22	1:A:23:PHE:HB3	2.04	0.40
1:A:860:TRP:CD1	1:A:860:TRP:C	2.94	0.40
1:A:766:TYR:CD1	1:A:797:PRO:HG3	2.57	0.40
1:A:6:ILE:H	1:A:6:ILE:HG12	1.80	0.40
1:A:632:PHE:CZ	1:A:636:ILE:HD11	2.57	0.40
1:A:176:ILE:HD13	1:A:670:ILE:CG1	2.51	0.40
1:A:517:PHE:O	1:A:517:PHE:CG	2.75	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	742/961 (77%)	665 (90%)	61 (8%)	16 (2%)	<div><div>8</div><div>49</div></div>

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	804	SER
1	A	15	GLU
1	A	540	ARG
1	A	897	SER
1	A	516	TYR
1	A	729	SER
1	A	668	VAL
1	A	960	ASN
1	A	117	PRO
1	A	442	GLN
1	A	781	ASN
1	A	806	LEU
1	A	129	VAL
1	A	511	VAL
1	A	770	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	666/863 (77%)	516 (78%)	150 (22%)	1 6

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	ILE
1	A	8	VAL
1	A	15	GLU
1	A	16	HIS
1	A	17	LEU
1	A	18	LEU
1	A	29	THR
1	A	30	LYS
1	A	31	ILE
1	A	33	SER
1	A	37	ARG
1	A	38	HIS
1	A	47	ASN
1	A	50	ASP
1	A	56	ILE
1	A	57	ARG
1	A	58	THR
1	A	61	TRP
1	A	65	ILE
1	A	77	ASP
1	A	87	ARG
1	A	89	VAL
1	A	94	ARG
1	A	103	GLN
1	A	105	VAL
1	A	116	GLN
1	A	118	LEU
1	A	119	LYS
1	A	122	LEU
1	A	126	SER
1	A	132	SER
1	A	140	ILE
1	A	146	ASP
1	A	168	MET

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Mol	Chain	Res	Type
1	A	177	GLU
1	A	178	THR
1	A	183	GLN
1	A	188	THR
1	A	190	LYS
1	A	407	ILE
1	A	413	LEU
1	A	422	ILE
1	A	426	HIS
1	A	429	TYR
1	A	433	HIS
1	A	439	THR
1	A	452	ASP
1	A	453	ASP
1	A	458	THR
1	A	469	ILE
1	A	473	ILE
1	A	481	GLN
1	A	490	SER
1	A	494	VAL
1	A	504	LYS
1	A	505	LEU
1	A	506	THR
1	A	513	MET
1	A	525	MET
1	A	530	LEU
1	A	532	ILE
1	A	537	ILE
1	A	548	LYS
1	A	550	THR
1	A	561	LEU
1	A	572	ILE
1	A	576	LEU
1	A	577	ARG
1	A	588	SER
1	A	589	THR
1	A	594	ILE
1	A	603	ILE
1	A	604	LEU
1	A	606	ARG
1	A	612	ILE
1	A	617	CYS

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Mol	Chain	Res	Type
1	A	625	THR
1	A	627	GLU
1	A	642	VAL
1	A	643	ARG
1	A	650	VAL
1	A	658	HIS
1	A	669	ASP
1	A	670	ILE
1	A	675	ILE
1	A	676	LEU
1	A	679	ASP
1	A	698	ILE
1	A	704	MET
1	A	710	LEU
1	A	712	VAL
1	A	719	THR
1	A	723	LEU
1	A	724	LEU
1	A	727	LEU
1	A	733	VAL
1	A	739	LEU
1	A	747	LEU
1	A	750	ASP
1	A	755	SER
1	A	757	ARG
1	A	760	SER
1	A	763	LEU
1	A	764	LEU
1	A	765	LEU
1	A	784	CYS
1	A	787	ILE
1	A	789	TYR
1	A	794	VAL
1	A	818	LEU
1	A	819	LYS
1	A	823	ASN
1	A	831	VAL
1	A	836	VAL
1	A	838	THR
1	A	839	LYS
1	A	842	LEU
1	A	845	THR

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Mol	Chain	Res	Type
1	A	849	SER
1	A	851	CYS
1	A	856	ASP
1	A	858	ILE
1	A	860	TRP
1	A	862	LEU
1	A	865	THR
1	A	875	GLU
1	A	880	ARG
1	A	881	VAL
1	A	885	ILE
1	A	886	ARG
1	A	889	ARG
1	A	896	LEU
1	A	899	ARG
1	A	914	GLU
1	A	916	THR
1	A	917	VAL
1	A	923	VAL
1	A	926	ARG
1	A	929	LYS
1	A	932	LEU
1	A	934	LYS
1	A	938	ASP
1	A	941	LEU
1	A	945	SER
1	A	955	LEU
1	A	956	THR
1	A	957	LYS
1	A	959	LEU
1	A	961	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	180	HIS
1	A	587	GLN

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](#)

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.