



wwPDB EM Map/Model Validation Report ⓘ

Apr 26, 2016 – 06:29 PM BST

PDB ID : 1DYL
EMDB ID: : EMD-1015
Title : 9 ANGSTROM RESOLUTION CRYO-EM RECONSTRUCTION STRUCTURE OF SEMLIKI FOREST VIRUS (SFV) AND FITTING OF THE CAPSID PROTEIN STRUCTURE IN THE EM DENSITY
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Deposited on : 2000-02-02
Resolution : 9.00 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) : trunk27461

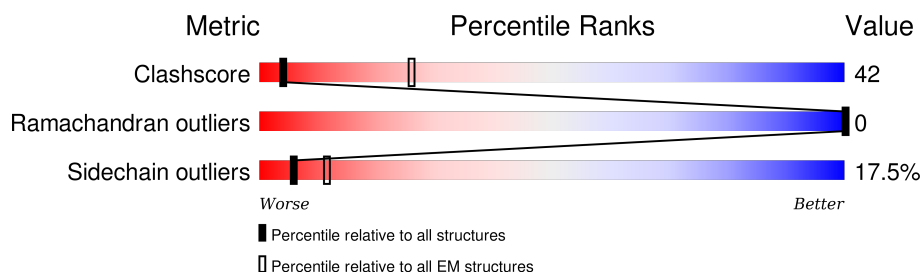
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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	149	63% 30% 7%
1	B	149	50% 43% 7%
1	C	149	58% 36% 7%
1	D	149	54% 38% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4563 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.

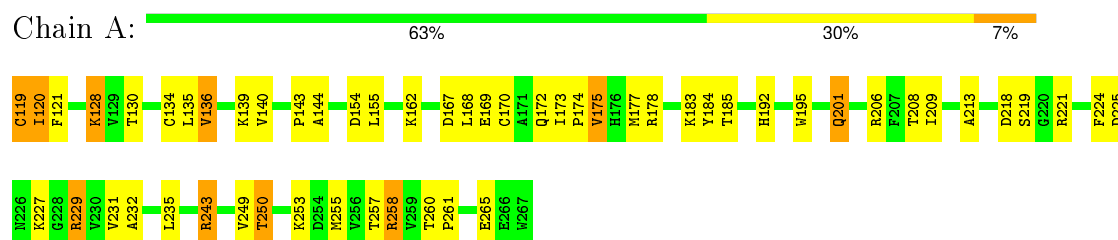
- Molecule 1 is a protein called NUCLEOCAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	149	Total	C	N	O	S	0	0
			1141	718	205	212	6		
1	B	149	Total	C	N	O	S	0	0
			1141	718	205	212	6		
1	C	149	Total	C	N	O	S	0	0
			1141	718	205	212	6		
1	D	149	Total	C	N	O	S	0	0
			1140	717	205	212	6		

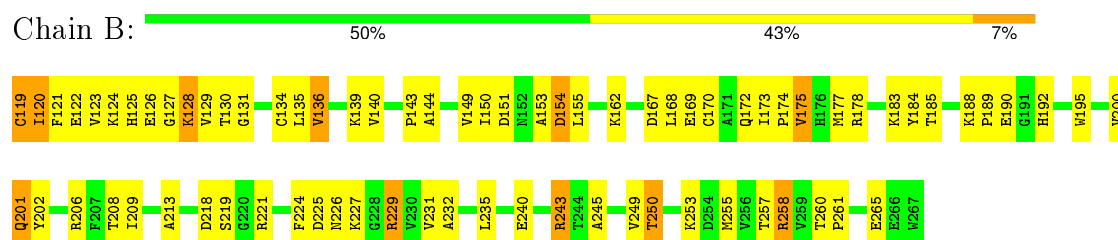
3 Residue-property plots [i](#)

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.

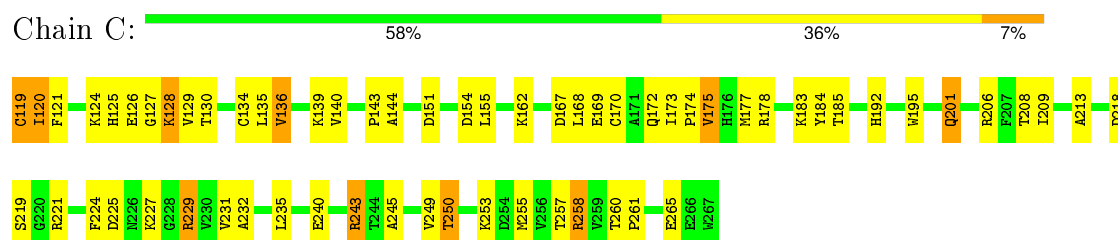
• Molecule 1: NUCLEOCAPSID PROTEIN



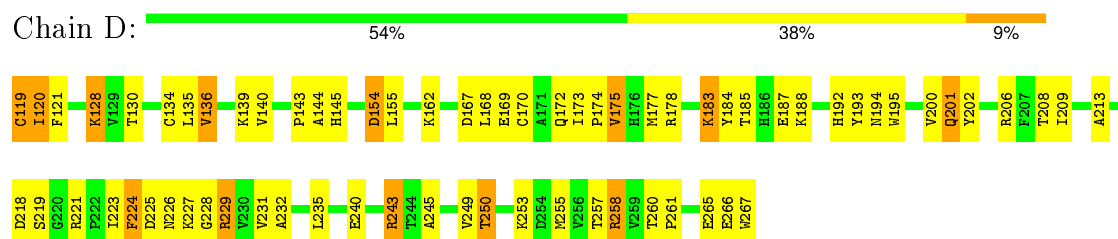
• Molecule 1: NUCLEOCAPSID PROTEIN



• Molecule 1: NUCLEOCAPSID PROTEIN



• Molecule 1: NUCLEOCAPSID PROTEIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI-CM200 FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1000	Depositor
Minimum defocus (nm)	975	Depositor
Maximum defocus (nm)	7600	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.63	0/1169	0.88	0/1579
1	B	0.64	0/1169	0.88	0/1579
1	C	0.64	0/1169	0.88	0/1579
1	D	0.63	0/1167	0.88	0/1576
All	All	0.63	0/4674	0.88	0/6313

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	1141	0	1119	33	0
1	B	1141	0	1110	276	0
1	C	1141	0	1117	112	0
1	D	1140	0	1111	199	0
All	All	4563	0	4457	380	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 42.

All (380) 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:128:LYS:CE	1:D:200:VAL:HB	1.12	1.56
1:B:190:GLU:HB2	1:C:125:HIS:CD2	1.42	1.51
1:B:128:LYS:CG	1:D:192:HIS:C	1.80	1.49
1:B:128:LYS:HE2	1:D:200:VAL:CB	1.00	1.45
1:B:128:LYS:NZ	1:D:193:TYR:C	1.70	1.45
1:B:192:HIS:HA	1:C:128:LYS:NZ	1.21	1.44
1:B:202:TYR:CE2	1:C:126:GLU:HB3	1.55	1.40
1:B:128:LYS:CD	1:D:193:TYR:HB2	1.17	1.40
1:B:189:PRO:HB2	1:C:125:HIS:CA	1.45	1.39
1:B:188:LYS:C	1:C:126:GLU:HA	1.18	1.31
1:B:126:GLU:C	1:D:231:VAL:CG1	1.87	1.29
1:B:128:LYS:HD2	1:D:193:TYR:CB	1.35	1.27
1:B:127:GLY:O	1:D:224:PHE:O	1.53	1.26
1:B:128:LYS:CD	1:D:193:TYR:CB	1.92	1.25
1:B:188:LYS:O	1:C:126:GLU:HA	1.32	1.24
1:B:128:LYS:CB	1:D:192:HIS:C	1.95	1.23
1:B:126:GLU:O	1:D:231:VAL:HG11	1.07	1.22
1:B:189:PRO:CB	1:C:125:HIS:HA	1.70	1.22
1:B:192:HIS:H	1:C:129:VAL:N	1.25	1.21
1:B:126:GLU:C	1:D:231:VAL:HG11	1.16	1.20
1:B:190:GLU:HB2	1:C:125:HIS:CG	1.79	1.16
1:B:192:HIS:N	1:C:129:VAL:H	1.44	1.15
1:B:188:LYS:C	1:C:126:GLU:CA	2.15	1.15
1:B:128:LYS:HB3	1:D:192:HIS:O	1.41	1.14
1:B:128:LYS:HB3	1:D:192:HIS:C	1.55	1.14
1:B:123:VAL:CA	1:D:227:LYS:HG3	1.78	1.14
1:B:190:GLU:CB	1:C:125:HIS:CD2	2.30	1.13
1:B:124:LYS:HA	1:D:226:ASN:N	1.58	1.12
1:B:124:LYS:CA	1:D:226:ASN:N	2.04	1.11
1:B:188:LYS:O	1:C:126:GLU:HG2	1.46	1.11
1:B:226:ASN:HB2	1:C:124:LYS:HZ2	1.06	1.10
1:B:226:ASN:H	1:C:124:LYS:NZ	1.49	1.10
1:B:124:LYS:CA	1:D:226:ASN:H	1.64	1.10
1:B:123:VAL:HA	1:D:227:LYS:CG	1.80	1.09
1:B:123:VAL:O	1:D:226:ASN:HB2	1.50	1.09
1:B:192:HIS:CA	1:C:128:LYS:NZ	2.15	1.08
1:B:124:LYS:NZ	1:D:228:GLY:HA2	1.68	1.08
1:B:128:LYS:HG2	1:D:192:HIS:HA	1.35	1.08
1:B:153:ALA:HB2	1:D:183:LYS:HE3	1.11	1.08
1:B:200:VAL:O	1:C:128:LYS:NZ	1.88	1.07
1:B:124:LYS:HA	1:D:226:ASN:H	0.91	1.06
1:B:128:LYS:HG2	1:D:192:HIS:CA	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:HIS:CG	1:D:193:TYR:OH	2.10	1.04
1:B:126:GLU:O	1:D:231:VAL:CG1	1.97	1.04
1:B:153:ALA:HB2	1:D:183:LYS:CE	1.86	1.04
1:B:128:LYS:CE	1:D:200:VAL:CA	2.34	1.04
1:B:226:ASN:HB2	1:C:124:LYS:NZ	1.72	1.03
1:B:188:LYS:O	1:C:126:GLU:CA	2.04	1.03
1:B:128:LYS:CD	1:D:193:TYR:N	2.19	1.03
1:B:128:LYS:HE3	1:D:200:VAL:CA	1.89	1.03
1:B:128:LYS:HG2	1:D:193:TYR:N	1.40	1.01
1:B:128:LYS:HE3	1:D:200:VAL:N	1.73	1.01
1:B:128:LYS:CD	1:D:193:TYR:H	1.73	1.00
1:B:125:HIS:N	1:D:225:ASP:CB	2.19	1.00
1:B:128:LYS:CE	1:D:200:VAL:CB	1.91	1.00
1:B:126:GLU:CA	1:D:231:VAL:CG1	2.42	0.98
1:B:192:HIS:CG	1:C:128:LYS:HZ2	1.81	0.97
1:B:188:LYS:O	1:C:126:GLU:CG	2.13	0.97
1:B:126:GLU:CA	1:D:231:VAL:HG11	1.95	0.96
1:B:190:GLU:O	1:C:125:HIS:CA	2.04	0.96
1:B:123:VAL:HG13	1:D:227:LYS:HE3	1.44	0.96
1:B:128:LYS:CG	1:D:193:TYR:N	0.82	0.96
1:D:267:TRP:CZ2	1:D:267:TRP:CZ3	2.39	0.95
1:B:202:TYR:CE2	1:C:126:GLU:CB	2.48	0.94
1:B:128:LYS:NZ	1:D:193:TYR:O	1.94	0.94
1:B:128:LYS:HE3	1:D:200:VAL:H	1.32	0.94
1:B:128:LYS:HE2	1:D:200:VAL:CA	1.98	0.93
1:B:128:LYS:CD	1:D:200:VAL:O	2.16	0.93
1:B:127:GLY:HA2	1:D:224:PHE:HA	1.50	0.93
1:B:128:LYS:CE	1:D:193:TYR:HB2	2.00	0.92
1:B:127:GLY:O	1:D:193:TYR:HB3	1.64	0.92
1:B:189:PRO:CB	1:C:125:HIS:CA	2.31	0.91
1:B:127:GLY:C	1:D:224:PHE:O	2.08	0.91
1:B:192:HIS:HA	1:C:128:LYS:HZ2	1.15	0.91
1:B:226:ASN:H	1:C:124:LYS:HZ3	1.12	0.91
1:B:149:VAL:O	1:D:227:LYS:HB2	1.72	0.89
1:B:151:ASP:HA	1:D:229:ARG:HD2	1.55	0.89
1:B:202:TYR:HE2	1:C:126:GLU:CB	1.85	0.89
1:B:124:LYS:HZ1	1:D:228:GLY:HA2	1.32	0.89
1:B:124:LYS:N	1:D:227:LYS:H	1.72	0.88
1:B:202:TYR:CD2	1:C:126:GLU:HB3	2.08	0.87
1:B:192:HIS:N	1:C:129:VAL:N	1.95	0.86
1:B:192:HIS:CA	1:C:128:LYS:HZ2	1.80	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:TYR:HE2	1:C:126:GLU:HB3	1.09	0.86
1:B:124:LYS:H	1:D:227:LYS:H	1.22	0.86
1:B:128:LYS:HG3	1:D:192:HIS:C	1.68	0.86
1:B:190:GLU:O	1:C:128:LYS:O	1.92	0.85
1:B:128:LYS:HZ1	1:D:193:TYR:C	1.67	0.85
1:B:124:LYS:HD3	1:D:224:PHE:HB2	1.58	0.85
1:B:226:ASN:N	1:C:124:LYS:NZ	2.24	0.85
1:B:153:ALA:CB	1:D:183:LYS:HE3	2.04	0.85
1:B:190:GLU:O	1:C:125:HIS:N	2.08	0.85
1:B:190:GLU:O	1:C:125:HIS:HB3	1.76	0.85
1:B:128:LYS:HE2	1:D:200:VAL:CG2	2.06	0.85
1:B:128:LYS:CG	1:D:193:TYR:H	0.82	0.84
1:B:123:VAL:C	1:D:226:ASN:HB2	1.97	0.83
1:B:190:GLU:O	1:C:125:HIS:CB	2.25	0.83
1:B:188:LYS:O	1:C:126:GLU:CB	2.26	0.83
1:B:192:HIS:C	1:C:127:GLY:O	2.17	0.82
1:B:226:ASN:CB	1:C:124:LYS:NZ	2.41	0.82
1:B:124:LYS:N	1:D:227:LYS:N	2.28	0.82
1:B:128:LYS:HD3	1:D:200:VAL:O	1.80	0.81
1:B:227:LYS:HE3	1:C:151:ASP:CG	2.00	0.81
1:B:128:LYS:NZ	1:D:194:ASN:N	2.28	0.81
1:B:128:LYS:CD	1:D:193:TYR:CA	2.38	0.80
1:B:129:VAL:HA	1:D:226:ASN:N	1.96	0.80
1:B:123:VAL:N	1:D:226:ASN:HB3	1.94	0.80
1:B:127:GLY:HA2	1:D:224:PHE:CA	2.12	0.80
1:B:128:LYS:CD	1:D:200:VAL:HB	2.10	0.79
1:B:192:HIS:CA	1:C:128:LYS:HZ3	1.87	0.79
1:B:128:LYS:NZ	1:D:193:TYR:CA	2.45	0.79
1:B:124:LYS:HD2	1:D:228:GLY:N	1.97	0.78
1:B:189:PRO:HB2	1:C:125:HIS:HA	0.79	0.77
1:B:128:LYS:CE	1:D:200:VAL:O	2.32	0.77
1:B:192:HIS:HA	1:C:128:LYS:HZ3	0.95	0.77
1:B:124:LYS:H	1:D:227:LYS:N	1.81	0.76
1:B:127:GLY:C	1:D:224:PHE:C	2.45	0.76
1:B:126:GLU:C	1:D:193:TYR:CE1	2.59	0.75
1:B:124:LYS:N	1:D:226:ASN:N	2.33	0.75
1:B:128:LYS:HE3	1:D:200:VAL:O	1.87	0.74
1:B:124:LYS:NZ	1:D:228:GLY:CA	2.50	0.73
1:B:126:GLU:HA	1:D:231:VAL:CG1	2.18	0.73
1:B:190:GLU:CB	1:C:125:HIS:CG	2.66	0.73
1:B:125:HIS:N	1:D:225:ASP:HB3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LYS:HZ2	1:D:227:LYS:HB2	1.51	0.72
1:C:232:ALA:HB2	1:C:250:THR:HG23	1.71	0.72
1:B:124:LYS:HZ2	1:D:228:GLY:HA2	1.50	0.72
1:B:128:LYS:HE3	1:D:200:VAL:C	2.09	0.72
1:B:232:ALA:HB2	1:B:250:THR:HG23	1.71	0.71
1:A:232:ALA:HB2	1:A:250:THR:HG23	1.71	0.71
1:B:127:GLY:O	1:D:224:PHE:C	2.27	0.71
1:B:124:LYS:CD	1:D:224:PHE:HB2	2.19	0.71
1:B:128:LYS:CE	1:D:200:VAL:N	2.50	0.71
1:D:232:ALA:HB2	1:D:250:THR:HG23	1.71	0.70
1:B:123:VAL:H	1:D:226:ASN:HB3	1.56	0.69
1:B:124:LYS:CE	1:D:224:PHE:HB2	2.22	0.69
1:B:190:GLU:CG	1:C:125:HIS:CD2	2.75	0.69
1:B:226:ASN:N	1:C:124:LYS:HZ1	1.87	0.69
1:B:190:GLU:HB2	1:C:125:HIS:HD2	1.47	0.69
1:B:128:LYS:HG2	1:D:192:HIS:C	1.73	0.69
1:B:226:ASN:H	1:C:124:LYS:HZ1	1.36	0.69
1:B:190:GLU:CA	1:C:126:GLU:HB2	2.14	0.68
1:B:126:GLU:HB2	1:D:193:TYR:CZ	2.28	0.68
1:B:192:HIS:H	1:C:129:VAL:H	0.69	0.68
1:B:128:LYS:CE	1:D:200:VAL:C	2.62	0.68
1:D:253:LYS:O	1:D:255:MET:SD	2.53	0.68
1:B:189:PRO:HA	1:C:126:GLU:HG3	1.75	0.67
1:B:128:LYS:CB	1:D:192:HIS:O	2.17	0.67
1:C:253:LYS:O	1:C:255:MET:SD	2.52	0.67
1:B:253:LYS:O	1:B:255:MET:SD	2.52	0.66
1:B:123:VAL:C	1:D:226:ASN:CB	2.64	0.66
1:A:253:LYS:O	1:A:255:MET:SD	2.52	0.66
1:B:123:VAL:N	1:D:226:ASN:CB	2.58	0.66
1:B:189:PRO:HB2	1:C:125:HIS:N	2.10	0.66
1:B:128:LYS:HG2	1:D:193:TYR:H	1.17	0.66
1:B:192:HIS:CB	1:C:128:LYS:HZ2	2.08	0.66
1:B:200:VAL:O	1:C:128:LYS:CE	2.44	0.66
1:B:128:LYS:NZ	1:D:193:TYR:CB	2.58	0.65
1:B:131:GLY:O	1:D:226:ASN:HB3	1.95	0.65
1:B:127:GLY:HA2	1:D:224:PHE:C	2.16	0.65
1:D:119:CYS:O	1:D:134:CYS:HA	1.98	0.64
1:B:124:LYS:HZ2	1:D:228:GLY:CA	2.10	0.64
1:B:126:GLU:C	1:D:193:TYR:CD1	2.71	0.64
1:B:190:GLU:HG3	1:C:125:HIS:NE2	2.12	0.64
1:A:119:CYS:O	1:A:134:CYS:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLU:N	1:D:231:VAL:HG21	2.02	0.64
1:B:128:LYS:CD	1:D:193:TYR:CD2	2.74	0.64
1:C:119:CYS:O	1:C:134:CYS:HA	1.98	0.63
1:B:124:LYS:HD2	1:D:228:GLY:H	1.62	0.63
1:B:119:CYS:O	1:B:134:CYS:HA	1.98	0.62
1:B:127:GLY:N	1:D:193:TYR:CD1	2.65	0.62
1:B:124:LYS:HD2	1:D:228:GLY:CA	2.30	0.62
1:B:190:GLU:N	1:C:125:HIS:CG	2.67	0.61
1:B:190:GLU:C	1:C:128:LYS:H	2.03	0.61
1:B:149:VAL:O	1:D:227:LYS:CB	2.35	0.61
1:B:128:LYS:C	1:D:192:HIS:O	2.38	0.61
1:B:122:GLU:HB2	1:D:226:ASN:CB	2.31	0.60
1:B:126:GLU:HA	1:D:231:VAL:HG13	1.83	0.60
1:B:218:ASP:O	1:B:221:ARG:HG3	2.02	0.60
1:B:227:LYS:HZ3	1:B:227:LYS:HB2	1.67	0.60
1:D:218:ASP:O	1:D:221:ARG:HG3	2.02	0.60
1:B:126:GLU:CA	1:D:231:VAL:HG13	2.32	0.59
1:B:226:ASN:CB	1:C:124:LYS:HZ1	2.12	0.59
1:A:218:ASP:O	1:A:221:ARG:HG3	2.02	0.59
1:C:218:ASP:O	1:C:221:ARG:HG3	2.02	0.59
1:B:125:HIS:CB	1:D:193:TYR:OH	2.51	0.59
1:B:128:LYS:CG	1:D:200:VAL:O	2.51	0.59
1:B:128:LYS:CG	1:D:192:HIS:CA	2.55	0.59
1:B:125:HIS:CD2	1:D:193:TYR:OH	2.54	0.58
1:B:125:HIS:N	1:D:225:ASP:HB2	1.56	0.58
1:B:128:LYS:CE	1:D:193:TYR:CA	2.81	0.58
1:B:127:GLY:CA	1:D:224:PHE:C	2.72	0.58
1:B:124:LYS:HG3	1:D:226:ASN:CA	2.01	0.58
1:B:131:GLY:O	1:D:226:ASN:ND2	2.37	0.58
1:B:149:VAL:HG11	1:D:187:GLU:OE1	2.03	0.58
1:B:192:HIS:CG	1:C:128:LYS:NZ	2.65	0.56
1:B:135:LEU:HD22	1:B:140:VAL:HG22	1.88	0.56
1:B:190:GLU:HA	1:C:126:GLU:HB2	1.87	0.56
1:A:135:LEU:HD22	1:A:140:VAL:HG22	1.88	0.56
1:B:192:HIS:NE2	1:B:201:GLN:HG2	2.21	0.56
1:B:189:PRO:HA	1:C:126:GLU:CG	2.36	0.56
1:C:192:HIS:NE2	1:C:201:GLN:HG2	2.21	0.56
1:D:192:HIS:NE2	1:D:201:GLN:HG2	2.21	0.55
1:A:192:HIS:NE2	1:A:201:GLN:HG2	2.21	0.55
1:B:123:VAL:HA	1:D:227:LYS:HG3	0.84	0.55
1:B:124:LYS:CD	1:D:228:GLY:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HD22	1:D:140:VAL:HG22	1.88	0.55
1:B:140:VAL:HG23	1:B:173:ILE:HG12	1.89	0.55
1:B:201:GLN:HB2	1:B:243:ARG:HH21	1.72	0.54
1:C:201:GLN:HB2	1:C:243:ARG:HH21	1.72	0.54
1:A:201:GLN:HB2	1:A:243:ARG:HH21	1.72	0.54
1:C:235:LEU:HD11	1:C:249:VAL:HG23	1.88	0.54
1:B:136:VAL:HG12	1:B:184:TYR:HB3	1.90	0.54
1:B:235:LEU:HD11	1:B:249:VAL:HG23	1.89	0.54
1:C:135:LEU:HD22	1:C:140:VAL:HG22	1.88	0.54
1:B:124:LYS:HE2	1:D:224:PHE:CD1	2.42	0.54
1:B:227:LYS:NZ	1:C:151:ASP:OD1	2.40	0.54
1:B:128:LYS:CE	1:D:193:TYR:CB	2.71	0.54
1:A:140:VAL:HG23	1:A:173:ILE:HG12	1.89	0.54
1:B:128:LYS:CD	1:D:193:TYR:HD2	2.21	0.54
1:A:235:LEU:HD11	1:A:249:VAL:HG23	1.89	0.54
1:C:136:VAL:HG12	1:C:184:TYR:HB3	1.90	0.54
1:B:125:HIS:H	1:D:225:ASP:CB	2.18	0.53
1:D:235:LEU:HD11	1:D:249:VAL:HG23	1.89	0.53
1:B:126:GLU:HB2	1:D:193:TYR:OH	2.08	0.53
1:D:140:VAL:HG23	1:D:173:ILE:HG12	1.89	0.53
1:D:136:VAL:HG12	1:D:184:TYR:HB3	1.90	0.53
1:C:140:VAL:HG23	1:C:173:ILE:HG12	1.89	0.53
1:B:175:VAL:HG22	1:B:178:ARG:NH1	2.24	0.53
1:C:175:VAL:HG22	1:C:178:ARG:NH1	2.24	0.53
1:D:201:GLN:HB2	1:D:243:ARG:HH21	1.72	0.52
1:B:201:GLN:NE2	1:C:128:LYS:HG2	2.24	0.52
1:A:136:VAL:HG12	1:A:184:TYR:HB3	1.90	0.52
1:B:124:LYS:HZ2	1:D:228:GLY:C	2.13	0.52
1:D:168:LEU:HD13	1:D:249:VAL:HG21	1.92	0.52
1:C:168:LEU:HD13	1:C:249:VAL:HG21	1.92	0.52
1:A:175:VAL:HG22	1:A:178:ARG:NH1	2.24	0.52
1:B:192:HIS:O	1:C:127:GLY:O	2.27	0.51
1:D:175:VAL:HG22	1:D:178:ARG:NH1	2.24	0.51
1:B:149:VAL:CG1	1:D:187:GLU:OE1	2.58	0.51
1:B:128:LYS:CE	1:D:200:VAL:CG2	2.77	0.51
1:B:153:ALA:HB2	1:D:183:LYS:NZ	2.26	0.51
1:A:168:LEU:HD13	1:A:249:VAL:HG21	1.92	0.51
1:B:128:LYS:CE	1:D:193:TYR:C	2.72	0.51
1:B:144:ALA:HB2	1:B:168:LEU:O	2.12	0.50
1:B:168:LEU:HD13	1:B:249:VAL:HG21	1.92	0.50
1:C:144:ALA:HB2	1:C:168:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:O	1:C:173:ILE:HD11	2.12	0.50
1:A:144:ALA:HB2	1:A:168:LEU:O	2.12	0.50
1:A:232:ALA:CB	1:A:250:THR:HG23	2.42	0.50
1:C:120:ILE:H	1:C:120:ILE:HD12	1.77	0.50
1:B:139:LYS:O	1:B:173:ILE:HD11	2.12	0.50
1:A:139:LYS:O	1:A:173:ILE:HD11	2.11	0.50
1:C:162:LYS:HE2	1:C:169:GLU:OE1	2.12	0.50
1:B:162:LYS:HE2	1:B:169:GLU:OE1	2.12	0.49
1:B:131:GLY:O	1:D:226:ASN:CB	2.59	0.49
1:D:139:LYS:O	1:D:173:ILE:HD11	2.12	0.49
1:B:120:ILE:HD12	1:B:120:ILE:H	1.77	0.49
1:B:127:GLY:HA3	1:D:223:ILE:HG22	1.94	0.49
1:B:124:LYS:HD2	1:D:228:GLY:C	2.33	0.49
1:D:162:LYS:HE2	1:D:169:GLU:OE1	2.12	0.49
1:D:232:ALA:HB2	1:D:250:THR:CG2	2.42	0.49
1:D:144:ALA:HB2	1:D:168:LEU:O	2.12	0.49
1:A:162:LYS:HE2	1:A:169:GLU:OE1	2.12	0.48
1:D:120:ILE:H	1:D:120:ILE:HD12	1.77	0.48
1:B:190:GLU:HG3	1:C:125:HIS:CD2	2.49	0.48
1:A:120:ILE:HD12	1:A:120:ILE:H	1.77	0.48
1:B:127:GLY:N	1:D:193:TYR:CE1	2.82	0.48
1:B:128:LYS:CE	1:D:193:TYR:H	2.26	0.48
1:B:192:HIS:CA	1:C:127:GLY:O	2.62	0.47
1:B:128:LYS:HD2	1:D:193:TYR:HB2	0.50	0.47
1:B:123:VAL:C	1:D:226:ASN:CA	2.83	0.47
1:B:175:VAL:HG22	1:B:178:ARG:HH12	1.79	0.47
1:B:125:HIS:CD2	1:D:193:TYR:HH	2.33	0.47
1:B:126:GLU:OE1	1:D:202:TYR:CE2	2.68	0.47
1:B:227:LYS:CE	1:C:151:ASP:CG	2.79	0.47
1:C:227:LYS:NZ	1:C:227:LYS:HB2	2.30	0.47
1:A:175:VAL:HG22	1:A:178:ARG:HH12	1.79	0.47
1:D:128:LYS:O	1:D:130:THR:HG23	2.15	0.47
1:B:124:LYS:NZ	1:D:224:PHE:CG	2.82	0.47
1:C:175:VAL:HG22	1:C:178:ARG:HH12	1.79	0.47
1:B:122:GLU:HB2	1:D:226:ASN:HB3	1.95	0.47
1:C:128:LYS:O	1:C:130:THR:HG23	2.15	0.46
1:B:232:ALA:CB	1:B:250:THR:HG23	2.42	0.46
1:B:150:ILE:HG13	1:D:227:LYS:HD3	1.42	0.46
1:D:121:PHE:HE2	1:D:135:LEU:HD11	1.81	0.46
1:A:227:LYS:NZ	1:A:227:LYS:HB2	2.30	0.46
1:A:128:LYS:O	1:A:130:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:TYR:CD2	1:C:126:GLU:CB	2.84	0.46
1:C:232:ALA:CB	1:C:250:THR:HG23	2.42	0.46
1:A:232:ALA:HB2	1:A:250:THR:CG2	2.42	0.46
1:C:209:ILE:HD12	1:C:213:ALA:HB3	1.97	0.46
1:D:175:VAL:HG22	1:D:178:ARG:HH12	1.80	0.46
1:B:128:LYS:O	1:B:130:THR:HG23	2.15	0.46
1:B:126:GLU:HA	1:D:231:VAL:HG22	1.51	0.46
1:A:227:LYS:HZ3	1:A:227:LYS:HB2	1.80	0.46
1:A:209:ILE:HD12	1:A:213:ALA:HB3	1.97	0.46
1:C:121:PHE:HE2	1:C:135:LEU:HD11	1.81	0.45
1:B:209:ILE:HD12	1:B:213:ALA:HB3	1.97	0.45
1:B:227:LYS:NZ	1:B:227:LYS:HB2	2.30	0.45
1:B:232:ALA:HB2	1:B:250:THR:CG2	2.42	0.45
1:D:209:ILE:HD12	1:D:213:ALA:HB3	1.97	0.45
1:B:201:GLN:HE21	1:C:128:LYS:HG2	1.80	0.45
1:D:232:ALA:CB	1:D:250:THR:HG23	2.42	0.45
1:C:232:ALA:HB2	1:C:250:THR:CG2	2.42	0.45
1:A:260:THR:HA	1:A:261:PRO:HD3	1.79	0.45
1:B:121:PHE:HE2	1:B:135:LEU:HD11	1.81	0.45
1:B:202:TYR:O	1:C:128:LYS:HB2	2.17	0.45
1:B:226:ASN:CA	1:C:124:LYS:NZ	2.80	0.45
1:B:227:LYS:HE3	1:C:151:ASP:OD1	2.16	0.44
1:D:225:ASP:OD2	1:D:229:ARG:HD3	2.18	0.44
1:B:124:LYS:N	1:D:226:ASN:H	2.08	0.44
1:B:126:GLU:CB	1:D:231:VAL:HG11	2.46	0.44
1:A:121:PHE:HE2	1:A:135:LEU:HD11	1.81	0.44
1:D:185:THR:HG21	1:D:229:ARG:NH1	2.33	0.43
1:B:185:THR:HG21	1:B:229:ARG:NH1	2.33	0.43
1:C:185:THR:HG21	1:C:229:ARG:NH1	2.34	0.43
1:B:124:LYS:N	1:D:226:ASN:CA	2.81	0.43
1:A:225:ASP:OD2	1:A:229:ARG:HD3	2.18	0.43
1:C:225:ASP:OD2	1:C:229:ARG:HD3	2.18	0.43
1:B:200:VAL:O	1:C:128:LYS:HE2	2.13	0.43
1:B:126:GLU:CA	1:D:193:TYR:CZ	2.96	0.43
1:B:192:HIS:CD2	1:C:128:LYS:HZ2	2.32	0.43
1:B:225:ASP:OD2	1:B:229:ARG:HD3	2.18	0.43
1:A:185:THR:HG21	1:A:229:ARG:NH1	2.33	0.43
1:A:140:VAL:CG2	1:A:173:ILE:HG12	2.49	0.43
1:C:140:VAL:CG2	1:C:173:ILE:HG12	2.49	0.43
1:C:167:ASP:HB2	1:C:258:ARG:HH12	1.84	0.43
1:B:124:LYS:NZ	1:D:224:PHE:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ASP:HB2	1:D:258:ARG:HH12	1.84	0.42
1:B:126:GLU:CB	1:D:193:TYR:CZ	2.98	0.42
1:B:167:ASP:HB2	1:B:258:ARG:HH12	1.84	0.42
1:B:227:LYS:CE	1:C:151:ASP:OD1	2.67	0.42
1:B:124:LYS:HD3	1:D:224:PHE:CB	2.41	0.42
1:D:154:ASP:OD1	1:D:154:ASP:N	2.52	0.42
1:B:189:PRO:HG2	1:C:124:LYS:HB3	2.01	0.42
1:B:202:TYR:HB3	1:C:128:LYS:HD2	1.90	0.42
1:A:175:VAL:HG13	1:A:178:ARG:HH11	1.85	0.42
1:D:143:PRO:HG2	1:D:219:SER:HB3	2.02	0.42
1:B:140:VAL:CG2	1:B:173:ILE:HG12	2.49	0.42
1:B:125:HIS:H	1:D:225:ASP:HB2	1.66	0.42
1:D:140:VAL:CG2	1:D:173:ILE:HG12	2.49	0.42
1:B:260:THR:HA	1:B:261:PRO:HD3	1.79	0.42
1:B:154:ASP:OD1	1:B:154:ASP:N	2.52	0.42
1:B:231:VAL:O	1:B:250:THR:HG22	2.20	0.42
1:D:175:VAL:HG13	1:D:178:ARG:HH11	1.85	0.42
1:A:167:ASP:HB2	1:A:258:ARG:HH12	1.84	0.42
1:B:149:VAL:HG23	1:D:227:LYS:NZ	2.35	0.41
1:B:143:PRO:HG2	1:B:219:SER:HB3	2.02	0.41
1:B:128:LYS:HD2	1:D:193:TYR:CD2	2.38	0.41
1:B:128:LYS:HG2	1:D:200:VAL:O	2.21	0.41
1:B:175:VAL:HG13	1:B:178:ARG:HH11	1.85	0.41
1:B:128:LYS:CE	1:D:193:TYR:O	2.67	0.41
1:B:129:VAL:N	1:D:194:ASN:ND2	2.67	0.41
1:B:130:THR:N	1:D:226:ASN:CG	2.69	0.41
1:A:143:PRO:HG2	1:A:219:SER:HB3	2.02	0.41
1:D:240:GLU:OE2	1:D:245:ALA:HB2	2.21	0.41
1:C:174:PRO:HG2	1:C:177:MET:HG3	2.03	0.41
1:D:231:VAL:O	1:D:250:THR:HG22	2.20	0.41
1:D:260:THR:HA	1:D:261:PRO:HD3	1.79	0.41
1:C:240:GLU:OE2	1:C:245:ALA:HB2	2.21	0.41
1:C:260:THR:HA	1:C:261:PRO:HD3	1.79	0.41
1:A:231:VAL:O	1:A:250:THR:HG22	2.20	0.41
1:C:175:VAL:HG13	1:C:178:ARG:HH11	1.85	0.41
1:B:240:GLU:OE2	1:B:245:ALA:HB2	2.21	0.41
1:B:126:GLU:N	1:D:188:LYS:HA	2.35	0.41
1:B:124:LYS:CB	1:D:227:LYS:H	2.34	0.41
1:B:174:PRO:HG2	1:B:177:MET:HG3	2.03	0.41
1:B:192:HIS:N	1:C:127:GLY:O	2.54	0.40
1:B:192:HIS:CE1	1:B:201:GLN:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:HIS:CG	1:D:193:TYR:HH	2.31	0.40
1:B:149:VAL:CG2	1:D:227:LYS:NZ	2.84	0.40
1:C:192:HIS:CE1	1:C:201:GLN:HG2	2.56	0.40
1:A:174:PRO:HG2	1:A:177:MET:HG3	2.03	0.40
1:D:174:PRO:HG2	1:D:177:MET:HG3	2.03	0.40
1:B:131:GLY:H	1:D:226:ASN:CG	2.25	0.40
1:C:143:PRO:HG2	1:C:219:SER:HB3	2.02	0.40
1:D:145:HIS:CD2	1:D:266:GLU:HB3	2.57	0.40
1:D:192:HIS:CE1	1:D:201:GLN:HG2	2.56	0.40
1:C:231:VAL:O	1:C:250:THR:HG22	2.20	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	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
1	B	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
1	C	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
1	D	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
All	All	588/596 (99%)	552 (94%)	36 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	120/120 (100%)	99 (82%)	21 (18%)	2	16
1	B	120/120 (100%)	99 (82%)	21 (18%)	2	16
1	C	120/120 (100%)	99 (82%)	21 (18%)	2	16
1	D	120/120 (100%)	99 (82%)	21 (18%)	2	16
All	All	480/480 (100%)	396 (82%)	84 (18%)	6	16

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	CYS
1	A	120	ILE
1	A	128	LYS
1	A	136	VAL
1	A	154	ASP
1	A	155	LEU
1	A	170	CYS
1	A	172	GLN
1	A	175	VAL
1	A	183	LYS
1	A	195	TRP
1	A	201	GLN
1	A	206	ARG
1	A	208	THR
1	A	224	PHE
1	A	229	ARG
1	A	243	ARG
1	A	250	THR
1	A	257	THR
1	A	258	ARG
1	A	265	GLU
1	B	119	CYS
1	B	120	ILE
1	B	128	LYS
1	B	136	VAL
1	B	154	ASP
1	B	155	LEU
1	B	170	CYS
1	B	172	GLN
1	B	175	VAL

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Mol	Chain	Res	Type
1	B	183	LYS
1	B	195	TRP
1	B	201	GLN
1	B	206	ARG
1	B	208	THR
1	B	224	PHE
1	B	229	ARG
1	B	243	ARG
1	B	250	THR
1	B	257	THR
1	B	258	ARG
1	B	265	GLU
1	C	119	CYS
1	C	120	ILE
1	C	128	LYS
1	C	136	VAL
1	C	154	ASP
1	C	155	LEU
1	C	170	CYS
1	C	172	GLN
1	C	175	VAL
1	C	183	LYS
1	C	195	TRP
1	C	201	GLN
1	C	206	ARG
1	C	208	THR
1	C	224	PHE
1	C	229	ARG
1	C	243	ARG
1	C	250	THR
1	C	257	THR
1	C	258	ARG
1	C	265	GLU
1	D	119	CYS
1	D	120	ILE
1	D	128	LYS
1	D	136	VAL
1	D	154	ASP
1	D	155	LEU
1	D	170	CYS
1	D	172	GLN
1	D	175	VAL

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Mol	Chain	Res	Type
1	D	183	LYS
1	D	195	TRP
1	D	201	GLN
1	D	206	ARG
1	D	208	THR
1	D	224	PHE
1	D	229	ARG
1	D	243	ARG
1	D	250	THR
1	D	257	THR
1	D	258	ARG
1	D	265	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	197	HIS
1	B	172	GLN
1	B	197	HIS
1	B	201	GLN
1	C	172	GLN
1	C	197	HIS
1	D	172	GLN
1	D	194	ASN
1	D	197	HIS

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 [i](#)

There are no ligands in this entry.

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.