



Full wwPDB EM Validation Report ⓘ

Jul 15, 2025 – 11:26 PM JST

PDB ID : 9L99 / pdb_00009L99
EMDB ID : EMD-62898
Title : Structure of Western equine encephalitis virus McMillan strain in complex with VLDLR LA1-2
Authors : Ma, B.; Cao, Z.; Ding, W.; Zhang, X.; Xiang, Y.; Cao, D.
Deposited on : 2024-12-29
Resolution : 3.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

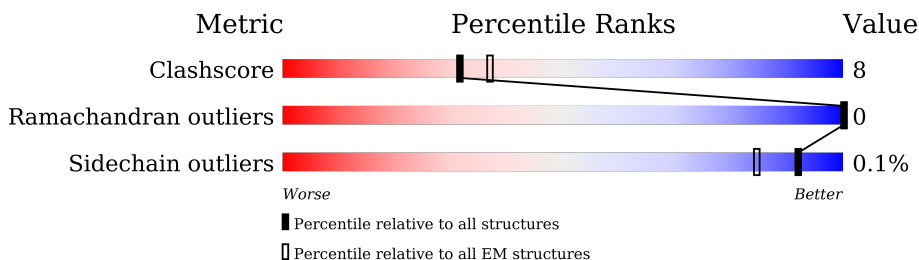
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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 ≥ 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	411	82%	18%
1	G	411	81%	19%
2	B	369	79%	21%
2	H	369	79%	21%
3	N	80	78%	22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12710 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 Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	411	Total	C	N	O	S	0	0
			3122	1980	525	598	19		
1	G	411	Total	C	N	O	S	0	0
			3122	1980	525	598	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	LYS	ARG	conflict	UNP P13897
A	349	THR	VAL	conflict	UNP P13897
G	50	LYS	ARG	conflict	UNP P13897
G	349	THR	VAL	conflict	UNP P13897

- Molecule 2 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	369	Total	C	N	O	S	0	0
			2929	1861	514	538	16		
2	H	369	Total	C	N	O	S	0	0
			2929	1861	514	538	16		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	TYR	PHE	conflict	UNP P13897
B	81	GLU	ASP	conflict	UNP P13897
B	146	GLN	HIS	conflict	UNP P13897
B	157	ARG	HIS	conflict	UNP P13897
B	181	LYS	GLU	conflict	UNP P13897
B	214	GLN	ARG	conflict	UNP P13897
B	224	ARG	LYS	conflict	UNP P13897
B	231	LEU	SER	conflict	UNP P13897
H	69	TYR	PHE	conflict	UNP P13897

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Chain	Residue	Modelled	Actual	Comment	Reference
H	81	GLU	ASP	conflict	UNP P13897
H	146	GLN	HIS	conflict	UNP P13897
H	157	ARG	HIS	conflict	UNP P13897
H	181	LYS	GLU	conflict	UNP P13897
H	214	GLN	ARG	conflict	UNP P13897
H	224	ARG	LYS	conflict	UNP P13897
H	231	LEU	SER	conflict	UNP P13897

- Molecule 3 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	80	Total	C	N	O	S	0	0
			606	356	104	133	13		

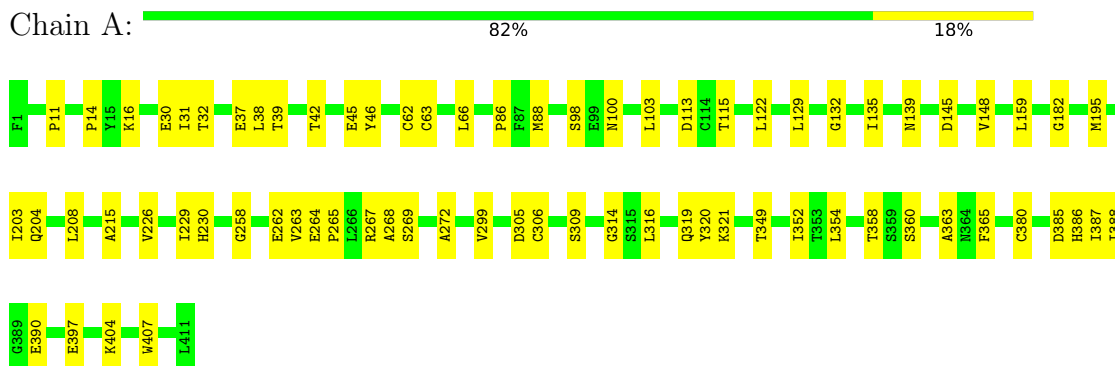
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	N	2	Total	Ca	0
			2	2	

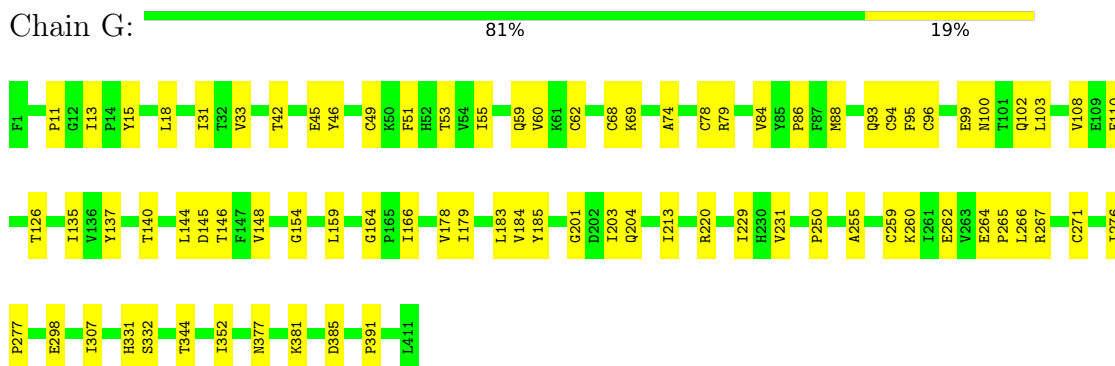
3 Residue-property plots

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: Spike glycoprotein E1



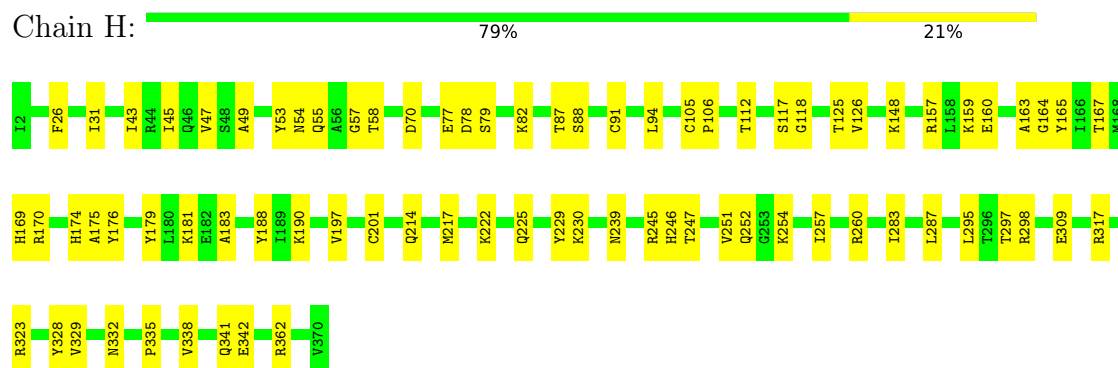
- Molecule 1: Spike glycoprotein E1



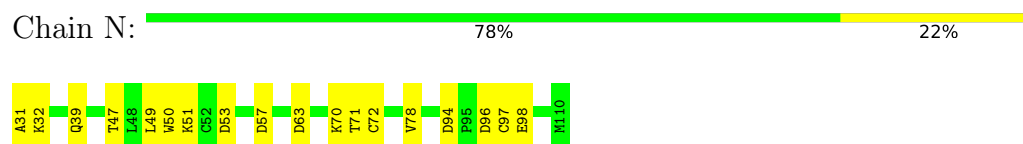
- Molecule 2: Spike glycoprotein E2



● Molecule 2: Spike glycoprotein E2



● Molecule 3: Very low-density lipoprotein receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180284	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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: CA

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	0.16	0/3203	0.40	0/4371
1	G	0.15	0/3203	0.39	0/4371
2	B	0.15	0/3016	0.37	0/4103
2	H	0.15	0/3016	0.39	0/4103
3	N	0.12	0/616	0.36	0/830
All	All	0.15	0/13054	0.39	0/17778

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	3122	0	3045	57	0
1	G	3122	0	3045	55	0
2	B	2929	0	2855	51	0
2	H	2929	0	2855	52	0
3	N	606	0	523	13	0
4	N	2	0	0	0	0
All	All	12710	0	12323	212	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 8.

All (212) 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:G:18:LEU:HD22	1:G:331:HIS:HD2	1.49	0.78
1:G:51:PHE:HB3	1:G:203:ILE:HD11	1.68	0.75
2:H:181:LYS:HB3	2:H:188:TYR:HB2	1.67	0.75
1:G:94:CYS:SG	1:G:100:ASN:ND2	2.60	0.74
1:G:179:ILE:HG12	1:G:184:VAL:HG12	1.68	0.74
1:A:258:GLY:HA2	2:B:298:ARG:HH12	1.53	0.73
1:G:18:LEU:HD22	1:G:331:HIS:CD2	2.22	0.72
1:G:68:CYS:HB3	1:G:103:LEU:HD11	1.71	0.71
1:A:385:ASP:O	2:B:341:GLN:NE2	2.25	0.70
2:B:321:VAL:HG23	2:B:340:ALA:HB2	1.75	0.68
1:G:144:LEU:HD11	1:G:159:LEU:HD23	1.76	0.68
1:G:385:ASP:O	2:H:341:GLN:NE2	2.21	0.67
1:G:264:GLU:HB3	1:G:265:PRO:HD3	1.76	0.67
2:H:181:LYS:HE3	2:H:183:ALA:HB2	1.75	0.66
2:H:47:VAL:HG23	2:H:49:ALA:H	1.61	0.66
2:B:31:ILE:HG22	2:B:47:VAL:HG12	1.77	0.66
2:B:47:VAL:HG23	2:B:49:ALA:H	1.61	0.65
2:B:68:SER:HB3	2:B:76:LYS:HD3	1.78	0.65
2:H:78:ASP:OD1	2:H:82:LYS:HD2	1.96	0.65
1:A:129:LEU:HD23	1:A:148:VAL:HG21	1.79	0.64
2:B:55:GLN:NE2	2:B:75:ILE:O	2.30	0.64
2:B:82:LYS:NZ	2:B:117:SER:O	2.29	0.64
1:A:358:THR:HG22	1:A:360:SER:H	1.63	0.63
2:H:342:GLU:HG2	2:H:362:ARG:HE	1.63	0.63
2:H:53:TYR:HB3	2:H:57:GLY:HA2	1.82	0.62
2:H:163:ALA:HB2	2:H:260:ARG:HB2	1.82	0.62
2:H:222:LYS:HB3	2:H:225:GLN:HG2	1.83	0.61
2:H:91:CYS:HA	2:H:105:CYS:HB3	1.81	0.61
1:A:203:ILE:HG13	1:A:215:ALA:HB2	1.83	0.61
3:N:63:ASP:OD1	3:N:63:ASP:N	2.35	0.60
2:B:40:ASP:HB2	2:B:154:VAL:HG12	1.84	0.60
1:G:183:LEU:HD13	1:G:250:PRO:HB3	1.83	0.60
1:G:259:CYS:HA	1:G:271:CYS:HB3	1.83	0.60
1:G:11:PRO:HA	1:G:33:VAL:HG23	1.84	0.59
2:H:283:ILE:HD11	2:H:338:VAL:HG11	1.84	0.59
1:G:144:LEU:HD11	1:G:159:LEU:CD2	2.32	0.59
2:H:82:LYS:HD3	2:H:117:SER:HB2	1.85	0.59
2:B:137:ARG:HD3	2:B:294:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LYS:HD2	2:B:202:LYS:O	2.02	0.58
2:B:43:ILE:HD11	2:B:130:ILE:HD12	1.86	0.58
1:A:63:CYS:H	1:A:100:ASN:HA	1.68	0.58
1:A:113:ASP:OD2	2:B:44:ARG:NH2	2.32	0.58
1:G:201:GLY:O	1:G:204:GLN:NE2	2.37	0.57
2:H:87:THR:HG23	2:H:88:SER:H	1.69	0.57
1:A:37:GLU:HA	1:A:269:SER:HA	1.86	0.57
1:A:264:GLU:HB3	1:A:265:PRO:HD2	1.87	0.57
1:G:96:CYS:SG	1:G:99:GLU:HB3	2.45	0.56
1:G:95:PHE:CD1	2:H:201:CYS:HA	2.41	0.56
1:A:14:PRO:HB3	1:A:32:THR:HG22	1.88	0.55
2:H:329:VAL:HG22	2:H:335:PRO:HB3	1.87	0.55
2:H:167:THR:HG21	2:H:251:VAL:HG22	1.89	0.55
3:N:51:LYS:HA	3:N:63:ASP:HB2	1.88	0.55
2:H:201:CYS:SG	2:H:217:MET:HE1	2.46	0.55
2:H:197:VAL:HA	2:H:230:LYS:HA	1.88	0.55
2:H:78:ASP:OD1	2:H:79:SER:N	2.40	0.55
2:H:164:GLY:HA3	2:H:257:ILE:HD12	1.89	0.54
2:H:287:LEU:HD11	2:H:295:LEU:HD22	1.89	0.54
2:H:55:GLN:N	2:H:77:GLU:OE2	2.41	0.54
1:A:226:VAL:HG21	1:A:230:HIS:HE1	1.71	0.54
1:G:74:ALA:HB2	1:G:213:ILE:HG13	1.90	0.53
1:A:195:MET:SD	1:A:195:MET:N	2.81	0.53
2:B:28:PRO:HD2	2:B:122:ASN:HD22	1.74	0.53
1:G:69:LYS:H	1:G:69:LYS:HD2	1.74	0.53
1:G:164:GLY:HA3	1:G:277:PRO:HG2	1.90	0.53
1:G:88:MET:HE2	2:H:174:HIS:ND1	2.24	0.53
1:G:135:ILE:HD12	1:G:144:LEU:HD12	1.90	0.53
2:B:152:CYS:N	2:B:264:THR:O	2.41	0.53
1:A:195:MET:HE3	1:A:204:GLN:HG3	1.90	0.52
2:H:31:ILE:HD11	2:H:126:VAL:HG22	1.91	0.52
1:G:148:VAL:HG21	1:G:166:ILE:HD11	1.91	0.52
1:G:55:ILE:HG21	1:G:231:VAL:HG21	1.92	0.51
2:H:31:ILE:HG22	2:H:47:VAL:HG12	1.92	0.51
1:A:86:PRO:HB3	1:A:229:ILE:HB	1.92	0.51
2:B:191:PRO:HB3	2:B:197:VAL:HG13	1.91	0.51
2:B:272:HIS:CE1	1:G:220:ARG:HH11	2.29	0.51
3:N:31:ALA:HB3	3:N:39:GLN:HG2	1.93	0.51
2:H:105:CYS:HB2	2:H:106:PRO:HD2	1.93	0.51
1:A:38:LEU:HG	1:A:268:ALA:HB3	1.93	0.51
2:H:297:THR:HG22	2:H:328:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:HG2	1:A:267:ARG:HG3	1.93	0.50
2:B:135:VAL:HG21	2:B:152:CYS:SG	2.50	0.50
1:A:182:GLY:HA2	1:A:263:VAL:HG11	1.94	0.50
1:G:59:GLN:HB2	2:H:245:ARG:HE	1.77	0.50
1:G:178:VAL:HG13	1:G:185:TYR:HB2	1.94	0.49
1:G:144:LEU:CD1	1:G:159:LEU:HD23	2.42	0.49
1:G:45:GLU:HG3	1:G:46:TYR:HD1	1.77	0.49
2:H:94:LEU:HD23	2:H:157:ARG:HE	1.78	0.49
2:B:163:ALA:HB2	2:B:260:ARG:HA	1.95	0.49
2:B:200:GLU:OE1	2:B:206:TYR:OH	2.31	0.49
2:B:283:ILE:HG22	2:B:319:PHE:HB2	1.94	0.49
1:G:145:ASP:N	1:G:145:ASP:OD1	2.44	0.49
1:A:320:TYR:HE2	1:A:352:ILE:HG12	1.77	0.48
2:H:31:ILE:HA	2:H:47:VAL:HA	1.95	0.48
1:G:86:PRO:HB3	1:G:229:ILE:HB	1.96	0.48
1:A:31:ILE:HG12	1:A:135:ILE:HG22	1.95	0.48
1:G:78:CYS:SG	1:G:79:ARG:N	2.87	0.48
1:A:385:ASP:OD1	1:A:385:ASP:N	2.47	0.48
2:B:203:CYS:HB3	2:B:225:GLN:HE21	1.79	0.48
1:G:62:CYS:HA	1:G:100:ASN:HB3	1.96	0.48
2:B:169:HIS:CD2	2:B:239:ASN:HB2	2.49	0.47
2:H:159:LYS:HG3	2:H:160:GLU:OE2	2.14	0.47
2:B:203:CYS:HB2	2:B:220:CYS:HB3	1.59	0.47
2:B:275:THR:HG23	2:B:286:HIS:HB2	1.96	0.47
1:G:137:TYR:O	1:G:140:THR:OG1	2.30	0.47
1:A:98:SER:O	1:A:98:SER:OG	2.30	0.47
1:G:13:ILE:HD11	1:G:391:PRO:HG2	1.95	0.47
1:G:60:VAL:HG12	1:G:102:GLN:HB2	1.97	0.47
1:G:377:ASN:OD1	1:G:377:ASN:N	2.46	0.47
1:A:262:GLU:OE2	1:A:267:ARG:NE	2.40	0.47
1:A:363:ALA:HB1	1:A:365:PHE:HE1	1.79	0.47
1:A:37:GLU:OE1	1:A:37:GLU:N	2.48	0.46
1:G:15:TYR:HE1	1:G:31:ILE:HB	1.80	0.46
1:G:53:THR:HG22	1:G:108:VAL:HG22	1.97	0.46
1:G:344:THR:HG21	1:G:352:ILE:HD13	1.97	0.46
1:A:45:GLU:HG3	1:A:46:TYR:HD1	1.81	0.46
2:B:321:VAL:HG12	2:B:326:LEU:HD22	1.98	0.46
1:G:255:ALA:O	2:H:298:ARG:NH1	2.48	0.46
2:H:54:ASN:ND2	2:H:58:THR:OG1	2.49	0.46
2:B:26:PHE:O	2:B:69:TYR:OH	2.22	0.46
1:A:45:GLU:HG3	1:A:46:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ILE:HG22	2:B:113:VAL:HG23	1.98	0.46
1:A:135:ILE:HD11	1:A:159:LEU:HG	1.98	0.46
2:B:222:LYS:HD2	2:B:223:ALA:H	1.80	0.46
2:H:323:ARG:NH1	2:H:342:GLU:OE2	2.50	0.45
2:B:149:LEU:HD23	2:B:267:PRO:HA	1.99	0.45
2:H:148:LYS:HD3	2:H:332:ASN:HB3	1.96	0.45
1:A:316:LEU:HD22	1:A:354:LEU:HD12	1.98	0.45
2:B:137:ARG:HH12	2:B:329:VAL:HG21	1.80	0.45
2:B:181:LYS:HB2	2:B:188:TYR:HB2	1.97	0.45
2:B:3:THR:N	2:B:254:LYS:O	2.49	0.45
3:N:32:LYS:HB2	3:N:39:GLN:HB2	1.98	0.45
2:H:176:TYR:HB2	2:H:179:TYR:CE2	2.52	0.45
1:G:84:VAL:HG21	1:G:102:GLN:HB3	1.99	0.45
2:H:117:SER:OG	2:H:118:GLY:N	2.50	0.45
1:A:132:GLY:HA2	1:A:145:ASP:HA	1.99	0.45
2:H:112:THR:HG22	2:H:125:THR:HG23	1.97	0.45
1:A:299:VAL:HA	1:A:319:GLN:O	2.17	0.45
2:H:190:LYS:NZ	3:N:96:ASP:OD2	2.50	0.45
1:A:38:LEU:HB3	1:A:129:LEU:HD12	1.98	0.44
1:A:363:ALA:HB1	1:A:365:PHE:CE1	2.52	0.44
1:G:42:THR:HG21	1:G:266:LEU:HD23	1.99	0.44
1:A:388:ILE:HG23	1:A:390:GLU:H	1.82	0.44
1:A:404:LYS:HA	1:A:407:TRP:HB2	2.00	0.44
3:N:50:TRP:HB3	3:N:57:ASP:OD2	2.17	0.44
1:G:49:CYS:SG	1:G:110:PHE:HD1	2.41	0.44
2:H:246:HIS:CD2	2:H:247:THR:HG22	2.53	0.44
1:A:115:THR:HA	1:A:208:LEU:HD21	1.99	0.44
3:N:47:THR:HG22	3:N:49:LEU:H	1.82	0.44
2:B:300:LEU:HD21	2:B:337:ARG:HH11	1.82	0.44
1:A:62:CYS:HA	1:A:100:ASN:HB3	2.00	0.44
2:B:165:TYR:HE1	2:B:254:LYS:HD3	1.83	0.44
2:B:311:ILE:HD11	2:B:330:TRP:CH2	2.52	0.44
1:A:305:ASP:OD1	1:A:305:ASP:N	2.51	0.43
3:N:97:CYS:SG	3:N:98:GLU:N	2.89	0.43
2:B:21:HIS:CD2	2:B:23:ALA:HB3	2.54	0.43
2:B:317:ARG:HA	2:B:317:ARG:HD3	1.90	0.43
1:G:100:ASN:OD1	1:G:100:ASN:N	2.43	0.43
2:H:70:ASP:OD1	2:H:70:ASP:C	2.62	0.43
2:H:175:ALA:HA	2:H:229:TYR:HB3	2.00	0.43
1:A:306:CYS:HB3	1:A:314:GLY:HA2	2.01	0.43
1:G:88:MET:HA	2:H:26:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:NZ	1:A:30:GLU:OE1	2.51	0.43
1:A:264:GLU:HB3	1:A:265:PRO:CD	2.48	0.43
1:A:306:CYS:H	1:A:380:CYS:HB2	1.84	0.43
2:B:191:PRO:HG3	2:B:197:VAL:HG22	2.00	0.43
2:H:43:ILE:HG22	2:H:45:ILE:HG13	2.00	0.43
2:H:165:TYR:CE1	2:H:254:LYS:HG2	2.54	0.43
2:H:170:ARG:HE	2:H:252:GLN:HE22	1.67	0.43
2:H:342:GLU:HG2	2:H:362:ARG:NE	2.33	0.43
1:A:42:THR:HB	1:A:122:LEU:HD23	2.01	0.43
1:A:139:ASN:C	1:A:139:ASN:OD1	2.62	0.43
1:A:321:LYS:HG2	1:A:349:THR:HG22	2.01	0.43
1:A:39:THR:HG22	1:A:267:ARG:HG2	2.01	0.42
2:B:236:TRP:CZ3	2:B:253:GLY:HA3	2.54	0.42
1:G:262:GLU:HG2	1:G:267:ARG:HH21	1.84	0.42
1:A:386:HIS:HB3	2:B:343:SER:OG	2.19	0.42
2:H:169:HIS:CE1	2:H:239:ASN:HD22	2.37	0.42
3:N:53:ASP:OD1	3:N:53:ASP:N	2.53	0.42
3:N:70:LYS:O	3:N:71:THR:OG1	2.31	0.42
2:B:201:CYS:HB3	2:B:226:CYS:HA	2.01	0.42
2:B:240:SER:HB3	2:B:243:LEU:HD23	2.01	0.42
1:A:63:CYS:H	1:A:100:ASN:CA	2.32	0.42
1:G:144:LEU:CD1	1:G:159:LEU:CD2	2.98	0.42
1:A:11:PRO:HD2	1:A:272:ALA:HB2	2.02	0.42
2:B:343:SER:OG	2:B:343:SER:O	2.37	0.42
1:G:331:HIS:ND1	1:G:332:SER:N	2.67	0.42
2:B:222:LYS:HD2	2:B:223:ALA:N	2.35	0.42
1:A:387:ILE:HB	2:B:278:LYS:HG2	2.02	0.41
1:A:309:SER:HB2	2:B:341:GLN:OE1	2.20	0.41
2:H:214:GLN:HE22	3:N:94:ASP:CG	2.28	0.41
1:A:63:CYS:H	1:A:100:ASN:HB3	1.84	0.41
1:G:126:THR:O	1:G:126:THR:HG23	2.21	0.41
2:H:170:ARG:HE	2:H:252:GLN:NE2	2.19	0.41
3:N:71:THR:HG22	3:N:72:CYS:N	2.35	0.41
1:A:88:MET:HE2	2:B:174:HIS:ND1	2.35	0.41
1:A:66:LEU:HD21	1:A:103:LEU:HD23	2.03	0.41
2:B:2:ILE:HA	2:B:254:LYS:HB2	2.02	0.41
2:B:87:THR:HG21	2:B:130:ILE:HD11	2.03	0.41
1:G:260:LYS:NZ	1:G:262:GLU:OE2	2.54	0.41
1:A:397:GLU:O	1:A:397:GLU:HG3	2.20	0.41
3:N:72:CYS:SG	3:N:78:VAL:HG22	2.61	0.41
1:G:146:THR:HG22	1:G:154:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:ILE:O	1:G:276:ILE:HG13	2.21	0.40
1:A:264:GLU:OE2	1:A:264:GLU:HA	2.21	0.40
1:G:298:GLU:O	1:G:298:GLU:OE2	2.39	0.40
1:G:307:ILE:HG13	1:G:381:LYS:O	2.22	0.40
1:A:226:VAL:HG21	1:A:230:HIS:CE1	2.53	0.40
1:G:88:MET:HG2	1:G:93:GLN:HG3	2.02	0.40
2:B:11:PRO:HD2	2:B:75:ILE:HD12	2.03	0.40
2:H:309:GLU:OE1	2:H:317:ARG:NH1	2.53	0.40
1:A:88:MET:HG2	1:A:229:ILE:HG21	2.01	0.40
2:H:342:GLU:HB3	2:H:362:ARG:HD2	2.04	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	409/411 (100%)	381 (93%)	28 (7%)	0	100	100
1	G	409/411 (100%)	386 (94%)	23 (6%)	0	100	100
2	B	367/369 (100%)	337 (92%)	30 (8%)	0	100	100
2	H	367/369 (100%)	342 (93%)	25 (7%)	0	100	100
3	N	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
All	All	1630/1640 (99%)	1520 (93%)	110 (7%)	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	346/346 (100%)	346 (100%)	0	100	100
1	G	346/346 (100%)	346 (100%)	0	100	100
2	B	323/323 (100%)	321 (99%)	2 (1%)	84	92
2	H	323/323 (100%)	323 (100%)	0	100	100
3	N	72/72 (100%)	72 (100%)	0	100	100
All	All	1410/1410 (100%)	1408 (100%)	2 (0%)	92	97

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

Mol	Chain	Res	Type
2	B	6	PHE
2	B	18	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	125	HIS
1	A	143	HIS
1	A	230	HIS
1	A	319	GLN
1	A	331	HIS
1	A	333	HIS
1	A	345	HIS
1	A	355	HIS
1	A	399	GLN
2	B	33	ASN
2	B	153	HIS
2	B	174	HIS
2	B	214	GLN
2	B	225	GLN
2	B	246	HIS
2	B	256	HIS
2	B	349	HIS
1	G	43	ASN
1	G	52	HIS
1	G	246	ASN

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Mol	Chain	Res	Type
1	G	275	HIS
1	G	331	HIS
1	G	392	HIS
2	H	96	HIS
2	H	169	HIS
2	H	174	HIS
2	H	214	GLN
2	H	246	HIS
2	H	252	GLN
2	H	361	HIS

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 [i](#)

Of 2 ligands modelled in this entry, 2 are 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 ⓘ

There are no chain breaks in this entry.