Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 02:51 PM JST

PDB ID	:	8YEO / pdb_00008yeo
EMDB ID	:	EMD-39200
Title	:	Type I-FHNH Cascade-dsDNA R-loop complex
Authors	:	Li, Z.
Deposited on	:	2024-02-22
Resolution	:	3.44 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:

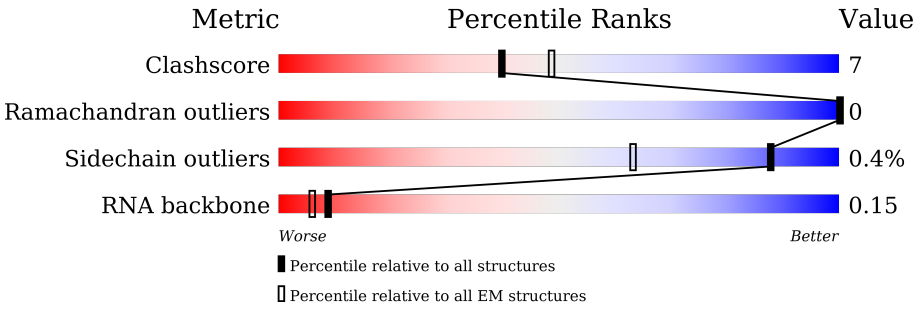
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.44 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
RNA backbone	6643	2191

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%

Mol	Chain	Length	Quality of chain
1	A	255	78% 22%
2	J	344	70% 28% ••
3	B	181	69% 28% • •
4	D	335	73% 15% 12%
4	E	335	84% 13% •
4	F	335	85% 11% •
4	G	335	79% 18% •
4	H	335	83% 13% •

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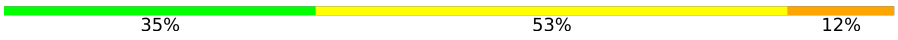
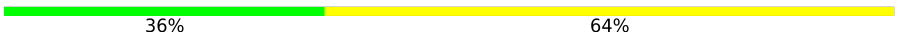
Mol	Chain	Length	Quality of chain
4	I	335	
5	C	60	
6	T	48	
7	N	11	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24197 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 Cas5f.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	255	Total	C	N	O	S	0	0
			2010	1281	338	377	14		

- Molecule 2 is a protein called Cas8f fusion with HNH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	340	Total	C	N	O	S	0	0
			2718	1719	468	518	13		

- Molecule 3 is a protein called Cas6f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	175	Total	C	N	O	S	0	0
			1415	913	239	258	5		

- Molecule 4 is a protein called Cas7f.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	324	Total	C	N	O	S	0	0
			2639	1688	436	500	15		
4	D	295	Total	C	N	O	S	0	0
			2412	1546	397	456	13		
4	E	322	Total	C	N	O	S	0	0
			2621	1677	433	496	15		
4	F	323	Total	C	N	O	S	0	0
			2630	1682	434	499	15		
4	G	323	Total	C	N	O	S	0	0
			2630	1682	434	499	15		
4	H	323	Total	C	N	O	S	0	0
			2630	1682	434	499	15		

- Molecule 5 is a RNA chain called 60-nt crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	60	Total 1287	C 577	N 240	O 411	P 59	0	0

- Molecule 6 is DNA/RNA hybrid called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	48	Total 975	C 468	N 168	O 291	P 48	0	0

- Molecule 7 is DNA/RNA hybrid called NTS.

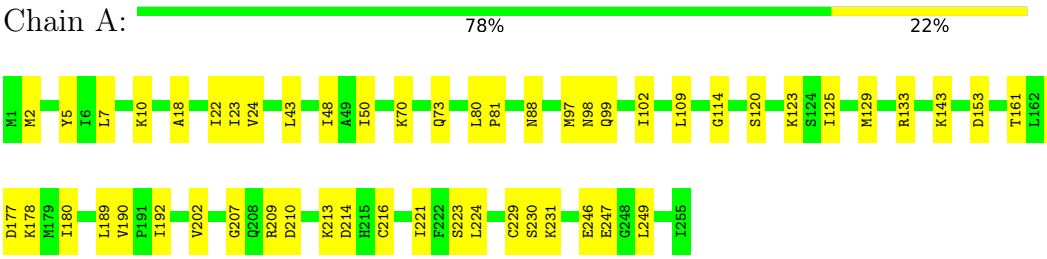
Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	11	Total 230	C 109	N 44	O 66	P 11	0	0

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.

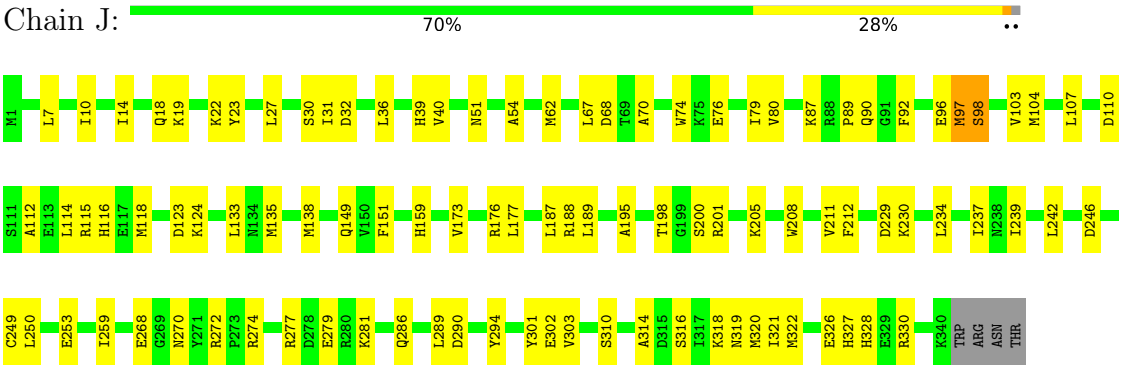
- Molecule 1: Cas5f

Chain A:



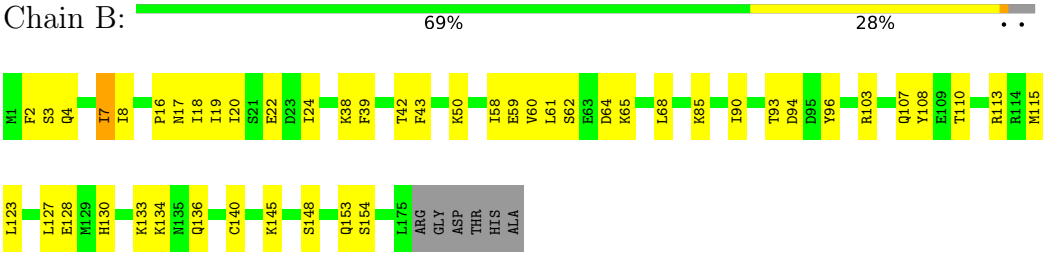
- Molecule 2: Cas8f fusion with HNH

Chain J:



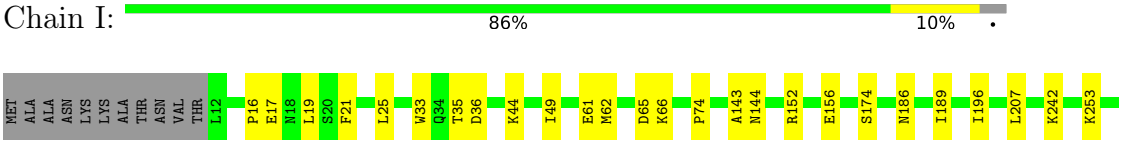
- Molecule 3: Cas6f

Chain B:



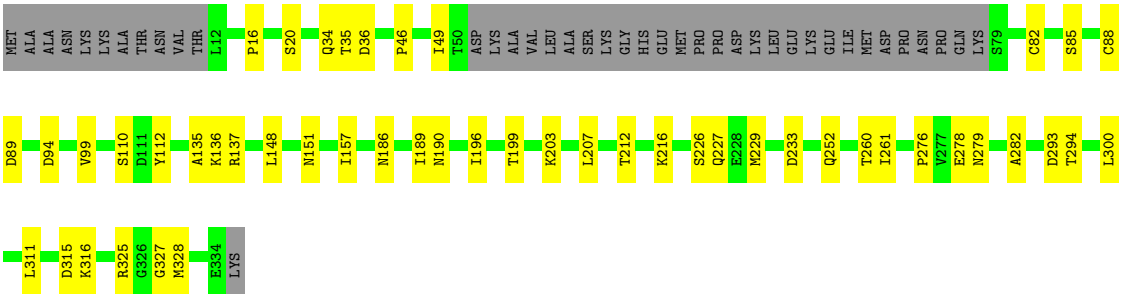
- Molecule 4: Cas7f

Chain I:



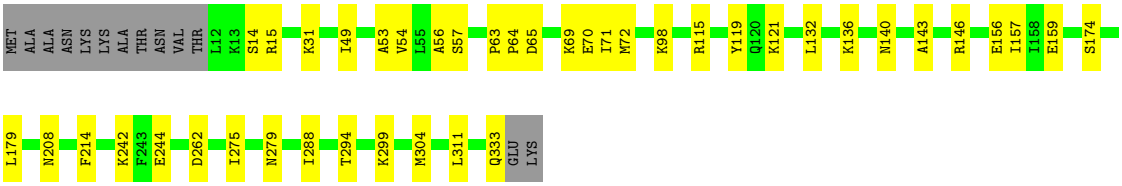
• Molecule 4: Cas7f

Chain D:



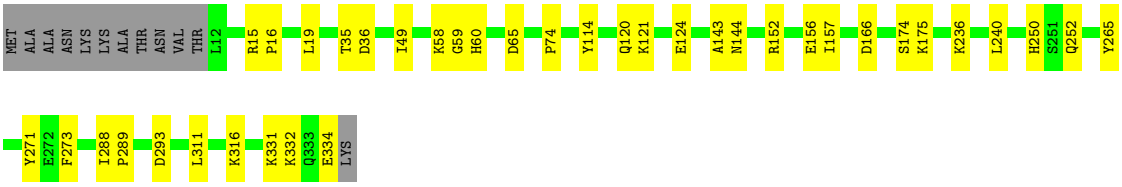
• Molecule 4: Cas7f

Chain E:



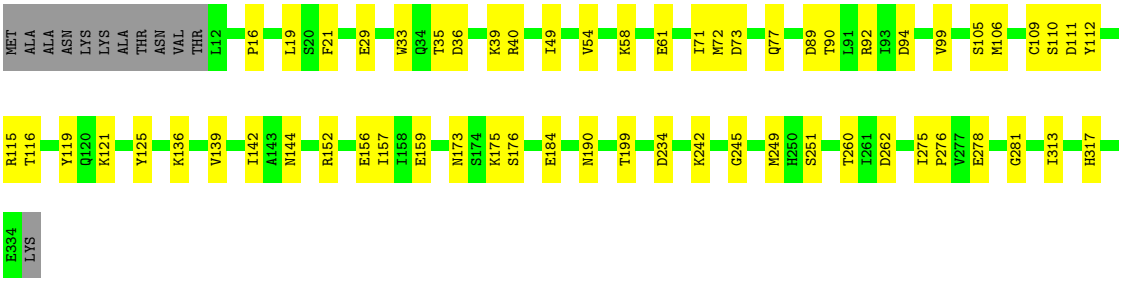
• Molecule 4: Cas7f

Chain F:



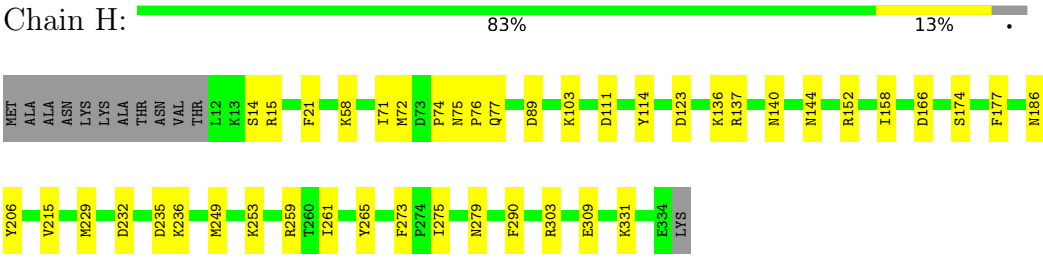
• Molecule 4: Cas7f

Chain G:



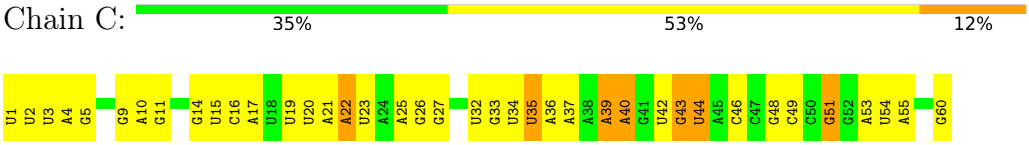
• Molecule 4: Cas7f

Chain H:



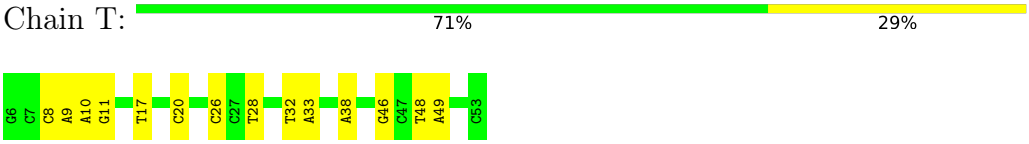
• Molecule 5: 60-nt crRNA

Chain C:



• Molecule 6: TS

Chain T:



• Molecule 7: NTS

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48756	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.12	0/2045	0.37	0/2756
2	J	0.14	0/2773	0.38	0/3745
3	B	0.17	0/1446	0.43	0/1945
4	D	0.12	0/2465	0.33	0/3327
4	E	0.11	0/2680	0.31	0/3618
4	F	0.12	0/2689	0.32	0/3630
4	G	0.11	0/2689	0.31	0/3630
4	H	0.10	0/2689	0.27	0/3630
4	I	0.10	0/2698	0.27	0/3641
5	C	0.15	0/1443	0.35	0/2250
6	T	0.20	0/1090	0.45	0/1678
7	N	0.15	0/258	0.34	0/397
All	All	0.13	0/24965	0.34	0/34247

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

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	2010	0	2030	41	0
2	J	2718	0	2708	72	0
3	B	1415	0	1437	35	0
4	D	2412	0	2379	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2621	0	2596	27	0
4	F	2630	0	2602	28	0
4	G	2630	0	2602	42	0
4	H	2630	0	2602	29	0
4	I	2639	0	2615	23	0
5	C	1287	0	645	24	0
6	T	975	0	545	16	0
7	N	230	0	125	4	0
All	All	24197	0	22886	326	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 7.

All (326) 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)
6:T:8:DC:H2"	6:T:9:DA:H5'	1.64	0.80
2:J:103:VAL:O	2:J:107:LEU:HB2	1.93	0.69
4:I:74:PRO:HG2	6:T:38:A:H1'	1.76	0.68
1:A:50:ILE:HG22	1:A:114:GLY:HA3	1.77	0.66
1:A:80:LEU:HD12	1:A:81:PRO:HD2	1.78	0.66
2:J:286:GLN:NE2	2:J:290:ASP:OD2	2.27	0.65
4:H:71:ILE:HG23	4:H:72:MET:HG2	1.80	0.64
1:A:43:LEU:HD22	1:A:48:ILE:HG13	1.80	0.64
2:J:79:ILE:HG22	2:J:90:GLN:HE21	1.64	0.63
4:G:106:MET:HE1	4:G:115:ARG:HG3	1.78	0.63
2:J:274:ARG:HG2	2:J:277:ARG:HH21	1.62	0.63
1:A:229:CYS:SG	1:A:230:SER:N	2.72	0.63
3:B:103:ARG:NH2	5:C:60:G:N7	2.47	0.63
6:T:28:DT:H5'	4:G:77:GLN:HE22	1.64	0.63
4:F:156:GLU:HG2	4:F:157:ILE:HG13	1.80	0.62
4:H:186:ASN:HB3	4:H:189:ILE:HB	1.81	0.62
2:J:40:VAL:HG21	2:J:80:VAL:HG21	1.82	0.62
1:A:98:ASN:HA	2:J:189:LEU:HD11	1.82	0.62
2:J:205:LYS:HZ3	7:N:19:A:HO3'	1.45	0.62
3:B:42:THR:HB	3:B:59:GLU:HB3	1.82	0.62
1:A:177:ASP:OD1	2:J:176:ARG:NH1	2.33	0.62
6:T:20:C:H1'	4:F:74:PRO:HG2	1.82	0.61
4:I:49:ILE:HD12	4:I:242:LYS:HG2	1.82	0.61
4:D:136:LYS:NZ	4:D:190:ASN:OD1	2.33	0.60
4:F:58:LYS:HD2	4:F:60:HIS:HE1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:TYR:HB2	4:E:288:ILE:HD11	1.85	0.59
2:J:289:LEU:HB3	2:J:294:TYR:HB2	1.84	0.59
2:J:314:ALA:O	2:J:319:ASN:ND2	2.36	0.58
2:J:112:ALA:O	2:J:116:HIS:ND1	2.32	0.58
4:D:229:MET:HG2	4:E:53:ALA:HB1	1.85	0.58
4:E:15:ARG:O	4:E:333:GLN:NE2	2.36	0.58
1:A:88:ASN:ND2	6:T:46:G:OP2	2.37	0.58
3:B:108:TYR:HE1	3:B:128:GLU:HG3	1.69	0.58
4:G:16:PRO:HG2	4:G:19:LEU:HB2	1.86	0.57
3:B:133:LYS:O	3:B:136:GLN:HB3	2.04	0.56
1:A:175:MET:HB3	2:J:67:LEU:HD13	1.86	0.56
4:I:311:LEU:O	4:I:316:LYS:NZ	2.38	0.56
3:B:110:THR:HA	3:B:113:ARG:HH12	1.68	0.56
5:C:51:G:N2	5:C:55:A:OP2	2.39	0.56
2:J:253:GLU:OE2	2:J:327:HIS:NE2	2.35	0.56
3:B:50:LYS:NZ	3:B:140:CYS:SG	2.79	0.56
3:B:130:HIS:O	3:B:133:LYS:HB2	2.06	0.56
4:E:65:ASP:O	4:E:69:LYS:NZ	2.38	0.56
4:E:159:GLU:HG2	4:E:214:PHE:HB2	1.88	0.56
4:D:135:ALA:HB1	4:D:196:ILE:HG23	1.89	0.55
4:D:279:ASN:OD1	4:D:325:ARG:NH2	2.40	0.55
2:J:149:GLN:OE1	5:C:4:A:N6	2.40	0.55
4:G:71:ILE:HG23	4:G:72:MET:HG2	1.88	0.55
4:F:288:ILE:HD12	4:F:289:PRO:HD2	1.89	0.55
4:H:76:PRO:O	4:H:77:GLN:NE2	2.39	0.55
2:J:274:ARG:HA	2:J:277:ARG:HB2	1.88	0.55
5:C:11:G:O2'	4:H:21:PHE:O	2.25	0.55
2:J:27:LEU:HD13	2:J:89:PRO:HG3	1.88	0.55
4:G:156:GLU:HG2	4:G:157:ILE:HG13	1.89	0.55
2:J:89:PRO:HA	2:J:92:PHE:HB3	1.89	0.54
4:E:262:ASP:HB3	4:E:275:ILE:HG13	1.89	0.54
1:A:97:MET:O	1:A:99:GLN:NE2	2.40	0.54
4:E:156:GLU:HG2	4:E:157:ILE:HG13	1.87	0.54
4:H:89:ASP:OD1	4:H:89:ASP:N	2.36	0.54
2:J:7:LEU:O	2:J:19:LYS:NZ	2.40	0.54
1:A:209:ARG:NH2	2:J:149:GLN:O	2.41	0.54
4:I:65:ASP:OD1	4:I:65:ASP:N	2.39	0.54
4:H:75:ASN:OD1	4:H:77:GLN:NE2	2.41	0.54
1:A:73:GLN:OE1	1:A:73:GLN:N	2.39	0.54
4:E:146:ARG:NH2	4:E:179:LEU:O	2.39	0.54
4:F:65:ASP:OD1	4:F:65:ASP:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:14:ILE:HG13	2:J:19:LYS:HG3	1.89	0.54
4:I:253:LYS:NZ	5:C:10:A:OP1	2.40	0.53
4:E:115:ARG:NH1	4:E:119:TYR:OH	2.41	0.53
4:G:262:ASP:HB3	4:G:275:ILE:HG13	1.91	0.53
4:D:260:THR:HA	4:D:276:PRO:HA	1.90	0.53
1:A:161:THR:OG1	1:A:163:ARG:NH1	2.42	0.53
4:G:136:LYS:NZ	4:G:190:ASN:OD1	2.42	0.53
4:E:304:MET:HB2	4:E:311:LEU:HD11	1.91	0.53
5:C:22:A:O2'	5:C:23:U:O4'	2.26	0.53
4:F:144:ASN:O	4:F:152:ARG:NH1	2.42	0.53
4:H:232:ASP:O	4:H:236:LYS:NZ	2.42	0.53
3:B:7:ILE:HG23	3:B:85:LYS:HB3	1.91	0.53
2:J:110:ASP:OD1	2:J:115:ARG:NH2	2.42	0.53
3:B:148:SER:HB2	3:B:153:GLN:H	1.75	0.52
3:B:18:ILE:O	3:B:22:GLU:HB2	2.09	0.52
4:F:15:ARG:NH2	4:G:61:GLU:OE1	2.41	0.52
3:B:148:SER:N	3:B:153:GLN:O	2.38	0.52
5:C:14:G:OP2	4:H:259:ARG:NH2	2.41	0.52
4:G:16:PRO:HB2	4:G:110:SER:HB3	1.92	0.52
4:H:136:LYS:O	4:H:140:ASN:ND2	2.42	0.52
1:A:178:LYS:HE2	2:J:62:MET:HE1	1.92	0.52
4:H:144:ASN:O	4:H:152:ARG:NH1	2.42	0.52
2:J:279:GLU:O	2:J:281:LYS:NZ	2.43	0.51
1:A:120:SER:HA	1:A:123:LYS:HD2	1.93	0.51
4:H:158:ILE:HG23	4:H:215:VAL:HG22	1.93	0.51
1:A:210:ASP:OD2	1:A:213:LYS:NZ	2.42	0.51
4:F:120:GLN:NE2	4:F:124:GLU:OE2	2.43	0.51
2:J:76:GLU:OE2	2:J:201:ARG:NH1	2.43	0.51
2:J:195:ALA:O	2:J:198:THR:OG1	2.28	0.51
4:D:252:GLN:HE21	4:E:54:VAL:HG12	1.76	0.51
4:G:94:ASP:OD1	4:G:94:ASP:N	2.43	0.51
4:G:242:LYS:NZ	4:G:245:GLY:O	2.44	0.51
4:G:260:THR:HA	4:G:276:PRO:HA	1.92	0.51
4:H:303:ARG:NH2	4:H:309:GLU:OE2	2.42	0.51
2:J:277:ARG:HD3	2:J:310:SER:HA	1.93	0.50
4:G:156:GLU:O	4:G:175:LYS:NZ	2.44	0.50
3:B:39:PHE:HA	3:B:61:LEU:O	2.12	0.50
1:A:190:VAL:HG23	1:A:192:ILE:HD11	1.93	0.50
4:D:311:LEU:O	4:D:316:LYS:NZ	2.44	0.50
4:F:143:ALA:O	4:F:174:SER:OG	2.27	0.50
1:A:176:LEU:HD21	2:J:176:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:233:ASP:OD1	4:D:233:ASP:N	2.37	0.50
4:I:21:PHE:O	5:C:5:G:O2'	2.27	0.50
1:A:246:GLU:HB2	1:A:249:LEU:HB2	1.94	0.49
4:G:144:ASN:O	4:G:152:ARG:NH1	2.45	0.49
4:G:136:LYS:HD3	4:G:184:GLU:HG3	1.94	0.49
5:C:10:A:O2'	5:C:11:G:O4'	2.28	0.49
5:C:14:G:N3	4:H:253:LYS:NZ	2.60	0.49
2:J:200:SER:OG	2:J:201:ARG:N	2.45	0.49
3:B:65:LYS:HE3	3:B:90:ILE:HB	1.94	0.49
3:B:116:ARG:NH1	3:B:122:GLU:OE1	2.45	0.49
4:F:16:PRO:HG2	4:F:19:LEU:HB2	1.94	0.49
4:G:40:ARG:NE	4:G:159:GLU:OE2	2.45	0.49
4:G:105:SER:OG	4:G:105:SER:O	2.30	0.49
4:I:186:ASN:HB3	4:I:189:ILE:HB	1.95	0.49
5:C:37:A:H1'	4:E:56:ALA:HB2	1.94	0.49
4:D:16:PRO:HB2	4:D:110:SER:HB3	1.95	0.49
4:I:16:PRO:HG2	4:I:19:LEU:HB2	1.93	0.49
4:E:31:LYS:NZ	4:E:244:GLU:OE1	2.45	0.49
1:A:2:MET:SD	1:A:2:MET:N	2.85	0.49
4:E:294:THR:HA	4:E:299:LYS:HG3	1.95	0.49
7:N:16:C:H2"	7:N:17:G:C8	2.47	0.49
4:D:49:ILE:HD13	4:D:82:CYS:HB2	1.95	0.48
4:D:89:ASP:OD1	4:D:89:ASP:N	2.46	0.48
4:D:94:ASP:OD1	4:D:212:THR:OG1	2.26	0.48
1:A:202:VAL:HG12	1:A:216:CYS:HB2	1.95	0.48
4:H:137:ARG:NH1	4:H:261:ILE:O	2.44	0.48
2:J:322:MET:SD	2:J:322:MET:N	2.86	0.48
4:G:33:TRP:HB2	4:G:92:ARG:HB3	1.96	0.48
4:F:156:GLU:O	4:F:175:LYS:NZ	2.47	0.48
1:A:133:ARG:O	5:C:2:U:N3	2.41	0.48
2:J:302:GLU:HB2	2:J:328:HIS:HD2	1.79	0.48
4:H:174:SER:HA	4:H:177:PHE:HD2	1.79	0.48
2:J:39:HIS:HB2	2:J:54:ALA:HB3	1.96	0.48
2:J:104:MET:SD	2:J:104:MET:N	2.86	0.48
2:J:32:ASP:N	2:J:32:ASP:OD1	2.38	0.48
3:B:8:ILE:HG21	3:B:16:PRO:HB3	1.96	0.48
4:F:35:THR:OG1	4:F:36:ASP:N	2.47	0.48
4:D:226:SER:OG	4:D:227:GLN:N	2.47	0.48
4:G:35:THR:O	4:G:90:THR:OG1	2.31	0.48
4:D:293:ASP:OD1	4:D:294:THR:N	2.47	0.47
4:D:282:ALA:HB1	4:E:72:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:136:LYS:O	4:E:140:ASN:ND2	2.46	0.47
1:A:10:LYS:HB2	1:A:143:LYS:HB2	1.97	0.47
1:A:223:SER:OG	1:A:224:LEU:N	2.47	0.47
2:J:90:GLN:HG2	2:J:201:ARG:HB3	1.96	0.47
2:J:70:ALA:H	2:J:74:TRP:HE1	1.63	0.47
6:T:8:DC:H2"	6:T:9:DA:H2'	1.97	0.47
4:F:311:LEU:O	4:F:316:LYS:NZ	2.47	0.47
4:H:235:ASP:OD1	4:H:236:LYS:N	2.47	0.47
4:I:144:ASN:O	4:I:152:ARG:NH1	2.47	0.47
4:F:252:GLN:HE21	4:G:54:VAL:HG12	1.79	0.47
2:J:51:ASN:OD1	2:J:51:ASN:N	2.48	0.47
4:G:49:ILE:HD12	4:G:242:LYS:HG2	1.97	0.47
4:G:58:LYS:HE3	4:G:73:ASP:HB2	1.96	0.47
4:D:203:LYS:HA	4:D:203:LYS:HD3	1.70	0.47
4:G:99:VAL:HG23	4:G:199:THR:HG21	1.97	0.46
2:J:230:LYS:HD3	2:J:230:LYS:HA	1.55	0.46
3:B:107:GLN:NE2	5:C:46:C:OP1	2.48	0.46
5:C:35:U:H1'	4:D:20:SER:HB3	1.98	0.46
4:G:139:VAL:HA	4:G:142:ILE:HG22	1.96	0.46
4:G:173:ASN:OD1	4:G:176:SER:OG	2.30	0.46
4:E:49:ILE:HD12	4:E:242:LYS:HG2	1.98	0.46
4:F:265:TYR:OH	4:F:273:PHE:O	2.33	0.46
2:J:246:ASP:HB2	2:J:249:CYS:HB3	1.97	0.46
4:D:278:GLU:OE1	4:E:57:SER:OG	2.34	0.46
4:G:234:ASP:OD1	4:G:234:ASP:N	2.49	0.46
2:J:250:LEU:O	2:J:301:TYR:OH	2.34	0.46
5:C:43:G:H1'	5:C:44:U:C2	2.51	0.46
4:G:73:ASP:OD1	4:G:73:ASP:N	2.49	0.46
4:H:111:ASP:OD2	4:H:114:TYR:N	2.47	0.46
7:N:14:A:H2"	7:N:15:G:C8	2.51	0.46
1:A:231:LYS:HB3	1:A:231:LYS:HE2	1.80	0.45
2:J:27:LEU:O	2:J:31:ILE:HG12	2.15	0.45
4:I:62:MET:HG2	4:I:66:LYS:HE2	1.98	0.45
6:T:8:DC:C2'	6:T:9:DA:H2'	2.46	0.45
4:I:33:TRP:CD2	4:I:44:LYS:HD2	2.51	0.45
4:F:293:ASP:OD1	4:F:293:ASP:N	2.47	0.45
2:J:36:LEU:HD22	2:J:135:MET:HG2	1.98	0.45
4:D:85:SER:OG	4:D:88:CYS:SG	2.69	0.45
1:A:70:LYS:HD2	1:A:70:LYS:HA	1.84	0.45
4:F:332:LYS:HE3	4:F:334:GLU:HG2	1.98	0.45
1:A:177:ASP:HA	1:A:180:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:62:SER:OG	3:B:64:ASP:O	2.34	0.45
3:B:134:LYS:HB3	3:B:134:LYS:HE2	1.79	0.45
4:I:156:GLU:OE1	4:H:206:TYR:OH	2.28	0.45
4:D:186:ASN:HB3	4:D:189:ILE:HB	1.98	0.45
5:C:39:A:H1'	5:C:40:A:C8	2.52	0.45
4:F:49:ILE:HD13	4:F:240:LEU:HB2	1.99	0.45
1:A:189:LEU:HD13	1:A:224:LEU:HD23	1.98	0.45
3:B:17:ASN:OD1	3:B:17:ASN:N	2.50	0.45
4:H:249:MET:HE2	4:H:249:MET:HB3	1.81	0.45
4:E:98:LYS:NZ	4:E:208:ASN:OD1	2.47	0.44
2:J:272:ARG:O	2:J:277:ARG:NH1	2.51	0.44
6:T:9:DA:H1'	6:T:10:DA:C8	2.51	0.44
4:F:121:LYS:HA	4:F:121:LYS:HD2	1.79	0.44
3:B:93:THR:HG23	3:B:96:TYR:HD2	1.81	0.44
2:J:97:MET:HE2	2:J:97:MET:HB2	1.74	0.44
2:J:173:VAL:HG13	2:J:177:LEU:HD23	1.99	0.44
2:J:87:LYS:NZ	2:J:200:SER:O	2.44	0.44
3:B:38:LYS:HE3	3:B:62:SER:HB2	1.99	0.44
1:A:5:TYR:HB3	1:A:109:LEU:HD11	1.99	0.44
2:J:30:SER:O	2:J:30:SER:OG	2.34	0.44
2:J:229:ASP:OD1	2:J:230:LYS:N	2.46	0.44
2:J:318:LYS:HE2	2:J:318:LYS:HB2	1.71	0.44
4:D:34:GLN:NE2	4:D:46:PRO:O	2.35	0.44
4:D:157:ILE:HG22	4:D:216:LYS:HB3	1.99	0.44
4:I:271:TYR:HB3	4:I:273:PHE:CE2	2.53	0.44
4:I:35:THR:OG1	4:I:36:ASP:N	2.51	0.44
4:I:196:ILE:HD13	4:I:207:LEU:HD23	1.98	0.44
4:I:259:ARG:NH2	4:I:278:GLU:OE2	2.51	0.44
4:D:199:THR:HG21	4:D:207:LEU:HB2	1.99	0.44
3:B:4:GLN:HB2	3:B:68:LEU:HD13	2.00	0.43
4:G:249:MET:HE3	4:G:249:MET:HB2	1.93	0.43
1:A:214:ASP:HB3	2:J:159:HIS:CD2	2.53	0.43
4:I:61:GLU:OE1	4:H:15:ARG:NH2	2.40	0.43
4:E:121:LYS:HA	4:E:121:LYS:HD2	1.80	0.43
3:B:94:ASP:OD1	3:B:94:ASP:N	2.50	0.43
3:B:127:LEU:O	3:B:130:HIS:ND1	2.44	0.43
5:C:51:G:O2'	5:C:55:A:N6	2.51	0.43
1:A:7:LEU:HD13	1:A:109:LEU:HD13	2.00	0.43
3:B:117:LYS:HA	3:B:117:LYS:HD2	1.72	0.43
4:D:99:VAL:HG11	4:D:196:ILE:HD11	2.00	0.43
2:J:151:PHE:HD2	5:C:1:U:H2'	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:279:ASN:ND2	4:F:59:GLY:O	2.52	0.43
1:A:207:GLY:HA2	4:I:17:GLU:HG3	2.00	0.43
3:B:153:GLN:OE1	3:B:154:SER:N	2.40	0.43
4:E:63:PRO:HA	4:E:64:PRO:HD3	1.92	0.43
4:H:166:ASP:OD1	4:H:166:ASP:N	2.52	0.43
6:T:8:DC:C4	6:T:9:DA:C6	3.06	0.43
6:T:17:DT:C2	4:D:328:MET:HE1	2.54	0.43
4:E:69:LYS:HG3	4:E:70:GLU:HG3	2.01	0.43
4:H:14:SER:OG	4:H:15:ARG:N	2.52	0.43
1:A:133:ARG:NH1	5:C:5:G:OP1	2.52	0.42
2:J:239:ILE:HD12	2:J:321:ILE:HD12	2.00	0.42
5:C:51:G:H22	5:C:55:A:P	2.42	0.42
3:B:20:ILE:HA	3:B:24:ILE:HD12	2.02	0.42
4:I:262:ASP:HB3	4:I:275:ILE:HG13	2.02	0.42
2:J:234:LEU:HD23	2:J:234:LEU:HA	1.92	0.42
2:J:326:GLU:O	2:J:330:ARG:HG2	2.19	0.42
4:F:236:LYS:HE2	4:F:236:LYS:HB2	1.84	0.42
4:G:35:THR:OG1	4:G:36:ASP:N	2.53	0.42
4:E:132:LEU:HG	4:E:136:LYS:HD2	2.01	0.42
4:F:331:LYS:HD2	4:F:331:LYS:HA	1.81	0.42
3:B:43:PHE:HE1	3:B:58:ILE:HD13	1.84	0.42
4:I:304:MET:HE3	4:I:311:LEU:HD12	2.02	0.42
6:T:48:DT:H2"	6:T:49:A:C8	2.55	0.42
4:D:35:THR:OG1	4:D:36:ASP:N	2.53	0.42
4:F:332:LYS:O	4:F:332:LYS:NZ	2.34	0.42
4:H:331:LYS:HA	4:H:331:LYS:HD3	1.83	0.42
2:J:188:ARG:HB2	2:J:208:TRP:CD2	2.55	0.42
3:B:3:SER:HA	3:B:60:VAL:O	2.18	0.42
4:I:284:ARG:HE	4:I:284:ARG:HB3	1.63	0.42
6:T:26:C:H4'	4:G:73:ASP:HB3	2.01	0.42
4:E:71:ILE:HG23	4:E:72:MET:SD	2.60	0.42
4:F:16:PRO:HD3	4:F:114:TYR:CD1	2.55	0.42
4:G:111:ASP:OD1	4:G:112:TYR:N	2.53	0.42
2:J:124:LYS:HD2	2:J:124:LYS:HA	1.76	0.42
4:G:39:LYS:HB2	4:G:39:LYS:HE3	1.87	0.42
4:H:103:LYS:NZ	4:H:123:ASP:OD1	2.43	0.42
1:A:22:ILE:HD12	1:A:23:ILE:HG12	2.02	0.41
2:J:114:LEU:O	2:J:118:MET:HG2	2.19	0.41
2:J:259:ILE:HD13	2:J:259:ILE:HA	1.89	0.41
3:B:2:PHE:HB3	3:B:90:ILE:HG22	2.01	0.41
3:B:145:LYS:HA	3:B:145:LYS:HD3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:205:GLU:HG2	4:H:206:TYR:HD1	1.84	0.41
4:H:265:TYR:OH	4:H:273:PHE:O	2.29	0.41
7:N:12:DT:H2'	7:N:13:DT:H71	2.01	0.41
2:J:188:ARG:HB2	2:J:208:TRP:CG	2.55	0.41
3:B:153:GLN:CD	3:B:154:SER:H	2.27	0.41
6:T:10:DA:H3'	6:T:11:DG:C8	2.55	0.41
2:J:22:LYS:HD3	2:J:22:LYS:HA	1.77	0.41
6:T:32:DT:H1'	4:H:74:PRO:HG2	2.02	0.41
4:G:29:GLU:OE1	4:G:251:SER:N	2.54	0.41
4:G:125:TYR:OH	4:G:317:HIS:ND1	2.50	0.41
1:A:18:ALA:HB2	1:A:102:ILE:HB	2.02	0.41
5:C:36:A:H2'	5:C:37:A:C8	2.55	0.41
6:T:33:A:OP1	4:H:58:LYS:NZ	2.50	0.41
4:D:148:LEU:O	4:D:151:ASN:ND2	2.49	0.41
4:G:116:THR:O	4:G:119:TYR:HB2	2.21	0.41
4:F:250:HIS:HB3	4:F:252:GLN:OE1	2.21	0.41
1:A:153:ASP:OD1	1:A:153:ASP:N	2.54	0.41
2:J:316:SER:O	2:J:320:MET:HE1	2.20	0.41
4:E:14:SER:OG	4:E:15:ARG:N	2.54	0.41
4:E:143:ALA:O	4:E:174:SER:OG	2.31	0.41
4:F:166:ASP:OD1	4:F:166:ASP:N	2.51	0.41
4:F:252:GLN:NE2	4:G:54:VAL:HG12	2.36	0.41
4:G:89:ASP:OD1	4:G:89:ASP:N	2.54	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.83	0.41
2:J:18:GLN:O	2:J:22:LYS:HG2	2.21	0.41
2:J:237:ILE:HG23	2:J:242:LEU:HD21	2.02	0.41
2:J:268:GLU:O	2:J:270:ASN:ND2	2.54	0.41
3:B:115:MET:HE2	3:B:115:MET:HB3	1.99	0.41
4:I:25:LEU:HD12	4:I:25:LEU:HA	1.96	0.41
5:C:35:U:O2'	4:D:327:GLY:O	2.39	0.41
4:D:300:LEU:HD23	4:D:315:ASP:HB3	2.03	0.41
4:F:271:TYR:HB3	4:F:273:PHE:CE2	2.56	0.41
4:G:106:MET:HE2	4:G:106:MET:HB3	1.86	0.41
4:G:278:GLU:OE1	4:G:281:GLY:N	2.54	0.41
4:H:275:ILE:HD13	4:H:290:PHE:HD2	1.86	0.41
1:A:247:GLU:H	1:A:247:GLU:HG2	1.66	0.41
2:J:10:ILE:HD11	2:J:23:TYR:HD1	1.85	0.40
2:J:133:LEU:HD23	2:J:133:LEU:HA	1.86	0.40
3:B:16:PRO:HA	3:B:19:ILE:HD12	2.03	0.40
4:G:121:LYS:HA	4:G:121:LYS:HD2	1.90	0.40
1:A:24:VAL:HG23	2:J:211:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:138:MET:SD	2:J:138:MET:N	2.94	0.40
3:B:123:LEU:HD13	5:C:54:U:N3	2.36	0.40
6:T:8:DC:H6	6:T:8:DC:H2'	1.72	0.40
4:G:313:ILE:HD12	4:G:313:ILE:HA	1.94	0.40
1:A:73:GLN:H	1:A:73:GLN:CD	2.28	0.40
2:J:177:LEU:HD21	2:J:212:PHE:CZ	2.57	0.40
2:J:320:MET:SD	2:J:320:MET:N	2.94	0.40
4:I:143:ALA:O	4:I:174:SER:OG	2.30	0.40
4:D:137:ARG:NH1	4:D:261:ILE:O	2.48	0.40
1:A:125:ILE:O	1:A:129:MET:HB2	2.22	0.40
1:A:221:ILE:HG22	2:J:68:ASP:HB3	2.02	0.40
2:J:97:MET:O	2:J:98:SER:C	2.65	0.40
5:C:17:A:O2'	4:G:21:PHE:O	2.35	0.40
2:J:303:VAL:HG13	2:J:320:MET:HG3	2.02	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	253/255 (99%)	236 (93%)	17 (7%)	0	100	100
2	J	338/344 (98%)	316 (94%)	22 (6%)	0	100	100
3	B	173/181 (96%)	153 (88%)	20 (12%)	0	100	100
4	D	291/335 (87%)	279 (96%)	12 (4%)	0	100	100
4	E	320/335 (96%)	305 (95%)	15 (5%)	0	100	100
4	F	321/335 (96%)	304 (95%)	17 (5%)	0	100	100
4	G	321/335 (96%)	308 (96%)	13 (4%)	0	100	100
4	H	321/335 (96%)	311 (97%)	10 (3%)	0	100	100
4	I	322/335 (96%)	314 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2660/2790 (95%)	2526 (95%)	134 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	219/219 (100%)	219 (100%)	0	100 100
2	J	299/304 (98%)	294 (98%)	5 (2%)	56 75
3	B	156/160 (98%)	155 (99%)	1 (1%)	84 91
4	D	265/299 (89%)	265 (100%)	0	100 100
4	E	289/299 (97%)	289 (100%)	0	100 100
4	F	290/299 (97%)	290 (100%)	0	100 100
4	G	290/299 (97%)	289 (100%)	1 (0%)	91 96
4	H	290/299 (97%)	288 (99%)	2 (1%)	81 89
4	I	291/299 (97%)	290 (100%)	1 (0%)	91 96
All	All	2389/2477 (96%)	2379 (100%)	10 (0%)	88 94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	96	GLU
2	J	97	MET
2	J	98	SER
2	J	123	ASP
2	J	187	LEU
3	B	7	ILE
4	I	284	ARG
4	G	109	CYS
4	H	229	MET
4	H	279	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	237	ASN
2	J	4	ASN
2	J	12	GLN
2	J	238	ASN
2	J	311	GLN
4	D	144	ASN
4	D	194	GLN
4	D	250	HIS
4	E	41	HIS
4	G	77	GLN
4	H	186	ASN
4	H	279	ASN
4	H	308	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	C	59/60 (98%)	24 (40%)	0
6	T	0/48	-	-
7	N	0/11	-	-
All	All	59/119 (49%)	24 (40%)	0

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	C	3	U
5	C	9	G
5	C	15	U
5	C	16	C
5	C	19	U
5	C	20	U
5	C	21	A
5	C	22	A
5	C	25	A
5	C	26	G
5	C	27	G
5	C	32	U
5	C	33	G
5	C	34	U

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Mol	Chain	Res	Type
5	C	35	U
5	C	39	A
5	C	40	A
5	C	42	U
5	C	43	G
5	C	44	U
5	C	48	G
5	C	49	C
5	C	51	G
5	C	53	A

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 oligosaccharides 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.