



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 29, 2017 – 09:04 PM EST

PDB ID : 6B44  
EMDB ID: : EMD-7048  
Title : Cryo-EM structure of Type I-F CRISPR crRNA-guided Csy surveillance complex with bound target dsDNA  
Authors : Guo, T.W.; Bartesaghi, A.; Yang, H.; Falconieri, V.; Rao, P.; Merk, A.; Fox, T.; Earl, L.; Patel, D.J.; Subramaniam, S.  
Deposited on : unknown  
Resolution : 2.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

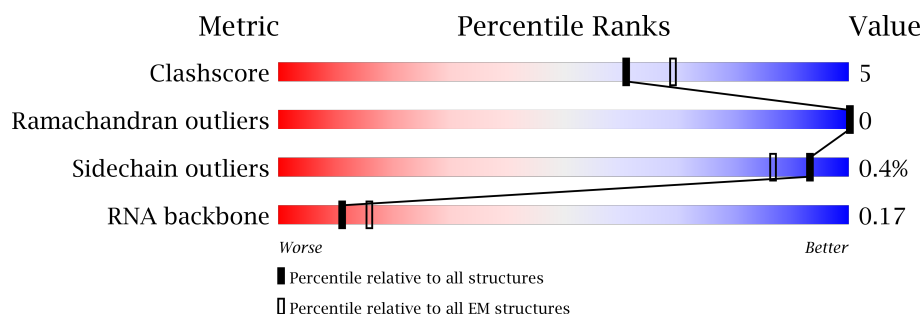
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	436	93% (Green) . . (Grey)
2	B	329	71% (Green) 21% (Yellow) 7% (Grey)
3	C	344	67% (Green) 18% (Yellow) 15% (Grey)
3	D	344	80% (Green) 17% (Yellow) . (Grey)
3	E	344	84% (Green) 13% (Yellow) . (Grey)
3	F	344	86% (Green) 11% (Yellow) . (Grey)
3	G	344	85% (Green) 11% (Yellow) . (Grey)
3	H	344	82% (Green) 15% (Yellow) . (Grey)

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L	189	<div><div></div><div>99%</div><div></div></div>
5	M	60	<div><div></div><div>30%</div><div></div><div>50%</div><div></div><div>18%</div><div></div></div>
6	N	49	<div><div></div><div>63%</div><div></div><div>18%</div><div></div><div>•</div><div>16%</div><div></div></div>
7	O	27	<div><div></div><div>30%</div><div></div><div>19%</div><div></div><div>52%</div><div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22681 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 CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	424	Total	C	N	O	0	0
			2079	1145	473	461		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q02ML9
A	0	SER	-	expression tag	UNP Q02ML9

- Molecule 2 is a protein called CRISPR-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	305	Total	C	N	O	S	0	0
			2374	1504	440	425	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP Q02MM0
B	0	ALA	-	expression tag	UNP Q02MM0

- Molecule 3 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		
3	D	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	E	334	Total	C	N	O	S	0	0
			2561	1611	466	482	2		
3	F	335	Total	C	N	O	S	0	0
			2566	1614	467	483	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	333	Total	C	N	O	S	0	0
			2557	1608	466	481	2		
3	H	333	Total	C	N	O	S	0	0
			2569	1613	469	485	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP Q02MM1
C	0	ALA	-	expression tag	UNP Q02MM1
D	-1	MET	-	initiating methionine	UNP Q02MM1
D	0	ALA	-	expression tag	UNP Q02MM1
E	-1	MET	-	initiating methionine	UNP Q02MM1
E	0	ALA	-	expression tag	UNP Q02MM1
F	-1	MET	-	initiating methionine	UNP Q02MM1
F	0	ALA	-	expression tag	UNP Q02MM1
G	-1	MET	-	initiating methionine	UNP Q02MM1
G	0	ALA	-	expression tag	UNP Q02MM1
H	-1	MET	-	initiating methionine	UNP Q02MM1
H	0	ALA	-	expression tag	UNP Q02MM1

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	189	Total	C	N	O	S	0	0
			761	382	189	189	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	MET	-	initiating methionine	UNP Q02MM2
L	0	ALA	-	expression tag	UNP Q02MM2

- Molecule 5 is a RNA chain called Pseudomonas aeruginosa strain SMC4485 CRISPR repeat sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	60	Total	C	N	O	P	0	0
			1276	569	223	424	60		

- Molecule 6 is a DNA chain called Target DNA strand (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	41	Total	C	N	O	P	0	0
			850	400	167	242	41		

- Molecule 7 is a DNA chain called Non-target DNA strand (5'-D(P\*CP\*AP\*GP\*TP\*CP\*AP\*TP\*CP\*AP\*CP\*CP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	13	Total	C	N	O	P	0	0
			262	125	49	75	13		





• Molecule 3: CRISPR-associated protein Csy3

Chain E: 84% 13% .



• Molecule 3: CRISPR-associated protein Csy3

Chain F: 86% 11% .



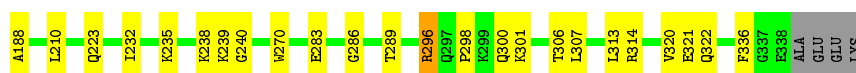
• Molecule 3: CRISPR-associated protein Csy3

Chain G: 85% 11% .



• Molecule 3: CRISPR-associated protein Csy3

Chain H: 82% 15% .



• Molecule 4: CRISPR-associated endonuclease Cas6/Csy4

Chain L: 99% .



• Molecule 5: Pseudomonas aeruginosa strain SMC4485 CRISPR repeat sequence



Chain M: 




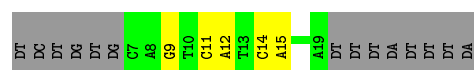
- Molecule 6: Target DNA strand (41-MER)

Chain N: 



- Molecule 7: Non-target DNA strand (5'-D(P\*CP\*AP\*GP\*TP\*CP\*AP\*TP\*CP\*AP\*CP\*CP\*AP\*A)-3')

Chain O: 



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39811	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k 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  >2	RMSZ	# Z  >2
1	A	0.27	0/2104	0.51	0/2715
2	B	0.32	0/2431	0.61	1/3310 (0.0%)
3	C	0.31	0/2315	0.66	1/3143 (0.0%)
3	D	0.33	0/2601	0.62	0/3532
3	E	0.36	0/2608	0.59	1/3540 (0.0%)
3	F	0.39	0/2613	0.61	1/3547 (0.0%)
3	G	0.37	0/2604	0.58	1/3533 (0.0%)
3	H	0.35	0/2616	0.58	1/3548 (0.0%)
4	L	0.23	0/760	0.49	0/949
5	M	0.63	0/1424	1.26	16/2217 (0.7%)
6	N	0.90	0/956	0.95	1/1475 (0.1%)
7	O	0.68	0/293	1.03	0/448
All	All	0.41	0/23325	0.69	23/31957 (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
3	D	0	1
3	H	0	1
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	42	U	C2-N1-C1'	9.81	129.47	117.70
5	M	42	U	N1-C2-O2	7.92	128.35	122.80
3	C	18	LEU	CA-CB-CG	7.82	133.28	115.30
5	M	47	U	C2-N1-C1'	7.27	126.42	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	42	U	N3-C2-O2	-7.02	117.29	122.20
5	M	29	C	O4'-C1'-N1	7.01	113.81	108.20
5	M	11	C	O4'-C1'-N1	6.64	113.51	108.20
5	M	23	G	O4'-C1'-N9	6.58	113.47	108.20
5	M	42	U	C6-N1-C1'	-6.54	112.04	121.20
5	M	42	U	C5-C6-N1	6.31	125.86	122.70
3	H	296	ARG	C-N-CA	6.29	137.44	121.70
5	M	20	C	N1-C2-O2	6.23	122.64	118.90
5	M	47	U	N1-C2-O2	6.18	127.13	122.80
3	G	251	ASP	CB-CG-OD1	5.71	123.44	118.30
5	M	47	U	C5-C6-N1	5.52	125.46	122.70
5	M	16	C	O4'-C1'-N1	5.50	112.60	108.20
3	E	231	LEU	CA-CB-CG	5.47	127.88	115.30
2	B	181	LEU	CA-CB-CG	5.46	127.85	115.30
5	M	20	C	N3-C2-O2	-5.27	118.21	121.90
3	F	251	ASP	CB-CG-OD1	5.20	122.98	118.30
5	M	43	U	C2-N1-C1'	5.16	123.89	117.70
5	M	1	C	C2-N1-C1'	5.14	124.46	118.80
6	N	38	DT	O4'-C1'-N1	5.14	111.60	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	248	SER	Peptide
3	H	300	GLN	Peptide

## 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	2079	0	1094	11	0
2	B	2374	0	2345	46	0
3	C	2272	0	2232	35	0
3	D	2554	0	2522	37	0
3	E	2561	0	2542	26	0
3	F	2566	0	2547	23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2557	0	2542	22	0
3	H	2569	0	2557	33	0
4	L	761	0	216	2	0
5	M	1276	0	646	15	0
6	N	850	0	458	11	0
7	O	262	0	146	4	0
All	All	22681	0	19847	223	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 5.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:ALA:O	3:H:110:ASN:ND2	2.29	0.66
3:F:265:ARG:NH2	5:M:20:C:OP2	2.31	0.64
3:D:166:ARG:HH12	3:D:208:HIS:HB3	1.63	0.64
2:B:213:LEU:HA	2:B:218:ARG:HH21	1.63	0.63
3:C:98:ARG:NH2	3:D:153:VAL:O	2.32	0.63
2:B:54:ILE:HA	2:B:115:GLY:HA3	1.82	0.62
3:C:296:ARG:HG3	3:C:302:LEU:HG	1.79	0.62
6:N:39:DG:H1	7:O:11:DC:H42	1.48	0.62
3:C:184:ARG:HD3	3:C:278:GLY:HA3	1.81	0.62
2:B:18:GLN:HE22	3:H:21:SER:HA	1.65	0.61
2:B:10:LEU:HB3	2:B:111:LEU:HB2	1.81	0.61
3:C:17:LYS:HE3	3:C:100:LEU:HB3	1.83	0.61
2:B:12:LEU:HB2	2:B:109:LEU:HB2	1.83	0.60
3:E:136:ARG:O	3:E:140:HIS:ND1	2.34	0.60
1:A:233:SER:OG	2:B:218:ARG:NH1	2.33	0.60
3:C:94:ARG:HA	3:C:214:VAL:HG12	1.84	0.60
2:B:148:CYS:SG	2:B:149:ASN:N	2.74	0.59
3:D:265:ARG:NH1	3:D:282:VAL:O	2.34	0.59
3:C:144:ASN:HD21	3:C:181:ILE:HB	1.66	0.59
3:G:30:TRP:HD1	3:G:90:THR:HG1	1.51	0.58
3:H:12:LEU:HB2	3:H:336:PHE:HB2	1.84	0.58
3:G:265:ARG:NH2	5:M:14:G:OP2	2.36	0.58
2:B:73:PRO:HG2	2:B:76:LYS:HB2	1.85	0.58
3:D:144:ASN:HA	3:D:178:ALA:HB1	1.84	0.58
3:F:265:ARG:NH1	3:F:282:VAL:O	2.38	0.57
3:E:184:ARG:NH2	3:E:276:GLY:O	2.37	0.57
3:E:265:ARG:NH2	5:M:26:G:OP2	2.36	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:VAL:HG21	2:B:277:LEU:HD22	1.86	0.57
2:B:46:ARG:NH2	5:M:1:C:O4'	2.38	0.57
1:A:171:SER:OG	1:A:177:GLN:NE2	2.38	0.56
3:H:144:ASN:ND2	3:H:182:GLY:O	2.39	0.56
2:B:219:ILE:HG23	2:B:240:GLN:H	1.70	0.56
3:C:307:LEU:HD13	3:C:326:VAL:HG22	1.88	0.56
3:H:232:ILE:HG21	3:H:235:LYS:HD3	1.88	0.56
2:B:72:GLN:NE2	2:B:76:LYS:O	2.38	0.56
3:H:172:ARG:NH1	3:H:173:ALA:O	2.39	0.56
3:F:164:HIS:HB3	3:F:172:ARG:HB3	1.88	0.56
3:C:228:SER:HB2	3:C:255:ILE:HG23	1.88	0.55
3:D:48:SER:HA	3:D:78:THR:HA	1.87	0.55
3:E:36:SER:O	3:E:92:LYS:NZ	2.38	0.55
3:D:57:LEU:HD13	3:D:67:LEU:HB2	1.88	0.55
3:C:137:ARG:NH2	3:C:267:ILE:O	2.39	0.55
3:C:133:GLU:OE1	3:C:136:ARG:NH2	2.39	0.55
3:G:129:GLN:HE22	3:G:320:VAL:HG13	1.72	0.54
2:B:159:LEU:HD21	2:B:176:LEU:HD11	1.88	0.54
2:B:248:LEU:HD23	2:B:288:GLU:HB3	1.89	0.54
1:A:216:LYS:HD3	1:A:219:ARG:HD3	1.89	0.54
2:B:17:ILE:HD11	2:B:105:LEU:HD12	1.88	0.54
3:C:142:LEU:HD22	3:C:213:VAL:HG21	1.89	0.54
3:C:145:ALA:HB1	3:C:148:LEU:HB2	1.90	0.54
3:E:33:ARG:NH1	3:E:159:GLU:OE1	2.40	0.53
3:G:10:SER:OG	3:G:110:ASN:ND2	2.42	0.53
3:E:296:ARG:HG3	3:E:302:LEU:HB3	1.91	0.53
3:F:36:SER:O	3:F:92:LYS:NZ	2.38	0.53
6:N:35:DT:H2"	6:N:36:DG:C8	2.44	0.53
3:E:164:HIS:HD2	3:E:171:ALA:HB3	1.74	0.53
3:C:146:ARG:NH2	3:C:183:LEU:O	2.41	0.53
3:C:166:ARG:HH22	3:C:209:VAL:HA	1.73	0.53
3:F:10:SER:OG	3:F:110:ASN:ND2	2.41	0.53
2:B:44:LEU:HD21	2:B:134:ALA:HB2	1.89	0.52
3:D:145:ALA:HB1	3:D:148:LEU:HD13	1.89	0.52
3:E:48:SER:HA	3:E:78:THR:HA	1.92	0.52
2:B:214:LEU:HD23	2:B:286:LEU:HD11	1.92	0.52
3:G:144:ASN:ND2	3:G:182:GLY:O	2.43	0.52
2:B:305:HIS:HD2	2:B:316:TRP:HB3	1.74	0.52
3:D:33:ARG:NH1	3:D:159:GLU:OE1	2.44	0.51
3:G:17:LYS:HG3	3:G:100:LEU:HB2	1.92	0.51
3:G:166:ARG:HH12	3:G:208:HIS:HB3	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:152:GLY:O	5:M:40:G:O2'	2.28	0.51
3:D:136:ARG:O	3:D:140:HIS:ND1	2.41	0.51
3:C:109:CYS:SG	3:C:110:ASN:N	2.84	0.51
3:D:258:GLN:NE2	5:M:33:U:OP1	2.42	0.51
1:A:195:PRO:HB2	1:A:198:LEU:HB3	1.93	0.51
3:E:167:GLN:HB2	3:E:169:GLU:HG3	1.93	0.51
3:D:229:GLN:OE1	5:M:33:U:O2'	2.29	0.51
1:A:199:VAL:O	1:A:203:HIS:HB2	2.11	0.50
2:B:88:LEU:HG	3:H:289:THR:HG22	1.92	0.50
3:H:62:ARG:NH2	3:H:63:ASP:O	2.43	0.50
3:G:265:ARG:NH1	3:G:282:VAL:O	2.44	0.50
2:B:220:ASN:H	2:B:240:GLN:HB2	1.76	0.50
3:F:137:ARG:NH2	3:F:269:THR:OG1	2.45	0.50
4:L:154:HIS:H	5:M:42:U:H4'	1.75	0.50
3:C:324:HIS:HA	3:C:327:ILE:HG22	1.94	0.50
3:E:104:GLY:HA3	3:E:122:VAL:HG11	1.94	0.50
3:D:30:TRP:HE1	3:D:218:ARG:HB2	1.77	0.49
3:E:270:TRP:CD1	3:E:321:GLU:HB2	2.47	0.49
2:B:242:ARG:HH12	2:B:245:PRO:HD3	1.77	0.49
3:F:73:SER:HB3	6:N:14:DA:H4'	1.93	0.49
1:A:207:ARG:NH1	1:A:257:GLU:O	2.46	0.49
2:B:34:PRO:HA	2:B:37:PHE:HD2	1.78	0.49
3:F:159:GLU:HB3	3:F:216:PHE:HB2	1.94	0.49
3:G:96:THR:OG1	3:H:223:GLN:NE2	2.45	0.49
3:E:137:ARG:NH2	3:E:269:THR:OG1	2.42	0.49
2:B:117:GLY:HA2	2:B:120:ASP:HB2	1.94	0.48
6:N:39:DG:N2	7:O:12:DA:N1	2.61	0.48
3:C:161:ARG:HE	3:C:175:ARG:HH21	1.61	0.48
3:G:57:LEU:HB3	3:G:67:LEU:HD21	1.95	0.48
3:C:14:PHE:HB2	3:C:333:GLY:HA2	1.95	0.48
3:C:299:LYS:HD3	3:D:62:ARG:HH22	1.79	0.48
3:G:266:THR:HA	3:G:281:ALA:HA	1.95	0.48
3:E:189:ASP:N	3:E:189:ASP:OD1	2.47	0.48
3:H:36:SER:O	3:H:92:LYS:NZ	2.43	0.48
3:F:296:ARG:NH1	3:F:322:GLN:OE1	2.38	0.48
3:D:144:ASN:HB2	3:D:152:ARG:HH12	1.76	0.48
3:G:8:THR:HG23	3:G:313:LEU:HD11	1.96	0.47
2:B:46:ARG:NH1	5:M:1:C:OP2	2.47	0.47
3:G:74:PRO:HG2	6:N:20:DA:H1'	1.94	0.47
3:C:10:SER:OG	3:C:110:ASN:OD1	2.32	0.47
3:D:156:GLU:HB2	3:D:218:ARG:HD2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ALA:HB1	2:B:156:ASN:HB2	1.96	0.47
2:B:90:ARG:HH21	3:H:298:PRO:HG2	1.78	0.47
3:F:104:GLY:HA3	3:F:122:VAL:HG11	1.97	0.47
3:D:109:CYS:SG	3:D:110:ASN:N	2.87	0.47
3:H:136:ARG:HH21	3:H:188:ALA:HB2	1.79	0.47
2:B:257:ALA:HA	2:B:280:VAL:HG12	1.97	0.47
3:C:319:ALA:HB3	3:C:322:GLN:HG2	1.95	0.47
3:D:184:ARG:HG2	3:D:278:GLY:HA3	1.96	0.47
3:D:229:GLN:NE2	5:M:35:U:OP2	2.44	0.47
3:D:158:VAL:HG22	3:D:179:LEU:HG	1.96	0.47
3:C:14:PHE:HE1	3:C:106:PRO:HB3	1.80	0.46
3:D:140:HIS:NE2	3:D:187:LYS:O	2.48	0.46
3:F:74:PRO:HG2	6:N:14:DA:H1'	1.97	0.46
3:G:289:THR:HG21	3:H:74:PRO:HB3	1.97	0.46
3:C:227:PRO:HG2	3:C:246:LEU:HB3	1.96	0.46
3:H:8:THR:HB	3:H:313:LEU:HD11	1.97	0.46
3:C:160:VAL:O	3:C:176:PHE:N	2.49	0.46
3:D:172:ARG:NH1	3:D:173:ALA:O	2.48	0.46
2:B:143:SER:HB2	3:H:98:ARG:HH21	1.81	0.46
2:B:38:THR:HA	2:B:41:VAL:HG12	1.98	0.46
2:B:10:LEU:HD23	2:B:111:LEU:HD12	1.96	0.45
3:D:283:GLU:O	3:D:325:TYR:OH	2.34	0.45
3:E:318:PRO:HB2	3:E:322:GLN:HB2	1.97	0.45
3:G:137:ARG:HB3	3:G:267:ILE:HD12	1.98	0.45
3:G:287:SER:HA	3:G:294:ALA:HA	1.97	0.45
3:H:283:GLU:HB2	3:H:286:GLY:HA2	1.98	0.45
2:B:207:ALA:HA	2:B:210:LEU:HD13	1.99	0.45
3:H:129:GLN:HE22	3:H:320:VAL:HG23	1.81	0.45
3:C:337:GLY:O	3:D:56:ARG:NE	2.50	0.45
3:E:266:THR:HA	3:E:281:ALA:HA	1.98	0.45
3:C:141:ASN:ND2	3:C:266:THR:OG1	2.49	0.45
3:E:321:GLU:HA	3:E:324:HIS:HD2	1.82	0.45
3:D:305:TYR:OH	3:E:54:SER:O	2.29	0.45
3:H:45:ARG:NH2	3:H:83:ASN:OD1	2.43	0.45
3:G:332:ARG:NH1	3:G:333:GLY:O	2.49	0.45
3:H:133:GLU:OE1	3:H:137:ARG:NH2	2.46	0.45
2:B:83:LEU:HD11	2:B:99:GLU:HA	1.99	0.44
2:B:178:ARG:HA	2:B:181:LEU:HD23	1.98	0.44
2:B:273:ARG:HE	3:H:110:ASN:HB3	1.82	0.44
3:C:91:LEU:HB3	3:C:217:ALA:HB3	1.99	0.44
3:H:238:LYS:HG2	3:H:240:GLY:H	1.82	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:42:DT:H4'	7:O:9:DG:H22	1.83	0.44
2:B:166:ASP:HA	2:B:169:ARG:HE	1.81	0.44
3:F:294:ALA:O	3:F:297:GLN:NE2	2.51	0.44
3:F:57:LEU:HD13	3:F:67:LEU:HD12	1.99	0.44
3:F:77:GLN:HG3	6:N:16:DA:C6	2.52	0.44
3:H:23:ALA:HB1	3:H:93:VAL:HG13	1.98	0.44
2:B:214:LEU:HD21	2:B:248:LEU:HD13	1.99	0.44
3:E:231:LEU:HD11	3:F:50:ARG:HB2	2.00	0.44
3:D:304:PHE:HE1	3:D:326:VAL:HG13	1.83	0.44
3:D:78:THR:O	3:D:243:SER:OG	2.34	0.44
3:H:301:LYS:HB3	3:H:306:THR:HG21	1.99	0.44
3:H:31:ALA:H	3:H:33:ARG:HH11	1.66	0.44
3:C:327:ILE:HD12	3:C:330:LEU:HD12	2.00	0.43
1:A:229:PRO:HA	2:B:221:PHE:H	1.82	0.43
3:C:148:LEU:HB3	3:C:151:ASN:HB2	2.00	0.43
2:B:52:LEU:HD13	2:B:126:ILE:HG12	1.99	0.43
3:D:294:ALA:H	3:E:72:GLN:HG2	1.83	0.43
3:H:148:LEU:HB2	3:H:152:ARG:HG3	1.99	0.43
3:G:184:ARG:HG3	3:G:278:GLY:HA2	2.00	0.43
2:B:47:ARG:HD2	2:B:133:GLN:NE2	2.34	0.43
3:H:307:LEU:HD13	3:H:322:GLN:HB3	2.00	0.43
3:C:301:LYS:HD3	3:C:306:THR:HG21	2.01	0.43
3:E:174:TRP:HD1	3:E:191:GLU:HG2	1.84	0.43
3:F:144:ASN:ND2	3:F:182:GLY:O	2.39	0.43
6:N:38:DT:H2''	6:N:39:DG:C8	2.54	0.43
3:H:11:VAL:N	3:H:110:ASN:OD1	2.52	0.42
2:B:82:ASN:HD22	3:H:232:ILE:HG12	1.84	0.42
3:C:126:VAL:HG22	3:C:131:PHE:HZ	1.84	0.42
3:E:96:THR:OG1	3:F:223:GLN:NE2	2.50	0.42
3:G:94:ARG:NE	3:G:212:GLU:OE2	2.39	0.42
3:D:164:HIS:HB3	3:D:172:ARG:HB3	2.02	0.42
3:D:11:VAL:HG22	6:N:12:DG:H1'	2.02	0.42
3:F:266:THR:HA	3:F:281:ALA:HA	2.01	0.42
3:C:78:THR:H	5:M:43:U:H3	1.67	0.42
3:D:149:TRP:CD1	3:D:259:LYS:HE2	2.55	0.42
3:E:294:ALA:O	3:E:297:GLN:NE2	2.49	0.42
3:E:51:GLY:N	3:E:75:ASN:O	2.41	0.42
3:H:270:TRP:CD1	3:H:321:GLU:HB3	2.55	0.42
3:H:296:ARG:NH1	3:H:322:GLN:OE1	2.50	0.42
3:E:249:VAL:HG12	3:E:250:ARG:HG2	2.01	0.42
3:F:283:GLU:OE2	3:F:287:SER:N	2.45	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:VAL:HG21	2:B:289:TRP:HE1	1.85	0.41
3:G:18:LEU:HD13	3:G:99:VAL:HG22	2.02	0.41
3:D:94:ARG:NH2	3:D:212:GLU:OE2	2.54	0.41
3:E:137:ARG:NH2	3:E:267:ILE:O	2.53	0.41
2:B:19:ASN:H	2:B:104:HIS:HD2	1.67	0.41
5:M:51:G:N7	5:M:55:A:N6	2.69	0.41
5:M:56:G:N2	5:M:57:G:O6	2.53	0.41
1:A:199:VAL:HA	1:A:202:VAL:HG12	2.02	0.41
3:C:270:TRP:CD1	3:C:321:GLU:HB2	2.55	0.41
3:D:50:ARG:O	5:M:37:C:O2'	2.36	0.41
3:D:288:VAL:HG12	3:D:291:GLN:H	1.85	0.41
2:B:146:PRO:HG3	3:H:210:LEU:HD11	2.02	0.41
3:H:239:LYS:HB3	6:N:27:DC:H2''	2.02	0.41
1:A:178:LEU:HD23	5:M:2:U:H5''	2.03	0.41
2:B:291:SER:H	2:B:294:ARG:NH1	2.19	0.41
3:D:166:ARG:NH1	3:D:208:HIS:HB3	2.33	0.41
3:F:242:LYS:HE2	3:F:242:LYS:HB3	1.90	0.41
1:A:182:LEU:HD22	2:B:309:PRO:HG3	2.03	0.41
1:A:243:PHE:HB2	1:A:254:LEU:HD21	2.02	0.41
3:F:14:PHE:HZ	3:F:118:LEU:HD21	1.86	0.41
3:G:57:LEU:HD22	3:G:67:LEU:HD11	2.02	0.41
3:D:227:PRO:HG2	3:D:246:LEU:HD22	2.04	0.40
3:D:266:THR:HA	3:D:281:ALA:HA	2.03	0.40
3:D:61:ASP:O	3:D:66:LYS:NZ	2.43	0.40
3:F:303:ASP:N	3:F:303:ASP:OD1	2.54	0.40
3:G:111:ASP:HB3	3:G:114:TYR:HB3	2.02	0.40
3:F:300:GLN:O	3:F:302:LEU:N	2.54	0.40
7:O:14:DC:H2''	7:O:15:DA:C8	2.56	0.40
3:C:96:THR:HA	3:C:212:GLU:HA	2.03	0.40
3:C:97:LEU:HB2	3:C:211:LEU:HB2	2.02	0.40
3:E:310:ASN:HB3	3:E:316:GLU:HG3	2.03	0.40
3:H:62:ARG:HH21	3:H:67:LEU:HB2	1.86	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	422/436 (97%)	352 (83%)	70 (17%)	0	100	100
2	B	301/329 (92%)	269 (89%)	32 (11%)	0	100	100
3	C	287/344 (83%)	255 (89%)	32 (11%)	0	100	100
3	D	331/344 (96%)	287 (87%)	44 (13%)	0	100	100
3	E	332/344 (96%)	305 (92%)	27 (8%)	0	100	100
3	F	333/344 (97%)	303 (91%)	30 (9%)	0	100	100
3	G	331/344 (96%)	301 (91%)	30 (9%)	0	100	100
3	H	331/344 (96%)	305 (92%)	26 (8%)	0	100	100
4	L	187/189 (99%)	152 (81%)	35 (19%)	0	100	100
All	All	2855/3018 (95%)	2529 (89%)	326 (11%)	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	78/366 (21%)	77 (99%)	1 (1%)	73	93
2	B	245/271 (90%)	245 (100%)	0	100	100
3	C	230/274 (84%)	230 (100%)	0	100	100
3	D	258/274 (94%)	256 (99%)	2 (1%)	85	96
3	E	259/274 (94%)	257 (99%)	2 (1%)	85	96
3	F	259/274 (94%)	258 (100%)	1 (0%)	93	98
3	G	259/274 (94%)	258 (100%)	1 (0%)	93	98
3	H	262/274 (96%)	261 (100%)	1 (0%)	93	98
4	L	1/161 (1%)	1 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1851/2442 (76%)	1843 (100%)	8 (0%)	93 98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ARG
3	D	187	LYS
3	D	331	ILE
3	E	16	ARG
3	E	331	ILE
3	F	331	ILE
3	G	331	ILE
3	H	314	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	18	GLN
2	B	42	HIS
2	B	82	ASN
2	B	104	HIS
2	B	172	ASN
2	B	305	HIS
3	C	144	ASN
3	D	83	ASN
3	D	223	GLN
3	D	329	ASN
3	E	83	ASN
3	E	164	HIS
3	E	223	GLN
3	F	110	ASN
3	G	110	ASN
3	G	120	GLN
3	G	129	GLN
3	H	129	GLN
3	H	223	GLN
3	H	310	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	M	59/60 (98%)	31 (52%)	0

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	M	3	A
5	M	8	A
5	M	9	U
5	M	10	U
5	M	15	G
5	M	16	C
5	M	19	G
5	M	21	U
5	M	22	U
5	M	27	U
5	M	28	C
5	M	32	G
5	M	33	U
5	M	34	C
5	M	37	C
5	M	39	U
5	M	40	G
5	M	41	G
5	M	43	U
5	M	45	A
5	M	47	U
5	M	48	G
5	M	49	C
5	M	50	C
5	M	51	G
5	M	52	U
5	M	54	U
5	M	55	A
5	M	57	G
5	M	59	A
5	M	60	G

There are no RNA pucker outliers to report.

## 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 [i](#)

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.