



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 7, 2019 – 05:58 PM EDT

PDB ID : 6RGL
EMDB ID: : EMD-4876
Title : Cryo-EM structure of the anti-feeding prophage (AFP) baseplate in contracted state
Authors : Desfosses, A.
Deposited on : 2019-04-16
Resolution : 5.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

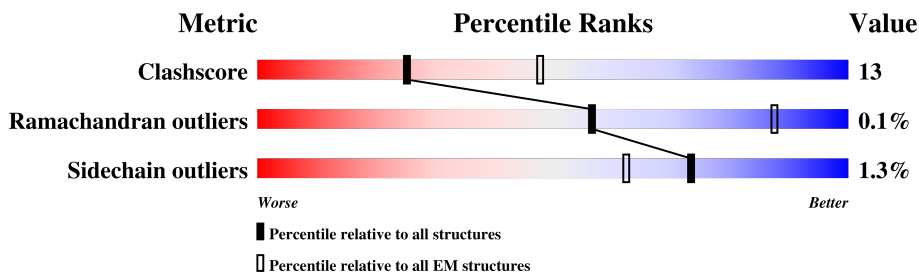
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	354	82% 15% ..
1	B	354	61% 36% ..
2	C	451	63% 15% 21%
3	D	417	52% 40% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11124 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 Afp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	348	Total	C	N	O	S	0	0
			2696	1726	446	518	6		
1	A	348	Total	C	N	O	S	0	0
			2696	1726	446	518	6		

- Molecule 2 is a protein called Afp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	355	Total	C	N	O	S	0	0
			2727	1741	461	519	6		

- Molecule 3 is a protein called Afp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	386	Total	C	N	O	S	0	0
			3005	1920	512	561	12		

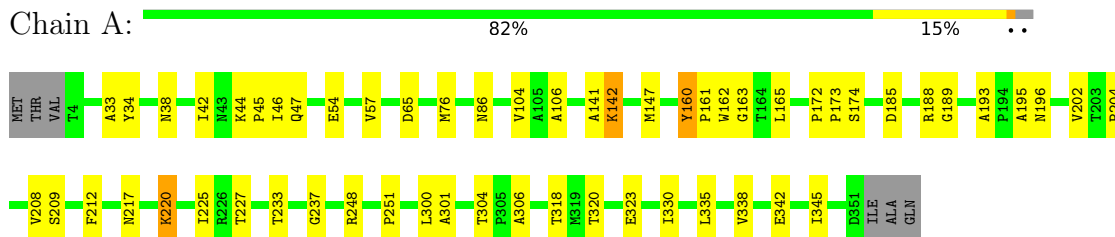
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

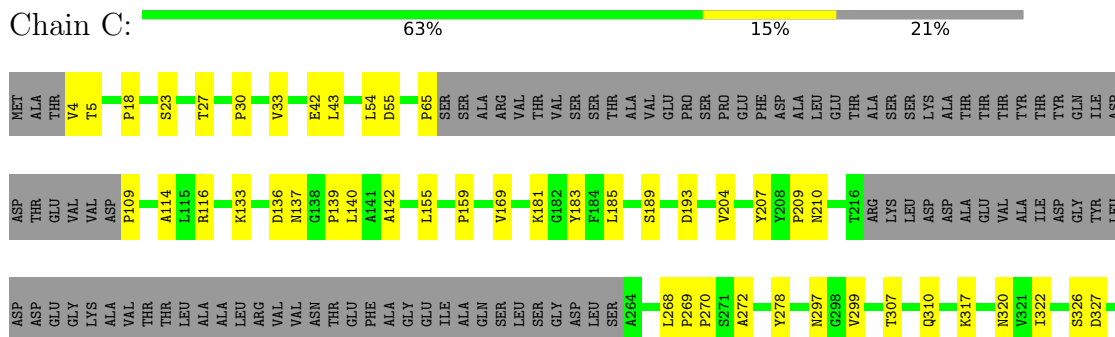
- Molecule 1: Afp2

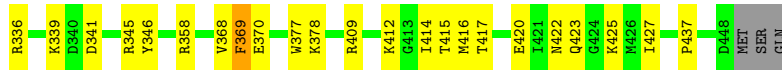


- Molecule 1: Afp2

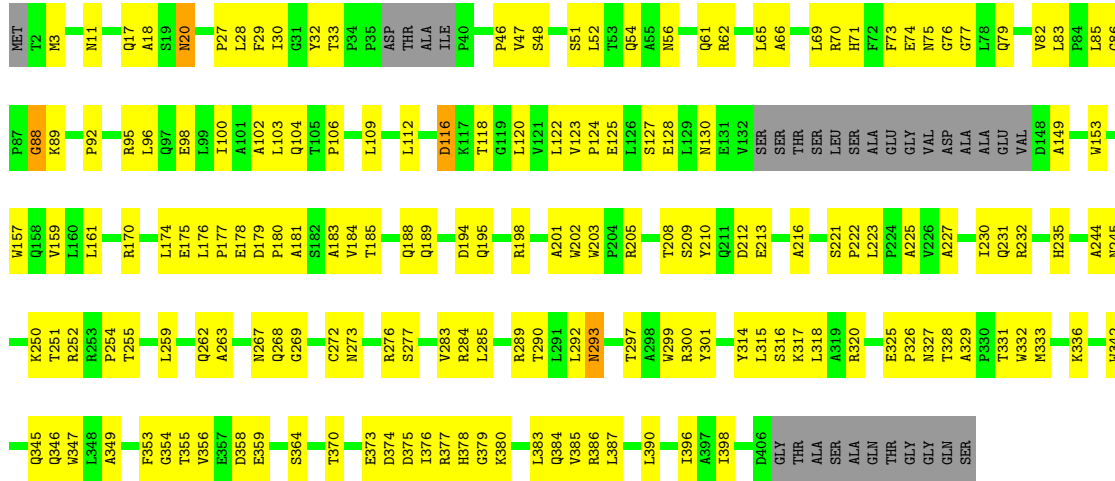


- Molecule 2: Afp3





• Molecule 3: Afp4



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	3816	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 ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	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	0.24	0/2767	0.48	0/3782
1	B	0.59	1/2767 (0.0%)	0.75	5/3782 (0.1%)
2	C	0.24	0/2790	0.46	0/3808
3	D	0.52	0/3073	0.75	4/4195 (0.1%)
All	All	0.43	1/11397 (0.0%)	0.63	9/15567 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
2	C	0	1
3	D	0	5
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	PHE	C-N	-7.97	1.15	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	PRO	C-N-CA	7.89	141.43	121.70
3	D	96	LEU	CA-CB-CG	6.30	129.79	115.30
3	D	116	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	253	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	272	PHE	C-N-CA	5.58	135.65	121.70
1	B	142	LYS	CA-CB-CG	5.48	125.46	113.40
3	D	179	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	194	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	73	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	TYR	Peptide
1	A	220	LYS	Peptide
1	B	160	TYR	Peptide
1	B	23	ASN	Peptide
1	B	247	TRP	Peptide
1	B	304	THR	Peptide
1	B	309	TRP	Peptide
2	C	317	LYS	Peptide
3	D	17	GLN	Peptide
3	D	20	ASN	Peptide
3	D	293	ASN	Peptide
3	D	299	TRP	Peptide
3	D	88	GLY	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	2696	0	2606	37	0
1	B	2696	0	2605	91	0
2	C	2727	0	2699	49	0
3	D	3005	0	3005	130	0
All	All	11124	0	10915	276	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 13.

All (276) 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:C:54:LEU:HD23	3:D:106:PRO:CB	1.87	1.05
2:C:54:LEU:HD23	3:D:106:PRO:HB2	1.43	0.99
2:C:54:LEU:CD2	3:D:106:PRO:HB2	1.95	0.95
2:C:326:SER:O	3:D:268:GLN:NE2	2.05	0.88
2:C:54:LEU:HD23	3:D:106:PRO:HB3	1.65	0.77
3:D:56:ASN:OD1	3:D:69:LEU:HD13	1.85	0.77
3:D:209:SER:HA	3:D:252:ARG:HE	1.51	0.75
2:C:23:SER:OG	3:D:378:HIS:NE2	2.16	0.74
3:D:364:SER:HB3	3:D:384:GLN:HB2	1.72	0.72
2:C:54:LEU:CD2	3:D:106:PRO:CB	2.60	0.70
3:D:56:ASN:OD1	3:D:69:LEU:CD1	2.39	0.70
1:A:42:ILE:HG22	1:A:44:LYS:H	1.55	0.70
3:D:56:ASN:OD1	3:D:69:LEU:HB3	1.91	0.69
1:A:248:ARG:HH22	2:C:423:GLN:HG3	1.57	0.69
3:D:61:GLN:HB3	3:D:70:ARG:HD2	1.75	0.69
2:C:159:PRO:HB3	2:C:272:ALA:HB2	1.74	0.67
1:A:161:PRO:HG2	1:A:225:ILE:H	1.60	0.66
3:D:27:PRO:HA	3:D:120:LEU:HB2	1.77	0.66
3:D:208:THR:HA	3:D:251:THR:HA	1.77	0.66
3:D:272:CYS:SG	3:D:273:ASN:N	2.68	0.66
3:D:71:HIS:O	3:D:75:ASN:ND2	2.28	0.66
3:D:73:PHE:HA	3:D:77:GLY:H	1.59	0.66
1:B:209:SER:O	1:B:226:ARG:NH1	2.28	0.66
1:A:345:ILE:HD11	2:C:427:ILE:HG13	1.76	0.66
2:C:268:LEU:HD22	2:C:269:PRO:HD2	1.75	0.66
3:D:170:ARG:O	3:D:198:ARG:NH1	2.29	0.65
1:A:208:VAL:HG13	1:A:209:SER:H	1.60	0.65
1:B:341:ALA:N	3:D:325:GLU:O	2.28	0.65
2:C:4:VAL:HG13	2:C:5:THR:HG23	1.79	0.65
1:A:248:ARG:NH2	2:C:422:ASN:O	2.30	0.65
1:B:163:GLY:HA2	1:B:204:PRO:HA	1.79	0.65
3:D:277:SER:HA	3:D:283:VAL:HA	1.79	0.64
3:D:297:THR:O	3:D:300:ARG:NH1	2.29	0.64
1:A:342:GLU:HG3	2:C:369:PHE:HE1	1.63	0.64
3:D:130:ASN:HD21	3:D:177:PRO:HA	1.64	0.63
2:C:409:ARG:HD3	2:C:414:ILE:HD12	1.81	0.63
3:D:358:ASP:O	3:D:386:ARG:NH2	2.32	0.63
1:A:45:PRO:HB2	1:A:46:ILE:HD12	1.81	0.62
1:B:227:THR:HG23	1:B:233:THR:H	1.64	0.62
3:D:56:ASN:OD1	3:D:69:LEU:CB	2.47	0.62
1:B:323:GLU:HA	1:B:326:GLN:HB2	1.82	0.62
1:B:317:LEU:HD12	1:B:318:THR:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:297:ASN:OD1	3:D:195:GLN:NE2	2.33	0.61
2:C:23:SER:HG	3:D:378:HIS:CD2	2.18	0.61
3:D:48:SER:OG	3:D:79:GLN:NE2	2.34	0.61
1:B:288:ASP:N	1:B:288:ASP:OD1	2.32	0.60
1:B:132:GLY:HA3	1:B:160:TYR:HA	1.83	0.60
1:B:136:LYS:N	1:B:160:TYR:OH	2.33	0.60
1:A:38:ASN:ND2	1:A:65:ASP:OD2	2.35	0.60
1:A:33:ALA:HB3	1:A:106:ALA:H	1.67	0.60
2:C:30:PRO:HB3	2:C:155:LEU:HB2	1.82	0.60
1:A:193:ALA:HB2	1:A:251:PRO:HG3	1.84	0.60
2:C:207:TYR:HH	2:C:278:TYR:HH	1.50	0.59
1:B:22:VAL:HG11	1:B:263:ILE:HG12	1.83	0.59
1:B:139:GLY:O	1:B:215:LYS:NZ	2.35	0.59
3:D:122:LEU:HD11	3:D:223:LEU:HB3	1.84	0.58
1:B:278:PRO:O	1:B:281:GLN:NE2	2.36	0.58
1:B:295:TRP:NE1	1:B:302:GLY:O	2.37	0.58
1:B:309:TRP:HA	1:B:335:LEU:HA	1.86	0.58
3:D:259:LEU:O	3:D:262:GLN:NE2	2.37	0.57
2:C:181:LYS:HD2	2:C:183:TYR:CZ	2.39	0.57
3:D:375:ASP:HB3	3:D:380:LYS:HB2	1.86	0.57
1:A:44:LYS:O	1:A:47:GLN:NE2	2.38	0.57
3:D:47:VAL:N	3:D:82:VAL:O	2.34	0.57
3:D:28:LEU:HB2	3:D:118:THR:HG21	1.85	0.57
3:D:33:THR:HG23	3:D:86:GLY:H	1.70	0.57
1:B:275:ASN:OD1	1:B:280:TRP:NE1	2.36	0.56
3:D:205:ARG:HA	3:D:222:PRO:HD3	1.87	0.56
3:D:345:GLN:O	3:D:349:ALA:N	2.38	0.56
1:B:209:SER:OG	1:B:213:GLN:N	2.34	0.56
2:C:320:ASN:HD21	2:C:336:ARG:H	1.53	0.56
1:B:38:ASN:ND2	1:B:65:ASP:OD2	2.37	0.56
3:D:205:ARG:HG3	3:D:221:SER:HA	1.87	0.56
1:B:347:GLN:O	3:D:385:VAL:N	2.37	0.56
1:B:23:ASN:O	1:B:265:LYS:NZ	2.37	0.56
3:D:178:GLU:OE2	3:D:255:THR:OG1	2.24	0.55
1:B:228:PHE:HB2	1:B:231:GLN:HG3	1.88	0.55
2:C:299:VAL:O	3:D:189:GLN:NE2	2.40	0.55
1:B:140:THR:OG1	1:B:142:LYS:NZ	2.39	0.55
3:D:51:SER:H	3:D:54:GLN:HB3	1.72	0.55
3:D:118:THR:OG1	3:D:170:ARG:NH1	2.35	0.55
3:D:175:GLU:HA	3:D:202:TRP:H	1.71	0.55
3:D:52:LEU:HD22	3:D:56:ASN:ND2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:N	1:B:54:GLU:OE2	2.36	0.55
3:D:347:TRP:NE1	3:D:354:GLY:O	2.35	0.55
1:B:46:ILE:HG23	1:B:85:VAL:HG12	1.89	0.54
3:D:227:ALA:HA	3:D:230:ILE:HD12	1.88	0.54
3:D:245:ASN:HA	3:D:284:ARG:HB3	1.89	0.54
3:D:176:LEU:HD12	3:D:203:TRP:HB2	1.89	0.54
1:A:227:THR:HG23	1:A:233:THR:H	1.72	0.54
1:B:164:THR:N	1:B:203:THR:O	2.40	0.54
1:A:320:THR:N	1:A:323:GLU:OE2	2.40	0.54
3:D:149:ALA:O	3:D:153:TRP:N	2.32	0.54
1:B:311:VAL:HA	1:B:333:ILE:HG22	1.90	0.53
2:C:416:MET:HG2	2:C:427:ILE:HD13	1.91	0.53
3:D:109:LEU:HA	3:D:112:LEU:HB2	1.88	0.53
1:B:225:ILE:HG23	1:B:235:VAL:HA	1.91	0.53
1:B:351:ASP:HB2	3:D:386:ARG:HD3	1.90	0.53
1:B:30:PRO:HB3	1:B:102:LEU:HB2	1.90	0.53
3:D:180:PRO:HB3	3:D:263:ALA:HB3	1.90	0.53
1:A:162:TRP:HA	1:A:173:PRO:HG3	1.91	0.53
1:B:46:ILE:HA	1:B:85:VAL:HA	1.91	0.53
1:B:31:LEU:HD23	1:B:100:ILE:HG21	1.91	0.52
2:C:65:PRO:HB3	2:C:109:PRO:HG3	1.91	0.52
3:D:326:PRO:HG2	3:D:331:THR:HG21	1.90	0.52
1:A:165:LEU:HD23	1:A:202:VAL:HG22	1.92	0.52
1:B:119:VAL:O	1:B:123:GLY:N	2.43	0.52
3:D:374:ASP:O	3:D:378:HIS:N	2.42	0.52
3:D:56:ASN:HB3	3:D:61:GLN:HG3	1.91	0.52
1:B:45:PRO:HB2	1:B:46:ILE:HD12	1.92	0.52
3:D:269:GLY:O	3:D:293:ASN:ND2	2.42	0.52
3:D:65:LEU:O	3:D:69:LEU:N	2.32	0.52
1:B:322:GLU:O	1:B:326:GLN:N	2.43	0.52
1:B:178:ALA:HA	1:B:181:ILE:HD12	1.92	0.51
3:D:52:LEU:HD13	3:D:70:ARG:HA	1.91	0.51
3:D:355:THR:N	3:D:359:GLU:OE2	2.43	0.51
1:B:31:LEU:HD13	1:B:85:VAL:HG22	1.91	0.51
1:B:36:SER:HB3	1:B:86:ASN:HB2	1.91	0.51
3:D:62:ARG:HH12	3:D:213:GLU:HB3	1.76	0.51
1:B:71:LEU:HA	1:B:74:TRP:HB3	1.93	0.51
1:B:160:TYR:HB3	1:B:224:MET:HG3	1.92	0.51
3:D:289:ARG:HA	3:D:301:TYR:H	1.76	0.51
3:D:314:TYR:HA	3:D:317:LYS:HZ3	1.76	0.51
1:B:341:ALA:HB3	3:D:325:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:HA	1:B:57:VAL:HG12	1.93	0.51
1:B:349:SER:N	3:D:385:VAL:O	2.44	0.51
1:B:293:SER:O	1:B:297:GLN:N	2.40	0.51
3:D:74:GLU:OE1	3:D:210:TYR:OH	2.23	0.50
1:B:136:LYS:H	1:B:160:TYR:HH	1.57	0.50
2:C:133:LYS:HB3	2:C:136:ASP:HB2	1.92	0.50
2:C:307:THR:H	2:C:310:GLN:NE2	2.09	0.50
2:C:417:THR:N	2:C:420:GLU:OE2	2.38	0.50
1:A:141:ALA:C	1:A:142:LYS:HD2	2.32	0.50
3:D:244:ALA:HA	3:D:285:LEU:HB2	1.94	0.50
1:B:117:THR:HG23	1:A:76:MET:SD	2.51	0.50
2:C:210:ASN:HA	2:C:270:PRO:HD3	1.93	0.50
1:B:320:THR:N	1:B:323:GLU:OE2	2.45	0.50
3:D:88:GLY:HA3	3:D:95:ARG:HH21	1.77	0.50
2:C:189:SER:OG	2:C:193:ASP:O	2.29	0.49
3:D:11:ASN:OD1	3:D:11:ASN:N	2.44	0.49
3:D:46:PRO:HG3	3:D:83:LEU:HD12	1.93	0.49
1:B:212:PHE:HA	1:B:215:LYS:HE2	1.94	0.49
1:B:216:TYR:HB3	1:B:222:LEU:HG	1.93	0.49
2:C:114:ALA:HB2	2:C:268:LEU:HD21	1.93	0.49
2:C:341:ASP:O	2:C:345:ARG:HG3	2.12	0.49
3:D:56:ASN:HD21	3:D:70:ARG:N	2.09	0.49
3:D:328:THR:O	3:D:331:THR:OG1	2.27	0.49
1:B:323:GLU:O	1:B:328:LYS:N	2.46	0.49
1:B:349:SER:O	3:D:386:ARG:HA	2.12	0.49
3:D:177:PRO:HG2	3:D:183:ALA:HB2	1.94	0.48
3:D:212:ASP:HB3	3:D:216:ALA:HB3	1.94	0.48
3:D:76:GLY:O	3:D:232:ARG:NE	2.35	0.48
3:D:28:LEU:HD11	3:D:83:LEU:HB2	1.95	0.48
3:D:231:GLN:O	3:D:235:HIS:N	2.40	0.48
1:A:209:SER:OG	1:A:212:PHE:N	2.34	0.48
1:B:164:THR:HA	1:B:170:ALA:HA	1.96	0.48
1:B:240:THR:HG22	1:B:248:ARG:HA	1.95	0.48
3:D:161:LEU:HB3	3:D:195:GLN:HB2	1.94	0.48
1:B:165:LEU:HD23	1:B:202:VAL:HG22	1.95	0.47
1:B:319:MET:HB3	1:B:330:ILE:H	1.79	0.47
2:C:414:ILE:O	2:C:415:THR:HG22	2.15	0.47
3:D:329:ALA:HA	3:D:332:TRP:CD2	2.48	0.47
1:B:211:ASP:O	1:B:215:LYS:N	2.38	0.47
1:A:300:LEU:HD22	1:A:335:LEU:HD13	1.97	0.47
1:B:171:VAL:HB	1:B:176:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HB	1:A:174:SER:HB3	1.96	0.47
1:B:44:LYS:HZ3	1:B:45:PRO:HD2	1.79	0.47
3:D:375:ASP:HA	3:D:378:HIS:HB2	1.97	0.47
3:D:29:PHE:HB2	3:D:82:VAL:HG22	1.97	0.47
3:D:123:VAL:HG12	3:D:125:GLU:H	1.80	0.47
1:B:291:LEU:O	1:B:295:TRP:N	2.44	0.47
2:C:209:PRO:HG2	2:C:322:ILE:HB	1.97	0.47
1:B:44:LYS:HZ2	1:B:46:ILE:HB	1.80	0.47
1:B:215:LYS:HE3	1:B:216:TYR:CZ	2.51	0.46
1:B:219:GLY:N	1:B:243:ASP:OD2	2.48	0.46
3:D:157:TRP:CD2	3:D:174:LEU:HD13	2.50	0.46
3:D:289:ARG:HG3	3:D:300:ARG:HB2	1.96	0.46
3:D:28:LEU:HG	3:D:30:ILE:HG12	1.97	0.46
3:D:290:THR:H	3:D:300:ARG:HA	1.80	0.46
3:D:92:PRO:HB3	3:D:128:GLU:OE1	2.15	0.46
2:C:42:GLU:HG2	2:C:43:LEU:HD22	1.98	0.46
1:B:182:THR:HG22	1:B:186:ARG:HH12	1.80	0.46
1:B:221:ALA:HB3	1:B:241:LEU:HD23	1.98	0.46
1:B:50:ARG:HA	1:B:81:LYS:HG3	1.97	0.46
3:D:56:ASN:ND2	3:D:70:ARG:HG3	2.31	0.46
3:D:66:ALA:HA	3:D:69:LEU:HD12	1.98	0.46
1:B:305:PRO:HB2	1:B:309:TRP:CZ3	2.51	0.45
3:D:254:PRO:HD2	3:D:277:SER:HB3	1.98	0.45
1:A:163:GLY:HA2	1:A:204:PRO:HA	1.99	0.45
1:B:185:ASP:OD1	1:B:186:ARG:N	2.49	0.45
1:B:187:THR:HG22	1:B:188:ARG:HG2	1.98	0.45
1:A:318:THR:HB	1:A:330:ILE:HD11	1.98	0.45
1:A:160:TYR:O	1:A:162:TRP:N	2.50	0.45
1:A:304:THR:O	1:A:306:ALA:N	2.50	0.45
3:D:185:THR:HA	3:D:188:GLN:HB2	1.98	0.45
3:D:89:LYS:H	3:D:95:ARG:HG2	1.82	0.45
3:D:29:PHE:O	3:D:83:LEU:N	2.40	0.45
3:D:77:GLY:O	3:D:232:ARG:NH2	2.49	0.44
3:D:79:GLN:H	3:D:231:GLN:NE2	2.15	0.44
1:B:339:ARG:HD3	3:D:377:ARG:HA	1.99	0.44
3:D:316:SER:O	3:D:320:ARG:NH1	2.50	0.44
3:D:370:THR:HG21	3:D:383:LEU:HA	2.00	0.44
1:B:117:THR:CG2	1:A:76:MET:SD	3.06	0.44
1:A:195:ALA:HB1	2:C:369:PHE:CD2	2.53	0.44
3:D:181:ALA:HA	3:D:184:VAL:HB	2.00	0.44
3:D:124:PRO:HA	3:D:223:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:HA	1:A:189:GLY:O	2.17	0.44
1:B:295:TRP:CE3	1:B:296:GLN:HG3	2.52	0.44
2:C:370:GLU:N	2:C:370:GLU:OE1	2.51	0.44
1:B:239:ARG:HA	1:B:249:TYR:H	1.83	0.43
2:C:185:LEU:HD21	2:C:204:VAL:HG12	2.00	0.43
3:D:276:ARG:O	3:D:284:ARG:N	2.50	0.43
1:B:184:THR:O	1:B:188:ARG:N	2.38	0.43
1:B:262:ASP:OD1	1:B:262:ASP:N	2.50	0.43
1:B:172:PRO:HA	1:B:173:PRO:HD3	1.87	0.43
3:D:29:PHE:HE1	3:D:122:LEU:HD23	1.84	0.43
3:D:52:LEU:HD22	3:D:56:ASN:HD21	1.83	0.43
3:D:98:GLU:O	3:D:102:ALA:N	2.45	0.43
2:C:327:ASP:HA	3:D:268:GLN:HG2	2.01	0.43
1:A:54:GLU:HA	1:A:57:VAL:HG12	2.01	0.43
1:B:329:MET:N	1:B:329:MET:SD	2.92	0.42
2:C:33:VAL:HG21	2:C:169:VAL:HG11	1.99	0.42
3:D:127:SER:OG	3:D:205:ARG:NH2	2.52	0.42
1:A:147:MET:HB3	1:A:220:LYS:HD3	2.02	0.42
1:B:211:ASP:OD1	1:B:211:ASP:N	2.49	0.42
1:B:215:LYS:O	1:B:218:GLN:NE2	2.52	0.42
3:D:32:TYR:HA	3:D:85:LEU:HB2	2.00	0.42
1:A:237:GLY:H	2:C:369:PHE:HE2	1.66	0.42
1:B:251:PRO:O	1:B:255:LEU:N	2.50	0.42
1:B:4:THR:OG1	1:B:5:THR:N	2.50	0.42
3:D:373:GLU:HA	3:D:376:ILE:HB	2.00	0.42
1:B:180:SER:HA	1:B:183:GLN:HE21	1.83	0.42
1:A:188:ARG:HH12	2:C:18:PRO:HD3	1.83	0.42
1:B:290:TYR:O	1:B:293:SER:OG	2.36	0.42
3:D:79:GLN:H	3:D:231:GLN:HE22	1.67	0.42
3:D:65:LEU:HG	3:D:69:LEU:HG	2.01	0.42
1:B:99:ASP:OD1	1:B:99:ASP:N	2.53	0.42
1:B:160:TYR:O	1:B:162:TRP:N	2.52	0.42
2:C:423:GLN:O	2:C:425:LYS:HG3	2.20	0.42
3:D:315:LEU:HA	3:D:315:LEU:HD23	1.87	0.42
3:D:333:MET:HA	3:D:336:LYS:HD3	2.00	0.42
1:B:225:ILE:HD12	1:B:235:VAL:HG12	2.02	0.42
1:B:134:LYS:HD2	1:B:134:LYS:HA	1.82	0.42
3:D:176:LEU:HB2	3:D:203:TRP:HA	2.02	0.42
3:D:396:ILE:HG22	3:D:398:ILE:HG12	2.02	0.42
1:B:66:ALA:O	1:B:70:SER:N	2.52	0.41
1:B:350:GLN:HA	3:D:387:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:370:THR:HG22	3:D:384:GLN:HG3	2.01	0.41
1:B:322:GLU:HA	1:B:325:ASN:HD22	1.84	0.41
2:C:346:TYR:CD2	2:C:437:PRO:HD2	2.55	0.41
3:D:100:ILE:O	3:D:104:GLN:N	2.51	0.41
3:D:342:TRP:O	3:D:346:GLN:HG2	2.20	0.41
3:D:71:HIS:CE1	3:D:225:ALA:HB2	2.56	0.41
1:A:196:ASN:HD21	2:C:368:VAL:HG12	1.85	0.41
3:D:356:VAL:HG23	3:D:359:GLU:H	1.85	0.41
1:A:142:LYS:O	1:A:142:LYS:HG2	2.21	0.41
1:A:172:PRO:HA	1:A:173:PRO:HD3	1.83	0.41
3:D:292:LEU:HA	3:D:292:LEU:HD23	1.82	0.41
1:B:339:ARG:O	3:D:327:ASN:N	2.50	0.41
3:D:373:GLU:HA	3:D:376:ILE:HD12	2.03	0.41
3:D:375:ASP:O	3:D:379:GLY:N	2.54	0.41
1:B:147:MET:HB3	1:B:220:LYS:HD3	2.03	0.40
3:D:174:LEU:HB2	3:D:201:ALA:HB2	2.03	0.40
3:D:353:PHE:HD1	3:D:390:LEU:HD23	1.86	0.40
1:A:301:ALA:HB2	1:A:338:VAL:HG12	2.03	0.40
1:B:339:ARG:NH2	3:D:373:GLU:OE2	2.54	0.40
2:C:377:TRP:CZ3	2:C:412:LYS:HB2	2.56	0.40
3:D:318:LEU:HG	3:D:318:LEU:H	1.69	0.40
2:C:55:ASP:OD1	2:C:55:ASP:N	2.54	0.40
3:D:398:ILE:HA	3:D:398:ILE:HD13	1.93	0.40
2:C:137:ASN:HA	2:C:140:LEU:HB2	2.04	0.40
2:C:139:PRO:HA	2:C:142:ALA:HB3	2.03	0.40
3:D:103:LEU:HB3	3:D:159:VAL:HG11	2.02	0.40
1:A:34:TYR:HB3	1:A:86:ASN:HA	2.03	0.40
1:B:47:GLN:N	1:B:84:LEU:O	2.36	0.40
2:C:27:THR:HG22	2:C:358:ARG:HH22	1.86	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	346/354 (98%)	306 (88%)	40 (12%)	0	100	100
1	B	346/354 (98%)	289 (84%)	57 (16%)	0	100	100
2	C	349/451 (77%)	303 (87%)	46 (13%)	0	100	100
3	D	380/417 (91%)	326 (86%)	52 (14%)	2 (0%)	31	74
All	All	1421/1576 (90%)	1224 (86%)	195 (14%)	2 (0%)	56	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	18	ALA
3	D	116	ASP

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	282/287 (98%)	280 (99%)	2 (1%)	85	93
1	B	282/287 (98%)	277 (98%)	5 (2%)	62	82
2	C	289/368 (78%)	285 (99%)	4 (1%)	69	85
3	D	324/345 (94%)	320 (99%)	4 (1%)	74	87
All	All	1177/1287 (92%)	1162 (99%)	15 (1%)	73	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142	LYS
1	B	217	ASN
1	B	265	LYS
1	B	270	LEU
1	B	345	ILE
1	A	142	LYS
1	A	217	ASN
2	C	116	ARG
2	C	339	LYS

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Mol	Chain	Res	Type
2	C	369	PHE
2	C	378	LYS
3	D	3	MET
3	D	20	ASN
3	D	250	LYS
3	D	267	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	196	ASN
1	B	197	GLN
1	B	217	ASN
1	B	325	ASN
1	A	196	ASN
1	A	217	ASN
1	A	321	GLN
2	C	179	GLN
2	C	308	ASN
2	C	320	ASN
3	D	20	ASN
3	D	79	GLN
3	D	189	GLN
3	D	211	GLN
3	D	231	GLN
3	D	267	ASN
3	D	345	GLN
3	D	346	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	272:PHE	C	273:GLU	N	1.15