



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 9, 2019 – 12:02 AM EST

PDB ID : 6IB1
EMDB ID: : EMD-4442
Title : Icosahedrally averaged capsid of empty particle of bacteriophage P68
Authors : Hrebik, D.; Skubnik, K.; Fuzik, T.; Plevka, P.
Deposited on : 2018-11-28
Resolution : 3.50 Å(reported)
Based on PDB ID : 6IAT

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

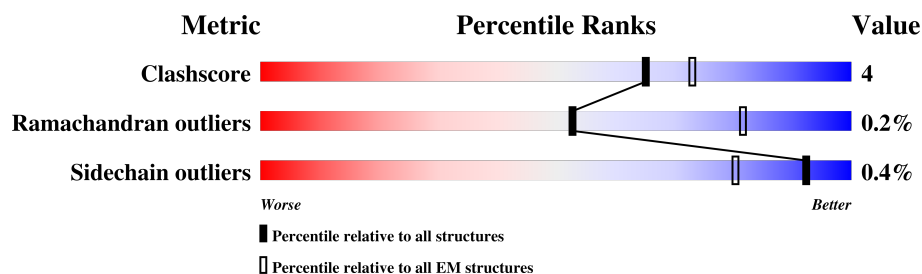
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	408	
1	B	408	
1	C	408	
1	D	408	
2	E	60	
2	F	60	
2	G	60	
2	H	60	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14150 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 Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	385	Total	C	N	O	S	0	0
			3126	2014	508	596	8		
1	D	392	Total	C	N	O	S	0	0
			3181	2045	518	610	8		
1	B	385	Total	C	N	O	S	0	0
			3126	2014	508	596	8		
1	A	393	Total	C	N	O	S	0	0
			3190	2050	520	612	8		

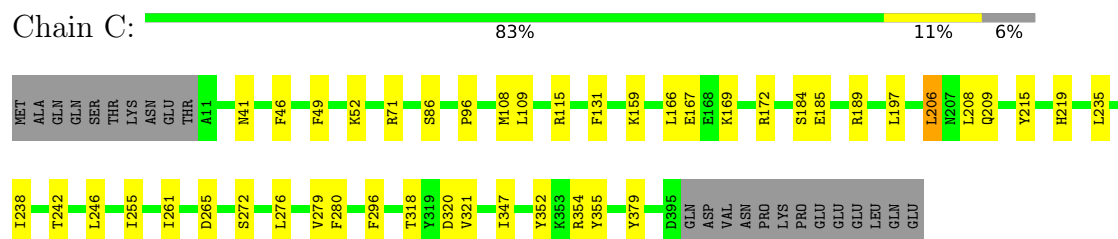
- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	54	Total	C	N	O	S	0	0
			433	258	76	94	5		
2	F	55	Total	C	N	O	S	0	0
			437	260	77	95	5		
2	G	27	Total	C	N	O	S	0	0
			221	130	41	46	4		
2	H	55	Total	C	N	O	S	0	0
			436	260	77	94	5		

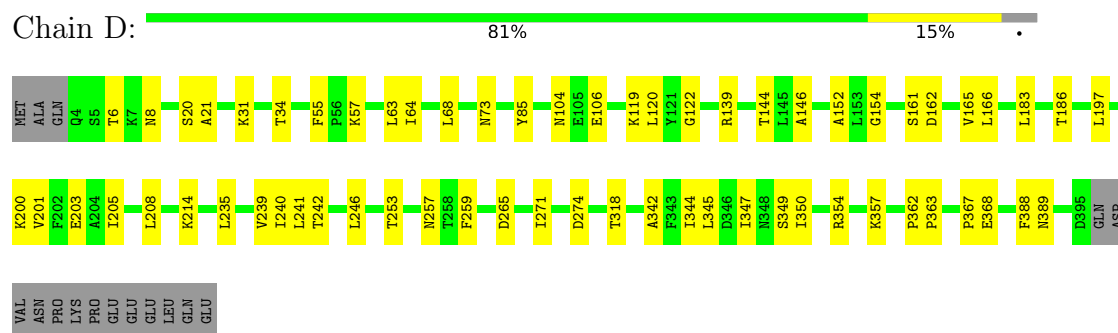
3 Residue-property plots

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.

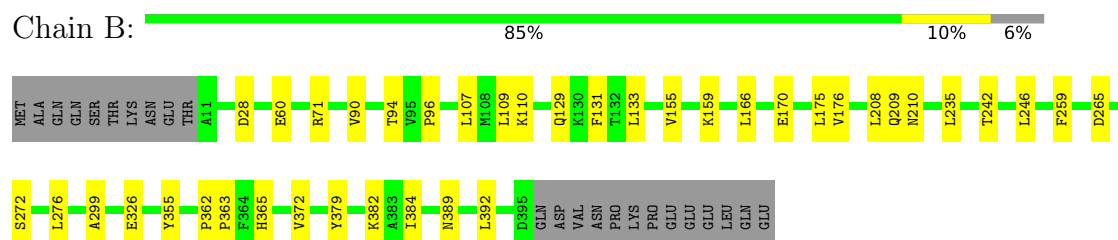
- Molecule 1: Major head protein



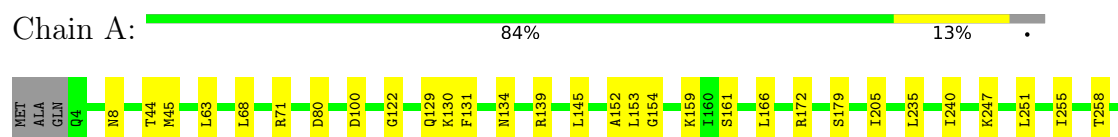
- Molecule 1: Major head protein



- Molecule 1: Major head protein



- Molecule 1: Major head protein





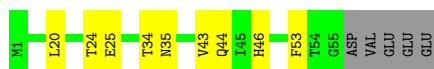
- Molecule 2: Uncharacterized protein

Chain E: 67% 22% • 10%



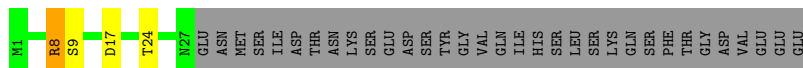
- Molecule 2: Uncharacterized protein

Chain F: 77% 15% 8%



- Molecule 2: Uncharacterized protein

Chain G: 38% 5% • 55%



- Molecule 2: Uncharacterized protein

Chain H: 80% 10% • 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8580	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 ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1.0	Depositor
Maximum defocus (nm)	3.0	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (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	0.38	0/3257	0.61	2/4400 (0.0%)
1	B	0.36	0/3193	0.60	4/4314 (0.1%)
1	C	0.38	0/3193	0.62	4/4314 (0.1%)
1	D	0.38	0/3247	0.62	4/4385 (0.1%)
2	E	0.35	0/437	0.83	1/582 (0.2%)
2	F	0.33	0/441	0.74	0/587
2	G	0.29	0/222	0.69	0/293
2	H	0.35	0/440	0.75	0/586
All	All	0.37	0/14430	0.63	15/19461 (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	C	0	2
2	E	0	2
2	F	0	3
2	G	0	2
2	H	0	1
All	All	0	10

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LEU	CA-CB-CG	8.72	135.35	115.30
1	B	326	GLU	N-CA-CB	-8.00	96.21	110.60
1	C	197	LEU	CA-CB-CG	7.34	132.18	115.30
1	B	326	GLU	N-CA-C	6.95	129.75	111.00
1	A	326	GLU	N-CA-CB	-6.33	99.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	40	SER	N-CA-C	6.27	127.93	111.00
1	C	166	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	166	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	265	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	235	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	265	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	265	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	392	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	183	LEU	CA-CB-CG	5.04	126.90	115.30
1	D	120	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	206	LEU	Peptide
1	C	347	ILE	Peptide
2	E	46	HIS	Peptide
2	E	9	SER	Peptide
2	F	24	THR	Peptide
2	F	25	GLU	Peptide
2	F	43	VAL	Peptide
2	G	24	THR	Peptide
2	G	9	SER	Peptide
2	H	44	GLN	Peptide

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	3190	0	3161	34	0
1	B	3126	0	3101	30	0
1	C	3126	0	3101	25	0
1	D	3181	0	3152	45	0
2	E	433	0	408	10	0
2	F	437	0	411	4	0
2	G	221	0	211	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	436	0	408	4	0
All	All	14150	0	13953	125	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 4.

All (125) 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:D:259:PHE:CE1	1:B:259:PHE:CE2	2.53	0.96
1:D:259:PHE:HE1	1:B:259:PHE:CE2	1.85	0.94
1:D:259:PHE:CE1	1:B:259:PHE:CD2	2.64	0.85
2:E:43:VAL:O	2:E:44:GLN:HG2	1.78	0.83
1:D:20:SER:HG	1:D:21:ALA:N	1.85	0.75
1:A:131:PHE:HB3	1:A:159:LYS:HE3	1.76	0.67
1:B:208:LEU:HD22	1:B:389:ASN:HB3	1.77	0.65
1:B:355:TYR:HB3	1:B:379:TYR:HB3	1.80	0.64
1:C:167:GLU:OE2	1:C:354:ARG:NH1	2.33	0.61
1:A:71:ARG:HD3	1:A:271:ILE:HD12	1.81	0.61
1:D:162:ASP:HA	1:D:165:VAL:HG22	1.82	0.61
1:C:169:LYS:HD2	1:C:318:THR:HG23	1.82	0.61
1:D:368:GLU:OE1	1:A:375:TRP:NE1	2.34	0.60
1:D:259:PHE:CZ	1:B:259:PHE:CZ	2.90	0.60
1:D:166:LEU:HG	1:B:96:PRO:HD2	1.84	0.59
1:C:167:GLU:OE2	1:C:352:TYR:OH	2.22	0.58
1:A:129:GLN:NE2	1:A:159:LYS:O	2.36	0.58
1:A:68:LEU:HB2	1:A:161:SER:HB3	1.86	0.57
2:E:43:VAL:O	2:E:44:GLN:CG	2.50	0.57
1:A:63:LEU:HD21	1:A:154:GLY:HA3	1.86	0.57
1:B:170:GLU:HG3	1:B:382:LYS:HE2	1.87	0.56
1:A:394:THR:HG23	1:A:396:GLN:H	1.69	0.56
1:D:271:ILE:HG22	2:H:45:ILE:HD11	1.88	0.56
1:C:115:ARG:NH2	1:B:299:ALA:O	2.39	0.55
1:D:259:PHE:CZ	1:B:259:PHE:CE2	2.93	0.55
1:D:259:PHE:HE1	1:B:259:PHE:CD2	2.10	0.55
1:D:367:PRO:O	1:A:377:HIS:NE2	2.38	0.55
1:C:255:ILE:HG23	1:C:261:ILE:HG12	1.89	0.55
1:D:139:ARG:NH2	2:G:17:ASP:OD2	2.39	0.55
1:A:8:ASN:HD21	1:A:44:THR:HB	1.72	0.54
1:A:235:LEU:HD22	1:A:264:ILE:HG21	1.90	0.54
1:B:129:GLN:NE2	1:B:159:LYS:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:HG21	1:C:246:LEU:HD12	1.90	0.53
1:B:71:ARG:NH1	1:B:272:SER:O	2.42	0.53
1:D:152:ALA:O	2:G:8:ARG:NH1	2.42	0.53
1:B:365:HIS:HA	1:B:372:VAL:HG23	1.90	0.52
1:D:34:THR:HG21	1:A:122:GLY:H	1.75	0.52
1:A:153:LEU:HD21	2:E:4:GLY:HA3	1.91	0.52
1:A:240:ILE:HG12	1:A:344:ILE:HG12	1.91	0.52
1:D:239:VAL:HG22	2:H:48:LEU:HD13	1.90	0.52
2:E:21:ASN:O	2:E:23:ARG:NH1	2.43	0.52
1:D:85:TYR:HD1	1:D:122:GLY:HA2	1.76	0.51
1:D:253:THR:O	1:D:257:ASN:HB2	2.11	0.51
1:D:205:ILE:HD11	1:D:240:ILE:HD11	1.92	0.51
1:B:209:GLN:HB3	2:F:34:THR:HB	1.93	0.51
1:A:152:ALA:HB1	2:E:8:ARG:HH22	1.77	0.50
1:A:279:VAL:HG22	1:A:318:THR:HA	1.94	0.50
1:D:345:LEU:HD11	1:D:350:ILE:HD11	1.93	0.50
1:A:145:LEU:HD23	2:E:16:GLU:HA	1.92	0.50
1:D:241:LEU:HD12	1:D:271:ILE:HD11	1.92	0.49
1:D:242:THR:HG21	1:D:246:LEU:HD12	1.95	0.49
1:D:239:VAL:HG21	1:D:347:ILE:HD13	1.94	0.48
1:A:179:SER:HG	1:A:341:TYR:HH	1.54	0.48
1:D:186:THR:HG21	1:D:214:LYS:HD2	1.95	0.48
1:D:55:PHE:O	1:D:57:LYS:NZ	2.39	0.48
1:C:131:PHE:HB3	1:C:159:LYS:HE2	1.96	0.48
1:C:189:ARG:NH2	1:C:215:TYR:OH	2.47	0.47
1:D:200:LYS:HA	1:D:203:GLU:HG3	1.95	0.47
1:D:73:ASN:HB2	1:D:354:ARG:HH22	1.79	0.47
2:E:39:ASP:N	2:E:39:ASP:OD2	2.42	0.47
1:B:176:VAL:HG21	1:B:276:LEU:HB3	1.96	0.47
1:D:259:PHE:HZ	1:B:259:PHE:CZ	2.31	0.47
1:B:362:PRO:HA	1:B:363:PRO:HD3	1.78	0.47
1:C:184:SER:OG	1:C:185:GLU:N	2.46	0.47
1:C:41:ASN:ND2	1:C:46:PHE:O	2.48	0.47
1:C:71:ARG:NH1	1:C:272:SER:O	2.48	0.47
1:C:172:ARG:HD2	1:C:276:LEU:HD23	1.96	0.47
1:D:104:ASN:ND2	1:D:106:GLU:OE2	2.48	0.47
1:C:355:TYR:HB3	1:C:379:TYR:HB3	1.96	0.46
2:H:45:ILE:HG23	2:H:46:HIS:CG	2.51	0.46
1:A:134:ASN:HB3	1:A:371:GLU:HB3	1.98	0.46
1:A:385:SER:O	1:A:390:LYS:NZ	2.42	0.46
1:C:209:GLN:NE2	1:C:235:LEU:HB2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:VAL:HG12	1:C:318:THR:HA	1.96	0.46
1:D:201:VAL:HG22	1:D:344:ILE:HD11	1.99	0.45
1:D:6:THR:HG22	1:D:8:ASN:H	1.81	0.45
1:B:28:ASP:OD1	1:B:28:ASP:N	2.50	0.45
1:B:107:LEU:HD12	1:B:110:LYS:HD3	1.98	0.45
2:H:40:SER:OG	2:H:41:TYR:N	2.47	0.45
1:A:71:ARG:HH11	1:A:271:ILE:HG23	1.81	0.45
1:D:64:ILE:HB	1:B:90:VAL:HG12	1.97	0.45
1:A:172:ARG:HH12	1:A:277:GLY:H	1.63	0.44
1:B:242:THR:HG21	1:B:246:LEU:HD12	1.99	0.44
1:D:68:LEU:HB2	1:D:161:SER:HB3	1.99	0.44
1:D:362:PRO:HA	1:D:363:PRO:HD3	1.86	0.44
1:A:130:LYS:HE3	1:A:373:THR:HG21	1.99	0.44
1:C:108:MET:HG3	1:C:109:LEU:HD12	1.99	0.44
1:C:96:PRO:HD2	1:B:166:LEU:HG	2.00	0.44
1:A:324:LEU:HB2	1:A:327:PHE:HD2	1.83	0.44
1:C:255:ILE:HG12	1:C:261:ILE:HD11	2.00	0.44
2:E:10:MET:O	2:E:14:SER:HB2	2.18	0.44
1:A:44:THR:OG1	1:A:45:MET:N	2.50	0.43
1:C:169:LYS:HG3	1:C:172:ARG:HH21	1.83	0.43
1:A:100:ASP:OD1	1:A:100:ASP:N	2.51	0.43
2:E:44:GLN:HB3	2:E:45:ILE:H	1.66	0.43
1:C:49:PHE:O	1:C:52:LYS:NZ	2.52	0.43
1:D:64:ILE:HG13	2:F:53:PHE:CD2	2.54	0.43
1:A:361:LYS:HE2	1:A:377:HIS:HB2	2.01	0.42
1:D:357:LYS:HG2	2:F:20:LEU:HD12	2.01	0.42
1:C:86:SER:HB2	1:B:60:GLU:HB2	2.00	0.42
1:A:255:ILE:HA	1:A:258:THR:HG22	2.02	0.42
1:A:265:ASP:OD1	1:A:265:ASP:N	2.48	0.42
1:B:133:LEU:HD21	1:B:155:VAL:HG11	2.00	0.42
1:C:184:SER:HB2	1:C:219:HIS:CE1	2.55	0.42
1:A:247:LYS:HE2	1:A:251:LEU:HD11	2.01	0.42
1:B:175:LEU:HD23	1:B:384:ILE:HD11	2.01	0.42
1:A:205:ILE:HD11	1:A:240:ILE:HD11	2.00	0.42
1:D:274:ASP:HB3	1:B:210:ASN:HD22	1.85	0.42
1:D:208:LEU:HD22	1:D:389:ASN:HB3	2.01	0.42
1:C:208:LEU:HD22	1:C:238:ILE:HG12	2.02	0.42
1:B:209:GLN:NE2	1:B:235:LEU:HB2	2.34	0.42
1:D:139:ARG:NH2	1:A:80:ASP:O	2.53	0.42
1:D:349:SER:HB2	1:D:388:PHE:HB2	2.01	0.42
1:A:139:ARG:NH1	2:E:14:SER:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LYS:HA	1:D:119:LYS:HD3	1.88	0.41
1:C:280:PHE:HE2	1:C:320:ASP:HA	1.85	0.41
1:A:361:LYS:HD3	1:A:377:HIS:HD2	1.86	0.41
1:B:131:PHE:HB3	1:B:159:LYS:HE2	2.02	0.41
1:C:296:PHE:HE2	1:C:321:VAL:HG23	1.85	0.41
1:D:68:LEU:HD12	1:D:161:SER:HB3	2.03	0.41
1:D:197:LEU:HD21	1:D:342:ALA:HB2	2.03	0.41
1:D:63:LEU:HD21	1:D:154:GLY:HA3	2.03	0.41
1:B:209:GLN:HB3	2:F:35:ASN:H	1.86	0.41
1:D:144:THR:HG22	1:D:146:ALA:H	1.86	0.40
1:A:274:ASP:OD1	1:A:274:ASP:N	2.55	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	391/408 (96%)	369 (94%)	22 (6%)	0	100	100
1	B	383/408 (94%)	348 (91%)	35 (9%)	0	100	100
1	C	383/408 (94%)	349 (91%)	34 (9%)	0	100	100
1	D	388/408 (95%)	357 (92%)	31 (8%)	0	100	100
2	E	52/60 (87%)	40 (77%)	11 (21%)	1 (2%)	9	43
2	F	53/60 (88%)	38 (72%)	13 (24%)	2 (4%)	3	28
2	G	25/60 (42%)	19 (76%)	6 (24%)	0	100	100
2	H	53/60 (88%)	37 (70%)	15 (28%)	1 (2%)	9	43
All	All	1728/1872 (92%)	1557 (90%)	167 (10%)	4 (0%)	53	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	44	GLN
2	E	44	GLN
2	H	45	ILE
2	F	46	HIS

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	353/367 (96%)	353 (100%)	0	100	100
1	B	345/367 (94%)	343 (99%)	2 (1%)	87	95
1	C	345/367 (94%)	345 (100%)	0	100	100
1	D	352/367 (96%)	350 (99%)	2 (1%)	87	95
2	E	51/56 (91%)	51 (100%)	0	100	100
2	F	51/56 (91%)	51 (100%)	0	100	100
2	G	25/56 (45%)	24 (96%)	1 (4%)	34	67
2	H	50/56 (89%)	49 (98%)	1 (2%)	58	82
All	All	1572/1692 (93%)	1566 (100%)	6 (0%)	92	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	31	LYS
1	D	318	THR
1	B	94	THR
1	B	109	LEU
2	G	8	ARG
2	H	22	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	20:SER	C	21:ALA	N	3.61