wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 13, 2016 – 04:24 PM EST

PDB ID	:	5ARA
EMDB ID:	:	EMD-3164
Title	:	Bovine mitochondrial ATP synthase state 1a
Authors	:	Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.
Deposited on	:	2015-09-24
Resolution	:	6.70 Å(reported)
Based on PDB ID	:	2CLY, 2XND, 2WSS

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

We welcome your comments at *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.

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 6.70 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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		4.6%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
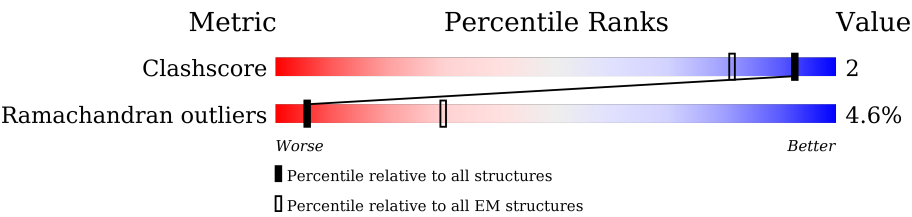
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	510	90% 10%
1	B	510	85% 9% • 6%
1	C	510	85% 9% • 5%
2	D	482	87% 9% • •
2	E	482	89% 8% •
2	F	482	85% 11% •
3	G	273	88% 7% • •
4	H	146	78% 12% 10%
5	I	50	82% 10% • 6%
6	J	72	97% •
6	K	72	99% •

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Mol	Chain	Length	Quality of chain
6	L	72	100%
6	M	72	97%
6	N	72	100%
6	O	72	99%
6	P	72	99%
6	Q	72	97%
7	S	190	60% 25% 12%
8	T	174	82% 14%
9	U	124	79% 15%
10	V	77	74% 10% 14%
11	W	217	88% 11%

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 18544 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	509	Total 2035	C 1018	N 509	O 508	0	0
1	B	480	Total 1918	C 960	N 480	O 478	0	0
1	C	487	Total 1947	C 974	N 487	O 486	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CONFLICT	UNP P19483
B	481	GLY	SER	CONFLICT	UNP P19483
C	481	GLY	SER	CONFLICT	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	467	Total 1867	C 934	N 467	O 466	0	0
2	E	466	Total 1863	C 932	N 466	O 465	0	0
2	F	466	Total 1863	C 932	N 466	O 465	0	0

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	264	Total 1053	C 528	N 264	O 261	0	0

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	131	Total 523	C 262	N 131	O 130	0	0

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	47	Total 187	C 94	N 47	O 46	0	0

- Molecule 6 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITO-CHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	72	Total 288	C 144	N 72	O 72	0	0
6	K	72	Total 288	C 144	N 72	O 72	0	0
6	L	72	Total 288	C 144	N 72	O 72	0	0
6	M	72	Total 288	C 144	N 72	O 72	0	0
6	N	72	Total 288	C 144	N 72	O 72	0	0
6	O	72	Total 288	C 144	N 72	O 72	0	0
6	P	72	Total 288	C 144	N 72	O 72	0	0
6	Q	72	Total 288	C 144	N 72	O 72	0	0

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	168	Total 669	C 334	N 168	O 167	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	CONFLICT	UNP P13621

- Molecule 8 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITO-CHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	T	174	697	348	174	175	0	0

- Molecule 9 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	122	485	242	122	121	0	1

- Molecule 10 is a protein called ATP SYNTHASE-COUPLING FACTOR 6, MITOCHON-DRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	V	66	264	132	66	66	0	0

- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

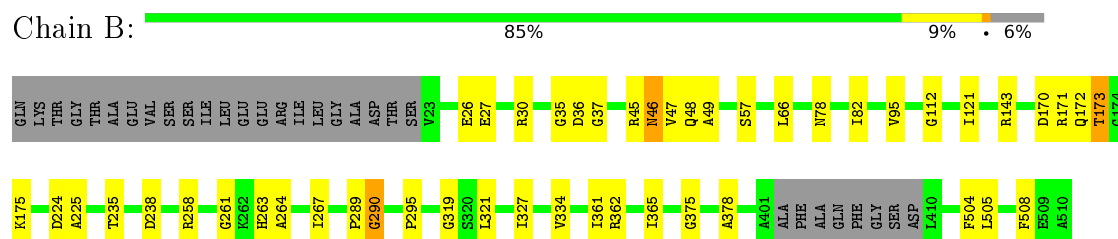| Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	217	869	434	217	218	0	0

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 errors 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.
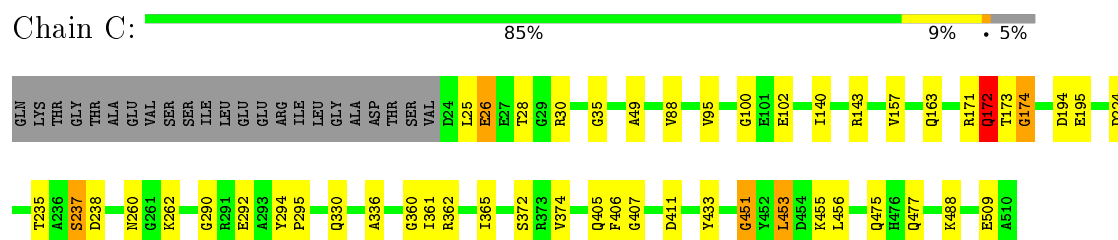
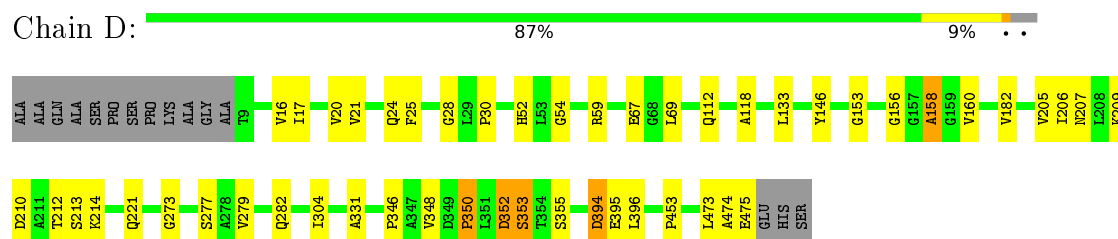- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:

90%	10%

GLN K2 T3 G4 T5 A6 I11 L12 E13 E14 D20 T21 D24 G35 V41 A49 D79 K80 L81 I82 V88 K89 V95 G100 S123 K124 A125 R126 P145 M146 R171 G174 K175 T176 G192 K198 D224 T235 D238 R258

D259 N260 G261 K262 D269 P289 P295 G319 I327 V334 S335 A336 S372 R373 V374 G407 S408 D409 A437 T485 D486 G487 K488 A510

- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:

85%	9%	6%

GLN LYS THR GLY THR ALA GLU VAL SER SER ILE LEU GLU GLU ARG ILE LEU GLY ALA ASP THR SER V23 E26 E27 R30 G35 D36 G37 R45 N46 V47 Q48 A49 S57 L66 N78 I82 V95 G112 I121 R143 D170 R171 Q172 T173 G174

K175 D224 A225 T235 D238 R258 G261 K262 H263 A264 I267 P289 Q290 P295 G319 S320 L321 I327 V334 I361 R362 I365 G375 A378 A401 ALA PHE ALA GLN PHE GLY SER ASP L410 F504 L505 F508 E509 A510

- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain C:

85%	9%	5%

GLN LYS THR GLY THR ALA GLU VAL SER SER ILE LEU GLU GLU ARG ILE LEU GLY ALA ASP THR SER VAL D24 L25 E26 E27 T28 G29 R30 G35 A49 V88 V95 G100 E101 E102 I140 R143 V157 Q163 R171 Q172 T173 G174 D194 E195 D224

T235 A236 S237 D238 N260 G261 K262 G290 R291 E292 A293 Y294 P295 Q330 A336 G360 I361 R362 I365 S372 R373 V374 Q405 F406 G407 D411 Y433 G451 Y452 L453 D454 K455 L456 Q475 H476 Q477 K488 E509 A510

- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:

87%	9%

ALA ALA GLN ALA SER PRO SER PRO LYS ALA GLY ALA T9 V16 I17 V20 V21 Q24 P25 G28 L29 P30 H52 L53 G54 R59 E67 G68 L69 Q112 A118 L133 Y146 G153 G156 G157 A158 G159 V160 V182 V205 I206 N207 L208 K209

D210 A211 T212 S213 K214 Q221 G273 S277 A278 V279 Q282 I304 A331 P346 A347 V348 D349 P350 L351 D352 S353 T354 S355 D394 E395 L396 P453 L473 A474 E475 GLU HIS SER
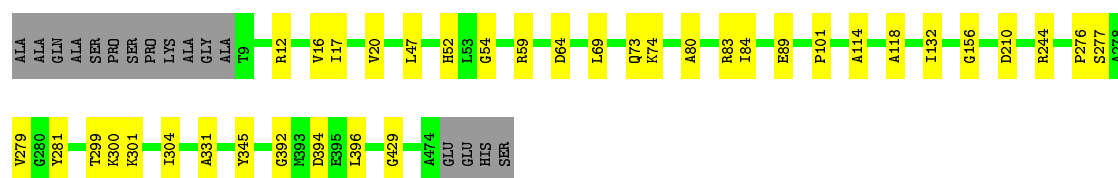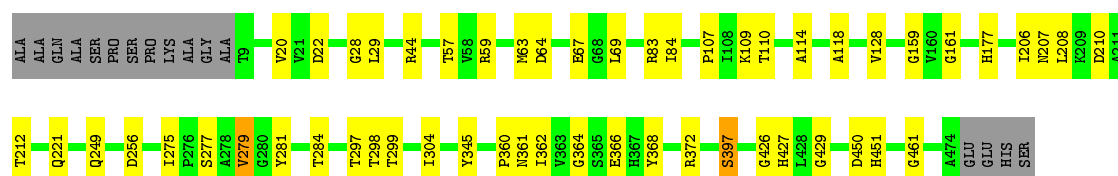
- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:

89%   8%   ·

• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:

85%   11%   ·

• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:

88%   7%   ·   ·
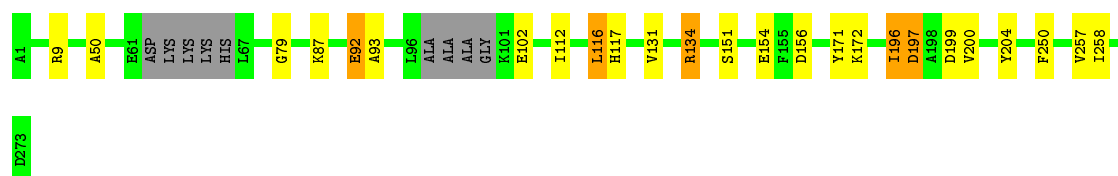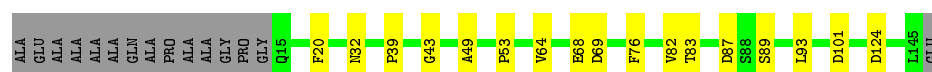

• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H:

78%   12%   10%

• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:

82%   10%   ·   6%

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain J:

97%   ·

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K: 99%   .

I2 P40 F73

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain L: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain M: 97%   .

I2 P40 I71 L72 F73

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain N: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O: 99%   .

I2 N39 F73

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain P: 99%   .

I2 P40 F73

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q: 97%   .

I2 P40 Q44 F73

• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S: 60%   25%   • •   12%

F1 V9 G13 G16 L46 K47 E48 P49 K61 K65 V66 K67 S68 L69 S70 D71 M72 T73 S79 P80 N92 S106 T107 M108 M109 S110 V111 H112 R113 G114 E115 V116 V120 T121 T122 A123 L126 D127 E128 T129 T132 K139 S140 F141 L142 S143 K144

G145 Q146 L150 E151 V152 K153 I154 D155 P156 S157 I158 M159 I163 V164 G167 E168 LYS TYR VAL ASP MET SER ALA LYS THR LYS ILE GLN LYS LEU SER ARG ALA MET ARG GLU ILE LEU
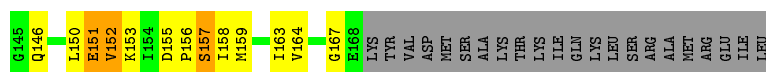
• Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T: 82%   14%   ·

P1 K15 T21 P22 E23 T24 F25 K51 R88 H89 Y90 L91 F92 D93 V94 Q95 A100 E104 E109 R110 E117 K135 E136 R147 V148 I152 Q155 Q156 E159 T160 I161 A162 K163 A166 S172 K173 K174

• Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U: 79%   15%   · ·

ALA GLY R3 K4 L5 A6 V13 G16 E17 I18 I19 P20 A50 V78 P79 I80 P81 Q88 E92 D96 C100 A101 L104 Q112 E113 Y114 E115 R122 N123 I124

• Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

Chain V: 74%   10%   ·   14%

PHE ASN LYS GLU L1 D2 P3 V4 S22 G23 G24 P25 V26 K42 N57 P63 E66 VAL VAL GLU LYS PRO GLN SER

• Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W: 88%   11%

I10 G16 N35 R36 N40 Q47 S63 L85 G86 L87 L88 P89 H90 S91 F92 K122 G132 V142 S148 Q152 L156 N163 G175 G176 S219 L220 Y221 L222 T226

4   Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	20104	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	30487	Depositor
Image detector	GATAN K2 (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	1.81	3/2034 (0.1%)	1.42	17/2541 (0.7%)
1	B	1.85	3/1916 (0.2%)	1.42	18/2392 (0.8%)
1	C	1.83	3/1946 (0.2%)	1.42	17/2431 (0.7%)
10	V	0.79	0/263	1.06	0/327
11	W	2.53	5/868 (0.6%)	1.21	6/1082 (0.6%)
2	D	1.82	2/1866 (0.1%)	1.47	23/2331 (1.0%)
2	E	1.79	5/1862 (0.3%)	1.43	16/2326 (0.7%)
2	F	1.87	2/1862 (0.1%)	1.53	22/2326 (0.9%)
3	G	1.78	1/1050 (0.1%)	1.37	8/1308 (0.6%)
4	H	1.81	0/522	1.61	10/651 (1.5%)
5	I	1.63	0/186	1.40	2/231 (0.9%)
6	J	0.30	0/287	0.41	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.30	0/287	0.45	0/357
6	M	0.29	0/287	0.44	0/357
6	N	0.28	0/287	0.40	0/357
6	O	0.30	0/287	0.41	0/357
6	P	0.29	0/287	0.43	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.63	3/668 (0.4%)	1.92	18/834 (2.2%)
8	T	1.24	6/696 (0.9%)	1.53	13/867 (1.5%)
9	U	0.87	0/484	1.37	4/604 (0.7%)
All	All	1.69	33/18519 (0.2%)	1.37	174/23107 (0.8%)

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	3
1	B	0	1
1	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	V	0	6
11	W	0	16
2	D	0	5
2	F	0	1
3	G	0	2
7	S	0	11
8	T	0	22
9	U	0	19
All	All	0	89

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	88	LEU	CA-C	62.36	3.15	1.52
11	W	88	LEU	N-CA	20.90	1.88	1.46
11	W	89	PRO	N-CA	-18.54	1.15	1.47
11	W	88	LEU	C-O	-14.20	0.96	1.23
8	T	160	THR	N-CA	9.37	1.65	1.46

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	73	THR	C-N-CA	16.48	162.91	121.70
7	S	110	SER	C-N-CA	-12.41	90.68	121.70
7	S	106	SER	CA-C-N	-12.23	90.30	117.20
11	W	89	PRO	N-CA-C	-10.49	84.82	112.10
9	U	78	VAL	CA-C-O	-9.60	99.94	120.10

There are no chirality outliers.

5 of 89 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	ALA	Mainchain,Peptide
1	A	485	THR	Mainchain
1	B	46	ASN	Mainchain
1	C	173	THR	Mainchain
1	C	336	ALA	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	2035	0	589	5	0
1	B	1918	0	553	7	0
1	C	1947	0	563	7	0
2	D	1867	0	533	4	0
2	E	1863	0	532	4	0
2	F	1863	0	532	8	0
3	G	1053	0	283	0	0
4	H	523	0	140	1	0
5	I	187	0	53	1	0
6	J	288	0	92	0	0
6	K	288	0	92	0	0
6	L	288	0	92	0	0
6	M	288	0	92	0	0
6	N	288	0	92	0	0
6	O	288	0	92	0	0
6	P	288	0	92	0	0
6	Q	288	0	92	0	0
7	S	669	0	178	8	0
8	T	697	0	182	1	0
9	U	485	0	118	0	0
10	V	264	0	71	0	0
11	W	869	0	226	4	0
All	All	18544	0	5289	43	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 2.

The worst 5 of 43 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)
11:W:88:LEU:CA	11:W:88:LEU:N	1.88	1.36
7:S:164:VAL:CA	7:S:167:GLY:O	2.28	0.80
2:F:84:ILE:H	2:F:114:ALA:H	1.42	0.68
1:B:49:ALA:H	2:F:69:LEU:H	1.43	0.67
1:A:49:ALA:H	2:E:69:LEU:N	2.00	0.59

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	507/510 (99%)	445 (88%)	35 (7%)	27 (5%)	2	29
1	B	476/510 (93%)	423 (89%)	30 (6%)	23 (5%)	3	32
1	C	485/510 (95%)	434 (90%)	28 (6%)	23 (5%)	3	32
2	D	465/482 (96%)	415 (89%)	30 (6%)	20 (4%)	3	34
2	E	464/482 (96%)	418 (90%)	34 (7%)	12 (3%)	7	45
2	F	464/482 (96%)	412 (89%)	32 (7%)	20 (4%)	3	34
3	G	258/273 (94%)	195 (76%)	43 (17%)	20 (8%)	1	20
4	H	129/146 (88%)	114 (88%)	10 (8%)	5 (4%)	4	36
5	I	45/50 (90%)	35 (78%)	7 (16%)	3 (7%)	1	24
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	6	43
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14	58
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100	100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	6	43
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100	100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14	58
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14	58
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	6	43
7	S	166/190 (87%)	110 (66%)	30 (18%)	26 (16%)	0	5
8	T	172/174 (99%)	154 (90%)	14 (8%)	4 (2%)	8	48
9	U	120/124 (97%)	95 (79%)	16 (13%)	9 (8%)	1	21
10	V	64/77 (83%)	51 (80%)	9 (14%)	4 (6%)	2	25
11	W	215/217 (99%)	192 (89%)	19 (9%)	4 (2%)	10	52
All	All	4590/4803 (96%)	3990 (87%)	391 (8%)	209 (5%)	5	32

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	13	GLU
1	A	14	GLU
1	A	20	ASP
1	A	24	ASP

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

There are no chain breaks in this entry.