wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Dec 13, 2016 – 03:56 PM EST

PDB ID	:	5FIL
EMDB ID:	:	EMD-3170
Title	:	Bovine mitochondrial ATP synthase state 3b
Authors	:	Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.
Deposited on	:	2015-09-28
Resolution	:	7.10 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 (i) symbol.

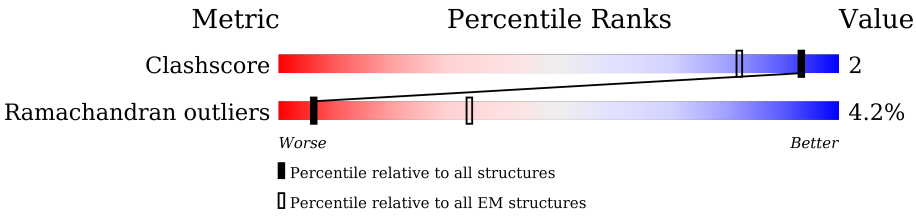
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 7.10 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.



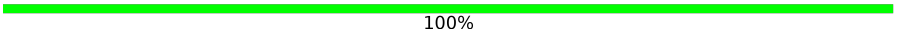
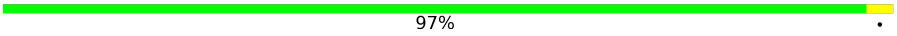
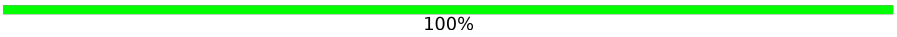
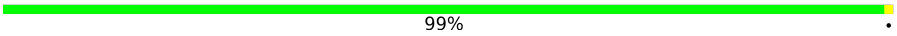
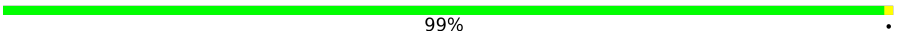
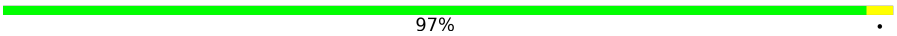
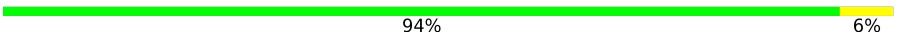
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726

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	88% 11% •
1	B	510	84% 9% • 6%
1	C	510	87% 7% • 5%
2	D	482	88% 9% •
2	E	482	86% 10% • •
2	F	482	88% 9% •
3	G	273	75% 19% • •
4	H	146	66% 24% 10%
5	I	50	72% 20% • 6%
6	J	72	97% •
6	K	72	99% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	L	72	
6	M	72	
6	N	72	
6	O	72	
6	P	72	
6	Q	72	
7	S	190	
8	T	174	
9	U	124	
10	V	77	
11	W	217	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18546 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 1948	C 974	N 487	O 487	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	C	N	O	0	0
			523	262	131	130		

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

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

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

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

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

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

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, MITOCHONDRIAL.

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	67	Total 265	C 132	N 67	O 66	0	1

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

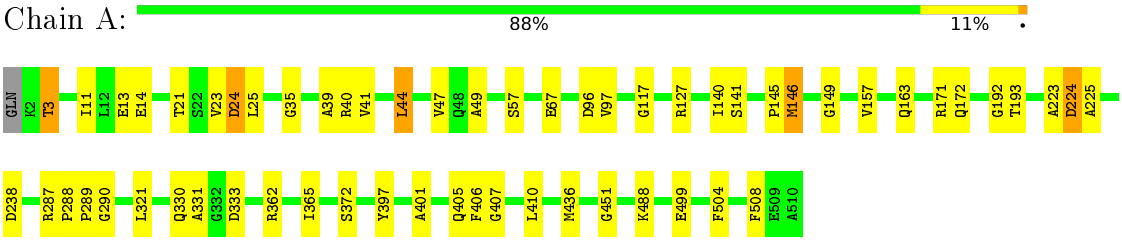
Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	217	Total 869	C 434	N 217	O 218	0	0

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 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.

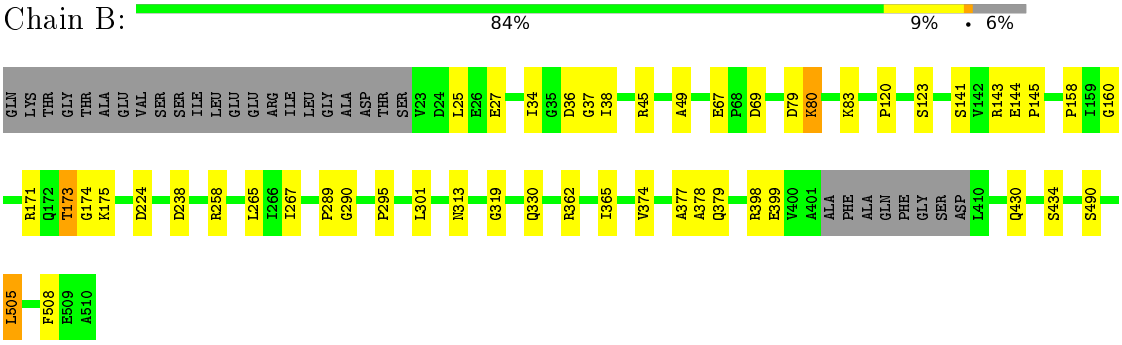
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



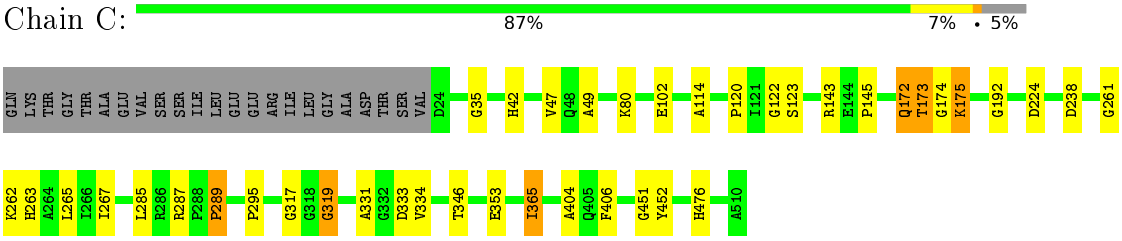
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:



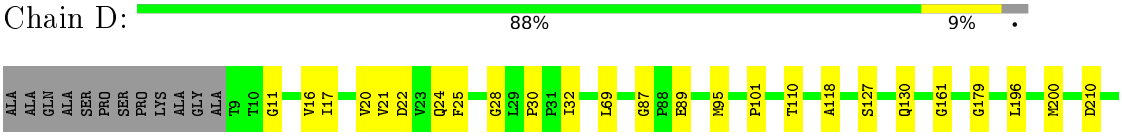
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain C:



- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:

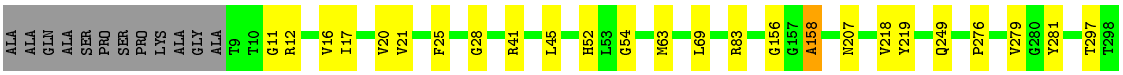


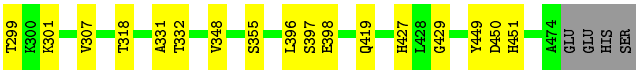
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:

• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

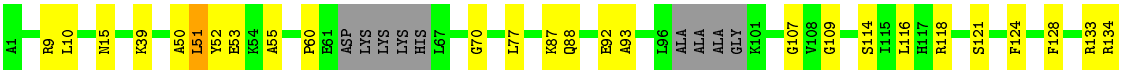
Chain F:

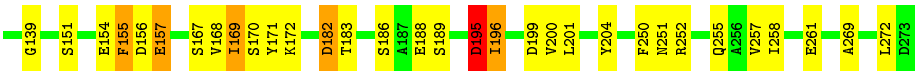




• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

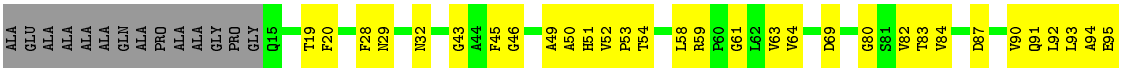
Chain G:

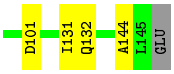




• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

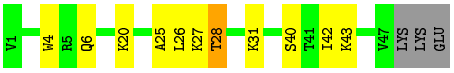
Chain H:



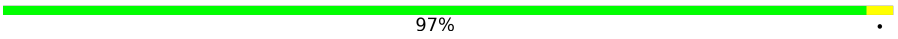


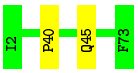
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:

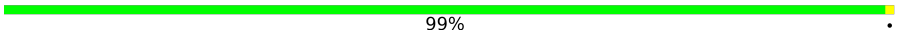


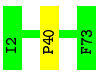
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain J: 

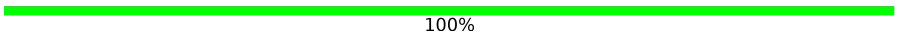


• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K: 

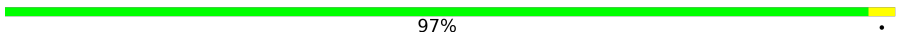


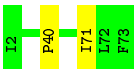
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain L: 

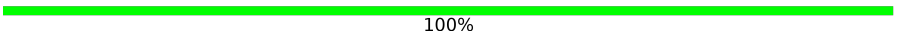
There are no outlier residues recorded for this chain.

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

Chain M: 

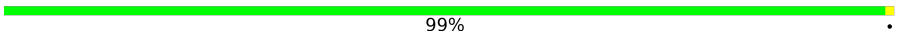


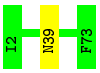
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain N: 

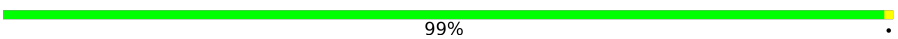
There are no outlier residues recorded for this chain.

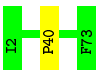
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O: 

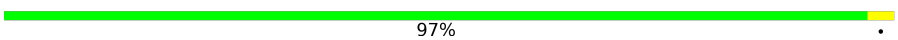


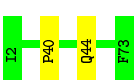
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain P: 



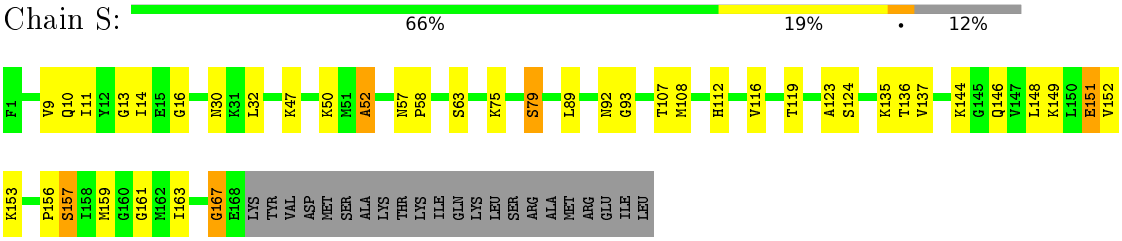
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q: 



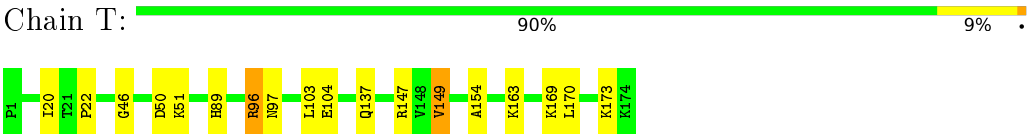
• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:



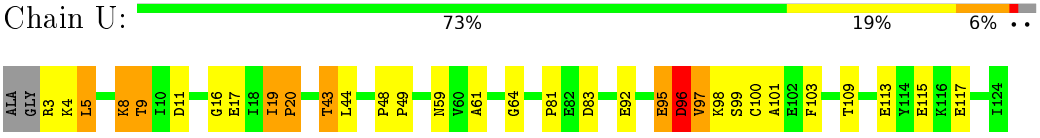
• Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:



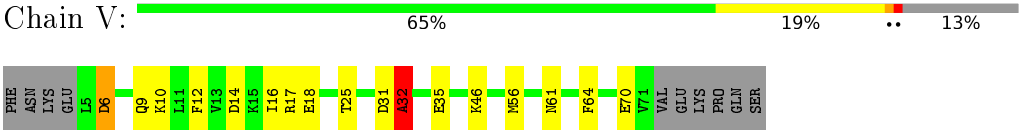
• Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:



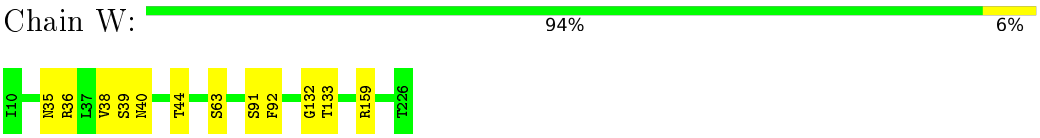
• Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

Chain V:



• Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	22117	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	1.82	4/2034 (0.2%)	1.49	24/2541 (0.9%)
1	B	1.83	3/1916 (0.2%)	1.49	17/2392 (0.7%)
1	C	1.78	6/1947 (0.3%)	1.43	12/2432 (0.5%)
10	V	0.78	0/264	1.13	2/329 (0.6%)
11	W	0.50	1/868 (0.1%)	0.77	2/1082 (0.2%)
2	D	1.80	3/1866 (0.2%)	1.47	21/2331 (0.9%)
2	E	1.84	5/1862 (0.3%)	1.52	21/2326 (0.9%)
2	F	1.78	1/1862 (0.1%)	1.49	25/2326 (1.1%)
3	G	2.01	10/1050 (1.0%)	1.68	22/1308 (1.7%)
4	H	2.23	11/522 (2.1%)	1.91	19/651 (2.9%)
5	I	1.93	1/186 (0.5%)	1.71	3/231 (1.3%)
6	J	0.30	0/287	0.41	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.31	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	1.67	0/668	1.75	14/834 (1.7%)
8	T	0.78	1/696 (0.1%)	0.91	1/867 (0.1%)
9	U	1.18	4/484 (0.8%)	1.56	9/604 (1.5%)
All	All	1.62	50/18521 (0.3%)	1.39	192/23110 (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	7
1	C	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
10	V	0	15
11	W	0	5
2	D	0	3
2	E	0	4
2	F	0	3
3	G	0	4
4	H	0	1
7	S	0	9
8	T	0	13
9	U	0	32
All	All	0	103

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	96	ASP	N-CA	13.61	1.73	1.46
9	U	9	THR	N-CA	9.92	1.66	1.46
3	G	261	GLU	CA-C	-6.93	1.34	1.52
4	H	46	GLY	CA-C	-6.57	1.41	1.51
2	E	161	GLY	N-CA	-6.51	1.36	1.46

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	U	96	ASP	N-CA-C	11.66	142.48	111.00
7	S	52	ALA	C-N-CA	-9.93	96.86	121.70
11	W	44	THR	CA-C-N	9.73	138.62	117.20
4	H	29	ASN	N-CA-C	-9.33	85.81	111.00
1	A	3	THR	N-CA-C	-9.04	86.59	111.00

There are no chirality outliers.

5 of 103 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ASP	Mainchain
1	A	333	ASP	Mainchain
1	A	406	PHE	Peptide
1	B	123	SER	Mainchain,Peptide
1	B	379	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	2035	0	589	6	0
1	B	1918	0	553	4	0
1	C	1948	0	563	6	0
2	D	1867	0	533	5	0
2	E	1863	0	532	3	0
2	F	1863	0	532	3	0
3	G	1053	0	283	4	0
4	H	523	0	140	1	0
5	I	187	0	53	2	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	179	3	0
8	T	697	0	182	3	0
9	U	485	0	118	3	0
10	V	265	0	68	1	0
11	W	869	0	226	2	0
All	All	18546	0	5287	40	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 40 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)
9:U:96:ASP:N	9:U:96:ASP:CA	1.73	1.46
7:S:163:ILE:O	7:S:167:GLY:O	1.88	0.90
1:B:173:THR:H	1:B:175:LYS:H	1.26	0.82
3:G:51:LEU:C	3:G:53:GLU:H	2.03	0.61
1:A:223:ALA:C	1:A:225:ALA:H	2.09	0.55

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%)	446 (88%)	37 (7%)	24 (5%)	3 32
1	B	476/510 (93%)	430 (90%)	24 (5%)	22 (5%)	3 32
1	C	485/510 (95%)	437 (90%)	29 (6%)	19 (4%)	4 36
2	D	465/482 (96%)	422 (91%)	32 (7%)	11 (2%)	7 47
2	E	464/482 (96%)	414 (89%)	29 (6%)	21 (4%)	3 33
2	F	464/482 (96%)	423 (91%)	31 (7%)	10 (2%)	8 49
3	G	258/273 (94%)	189 (73%)	42 (16%)	27 (10%)	1 12
4	H	129/146 (88%)	111 (86%)	9 (7%)	9 (7%)	1 22
5	I	45/50 (90%)	31 (69%)	10 (22%)	4 (9%)	1 17
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%)	107 (64%)	39 (24%)	20 (12%)	0 8
8	T	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	11 55
9	U	120/124 (97%)	95 (79%)	16 (13%)	9 (8%)	1 21
10	V	65/77 (84%)	50 (77%)	12 (18%)	3 (5%)	3 32
11	W	215/217 (99%)	195 (91%)	17 (8%)	3 (1%)	14 58
All	All	4591/4803 (96%)	4011 (87%)	386 (8%)	194 (4%)	6 34

5 of 194 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	21	THR
1	A	141	SER
1	A	289	PRO

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.