



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 05:06 AM EDT

PDB ID : 5ARI
EMDB ID: : EMD-3167
Title : Bovine mitochondrial ATP synthase state 2b
Authors : Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.
Deposited on : unknown
Resolution : 7.40 Å(reported)
Based on PDB ID : 2CLY, 2XND, 2WSS

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

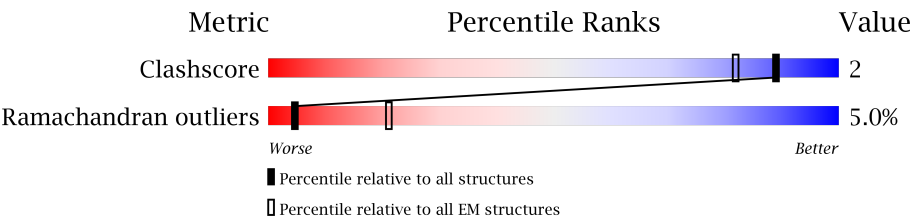
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

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 7.40 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	125131	1336
Ramachandran outliers	121729	1120

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	510	<div><div>86%13%.</div></div>
1	B	510	<div><div>82%11%.6%</div></div>
1	C	510	<div><div>86%10%5%</div></div>
2	D	482	<div><div>85%11%..</div></div>
2	E	482	<div><div>84%11%..</div></div>
2	F	482	<div><div>85%11%..</div></div>
3	G	273	<div><div>78%16%..</div></div>
4	H	146	<div><div>71%18%.10%</div></div>
5	I	50	<div><div>76%16%.6%</div></div>
6	J	72	<div><div>97%..</div></div>
6	K	72	<div><div>99%..</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	L	72	<div><div></div><div>100%</div></div>
6	M	72	<div><div></div><div>97%</div><div>.</div></div>
6	N	72	<div><div></div><div>100%</div></div>
6	O	72	<div><div></div><div>99%</div><div>.</div></div>
6	P	72	<div><div></div><div>99%</div><div>.</div></div>
6	Q	72	<div><div></div><div>97%</div><div>.</div></div>
7	S	190	<div><div></div><div>64%</div><div>19%</div><div>5%</div><div>12%</div></div>
8	T	174	<div><div></div><div>87%</div><div>11%</div><div>..</div></div>
9	U	124	<div><div></div><div>95%</div><div>...</div></div>
10	V	77	<div><div></div><div>60%</div><div>23%</div><div>.</div><div>13%</div></div>
11	W	217	<div><div></div><div>96%</div><div>.</div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 18545 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	C	N	O	0	0
			2035	1018	509	508		
1	B	480	Total	C	N	O	0	0
			1918	960	480	478		
1	C	487	Total	C	N	O	0	0
			1947	974	487	486		

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	C	N	O	0	0
			1867	934	467	466		
2	E	466	Total	C	N	O	0	0
			1863	932	466	465		
2	F	466	Total	C	N	O	0	0
			1863	932	466	465		

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

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

- 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	C	N	O	0	0
			697	348	174	175		

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

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

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

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

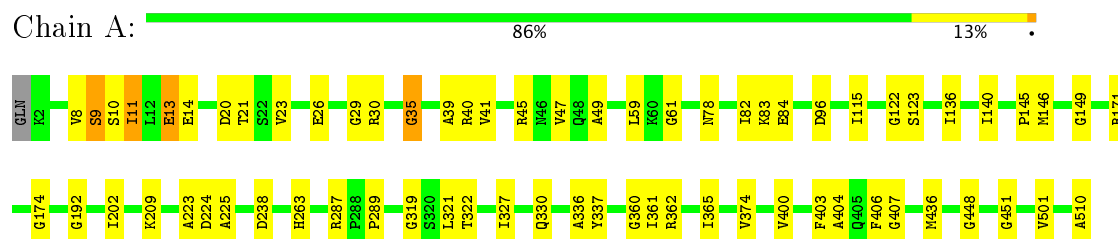
- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

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

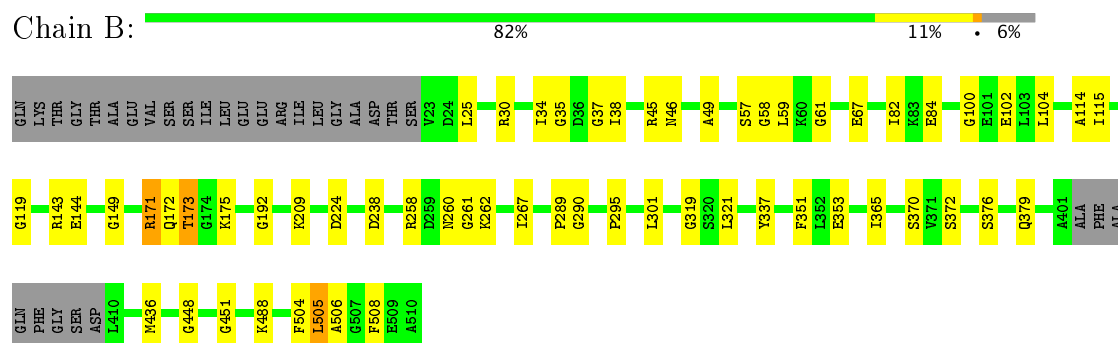
3 Residue-property plots

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.

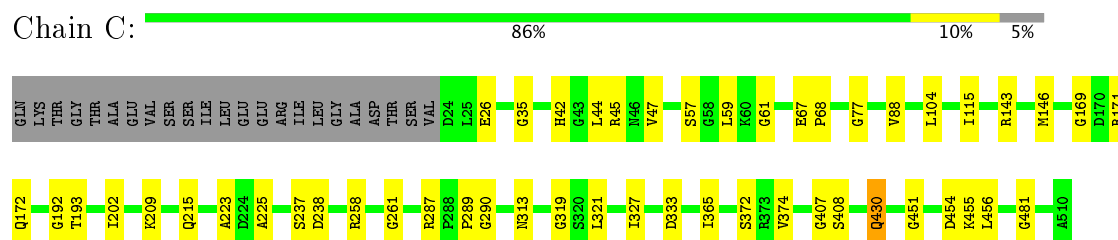
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



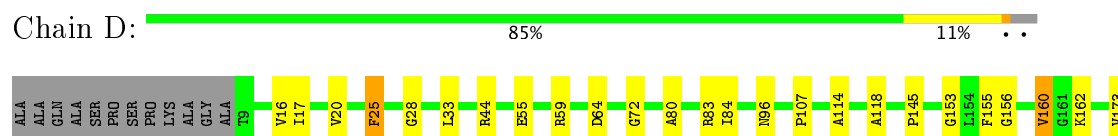
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

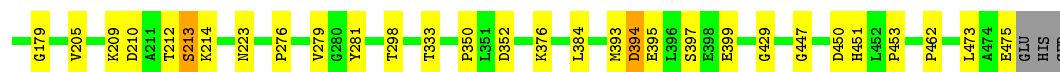


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



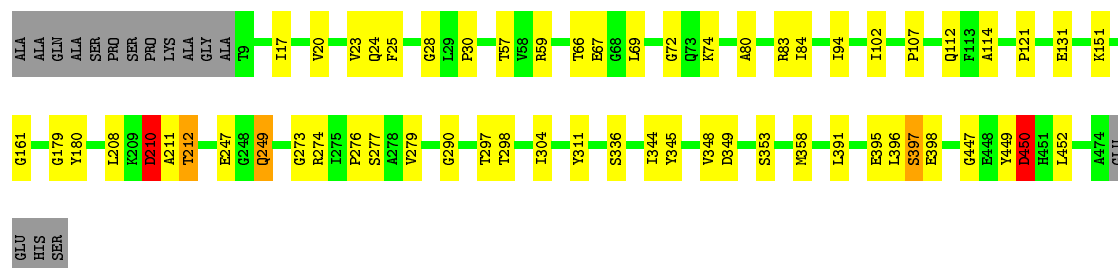
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





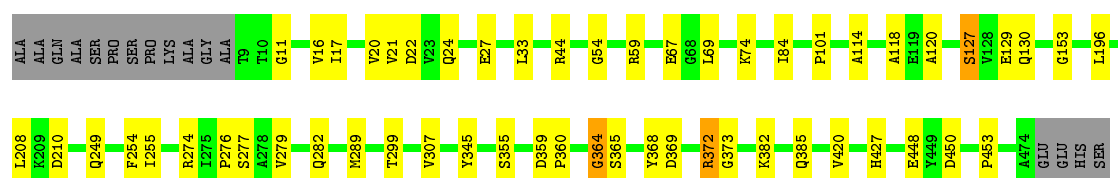
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 84% 11% . .



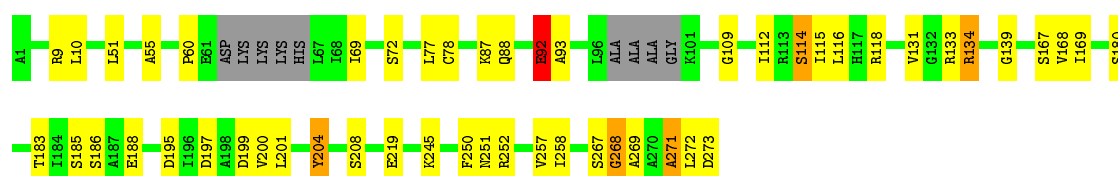
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F: 85% 11% . .



• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G: 78% 16% . .





- 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%



- 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%



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

Chain N: 100%

There are no outlier residues recorded for this chain.

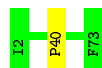
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O: 99%



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

Chain P: 99%



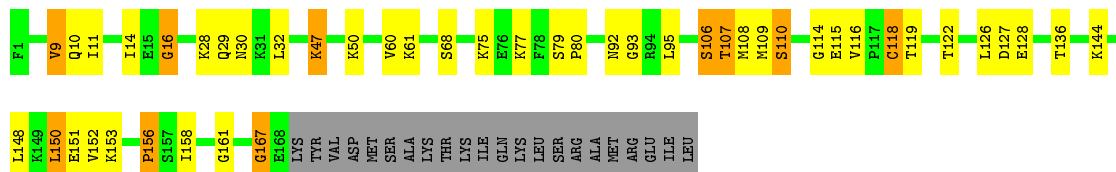
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q:  97% .




- Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:  64% 19% 5% 12%



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

Chain T:  87% 11% ..



- Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:  95% ...



- Molecule 10: ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL

Chain V:  60% 23% . 13%



- Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W:  96% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17610	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.3	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	1.83	9/2034 (0.4%)	1.55	29/2541 (1.1%)
1	B	1.90	7/1916 (0.4%)	1.53	19/2392 (0.8%)
1	C	1.85	4/1946 (0.2%)	1.50	23/2431 (0.9%)
10	V	0.70	0/264	1.19	0/329
11	W	0.43	0/868	0.73	0/1082
2	D	1.84	4/1866 (0.2%)	1.55	20/2331 (0.9%)
2	E	1.81	3/1862 (0.2%)	1.54	27/2326 (1.2%)
2	F	1.82	9/1862 (0.5%)	1.53	18/2326 (0.8%)
3	G	1.98	7/1050 (0.7%)	1.58	10/1308 (0.8%)
4	H	2.09	5/522 (1.0%)	1.80	12/651 (1.8%)
5	I	1.91	1/186 (0.5%)	1.70	4/231 (1.7%)
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	0.31	0/287	0.41	0/357
6	P	0.29	0/287	0.42	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.72	1/668 (0.1%)	2.43	11/834 (1.3%)
8	T	0.70	0/696	1.11	3/867 (0.3%)
9	U	0.56	0/484	2.57	1/604 (0.2%)
All	All	1.63	50/18520 (0.3%)	1.49	177/23109 (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	6
1	B	0	2
1	C	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
10	V	0	20
11	W	0	5
2	D	0	6
2	E	0	3
2	F	0	2
3	G	0	2
7	S	0	11
8	T	0	18
9	U	0	2
All	All	0	78

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLY	N-CA	-7.25	1.35	1.46
3	G	252	ARG	CA-C	-6.38	1.36	1.52
1	C	261	GLY	CA-C	-5.94	1.42	1.51
4	H	28	PHE	CA-C	-5.93	1.37	1.52
1	A	451	GLY	CA-C	-5.92	1.42	1.51
1	C	215	GLN	N-CA	-5.92	1.34	1.46
2	E	74	LYS	CA-C	-5.64	1.38	1.52
2	F	364	GLY	CA-C	-5.63	1.42	1.51
1	A	174	GLY	N-CA	-5.62	1.37	1.46
1	A	35	GLY	CA-C	-5.61	1.42	1.51
1	B	451	GLY	CA-C	-5.57	1.43	1.51
3	G	109	GLY	N-CA	-5.46	1.37	1.46
1	C	481	GLY	CA-C	-5.46	1.43	1.51
3	G	268	GLY	CA-C	-5.41	1.43	1.51
2	D	153	GLY	CA-C	-5.39	1.43	1.51
2	F	373	GLY	CA-C	-5.39	1.43	1.51
7	S	16	GLY	N-CA	-5.37	1.38	1.46
3	G	252	ARG	N-CA	-5.36	1.35	1.46
2	D	173	VAL	CA-C	-5.34	1.39	1.52
1	A	448	GLY	CA-C	-5.34	1.43	1.51
4	H	132	GLN	N-CA	-5.32	1.35	1.46
2	F	373	GLY	N-CA	-5.31	1.38	1.46
2	E	290	GLY	CA-C	-5.31	1.43	1.51
2	F	196	LEU	CA-C	-5.25	1.39	1.52
1	B	35	GLY	CA-C	-5.22	1.43	1.51
1	B	337	TYR	CA-C	-5.19	1.39	1.52
4	H	19	THR	CA-C	-5.19	1.39	1.52
3	G	219	GLU	N-CA	-5.19	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	20	PHE	N-CA	-5.18	1.35	1.46
4	H	19	THR	N-CA	-5.18	1.35	1.46
1	A	319	GLY	CA-C	-5.18	1.43	1.51
1	A	501	VAL	CA-C	-5.18	1.39	1.52
2	E	72	GLY	N-CA	-5.13	1.38	1.46
2	D	447	GLY	CA-C	-5.11	1.43	1.51
3	G	251	ASN	CA-C	-5.11	1.39	1.52
1	B	261	GLY	CA-C	-5.10	1.43	1.51
2	F	153	GLY	CA-C	-5.10	1.43	1.51
1	B	448	GLY	CA-C	-5.09	1.43	1.51
1	C	451	GLY	CA-C	-5.08	1.43	1.51
1	A	337	TYR	CA-C	-5.07	1.39	1.52
2	F	369	ASP	CA-C	-5.05	1.39	1.52
3	G	245	LYS	CA-C	-5.05	1.39	1.52
5	I	14	TYR	N-CA	-5.05	1.36	1.46
2	D	376	LYS	N-CA	-5.05	1.36	1.46
2	F	74	LYS	CA-C	-5.04	1.39	1.52
2	F	372	ARG	CA-C	-5.04	1.39	1.52
1	A	26	GLU	CA-C	-5.03	1.39	1.52
1	B	301	LEU	CA-C	-5.03	1.39	1.52
2	F	289	MET	N-CA	-5.02	1.36	1.46
1	B	267	ILE	N-CA	-5.01	1.36	1.46

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	121	ASN	O-C-N	-59.23	27.93	122.70
7	S	167	GLY	O-C-N	-48.08	45.78	122.70
7	S	110	SER	C-N-CA	12.85	153.84	121.70
7	S	107	THR	C-N-CA	9.54	145.54	121.70
1	A	35	GLY	N-CA-C	-8.91	90.83	113.10
2	E	210	ASP	N-CA-C	-8.17	88.93	111.00
2	D	395	GLU	N-CA-C	-8.03	89.32	111.00
8	T	93	ASP	N-CA-C	-7.91	89.65	111.00
1	A	362	ARG	N-CA-C	-7.79	89.95	111.00
2	F	20	VAL	N-CA-C	-7.71	90.19	111.00
2	F	345	TYR	N-CA-C	-7.70	90.21	111.00
7	S	150	LEU	N-CA-C	-7.66	90.31	111.00
2	F	17	ILE	N-CA-C	-7.64	90.36	111.00
1	B	100	GLY	N-CA-C	-7.61	94.08	113.10
3	G	134	ARG	N-CA-C	-7.61	90.46	111.00
1	A	327	ILE	N-CA-C	-7.52	90.70	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	GLY	N-CA-C	-7.50	94.35	113.10
2	E	298	THR	N-CA-C	-7.07	91.90	111.00
1	A	140	ILE	N-CA-C	-6.96	92.22	111.00
2	E	349	ASP	N-CA-C	-6.90	92.37	111.00
2	D	429	GLY	N-CA-C	-6.88	95.89	113.10
2	D	17	ILE	N-CA-C	-6.84	92.53	111.00
1	C	407	GLY	N-CA-C	-6.80	96.11	113.10
3	G	109	GLY	N-CA-C	-6.77	96.17	113.10
5	I	42	ILE	N-CA-C	-6.77	92.71	111.00
1	C	67	GLU	N-CA-C	-6.71	92.88	111.00
1	A	123	SER	N-CA-C	-6.67	92.99	111.00
2	E	24	GLN	N-CA-C	-6.66	93.02	111.00
5	I	8	GLY	N-CA-C	-6.64	96.49	113.10
1	C	61	GLY	N-CA-C	-6.64	96.50	113.10
2	D	298	THR	N-CA-C	-6.63	93.09	111.00
1	B	488	LYS	N-CA-C	-6.63	93.09	111.00
1	B	25	LEU	N-CA-C	-6.63	93.11	111.00
4	H	36	VAL	N-CA-C	-6.60	93.18	111.00
1	C	146	MET	N-CA-C	-6.58	93.25	111.00
4	H	93	LEU	N-CA-C	-6.56	93.28	111.00
1	B	290	GLY	N-CA-C	-6.54	96.76	113.10
4	H	91	GLN	N-CA-C	-6.51	93.42	111.00
2	F	22	ASP	N-CA-C	-6.50	93.44	111.00
3	G	77	LEU	C-N-CA	6.50	137.95	121.70
1	C	42	HIS	C-N-CA	6.47	135.88	122.30
4	H	84	VAL	N-CA-C	-6.40	93.72	111.00
1	B	38	ILE	N-CA-C	-6.40	93.73	111.00
1	B	267	ILE	N-CA-C	-6.39	93.75	111.00
1	A	61	GLY	N-CA-C	-6.23	97.53	113.10
2	F	208	LEU	C-N-CA	6.21	137.22	121.70
2	E	397	SER	N-CA-C	-6.21	94.24	111.00
2	F	16	VAL	N-CA-C	-6.20	94.27	111.00
2	D	59	ARG	N-CA-C	-6.18	94.32	111.00
7	S	106	SER	C-N-CA	-6.16	106.30	121.70
2	E	345	TYR	N-CA-C	-6.15	94.39	111.00
2	F	255	ILE	N-CA-C	-6.13	94.44	111.00
2	E	80	ALA	N-CA-C	-6.13	94.46	111.00
2	E	450	ASP	N-CA-C	-6.12	94.47	111.00
2	E	273	GLY	N-CA-C	-6.09	97.89	113.10
2	E	23	VAL	N-CA-C	-6.08	94.60	111.00
1	B	35	GLY	N-CA-C	-6.07	97.93	113.10
3	G	139	GLY	C-N-CA	6.06	136.86	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	83	ARG	N-CA-C	-6.06	94.63	111.00
1	B	61	GLY	N-CA-C	-6.05	97.97	113.10
1	A	29	GLY	N-CA-C	-6.05	97.97	113.10
4	H	67	ALA	C-N-CA	6.05	136.82	121.70
1	B	192	GLY	N-CA-C	-6.04	98.00	113.10
2	F	307	VAL	N-CA-C	-6.04	94.70	111.00
2	D	20	VAL	N-CA-C	-6.03	94.73	111.00
4	H	76	PHE	N-CA-C	-6.01	94.78	111.00
1	C	287	ARG	N-CA-C	-5.99	94.83	111.00
1	C	430	GLN	N-CA-C	-5.97	94.88	111.00
2	D	399	GLU	N-CA-C	-5.94	94.96	111.00
1	B	506	ALA	C-N-CA	5.93	134.76	122.30
1	A	8	VAL	C-N-CA	5.93	136.51	121.70
2	E	17	ILE	N-CA-C	-5.93	95.00	111.00
2	D	393	MET	C-N-CA	5.92	136.50	121.70
2	F	127	SER	N-CA-C	-5.89	95.11	111.00
4	H	22	SER	N-CA-C	-5.88	95.11	111.00
2	D	394	ASP	CA-C-N	-5.88	104.26	117.20
1	A	263	HIS	N-CA-C	-5.88	95.12	111.00
1	A	287	ARG	N-CA-C	-5.82	95.29	111.00
7	S	118	CYS	N-CA-C	-5.82	95.29	111.00
1	A	330	GLN	N-CA-C	-5.82	95.30	111.00
3	G	204	TYR	N-CA-C	-5.81	95.32	111.00
2	E	57	THR	N-CA-C	-5.78	95.39	111.00
2	E	311	TYR	N-CA-C	-5.77	95.42	111.00
1	A	39	ALA	N-CA-C	-5.75	95.48	111.00
1	A	96	ASP	N-CA-C	-5.75	95.48	111.00
1	A	122	GLY	N-CA-C	-5.75	98.73	113.10
2	E	336	SER	N-CA-C	-5.74	95.50	111.00
2	F	355	SER	N-CA-C	-5.73	95.54	111.00
2	F	254	PHE	N-CA-C	-5.71	95.58	111.00
2	F	21	VAL	N-CA-C	-5.71	95.58	111.00
8	T	170	LEU	O-C-N	-5.70	113.58	122.70
4	H	39	PRO	N-CA-C	-5.69	97.30	112.10
1	C	192	GLY	N-CA-C	-5.68	98.89	113.10
1	A	224	ASP	C-N-CA	5.66	135.84	121.70
2	E	449	TYR	N-CA-C	-5.62	95.82	111.00
7	S	144	LYS	N-CA-C	-5.62	95.83	111.00
5	I	41	THR	C-N-CA	5.62	135.74	121.70
2	E	59	ARG	N-CA-C	-5.61	95.85	111.00
2	D	80	ALA	N-CA-C	-5.61	95.86	111.00
2	E	112	GLN	N-CA-C	-5.58	95.94	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	20	VAL	N-CA-C	-5.58	95.94	111.00
1	C	333	ASP	CA-C-N	-5.57	104.94	117.20
3	G	131	VAL	N-CA-C	-5.57	95.96	111.00
2	D	16	VAL	N-CA-C	-5.54	96.03	111.00
2	D	96	ASN	N-CA-C	-5.53	96.07	111.00
1	C	321	LEU	N-CA-C	-5.53	96.08	111.00
1	B	119	GLY	N-CA-C	-5.50	99.34	113.10
7	S	16	GLY	N-CA-C	-5.50	99.34	113.10
2	D	145	PRO	N-CA-C	-5.50	97.80	112.10
2	F	27	GLU	N-CA-C	-5.49	96.17	111.00
4	H	43	GLY	N-CA-C	-5.48	99.39	113.10
2	F	210	ASP	N-CA-C	-5.48	96.21	111.00
7	S	9	VAL	C-N-CA	5.48	135.39	121.70
3	G	114	SER	N-CA-C	-5.45	96.27	111.00
1	C	202	ILE	N-CA-C	-5.44	96.31	111.00
1	B	67	GLU	N-CA-C	-5.44	96.32	111.00
1	A	407	GLY	N-CA-C	5.43	126.68	113.10
1	A	35	GLY	CA-C-N	-5.42	105.27	117.20
3	G	273	ASP	N-CA-C	-5.42	96.36	111.00
1	A	202	ILE	N-CA-C	-5.42	96.36	111.00
1	A	30	ARG	N-CA-C	-5.42	96.37	111.00
1	C	372	SER	N-CA-C	-5.42	96.38	111.00
1	A	192	GLY	N-CA-C	-5.40	99.61	113.10
1	C	193	THR	N-CA-C	-5.38	96.47	111.00
2	E	391	LEU	CA-C-N	5.37	126.95	116.20
2	F	54	GLY	N-CA-C	-5.36	99.70	113.10
2	E	304	ILE	N-CA-C	-5.35	96.55	111.00
1	A	360	GLY	N-CA-C	-5.35	99.73	113.10
1	B	504	PHE	C-N-CA	5.34	135.06	121.70
2	E	211	ALA	C-N-CA	5.34	135.05	121.70
2	F	274	ARG	N-CA-C	-5.33	96.62	111.00
2	D	394	ASP	C-N-CA	5.32	134.99	121.70
3	G	271	ALA	N-CA-C	-5.31	96.66	111.00
2	F	59	ARG	N-CA-C	-5.31	96.66	111.00
1	A	83	LYS	N-CA-C	-5.30	96.69	111.00
2	D	213	SER	N-CA-C	-5.30	96.70	111.00
2	E	353	SER	N-CA-C	-5.29	96.71	111.00
5	I	43	LYS	CA-C-N	-5.29	105.57	117.20
1	B	34	ILE	N-CA-C	-5.28	96.75	111.00
2	E	83	ARG	N-CA-C	-5.25	96.82	111.00
1	B	173	THR	N-CA-C	-5.25	96.83	111.00
1	B	30	ARG	N-CA-C	-5.23	96.88	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	LEU	N-CA-C	-5.22	96.91	111.00
1	C	290	GLY	N-CA-C	-5.21	100.08	113.10
2	E	151	LYS	N-CA-C	-5.19	96.98	111.00
7	S	119	THR	N-CA-C	-5.19	96.99	111.00
1	A	510	ALA	N-CA-C	-5.19	97.00	111.00
1	C	237	SER	N-CA-C	-5.19	97.00	111.00
7	S	47	LYS	N-CA-C	5.18	124.99	111.00
2	D	210	ASP	N-CA-C	-5.18	97.02	111.00
1	A	8	VAL	O-C-N	5.18	130.98	122.70
1	C	327	ILE	N-CA-C	-5.17	97.03	111.00
2	D	118	ALA	N-CA-C	-5.17	97.04	111.00
4	H	72	THR	N-CA-C	-5.17	97.05	111.00
2	D	25	PHE	CA-C-N	-5.17	105.83	117.20
1	C	88	VAL	N-CA-C	-5.16	97.07	111.00
1	C	454	ASP	C-N-CA	5.16	134.59	121.70
4	H	41	GLN	N-CA-C	-5.13	97.14	111.00
2	D	156	GLY	N-CA-C	-5.13	100.28	113.10
1	C	313	ASN	C-N-CA	5.13	134.51	121.70
1	B	58	GLY	C-N-CA	5.11	134.48	121.70
2	E	66	THR	C-N-CA	5.10	134.45	121.70
2	F	365	SER	CA-C-N	5.10	128.41	117.20
1	C	104	LEU	N-CA-C	-5.09	97.24	111.00
1	A	403	PHE	N-CA-C	-5.08	97.27	111.00
1	A	40	ARG	N-CA-C	-5.08	97.28	111.00
1	C	77	GLY	N-CA-C	-5.08	100.41	113.10
8	T	170	LEU	CA-C-N	5.08	128.37	117.20
1	B	321	LEU	N-CA-C	-5.07	97.32	111.00
1	B	372	SER	N-CA-C	-5.07	97.32	111.00
3	G	92	GLU	C-N-CA	5.05	134.34	121.70
1	A	41	VAL	N-CA-C	-5.04	97.39	111.00
2	E	94	ILE	N-CA-C	-5.03	97.43	111.00
2	E	398	GLU	N-CA-C	5.03	124.58	111.00
1	C	407	GLY	C-N-CA	5.02	134.24	121.70
1	A	322	THR	N-CA-C	-5.01	97.48	111.00
4	H	20	PHE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	THR	Peptide
1	A	336	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	35	GLY	Peptide
1	A	400	VAL	Mainchain
1	A	404	ALA	Mainchain
1	A	406	PHE	Mainchain
1	B	379	GLN	Peptide
1	B	505	LEU	Mainchain
1	C	169	GLY	Mainchain
2	D	160	VAL	Mainchain
2	D	205	VAL	Peptide
2	D	25	PHE	Mainchain
2	D	384	LEU	Mainchain
2	D	397	SER	Mainchain
2	D	72	GLY	Mainchain
2	E	249	GLN	Mainchain
2	E	25	PHE	Mainchain
2	E	397	SER	Mainchain
2	F	130	GLN	Mainchain
2	F	249	GLN	Peptide
3	G	92	GLU	Mainchain,Peptide
7	S	107	THR	Peptide
7	S	118	CYS	Mainchain
7	S	122	THR	Peptide
7	S	150	LEU	Mainchain,Peptide
7	S	151	GLU	Peptide
7	S	152	VAL	Peptide
7	S	156	PRO	Mainchain,Peptide
7	S	161	GLY	Mainchain
7	S	167	GLY	Mainchain
8	T	113	ARG	Mainchain
8	T	121	ARG	Mainchain
8	T	140	MET	Mainchain
8	T	144	VAL	Mainchain
8	T	149	VAL	Peptide
8	T	154	ALA	Peptide
8	T	155	GLN	Mainchain
8	T	158	LYS	Mainchain
8	T	166	ALA	Mainchain
8	T	168	LEU	Peptide
8	T	172	SER	Peptide
8	T	18	TYR	Mainchain
8	T	51	LYS	Mainchain
8	T	84	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	T	86	GLN	Mainchain
8	T	87	LYS	Mainchain
8	T	89	HIS	Mainchain
8	T	98	ASN	Mainchain
9	U	121	ASN	Mainchain
9	U	18	PRO	Mainchain
10	V	12	PHE	Mainchain
10	V	14	ASP	Mainchain
10	V	18	GLU	Mainchain
10	V	19	TYR	Mainchain
10	V	20	ARG	Mainchain
10	V	27	GLY	Peptide
10	V	29	PRO	Mainchain
10	V	32	ALA	Mainchain
10	V	33	GLY	Mainchain
10	V	35	GLU	Mainchain
10	V	49	GLN	Mainchain
10	V	50	MET	Peptide
10	V	54	ALA	Mainchain
10	V	56	MET	Mainchain
10	V	6	ASP	Mainchain,Peptide
10	V	63	THR	Mainchain
10	V	7	PRO	Mainchain,Peptide
10	V	70	GLU	Mainchain
11	W	176	GLY	Mainchain
11	W	35	ASN	Peptide
11	W	48	TRP	Mainchain
11	W	87	LEU	Mainchain
11	W	91	SER	Mainchain

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	2035	0	589	6	0
1	B	1918	0	553	11	0
1	C	1947	0	563	2	0
2	D	1867	0	533	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1863	0	532	7	0
2	F	1863	0	532	7	0
3	G	1053	0	283	5	0
4	H	523	0	140	1	0
5	I	187	0	53	0	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	5	0
8	T	697	0	182	1	0
9	U	485	0	121	0	0
10	V	265	0	68	0	0
11	W	869	0	226	0	0
All	All	18545	0	5289	49	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.

All (49) 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)
3:G:267:SER:H	3:G:271:ALA:H	1.25	0.82
1:B:49:ALA:H	2:F:69:LEU:H	1.33	0.74
1:A:149:GLY:HA3	1:A:436:MET:H	1.54	0.72
1:B:149:GLY:HA3	1:B:436:MET:H	1.56	0.71
7:S:106:SER:O	7:S:108:MET:N	2.28	0.66
1:B:173:THR:N	1:B:175:LYS:H	1.96	0.63
3:G:267:SER:H	3:G:271:ALA:N	1.93	0.63
1:B:173:THR:H	1:B:175:LYS:H	1.51	0.59
7:S:30:ASN:C	7:S:32:LEU:H	2.06	0.57
2:D:160:VAL:H	2:D:162:LYS:H	1.52	0.56
3:G:167:SER:C	3:G:169:ILE:H	2.08	0.55
1:A:223:ALA:C	1:A:225:ALA:H	2.10	0.54
2:E:84:ILE:H	2:E:114:ALA:H	1.55	0.54
2:E:450:ASP:H	2:E:452:LEU:H	1.57	0.53
1:A:149:GLY:CA	1:A:436:MET:H	2.21	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:473:LEU:C	2:D:475:GLU:H	2.15	0.50
2:D:160:VAL:N	2:D:162:LYS:H	2.10	0.49
2:F:127:SER:C	2:F:129:GLU:H	2.15	0.49
7:S:28:LYS:C	7:S:30:ASN:H	2.15	0.49
2:E:210:ASP:C	2:E:212:THR:H	2.16	0.48
1:C:223:ALA:C	1:C:225:ALA:H	2.18	0.47
7:S:115:GLU:N	7:S:127:ASP:H	2.13	0.45
1:B:149:GLY:CA	1:B:436:MET:H	2.25	0.45
2:F:84:ILE:H	2:F:114:ALA:H	1.64	0.44
2:F:382:LYS:C	2:F:385:GLN:H	2.21	0.44
2:D:84:ILE:H	2:D:114:ALA:H	1.65	0.44
3:G:204:TYR:O	3:G:208:SER:N	2.50	0.44
7:S:93:GLY:C	7:S:95:LEU:H	2.21	0.43
1:A:49:ALA:H	2:E:69:LEU:N	2.16	0.43
2:F:448:GLU:C	2:F:450:ASP:H	2.21	0.43
1:A:9:SER:O	1:A:11:ILE:N	2.51	0.43
1:B:258:ARG:O	1:B:319:GLY:HA3	2.18	0.43
1:B:351:PHE:H	1:B:370:SER:CA	2.32	0.43
1:B:353:GLU:H	1:B:365:ILE:CA	2.32	0.43
1:C:258:ARG:O	1:C:319:GLY:HA3	2.19	0.42
2:E:208:LEU:C	2:E:210:ASP:H	2.22	0.42
2:E:247:GLU:C	2:E:249:GLN:H	2.22	0.42
2:E:450:ASP:H	2:E:452:LEU:N	2.17	0.42
8:T:166:ALA:O	8:T:170:LEU:N	2.51	0.42
1:A:9:SER:C	1:A:13:GLU:H	2.22	0.42
3:G:112:ILE:C	3:G:114:SER:H	2.22	0.42
2:F:368:TYR:O	2:F:372:ARG:N	2.51	0.41
1:B:260:ASN:C	1:B:262:LYS:H	2.23	0.41
1:B:102:GLU:C	1:B:104:LEU:H	2.23	0.41
4:H:107:ALA:O	4:H:111:ASN:N	2.53	0.41
2:D:350:PRO:C	2:D:352:ASP:H	2.24	0.41
2:D:155:PHE:N	2:D:333:THR:O	2.53	0.40
1:B:171:ARG:O	1:B:173:THR:N	2.54	0.40
2:F:11:GLY:HA2	2:F:24:GLN:O	2.22	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	507/510 (99%)	442 (87%)	41 (8%)	24 (5%)	3	28
1	B	476/510 (93%)	425 (89%)	30 (6%)	21 (4%)	3	29
1	C	485/510 (95%)	434 (90%)	31 (6%)	20 (4%)	3	30
2	D	465/482 (96%)	407 (88%)	38 (8%)	20 (4%)	3	29
2	E	464/482 (96%)	406 (88%)	34 (7%)	24 (5%)	2	26
2	F	464/482 (96%)	416 (90%)	31 (7%)	17 (4%)	4	33
3	G	258/273 (94%)	191 (74%)	33 (13%)	34 (13%)	0	6
4	H	129/146 (88%)	105 (81%)	12 (9%)	12 (9%)	1	14
5	I	45/50 (90%)	32 (71%)	8 (18%)	5 (11%)	0	9
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	5	38
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	13	54
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100	100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	5	38
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100	100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	13	54
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	13	54
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	5	38
7	S	166/190 (87%)	107 (64%)	32 (19%)	27 (16%)	0	4
8	T	172/174 (99%)	152 (88%)	16 (9%)	4 (2%)	7	43
9	U	120/124 (97%)	108 (90%)	10 (8%)	2 (2%)	11	50
10	V	65/77 (84%)	51 (78%)	8 (12%)	6 (9%)	1	14
11	W	215/217 (99%)	193 (90%)	18 (8%)	4 (2%)	9	47
All	All	4591/4803 (96%)	3966 (86%)	396 (9%)	229 (5%)	5	27

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	SER
1	A	13	GLU
1	A	14	GLU
1	A	20	ASP
1	A	45	ARG
1	A	47	VAL
1	A	59	LEU
1	A	78	ASN
1	A	84	GLU
1	A	238	ASP
1	A	361	ILE
1	A	365	ILE
1	A	374	VAL
1	B	45	ARG
1	B	57	SER
1	B	59	LEU
1	B	114	ALA
1	B	144	GLU
1	B	171	ARG
1	B	172	GLN
1	B	238	ASP
1	B	376	SER
1	C	289	PRO
1	C	365	ILE
1	C	374	VAL
1	C	408	SER
1	C	455	LYS
1	C	456	LEU
2	D	214	LYS
2	D	281	TYR
2	D	450	ASP
2	D	451	HIS
2	E	180	TYR
2	E	210	ASP
2	E	274	ARG
2	E	344	ILE
2	E	348	VAL
2	E	358	MET
2	F	67	GLU
2	F	277	SER
2	F	299	THR
2	F	364	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	55	ALA
3	G	60	PRO
3	G	78	CYS
3	G	93	ALA
3	G	115	ILE
3	G	134	ARG
3	G	183	THR
3	G	186	SER
3	G	199	ASP
3	G	250	PHE
4	H	42	THR
4	H	45	PHE
4	H	49	ALA
4	H	50	ALA
4	H	51	HIS
4	H	52	VAL
4	H	68	GLU
4	H	69	ASP
4	H	87	ASP
4	H	95	GLU
4	H	101	ASP
5	I	28	THR
5	I	41	THR
7	S	10	GLN
7	S	11	ILE
7	S	47	LYS
7	S	50	LYS
7	S	75	LYS
7	S	80	PRO
7	S	109	MET
7	S	110	SER
7	S	126	LEU
7	S	136	THR
7	S	153	LYS
9	U	98	CYS
10	V	54	ALA
10	V	67	PRO
10	V	70	GLU
1	A	11	ILE
1	A	23	VAL
1	A	82	ILE
1	A	171	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	46	ASN
1	B	82	ILE
1	B	84	GLU
1	B	115	ILE
1	B	143	ARG
1	B	209	LYS
1	B	224	ASP
1	B	289	PRO
1	B	505	LEU
1	C	26	GLU
1	C	44	LEU
1	C	45	ARG
1	C	115	ILE
1	C	143	ARG
1	C	172	GLN
1	C	209	LYS
2	D	28	GLY
2	D	107	PRO
2	D	179	GLY
2	D	212	THR
2	D	276	PRO
2	D	394	ASP
2	E	28	GLY
2	E	67	GLU
2	E	102	ILE
2	E	450	ASP
2	F	420	VAL
2	F	453	PRO
3	G	9	ARG
3	G	51	LEU
3	G	69	ILE
3	G	87	LYS
3	G	116	LEU
3	G	180	SER
3	G	185	SER
3	G	200	VAL
3	G	257	VAL
3	G	272	LEU
7	S	68	SER
7	S	114	GLY
7	S	158	ILE
8	T	147	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	MET
1	A	289	PRO
1	B	37	GLY
1	B	508	PHE
1	C	68	PRO
1	C	171	ARG
1	C	238	ASP
1	C	430	GLN
2	D	55	GLU
2	D	209	LYS
2	D	462	PRO
2	E	212	THR
2	E	395	GLU
2	F	44	ARG
2	F	118	ALA
2	F	282	GLN
2	F	359	ASP
2	F	427	HIS
3	G	88	GLN
3	G	195	ASP
3	G	197	ASP
3	G	268	GLY
3	G	269	ALA
6	J	45	GLN
7	S	16	GLY
7	S	29	GLN
7	S	79	SER
10	V	55	ASP
11	W	36	ARG
1	A	136	ILE
1	A	209	LYS
1	C	57	SER
2	D	44	ARG
2	D	453	PRO
2	E	277	SER
2	E	447	GLY
2	F	101	PRO
3	G	72	SER
3	G	92	GLU
3	G	188	GLU
5	I	33	ASN
5	I	38	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	P	40	PRO
6	Q	44	GLN
7	S	61	LYS
7	S	77	LYS
8	T	149	VAL
8	T	170	LEU
11	W	40	ASN
1	A	145	PRO
1	C	59	LEU
2	D	33	LEU
2	E	276	PRO
2	E	396	LEU
2	F	33	LEU
2	F	360	PRO
3	G	10	LEU
3	G	133	ARG
3	G	201	LEU
3	G	258	ILE
4	H	39	PRO
6	O	39	ASN
7	S	14	ILE
7	S	92	ASN
7	S	128	GLU
7	S	148	LEU
10	V	31	ASP
11	W	92	PHE
2	D	64	ASP
2	D	213	SER
2	D	223	ASN
2	D	279	VAL
2	E	107	PRO
2	E	131	GLU
2	E	179	GLY
2	E	297	THR
3	G	118	ARG
6	M	40	PRO
9	U	45	LYS
1	A	115	ILE
2	E	161	GLY
2	E	279	VAL
2	F	279	VAL
7	S	116	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	V	6	ASP
1	B	295	PRO
2	E	30	PRO
2	E	121	PRO
7	S	156	PRO
2	F	120	ALA
3	G	168	VAL
7	S	9	VAL
8	T	19	VAL
1	C	47	VAL
2	F	276	PRO
6	J	40	PRO
6	M	71	ILE
11	W	88	LEU
5	I	39	GLY
7	S	60	VAL
6	K	40	PRO
6	Q	40	PRO

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.