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

Dec 13, 2016 – 11:01 AM EST

PDB ID	:	5FIJ
EMDB ID:	:	EMD-3168
Title	:	Bovine mitochondrial ATP synthase state 2c
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	:	7.40 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 (i) symbol.

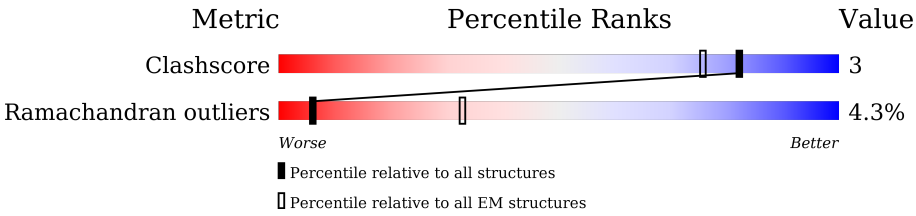
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 7.40 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	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	91% 7% •
1	B	510	85% 9% 6%
1	C	510	87% 7% • 5%
2	D	482	86% 10% •
2	E	482	88% 9% •
2	F	482	86% 10% • •
3	G	273	80% 14% • •
4	H	146	77% 13% 10%
5	I	50	72% 20% • 6%
6	J	72	97% •
6	K	72	99% •

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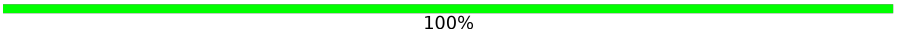
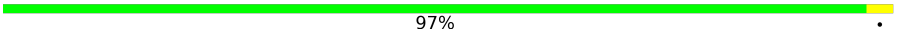
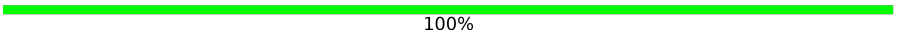
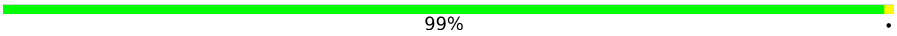
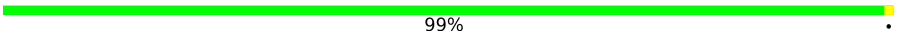
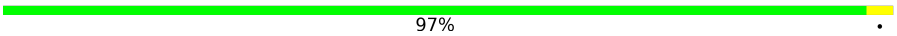
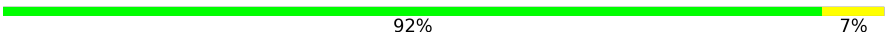
Mol	Chain	Length	Quality of chain
6	L	72	
6	M	72	
6	N	72	
6	O	72	
6	P	72	
6	Q	72	
7	S	190	
8	T	174	
9	U	124	
10	V	77	
11	W	217	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18543 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	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	121	Total 484	C 242	N 121	O 121	0	0

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

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

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

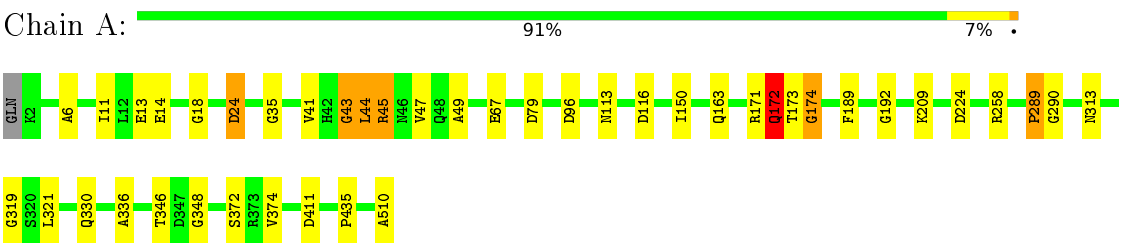
Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	217	Total 869	C 434	N 217	O 218	0	0

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.

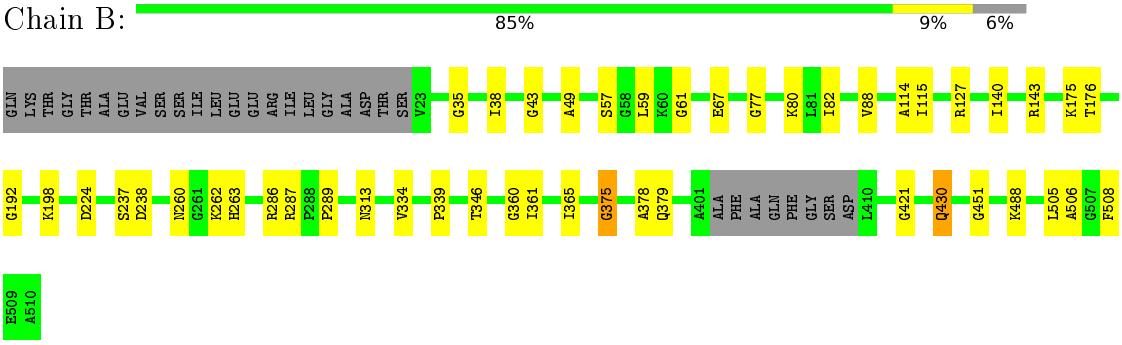
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



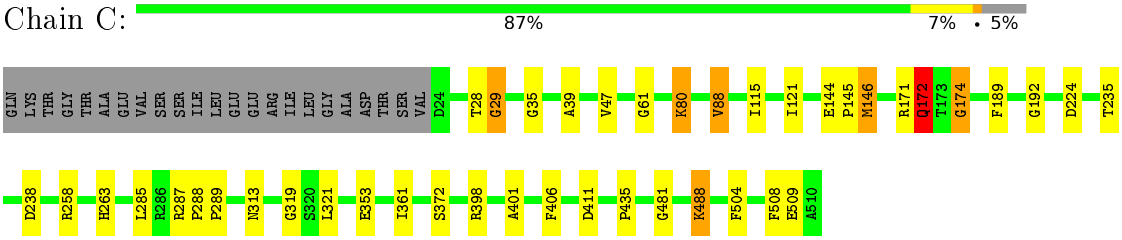
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:



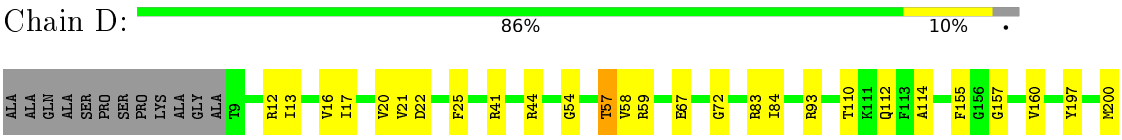
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

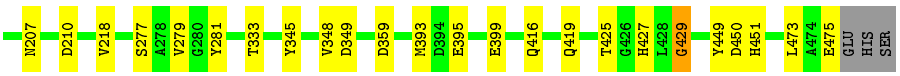
Chain C:



- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:



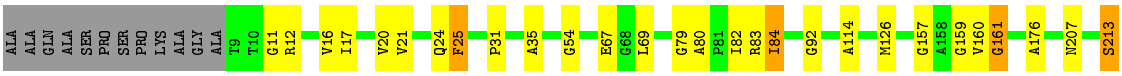


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:

• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:

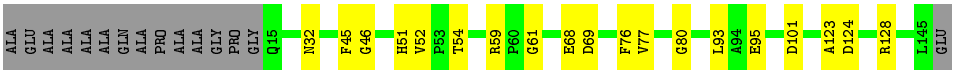


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:

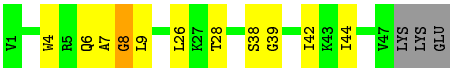
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H:



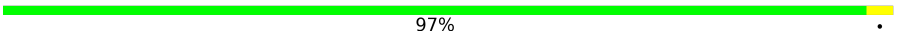
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

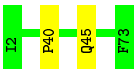
Chain I:



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

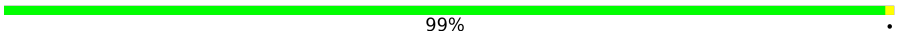
Chain J:





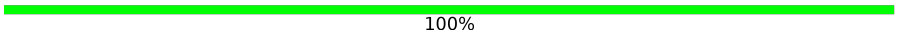
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K:



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

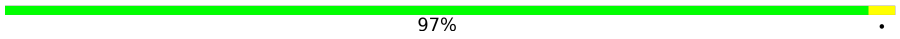
Chain L:

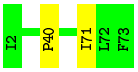


There are no outlier residues recorded for this chain.

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

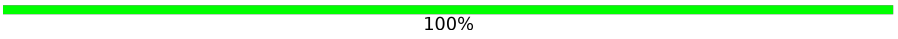
Chain M:





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

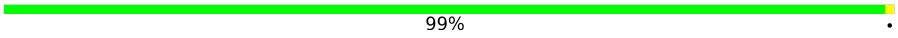
Chain N:



There are no outlier residues recorded for this chain.

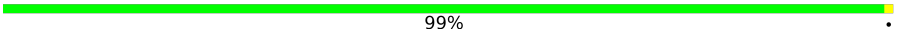
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O:



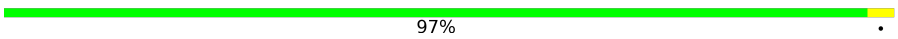
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain P:



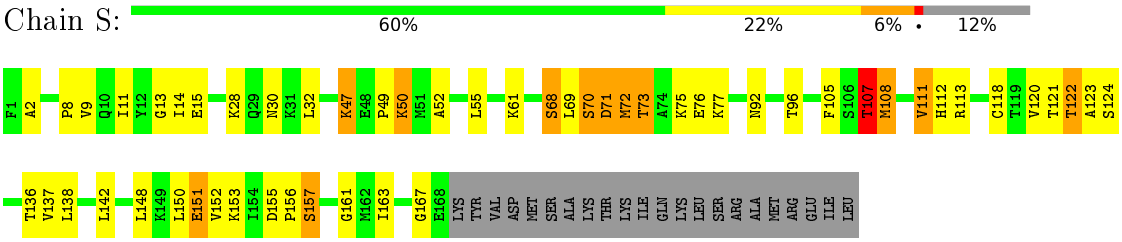
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q:



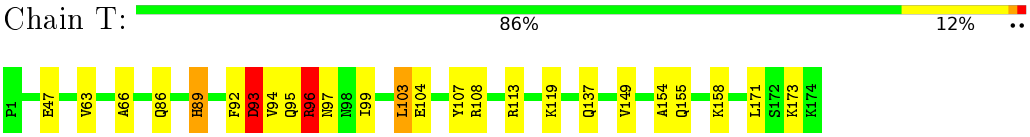
• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:



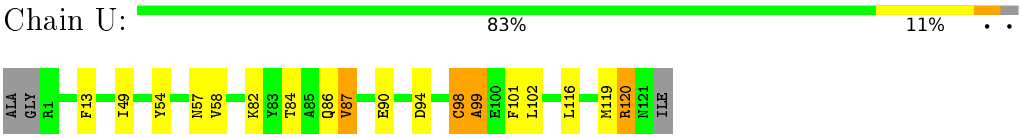
• Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:



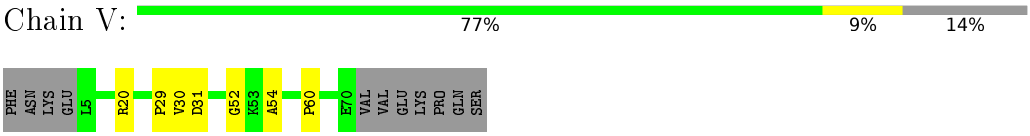
• Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:



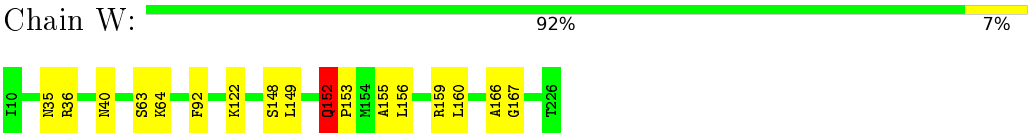
• Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

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	18899	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	1.76	4/2034 (0.2%)	1.43	17/2541 (0.7%)
1	B	1.83	6/1916 (0.3%)	1.48	18/2392 (0.8%)
1	C	1.77	1/1946 (0.1%)	1.44	19/2431 (0.8%)
10	V	0.63	0/263	0.93	0/327
11	W	0.79	1/868 (0.1%)	0.91	1/1082 (0.1%)
2	D	1.80	4/1866 (0.2%)	1.50	22/2331 (0.9%)
2	E	1.67	2/1862 (0.1%)	1.47	16/2326 (0.7%)
2	F	1.82	9/1862 (0.5%)	1.46	16/2326 (0.7%)
3	G	1.93	6/1050 (0.6%)	1.57	14/1308 (1.1%)
4	H	2.05	2/522 (0.4%)	1.76	6/651 (0.9%)
5	I	1.86	0/186	1.50	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	0.31	0/287	0.41	0/357
6	P	0.29	0/287	0.43	0/357
6	Q	0.29	0/287	0.44	0/357
7	S	1.70	3/668 (0.4%)	1.74	13/834 (1.6%)
8	T	1.14	2/696 (0.3%)	1.33	10/867 (1.2%)
9	U	0.33	0/483	0.47	0/602
All	All	1.59	40/18518 (0.2%)	1.35	154/23105 (0.7%)

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	1
1	B	0	2
10	V	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	W	0	9
2	D	0	2
2	E	0	3
2	F	0	5
3	G	0	3
4	H	0	1
5	I	0	1
7	S	0	9
8	T	0	17
9	U	0	2
All	All	0	58

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	93	ASP	N-CA	15.12	1.76	1.46
8	T	96	ARG	CA-C	13.65	1.88	1.52
3	G	109	GLY	CA-C	-7.87	1.39	1.51
7	S	72	MET	N-CA	7.27	1.60	1.46
3	G	261	GLU	CA-C	-6.83	1.35	1.52
2	F	11	GLY	CA-C	-6.11	1.42	1.51
2	F	364	GLY	CA-C	-6.00	1.42	1.51
3	G	252	ARG	CA-C	-5.99	1.37	1.52
1	B	339	PRO	CA-C	-5.98	1.40	1.52
4	H	46	GLY	CA-C	-5.89	1.42	1.51
2	F	12	ARG	N-CA	-5.82	1.34	1.46
2	F	246	GLN	CA-C	-5.67	1.38	1.52
2	F	366	GLU	CA-C	-5.63	1.38	1.52
1	B	176	THR	N-CA	-5.59	1.35	1.46
1	B	451	GLY	CA-C	-5.54	1.43	1.51
1	A	174	GLY	N-CA	-5.53	1.37	1.46
2	D	429	GLY	CA-C	-5.49	1.43	1.51
2	F	364	GLY	N-CA	-5.49	1.37	1.46
2	E	12	ARG	CA-C	-5.48	1.38	1.52
2	D	54	GLY	CA-C	-5.44	1.43	1.51
7	S	71	ASP	C-N	5.42	1.46	1.34
3	G	158	GLY	CA-C	-5.41	1.43	1.51
1	B	43	GLY	CA-C	-5.35	1.43	1.51
1	C	481	GLY	CA-C	-5.25	1.43	1.51
11	W	152	GLN	N-CA	-5.22	1.35	1.46
2	D	58	VAL	N-CA	-5.20	1.35	1.46
7	S	72	MET	CA-C	5.20	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLY	N-CA	-5.11	1.38	1.46
3	G	172	LYS	N-CA	-5.10	1.36	1.46
3	G	266	ILE	CA-C	-5.10	1.39	1.52
1	A	290	GLY	CA-C	-5.10	1.43	1.51
1	B	175	LYS	CA-C	-5.08	1.39	1.52
2	F	429	GLY	CA-C	-5.08	1.43	1.51
1	A	43	GLY	N-CA	-5.05	1.38	1.46
2	E	290	GLY	CA-C	-5.05	1.43	1.51
2	F	79	GLY	CA-C	-5.04	1.43	1.51
2	F	12	ARG	CA-C	-5.04	1.39	1.52
2	D	12	ARG	CA-C	-5.03	1.39	1.52
1	B	421	GLY	CA-C	-5.02	1.43	1.51
4	H	128	ARG	CA-C	-5.01	1.40	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	96	ARG	O-C-N	-14.33	99.77	122.70
8	T	92	PHE	C-N-CA	10.34	147.54	121.70
8	T	96	ARG	CA-C-N	10.23	139.70	117.20
7	S	71	ASP	C-N-CA	9.34	145.06	121.70
8	T	103	LEU	CA-C-O	-9.06	101.07	120.10
1	A	35	GLY	N-CA-C	-8.49	91.87	113.10
2	F	256	ASP	N-CA-C	-7.86	89.79	111.00
7	S	72	MET	C-N-CA	7.73	141.03	121.70
2	D	16	VAL	N-CA-C	-7.71	90.17	111.00
3	G	268	GLY	N-CA-C	-7.69	93.88	113.10
1	C	35	GLY	N-CA-C	-7.62	94.06	113.10
7	S	157	SER	N-CA-C	-7.61	90.45	111.00
2	F	345	TYR	N-CA-C	-7.47	90.83	111.00
2	F	83	ARG	N-CA-C	-7.29	91.32	111.00
2	E	54	GLY	N-CA-C	-7.20	95.09	113.10
7	S	107	THR	CA-C-N	7.20	133.05	117.20
2	E	355	SER	N-CA-C	-7.17	91.64	111.00
8	T	96	ARG	N-CA-C	-7.13	91.74	111.00
2	D	349	ASP	N-CA-C	-6.98	92.16	111.00
2	D	17	ILE	N-CA-C	-6.79	92.68	111.00
2	E	461	GLY	N-CA-C	-6.79	96.13	113.10
2	D	207	ASN	N-CA-C	-6.73	92.83	111.00
2	F	17	ILE	N-CA-C	-6.71	92.87	111.00
1	B	430	GLN	N-CA-C	-6.67	92.99	111.00
2	D	449	TYR	N-CA-C	-6.65	93.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	93	LEU	N-CA-C	-6.60	93.17	111.00
8	T	104	GLU	N-CA-C	6.58	128.76	111.00
3	G	171	TYR	N-CA-C	-6.56	93.30	111.00
1	B	38	ILE	N-CA-C	-6.52	93.39	111.00
1	A	330	GLN	N-CA-C	-6.50	93.46	111.00
1	A	41	VAL	N-CA-C	-6.49	93.49	111.00
2	D	57	THR	CA-C-N	-6.44	103.03	117.20
1	A	24	ASP	N-CA-C	-6.36	93.82	111.00
5	I	39	GLY	N-CA-C	-6.35	97.22	113.10
1	B	35	GLY	N-CA-C	-6.33	97.28	113.10
2	D	112	GLN	N-CA-C	-6.32	93.93	111.00
2	F	304	ILE	N-CA-C	-6.31	93.97	111.00
1	B	360	GLY	N-CA-C	-6.24	97.50	113.10
3	G	105	ILE	N-CA-C	-6.23	94.19	111.00
2	D	57	THR	N-CA-C	-6.19	94.28	111.00
1	A	174	GLY	N-CA-C	-6.18	97.64	113.10
2	D	20	VAL	N-CA-C	-6.17	94.35	111.00
3	G	197	ASP	N-CA-C	6.15	127.60	111.00
2	F	84	ILE	N-CA-C	-6.14	94.42	111.00
7	S	70	SER	C-N-CA	6.14	137.05	121.70
2	F	450	ASP	N-CA-C	-6.12	94.48	111.00
4	H	54	THR	N-CA-C	-6.09	94.55	111.00
8	T	93	ASP	O-C-N	-6.02	113.06	122.70
2	E	52	HIS	N-CA-C	-6.00	94.81	111.00
1	C	353	GLU	C-N-CA	5.99	136.67	121.70
2	D	22	ASP	N-CA-C	-5.94	94.95	111.00
2	E	57	THR	N-CA-C	-5.92	95.02	111.00
3	G	51	LEU	N-CA-C	-5.90	95.06	111.00
2	D	41	ARG	C-N-CA	5.89	136.43	121.70
5	I	8	GLY	N-CA-C	-5.89	98.39	113.10
7	S	122	THR	N-CA-C	5.87	126.85	111.00
3	G	93	ALA	N-CA-C	5.85	126.81	111.00
2	E	145	PRO	N-CA-C	-5.85	96.90	112.10
2	E	118	ALA	N-CA-C	-5.82	95.28	111.00
1	B	88	VAL	N-CA-C	-5.82	95.29	111.00
2	F	257	ASN	N-CA-C	-5.81	95.30	111.00
1	A	289	PRO	N-CA-C	-5.79	97.05	112.10
2	D	218	VAL	N-CA-C	-5.79	95.37	111.00
7	S	121	THR	C-N-CA	5.77	136.12	121.70
2	D	345	TYR	N-CA-C	-5.74	95.50	111.00
2	D	157	GLY	C-N-CA	5.72	135.99	121.70
4	H	76	PHE	N-CA-C	-5.71	95.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	506	ALA	C-N-CA	5.70	134.26	122.30
2	F	24	GLN	N-CA-C	-5.69	95.64	111.00
2	D	83	ARG	N-CA-C	-5.69	95.65	111.00
1	C	321	LEU	N-CA-C	-5.67	95.68	111.00
8	T	96	ARG	C-N-CA	5.65	135.82	121.70
7	S	76	GLU	C-N-CA	5.64	135.81	121.70
1	A	44	LEU	C-N-CA	5.63	135.78	121.70
2	E	218	VAL	N-CA-C	-5.63	95.80	111.00
1	A	290	GLY	N-CA-C	-5.62	99.04	113.10
1	B	140	ILE	N-CA-C	-5.62	95.83	111.00
1	C	488	LYS	N-CA-C	-5.61	95.84	111.00
1	A	172	GLN	CA-C-N	-5.59	104.90	117.20
1	B	237	SER	C-N-CA	5.58	135.66	121.70
4	H	61	GLY	N-CA-C	-5.56	99.21	113.10
2	D	54	GLY	N-CA-C	-5.55	99.21	113.10
2	E	47	LEU	N-CA-C	-5.55	96.01	111.00
2	F	20	VAL	N-CA-C	-5.55	96.01	111.00
1	A	313	ASN	C-N-CA	5.54	135.55	121.70
2	F	16	VAL	N-CA-C	-5.53	96.07	111.00
2	D	25	PHE	N-CA-C	-5.52	96.10	111.00
2	E	446	ALA	C-N-CA	5.52	133.89	122.30
3	G	154	GLU	CA-C-N	-5.52	105.06	117.20
1	C	88	VAL	N-CA-C	-5.50	96.14	111.00
1	B	77	GLY	N-CA-C	-5.50	99.35	113.10
3	G	70	GLY	N-CA-C	-5.50	99.35	113.10
1	C	29	GLY	N-CA-C	-5.49	99.37	113.10
1	C	372	SER	N-CA-C	-5.48	96.21	111.00
1	C	61	GLY	N-CA-C	-5.47	99.42	113.10
1	A	372	SER	N-CA-C	-5.47	96.23	111.00
1	C	39	ALA	N-CA-C	-5.47	96.24	111.00
2	D	59	ARG	N-CA-C	-5.46	96.25	111.00
4	H	32	ASN	C-N-CA	5.45	135.31	121.70
2	E	345	TYR	N-CA-C	-5.44	96.32	111.00
1	C	172	GLN	CA-C-N	-5.43	105.24	117.20
1	C	263	HIS	N-CA-C	-5.43	96.33	111.00
1	C	146	MET	N-CA-C	-5.42	96.37	111.00
1	B	175	LYS	CA-C-N	-5.42	105.28	117.20
4	H	77	VAL	N-CA-C	-5.41	96.40	111.00
1	B	488	LYS	N-CA-C	-5.39	96.44	111.00
3	G	167	SER	N-CA-C	-5.38	96.48	111.00
7	S	111	VAL	N-CA-C	-5.38	96.48	111.00
2	D	21	VAL	N-CA-C	-5.34	96.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	313	ASN	C-N-CA	5.34	135.05	121.70
1	A	321	LEU	N-CA-C	-5.34	96.58	111.00
7	S	150	LEU	C-N-CA	5.33	135.03	121.70
8	T	93	ASP	N-CA-C	-5.32	96.64	111.00
2	D	416	GLN	N-CA-C	-5.32	96.64	111.00
1	A	150	ILE	N-CA-C	-5.30	96.70	111.00
1	A	510	ALA	N-CA-C	-5.30	96.70	111.00
3	G	270	ALA	N-CA-C	-5.29	96.70	111.00
2	E	418	PHE	C-N-CA	5.29	134.93	121.70
3	G	267	SER	CA-C-N	-5.26	105.68	116.20
2	D	399	GLU	N-CA-C	-5.25	96.82	111.00
2	F	21	VAL	N-CA-C	-5.25	96.83	111.00
1	C	411	ASP	N-CA-C	-5.25	96.84	111.00
1	C	509	GLU	N-CA-C	-5.25	96.84	111.00
2	D	110	THR	C-N-CA	5.23	134.79	121.70
1	A	67	GLU	N-CA-C	-5.21	96.93	111.00
1	A	113	ASN	N-CA-C	-5.21	96.94	111.00
3	G	129	LYS	N-CA-C	-5.20	96.96	111.00
3	G	134	ARG	N-CA-C	-5.20	96.97	111.00
1	B	198	LYS	N-CA-C	-5.19	96.99	111.00
2	F	207	ASN	N-CA-C	-5.18	97.00	111.00
7	S	47	LYS	N-CA-C	5.18	124.99	111.00
11	W	148	SER	CA-C-O	-5.17	109.23	120.10
2	F	25	PHE	CA-C-N	-5.16	105.84	117.20
1	C	28	THR	N-CA-C	-5.14	97.12	111.00
2	E	182	VAL	N-CA-C	-5.13	97.15	111.00
1	A	96	ASP	N-CA-C	-5.12	97.16	111.00
2	E	331	ALA	N-CA-C	-5.12	97.19	111.00
1	B	313	ASN	C-N-CA	5.11	134.49	121.70
1	B	127	ARG	N-CA-C	-5.08	97.28	111.00
1	C	80	LYS	C-N-CA	5.08	134.40	121.70
2	F	54	GLY	N-CA-C	-5.08	100.41	113.10
1	B	263	HIS	N-CA-C	-5.06	97.33	111.00
8	T	89	HIS	O-C-N	-5.06	114.60	122.70
1	C	406	PHE	N-CA-C	-5.06	97.34	111.00
1	B	61	GLY	N-CA-C	-5.05	100.48	113.10
2	E	59	ARG	N-CA-C	-5.04	97.38	111.00
3	G	204	TYR	N-CA-C	-5.04	97.38	111.00
7	S	50	LYS	C-N-CA	5.04	134.31	121.70
1	B	67	GLU	N-CA-C	-5.04	97.40	111.00
1	C	174	GLY	N-CA-C	-5.02	100.55	113.10
2	E	183	PHE	N-CA-C	-5.02	97.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	72	MET	N-CA-C	5.01	124.54	111.00
1	B	192	GLY	N-CA-C	-5.01	100.58	113.10
2	F	161	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	THR	Mainchain
1	B	375	GLY	Peptide
1	B	379	GLN	Peptide
2	D	160	VAL	Mainchain
2	D	57	THR	Mainchain
2	E	180	TYR	Mainchain
2	E	397	SER	Mainchain
2	E	433	PRO	Peptide
2	F	126	MET	Peptide
2	F	25	PHE	Mainchain
2	F	319	ASP	Mainchain,Peptide
2	F	329	LEU	Mainchain
3	G	112	ILE	Mainchain
3	G	154	GLU	Mainchain
3	G	53	GLU	Mainchain
4	H	59	ARG	Mainchain
5	I	38	SER	Peptide
7	S	148	LEU	Peptide
7	S	151	GLU	Peptide
7	S	152	VAL	Peptide
7	S	156	PRO	Peptide
7	S	157	SER	Mainchain
7	S	161	GLY	Mainchain
7	S	70	SER	Mainchain
7	S	73	THR	Peptide
7	S	96	THR	Mainchain
8	T	103	LEU	Mainchain
8	T	107	TYR	Mainchain
8	T	108	ARG	Mainchain
8	T	113	ARG	Mainchain
8	T	119	LYS	Mainchain
8	T	137	GLN	Mainchain
8	T	154	ALA	Peptide
8	T	155	GLN	Mainchain

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Mol	Chain	Res	Type	Group
8	T	158	LYS	Mainchain
8	T	173	LYS	Peptide
8	T	47	GLU	Peptide
8	T	63	VAL	Mainchain
8	T	86	GLN	Mainchain
8	T	89	HIS	Mainchain
8	T	93	ASP	Mainchain
8	T	96	ARG	Mainchain
8	T	97	ASN	Mainchain
9	U	120	ARG	Peptide
9	U	57	ASN	Peptide
10	V	20	ARG	Mainchain
10	V	29	PRO	Peptide
10	V	52	GLY	Mainchain
11	W	122	LYS	Mainchain
11	W	149	LEU	Mainchain
11	W	152	GLN	Mainchain
11	W	159	ARG	Mainchain
11	W	166	ALA	Mainchain
11	W	167	GLY	Mainchain
11	W	35	ASN	Peptide
11	W	63	SER	Mainchain
11	W	64	LYS	Mainchain

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	2	0
1	C	1947	0	563	7	0
2	D	1867	0	533	8	0
2	E	1863	0	532	5	0
2	F	1863	0	532	7	0
3	G	1053	0	283	3	0
4	H	523	0	140	1	0
5	I	187	0	53	2	0
6	J	288	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17	0
8	T	697	0	182	9	0
9	U	484	0	121	9	0
10	V	264	0	68	0	0
11	W	869	0	226	2	0
All	All	18543	0	5290	74	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 3.

All (74) 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)
8:T:93:ASP:N	8:T:93:ASP:CA	1.76	1.46
8:T:96:ARG:C	8:T:96:ARG:CA	1.88	1.40
7:S:163:ILE:O	7:S:167:GLY:O	1.76	1.03
3:G:267:SER:H	3:G:270:ALA:H	1.22	0.82
9:U:116:LEU:O	9:U:120:ARG:N	2.16	0.78
9:U:98:CYS:O	9:U:102:LEU:N	2.15	0.78
8:T:93:ASP:C	8:T:93:ASP:N	2.38	0.77
8:T:96:ARG:C	8:T:96:ARG:N	2.39	0.76
2:F:84:ILE:H	2:F:114:ALA:H	1.34	0.72
9:U:98:CYS:O	9:U:101:PHE:N	2.26	0.68
8:T:93:ASP:N	8:T:94:VAL:N	2.42	0.67
7:S:69:LEU:CA	7:S:72:MET:H	2.09	0.64
7:S:69:LEU:O	7:S:72:MET:N	2.31	0.62
7:S:107:THR:O	7:S:111:VAL:N	2.33	0.61
3:G:267:SER:H	3:G:270:ALA:N	1.97	0.61
2:D:84:ILE:H	2:D:114:ALA:H	1.47	0.61
7:S:68:SER:C	7:S:72:MET:H	2.06	0.58
9:U:98:CYS:O	9:U:99:ALA:C	2.43	0.56
7:S:69:LEU:O	7:S:73:THR:N	2.39	0.55
2:F:92:GLY:HA3	2:F:213:SER:H	1.71	0.55
8:T:66:ALA:O	9:U:119:MET:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:419:GLN:H	2:E:429:GLY:H	1.56	0.53
2:D:473:LEU:C	2:D:475:GLU:H	2.13	0.51
1:C:285:LEU:C	1:C:287:ARG:H	2.13	0.51
8:T:95:GLN:C	8:T:96:ARG:C	2.69	0.50
1:A:49:ALA:H	2:E:69:LEU:N	2.08	0.50
1:A:43:GLY:C	1:A:45:ARG:H	2.15	0.50
7:S:136:THR:C	7:S:138:LEU:H	2.15	0.50
1:C:172:GLN:C	1:C:174:GLY:H	2.16	0.49
1:C:258:ARG:O	1:C:319:GLY:HA3	2.14	0.48
2:E:419:GLN:N	2:E:429:GLY:H	2.11	0.48
1:C:398:ARG:C	1:C:401:ALA:H	2.17	0.48
7:S:108:MET:CA	7:S:111:VAL:O	2.62	0.48
2:E:417:PRO:O	2:E:429:GLY:HA2	2.14	0.47
1:B:260:ASN:C	1:B:262:LYS:H	2.17	0.47
4:H:80:GLY:HA3	4:H:95:GLU:H	1.79	0.47
7:S:69:LEU:C	7:S:71:ASP:N	2.67	0.47
2:D:419:GLN:CA	2:D:429:GLY:H	2.27	0.47
7:S:73:THR:C	7:S:75:LYS:H	2.17	0.47
1:B:49:ALA:H	2:F:69:LEU:N	2.13	0.47
1:A:258:ARG:O	1:A:319:GLY:HA3	2.15	0.46
7:S:105:PHE:O	7:S:108:MET:N	2.48	0.46
1:A:189:PHE:C	1:A:192:GLY:H	2.20	0.46
8:T:96:ARG:O	8:T:99:ILE:N	2.49	0.46
9:U:54:TYR:O	9:U:58:VAL:N	2.29	0.45
1:A:172:GLN:C	1:A:174:GLY:H	2.20	0.45
11:W:152:GLN:O	11:W:155:ALA:N	2.50	0.44
7:S:69:LEU:N	7:S:72:MET:H	2.16	0.44
7:S:28:LYS:C	7:S:30:ASN:H	2.21	0.43
7:S:13:GLY:C	7:S:15:GLU:H	2.21	0.43
1:C:189:PHE:C	1:C:192:GLY:H	2.22	0.43
11:W:156:LEU:O	11:W:160:LEU:N	2.51	0.43
9:U:90:GLU:O	9:U:94:ASP:N	2.49	0.43
5:I:4:TRP:C	5:I:7:ALA:H	2.22	0.43
5:I:6:GLN:C	5:I:8:GLY:H	2.21	0.42
7:S:69:LEU:CA	7:S:72:MET:N	2.80	0.42
3:G:51:LEU:C	3:G:54:LYS:H	2.23	0.42
7:S:105:PHE:O	7:S:108:MET:CA	2.68	0.42
8:T:66:ALA:C	9:U:119:MET:O	2.59	0.41
2:F:159:GLY:C	2:F:161:GLY:H	2.23	0.41
1:C:29:GLY:N	1:C:88:VAL:O	2.54	0.41
2:D:155:PHE:N	2:D:333:THR:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ALA:H	2:F:80:ALA:C	2.23	0.41
2:D:13:ILE:O	2:D:72:GLY:N	2.50	0.41
1:C:504:PHE:O	1:C:508:PHE:N	2.53	0.41
2:D:425:THR:C	2:D:427:HIS:H	2.24	0.41
7:S:30:ASN:C	7:S:32:LEU:H	2.22	0.41
9:U:86:GLN:O	9:U:87:VAL:C	2.59	0.41
2:F:92:GLY:H	2:F:215:VAL:H	1.68	0.41
2:E:277:SER:H	2:E:283:PRO:N	2.19	0.40
2:D:197:TYR:C	2:D:200:MET:H	2.25	0.40
2:D:393:MET:C	2:D:395:GLU:H	2.23	0.40
1:A:346:THR:C	1:A:348:GLY:H	2.24	0.40
2:F:362:ILE:C	2:F:364:GLY:H	2.25	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	507/510 (99%)	451 (89%)	35 (7%)	21 (4%)	3 35
1	B	476/510 (93%)	424 (89%)	31 (6%)	21 (4%)	3 33
1	C	485/510 (95%)	440 (91%)	28 (6%)	17 (4%)	4 39
2	D	465/482 (96%)	417 (90%)	37 (8%)	11 (2%)	7 47
2	E	464/482 (96%)	416 (90%)	33 (7%)	15 (3%)	5 41
2	F	464/482 (96%)	410 (88%)	34 (7%)	20 (4%)	3 34
3	G	258/273 (94%)	196 (76%)	37 (14%)	25 (10%)	1 14
4	H	129/146 (88%)	111 (86%)	10 (8%)	8 (6%)	2 26
5	I	45/50 (90%)	35 (78%)	5 (11%)	5 (11%)	0 11
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	6 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	112 (68%)	26 (16%)	28 (17%)	0 5
8	T	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	16 61
9	U	119/124 (96%)	97 (82%)	15 (13%)	7 (6%)	2 27
10	V	64/77 (83%)	50 (78%)	10 (16%)	4 (6%)	2 25
11	W	215/217 (99%)	187 (87%)	23 (11%)	5 (2%)	8 48
All	All	4589/4803 (96%)	3996 (87%)	395 (9%)	198 (4%)	6 34

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	45	ARG
1	A	47	VAL
1	A	171	ARG
1	A	289	PRO
1	A	374	VAL
1	A	435	PRO
1	B	57	SER
1	B	59	LEU
1	B	80	LYS
1	B	143	ARG
1	B	224	ASP
1	B	238	ASP
1	B	289	PRO
1	B	346	THR
1	B	361	ILE
1	B	365	ILE
1	B	378	ALA
1	C	47	VAL
1	C	80	LYS

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Mol	Chain	Res	Type
1	C	121	ILE
1	C	146	MET
1	C	289	PRO
1	C	361	ILE
1	C	488	LYS
2	D	277	SER
2	D	281	TYR
2	D	450	ASP
2	D	451	HIS
2	E	249	GLN
2	E	282	GLN
2	E	348	VAL
2	E	395	GLU
2	E	447	GLY
2	F	213	SER
2	F	277	SER
2	F	450	ASP
2	F	451	HIS
3	G	73	SER
3	G	93	ALA
3	G	118	ARG
3	G	134	ARG
3	G	196	ILE
3	G	197	ASP
3	G	199	ASP
3	G	250	PHE
3	G	257	VAL
4	H	45	PHE
4	H	69	ASP
4	H	101	ASP
5	I	28	THR
5	I	42	ILE
7	S	2	ALA
7	S	47	LYS
7	S	52	ALA
7	S	108	MET
7	S	112	HIS
7	S	113	ARG
7	S	118	CYS
7	S	122	THR
7	S	124	SER
7	S	142	LEU

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Mol	Chain	Res	Type
7	S	151	GLU
7	S	153	LYS
8	T	149	VAL
10	V	54	ALA
10	V	60	PRO
11	W	152	GLN
1	A	11	ILE
1	A	24	ASP
1	A	116	ASP
1	A	163	GLN
1	A	172	GLN
1	A	224	ASP
1	B	114	ALA
1	B	115	ILE
1	B	505	LEU
1	B	508	PHE
1	C	172	GLN
1	C	224	ASP
1	C	238	ASP
2	D	67	GLU
2	D	93	ARG
2	E	73	GLN
2	E	102	ILE
2	E	132	ILE
2	E	213	SER
2	E	297	THR
2	E	392	GLY
2	F	82	ILE
2	F	282	GLN
2	F	419	GLN
3	G	9	ARG
3	G	87	LYS
3	G	114	SER
3	G	122	ASP
3	G	157	GLU
3	G	187	ALA
3	G	200	VAL
4	H	68	GLU
7	S	8	PRO
7	S	50	LYS
7	S	77	LYS
7	S	123	ALA

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Mol	Chain	Res	Type
9	U	49	ILE
9	U	98	CYS
10	V	30	VAL
10	V	31	ASP
1	A	411	ASP
1	B	82	ILE
1	B	286	ARG
1	B	430	GLN
1	C	171	ARG
2	D	348	VAL
2	E	391	LEU
2	F	31	PRO
2	F	223	ASN
2	F	317	LEU
3	G	92	GLU
3	G	116	LEU
3	G	272	LEU
4	H	51	HIS
4	H	123	ALA
4	H	124	ASP
5	I	26	LEU
6	J	45	GLN
7	S	14	ILE
7	S	55	LEU
7	S	68	SER
7	S	155	ASP
9	U	82	LYS
9	U	99	ALA
11	W	40	ASN
1	A	6	ALA
1	A	18	GLY
1	A	79	ASP
1	B	287	ARG
1	B	375	GLY
1	C	235	THR
2	D	210	ASP
2	F	67	GLU
2	F	297	THR
2	F	364	GLY
3	G	88	GLN
3	G	201	LEU
5	I	9	LEU

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Mol	Chain	Res	Type
6	P	40	PRO
6	Q	44	GLN
7	S	11	ILE
7	S	92	ASN
7	S	107	THR
7	S	137	VAL
8	T	171	LEU
9	U	84	THR
9	U	87	VAL
11	W	36	ARG
11	W	92	PHE
11	W	153	PRO
1	A	44	LEU
1	A	336	ALA
2	D	44	ARG
2	E	359	ASP
2	F	157	GLY
2	F	176	ALA
3	G	133	ARG
3	G	150	ASN
3	G	258	ILE
3	G	269	ALA
6	O	39	ASN
7	S	9	VAL
7	S	49	PRO
7	S	61	LYS
7	S	120	VAL
9	U	13	PHE
1	A	209	LYS
1	C	435	PRO
2	D	279	VAL
2	F	359	ASP
2	F	363	VAL
5	I	44	ILE
1	C	115	ILE
1	C	288	PRO
2	E	279	VAL
2	F	160	VAL
2	F	279	VAL
6	M	40	PRO
1	B	334	VAL
1	C	144	GLU

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Mol	Chain	Res	Type
2	E	453	PRO
4	H	52	VAL
6	J	40	PRO
1	C	145	PRO
2	D	359	ASP
2	F	420	VAL
6	M	71	ILE
6	K	40	PRO
6	Q	40	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.