



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

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 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.

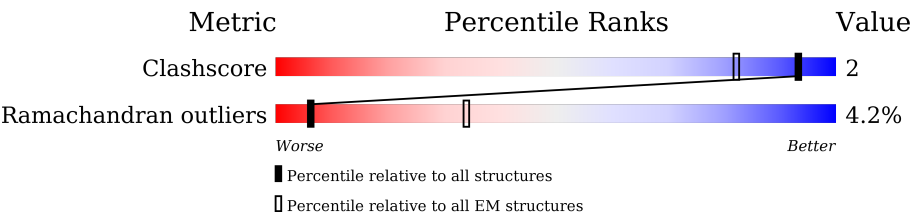
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

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 $\leq 5\%$

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% .

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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>66%</div><div>19%</div><div>.</div><div>12%</div></div>
8	T	174	<div><div></div><div>90%</div><div>9%</div><div>.</div></div>
9	U	124	<div><div></div><div>73%</div><div>19%</div><div>6%</div><div>..</div></div>
10	V	77	<div><div></div><div>65%</div><div>19%</div><div>..</div><div>13%</div></div>
11	W	217	<div><div></div><div>94%</div><div>6%</div></div>

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	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
			1948	974	487	487		

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		

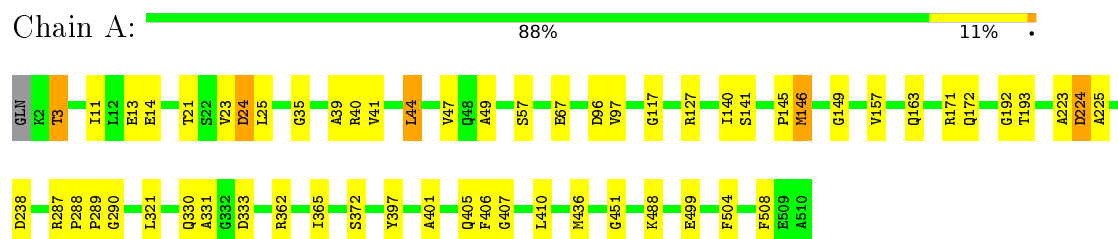
- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

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

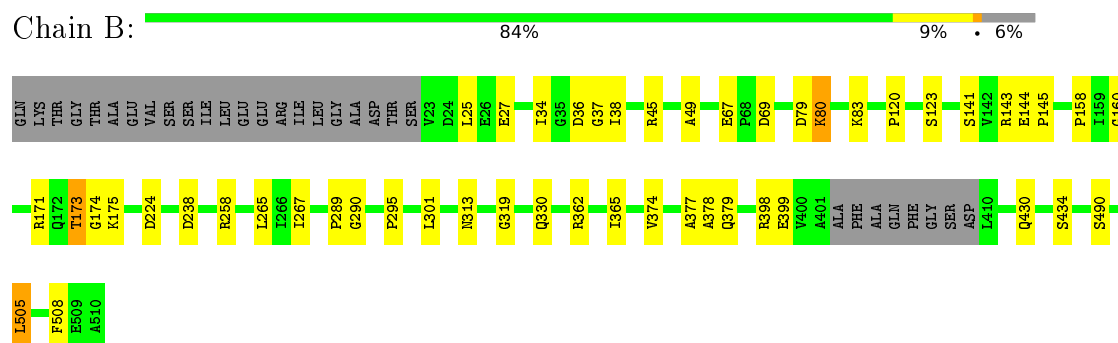
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

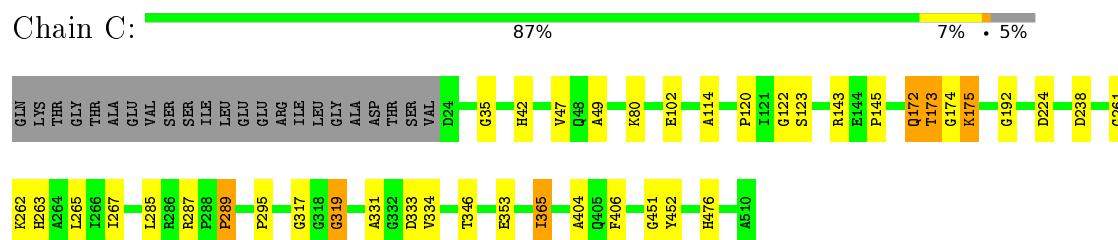
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



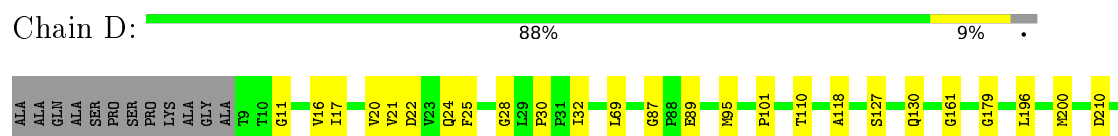
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



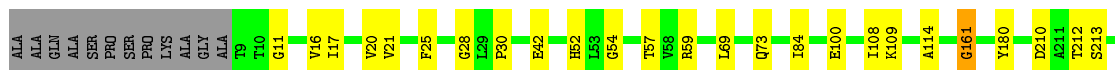
- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





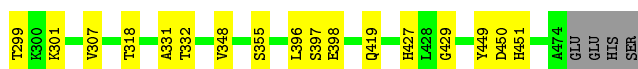
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 86% 10% . .



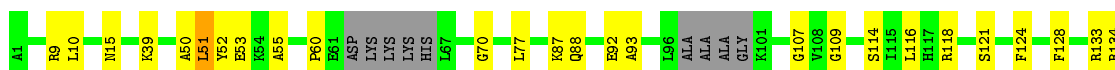
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F: 88% 9% .



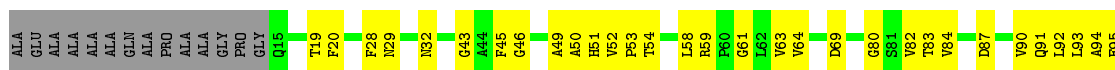
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G: 75% 19% . .



• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H: 66% 24% 10%



• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I: 72% 20% 6%



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

Chain J:  97%



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

Chain K:  99%



- 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%

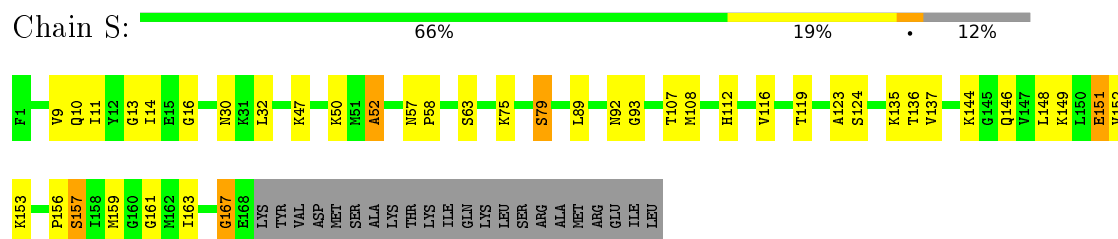


- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

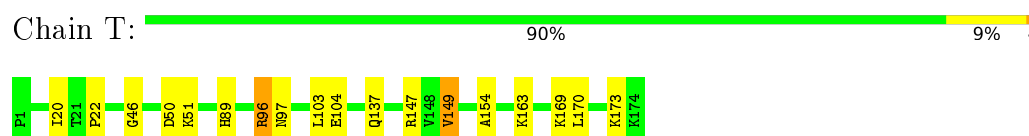
Chain Q:  97%



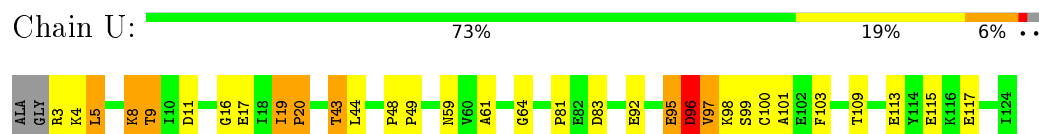
- Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



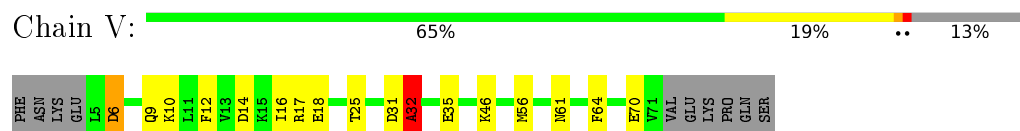
- Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL



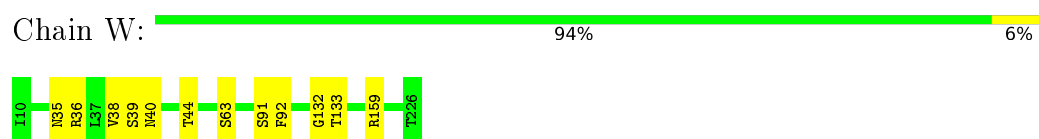
- Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



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



- Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

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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

All (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
3	G	252	ARG	CA-C	-6.39	1.36	1.52
2	E	54	GLY	CA-C	-6.37	1.41	1.51
2	D	11	GLY	CA-C	-6.31	1.41	1.51
1	A	35	GLY	N-CA	-6.26	1.36	1.46
11	W	44	THR	C-O	-6.24	1.11	1.23
3	G	172	LYS	N-CA	-6.18	1.33	1.46
4	H	43	GLY	CA-C	-6.14	1.42	1.51
9	U	95	GLU	C-N	6.11	1.48	1.34
3	G	252	ARG	N-CA	-6.09	1.34	1.46
3	G	139	GLY	CA-C	-6.09	1.42	1.51
3	G	15	ASN	CA-C	-5.91	1.37	1.52
1	A	35	GLY	CA-C	-5.81	1.42	1.51
4	H	132	GLN	N-CA	-5.74	1.34	1.46
1	A	451	GLY	CA-C	-5.68	1.42	1.51
2	E	429	GLY	CA-C	-5.66	1.42	1.51
2	D	161	GLY	N-CA	-5.66	1.37	1.46
4	H	28	PHE	CA-C	-5.64	1.38	1.52
4	H	92	LEU	N-CA	-5.62	1.35	1.46
1	C	175	LYS	CA-C	-5.62	1.38	1.52
1	C	35	GLY	CA-C	-5.48	1.43	1.51
5	I	20	LYS	CA-C	-5.48	1.38	1.52
4	H	131	ILE	CA-C	-5.48	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	451	GLY	CA-C	-5.44	1.43	1.51
8	T	103	LEU	N-CA	-5.39	1.35	1.46
4	H	84	VAL	CA-C	-5.38	1.39	1.52
2	E	11	GLY	CA-C	-5.34	1.43	1.51
3	G	251	ASN	CA-C	-5.33	1.39	1.52
4	H	46	GLY	N-CA	-5.25	1.38	1.46
1	C	172	GLN	N-CA	-5.24	1.35	1.46
2	E	440	GLY	CA-C	-5.21	1.43	1.51
2	D	11	GLY	N-CA	-5.21	1.38	1.46
3	G	255	GLN	CA-C	-5.18	1.39	1.52
1	C	35	GLY	N-CA	-5.17	1.38	1.46
4	H	53	PRO	N-CA	-5.16	1.38	1.47
3	G	171	TYR	N-CA	-5.13	1.36	1.46
1	B	174	GLY	N-CA	-5.13	1.38	1.46
3	G	172	LYS	CA-C	-5.12	1.39	1.52
1	B	67	GLU	C-N	-5.12	1.24	1.34
4	H	91	GLN	CA-C	-5.11	1.39	1.52
1	B	301	LEU	CA-C	-5.09	1.39	1.52
1	A	499	GLU	CA-C	-5.07	1.39	1.52
9	U	96	ASP	CA-C	5.06	1.66	1.52
4	H	19	THR	N-CA	-5.05	1.36	1.46
1	C	172	GLN	CA-C	-5.04	1.39	1.52
2	F	12	ARG	CA-C	-5.00	1.40	1.52

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
7	S	107	THR	C-N-CA	8.62	143.25	121.70
1	A	362	ARG	N-CA-C	-8.41	88.28	111.00
9	U	95	GLU	C-N-CA	8.38	142.64	121.70
1	B	173	THR	N-CA-C	-8.26	88.69	111.00
7	S	157	SER	N-CA-C	-8.24	88.76	111.00
11	W	44	THR	O-C-N	-8.19	109.59	122.70
2	F	449	TYR	N-CA-C	-8.08	89.18	111.00
4	H	93	LEU	N-CA-C	-8.07	89.22	111.00
9	U	95	GLU	CA-C-O	-7.74	103.84	120.10
2	E	16	VAL	N-CA-C	-7.68	90.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLY	N-CA-C	-7.59	94.12	113.10
2	D	161	GLY	N-CA-C	-7.54	94.25	113.10
7	S	112	HIS	C-N-CA	7.47	140.37	121.70
1	A	290	GLY	N-CA-C	-7.38	94.64	113.10
2	E	17	ILE	N-CA-C	-7.33	91.22	111.00
1	C	35	GLY	N-CA-C	-7.32	94.80	113.10
2	E	353	SER	N-CA-C	-7.22	91.51	111.00
3	G	171	TYR	N-CA-C	-7.21	91.53	111.00
2	D	353	SER	N-CA-C	-7.15	91.70	111.00
2	D	20	VAL	N-CA-C	-7.11	91.82	111.00
1	A	39	ALA	N-CA-C	-7.08	91.88	111.00
1	B	430	GLN	N-CA-C	-7.02	92.03	111.00
3	G	156	ASP	C-N-CA	7.02	139.24	121.70
2	F	355	SER	N-CA-C	-6.99	92.12	111.00
9	U	96	ASP	O-C-N	-6.93	111.61	122.70
2	F	398	GLU	N-CA-C	6.86	129.52	111.00
1	A	146	MET	N-CA-C	-6.84	92.52	111.00
2	F	28	GLY	N-CA-C	-6.81	96.07	113.10
7	S	50	LYS	N-CA-C	-6.81	92.62	111.00
2	E	161	GLY	N-CA-C	-6.62	96.54	113.10
2	D	304	ILE	N-CA-C	-6.60	93.18	111.00
2	E	210	ASP	N-CA-C	-6.57	93.25	111.00
2	F	207	ASN	N-CA-C	-6.57	93.27	111.00
1	A	330	GLN	N-CA-C	-6.52	93.39	111.00
2	F	332	THR	N-CA-C	-6.52	93.40	111.00
4	H	43	GLY	N-CA-C	-6.51	96.83	113.10
9	U	97	VAL	N-CA-C	6.50	128.54	111.00
7	S	16	GLY	N-CA-C	-6.49	96.86	113.10
7	S	135	LYS	C-N-CA	6.45	137.84	121.70
2	E	213	SER	N-CA-C	-6.41	93.69	111.00
1	A	321	LEU	N-CA-C	-6.39	93.74	111.00
4	H	83	THR	N-CA-C	-6.39	93.76	111.00
8	T	96	ARG	CA-C-N	-6.38	103.17	117.20
1	A	96	ASP	N-CA-C	-6.34	93.88	111.00
1	B	313	ASN	C-N-CA	6.34	137.54	121.70
2	D	21	VAL	N-CA-C	-6.34	93.89	111.00
2	E	59	ARG	N-CA-C	-6.33	93.92	111.00
1	B	362	ARG	N-CA-C	-6.31	93.96	111.00
1	C	289	PRO	N-CA-C	-6.27	95.79	112.10
5	I	27	LYS	C-N-CA	6.25	137.33	121.70
2	E	20	VAL	N-CA-C	-6.25	94.13	111.00
1	C	122	GLY	N-CA-C	-6.21	97.59	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ILE	N-CA-C	-6.20	94.27	111.00
9	U	8	LYS	C-N-CA	6.17	137.13	121.70
1	A	193	THR	N-CA-C	-6.16	94.38	111.00
4	H	61	GLY	N-CA-C	-6.16	97.71	113.10
1	B	25	LEU	N-CA-C	-6.14	94.41	111.00
2	F	218	VAL	N-CA-C	-6.14	94.41	111.00
3	G	92	GLU	C-N-CA	6.14	137.06	121.70
4	H	54	THR	N-CA-C	-6.12	94.46	111.00
3	G	70	GLY	N-CA-C	-6.10	97.84	113.10
2	F	45	LEU	N-CA-C	-6.10	94.53	111.00
1	B	330	GLN	N-CA-C	-6.06	94.64	111.00
1	A	372	SER	N-CA-C	-6.03	94.71	111.00
9	U	8	LYS	CA-C-O	-6.01	107.47	120.10
1	B	83	LYS	N-CA-C	-5.97	94.87	111.00
3	G	188	GLU	C-N-CA	5.96	136.60	121.70
2	F	17	ILE	N-CA-C	-5.92	95.00	111.00
3	G	134	ARG	N-CA-C	-5.92	95.01	111.00
2	E	109	LYS	N-CA-C	-5.92	95.02	111.00
2	D	24	GLN	N-CA-C	-5.92	95.03	111.00
1	A	410	LEU	N-CA-C	-5.89	95.08	111.00
1	B	34	ILE	N-CA-C	-5.89	95.09	111.00
3	G	272	LEU	N-CA-C	-5.89	95.10	111.00
1	A	41	VAL	N-CA-C	-5.86	95.17	111.00
1	A	157	VAL	N-CA-C	-5.84	95.23	111.00
1	A	67	GLU	N-CA-C	-5.83	95.25	111.00
2	F	331	ALA	N-CA-C	-5.82	95.28	111.00
2	E	307	VAL	N-CA-C	-5.80	95.34	111.00
4	H	64	VAL	N-CA-C	-5.80	95.35	111.00
1	A	97	VAL	N-CA-C	-5.79	95.36	111.00
1	A	192	GLY	N-CA-C	-5.79	98.62	113.10
4	H	84	VAL	N-CA-C	-5.79	95.36	111.00
1	A	24	ASP	N-CA-C	-5.77	95.43	111.00
4	H	46	GLY	N-CA-C	-5.77	98.69	113.10
2	D	118	ALA	N-CA-C	-5.76	95.45	111.00
2	F	52	HIS	N-CA-C	-5.74	95.49	111.00
2	F	83	ARG	N-CA-C	-5.73	95.53	111.00
2	F	20	VAL	N-CA-C	-5.73	95.53	111.00
3	G	109	GLY	N-CA-C	-5.72	98.79	113.10
2	F	21	VAL	N-CA-C	-5.71	95.58	111.00
7	S	9	VAL	C-N-CA	5.70	135.94	121.70
7	S	167	GLY	N-CA-C	-5.68	98.89	113.10
2	D	32	ILE	N-CA-C	-5.66	95.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	399	GLU	N-CA-C	-5.64	95.76	111.00
1	C	173	THR	C-N-CA	5.64	134.14	122.30
2	E	21	VAL	N-CA-C	-5.63	95.80	111.00
5	I	43	LYS	N-CA-C	-5.63	95.81	111.00
4	H	90	VAL	N-CA-C	-5.61	95.84	111.00
2	E	431	LEU	N-CA-C	-5.61	95.86	111.00
1	C	334	VAL	C-N-CA	5.60	135.69	121.70
7	S	50	LYS	C-N-CA	5.60	135.69	121.70
2	D	22	ASP	N-CA-C	-5.59	95.91	111.00
1	B	290	GLY	N-CA-C	-5.57	99.17	113.10
1	C	263	HIS	N-CA-C	-5.57	95.96	111.00
4	H	32	ASN	C-N-CA	5.56	135.60	121.70
2	D	17	ILE	N-CA-C	-5.55	96.01	111.00
2	F	54	GLY	N-CA-C	-5.55	99.22	113.10
2	F	41	ARG	C-N-CA	5.55	135.57	121.70
2	E	28	GLY	N-CA-C	-5.55	99.23	113.10
5	I	28	THR	N-CA-C	5.54	125.97	111.00
3	G	204	TYR	N-CA-C	-5.54	96.04	111.00
1	B	490	SER	C-N-CA	5.53	135.53	121.70
2	E	331	ALA	N-CA-C	-5.53	96.07	111.00
3	G	107	GLY	N-CA-C	-5.53	99.28	113.10
7	S	79	SER	CA-C-N	5.53	132.57	117.10
10	V	16	ILE	O-C-N	-5.52	113.87	122.70
10	V	32	ALA	O-C-N	-5.51	113.83	123.20
2	F	307	VAL	N-CA-C	-5.50	96.14	111.00
2	D	25	PHE	N-CA-C	-5.50	96.16	111.00
9	U	96	ASP	C-N-CA	5.49	135.43	121.70
3	G	196	ILE	N-CA-C	-5.49	96.17	111.00
4	H	94	ALA	N-CA-C	-5.49	96.18	111.00
7	S	13	GLY	N-CA-C	-5.48	99.40	113.10
4	H	20	PHE	N-CA-C	-5.48	96.21	111.00
4	H	28	PHE	N-CA-C	-5.47	96.22	111.00
1	B	79	ASP	C-N-CA	5.47	135.37	121.70
9	U	4	LYS	C-N-CA	5.45	135.32	121.70
2	F	63	MET	C-N-CA	5.45	135.32	121.70
1	B	158	PRO	N-CA-C	-5.44	97.95	112.10
2	D	130	GLN	N-CA-C	-5.44	96.30	111.00
2	E	311	TYR	N-CA-C	-5.43	96.34	111.00
3	G	128	PHE	N-CA-C	-5.40	96.42	111.00
2	D	210	ASP	N-CA-C	-5.39	96.43	111.00
3	G	195	ASP	CA-C-N	-5.38	105.36	117.20
4	H	92	LEU	N-CA-C	-5.36	96.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	ILE	N-CA-C	-5.33	96.61	111.00
1	C	42	HIS	CA-C-N	-5.32	105.55	116.20
7	S	119	THR	N-CA-C	-5.32	96.64	111.00
2	F	156	GLY	N-CA-C	-5.32	99.81	113.10
3	G	154	GLU	N-CA-C	-5.32	96.64	111.00
3	G	182	ASP	N-CA-C	-5.30	96.70	111.00
2	F	219	TYR	N-CA-C	-5.28	96.73	111.00
2	D	95	MET	N-CA-C	-5.28	96.75	111.00
2	E	256	ASP	N-CA-C	-5.25	96.82	111.00
2	D	301	LYS	N-CA-C	-5.24	96.85	111.00
1	A	407	GLY	N-CA-C	-5.24	100.00	113.10
7	S	112	HIS	N-CA-C	-5.23	96.87	111.00
2	D	127	SER	N-CA-C	-5.23	96.88	111.00
2	F	41	ARG	CA-C-N	-5.20	105.76	117.20
1	B	80	LYS	N-CA-C	-5.17	97.04	111.00
1	C	333	ASP	N-CA-C	-5.17	97.05	111.00
2	F	16	VAL	N-CA-C	-5.17	97.05	111.00
1	A	127	ARG	N-CA-C	-5.16	97.06	111.00
2	D	331	ALA	N-CA-C	-5.16	97.08	111.00
3	G	52	TYR	C-N-CA	5.15	134.58	121.70
2	D	393	MET	CA-C-N	-5.14	105.88	117.20
3	G	39	LYS	N-CA-C	5.14	124.88	111.00
1	A	140	ILE	N-CA-C	-5.14	97.12	111.00
1	C	102	GLU	C-N-CA	5.14	134.54	121.70
3	G	114	SER	N-CA-C	-5.14	97.13	111.00
4	H	19	THR	N-CA-C	-5.14	97.13	111.00
2	F	11	GLY	N-CA-C	-5.12	100.30	113.10
3	G	170	SER	CA-C-N	-5.11	105.96	117.20
2	F	450	ASP	N-CA-C	-5.10	97.23	111.00
2	D	249	GLN	CA-C-N	-5.10	105.99	117.20
3	G	55	ALA	N-CA-C	-5.09	97.25	111.00
1	B	67	GLU	N-CA-C	-5.09	97.26	111.00
4	H	82	VAL	N-CA-C	-5.08	97.27	111.00
2	D	16	VAL	N-CA-C	-5.08	97.29	111.00
1	B	265	LEU	N-CA-C	-5.07	97.31	111.00
2	E	248	GLY	C-N-CA	5.07	134.38	121.70
2	E	108	ILE	N-CA-C	-5.07	97.31	111.00
1	A	488	LYS	N-CA-C	-5.07	97.32	111.00
3	G	124	PHE	N-CA-C	-5.07	97.32	111.00
1	A	224	ASP	C-N-CA	5.06	134.35	121.70
4	H	63	VAL	N-CA-C	-5.05	97.38	111.00
1	C	265	LEU	N-CA-C	-5.04	97.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	THR	N-CA-C	-5.03	97.42	111.00
3	G	172	LYS	N-CA-C	-5.03	97.42	111.00
1	A	40	ARG	N-CA-C	-5.02	97.45	111.00
2	F	25	PHE	N-CA-C	-5.02	97.45	111.00
2	E	304	ILE	N-CA-C	-5.01	97.46	111.00
4	H	87	ASP	CA-C-N	-5.01	106.19	117.20
1	C	192	GLY	N-CA-C	-5.00	100.59	113.10
1	B	38	ILE	N-CA-C	-5.00	97.50	111.00
2	E	52	HIS	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (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
1	B	398	ARG	Mainchain
1	B	399	GLU	Mainchain,Peptide
1	B	505	LEU	Mainchain
1	C	173	THR	Mainchain
1	C	174	GLY	Mainchain,Peptide
1	C	476	HIS	Peptide
2	D	319	ASP	Mainchain
2	D	393	MET	Mainchain
2	D	397	SER	Mainchain
2	E	25	PHE	Mainchain,Peptide
2	E	311	TYR	Mainchain
2	E	397	SER	Mainchain
2	F	158	ALA	Peptide
2	F	318	THR	Mainchain
2	F	397	SER	Mainchain
3	G	155	PHE	Mainchain
3	G	182	ASP	Mainchain
3	G	195	ASP	Mainchain,Peptide
4	H	144	ALA	Peptide
7	S	151	GLU	Peptide
7	S	152	VAL	Peptide
7	S	156	PRO	Peptide
7	S	157	SER	Mainchain

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Mol	Chain	Res	Type	Group
7	S	159	MET	Mainchain
7	S	161	GLY	Mainchain
7	S	52	ALA	Peptide
7	S	57	ASN	Mainchain
7	S	89	LEU	Mainchain
8	T	137	GLN	Mainchain
8	T	149	VAL	Peptide
8	T	154	ALA	Peptide
8	T	163	LYS	Mainchain
8	T	169	LYS	Mainchain
8	T	173	LYS	Peptide
8	T	22	PRO	Peptide
8	T	46	GLY	Mainchain
8	T	50	ASP	Peptide
8	T	51	LYS	Mainchain
8	T	89	HIS	Mainchain
8	T	96	ARG	Mainchain
8	T	97	ASN	Mainchain
9	U	103	PHE	Peptide
9	U	109	THR	Mainchain
9	U	11	ASP	Peptide
9	U	113	GLU	Mainchain
9	U	115	GLU	Mainchain,Peptide
9	U	117	GLU	Mainchain
9	U	16	GLY	Peptide
9	U	17	GLU	Peptide
9	U	19	ILE	Mainchain
9	U	20	PRO	Mainchain,Peptide
9	U	3	ARG	Mainchain,Peptide
9	U	43	THR	Mainchain
9	U	44	LEU	Peptide
9	U	59	ASN	Mainchain,Peptide
9	U	61	ALA	Peptide
9	U	64	GLY	Mainchain
9	U	8	LYS	Mainchain,Peptide
9	U	81	PRO	Mainchain
9	U	83	ASP	Peptide
9	U	9	THR	Mainchain
9	U	92	GLU	Mainchain
9	U	95	GLU	Mainchain,Peptide
9	U	96	ASP	Mainchain,Peptide
9	U	97	VAL	Peptide

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Mol	Chain	Res	Type	Group
9	U	98	LYS	Peptide
10	V	12	PHE	Mainchain
10	V	17	ARG	Mainchain
10	V	18	GLU	Mainchain,Peptide
10	V	25	THR	Peptide
10	V	31	ASP	Peptide
10	V	32	ALA	Mainchain
10	V	35	GLU	Mainchain
10	V	46	LYS	Mainchain
10	V	6	ASP	Peptide
10	V	61	ASN	Peptide
10	V	64	PHE	Mainchain,Peptide
10	V	70	GLU	Mainchain
10	V	9	GLN	Peptide
11	W	132	GLY	Mainchain
11	W	133	THR	Mainchain
11	W	159	ARG	Mainchain
11	W	35	ASN	Peptide
11	W	63	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:149:GLY:HA3	1:A:436:MET:H	1.73	0.54
1:C:285:LEU:C	1:C:287:ARG:H	2.10	0.53
2:D:473:LEU:C	2:D:475:GLU:H	2.13	0.52
2:D:179:GLY:HA2	2:D:250:ASP:O	2.11	0.51
3:G:155:PHE:C	3:G:157:GLU:H	2.14	0.49
1:C:353:GLU:H	1:C:365:ILE:N	2.09	0.49
2:D:87:GLY:C	2:D:89:GLU:H	2.16	0.48
1:C:261:GLY:O	1:C:319:GLY:HA2	2.13	0.48
1:C:49:ALA:H	2:D:69:LEU:N	2.11	0.48
5:I:40:SER:C	5:I:42:ILE:H	2.17	0.48
3:G:167:SER:C	3:G:169:ILE:H	2.17	0.47
8:T:20:ILE:H	11:W:91:SER:H	1.62	0.47
1:B:144:GLU:O	1:B:160:GLY:HA2	2.15	0.47
10:V:10:LYS:O	10:V:14:ASP:N	2.48	0.47
1:A:25:LEU:C	1:A:44:LEU:H	2.19	0.47
8:T:104:GLU:N	9:U:5:LEU:H	2.12	0.47
7:S:146:GLN:C	7:S:148:LEU:H	2.20	0.46
1:C:261:GLY:HA2	1:C:317:GLY:HA3	1.97	0.45
1:B:49:ALA:H	2:F:69:LEU:H	1.63	0.45
4:H:80:GLY:HA3	4:H:95:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TYR:O	1:A:401:ALA:N	2.50	0.44
2:D:196:LEU:O	2:D:200:MET:N	2.51	0.43
3:G:183:THR:C	3:G:186:SER:H	2.21	0.43
1:A:49:ALA:H	2:E:69:LEU:N	2.17	0.43
1:C:172:GLN:CA	1:C:175:LYS:H	2.32	0.42
8:T:104:GLU:CA	9:U:5:LEU:H	2.32	0.42
1:A:504:PHE:O	1:A:508:PHE:N	2.52	0.42
2:F:419:GLN:N	2:F:429:GLY:H	2.18	0.42
5:I:28:THR:C	5:I:31:LYS:H	2.22	0.42
2:E:84:ILE:H	2:E:114:ALA:H	1.67	0.41
11:W:38:VAL:H	11:W:39:SER:CA	2.33	0.41
2:E:417:PRO:C	2:E:429:GLY:HA2	2.41	0.41
2:F:299:THR:C	2:F:301:LYS:H	2.23	0.41
7:S:30:ASN:C	7:S:32:LEU:H	2.24	0.41
1:B:258:ARG:O	1:B:319:GLY:HA3	2.22	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%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	B	45	ARG
1	B	80	LYS
1	B	171	ARG
1	B	224	ASP
1	B	377	ALA
1	B	434	SER
1	B	508	PHE
1	C	80	LYS
1	C	120	PRO
1	C	238	ASP
1	C	262	LYS
1	C	289	PRO
1	C	319	GLY

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Mol	Chain	Res	Type
1	C	331	ALA
1	C	365	ILE
1	C	406	PHE
2	D	276	PRO
2	D	427	HIS
2	D	451	HIS
2	E	180	TYR
2	E	277	SER
2	E	348	VAL
2	E	393	MET
2	E	394	ASP
2	E	397	SER
2	E	451	HIS
2	F	281	TYR
2	F	427	HIS
2	F	451	HIS
3	G	50	ALA
3	G	60	PRO
3	G	93	ALA
3	G	118	ARG
3	G	157	GLU
3	G	189	SER
3	G	196	ILE
3	G	199	ASP
3	G	250	PHE
4	H	45	PHE
4	H	49	ALA
4	H	50	ALA
4	H	51	HIS
4	H	58	LEU
4	H	59	ARG
4	H	69	ASP
4	H	101	ASP
5	I	6	GLN
7	S	47	LYS
7	S	79	SER
7	S	108	MET
7	S	116	VAL
7	S	123	ALA
7	S	124	SER
8	T	149	VAL
9	U	5	LEU

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Mol	Chain	Res	Type
9	U	100	CYS
1	A	3	THR
1	A	11	ILE
1	A	24	ASP
1	A	163	GLN
1	A	288	PRO
1	A	331	ALA
1	B	36	ASP
1	B	69	ASP
1	B	238	ASP
1	B	365	ILE
1	B	505	LEU
1	C	143	ARG
1	C	295	PRO
2	D	28	GLY
2	D	462	PRO
2	E	73	GLN
2	E	100	GLU
2	E	297	THR
2	E	392	GLY
2	F	158	ALA
2	F	276	PRO
2	F	348	VAL
3	G	9	ARG
3	G	77	LEU
3	G	87	LYS
3	G	116	LEU
3	G	195	ASP
3	G	200	VAL
3	G	257	VAL
7	S	11	ILE
7	S	93	GLY
7	S	136	THR
8	T	147	ARG
8	T	170	LEU
9	U	19	ILE
9	U	101	ALA
10	V	32	ALA
1	A	57	SER
1	A	171	ARG
1	A	172	GLN
1	A	224	ASP

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Mol	Chain	Res	Type
1	C	224	ASP
1	C	346	THR
1	C	452	TYR
2	D	297	THR
2	E	161	GLY
2	E	212	THR
2	E	249	GLN
2	E	282	GLN
2	E	350	PRO
2	E	357	ILE
2	F	249	GLN
3	G	88	GLN
3	G	133	ARG
3	G	151	SER
3	G	258	ILE
3	G	269	ALA
6	J	45	GLN
7	S	10	GLN
7	S	58	PRO
7	S	63	SER
7	S	92	ASN
7	S	144	LYS
7	S	153	LYS
10	V	56	MET
1	A	23	VAL
1	A	47	VAL
1	A	146	MET
1	B	37	GLY
1	B	143	ARG
1	B	378	ALA
1	C	114	ALA
1	C	123	SER
2	D	30	PRO
2	E	42	GLU
3	G	10	LEU
3	G	51	LEU
3	G	121	SER
3	G	201	LEU
5	I	4	TRP
5	I	26	LEU
6	P	40	PRO
6	Q	44	GLN

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Mol	Chain	Res	Type
7	S	75	LYS
7	S	149	LYS
7	S	151	GLU
9	U	20	PRO
9	U	43	THR
9	U	99	SER
11	W	36	ARG
11	W	40	ASN
11	W	92	PHE
1	A	287	ARG
1	A	365	ILE
1	A	405	GLN
1	B	27	GLU
1	B	120	PRO
1	B	141	SER
1	B	289	PRO
1	C	145	PRO
1	C	404	ALA
2	D	110	THR
2	D	223	ASN
2	D	279	VAL
2	E	462	PRO
2	F	297	THR
2	F	396	LEU
5	I	25	ALA
6	O	39	ASN
9	U	49	PRO
1	A	44	LEU
1	A	117	GLY
1	B	295	PRO
2	D	101	PRO
3	G	169	ILE
1	B	145	PRO
1	C	47	VAL
2	E	30	PRO
2	E	279	VAL
2	F	279	VAL
6	M	40	PRO
9	U	48	PRO
10	V	6	ASP
1	A	145	PRO
1	B	374	VAL

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Mol	Chain	Res	Type
7	S	14	ILE
3	G	168	VAL
6	J	40	PRO
6	M	71	ILE
7	S	137	VAL
4	H	52	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.