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

Dec 13, 2016 – 04:24 PM EST

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

This is a 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.

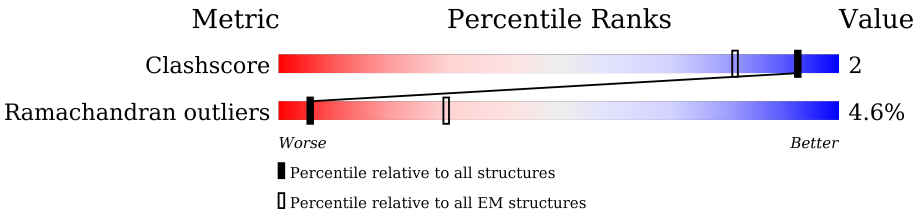
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 6.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

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

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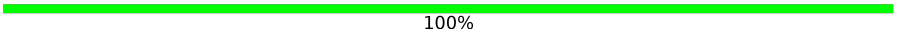
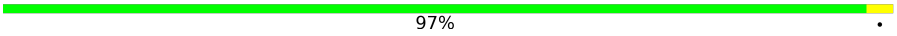
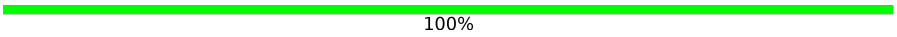
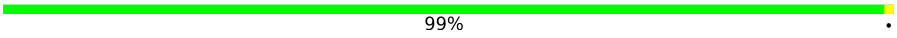
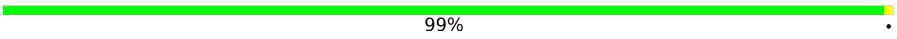
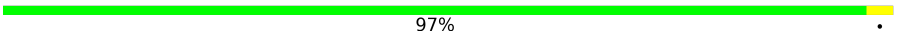
Mol	Chain	Length	Quality of chain
6	L	72	
6	M	72	
6	N	72	
6	O	72	
6	P	72	
6	Q	72	
7	S	190	
8	T	174	
9	U	124	
10	V	77	
11	W	217	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18544 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

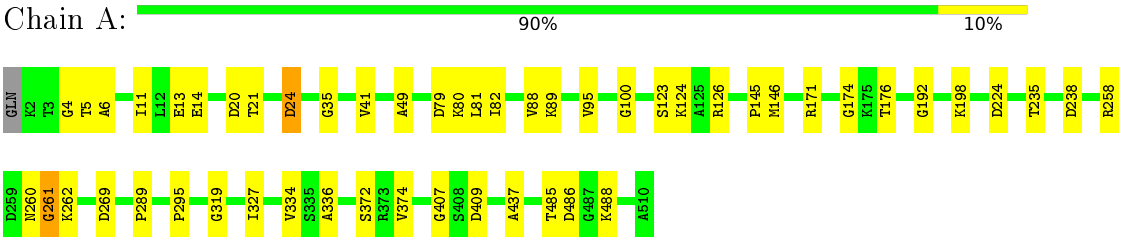
Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	217	Total 869	C 434	N 217	O 218	0	0

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.

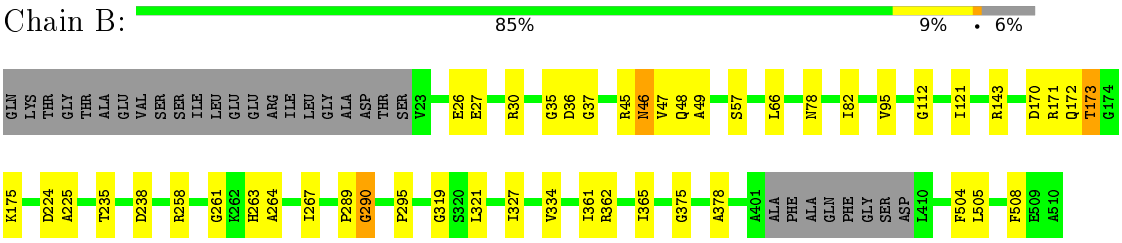
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



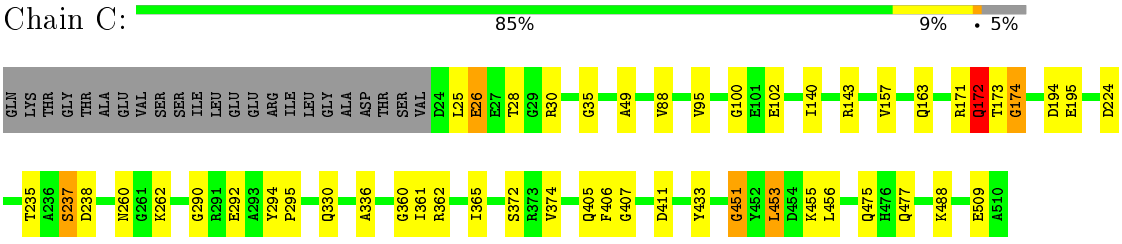
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:



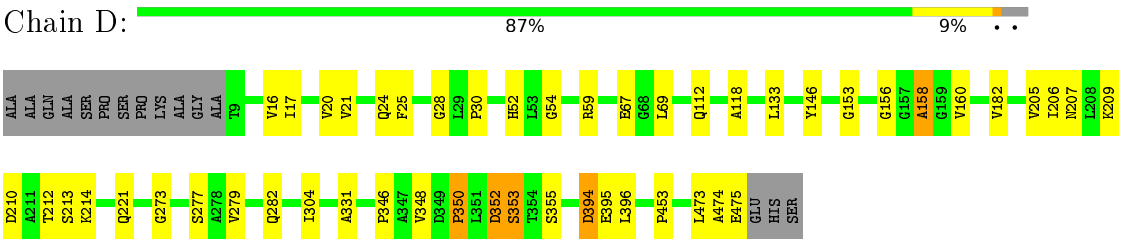
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain C:



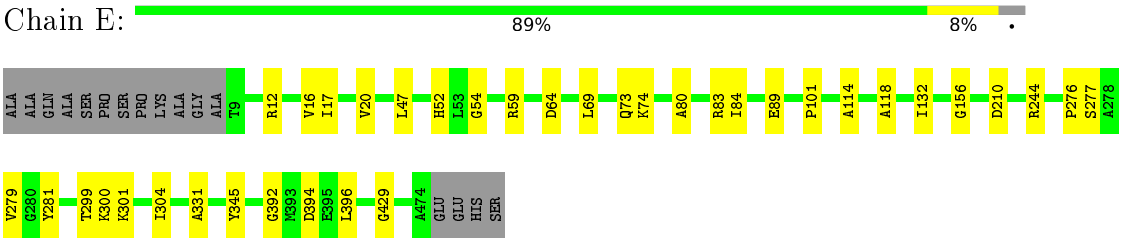
- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:



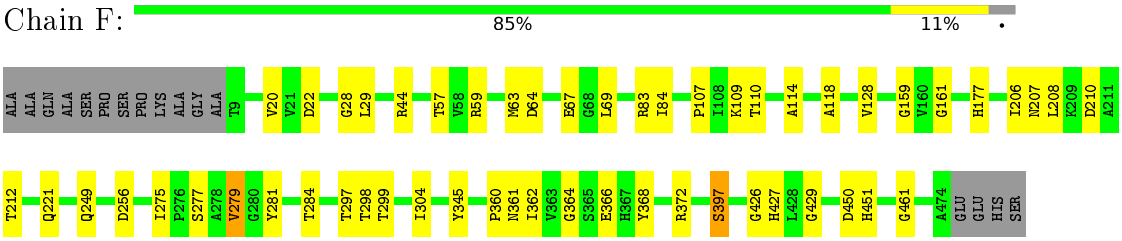
- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:



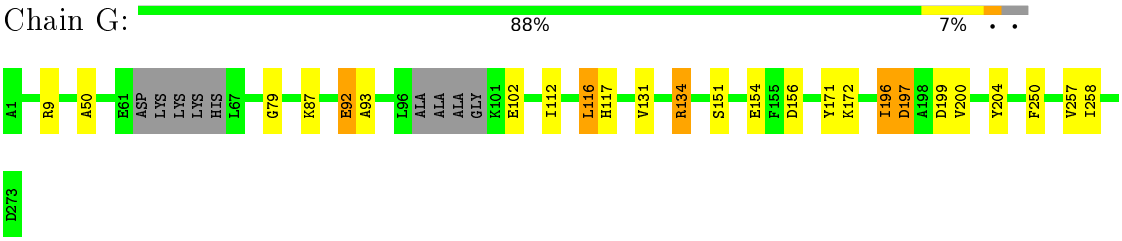
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:



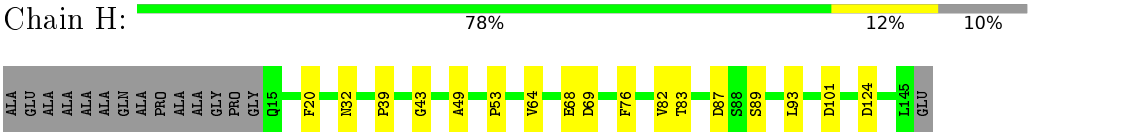
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:



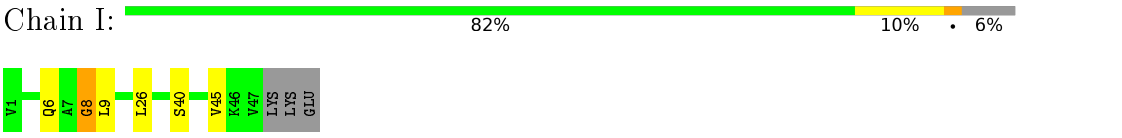
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H:



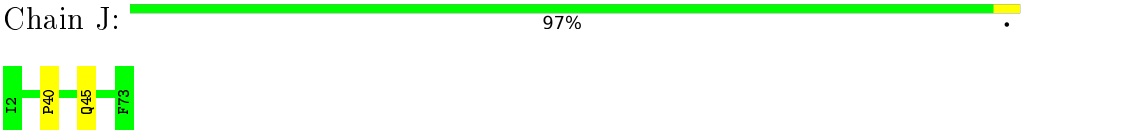
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:



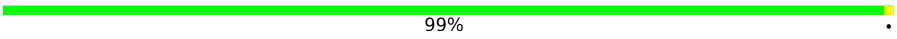
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain J:



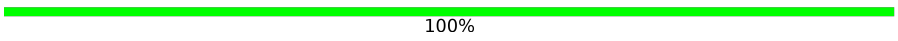
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K:



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

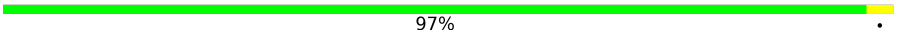
Chain L:

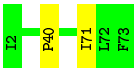


There are no outlier residues recorded for this chain.

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

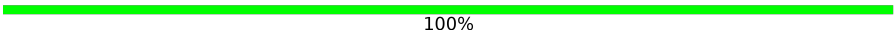
Chain M:





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

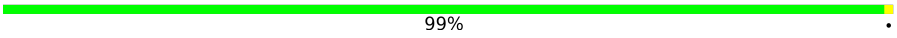
Chain N:



There are no outlier residues recorded for this chain.

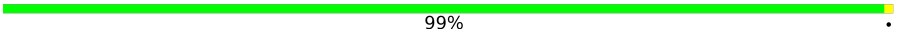
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O:



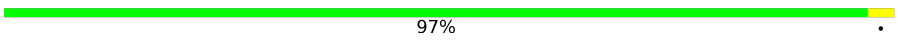
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

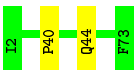
Chain P:



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

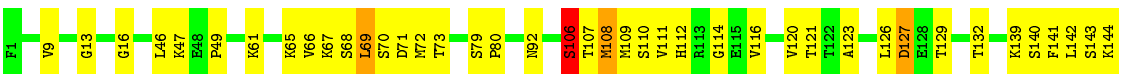
Chain Q:





• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:

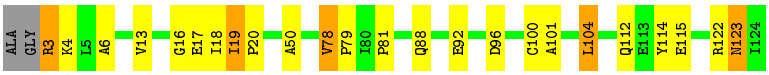


- Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:

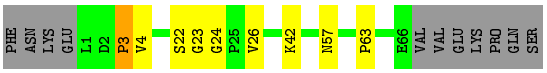
- Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

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	20104	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	30487	Depositor
Image detector	GATAN K2 (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	1.81	3/2034 (0.1%)	1.42	17/2541 (0.7%)
1	B	1.85	3/1916 (0.2%)	1.42	18/2392 (0.8%)
1	C	1.83	3/1946 (0.2%)	1.42	17/2431 (0.7%)
10	V	0.79	0/263	1.06	0/327
11	W	2.53	5/868 (0.6%)	1.21	6/1082 (0.6%)
2	D	1.82	2/1866 (0.1%)	1.47	23/2331 (1.0%)
2	E	1.79	5/1862 (0.3%)	1.43	16/2326 (0.7%)
2	F	1.87	2/1862 (0.1%)	1.53	22/2326 (0.9%)
3	G	1.78	1/1050 (0.1%)	1.37	8/1308 (0.6%)
4	H	1.81	0/522	1.61	10/651 (1.5%)
5	I	1.63	0/186	1.40	2/231 (0.9%)
6	J	0.30	0/287	0.41	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.30	0/287	0.45	0/357
6	M	0.29	0/287	0.44	0/357
6	N	0.28	0/287	0.40	0/357
6	O	0.30	0/287	0.41	0/357
6	P	0.29	0/287	0.43	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.63	3/668 (0.4%)	1.92	18/834 (2.2%)
8	T	1.24	6/696 (0.9%)	1.53	13/867 (1.5%)
9	U	0.87	0/484	1.37	4/604 (0.7%)
All	All	1.69	33/18519 (0.2%)	1.37	174/23107 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	3

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	88	LEU	CA-C	62.36	3.15	1.52
11	W	88	LEU	N-CA	20.90	1.88	1.46
11	W	89	PRO	N-CA	-18.54	1.15	1.47
11	W	88	LEU	C-O	-14.20	0.96	1.23
8	T	160	THR	N-CA	9.37	1.65	1.46
8	T	110	ARG	N-CA	-8.32	1.29	1.46
8	T	135	LYS	CA-C	7.46	1.72	1.52
2	D	273	GLY	CA-C	-7.40	1.40	1.51
7	S	107	THR	CA-C	-6.09	1.37	1.52
8	T	163	LYS	N-CA	6.02	1.58	1.46
2	E	74	LYS	CA-C	-5.95	1.37	1.52
7	S	108	MET	N-CA	-5.93	1.34	1.46
2	F	364	GLY	CA-C	-5.92	1.42	1.51
2	E	429	GLY	CA-C	-5.91	1.42	1.51
2	F	366	GLU	CA-C	-5.66	1.38	1.52
1	B	290	GLY	N-CA	-5.66	1.37	1.46
1	B	290	GLY	CA-C	-5.52	1.43	1.51
8	T	109	GLU	CA-C	-5.51	1.38	1.52
1	C	451	GLY	CA-C	-5.49	1.43	1.51
1	A	174	GLY	N-CA	-5.47	1.37	1.46
2	E	54	GLY	CA-C	-5.40	1.43	1.51
2	E	12	ARG	CA-C	-5.39	1.39	1.52
1	C	35	GLY	N-CA	-5.33	1.38	1.46
1	A	176	THR	N-CA	-5.31	1.35	1.46
2	D	153	GLY	CA-C	-5.31	1.43	1.51
1	A	35	GLY	CA-C	-5.29	1.43	1.51
1	B	35	GLY	CA-C	-5.28	1.43	1.51
7	S	16	GLY	N-CA	-5.27	1.38	1.46
1	C	172	GLN	CA-C	-5.22	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	244	ARG	CA-C	-5.22	1.39	1.52
8	T	100	ALA	N-CA	-5.14	1.36	1.46
3	G	172	LYS	N-CA	-5.04	1.36	1.46
11	W	132	GLY	N-CA	-5.02	1.38	1.46

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	73	THR	C-N-CA	16.48	162.91	121.70
7	S	110	SER	C-N-CA	-12.41	90.68	121.70
7	S	106	SER	CA-C-N	-12.23	90.30	117.20
11	W	89	PRO	N-CA-C	-10.49	84.82	112.10
9	U	78	VAL	CA-C-O	-9.60	99.94	120.10
8	T	88	ARG	CA-C-O	-9.58	99.99	120.10
8	T	159	GLU	CA-C-O	-9.01	101.18	120.10
11	W	90	HIS	O-C-N	-8.89	108.48	122.70
8	T	160	THR	CA-C-N	-8.62	98.24	117.20
8	T	159	GLU	C-N-CA	8.06	141.85	121.70
1	A	4	GLY	N-CA-C	-7.69	93.87	113.10
7	S	69	LEU	CA-C-N	-7.69	100.28	117.20
3	G	116	LEU	N-CA-C	-7.51	90.72	111.00
2	D	28	GLY	N-CA-C	-7.28	94.91	113.10
7	S	158	ILE	N-CA-C	-7.21	91.53	111.00
7	S	106	SER	O-C-N	7.17	134.17	122.70
2	D	394	ASP	N-CA-C	-7.17	91.65	111.00
1	A	35	GLY	N-CA-C	-7.16	95.19	113.10
2	F	345	TYR	N-CA-C	-7.12	91.78	111.00
2	E	345	TYR	N-CA-C	-7.08	91.89	111.00
1	C	35	GLY	N-CA-C	-7.06	95.45	113.10
2	D	353	SER	N-CA-C	-6.94	92.27	111.00
8	T	104	GLU	CA-C-N	-6.89	102.04	117.20
2	D	156	GLY	N-CA-C	-6.81	96.08	113.10
2	F	207	ASN	N-CA-C	-6.80	92.64	111.00
8	T	91	LEU	C-N-CA	6.80	138.70	121.70
2	D	17	ILE	N-CA-C	-6.75	92.79	111.00
2	F	109	LYS	N-CA-C	-6.67	92.98	111.00
2	E	16	VAL	N-CA-C	-6.66	93.01	111.00
1	C	237	SER	C-N-CA	6.65	138.32	121.70
7	S	73	THR	CA-C-N	-6.64	102.59	117.20
3	G	196	ILE	C-N-CA	6.61	138.22	121.70
2	D	304	ILE	N-CA-C	-6.60	93.18	111.00
1	C	174	GLY	N-CA-C	-6.59	96.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	134	ARG	N-CA-C	-6.54	93.33	111.00
1	C	100	GLY	N-CA-C	-6.53	96.77	113.10
7	S	107	THR	C-N-CA	-6.51	105.41	121.70
2	D	355	SER	N-CA-C	-6.49	93.47	111.00
2	F	20	VAL	N-CA-C	-6.47	93.52	111.00
2	D	16	VAL	N-CA-C	-6.46	93.56	111.00
8	T	159	GLU	O-C-N	6.45	133.01	122.70
11	W	85	LEU	CA-C-O	-6.43	106.59	120.10
2	E	210	ASP	N-CA-C	-6.40	93.72	111.00
2	E	83	ARG	N-CA-C	-6.30	93.99	111.00
1	B	263	HIS	N-CA-C	-6.25	94.12	111.00
2	F	304	ILE	N-CA-C	-6.24	94.14	111.00
1	C	406	PHE	N-CA-C	-6.23	94.19	111.00
3	G	171	TYR	N-CA-C	-6.22	94.20	111.00
2	E	54	GLY	N-CA-C	-6.22	97.55	113.10
11	W	88	LEU	O-C-N	6.21	132.91	121.10
2	F	83	ARG	N-CA-C	-6.20	94.26	111.00
2	E	17	ILE	N-CA-C	-6.18	94.31	111.00
2	F	461	GLY	N-CA-C	-6.16	97.69	113.10
2	D	210	ASP	N-CA-C	-6.14	94.42	111.00
2	F	397	SER	C-N-CA	6.13	137.03	121.70
1	C	25	LEU	C-N-CA	6.12	136.99	121.70
4	H	124	ASP	N-CA-C	-6.09	94.57	111.00
1	C	372	SER	N-CA-C	-6.07	94.60	111.00
1	A	192	GLY	N-CA-C	-6.07	97.93	113.10
2	F	28	GLY	N-CA-C	-6.05	97.97	113.10
1	A	81	LEU	C-N-CA	6.05	136.82	121.70
1	B	327	ILE	N-CA-C	-6.05	94.66	111.00
7	S	71	ASP	C-N-CA	6.05	136.83	121.70
2	E	20	VAL	N-CA-C	-6.04	94.69	111.00
7	S	106	SER	C-N-CA	6.01	136.72	121.70
7	S	150	LEU	N-CA-C	-5.99	94.82	111.00
8	T	95	GLN	CA-C-N	5.99	130.39	117.20
8	T	156	GLN	O-C-N	-5.99	113.11	122.70
3	G	197	ASP	N-CA-C	5.97	127.11	111.00
2	F	44	ARG	N-CA-C	-5.94	94.97	111.00
2	E	52	HIS	N-CA-C	-5.88	95.14	111.00
11	W	89	PRO	CA-C-N	-5.87	104.28	117.20
1	A	488	LYS	N-CA-C	-5.86	95.17	111.00
8	T	135	LYS	O-C-N	-5.84	113.35	122.70
2	D	52	HIS	N-CA-C	-5.84	95.23	111.00
1	C	362	ARG	N-CA-C	-5.84	95.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	24	GLN	N-CA-C	-5.83	95.27	111.00
4	H	53	PRO	N-CA-C	-5.81	96.99	112.10
1	B	30	ARG	N-CA-C	-5.81	95.32	111.00
4	H	93	LEU	N-CA-C	-5.80	95.34	111.00
2	E	59	ARG	N-CA-C	-5.76	95.44	111.00
2	F	29	LEU	N-CA-C	-5.75	95.49	111.00
1	B	508	PHE	N-CA-C	-5.73	95.53	111.00
1	B	267	ILE	N-CA-C	-5.73	95.54	111.00
1	C	488	LYS	N-CA-C	-5.68	95.66	111.00
2	D	213	SER	N-CA-C	-5.67	95.69	111.00
1	A	372	SER	N-CA-C	-5.66	95.72	111.00
1	C	88	VAL	N-CA-C	-5.65	95.74	111.00
1	B	112	GLY	N-CA-C	-5.64	99.00	113.10
7	S	46	LEU	C-N-CA	5.62	135.76	121.70
1	C	360	GLY	N-CA-C	-5.61	99.07	113.10
7	S	109	MET	N-CA-C	-5.61	95.84	111.00
3	G	154	GLU	N-CA-C	-5.61	95.86	111.00
5	I	45	VAL	N-CA-C	-5.58	95.93	111.00
9	U	3	ARG	CA-C-O	-5.58	108.38	120.10
2	D	59	ARG	N-CA-C	-5.55	96.00	111.00
1	B	78	ASN	N-CA-C	-5.54	96.06	111.00
2	F	275	ILE	N-CA-C	-5.53	96.06	111.00
2	F	118	ALA	N-CA-C	-5.51	96.11	111.00
1	C	102	GLU	C-N-CA	5.50	135.45	121.70
1	A	41	VAL	N-CA-C	-5.49	96.17	111.00
2	D	118	ALA	N-CA-C	-5.49	96.18	111.00
2	D	207	ASN	N-CA-C	-5.47	96.22	111.00
2	F	256	ASP	N-CA-C	-5.45	96.28	111.00
2	D	20	VAL	N-CA-C	-5.43	96.33	111.00
4	H	43	GLY	N-CA-C	-5.42	99.56	113.10
2	E	118	ALA	N-CA-C	-5.40	96.42	111.00
2	F	426	GLY	N-CA-C	-5.40	99.60	113.10
2	F	63	MET	C-N-CA	5.39	135.19	121.70
9	U	3	ARG	O-C-N	5.38	131.30	122.70
2	D	54	GLY	N-CA-C	-5.38	99.66	113.10
1	A	327	ILE	N-CA-C	-5.37	96.51	111.00
1	A	89	LYS	N-CA-C	-5.36	96.52	111.00
4	H	83	THR	N-CA-C	-5.36	96.52	111.00
1	C	330	GLN	N-CA-C	-5.34	96.57	111.00
1	B	225	ALA	N-CA-C	-5.34	96.58	111.00
1	A	261	GLY	C-N-CA	5.33	135.04	121.70
1	A	24	ASP	N-CA-C	-5.33	96.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	80	ALA	N-CA-C	-5.33	96.61	111.00
2	D	182	VAL	N-CA-C	-5.33	96.62	111.00
2	F	360	PRO	C-N-CA	5.31	134.98	121.70
2	E	89	GLU	C-N-CA	5.30	134.95	121.70
4	H	32	ASN	C-N-CA	5.29	134.91	121.70
1	B	173	THR	N-CA-C	-5.28	96.73	111.00
1	B	504	PHE	C-N-CA	5.27	134.88	121.70
2	E	47	LEU	N-CA-C	-5.27	96.78	111.00
1	A	100	GLY	N-CA-C	-5.26	99.94	113.10
1	B	334	VAL	C-N-CA	5.26	134.86	121.70
2	F	298	THR	N-CA-C	-5.25	96.83	111.00
8	T	174	LYS	CA-C-O	-5.24	109.09	120.10
11	W	89	PRO	C-N-CA	-5.23	108.62	121.70
4	H	64	VAL	N-CA-C	-5.22	96.89	111.00
1	C	30	ARG	N-CA-C	-5.21	96.93	111.00
7	S	120	VAL	C-N-CA	5.21	134.72	121.70
4	H	20	PHE	N-CA-C	-5.20	96.96	111.00
7	S	110	SER	CA-C-N	5.20	128.64	117.20
7	S	123	ALA	N-CA-C	-5.18	97.00	111.00
1	A	486	ASP	N-CA-C	5.18	124.99	111.00
2	D	153	GLY	N-CA-C	-5.17	100.16	113.10
5	I	8	GLY	C-N-CA	5.17	134.64	121.70
3	G	204	TYR	N-CA-C	-5.17	97.04	111.00
1	C	140	ILE	N-CA-C	-5.17	97.05	111.00
2	F	22	ASP	N-CA-C	-5.16	97.06	111.00
2	F	57	THR	N-CA-C	-5.16	97.08	111.00
1	B	66	LEU	N-CA-C	-5.16	97.08	111.00
2	E	300	LYS	N-CA-C	-5.15	97.09	111.00
1	A	126	ARG	N-CA-C	-5.15	97.10	111.00
2	F	59	ARG	N-CA-C	-5.14	97.12	111.00
7	S	155	ASP	CA-C-N	5.14	131.49	117.10
1	A	198	LYS	N-CA-C	-5.13	97.16	111.00
2	F	206	ILE	C-N-CA	5.12	134.49	121.70
7	S	157	SER	N-CA-C	-5.12	97.18	111.00
1	B	321	LEU	N-CA-C	-5.10	97.23	111.00
1	C	157	VAL	N-CA-C	-5.10	97.24	111.00
2	D	395	GLU	N-CA-C	5.09	124.75	111.00
2	D	206	ILE	C-N-CA	5.09	134.43	121.70
8	T	89	HIS	CA-C-O	5.09	130.78	120.10
4	H	76	PHE	N-CA-C	-5.08	97.27	111.00
1	B	362	ARG	N-CA-C	-5.08	97.28	111.00
1	A	88	VAL	N-CA-C	-5.08	97.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	453	LEU	C-N-CA	5.07	134.38	121.70
3	G	92	GLU	C-N-CA	5.07	134.38	121.70
2	D	331	ALA	N-CA-C	-5.06	97.33	111.00
1	A	269	ASP	N-CA-C	-5.06	97.33	111.00
4	H	82	VAL	N-CA-C	-5.06	97.34	111.00
1	B	264	ALA	N-CA-C	-5.05	97.36	111.00
1	B	290	GLY	N-CA-C	-5.05	100.48	113.10
1	B	224	ASP	CA-C-N	-5.04	106.11	117.20
2	E	331	ALA	N-CA-C	-5.04	97.40	111.00
1	B	170	ASP	C-N-CA	5.03	134.28	121.70
2	D	21	VAL	N-CA-C	-5.03	97.41	111.00
9	U	78	VAL	CA-C-N	5.03	131.18	117.10
2	E	304	ILE	N-CA-C	-5.02	97.44	111.00
8	T	109	GLU	CA-C-N	-5.02	106.16	117.20

There are no chirality outliers.

All (89) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	ALA	Mainchain,Peptide
1	A	485	THR	Mainchain
1	B	46	ASN	Mainchain
1	C	173	THR	Mainchain
1	C	336	ALA	Peptide
1	C	509	GLU	Peptide
2	D	158	ALA	Peptide
2	D	205	VAL	Peptide
2	D	209	LYS	Mainchain
2	D	25	PHE	Mainchain,Peptide
2	F	284	THR	Mainchain
3	G	156	ASP	Mainchain,Peptide
7	S	106	SER	Mainchain
7	S	13	GLY	Mainchain,Peptide
7	S	142	LEU	Peptide
7	S	151	GLU	Peptide
7	S	152	VAL	Peptide
7	S	156	PRO	Peptide
7	S	157	SER	Mainchain
7	S	49	PRO	Mainchain
7	S	69	LEU	Mainchain,Peptide
8	T	104	GLU	Mainchain
8	T	117	GLU	Mainchain

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Mol	Chain	Res	Type	Group
8	T	136	GLU	Mainchain
8	T	148	VAL	Mainchain,Peptide
8	T	155	GLN	Mainchain
8	T	156	GLN	Mainchain
8	T	160	THR	Mainchain
8	T	162	ALA	Mainchain,Peptide
8	T	166	ALA	Mainchain
8	T	172	SER	Peptide
8	T	173	LYS	Peptide
8	T	21	THR	Mainchain
8	T	23	GLU	Mainchain
8	T	25	PHE	Mainchain
8	T	51	LYS	Mainchain
8	T	88	ARG	Mainchain
8	T	90	TYR	Mainchain
8	T	91	LEU	Mainchain
8	T	92	PHE	Mainchain
8	T	93	ASP	Mainchain
9	U	104	LEU	Peptide
9	U	112	GLN	Mainchain
9	U	115	GLU	Mainchain
9	U	122	ARG	Mainchain
9	U	123	ASN	Mainchain
9	U	13	VAL	Mainchain
9	U	16	GLY	Peptide
9	U	17	GLU	Mainchain
9	U	19	ILE	Peptide
9	U	3	ARG	Peptide
9	U	50	ALA	Mainchain
9	U	6	ALA	Peptide
9	U	78	VAL	Mainchain
9	U	79	PRO	Mainchain
9	U	81	PRO	Mainchain,Peptide
9	U	88	GLN	Mainchain
9	U	92	GLU	Mainchain
9	U	96	ASP	Mainchain
10	V	22	SER	Peptide
10	V	23	GLY	Peptide
10	V	3	PRO	Mainchain
10	V	4	VAL	Mainchain
10	V	42	LYS	Mainchain
10	V	57	ASN	Mainchain

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Mol	Chain	Res	Type	Group
11	W	10	ILE	Mainchain
11	W	122	LYS	Mainchain
11	W	142	VAL	Mainchain
11	W	148	SER	Mainchain
11	W	16	GLY	Mainchain
11	W	163	ASN	Mainchain
11	W	175	GLY	Mainchain
11	W	176	GLY	Mainchain
11	W	219	SER	Mainchain
11	W	220	LEU	Mainchain
11	W	35	ASN	Peptide
11	W	47	GLN	Mainchain
11	W	63	SER	Mainchain
11	W	86	GLY	Mainchain
11	W	90	HIS	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	5	0
1	B	1918	0	553	7	0
1	C	1947	0	563	7	0
2	D	1867	0	533	4	0
2	E	1863	0	532	4	0
2	F	1863	0	532	8	0
3	G	1053	0	283	0	0
4	H	523	0	140	1	0
5	I	187	0	53	1	0
6	J	288	0	92	0	0
6	K	288	0	92	0	0
6	L	288	0	92	0	0
6	M	288	0	92	0	0
6	N	288	0	92	0	0
6	O	288	0	92	0	0
6	P	288	0	92	0	0
6	Q	288	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	669	0	178	8	0
8	T	697	0	182	1	0
9	U	485	0	118	0	0
10	V	264	0	71	0	0
11	W	869	0	226	4	0
All	All	18544	0	5289	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:88:LEU:CA	11:W:88:LEU:N	1.88	1.36
7:S:164:VAL:CA	7:S:167:GLY:O	2.28	0.80
2:F:84:ILE:H	2:F:114:ALA:H	1.42	0.68
1:B:49:ALA:H	2:F:69:LEU:H	1.43	0.67
1:A:49:ALA:H	2:E:69:LEU:N	2.00	0.59
2:E:84:ILE:H	2:E:114:ALA:H	1.52	0.58
1:B:173:THR:H	1:B:175:LYS:H	1.53	0.57
7:S:114:GLY:HA2	7:S:127:ASP:H	1.74	0.52
2:D:350:PRO:C	2:D:352:ASP:H	2.13	0.52
7:S:108:MET:CA	7:S:111:VAL:H	2.23	0.51
1:A:260:ASN:C	1:A:262:LYS:H	2.15	0.50
7:S:163:ILE:O	7:S:167:GLY:O	2.30	0.49
1:C:49:ALA:H	2:D:69:LEU:N	2.10	0.49
2:D:473:LEU:C	2:D:475:GLU:H	2.17	0.49
1:A:49:ALA:H	2:E:69:LEU:H	1.62	0.47
1:C:290:GLY:H	1:C:295:PRO:N	2.13	0.46
1:B:290:GLY:HA3	2:F:279:VAL:O	2.15	0.46
7:S:114:GLY:CA	7:S:127:ASP:H	2.28	0.46
7:S:65:LYS:C	7:S:67:LYS:H	2.18	0.46
7:S:139:LYS:C	7:S:141:PHE:H	2.19	0.46
7:S:164:VAL:C	7:S:167:GLY:O	2.53	0.46
2:F:368:TYR:O	2:F:372:ARG:N	2.49	0.45
1:B:258:ARG:O	1:B:319:GLY:HA3	2.16	0.45
1:B:173:THR:N	1:B:175:LYS:H	2.13	0.45
8:T:15:LYS:CA	11:W:90:HIS:C	2.86	0.44
1:B:49:ALA:N	2:F:69:LEU:H	2.11	0.43
1:C:26:GLU:C	1:C:28:THR:H	2.22	0.43
4:H:87:ASP:C	4:H:89:SER:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:6:GLN:C	5:I:8:GLY:H	2.21	0.43
1:C:260:ASN:C	1:C:262:LYS:H	2.23	0.43
1:A:261:GLY:O	1:A:319:GLY:HA2	2.19	0.42
1:C:475:GLN:C	1:C:477:GLN:H	2.23	0.42
11:W:88:LEU:O	11:W:90:HIS:N	2.52	0.42
2:D:133:LEU:N	2:D:146:TYR:O	2.52	0.42
1:B:26:GLU:C	1:B:46:ASN:H	2.24	0.41
2:F:159:GLY:C	2:F:161:GLY:H	2.23	0.41
1:C:292:GLU:C	1:C:294:TYR:H	2.23	0.41
1:C:172:GLN:C	1:C:174:GLY:H	2.23	0.41
2:F:210:ASP:C	2:F:212:THR:H	2.23	0.41
2:E:277:SER:N	2:E:281:TYR:O	2.55	0.40
11:W:152:GLN:O	11:W:156:LEU:N	2.50	0.40
1:A:258:ARG:O	1:A:319:GLY:HA3	2.22	0.40
2:F:208:LEU:C	2:F:210:ASP:H	2.24	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%)	445 (88%)	35 (7%)	27 (5%)	2 29
1	B	476/510 (93%)	423 (89%)	30 (6%)	23 (5%)	3 32
1	C	485/510 (95%)	434 (90%)	28 (6%)	23 (5%)	3 32
2	D	465/482 (96%)	415 (89%)	30 (6%)	20 (4%)	3 34
2	E	464/482 (96%)	418 (90%)	34 (7%)	12 (3%)	7 45
2	F	464/482 (96%)	412 (89%)	32 (7%)	20 (4%)	3 34
3	G	258/273 (94%)	195 (76%)	43 (17%)	20 (8%)	1 20
4	H	129/146 (88%)	114 (88%)	10 (8%)	5 (4%)	4 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	I	45/50 (90%)	35 (78%)	7 (16%)	3 (7%)	1 24
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	6 43
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14 58
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100 100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	6 43
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100 100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14 58
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14 58
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	6 43
7	S	166/190 (87%)	110 (66%)	30 (18%)	26 (16%)	0 5
8	T	172/174 (99%)	154 (90%)	14 (8%)	4 (2%)	8 48
9	U	120/124 (97%)	95 (79%)	16 (13%)	9 (8%)	1 21
10	V	64/77 (83%)	51 (80%)	9 (14%)	4 (6%)	2 25
11	W	215/217 (99%)	192 (89%)	19 (9%)	4 (2%)	10 52
All	All	4590/4803 (96%)	3990 (87%)	391 (8%)	209 (5%)	5 32

All (209) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	13	GLU
1	A	14	GLU
1	A	20	ASP
1	A	24	ASP
1	A	80	LYS
1	A	82	ILE
1	A	171	ARG
1	A	224	ASP
1	A	238	ASP
1	A	289	PRO
1	A	334	VAL
1	A	374	VAL
1	B	45	ARG
1	B	57	SER
1	B	143	ARG
1	B	171	ARG
1	B	172	GLN

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Mol	Chain	Res	Type
1	B	238	ASP
1	B	361	ILE
1	C	26	GLU
1	C	171	ARG
1	C	195	GLU
1	C	237	SER
1	C	238	ASP
1	C	361	ILE
2	D	214	LYS
2	D	277	SER
2	D	350	PRO
2	D	352	ASP
2	D	353	SER
2	D	394	ASP
2	E	392	GLY
2	F	67	GLU
2	F	249	GLN
2	F	277	SER
2	F	299	THR
2	F	361	ASN
2	F	450	ASP
2	F	451	HIS
3	G	9	ARG
3	G	93	ALA
3	G	112	ILE
3	G	116	LEU
3	G	151	SER
3	G	196	ILE
3	G	197	ASP
3	G	199	ASP
3	G	250	PHE
4	H	69	ASP
4	H	101	ASP
5	I	9	LEU
7	S	9	VAL
7	S	47	LYS
7	S	79	SER
7	S	106	SER
7	S	112	HIS
7	S	116	VAL
7	S	127	ASP
7	S	129	THR

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Mol	Chain	Res	Type
7	S	143	SER
7	S	146	GLN
7	S	152	VAL
7	S	153	LYS
7	S	159	MET
9	U	4	LYS
9	U	18	ILE
9	U	19	ILE
9	U	100	CYS
10	V	3	PRO
10	V	26	VAL
10	V	63	PRO
1	A	6	ALA
1	A	235	THR
1	A	295	PRO
1	A	336	ALA
1	B	27	GLU
1	B	36	ASP
1	B	48	GLN
1	B	378	ALA
1	C	143	ARG
1	C	172	GLN
1	C	194	ASP
1	C	224	ASP
1	C	235	THR
1	C	455	LYS
1	C	456	LEU
2	D	67	GLU
2	D	158	ALA
2	D	221	GLN
2	D	348	VAL
2	D	396	LEU
2	D	453	PRO
2	E	132	ILE
2	E	299	THR
2	E	394	ASP
2	F	64	ASP
2	F	177	HIS
2	F	281	TYR
2	F	397	SER
2	F	427	HIS
3	G	79	GLY

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Mol	Chain	Res	Type
3	G	87	LYS
3	G	134	ARG
3	G	200	VAL
4	H	68	GLU
5	I	26	LEU
5	I	40	SER
7	S	121	THR
7	S	144	LYS
8	T	155	GLN
8	T	163	LYS
9	U	104	LEU
9	U	114	TYR
1	A	21	THR
1	A	95	VAL
1	A	123	SER
1	A	407	GLY
1	B	47	VAL
1	B	95	VAL
1	B	121	ILE
1	B	289	PRO
1	B	375	GLY
1	B	505	LEU
1	C	365	ILE
1	C	405	GLN
1	C	407	GLY
2	D	30	PRO
2	D	112	GLN
2	D	212	THR
2	E	64	ASP
2	E	276	PRO
2	E	301	LYS
2	E	396	LEU
2	F	110	THR
2	F	221	GLN
3	G	50	ALA
3	G	92	GLU
3	G	117	HIS
3	G	257	VAL
4	H	39	PRO
6	J	45	GLN
7	S	70	SER
7	S	92	ASN

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Mol	Chain	Res	Type
7	S	126	LEU
7	S	132	THR
8	T	147	ARG
9	U	101	ALA
11	W	40	ASN
1	A	11	ILE
1	A	79	ASP
1	A	124	LYS
1	A	146	MET
1	A	409	ASP
1	B	365	ILE
1	C	453	LEU
2	D	282	GLN
2	D	346	PRO
2	E	73	GLN
2	E	156	GLY
3	G	102	GLU
4	H	49	ALA
6	P	40	PRO
6	Q	44	GLN
7	S	72	MET
7	S	151	GLU
10	V	24	GLY
11	W	36	ARG
11	W	92	PHE
1	B	37	GLY
1	B	235	THR
1	B	295	PRO
1	C	163	GLN
1	C	433	TYR
2	D	474	ALA
2	F	297	THR
6	O	39	ASN
7	S	61	LYS
7	S	140	SER
1	C	374	VAL
1	C	411	ASP
2	F	107	PRO
3	G	131	VAL
3	G	258	ILE
7	S	68	SER
9	U	123	ASN

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Mol	Chain	Res	Type
11	W	222	LEU
1	C	95	VAL
2	D	279	VAL
2	E	279	VAL
2	F	279	VAL
2	F	362	ILE
2	F	429	GLY
6	M	40	PRO
7	S	80	PRO
1	B	82	ILE
1	C	451	GLY
9	U	20	PRO
1	A	145	PRO
1	B	261	GLY
2	D	160	VAL
2	F	128	VAL
6	J	40	PRO
6	M	71	ILE
7	S	66	VAL
8	T	152	ILE
2	E	101	PRO
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

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.