



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 9, 2019 – 03:03 AM EST

PDB ID : 6RDB
EMDB ID: : EMD-4812
Title : CryoEM structure of Polytomella F-ATP synthase, Primary rotary state 1, focussed refinement of F1 head and rotor
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 2.80 Å(reported)

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

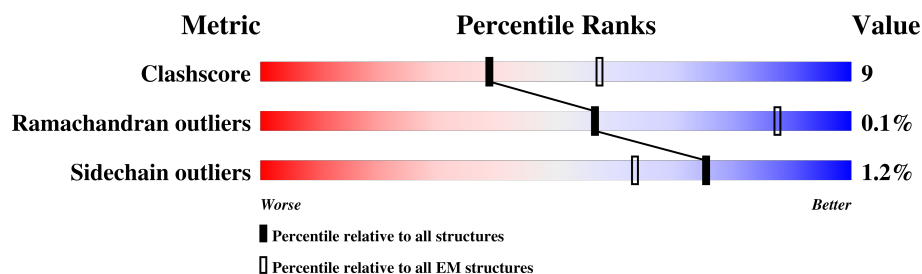
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	127	45% 13% 42%
1	B	127	48% 10% 42%
1	C	127	46% 13% 42%
1	D	127	50% 9% 42%
1	E	127	46% 12% 42%
1	F	127	42% 17% 42%
1	G	127	46% 12% 42%
1	H	127	49% 9% 42%
1	I	127	47% 11% 42%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	127	 47%11%42%
2	P	229	 42%7%51%
3	Q	74	 82%15%.
4	R	199	 80%9%11%
5	S	317	 74%14%13%
6	T	562	 68%17%.14%
6	U	562	 76%16%.7%
6	V	562	 75%16%.7%
7	X	574	 75%18%.6%
7	Y	574	 72%19%.9%
7	Z	574	 80%13%6%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 33961 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 Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 2 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	113	Total	C	N	O	S	0	0
			886	570	145	170	1		

- Molecule 3 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 4 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 5 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

- Molecule 6 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	483	Total	C	N	O	S	0	0
			3649	2322	647	669	11		
6	U	523	Total	C	N	O	S	0	0
			3980	2537	703	729	11		
6	V	520	Total	C	N	O	S	0	0
			3961	2527	700	723	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 7 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	542	Total	C	N	O	S	0	0
			4115	2586	696	820	13		
7	Y	521	Total	C	N	O	S	0	0
			3957	2485	670	789	13		
7	Z	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		

There are 6 discrepancies between the modelled and reference sequences:

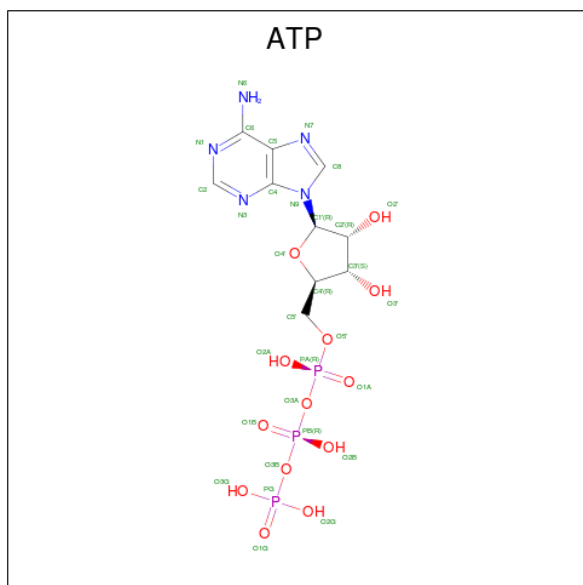
Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
8	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

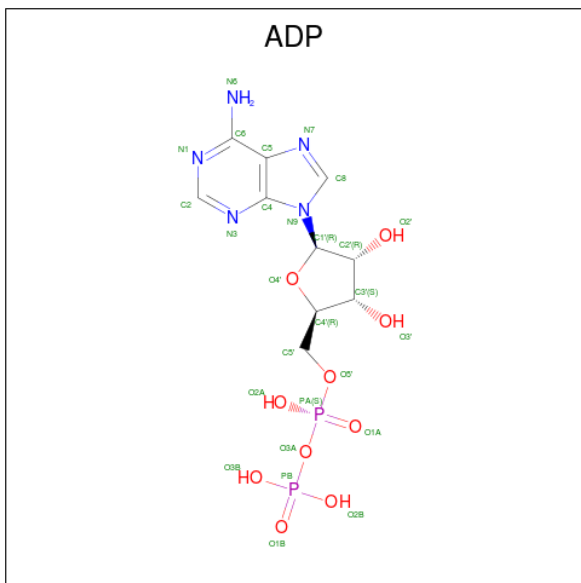
Mol	Chain	Residues	Atoms		AltConf
9	X	1	Total	Mg	0
			1	1	
9	Y	1	Total	Mg	0
			1	1	
9	T	1	Total	Mg	0
			1	1	
9	V	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	U	1	Total Mg 1 1	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
10	X	1	Total 27	C 10	N 5	O 10	P 2	0
10	Y	1	Total 27	C 10	N 5	O 10	P 2	0

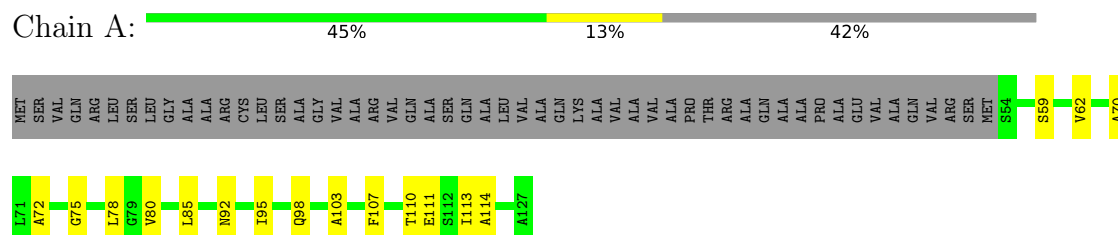
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	AltConf
11	T	7	Total O 7 7	0
11	U	9	Total O 9 9	0
11	V	7	Total O 7 7	0
11	X	9	Total O 9 9	0
11	Y	6	Total O 6 6	0
11	Z	2	Total O 2 2	0

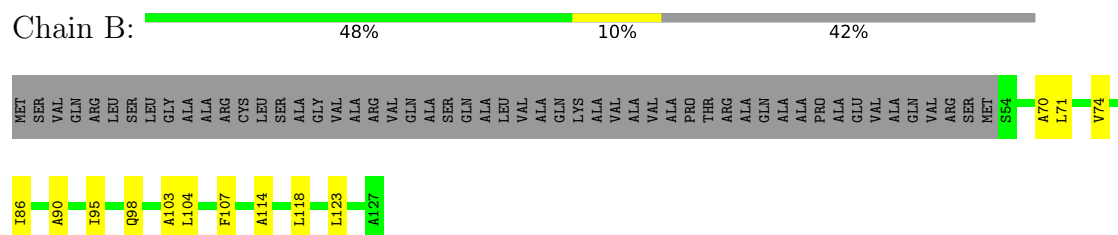
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

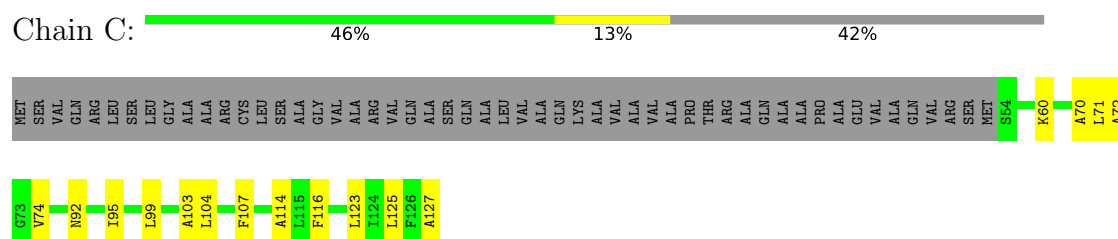
- Molecule 1: Mitochondrial ATP synthase subunit c



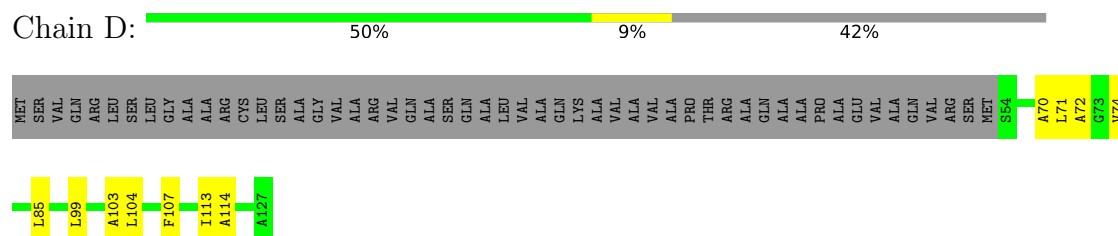
- Molecule 1: Mitochondrial ATP synthase subunit c



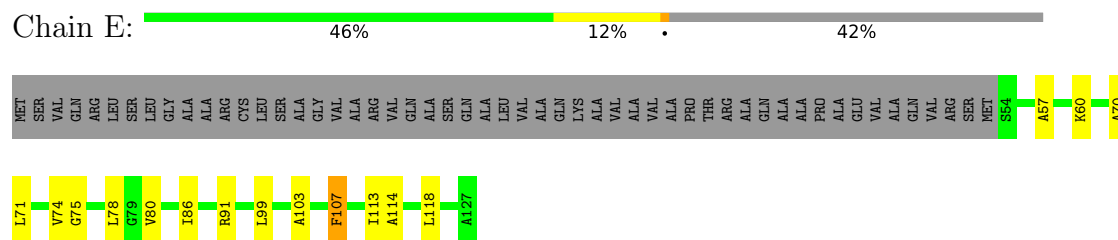
- Molecule 1: Mitochondrial ATP synthase subunit c



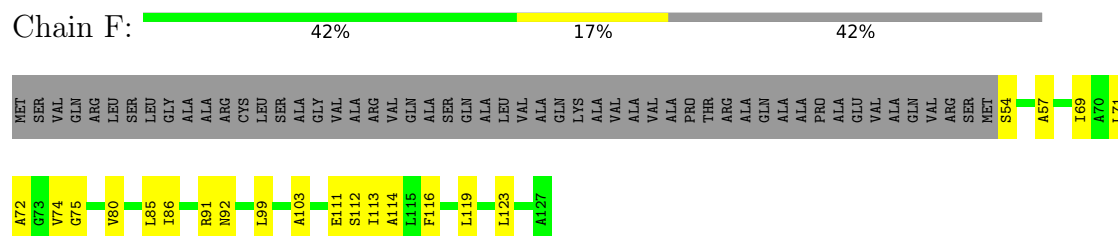
- Molecule 1: Mitochondrial ATP synthase subunit c



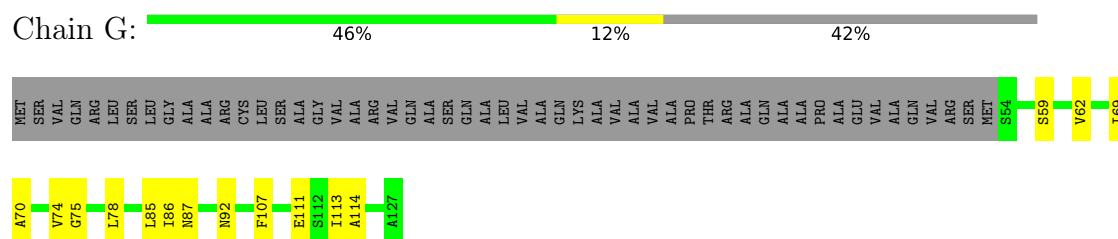
- Molecule 1: Mitochondrial ATP synthase subunit c



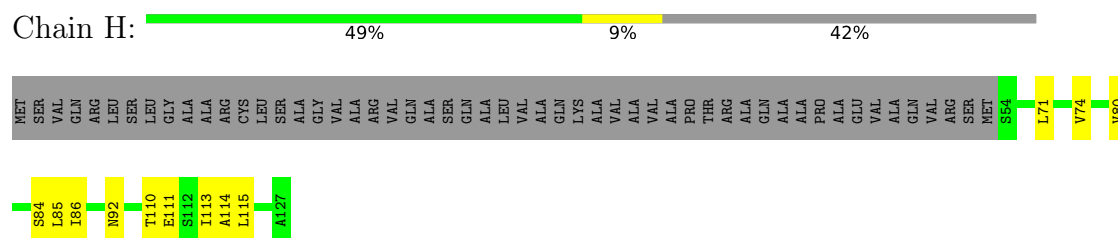
- Molecule 1: Mitochondrial ATP synthase subunit c



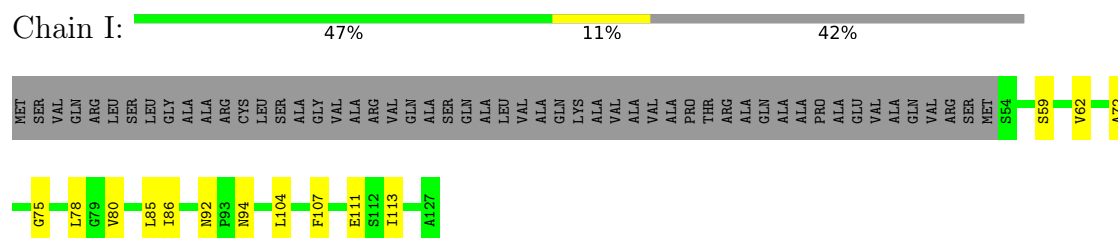
- Molecule 1: Mitochondrial ATP synthase subunit c



- Molecule 1: Mitochondrial ATP synthase subunit c

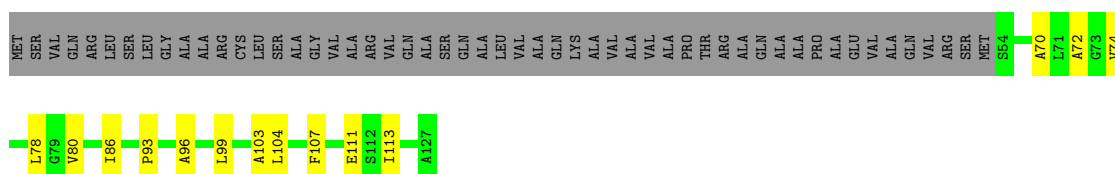


- Molecule 1: Mitochondrial ATP synthase subunit c

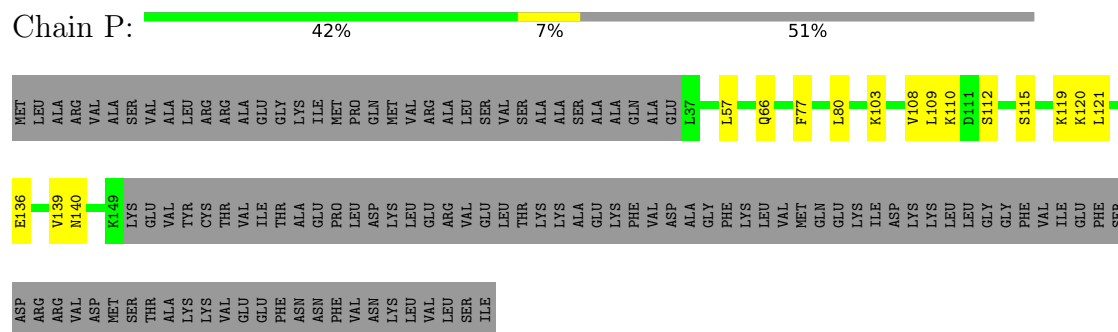


- Molecule 1: Mitochondrial ATP synthase subunit c

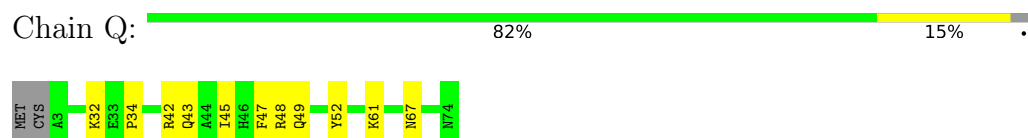




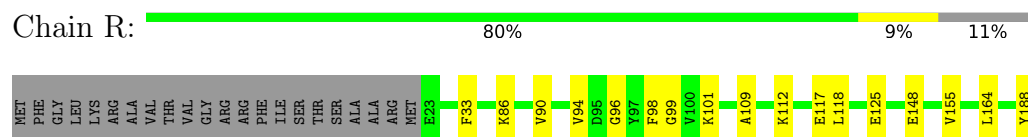
- Molecule 2: Mitochondrial ATP synthase subunit OSCP



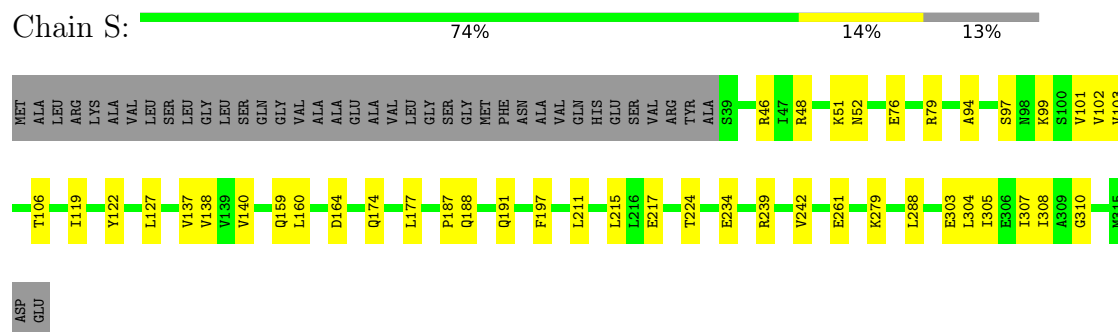
- Molecule 3: epsilon: *Polytomella* F-ATP synthase epsilon subunit



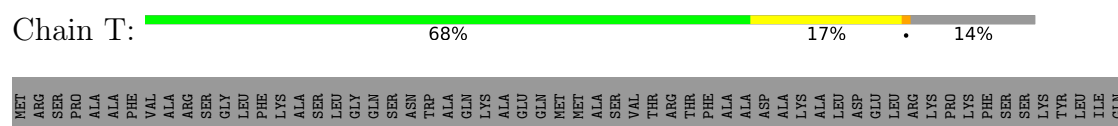
- Molecule 4: Mitochondrial ATP synthase subunit delta

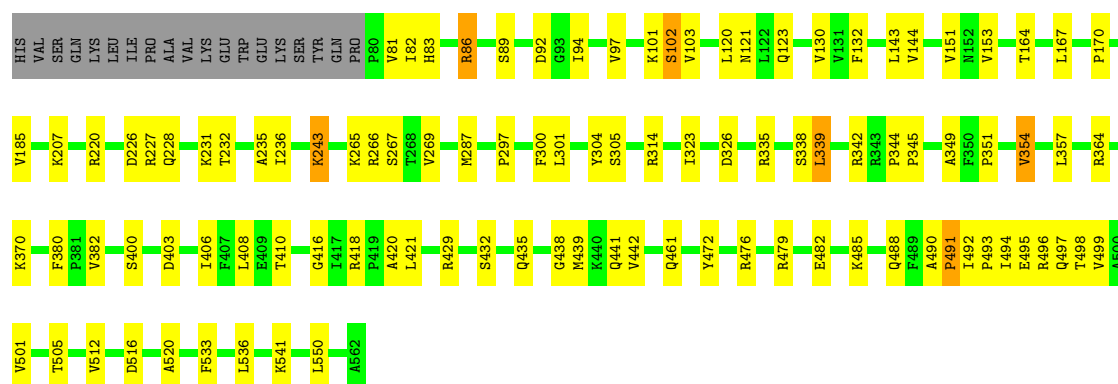


- Molecule 5: ATP synthase gamma chain, mitochondrial



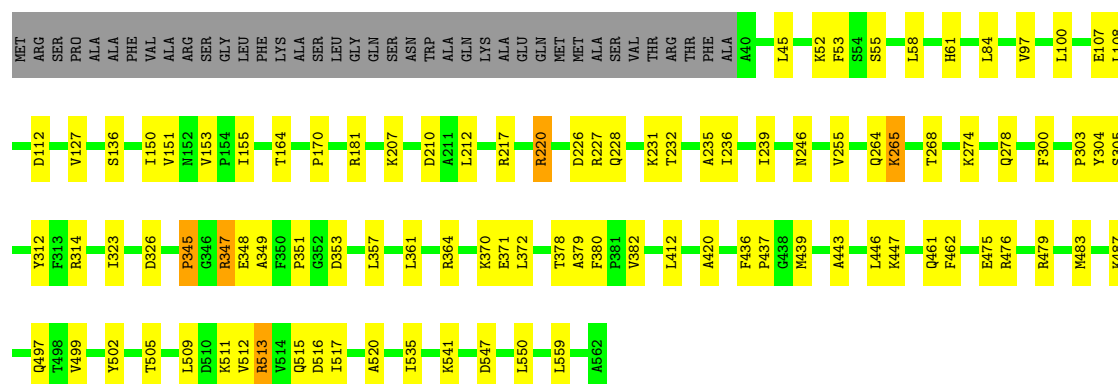
- Molecule 6: ATP synthase subunit alpha





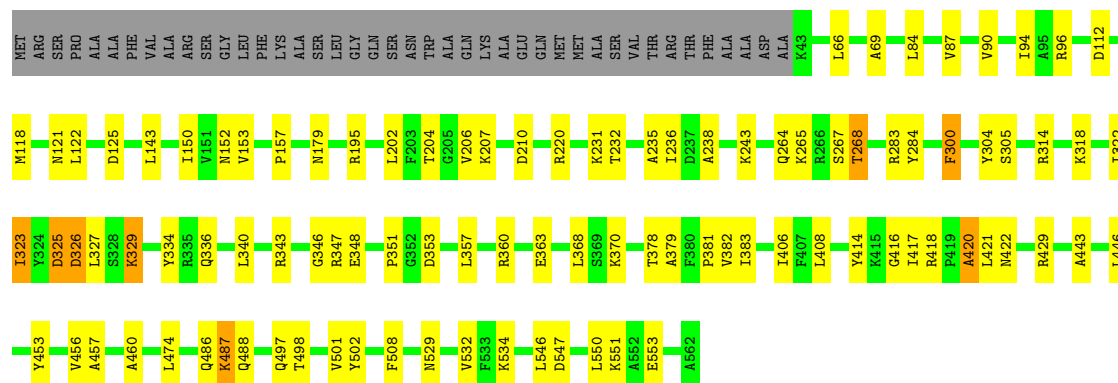
• Molecule 6: ATP synthase subunit alpha

Chain U: 76% 16% • 7%



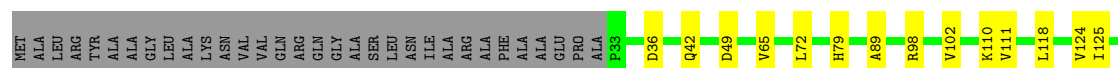
• Molecule 6: ATP synthase subunit alpha

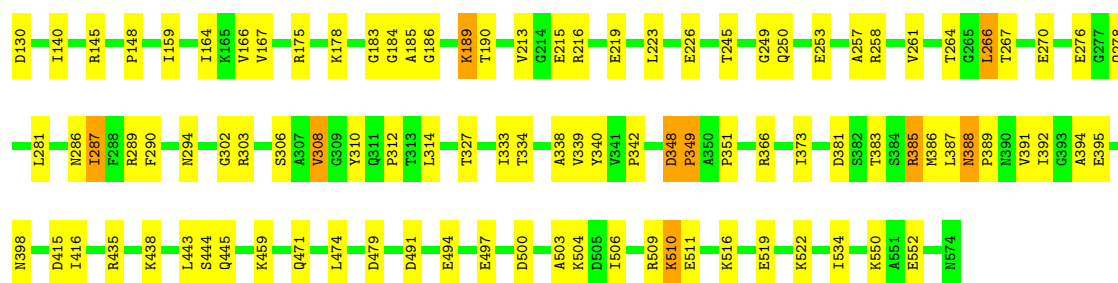
Chain V: 75% 16% • 7%



• Molecule 7: ATP synthase subunit beta

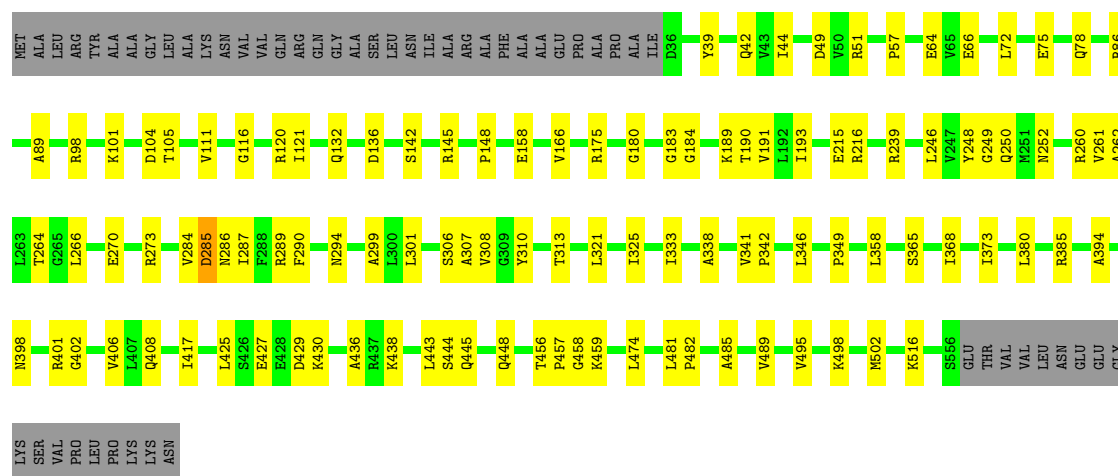
Chain X: 75% 18% • 6%





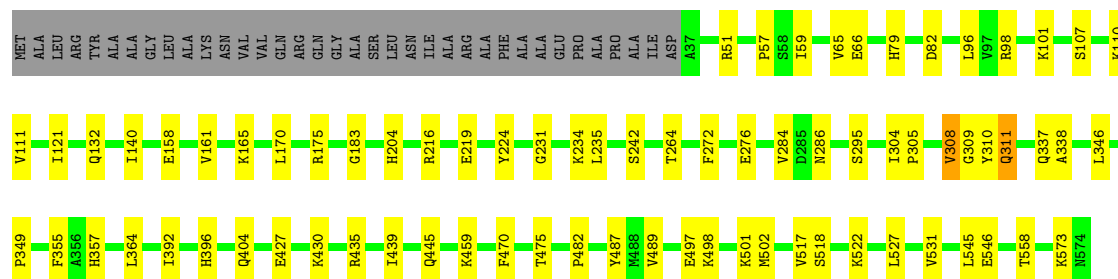
• Molecule 7: ATP synthase subunit beta

Chain Y: 72% 19% 9%



• Molecule 7: ATP synthase subunit beta

Chain Z: 80% 13% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	400918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	0.31	0/520	0.50	0/704
1	B	0.30	0/520	0.57	1/704 (0.1%)
1	C	0.30	0/519	0.57	1/701 (0.1%)
1	D	0.28	0/520	0.57	0/704
1	E	0.29	0/520	0.60	0/704
1	F	0.29	0/520	0.59	0/704
1	G	0.31	0/520	0.56	0/704
1	H	0.30	0/520	0.64	0/704
1	I	0.30	0/520	0.55	0/704
1	J	0.31	0/520	0.56	0/704
2	P	0.34	0/899	0.53	0/1218
3	Q	0.31	0/574	0.51	0/774
4	R	0.34	0/1336	0.52	0/1827
5	S	0.35	0/2153	0.55	0/2901
6	T	0.46	0/3709	0.59	2/5023 (0.0%)
6	U	0.44	0/4048	0.58	0/5477
6	V	0.42	0/4030	0.56	0/5456
7	X	0.48	2/4176 (0.0%)	0.59	3/5659 (0.1%)
7	Y	0.41	0/4015	0.55	0/5440
7	Z	0.39	0/4147	0.55	0/5619
All	All	0.40	2/34286 (0.0%)	0.57	7/46431 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	349	PRO	N-CA	12.98	1.69	1.47
7	X	348	ASP	C-N	5.79	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	36	ASP	CB-CG-OD1	9.50	126.85	118.30
7	X	349	PRO	CA-N-CD	-8.42	99.71	111.50
6	T	167	LEU	CA-CB-CG	7.83	133.32	115.30
1	C	95	ILE	CG1-CB-CG2	-5.82	98.60	111.40
1	B	123	LEU	CA-CB-CG	5.53	128.02	115.30
7	X	266	LEU	CA-CB-CG	5.18	127.22	115.30
6	T	550	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

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	514	0	554	13	0
1	B	514	0	554	10	0
1	C	514	0	553	12	0
1	D	514	0	554	8	0
1	E	514	0	554	14	0
1	F	514	0	554	20	0
1	G	514	0	554	15	0
1	H	514	0	554	12	0
1	I	514	0	554	13	0
1	J	514	0	554	14	0
2	P	886	0	921	13	0
3	Q	561	0	565	8	0
4	R	1303	0	1266	13	0
5	S	2130	0	2180	45	0
6	T	3649	0	3777	94	0
6	U	3980	0	4120	74	0
6	V	3961	0	4104	87	0
7	X	4115	0	4137	97	0
7	Y	3957	0	3967	84	0
7	Z	4087	0	4110	56	0
8	T	31	0	12	6	0
8	U	31	0	12	1	0
8	V	31	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	T	1	0	0	0	0
9	U	1	0	0	0	0
9	V	1	0	0	0	0
9	X	1	0	0	1	0
9	Y	1	0	0	0	0
10	X	27	0	12	3	0
10	Y	27	0	12	5	0
11	T	7	0	0	0	0
11	U	9	0	0	1	0
11	V	7	0	0	0	0
11	X	9	0	0	6	0
11	Y	6	0	0	1	0
11	Z	2	0	0	0	0
All	All	33961	0	34746	591	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 9.

All (591) 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)
7:X:349:PRO:CA	7:X:349:PRO:N	1.69	1.43
5:S:305:ILE:CD1	6:U:345:PRO:HB2	1.67	1.24
7:X:215:GLU:OE2	11:X:701:HOH:O	1.60	1.14
7:X:183:GLY:HA3	7:X:189:LYS:HD3	1.29	1.13
6:V:265:LYS:HG3	6:V:268:THR:HG22	1.21	1.10
9:X:602:MG:MG	11:X:703:HOH:O	0.35	1.09
6:U:347:ARG:NH2	7:X:348:ASP:OD2	1.85	1.07
7:X:310:TYR:CE2	7:X:349:PRO:HG2	1.93	1.03
7:X:286:ASN:OD1	11:X:702:HOH:O	1.74	1.02
5:S:305:ILE:HD11	6:U:345:PRO:HB2	1.37	1.02
6:V:406:ILE:HG23	6:V:421:LEU:CD2	1.90	1.01
7:X:503:ALA:O	7:X:506:ILE:HG12	1.61	1.00
6:V:265:LYS:HG3	6:V:268:THR:CG2	1.95	0.97
7:Z:295:SER:HA	7:Z:311:GLN:HG2	1.48	0.95
7:X:190:THR:OG1	11:X:703:HOH:O	1.84	0.94
6:T:207:LYS:HB3	6:T:497:GLN:HE21	1.33	0.92
6:V:406:ILE:HG23	6:V:421:LEU:HD21	1.49	0.92
6:T:227:ARG:O	8:T:1001:ATP:O2G	1.87	0.91
7:X:388:ASN:ND2	7:X:389:PRO:HD2	1.84	0.91
7:X:183:GLY:CA	7:X:189:LYS:HD3	2.00	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:207:LYS:HA	6:T:497:GLN:NE2	1.88	0.88
6:V:265:LYS:CG	6:V:268:THR:HG22	2.02	0.88
6:T:207:LYS:CB	6:T:497:GLN:HE21	1.87	0.87
7:X:215:GLU:OE1	7:X:286:ASN:OD1	1.94	0.86
6:T:228:GLN:OE1	7:X:383:THR:HG21	1.76	0.85
7:X:310:TYR:CD2	7:X:349:PRO:HG2	2.11	0.85
6:V:336:GLN:NE2	7:Y:313:THR:HG22	1.91	0.84
7:Y:183:GLY:O	7:Y:189:LYS:HE2	1.78	0.83
6:V:327:LEU:HD22	6:V:381:PRO:HB3	1.62	0.82
6:T:207:LYS:HB3	6:T:497:GLN:NE2	1.94	0.81
6:V:207:LYS:H	6:V:486:GLN:HE22	1.26	0.81
6:V:231:LYS:HD2	6:V:382:VAL:HG13	1.61	0.81
7:X:183:GLY:HA3	7:X:189:LYS:CD	2.10	0.81
6:T:92:ASP:OD2	7:X:303:ARG:NH2	2.13	0.80
6:V:326:ASP:HB3	6:V:329:LYS:HB2	1.63	0.80
7:X:388:ASN:HD22	7:X:389:PRO:HD2	1.46	0.80
5:S:305:ILE:CG1	6:U:345:PRO:HB2	2.12	0.79
7:Z:295:SER:HA	7:Z:311:GLN:CG	2.12	0.79
6:V:334:TYR:CE2	6:V:351:PRO:HG2	2.18	0.78
6:U:265:LYS:NZ	7:Z:357:HIS:O	2.16	0.78
6:T:86:ARG:HG2	6:T:86:ARG:HH21	1.48	0.78
6:U:345:PRO:HB3	6:U:349:ALA:HA	1.66	0.77
6:V:121:ASN:ND2	6:V:343:ARG:HH11	1.82	0.77
6:T:207:LYS:HA	6:T:497:GLN:HE22	1.48	0.77
6:T:269:VAL:HG13	6:T:287:MET:CE	2.14	0.77
6:T:498:THR:CG2	6:T:536:LEU:HD21	2.15	0.77
6:T:207:LYS:CA	6:T:497:GLN:NE2	2.49	0.75
6:T:335:ARG:HD2	6:T:349:ALA:O	1.85	0.75
6:T:269:VAL:HG13	6:T:287:MET:HE2	1.68	0.75
6:V:414:TYR:CZ	7:Y:380:LEU:O	2.39	0.75
7:Y:498:LYS:O	7:Y:502:MET:HG3	1.88	0.74
7:Y:191:VAL:HG11	10:Y:601:ADP:C5	2.24	0.73
6:T:416:GLY:O	6:T:485:LYS:HE3	1.88	0.73
6:V:232:THR:HG22	6:V:236:ILE:HG12	1.70	0.73
6:V:264:GLN:OE1	6:V:325:ASP:HB3	1.89	0.72
7:Y:191:VAL:HG11	10:Y:601:ADP:C6	2.24	0.72
6:V:231:LYS:HD2	6:V:382:VAL:CG1	2.19	0.72
6:V:327:LEU:HD22	6:V:381:PRO:CB	2.20	0.72
5:S:305:ILE:HD11	6:U:345:PRO:CB	2.18	0.72
5:S:305:ILE:HD13	6:U:345:PRO:HB2	1.67	0.72
7:Y:249:GLY:HA3	7:Y:261:VAL:HG21	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:228:GLN:NE2	8:T:1001:ATP:O3G	2.23	0.71
1:G:111:GLU:OE2	1:H:113:ILE:HD11	1.89	0.71
7:Y:456:THR:HG22	7:Y:457:PRO:HD2	1.71	0.71
7:Y:66:GLU:OE2	7:Y:101:LYS:HD3	1.90	0.71
6:U:231:LYS:HB2	8:U:1001:ATP:O1B	1.91	0.71
6:V:406:ILE:HG23	6:V:421:LEU:HD23	1.72	0.71
10:X:601:ADP:O2B	11:X:703:HOH:O	2.09	0.70
5:S:305:ILE:HG12	6:U:345:PRO:CG	2.20	0.70
6:T:335:ARG:CD	6:T:349:ALA:O	2.40	0.70
6:U:232:THR:HG22	6:U:236:ILE:HG12	1.73	0.69
6:V:406:ILE:CG2	6:V:421:LEU:CD2	2.70	0.69
6:T:207:LYS:CB	6:T:497:GLN:NE2	2.54	0.69
3:Q:32:LYS:HG3	3:Q:34:PRO:HD2	1.75	0.68
7:X:314:LEU:HD23	7:X:314:LEU:O	1.93	0.68
6:T:493:PRO:HD2	6:T:496:ARG:HG3	1.75	0.68
7:X:310:TYR:CD2	7:X:349:PRO:CG	2.78	0.67
6:T:499:VAL:HG21	6:T:533:PHE:HE1	1.58	0.67
6:T:498:THR:HG23	6:T:536:LEU:HD21	1.77	0.67
7:X:510:LYS:HD2	7:X:511:GLU:H	1.60	0.67
6:V:414:TYR:OH	7:Y:380:LEU:O	2.12	0.67
6:T:153:VAL:HG11	6:T:305:SER:HB2	1.77	0.66
1:E:75:GLY:HA3	1:F:74:VAL:HG12	1.76	0.66
7:Y:184:GLY:O	7:Y:189:LYS:HE3	1.95	0.66
7:Y:183:GLY:O	7:Y:189:LYS:CE	2.44	0.66
7:Y:308:VAL:HG21	7:Y:349:PRO:CD	2.26	0.65
6:V:207:LYS:H	6:V:486:GLN:NE2	1.92	0.65
7:X:388:ASN:HD22	7:X:389:PRO:CD	2.09	0.65
7:X:216:ARG:NH1	7:X:219:GLU:OE1	2.27	0.65
5:S:305:ILE:HG12	6:U:345:PRO:HG2	1.79	0.65
6:U:210:ASP:HB2	6:U:497:GLN:HE22	1.62	0.65
1:G:75:GLY:HA3	1:H:74:VAL:HG22	1.79	0.64
6:V:264:GLN:OE1	6:V:325:ASP:CB	2.45	0.64
7:X:186:GLY:N	10:X:601:ADP:O1B	2.30	0.64
7:Y:456:THR:CG2	7:Y:457:PRO:HD2	2.27	0.64
6:T:228:GLN:OE1	7:X:383:THR:CG2	2.46	0.64
6:T:488:GLN:OE1	8:T:1001:ATP:O2'	2.14	0.64
6:U:231:LYS:HD2	6:U:382:VAL:HG13	1.80	0.64
6:T:344:PRO:CG	7:Y:299:ALA:HB1	2.28	0.63
6:V:235:ALA:HB1	6:V:323:ILE:HG21	1.79	0.63
1:B:74:VAL:HG11	1:B:114:ALA:HB2	1.80	0.63
6:T:86:ARG:HH21	6:T:86:ARG:CG	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:281:LEU:HD23	7:X:334:THR:HB	1.80	0.63
1:I:75:GLY:HA3	1:J:74:VAL:HG12	1.81	0.62
7:X:185:ALA:HB2	7:X:340:TYR:HE1	1.62	0.62
4:R:86:LYS:HG3	4:R:118:LEU:HD12	1.80	0.62
5:S:305:ILE:HG12	6:U:345:PRO:HB2	1.80	0.62
6:T:344:PRO:HG2	7:Y:299:ALA:HB1	1.82	0.62
7:X:327:THR:HG22	7:X:333:ILE:H	1.63	0.62
6:V:121:ASN:HD21	6:V:343:ARG:HE	1.47	0.62
5:S:304:LEU:CD2	7:Z:309:GLY:HA2	2.30	0.62
6:T:86:ARG:HD3	6:T:143:LEU:HD23	1.82	0.61
6:U:227:ARG:HG2	6:U:228:GLN:HG2	1.81	0.61
7:Y:308:VAL:HG12	7:Y:308:VAL:O	2.01	0.61
6:T:400:SER:HB3	7:Y:289:ARG:HH22	1.65	0.61
7:X:373:ILE:HG23	7:X:444:SER:HB3	1.81	0.61
1:D:74:VAL:HG11	1:D:114:ALA:HB2	1.82	0.61
6:V:195:ARG:NH2	6:V:363:GLU:O	2.34	0.61
6:V:265:LYS:O	6:V:268:THR:HG23	2.01	0.60
1:G:74:VAL:HG11	1:G:114:ALA:HB2	1.82	0.60
6:V:406:ILE:CG2	6:V:421:LEU:HD23	2.32	0.60
7:X:308:VAL:O	7:X:308:VAL:HG12	2.01	0.60
6:V:508:PHE:HZ	6:V:551:LYS:HG3	1.67	0.59
6:V:488:GLN:NE2	8:V:1001:ATP:O2'	2.35	0.59
6:V:210:ASP:HB2	6:V:497:GLN:HE22	1.67	0.59
7:X:216:ARG:O	7:X:250:GLN:NE2	2.35	0.59
5:S:305:ILE:HG12	6:U:345:PRO:CB	2.32	0.59
7:X:500:ASP:O	7:X:504:LYS:HG3	2.02	0.59
6:U:207:LYS:NZ	6:U:483:MET:SD	2.74	0.59
6:U:303:PRO:HB2	6:U:361:LEU:HD11	1.84	0.59
7:Y:425:LEU:HB2	7:Y:430:LYS:HG3	1.83	0.59
5:S:308:ILE:HD11	7:Z:305:PRO:HG2	1.84	0.59
7:X:388:ASN:HB3	7:X:391:VAL:HG23	1.83	0.59
6:T:406:ILE:HG23	6:T:421:LEU:HD12	1.84	0.58
7:X:184:GLY:O	7:X:366:ARG:NH2	2.37	0.58
6:V:416:GLY:HA2	7:Y:401:ARG:HH12	1.68	0.58
6:V:265:LYS:CG	6:V:268:THR:CG2	2.70	0.58
6:T:499:VAL:HG21	6:T:533:PHE:CE1	2.38	0.58
6:U:513:ARG:HH11	6:U:515:GLN:HB2	1.68	0.58
7:X:387:LEU:HA	7:X:392:ILE:HD13	1.86	0.58
6:T:323:ILE:HG12	6:T:380:PHE:HB2	1.85	0.57
7:Y:438:LYS:NZ	7:Y:481:LEU:O	2.37	0.57
5:S:48:ARG:O	5:S:52:ASN:ND2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ILE:HG21	1:F:85:LEU:HA	1.86	0.57
5:S:46:ARG:NH1	7:X:415:ASP:OD1	2.38	0.57
7:Y:427:GLU:HA	7:Y:430:LYS:HB2	1.86	0.57
6:V:207:LYS:N	6:V:486:GLN:HE22	2.00	0.56
7:X:503:ALA:O	7:X:506:ILE:CG1	2.44	0.56
7:Z:310:TYR:CD2	7:Z:349:PRO:HG2	2.40	0.56
1:G:86:ILE:HG21	1:H:85:LEU:HA	1.88	0.56
6:T:441:GLN:HE22	6:T:541:LYS:HG3	1.70	0.56
7:X:249:GLY:HA3	7:X:261:VAL:HG11	1.86	0.56
5:S:102:VAL:HA	5:S:191:GLN:HB2	1.88	0.56
7:Z:286:ASN:H	7:Z:338:ALA:HB3	1.70	0.56
7:Z:158:GLU:OE2	7:Z:175:ARG:NH1	2.38	0.56
7:X:287:ILE:CG2	7:X:339:VAL:HG22	2.36	0.56
7:Y:425:LEU:HB3	7:Y:429:ASP:HB2	1.88	0.56
1:B:90:ALA:O	1:C:92:ASN:ND2	2.38	0.56
1:F:86:ILE:HG21	1:G:85:LEU:HA	1.88	0.55
1:I:104:LEU:HA	1:I:107:PHE:HB3	1.88	0.55
7:X:286:ASN:HB3	7:X:289:ARG:HG2	1.87	0.55
1:C:74:VAL:HG11	1:C:114:ALA:HB2	1.88	0.55
6:V:460:ALA:HB2	6:V:474:LEU:HD11	1.87	0.55
7:Y:290:PHE:O	7:Y:294:ASN:ND2	2.38	0.55
6:U:476:ARG:NH1	6:U:505:THR:O	2.40	0.55
7:X:42:GLN:HG2	7:X:49:ASP:HB2	1.88	0.55
1:A:72:ALA:HB2	1:B:70:ALA:HA	1.89	0.55
7:Y:417:ILE:HD11	7:Y:425:LEU:HD11	1.87	0.55
6:T:151:VAL:HG11	6:T:301:LEU:HD21	1.88	0.55
1:E:74:VAL:HG11	1:E:114:ALA:HB2	1.87	0.55
6:T:269:VAL:HG13	6:T:287:MET:HE1	1.86	0.55
7:X:124:VAL:HG13	7:X:125:ILE:HG23	1.88	0.55
6:T:335:ARG:HG3	6:T:349:ALA:O	2.07	0.55
6:V:357:LEU:HA	6:V:360:ARG:HH11	1.72	0.55
7:X:506:ILE:O	7:X:509:ARG:NH2	2.39	0.55
7:X:395:GLU:OE2	7:X:471:GLN:NE2	2.40	0.55
1:C:123:LEU:O	1:C:127:ALA:N	2.40	0.54
1:H:111:GLU:O	1:H:114:ALA:N	2.40	0.54
6:V:150:ILE:O	6:V:152:ASN:ND2	2.40	0.54
7:Z:231:GLY:O	7:Z:234:LYS:NZ	2.39	0.54
6:T:335:ARG:CG	6:T:349:ALA:O	2.56	0.54
6:T:354:VAL:O	6:T:357:LEU:HB3	2.07	0.54
6:U:351:PRO:HB2	6:U:353:ASP:OD1	2.08	0.54
7:X:253:GLU:O	7:X:258:ARG:NH1	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:385:ARG:NH1	11:Y:701:HOH:O	2.39	0.54
1:H:86:ILE:HG21	1:I:85:LEU:HA	1.89	0.54
5:S:138:VAL:HG13	5:S:159:GLN:HB2	1.90	0.54
7:Z:308:VAL:O	7:Z:308:VAL:HG12	2.08	0.54
6:V:202:LEU:HD22	6:V:378:THR:HG21	1.90	0.54
1:A:103:ALA:O	1:A:107:PHE:N	2.39	0.54
7:X:65:VAL:HG22	7:X:102:VAL:HG22	1.90	0.54
7:Z:132:GLN:HE22	7:Z:235:LEU:HD22	1.72	0.54
6:U:136:SER:HA	7:Z:59:ILE:HB	1.90	0.54
6:V:408:LEU:HA	6:V:420:ALA:O	2.08	0.54
7:X:314:LEU:C	7:X:314:LEU:HD23	2.28	0.54
1:A:85:LEU:HA	1:J:86:ILE:HG21	1.89	0.53
6:U:475:GLU:HG3	6:U:479:ARG:HH11	1.73	0.53
7:X:290:PHE:O	7:X:294:ASN:ND2	2.41	0.53
7:Y:166:VAL:HG23	7:Y:443:LEU:HD22	1.90	0.53
1:B:86:ILE:HG23	1:C:99:LEU:HB2	1.89	0.53
6:U:212:LEU:HA	6:U:447:LYS:HE2	1.90	0.53
6:T:266:ARG:NH1	7:X:148:PRO:O	2.41	0.53
6:T:123:GLN:HA	7:Y:42:GLN:HG3	1.89	0.53
6:T:231:LYS:HG2	6:T:408:LEU:HD12	1.90	0.53
6:T:439:MET:HE3	6:T:494:ILE:HD11	1.89	0.53
6:T:101:LYS:HA	7:Y:98:ARG:NH2	2.23	0.53
7:Y:286:ASN:H	7:Y:338:ALA:HB3	1.73	0.53
7:Z:183:GLY:HA2	7:Z:364:LEU:HB2	1.89	0.53
7:Z:518:SER:HB3	7:Z:522:LYS:HB2	1.90	0.53
7:X:276:GLU:HB3	7:X:278:GLN:HE21	1.73	0.53
6:U:479:ARG:NH2	6:U:512:VAL:O	2.30	0.53
7:Z:110:LYS:HB3	7:Z:140:ILE:HG22	1.89	0.53
6:U:226:ASP:O	6:U:231:LYS:NZ	2.41	0.52
2:P:136:GLU:O	2:P:140:ASN:ND2	2.40	0.52
5:S:304:LEU:HD21	7:Z:309:GLY:HA2	1.89	0.52
6:U:246:ASN:HD21	6:U:255:VAL:H	1.56	0.52
6:U:437:PRO:HB2	6:U:541:LYS:HB3	1.91	0.52
6:T:235:ALA:HB1	6:T:323:ILE:HD13	1.91	0.52
6:T:472:TYR:OH	6:T:476:ARG:NH1	2.43	0.52
6:U:231:LYS:HD2	6:U:382:VAL:CG1	2.39	0.52
6:V:529:ASN:HD21	7:Z:527:LEU:HD23	1.74	0.52
5:S:79:ARG:NH2	5:S:197:PHE:O	2.42	0.52
6:T:495:GLU:HG3	6:T:533:PHE:HB3	1.92	0.52
6:U:235:ALA:HB1	6:U:323:ILE:HG12	1.91	0.52
1:F:91:ARG:HE	4:R:98:PHE:HB3	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:283:ARG:NH2	6:V:284:TYR:OH	2.43	0.52
7:X:340:TYR:CE2	7:X:342:PRO:HA	2.45	0.52
7:Y:57:PRO:HB3	7:Y:104:ASP:OD2	2.10	0.52
4:R:33:PHE:HD2	5:S:94:ALA:HB2	1.74	0.52
6:T:408:LEU:HA	6:T:420:ALA:O	2.10	0.52
7:X:306:SER:HB2	7:X:312:PRO:HA	1.91	0.52
3:Q:49:GLN:HG2	3:Q:61:LYS:HB3	1.91	0.52
6:V:318:LYS:HE3	7:Z:545:LEU:HG	1.92	0.52
1:D:104:LEU:HA	1:D:107:PHE:HB3	1.91	0.52
1:E:118:LEU:HD11	1:F:116:PHE:HB3	1.93	0.51
3:Q:43:GLN:NE2	3:Q:67:ASN:O	2.44	0.51
6:T:479:ARG:NH1	6:T:512:VAL:O	2.44	0.51
5:S:76:GLU:HA	5:S:79:ARG:HD2	1.92	0.51
6:T:86:ARG:NH2	6:T:86:ARG:CG	2.73	0.51
6:U:58:LEU:HA	6:U:61:HIS:HB3	1.91	0.51
7:Y:266:LEU:HD11	7:Y:325:ILE:HG12	1.91	0.51
1:F:71:LEU:HA	1:F:74:VAL:HG22	1.92	0.51
1:F:72:ALA:HB2	1:G:70:ALA:HA	1.93	0.51
2:P:77:PHE:HZ	2:P:109:LEU:HD11	1.74	0.51
5:S:211:LEU:HB2	5:S:217:GLU:HB2	1.91	0.51
6:V:456:VAL:HG12	6:V:474:LEU:HD13	1.92	0.51
7:X:110:LYS:HB3	7:X:140:ILE:HG22	1.93	0.51
6:V:206:VAL:HA	6:V:486:GLN:HE22	1.76	0.51
1:A:59:SER:HA	1:A:62:VAL:HG12	1.93	0.51
1:C:60:LYS:HB3	1:C:125:LEU:HD23	1.92	0.51
6:U:499:VAL:HG13	6:U:550:LEU:HD21	1.93	0.51
8:T:1001:ATP:O2A	7:X:385:ARG:NH2	2.44	0.51
6:U:314:ARG:NH2	6:U:364:ARG:O	2.44	0.51
7:Y:158:GLU:HG3	7:Y:175:ARG:HB3	1.92	0.51
6:V:348:GLU:O	7:Y:307:ALA:HB2	2.10	0.51
1:D:72:ALA:HB2	1:E:70:ALA:HA	1.93	0.50
5:S:99:LYS:HB3	5:S:187:PRO:HA	1.93	0.50
1:F:91:ARG:O	4:R:99:GLY:N	2.38	0.50
6:V:429:ARG:NH2	7:Z:219:GLU:OE2	2.44	0.50
6:U:479:ARG:NH2	6:U:509:LEU:O	2.44	0.50
1:F:74:VAL:HG21	1:F:114:ALA:HB2	1.92	0.50
1:F:54:SER:HB3	1:F:57:ALA:HB3	1.93	0.50
6:T:403:ASP:O	6:T:429:ARG:NH2	2.37	0.50
7:X:189:LYS:N	10:X:601:ADP:O3B	2.36	0.50
6:T:488:GLN:NE2	8:T:1001:ATP:O2'	2.45	0.50
6:V:498:THR:HA	6:V:501:VAL:HG12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:SER:HB2	5:S:188:GLN:HB2	1.94	0.50
7:X:435:ARG:NH1	7:X:474:LEU:O	2.44	0.50
7:X:519:GLU:HB2	7:X:522:LYS:HE3	1.93	0.50
7:Z:170:LEU:HD22	7:Z:404:GLN:HG3	1.94	0.50
6:T:227:ARG:NH2	7:X:381:ASP:OD1	2.45	0.50
6:V:179:ASN:ND2	7:Z:546:GLU:OE2	2.44	0.50
1:D:71:LEU:HD12	1:E:113:ILE:HG23	1.93	0.50
7:Y:184:GLY:O	7:Y:189:LYS:CE	2.59	0.50
7:Z:439:ILE:HG23	7:Z:470:PHE:HE1	1.77	0.50
5:S:188:GLN:HG2	5:S:215:LEU:HB3	1.93	0.49
6:T:304:TYR:OH	6:T:357:LEU:O	2.25	0.49
6:T:314:ARG:NH1	6:T:364:ARG:O	2.45	0.49
6:U:108:LEU:HG	6:U:151:VAL:HA	1.95	0.49
6:V:353:ASP:OD1	6:V:353:ASP:N	2.40	0.49
6:T:265:LYS:HD2	7:X:178:LYS:HE3	1.94	0.49
7:Y:39:TYR:OH	7:Y:51:ARG:HD3	2.13	0.49
1:G:59:SER:HA	1:G:62:VAL:HG12	1.95	0.49
5:S:310:GLY:HA2	6:T:345:PRO:HD2	1.94	0.49
6:T:488:GLN:CD	8:T:1001:ATP:O2'	2.51	0.49
7:X:491:ASP:OD1	7:X:491:ASP:N	2.46	0.49
7:Y:406:VAL:HG12	7:Y:436:ALA:HB2	1.93	0.49
1:E:80:VAL:HG22	1:F:80:VAL:HG11	1.94	0.49
4:R:164:LEU:HD13	4:R:188:TYR:HB2	1.95	0.49
7:X:145:ARG:HH12	7:X:267:THR:HG23	1.76	0.49
6:T:92:ASP:CG	7:X:303:ARG:HH21	2.11	0.49
7:Y:189:LYS:HG3	10:Y:601:ADP:O1B	2.11	0.49
6:V:336:GLN:CD	7:Y:313:THR:HG22	2.32	0.49
5:S:239:ARG:HA	5:S:242:VAL:HG12	1.95	0.49
7:Z:482:PRO:HB2	7:Z:502:MET:HE1	1.93	0.49
1:C:72:ALA:HB2	1:D:70:ALA:HA	1.94	0.49
1:J:104:LEU:HA	1:J:107:PHE:HB3	1.94	0.49
6:V:314:ARG:HH21	6:V:368:LEU:HD21	1.78	0.49
6:V:532:VAL:HG21	6:V:550:LEU:HB3	1.93	0.49
7:X:213:VAL:HG22	7:X:261:VAL:HG13	1.94	0.49
6:U:232:THR:O	6:U:236:ILE:HG12	2.13	0.49
7:X:216:ARG:NH1	11:X:704:HOH:O	2.43	0.49
7:Z:51:ARG:NH2	7:Z:82:ASP:O	2.46	0.48
1:G:87:ASN:OD1	1:H:84:SER:OG	2.27	0.48
7:Y:42:GLN:HB3	7:Y:49:ASP:HB2	1.95	0.48
1:C:104:LEU:HA	1:C:107:PHE:HB3	1.96	0.48
7:Z:517:VAL:HG23	7:Z:522:LYS:HD2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:ILE:HG23	1:J:99:LEU:HB3	1.95	0.48
7:X:310:TYR:HE2	7:X:349:PRO:HG2	1.62	0.48
7:Y:180:GLY:HA3	7:Y:358:LEU:HD13	1.95	0.48
6:U:217:ARG:O	6:U:378:THR:OG1	2.30	0.48
1:I:111:GLU:OE2	1:J:113:ILE:HD11	2.13	0.48
5:S:303:GLU:O	5:S:307:ILE:HD12	2.13	0.48
6:U:100:LEU:O	7:X:98:ARG:NH2	2.47	0.48
7:Y:120:ARG:NH1	7:Y:132:GLN:O	2.47	0.48
6:T:438:GLY:O	6:T:498:THR:OG1	2.31	0.48
6:U:323:ILE:HG13	6:U:380:PHE:HB2	1.95	0.48
6:V:84:LEU:HD23	6:V:143:LEU:HD22	1.95	0.48
7:X:189:LYS:HB2	7:X:189:LYS:HE2	1.59	0.48
7:Y:216:ARG:O	7:Y:250:GLN:NE2	2.45	0.48
5:S:140:VAL:HG13	5:S:160:LEU:HB3	1.96	0.48
6:U:274:LYS:NZ	6:U:278:GLN:OE1	2.46	0.48
7:Y:273:ARG:HD3	7:Y:333:ILE:HG13	1.95	0.48
1:E:86:ILE:HG23	1:F:99:LEU:HB3	1.96	0.48
3:Q:42:ARG:NH2	4:R:148:GLU:OE2	2.47	0.48
6:T:326:ASP:H	6:T:382:VAL:HB	1.78	0.48
7:X:223:LEU:HA	7:X:226:GLU:HG2	1.95	0.48
5:S:101:VAL:HG22	5:S:138:VAL:HB	1.95	0.48
1:J:107:PHE:CE1	1:J:111:GLU:HG3	2.49	0.47
6:U:112:ASP:OD2	6:U:112:ASP:N	2.44	0.47
6:U:535:ILE:HD13	7:X:534:ILE:HD11	1.96	0.47
1:J:93:PRO:HA	1:J:96:ALA:HB2	1.96	0.47
7:Z:234:LYS:H	7:Z:242:SER:HB3	1.79	0.47
1:C:103:ALA:O	1:C:107:PHE:N	2.45	0.47
4:R:90:VAL:HB	4:R:117:GLU:HB2	1.96	0.47
5:S:119:ILE:HA	5:S:122:TYR:HB2	1.96	0.47
6:T:153:VAL:HG22	6:T:185:VAL:HG12	1.96	0.47
7:Y:116:GLY:HA3	7:Y:136:ASP:HB2	1.96	0.47
7:Y:373:ILE:HG23	7:Y:444:SER:HB2	1.96	0.47
1:J:107:PHE:CZ	1:J:111:GLU:HG3	2.49	0.47
6:V:304:TYR:OH	6:V:357:LEU:O	2.28	0.47
1:A:75:GLY:HA3	1:B:74:VAL:HG22	1.97	0.47
7:Z:65:VAL:HG11	7:Z:96:LEU:HD11	1.96	0.47
6:T:164:THR:HA	6:T:170:PRO:HA	1.95	0.47
5:S:304:LEU:CD1	6:V:346:GLY:O	2.63	0.47
7:Y:445:GLN:NE2	7:Y:459:LYS:O	2.45	0.47
7:Z:435:ARG:NH1	7:Z:475:THR:O	2.47	0.47
6:U:326:ASP:H	6:U:382:VAL:HB	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:ASN:N	1:F:92:ASN:OD1	2.47	0.47
6:T:92:ASP:OD1	7:X:303:ARG:NE	2.44	0.47
6:U:371:GLU:HG2	6:U:372:LEU:HD12	1.96	0.47
6:U:502:TYR:OH	6:U:547:ASP:OD1	2.33	0.47
7:Y:482:PRO:HB2	7:Y:502:MET:HE1	1.96	0.47
6:T:226:ASP:OD2	6:T:410:THR:OG1	2.30	0.47
6:T:345:PRO:HB3	6:T:349:ALA:HA	1.95	0.47
6:V:326:ASP:CB	6:V:329:LYS:HD2	2.45	0.47
7:Z:165:LYS:NZ	7:Z:489:VAL:O	2.44	0.47
6:V:446:LEU:HD22	6:V:501:VAL:HG21	1.95	0.47
6:V:453:TYR:O	6:V:457:ALA:N	2.47	0.47
7:Z:487:TYR:O	7:Z:498:LYS:NZ	2.45	0.47
1:F:71:LEU:HB2	1:G:70:ALA:HB1	1.98	0.46
3:Q:47:PHE:HB3	5:S:174:GLN:HE21	1.80	0.46
6:U:265:LYS:HD3	7:Z:357:HIS:HA	1.96	0.46
7:Z:161:VAL:O	7:Z:204:HIS:NE2	2.45	0.46
7:X:387:LEU:HD12	7:X:392:ILE:CD1	2.45	0.46
7:Y:402:GLY:HA3	7:Y:474:LEU:HD21	1.96	0.46
7:Z:57:PRO:O	7:Z:79:HIS:NE2	2.43	0.46
1:A:92:ASN:N	1:A:92:ASN:OD1	2.49	0.46
7:Y:308:VAL:CG2	7:Y:349:PRO:HG3	2.45	0.46
2:P:110:LYS:O	6:U:61:HIS:NE2	2.48	0.46
6:V:153:VAL:HG11	6:V:305:SER:HB3	1.97	0.46
7:X:216:ARG:HB2	7:X:219:GLU:CD	2.36	0.46
7:Y:75:GLU:OE2	7:Y:260:ARG:NE	2.46	0.46
7:Z:111:VAL:HG11	7:Z:264:THR:HG23	1.96	0.46
1:A:95:ILE:HG22	1:A:98:GLN:HB3	1.97	0.46
6:T:482:GLU:HA	6:T:485:LYS:HD2	1.98	0.46
1:I:94:ASN:ND2	5:S:224:THR:O	2.48	0.46
7:X:118:LEU:HA	7:X:245:THR:HB	1.97	0.46
7:Y:72:LEU:HD11	7:Y:89:ALA:HB1	1.96	0.46
1:A:80:VAL:HG11	1:J:80:VAL:HG22	1.97	0.46
1:G:107:PHE:O	1:G:111:GLU:HG2	2.16	0.46
6:V:443:ALA:HA	6:V:446:LEU:HB3	1.97	0.46
7:X:286:ASN:HA	7:X:286:ASN:HD22	1.46	0.46
7:Z:497:GLU:O	7:Z:501:LYS:HG2	2.16	0.46
1:H:92:ASN:OD1	1:H:92:ASN:N	2.49	0.46
1:A:70:ALA:HA	1:J:72:ALA:HB2	1.98	0.46
6:T:220:ARG:H	6:T:220:ARG:HG2	1.49	0.46
6:U:304:TYR:OH	6:U:357:LEU:O	2.30	0.46
6:V:112:ASP:N	6:V:112:ASP:OD1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:94:VAL:HG12	4:R:112:LYS:HG3	1.98	0.45
6:U:53:PHE:HD2	6:U:55:SER:H	1.64	0.45
1:A:110:THR:HG22	1:J:78:LEU:HB3	1.98	0.45
6:T:243:LYS:HB3	6:T:243:LYS:HE3	1.73	0.45
6:T:338:SER:CB	6:T:351:PRO:HG3	2.47	0.45
7:Z:482:PRO:HG2	7:Z:502:MET:HE2	1.97	0.45
6:T:476:ARG:NH2	6:T:505:THR:O	2.48	0.45
1:I:59:SER:HA	1:I:62:VAL:HG12	1.98	0.45
4:R:155:VAL:HG11	4:R:191:LEU:HD11	1.98	0.45
3:Q:48:ARG:HG2	5:S:164:ASP:HB2	1.98	0.45
7:X:287:ILE:HG22	7:X:339:VAL:HG22	1.98	0.45
6:T:121:ASN:HB2	7:Y:44:ILE:HG12	1.98	0.45
2:P:57:LEU:HD13	2:P:121:LEU:HD22	1.98	0.45
6:V:550:LEU:HA	6:V:553:GLU:HB2	1.99	0.45
7:Y:78:GLN:HE21	7:Y:86:ARG:HD2	1.82	0.45
6:U:164:THR:HA	6:U:170:PRO:HA	1.99	0.45
6:U:487:LYS:HE2	6:U:487:LYS:HB3	1.76	0.45
6:V:94:ILE:HG13	6:V:340:LEU:HB3	1.98	0.45
6:V:353:ASP:O	6:V:357:LEU:N	2.49	0.45
1:E:57:ALA:HA	1:E:60:LYS:HE2	1.97	0.45
1:H:111:GLU:O	1:H:115:LEU:N	2.38	0.45
1:H:80:VAL:HG22	1:I:80:VAL:HG11	1.99	0.45
6:U:461:GLN:HG2	6:U:462:PHE:HD2	1.82	0.45
1:F:99:LEU:O	1:F:103:ALA:N	2.49	0.45
7:Y:190:THR:HB	10:Y:601:ADP:O1A	2.17	0.45
1:G:78:LEU:HB3	1:H:110:THR:HG22	1.98	0.45
6:T:408:LEU:HD23	6:T:421:LEU:HA	1.99	0.45
6:U:155:ILE:HD12	6:U:312:TYR:HB2	1.99	0.45
6:U:511:LYS:HD2	6:U:559:LEU:HD12	1.98	0.45
6:T:416:GLY:HA2	6:T:418:ARG:NH2	2.31	0.45
6:V:370:LYS:HA	6:V:370:LYS:HD3	1.81	0.45
2:P:121:LEU:HD13	6:V:66:LEU:HD11	1.99	0.45
7:Y:485:ALA:HA	7:Y:498:LYS:HD3	1.99	0.45
6:U:443:ALA:HA	6:U:446:LEU:HB3	1.98	0.44
6:V:414:TYR:HB2	7:Y:408:GLN:OE1	2.17	0.44
6:V:534:LYS:HD2	7:Z:531:VAL:HG13	1.99	0.44
5:S:279:LYS:HD2	5:S:279:LYS:HA	1.76	0.44
6:T:120:LEU:HD23	6:T:120:LEU:HA	1.85	0.44
6:T:344:PRO:HG2	7:Y:299:ALA:CB	2.46	0.44
7:Y:310:TYR:CD1	7:Y:349:PRO:HG2	2.52	0.44
6:T:516:ASP:O	6:T:520:ALA:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:122:LEU:HB3	7:Z:98:ARG:HD3	2.00	0.44
6:V:87:VAL:HG11	6:V:90:VAL:HG22	2.00	0.44
7:Y:448:GLN:HG2	7:Y:458:GLY:HA3	1.99	0.44
3:Q:52:TYR:N	5:S:159:GLN:O	2.42	0.44
6:U:370:LYS:HD3	6:U:370:LYS:HA	1.72	0.44
7:X:266:LEU:O	7:X:270:GLU:N	2.48	0.44
4:R:109:ALA:HA	5:S:234:GLU:HB3	1.98	0.44
7:Y:365:SER:HB3	7:Y:368:ILE:HG12	2.00	0.44
7:Z:284:VAL:HB	7:Z:337:GLN:HG2	2.00	0.44
1:A:111:GLU:O	1:A:114:ALA:N	2.51	0.44
1:B:103:ALA:O	1:B:107:PHE:N	2.47	0.44
6:T:492:ILE:CG2	6:T:496:ARG:HB2	2.47	0.44
6:V:487:LYS:HD3	6:V:487:LYS:HA	1.33	0.44
3:Q:45:ILE:HG21	5:S:177:LEU:HD12	1.99	0.44
7:X:111:VAL:HG11	7:X:264:THR:HG23	2.00	0.44
7:X:287:ILE:O	7:X:287:ILE:HD12	2.18	0.44
7:X:72:LEU:HD11	7:X:89:ALA:HB1	2.00	0.44
7:Z:107:SER:OG	7:Z:110:LYS:NZ	2.46	0.44
1:D:103:ALA:O	1:D:107:PHE:N	2.50	0.44
5:S:103:VAL:HG22	5:S:140:VAL:HB	1.98	0.44
6:U:220:ARG:HG3	6:U:379:ALA:HB3	2.00	0.43
1:E:103:ALA:O	1:E:107:PHE:N	2.46	0.43
2:P:120:LYS:HG3	6:V:69:ALA:HB2	1.98	0.43
6:V:232:THR:HG22	6:V:236:ILE:CG1	2.45	0.43
7:X:175:ARG:O	7:X:334:THR:OG1	2.34	0.43
1:G:92:ASN:HB2	4:R:101:LYS:HB2	2.00	0.43
5:S:308:ILE:HD13	7:Z:304:ILE:HG23	1.99	0.43
7:Z:310:TYR:CE2	7:Z:349:PRO:HG2	2.53	0.43
1:C:92:ASN:OD1	1:C:92:ASN:N	2.52	0.43
1:G:113:ILE:HD12	1:G:113:ILE:HA	1.83	0.43
2:P:108:VAL:HG23	2:P:109:LEU:HD12	2.00	0.43
2:P:119:LYS:HE2	2:P:119:LYS:HB3	1.85	0.43
6:V:360:ARG:HE	6:V:360:ARG:HB3	1.58	0.43
6:U:232:THR:HG22	6:U:236:ILE:CG1	2.46	0.43
7:X:286:ASN:H	7:X:338:ALA:HB3	1.84	0.43
5:S:308:ILE:HD11	7:Z:305:PRO:CG	2.48	0.43
6:U:436:PHE:HB3	6:U:439:MET:HB3	2.00	0.43
6:V:421:LEU:C	6:V:421:LEU:HD13	2.39	0.43
7:Y:136:ASP:OD2	7:Y:239:ARG:NH2	2.52	0.43
7:Y:341:VAL:HA	7:Y:342:PRO:HD3	1.86	0.43
7:Z:427:GLU:HA	7:Z:430:LYS:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:132:PHE:HE1	6:T:297:PRO:HB2	1.83	0.43
6:T:406:ILE:HG23	6:T:421:LEU:CD1	2.48	0.43
6:V:204:THR:HG23	6:V:238:ALA:HB2	2.00	0.43
7:X:445:GLN:NE2	7:X:459:LYS:O	2.51	0.43
7:Y:190:THR:HA	7:Y:193:ILE:HG22	2.00	0.43
6:T:83:HIS:CG	6:T:102:SER:OG	2.72	0.43
7:Y:266:LEU:O	7:Y:270:GLU:N	2.51	0.43
5:S:127:LEU:HD21	5:S:137:VAL:HG11	2.01	0.43
6:T:232:THR:O	6:T:236:ILE:HG12	2.19	0.43
7:Y:189:LYS:HZ2	10:Y:601:ADP:PB	2.42	0.43
7:Y:310:TYR:CE1	7:Y:349:PRO:HG2	2.54	0.43
1:B:118:LEU:HD11	1:C:116:PHE:HB3	2.00	0.43
1:F:75:GLY:HA3	1:G:74:VAL:HG22	2.00	0.43
6:U:153:VAL:HG11	6:U:305:SER:HB3	2.01	0.43
6:V:322:ILE:HG23	6:V:379:ALA:HA	2.01	0.43
7:X:500:ASP:HB3	7:X:504:LYS:HE3	2.00	0.43
1:H:111:GLU:OE1	1:I:113:ILE:HD11	2.18	0.42
4:R:118:LEU:HB2	4:R:125:GLU:HG2	2.00	0.42
6:U:479:ARG:HG3	6:U:517:ILE:HD13	1.99	0.42
7:Z:66:GLU:HB3	7:Z:101:LYS:HB3	2.00	0.42
1:E:71:LEU:HD23	1:F:113:ILE:HG23	2.02	0.42
1:F:111:GLU:O	1:F:112:SER:C	2.57	0.42
1:F:69:ILE:HD13	1:G:69:ILE:HD11	2.01	0.42
6:T:344:PRO:HA	6:T:345:PRO:HD3	1.86	0.42
6:T:442:VAL:HG12	6:T:501:VAL:HG12	2.01	0.42
6:U:97:VAL:HB	6:U:127:VAL:HG13	2.01	0.42
7:Y:246:LEU:HD13	7:Y:248:TYR:HE2	1.83	0.42
7:Y:308:VAL:HG21	7:Y:349:PRO:CG	2.49	0.42
1:J:103:ALA:O	1:J:107:PHE:N	2.49	0.42
6:V:334:TYR:CD2	6:V:351:PRO:HG2	2.52	0.42
6:V:327:LEU:HB3	6:V:383:ILE:HD11	2.01	0.42
6:V:421:LEU:HD13	6:V:422:ASN:N	2.35	0.42
7:X:438:LYS:HE2	7:X:479:ASP:HA	2.01	0.42
7:Y:142:SER:O	7:Y:145:ARG:NH2	2.52	0.42
6:T:339:LEU:HD12	6:T:339:LEU:HA	1.82	0.42
1:A:113:ILE:HG21	1:J:74:VAL:HG23	2.00	0.42
6:U:207:LYS:HA	6:U:497:GLN:NE2	2.35	0.42
7:X:348:ASP:HA	7:X:349:PRO:HD2	1.89	0.42
7:Y:516:LYS:HA	7:Y:516:LYS:HD2	1.80	0.42
1:B:95:ILE:HG12	1:B:98:GLN:HB3	2.01	0.42
5:S:197:PHE:N	5:S:261:GLU:OE1	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:139:VAL:HG21	6:U:45:LEU:HG	2.01	0.42
1:F:119:LEU:O	1:F:123:LEU:N	2.49	0.42
6:T:432:SER:OG	6:T:435:GLN:NE2	2.46	0.42
6:V:243:LYS:HE3	6:V:243:LYS:HB3	1.79	0.42
7:X:130:ASP:N	7:X:130:ASP:OD1	2.51	0.42
7:X:253:GLU:HB3	7:X:257:ALA:HB3	2.00	0.42
6:U:107:GLU:HA	6:U:150:ILE:HA	2.01	0.42
6:U:239:ILE:HD11	6:U:323:ILE:HD13	2.01	0.42
6:U:52:LYS:HB3	6:U:52:LYS:HE2	1.85	0.42
1:E:99:LEU:O	1:E:103:ALA:N	2.53	0.42
6:T:132:PHE:CE1	6:T:297:PRO:HB2	2.54	0.42
6:T:342:ARG:NH1	7:X:302:GLY:O	2.53	0.42
7:Y:489:VAL:HG21	7:Y:495:VAL:HG22	2.01	0.42
7:Z:295:SER:HB2	7:Z:311:GLN:HE21	1.85	0.42
1:B:71:LEU:HB2	1:C:70:ALA:HB1	2.01	0.42
2:P:103:LYS:HD2	2:P:103:LYS:HA	1.81	0.42
6:T:97:VAL:CG2	6:T:144:VAL:HG21	2.50	0.42
6:V:327:LEU:HA	6:V:327:LEU:HD12	1.77	0.42
7:Y:64:GLU:OE2	7:Y:105:THR:CG2	2.68	0.42
7:Z:346:LEU:HD22	7:Z:355:PHE:HE1	1.84	0.42
7:Z:573:LYS:HD3	7:Z:573:LYS:HA	1.88	0.42
1:B:104:LEU:HA	1:B:107:PHE:HB3	2.02	0.41
5:S:51:LYS:HE3	5:S:51:LYS:HB2	1.90	0.41
7:X:164:ILE:HB	7:X:167:VAL:HB	2.01	0.41
7:Y:215:GLU:HG3	7:Y:285:ASP:OD2	2.20	0.41
1:D:99:LEU:O	1:D:103:ALA:N	2.50	0.41
5:S:106:THR:HG22	5:S:119:ILE:HD11	2.02	0.41
6:T:269:VAL:CG1	6:T:287:MET:HE2	2.44	0.41
6:U:412:LEU:HB2	6:U:420:ALA:HB1	2.02	0.41
6:V:118:MET:HE1	6:V:300:PHE:HE2	1.84	0.41
7:Z:445:GLN:NE2	7:Z:459:LYS:O	2.53	0.41
7:Z:392:ILE:HB	7:Z:396:HIS:HD1	1.85	0.41
2:P:66:GLN:OE1	2:P:115:SER:OG	2.33	0.41
7:X:394:ALA:O	7:X:398:ASN:ND2	2.53	0.41
7:Y:284:VAL:HG11	7:Y:287:ILE:HD13	2.01	0.41
7:Y:66:GLU:OE2	7:Y:101:LYS:CD	2.64	0.41
1:E:78:LEU:HA	1:E:78:LEU:HD23	1.83	0.41
5:S:46:ARG:HB3	5:S:288:LEU:HD21	2.03	0.41
1:C:71:LEU:HD22	1:D:113:ILE:HG23	2.02	0.41
2:P:77:PHE:HA	2:P:80:LEU:HB2	2.03	0.41
7:Y:262:ALA:HB3	7:Y:321:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:66:GLU:HG2	7:Z:101:LYS:HD3	2.01	0.41
6:V:220:ARG:HH12	7:Z:216:ARG:HB3	1.86	0.41
1:H:71:LEU:HD23	1:I:113:ILE:HG23	2.03	0.41
6:V:125:ASP:OD1	6:V:125:ASP:N	2.45	0.41
6:T:490:ALA:HA	6:T:491:PRO:HD3	1.93	0.41
6:V:502:TYR:OH	6:V:547:ASP:OD1	2.32	0.41
7:X:516:LYS:O	7:X:522:LYS:NZ	2.49	0.41
6:U:181:ARG:HA	7:X:552:GLU:HG2	2.03	0.41
7:Y:394:ALA:O	7:Y:398:ASN:ND2	2.54	0.41
7:Y:111:VAL:HG11	7:Y:264:THR:HG23	2.03	0.41
1:E:91:ARG:HG2	4:R:96:GLY:HA3	2.02	0.41
1:I:72:ALA:HB2	1:J:70:ALA:HA	2.03	0.41
2:P:112:SER:HB3	6:U:61:HIS:CD2	2.56	0.41
6:U:264:GLN:NE2	11:U:1102:HOH:O	2.43	0.41
7:X:183:GLY:HA3	7:X:189:LYS:CG	2.49	0.41
6:T:89:SER:HB2	7:X:79:HIS:O	2.21	0.41
6:U:516:ASP:O	6:U:520:ALA:N	2.51	0.41
7:X:494:GLU:HA	7:X:497:GLU:HB2	2.03	0.41
6:V:157:PRO:HB3	7:Z:545:LEU:HB3	2.03	0.41
1:I:78:LEU:HD23	1:I:78:LEU:HA	1.90	0.40
6:T:94:ILE:HD13	6:T:130:VAL:HG12	2.02	0.40
6:V:532:VAL:HG23	6:V:546:LEU:HD11	2.03	0.40
7:Z:121:ILE:HD11	7:Z:224:TYR:CG	2.56	0.40
6:U:232:THR:O	6:U:236:ILE:N	2.46	0.40
7:X:348:ASP:HB3	7:X:351:PRO:HD2	2.03	0.40
7:Y:78:GLN:NE2	7:Y:301:LEU:O	2.44	0.40
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.93	0.40
6:T:370:LYS:HB2	6:T:370:LYS:HE2	1.94	0.40
7:Y:121:ILE:HG12	7:Y:246:LEU:HD12	2.02	0.40
7:Y:252:ASN:N	7:Y:252:ASN:OD1	2.54	0.40
7:Y:308:VAL:HB	7:Y:310:TYR:CD1	2.57	0.40
1:I:92:ASN:N	1:I:92:ASN:OD1	2.55	0.40
6:T:461:GLN:HG3	7:X:416:ILE:HD11	2.04	0.40
7:X:159:ILE:HA	7:X:386:MET:HE2	2.03	0.40
7:X:166:VAL:HG23	7:X:443:LEU:HD22	2.04	0.40
7:Y:341:VAL:HG11	7:Y:346:LEU:HD23	2.03	0.40
7:Z:272:PHE:HD1	7:Z:276:GLU:HG3	1.85	0.40
7:Z:311:GLN:H	7:Z:311:GLN:HG3	1.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/127 (57%)	72 (100%)	0	0	100	100
1	B	72/127 (57%)	72 (100%)	0	0	100	100
1	C	71/127 (56%)	71 (100%)	0	0	100	100
1	D	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	E	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	G	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	H	72/127 (57%)	72 (100%)	0	0	100	100
1	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
2	P	111/229 (48%)	103 (93%)	8 (7%)	0	100	100
3	Q	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
4	R	175/199 (88%)	162 (93%)	13 (7%)	0	100	100
5	S	275/317 (87%)	265 (96%)	10 (4%)	0	100	100
6	T	481/562 (86%)	468 (97%)	12 (2%)	1 (0%)	49	81
6	U	519/562 (92%)	493 (95%)	25 (5%)	1 (0%)	49	81
6	V	518/562 (92%)	507 (98%)	10 (2%)	1 (0%)	49	81
7	X	540/574 (94%)	502 (93%)	37 (7%)	1 (0%)	49	81
7	Y	519/574 (90%)	486 (94%)	32 (6%)	1 (0%)	49	81
7	Z	536/574 (93%)	510 (95%)	25 (5%)	1 (0%)	49	81
All	All	4463/5497 (81%)	4275 (96%)	182 (4%)	6 (0%)	56	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	V	420	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	X	308	VAL
7	Z	308	VAL
6	U	513	ARG
7	Y	148	PRO
6	T	491	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/86 (58%)	50 (100%)	0	100	100
1	B	50/86 (58%)	50 (100%)	0	100	100
1	C	50/86 (58%)	50 (100%)	0	100	100
1	D	50/86 (58%)	49 (98%)	1 (2%)	58	86
1	E	50/86 (58%)	49 (98%)	1 (2%)	58	86
1	F	50/86 (58%)	50 (100%)	0	100	100
1	G	50/86 (58%)	50 (100%)	0	100	100
1	H	50/86 (58%)	50 (100%)	0	100	100
1	I	50/86 (58%)	50 (100%)	0	100	100
1	J	50/86 (58%)	50 (100%)	0	100	100
2	P	98/196 (50%)	98 (100%)	0	100	100
3	Q	56/58 (97%)	56 (100%)	0	100	100
4	R	134/151 (89%)	134 (100%)	0	100	100
5	S	235/265 (89%)	235 (100%)	0	100	100
6	T	383/448 (86%)	373 (97%)	10 (3%)	49	81
6	U	419/448 (94%)	411 (98%)	8 (2%)	60	87
6	V	418/448 (93%)	406 (97%)	12 (3%)	45	79
7	X	449/469 (96%)	443 (99%)	6 (1%)	71	92
7	Y	430/469 (92%)	428 (100%)	2 (0%)	90	97
7	Z	446/469 (95%)	444 (100%)	2 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3568/4281 (83%)	3526 (99%)	42 (1%)	75	93

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	85	LEU
1	E	107	PHE
6	T	81	VAL
6	T	82	ILE
6	T	86	ARG
6	T	102	SER
6	T	103	VAL
6	T	243	LYS
6	T	267	SER
6	T	300	PHE
6	T	339	LEU
6	T	354	VAL
6	U	84	LEU
6	U	220	ARG
6	U	265	LYS
6	U	268	THR
6	U	300	PHE
6	U	345	PRO
6	U	347	ARG
6	U	348	GLU
6	V	96	ARG
6	V	267	SER
6	V	268	THR
6	V	300	PHE
6	V	323	ILE
6	V	325	ASP
6	V	326	ASP
6	V	329	LYS
6	V	347	ARG
6	V	417	ILE
6	V	418	ARG
6	V	487	LYS
7	X	189	LYS
7	X	287	ILE
7	X	385	ARG
7	X	388	ASN
7	X	510	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	X	550	LYS
7	Y	285	ASP
7	Y	306	SER
7	Z	311	GLN
7	Z	558	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	94	ASN
4	R	38	ASN
4	R	66	HIS
4	R	73	ASN
4	R	85	GLN
4	R	171	GLN
5	S	174	GLN
5	S	262	ASN
5	S	293	ASN
5	S	297	GLN
6	T	386	GLN
6	T	435	GLN
6	T	441	GLN
6	T	497	GLN
6	T	539	ASN
6	U	242	GLN
6	U	246	ASN
6	U	248	GLN
6	U	319	HIS
6	U	441	GLN
6	U	497	GLN
6	V	121	ASN
6	V	126	HIS
6	V	139	HIS
6	V	152	ASN
6	V	244	ASN
6	V	278	GLN
6	V	486	GLN
6	V	488	GLN
6	V	497	GLN
6	V	529	ASN
7	X	198	ASN
7	X	199	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	X	241	ASN
7	X	278	GLN
7	X	286	ASN
7	X	337	GLN
7	X	388	ASN
7	X	398	ASN
7	X	471	GLN
7	Y	174	GLN
7	Y	241	ASN
7	Y	398	ASN
7	Z	132	GLN
7	Z	144	HIS
7	Z	199	ASN
7	Z	241	ASN
7	Z	250	GLN
7	Z	278	GLN
7	Z	294	ASN
7	Z	398	ASN

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](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ATP	T	1001	9	26,33,33	0.70	0	27,52,52	0.76	1 (3%)
8	ATP	U	1001	9	26,33,33	0.67	0	27,52,52	0.74	1 (3%)
8	ATP	V	1001	9	26,33,33	0.69	0	27,52,52	0.76	1 (3%)
10	ADP	X	601	9	24,29,29	0.67	0	25,45,45	0.72	1 (4%)
10	ADP	Y	601	9	24,29,29	0.67	0	25,45,45	0.72	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	T	1001	9	-	5/18/38/38	0/3/3/3
8	ATP	U	1001	9	-	2/18/38/38	0/3/3/3
8	ATP	V	1001	9	-	3/18/38/38	0/3/3/3
10	ADP	X	601	9	-	6/12/32/32	0/3/3/3
10	ADP	Y	601	9	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	1001	ATP	C5-C6-N6	2.21	123.84	120.38
10	X	601	ADP	C5-C6-N6	2.17	123.79	120.38
10	Y	601	ADP	C5-C6-N6	2.16	123.78	120.38
8	U	1001	ATP	C5-C6-N6	2.16	123.78	120.38
8	T	1001	ATP	C5-C6-N6	2.16	123.77	120.38

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	X	601	ADP	C5'-O5'-PA-O3A
8	V	1001	ATP	C5'-O5'-PA-O2A
10	Y	601	ADP	C3'-C4'-C5'-O5'
10	X	601	ADP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

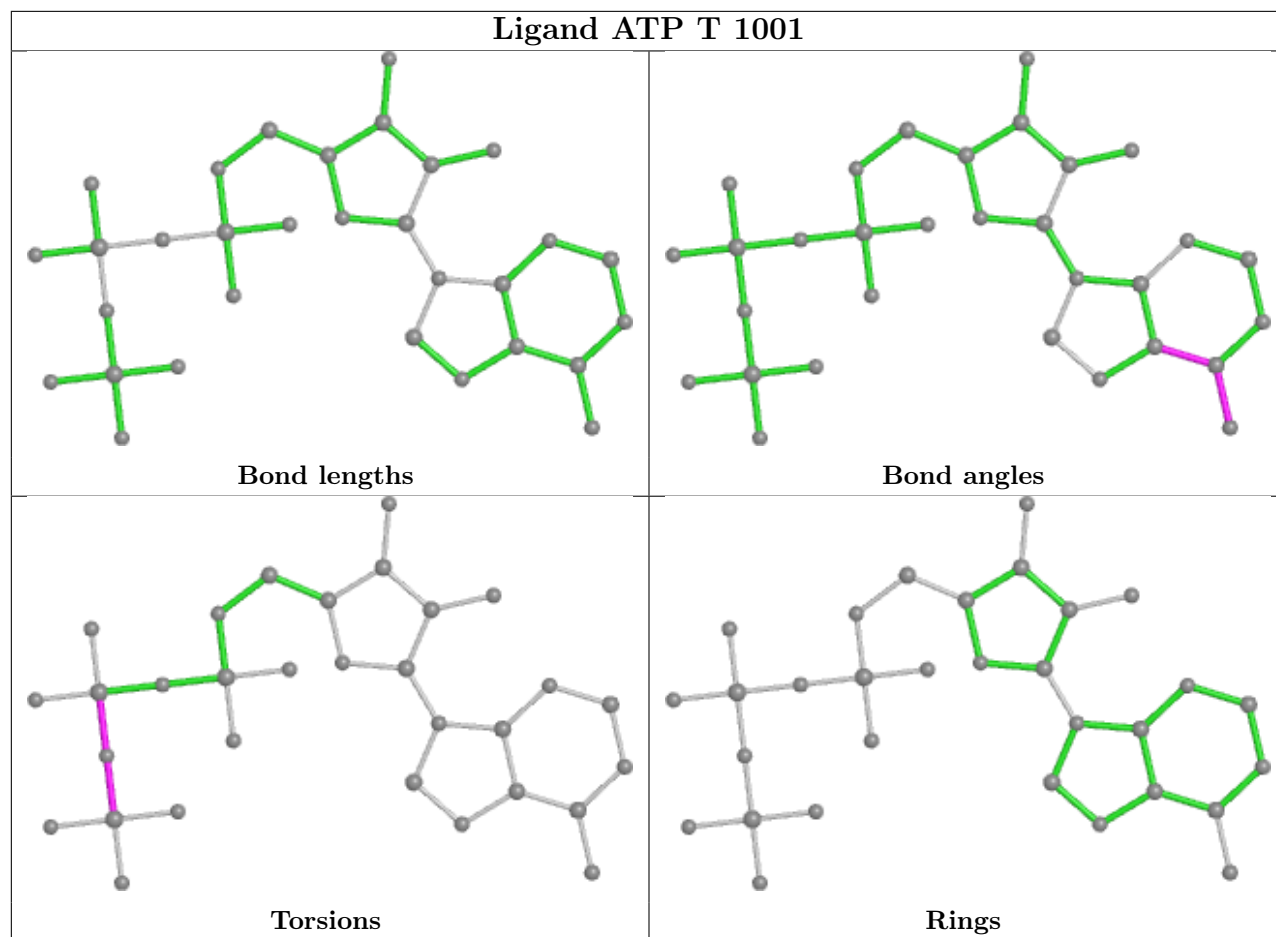
Mol	Chain	Res	Type	Atoms
10	Y	601	ADP	O4'-C4'-C5'-O5'
10	X	601	ADP	O4'-C4'-C5'-O5'
8	V	1001	ATP	C5'-O5'-PA-O3A
10	X	601	ADP	C5'-O5'-PA-O1A
10	X	601	ADP	C5'-O5'-PA-O2A
8	V	1001	ATP	C5'-O5'-PA-O1A
10	Y	601	ADP	PA-O3A-PB-O1B
8	T	1001	ATP	PB-O3B-PG-O1G
8	U	1001	ATP	PA-O3A-PB-O2B
8	T	1001	ATP	PG-O3B-PB-O1B
10	X	601	ADP	PB-O3A-PA-O1A
8	T	1001	ATP	PG-O3B-PB-O2B
8	U	1001	ATP	PB-O3B-PG-O3G
8	T	1001	ATP	PB-O3B-PG-O2G
8	T	1001	ATP	PB-O3B-PG-O3G

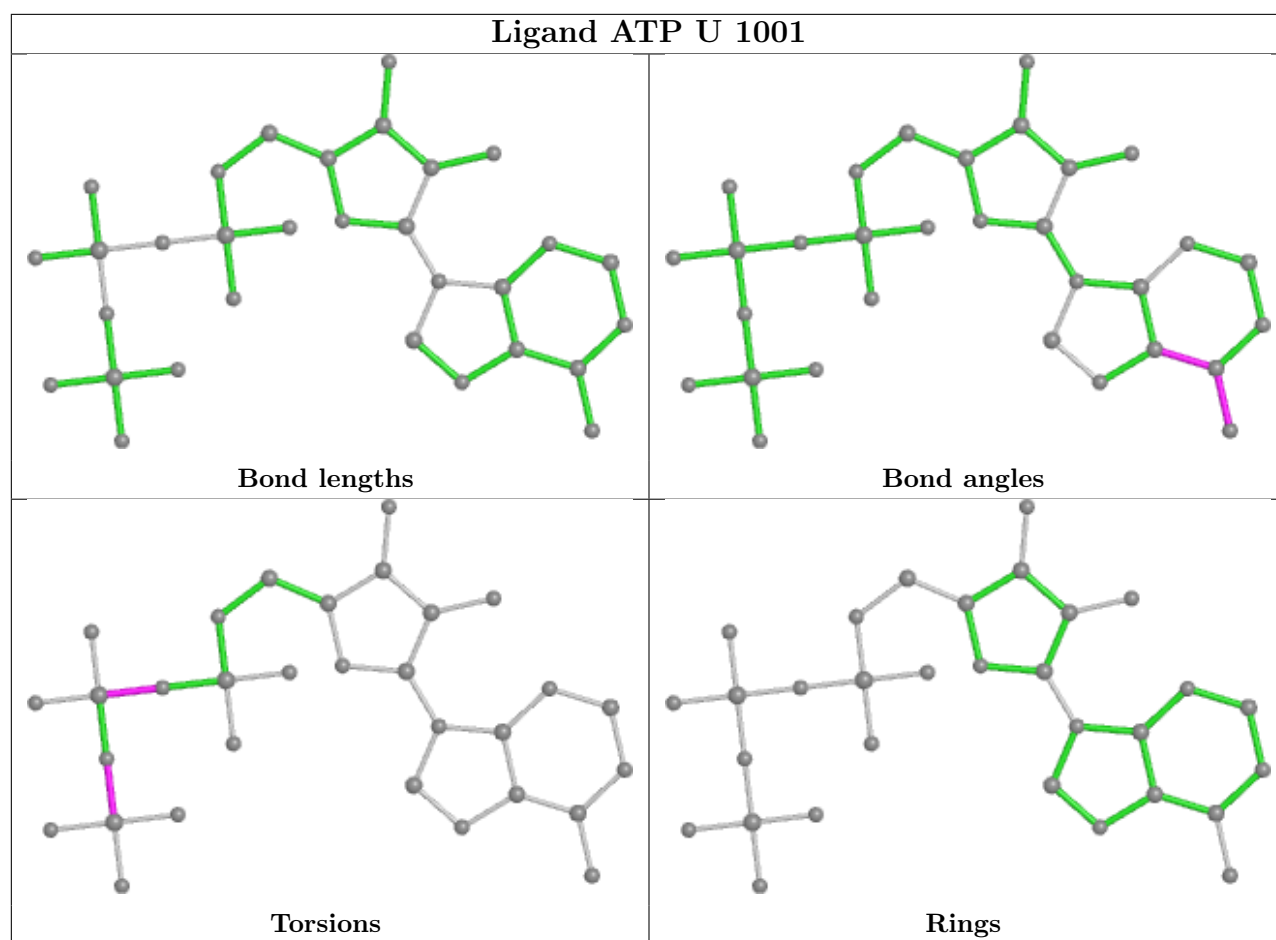
There are no ring outliers.

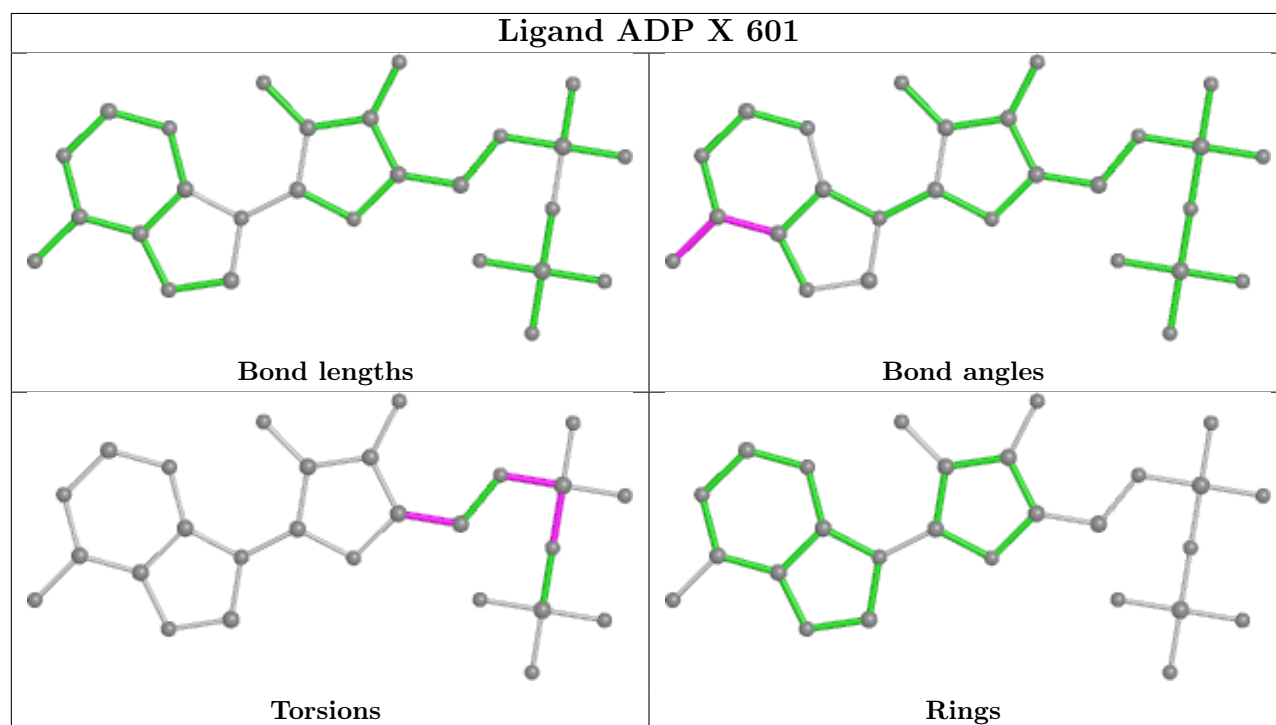
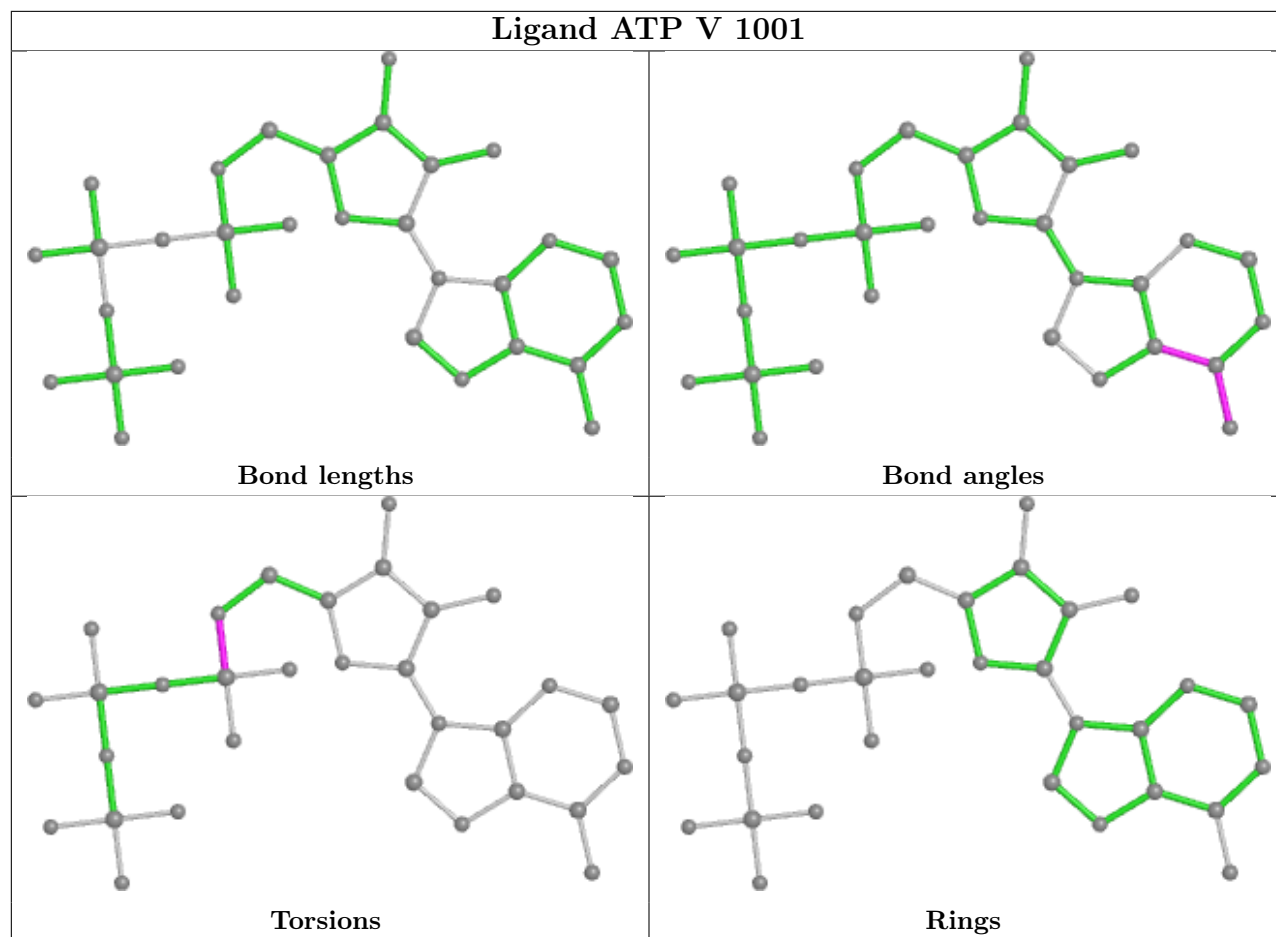
5 monomers are involved in 16 short contacts:

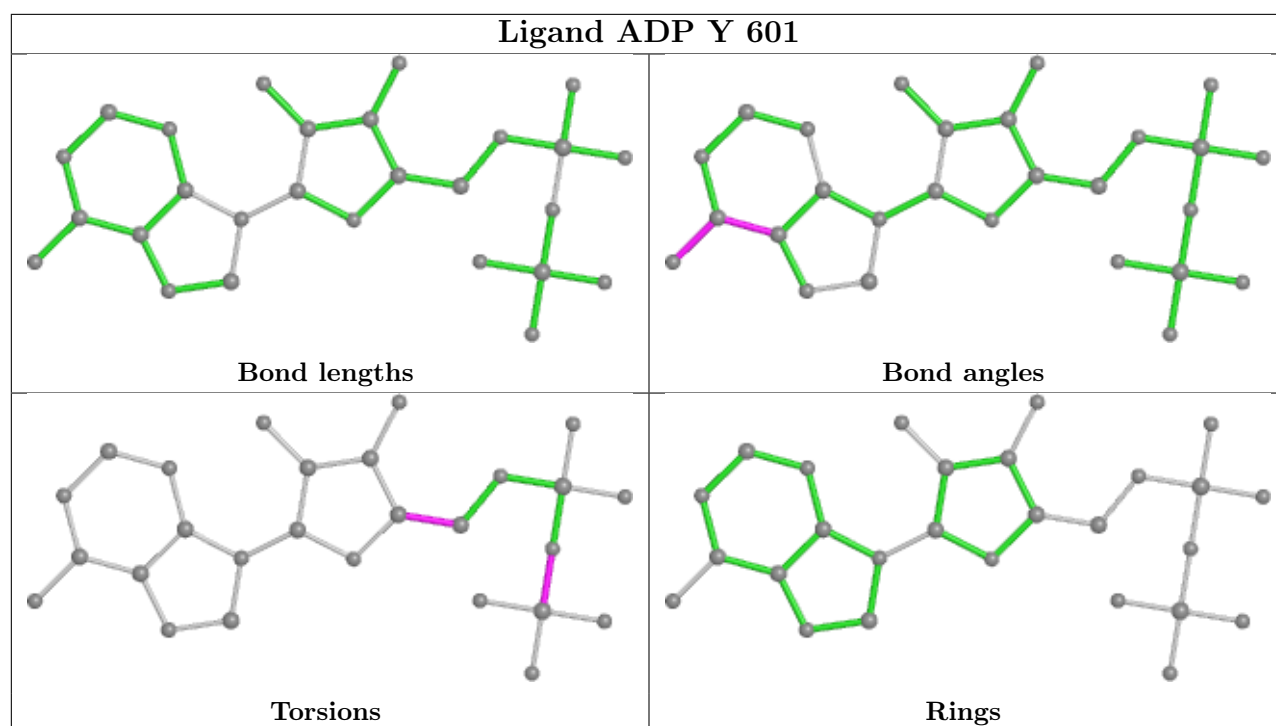
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	1001	ATP	6	0
8	U	1001	ATP	1	0
8	V	1001	ATP	1	0
10	X	601	ADP	3	0
10	Y	601	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
6	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.30
1	U	344:PRO	C	345:PRO	N	3.23