



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 2, 2017 – 06:35 PM EDT

PDB ID : 5U6Y
EMDB ID: : EMD-8514
Title : Pseudo-atomic model of the CaMKIIa holoenzyme.
Authors : Myers, J.; Reichow, S.L.
Deposited on : unknown
Resolution : 20.00 Å(reported)
Based on PDB ID : 51G3, 2VZ6

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

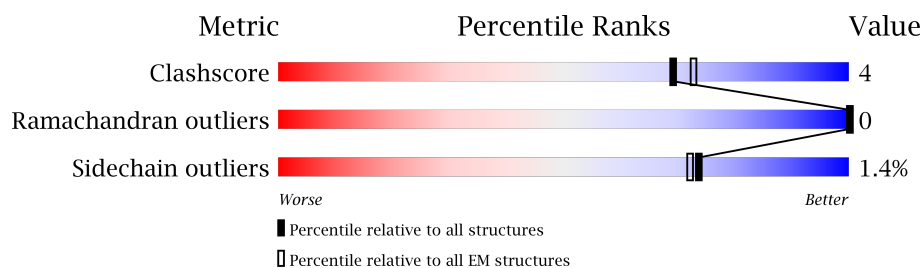
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	461	89% 10%
1	B	461	87% 12%
1	C	461	89% 10%
1	D	461	87% 12%
1	E	461	87% 12%
1	F	461	88% 11%
1	G	461	87% 12% .
1	H	461	88% 11%
1	I	461	88% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	461	 87%13%
1	K	461	 87%13%
1	L	461	 89%11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 87197 atoms, of which 43301 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	459	Total	C	H	N	O	S	3	0
			7248	2321	3590	644	676	17		
1	B	459	Total	C	H	N	O	S	3	0
			7251	2321	3593	644	676	17		
1	C	459	Total	C	H	N	O	S	3	0
			7280	2321	3622	644	676	17		
1	D	459	Total	C	H	N	O	S	3	0
			7248	2321	3590	644	676	17		
1	E	459	Total	C	H	N	O	S	3	0
			7254	2321	3596	644	676	17		
1	F	459	Total	C	H	N	O	S	3	0
			7267	2321	3609	644	676	17		
1	G	459	Total	C	H	N	O	S	3	0
			7272	2321	3614	644	676	17		
1	H	459	Total	C	H	N	O	S	3	0
			7284	2321	3626	644	676	17		
1	I	459	Total	C	H	N	O	S	3	0
			7284	2321	3626	644	676	17		
1	J	459	Total	C	H	N	O	S	3	0
			7272	2321	3614	644	676	17		
1	K	459	Total	C	H	N	O	S	3	0
			7272	2321	3614	644	676	17		
1	L	459	Total	C	H	N	O	S	3	0
			7265	2321	3607	644	676	17		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P11275
A	324	SER	ASN	conflict	UNP P11275
B	0	MET	-	initiating methionine	UNP P11275
B	324	SER	ASN	conflict	UNP P11275
C	0	MET	-	initiating methionine	UNP P11275

Continued on next page...

Continued from previous page...

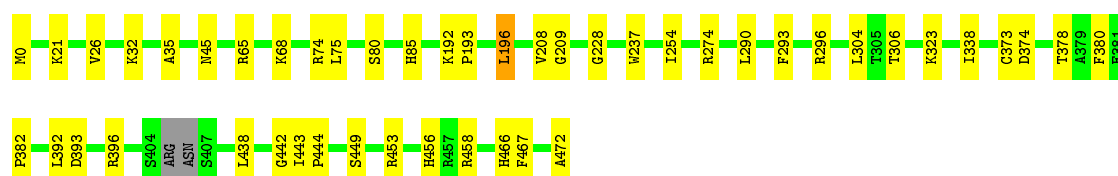
Chain	Residue	Modelled	Actual	Comment	Reference
C	324	SER	ASN	conflict	UNP P11275
D	0	MET	-	initiating methionine	UNP P11275
D	324	SER	ASN	conflict	UNP P11275
E	0	MET	-	initiating methionine	UNP P11275
E	324	SER	ASN	conflict	UNP P11275
F	0	MET	-	initiating methionine	UNP P11275
F	324	SER	ASN	conflict	UNP P11275
G	0	MET	-	initiating methionine	UNP P11275
G	324	SER	ASN	conflict	UNP P11275
H	0	MET	-	initiating methionine	UNP P11275
H	324	SER	ASN	conflict	UNP P11275
I	0	MET	-	initiating methionine	UNP P11275
I	324	SER	ASN	conflict	UNP P11275
J	0	MET	-	initiating methionine	UNP P11275
J	324	SER	ASN	conflict	UNP P11275
K	0	MET	-	initiating methionine	UNP P11275
K	324	SER	ASN	conflict	UNP P11275
L	0	MET	-	initiating methionine	UNP P11275
L	324	SER	ASN	conflict	UNP P11275

3 Residue-property plots

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

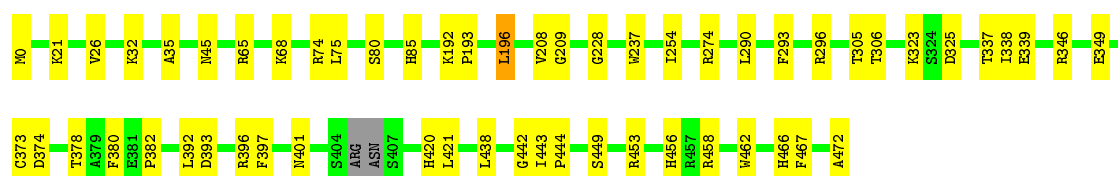
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain A: 



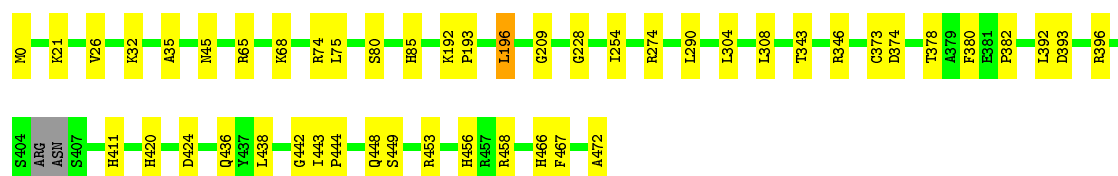
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain B: 




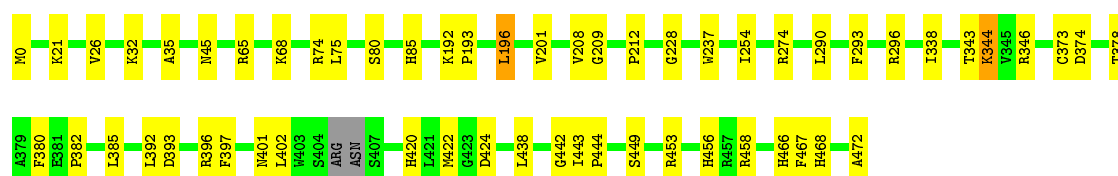
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain C: 

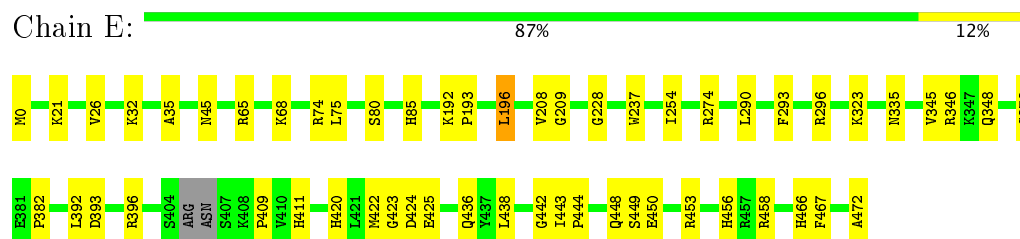


- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

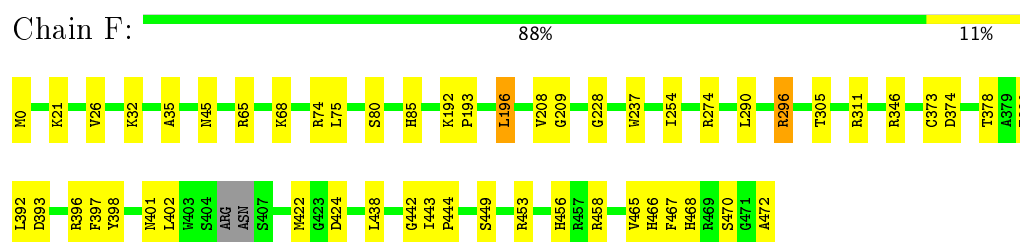
Chain D: 



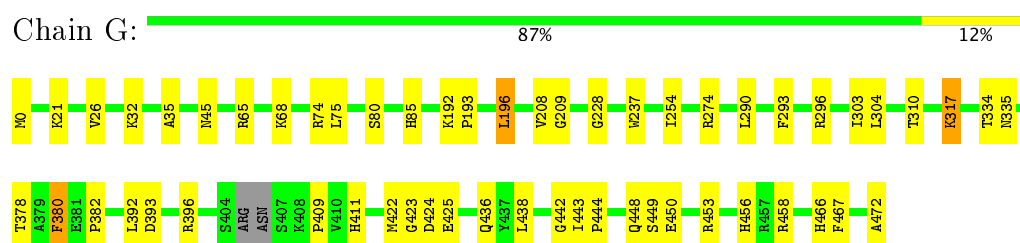
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



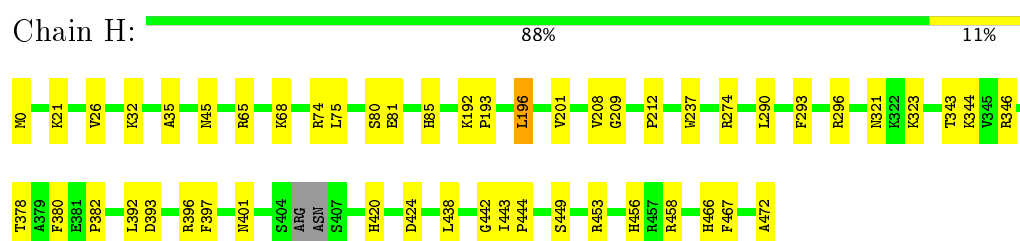
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



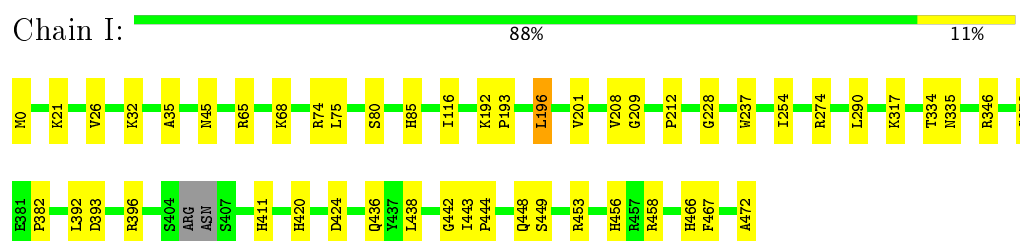
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha




- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

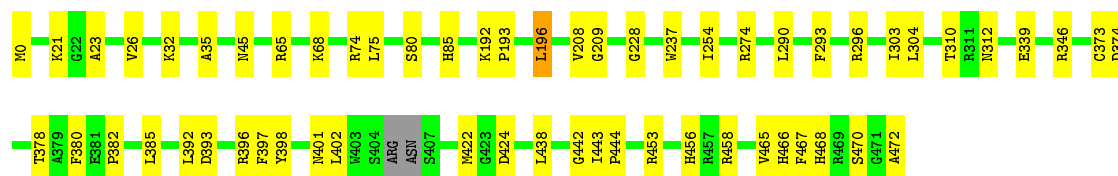


- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha




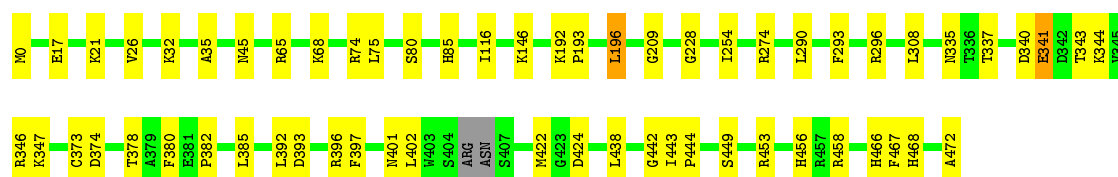
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain J:  87% 13%




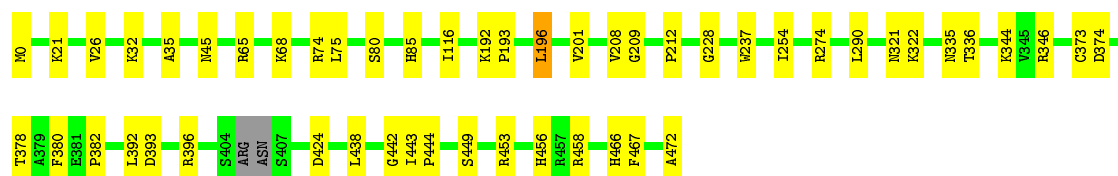
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain K:  87% 13%



- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain L:  89% 11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	2000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Performed in EMAN2	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	49000	Depositor
Image detector	FEI EAGLE (2k x 2k)	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	0.66	0/3742	0.73	2/5057 (0.0%)
1	B	0.66	0/3742	0.73	2/5057 (0.0%)
1	C	0.64	0/3742	0.73	2/5057 (0.0%)
1	D	0.65	0/3742	0.73	2/5057 (0.0%)
1	E	0.66	0/3742	0.74	2/5057 (0.0%)
1	F	0.66	0/3742	0.74	2/5057 (0.0%)
1	G	0.66	0/3742	0.74	2/5057 (0.0%)
1	H	0.65	0/3742	0.73	2/5057 (0.0%)
1	I	0.63	0/3742	0.73	2/5057 (0.0%)
1	J	0.65	0/3742	0.72	2/5057 (0.0%)
1	K	0.66	0/3742	0.73	2/5057 (0.0%)
1	L	0.67	0/3742	0.74	2/5057 (0.0%)
All	All	0.65	0/44904	0.73	24/60684 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	L	274	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	G	274	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	F	274	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	J	274	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	B	274	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	D	274	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	A	274	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	E	274	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	H	274	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	K	274	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	I	274	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	D	196	LEU	CA-CB-CG	-6.79	99.68	115.30
1	C	196	LEU	CA-CB-CG	-6.78	99.70	115.30
1	H	196	LEU	CA-CB-CG	-6.78	99.71	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	LEU	CA-CB-CG	-6.77	99.73	115.30
1	J	196	LEU	CA-CB-CG	-6.76	99.75	115.30
1	I	196	LEU	CA-CB-CG	-6.75	99.78	115.30
1	L	196	LEU	CA-CB-CG	-6.74	99.80	115.30
1	A	196	LEU	CA-CB-CG	-6.74	99.80	115.30
1	F	196	LEU	CA-CB-CG	-6.74	99.81	115.30
1	E	196	LEU	CA-CB-CG	-6.73	99.81	115.30
1	K	196	LEU	CA-CB-CG	-6.73	99.82	115.30
1	G	196	LEU	CA-CB-CG	-6.73	99.83	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	3658	3590	3619	24	0
1	B	3658	3593	3619	40	0
1	C	3658	3622	3619	30	0
1	D	3658	3590	3619	38	0
1	E	3658	3596	3619	40	0
1	F	3658	3609	3619	42	0
1	G	3658	3614	3616	41	0
1	H	3658	3626	3619	32	0
1	I	3658	3626	3619	33	0
1	J	3658	3614	3619	45	0
1	K	3658	3614	3619	43	0
1	L	3658	3607	3619	29	0
All	All	43896	43301	43425	378	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 4.

All (378) 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)
1:B:346:ARG:HB2	1:B:421:LEU:HD13	1.36	1.06
1:E:374:ASP:OD2	1:E:458:ARG:NH1	1.90	1.05
1:H:374:ASP:OD2	1:H:458:ARG:NH1	1.90	1.04
1:J:374:ASP:OD2	1:J:458:ARG:NH1	1.90	1.04
1:L:374:ASP:OD2	1:L:458:ARG:NH1	1.90	1.04
1:K:374:ASP:OD2	1:K:458:ARG:NH1	1.90	1.04
1:A:374:ASP:OD2	1:A:458:ARG:NH1	1.90	1.04
1:B:374:ASP:OD2	1:B:458:ARG:NH1	1.90	1.04
1:D:374:ASP:OD2	1:D:458:ARG:NH1	1.90	1.03
1:G:374:ASP:OD2	1:G:458:ARG:NH1	1.90	1.03
1:I:374:ASP:OD2	1:I:458:ARG:NH1	1.90	1.03
1:C:374:ASP:OD2	1:C:458:ARG:NH1	1.90	1.03
1:F:374:ASP:OD2	1:F:458:ARG:NH1	1.90	1.03
1:B:346:ARG:HB2	1:B:421:LEU:CD1	1.93	0.98
1:B:349:GLU:CD	1:B:462:TRP:HE1	1.73	0.92
1:B:346:ARG:CB	1:B:421:LEU:HD13	2.09	0.80
1:B:349:GLU:OE2	1:B:462:TRP:NE1	2.14	0.79
1:D:346:ARG:NH1	1:D:424:ASP:O	2.25	0.70
1:J:346:ARG:NH1	1:J:424:ASP:O	2.24	0.70
1:L:346:ARG:NH1	1:L:424:ASP:O	2.25	0.69
1:C:346:ARG:NH1	1:C:424:ASP:O	2.24	0.69
1:E:346:ARG:NH1	1:E:424:ASP:O	2.25	0.69
1:I:346:ARG:NH1	1:I:424:ASP:O	2.26	0.69
1:F:346:ARG:NH1	1:F:424:ASP:O	2.25	0.68
1:G:346:ARG:NH1	1:G:424:ASP:O	2.25	0.68
1:E:345:VAL:HG12	1:E:348:GLN:H	1.59	0.67
1:H:346:ARG:NH1	1:H:424:ASP:O	2.25	0.67
1:K:346:ARG:NH1	1:K:424:ASP:O	2.27	0.67
1:B:346:ARG:NE	1:B:421:LEU:HD13	2.14	0.63
1:F:296:ARG:O	1:F:296:ARG:HD3	1.97	0.63
1:B:209:GLY:HA2	1:B:290:LEU:HD13	1.83	0.61
1:A:209:GLY:HA2	1:A:290:LEU:HD13	1.83	0.60
1:K:346:ARG:NH1	1:K:424:ASP:HA	2.16	0.60
1:H:209:GLY:HA2	1:H:290:LEU:HD13	1.83	0.60
1:C:209:GLY:HA2	1:C:290:LEU:HD13	1.83	0.60
1:B:346:ARG:HB2	1:B:421:LEU:HD11	1.81	0.60
1:H:346:ARG:NH1	1:H:424:ASP:HA	2.17	0.60
1:F:209:GLY:HA2	1:F:290:LEU:HD13	1.83	0.60
1:G:209:GLY:HA2	1:G:290:LEU:HD13	1.83	0.60
1:G:436:GLN:HB3	1:J:397:PHE:CD2	2.37	0.60
1:K:209:GLY:HA2	1:K:290:LEU:HD13	1.83	0.60
1:I:209:GLY:HA2	1:I:290:LEU:HD13	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:436:GLN:HB3	1:F:397:PHE:CD2	2.37	0.59
1:D:209:GLY:HA2	1:D:290:LEU:HD13	1.83	0.59
1:J:209:GLY:HA2	1:J:290:LEU:HD13	1.83	0.59
1:L:209:GLY:HA2	1:L:290:LEU:HD13	1.83	0.59
1:E:209:GLY:HA2	1:E:290:LEU:HD13	1.83	0.59
1:I:436:GLN:HB3	1:K:397:PHE:CD2	2.37	0.59
1:C:346:ARG:NH1	1:C:424:ASP:HA	2.18	0.59
1:B:378:THR:HG1	1:I:420:HIS:HE2	0.61	0.59
1:L:346:ARG:NH1	1:L:424:ASP:HA	2.18	0.59
1:I:346:ARG:NH1	1:I:424:ASP:HA	2.18	0.59
1:C:436:GLN:HB3	1:D:397:PHE:CD2	2.38	0.58
1:A:338:ILE:HG22	1:A:338:ILE:O	2.02	0.58
1:D:346:ARG:NH1	1:D:424:ASP:HA	2.18	0.58
1:J:346:ARG:NH1	1:J:424:ASP:HA	2.18	0.58
1:E:346:ARG:NH1	1:E:424:ASP:HA	2.18	0.58
1:F:346:ARG:NH1	1:F:424:ASP:HA	2.18	0.57
1:G:346:ARG:NH1	1:G:424:ASP:HA	2.19	0.57
1:I:444:PRO:HG3	1:K:402:LEU:HB2	1.87	0.56
1:D:32:LYS:HB3	1:D:35:ALA:HB3	1.87	0.56
1:E:448:GLN:HB2	1:F:385:LEU:HD12	1.86	0.56
1:B:420:HIS:NE2	1:I:378:THR:OG1	2.25	0.56
1:K:293:PHE:O	1:K:296:ARG:HG2	2.06	0.56
1:D:293:PHE:O	1:D:296:ARG:HG2	2.06	0.56
1:H:293:PHE:O	1:H:296:ARG:HG2	2.06	0.56
1:A:293:PHE:O	1:A:296:ARG:HG2	2.06	0.56
1:F:32:LYS:HB3	1:F:35:ALA:HB3	1.87	0.56
1:H:32:LYS:HB3	1:H:35:ALA:HB3	1.88	0.56
1:I:32:LYS:HB3	1:I:35:ALA:HB3	1.87	0.56
1:J:293:PHE:O	1:J:296:ARG:HG2	2.06	0.56
1:B:349:GLU:CD	1:B:462:TRP:NE1	2.53	0.56
1:E:293:PHE:O	1:E:296:ARG:HG2	2.06	0.56
1:L:32:LYS:HB3	1:L:35:ALA:HB3	1.87	0.56
1:B:293:PHE:O	1:B:296:ARG:HG2	2.06	0.55
1:F:296:ARG:C	1:F:296:ARG:HD3	2.27	0.55
1:J:32:LYS:HB3	1:J:35:ALA:HB3	1.87	0.55
1:C:32:LYS:HB3	1:C:35:ALA:HB3	1.87	0.55
1:B:32:LYS:HB3	1:B:35:ALA:HB3	1.87	0.55
1:G:293:PHE:O	1:G:296:ARG:HG2	2.06	0.55
1:C:444:PRO:HG3	1:D:402:LEU:HB2	1.88	0.55
1:G:32:LYS:HB3	1:G:35:ALA:HB3	1.87	0.55
1:C:378:THR:OG1	1:H:420:HIS:NE2	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:GLN:HB2	1:J:385:LEU:HD12	1.87	0.55
1:A:32:LYS:HB3	1:A:35:ALA:HB3	1.87	0.54
1:B:378:THR:O	1:B:466:HIS:HA	2.08	0.54
1:E:378:THR:O	1:E:466:HIS:HA	2.08	0.54
1:H:378:THR:O	1:H:466:HIS:HA	2.08	0.54
1:K:32:LYS:HB3	1:K:35:ALA:HB3	1.88	0.54
1:K:378:THR:O	1:K:466:HIS:HA	2.08	0.54
1:F:393:ASP:OD1	1:F:396:ARG:NH1	2.41	0.54
1:F:378:THR:O	1:F:466:HIS:HA	2.08	0.54
1:I:393:ASP:OD1	1:I:396:ARG:NH1	2.41	0.54
1:L:393:ASP:OD1	1:L:396:ARG:NH1	2.41	0.54
1:E:32:LYS:HB3	1:E:35:ALA:HB3	1.87	0.54
1:H:393:ASP:OD1	1:H:396:ARG:NH1	2.41	0.54
1:J:393:ASP:OD1	1:J:396:ARG:NH1	2.41	0.54
1:J:378:THR:O	1:J:466:HIS:HA	2.08	0.54
1:A:378:THR:O	1:A:466:HIS:HA	2.08	0.54
1:C:378:THR:O	1:C:466:HIS:HA	2.08	0.54
1:C:393:ASP:OD1	1:C:396:ARG:NH1	2.40	0.54
1:D:393:ASP:OD1	1:D:396:ARG:NH1	2.41	0.54
1:E:393:ASP:OD1	1:E:396:ARG:NH1	2.41	0.54
1:K:344:LYS:HG2	1:K:346:ARG:H	1.72	0.54
1:D:378:THR:O	1:D:466:HIS:HA	2.08	0.54
1:L:378:THR:O	1:L:466:HIS:HA	2.08	0.54
1:H:397:PHE:HE2	1:J:444:PRO:HB2	1.73	0.53
1:G:393:ASP:OD1	1:G:396:ARG:NH1	2.41	0.53
1:A:393:ASP:OD1	1:A:396:ARG:NH1	2.40	0.53
1:C:420:HIS:HE2	1:H:378:THR:HG1	0.59	0.53
1:E:448:GLN:HB2	1:F:385:LEU:CD1	2.38	0.53
1:G:378:THR:O	1:G:466:HIS:HA	2.08	0.53
1:I:378:THR:O	1:I:466:HIS:HA	2.08	0.53
1:K:393:ASP:OD1	1:K:396:ARG:NH1	2.40	0.53
1:D:343:THR:OG1	1:D:344:LYS:N	2.42	0.53
1:B:393:ASP:OD1	1:B:396:ARG:NH1	2.41	0.53
1:B:397:PHE:HE2	1:F:444:PRO:HB2	1.73	0.53
1:H:442:GLY:HA2	1:H:443:ILE:HB	1.91	0.53
1:H:397:PHE:HE2	1:J:444:PRO:CB	2.22	0.53
1:B:382:PRO:HG2	1:B:472:ALA:H	1.74	0.53
1:A:382:PRO:HG2	1:A:472:ALA:H	1.74	0.53
1:C:442:GLY:HA2	1:C:443:ILE:HB	1.91	0.53
1:B:397:PHE:HE2	1:F:444:PRO:CB	2.22	0.53
1:H:382:PRO:HG2	1:H:472:ALA:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:382:PRO:HG2	1:G:472:ALA:H	1.74	0.52
1:L:382:PRO:HG2	1:L:472:ALA:H	1.74	0.52
1:J:304:LEU:HD22	1:J:304:LEU:N	2.24	0.52
1:G:448:GLN:HB2	1:J:385:LEU:CD1	2.39	0.52
1:F:382:PRO:HG2	1:F:472:ALA:H	1.74	0.52
1:I:382:PRO:HG2	1:I:472:ALA:H	1.74	0.52
1:E:382:PRO:HG2	1:E:472:ALA:H	1.74	0.52
1:F:442:GLY:HA2	1:F:443:ILE:HB	1.91	0.52
1:J:23:ALA:HB1	1:J:303:ILE:HD12	1.91	0.52
1:E:442:GLY:HA2	1:E:443:ILE:HB	1.91	0.52
1:B:442:GLY:HA2	1:B:443:ILE:HB	1.91	0.52
1:C:382:PRO:HG2	1:C:472:ALA:H	1.74	0.52
1:K:382:PRO:HG2	1:K:472:ALA:H	1.74	0.52
1:K:442:GLY:HA2	1:K:443:ILE:HB	1.91	0.52
1:D:382:PRO:HG2	1:D:472:ALA:H	1.74	0.52
1:G:442:GLY:HA2	1:G:443:ILE:HB	1.91	0.52
1:J:382:PRO:HG2	1:J:472:ALA:H	1.74	0.51
1:B:346:ARG:HE	1:B:421:LEU:HB3	1.75	0.51
1:I:442:GLY:HA2	1:I:443:ILE:HB	1.91	0.51
1:J:442:GLY:HA2	1:J:443:ILE:HB	1.91	0.51
1:D:442:GLY:HA2	1:D:443:ILE:HB	1.91	0.51
1:G:335:ASN:HD22	1:G:335:ASN:N	2.07	0.51
1:A:442:GLY:HA2	1:A:443:ILE:HB	1.91	0.51
1:L:442:GLY:HA2	1:L:443:ILE:HB	1.91	0.51
1:L:344:LYS:C	1:L:346:ARG:H	2.15	0.51
1:J:339:GLU:OE1	1:J:339:GLU:N	2.44	0.50
1:I:80:SER:HB3	1:I:85:HIS:HD1	1.78	0.49
1:L:80:SER:HB3	1:L:85:HIS:HD1	1.78	0.49
1:B:349:GLU:OE2	1:B:462:TRP:CD1	2.65	0.48
1:K:80:SER:HB3	1:K:85:HIS:HD1	1.78	0.48
1:B:346:ARG:HE	1:B:421:LEU:HD13	1.77	0.48
1:E:425:GLU:OE2	1:G:423:GLY:HA3	2.13	0.48
1:E:423:GLY:HA3	1:G:425:GLU:OE2	2.13	0.48
1:F:80:SER:HB3	1:F:85:HIS:HD1	1.78	0.48
1:G:80:SER:HB3	1:G:85:HIS:HD1	1.78	0.48
1:H:80:SER:HB3	1:H:85:HIS:HD1	1.78	0.48
1:J:80:SER:HB3	1:J:85:HIS:HD1	1.78	0.48
1:A:80:SER:HB3	1:A:85:HIS:HD1	1.78	0.48
1:C:80:SER:HB3	1:C:85:HIS:HD1	1.78	0.48
1:E:436:GLN:NE2	1:F:398:TYR:CE2	2.82	0.48
1:D:80:SER:HB3	1:D:85:HIS:HD1	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:SER:HB3	1:E:85:HIS:HD1	1.78	0.48
1:D:422:MET:SD	1:J:465:VAL:HG21	2.53	0.48
1:B:80:SER:HB3	1:B:85:HIS:HD1	1.78	0.47
1:E:335:ASN:N	1:E:335:ASN:HD22	2.10	0.47
1:G:317:LYS:HD2	1:G:317:LYS:H	1.78	0.47
1:G:436:GLN:NE2	1:J:398:TYR:CE2	2.82	0.47
1:I:438:LEU:HD11	1:K:401:ASN:OD1	2.15	0.47
1:K:341:GLU:OE2	1:K:343:THR:N	2.47	0.47
1:B:373:CYS:HB2	1:B:392:LEU:HD21	1.97	0.47
1:I:334:THR:OG1	1:I:335:ASN:N	2.47	0.47
1:D:65:ARG:HG3	1:D:75:LEU:HD23	1.97	0.47
1:J:65:ARG:HG3	1:J:75:LEU:HD23	1.97	0.47
1:A:373:CYS:HB2	1:A:392:LEU:HD21	1.97	0.47
1:C:65:ARG:HG3	1:C:75:LEU:HD23	1.97	0.47
1:C:373:CYS:HB2	1:C:392:LEU:HD21	1.97	0.47
1:F:373:CYS:HB2	1:F:392:LEU:HD21	1.97	0.47
1:H:373:CYS:HB2	1:H:392:LEU:HD21	1.97	0.47
1:I:373:CYS:HB2	1:I:392:LEU:HD21	1.97	0.47
1:K:373:CYS:HB2	1:K:392:LEU:HD21	1.97	0.47
1:C:308:LEU:N	1:C:308:LEU:HD12	2.30	0.46
1:J:373:CYS:HB2	1:J:392:LEU:HD21	1.97	0.46
1:I:411:HIS:NE2	1:K:393:ASP:OD1	2.48	0.46
1:K:65:ARG:HG3	1:K:75:LEU:HD23	1.97	0.46
1:E:373:CYS:HB2	1:E:392:LEU:HD21	1.97	0.46
1:E:436:GLN:HB3	1:F:397:PHE:CE2	2.51	0.46
1:E:444:PRO:HG3	1:F:402:LEU:HD22	1.98	0.46
1:G:373:CYS:HB2	1:G:392:LEU:HD21	1.97	0.46
1:G:65:ARG:HG3	1:G:75:LEU:HD23	1.97	0.46
1:G:436:GLN:HB3	1:J:397:PHE:CE2	2.51	0.46
1:L:373:CYS:HB2	1:L:392:LEU:HD21	1.97	0.46
1:D:373:CYS:HB2	1:D:392:LEU:HD21	1.97	0.46
1:H:65:ARG:HG3	1:H:75:LEU:HD23	1.97	0.46
1:A:65:ARG:HG3	1:A:75:LEU:HD23	1.97	0.46
1:B:65:ARG:HG3	1:B:75:LEU:HD23	1.97	0.46
1:F:465:VAL:HG21	1:K:422:MET:SD	2.56	0.46
1:H:81:GLU:OE2	1:H:323:LYS:HE2	2.16	0.46
1:F:65:ARG:HG3	1:F:75:LEU:HD23	1.97	0.46
1:K:344:LYS:HB2	1:K:344:LYS:NZ	2.30	0.46
1:E:65:ARG:HG3	1:E:75:LEU:HD23	1.97	0.46
1:G:304:LEU:N	1:G:304:LEU:HD12	2.31	0.46
1:H:81:GLU:OE2	1:H:323:LYS:CE	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HG2	1:A:26:VAL:HG12	1.98	0.46
1:B:21:LYS:HG2	1:B:26:VAL:HG12	1.98	0.46
1:G:444:PRO:HG3	1:J:402:LEU:HD22	1.98	0.45
1:L:21:LYS:HG2	1:L:26:VAL:HG12	1.98	0.45
1:E:68:LYS:HD2	1:E:74:ARG:NH2	2.32	0.45
1:E:411:HIS:NE2	1:F:393:ASP:OD1	2.50	0.45
1:F:68:LYS:HD2	1:F:74:ARG:NH2	2.32	0.45
1:I:65:ARG:HG3	1:I:75:LEU:HD23	1.97	0.45
1:A:304:LEU:N	1:A:304:LEU:HD12	2.31	0.45
1:H:21:LYS:HG2	1:H:26:VAL:HG12	1.98	0.45
1:K:146:LYS:NZ	1:K:308:LEU:O	2.48	0.45
1:C:68:LYS:HD2	1:C:74:ARG:NH2	2.32	0.45
1:G:411:HIS:NE2	1:J:393:ASP:OD1	2.50	0.45
1:H:68:LYS:HD2	1:H:74:ARG:NH2	2.32	0.45
1:I:21:LYS:HG2	1:I:26:VAL:HG12	1.98	0.45
1:I:438:LEU:HD23	1:I:444:PRO:HA	1.99	0.45
1:K:344:LYS:HD3	1:K:346:ARG:HB3	1.99	0.45
1:L:438:LEU:HD23	1:L:444:PRO:HA	1.99	0.45
1:C:438:LEU:HD11	1:D:401:ASN:OD1	2.17	0.45
1:K:68:LYS:HD2	1:K:74:ARG:NH2	2.32	0.45
1:L:344:LYS:C	1:L:346:ARG:N	2.70	0.45
1:G:438:LEU:HD23	1:G:444:PRO:HA	1.99	0.45
1:J:68:LYS:HD2	1:J:74:ARG:NH2	2.32	0.45
1:K:337:THR:O	1:K:337:THR:OG1	2.29	0.45
1:B:68:LYS:HD2	1:B:74:ARG:NH2	2.32	0.45
1:I:436:GLN:HB3	1:K:397:PHE:CE2	2.52	0.45
1:A:438:LEU:HD23	1:A:444:PRO:HA	1.99	0.45
1:C:448:GLN:HB2	1:D:385:LEU:HD12	1.98	0.45
1:F:470:SER:OG	1:K:468:HIS:CE1	2.70	0.45
1:G:68:LYS:HD2	1:G:74:ARG:NH2	2.32	0.45
1:D:420:HIS:CD2	1:J:378:THR:HG1	2.18	0.45
1:H:401:ASN:OD1	1:J:438:LEU:HD11	2.17	0.45
1:K:438:LEU:HD23	1:K:444:PRO:HA	1.99	0.45
1:A:68:LYS:HD2	1:A:74:ARG:NH2	2.32	0.45
1:C:438:LEU:HD23	1:C:444:PRO:HA	1.99	0.45
1:B:401:ASN:OD1	1:F:438:LEU:HD11	2.17	0.44
1:C:436:GLN:HB3	1:D:397:PHE:CE2	2.52	0.44
1:D:68:LYS:HD2	1:D:74:ARG:NH2	2.32	0.44
1:E:21:LYS:HG2	1:E:26:VAL:HG12	1.98	0.44
1:E:422:MET:HG2	1:G:456:HIS:CD2	2.52	0.44
1:G:21:LYS:HG2	1:G:26:VAL:HG12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:322:LYS:NZ	1:L:322:LYS:HB3	2.31	0.44
1:L:65:ARG:HG3	1:L:75:LEU:HD23	1.97	0.44
1:D:468:HIS:CE1	1:J:470:SER:OG	2.70	0.44
1:G:192:LYS:N	1:G:193:PRO:CD	2.81	0.44
1:J:192:LYS:N	1:J:193:PRO:CD	2.81	0.44
1:A:192:LYS:N	1:A:193:PRO:CD	2.81	0.44
1:B:192:LYS:N	1:B:193:PRO:CD	2.81	0.44
1:E:438:LEU:HD23	1:E:444:PRO:HA	1.99	0.44
1:F:311:ARG:HA	1:F:311:ARG:NE	2.32	0.44
1:F:456:HIS:CD2	1:F:458:ARG:HE	2.36	0.44
1:F:470:SER:OG	1:K:468:HIS:HE1	1.99	0.44
1:H:456:HIS:CD2	1:H:458:ARG:HE	2.36	0.44
1:I:456:HIS:CD2	1:I:458:ARG:HE	2.36	0.44
1:I:68:LYS:HD2	1:I:74:ARG:NH2	2.32	0.44
1:K:456:HIS:CD2	1:K:458:ARG:HE	2.36	0.44
1:C:21:LYS:HG2	1:C:26:VAL:HG12	1.98	0.44
1:C:456:HIS:CD2	1:C:458:ARG:HE	2.36	0.44
1:D:468:HIS:HE1	1:J:470:SER:OG	1.99	0.44
1:E:192:LYS:N	1:E:193:PRO:CD	2.81	0.44
1:E:456:HIS:CD2	1:E:458:ARG:HE	2.36	0.44
1:F:21:LYS:HG2	1:F:26:VAL:HG12	1.98	0.44
1:K:21:LYS:HG2	1:K:26:VAL:HG12	1.98	0.44
1:L:192:LYS:N	1:L:193:PRO:CD	2.81	0.44
1:A:456:HIS:CD2	1:A:458:ARG:HE	2.36	0.44
1:B:438:LEU:HD23	1:B:444:PRO:HA	1.99	0.44
1:L:68:LYS:HD2	1:L:74:ARG:NH2	2.32	0.44
1:C:192:LYS:N	1:C:193:PRO:CD	2.81	0.44
1:D:192:LYS:N	1:D:193:PRO:CD	2.81	0.44
1:J:312:ASN:HD22	1:J:312:ASN:N	2.14	0.44
1:B:456:HIS:CD2	1:B:458:ARG:HE	2.36	0.44
1:H:192:LYS:N	1:H:193:PRO:CD	2.81	0.44
1:I:192:LYS:N	1:I:193:PRO:CD	2.81	0.44
1:D:456:HIS:CD2	1:J:422:MET:HG2	2.53	0.44
1:F:438:LEU:HD23	1:F:444:PRO:HA	1.99	0.44
1:L:456:HIS:CD2	1:L:458:ARG:HE	2.36	0.44
1:H:438:LEU:HD23	1:H:444:PRO:HA	1.99	0.44
1:E:409:PRO:CG	1:F:401:ASN:OD1	2.66	0.43
1:J:438:LEU:HD23	1:J:444:PRO:HA	1.99	0.43
1:K:192:LYS:N	1:K:193:PRO:CD	2.81	0.43
1:K:340:ASP:OD2	1:K:347:LYS:NZ	2.37	0.43
1:D:438:LEU:HD23	1:D:444:PRO:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:456:HIS:CD2	1:G:458:ARG:HE	2.36	0.43
1:I:448:GLN:HB2	1:K:385:LEU:HD12	2.00	0.43
1:D:21:LYS:HG2	1:D:26:VAL:HG12	1.98	0.43
1:J:456:HIS:CD2	1:J:458:ARG:HE	2.36	0.43
1:L:335:ASN:OD1	1:L:336:THR:N	2.51	0.43
1:F:192:LYS:N	1:F:193:PRO:CD	2.81	0.43
1:E:456:HIS:CD2	1:G:422:MET:HG2	2.52	0.43
1:J:21:LYS:HG2	1:J:26:VAL:HG12	1.98	0.43
1:J:74:ARG:CG	1:J:75:LEU:N	2.82	0.43
1:B:74:ARG:CG	1:B:75:LEU:N	2.82	0.43
1:D:74:ARG:CG	1:D:75:LEU:N	2.82	0.43
1:A:74:ARG:CG	1:A:75:LEU:N	2.82	0.43
1:C:411:HIS:NE2	1:D:393:ASP:OD1	2.51	0.43
1:D:456:HIS:CD2	1:D:458:ARG:HE	2.36	0.43
1:B:397:PHE:CE2	1:F:444:PRO:CB	3.02	0.42
1:G:409:PRO:CG	1:J:401:ASN:OD1	2.67	0.42
1:H:397:PHE:CE2	1:J:444:PRO:CB	3.03	0.42
1:F:74:ARG:CG	1:F:75:LEU:N	2.82	0.42
1:J:453:ARG:HD3	1:J:467:PHE:HB2	2.02	0.42
1:K:74:ARG:CG	1:K:75:LEU:N	2.82	0.42
1:A:323:LYS:HD3	1:A:323:LYS:N	2.33	0.42
1:G:74:ARG:CG	1:G:75:LEU:N	2.82	0.42
1:H:344:LYS:HE3	1:H:349:GLU:HA	2.01	0.42
1:K:335:ASN:HB2	1:K:344:LYS:HE2	2.01	0.42
1:F:422:MET:HG2	1:K:456:HIS:CD2	2.55	0.42
1:L:321:ASN:N	1:L:321:ASN:HD22	2.15	0.42
1:C:74:ARG:CG	1:C:75:LEU:N	2.82	0.42
1:E:74:ARG:CG	1:E:75:LEU:N	2.82	0.42
1:L:74:ARG:CG	1:L:75:LEU:N	2.82	0.42
1:D:453:ARG:HD3	1:D:467:PHE:HB2	2.02	0.42
1:H:74:ARG:CG	1:H:75:LEU:N	2.82	0.42
1:C:449:SER:HB3	1:C:472:ALA:HB2	2.02	0.42
1:E:380:PHE:CZ	1:G:450:GLU:HB3	2.55	0.42
1:E:453:ARG:HD3	1:E:467:PHE:HB2	2.02	0.42
1:L:116:ILE:HD12	1:L:116:ILE:HA	2.00	0.42
1:E:450:GLU:HB3	1:G:380:PHE:CZ	2.55	0.42
1:F:453:ARG:HD3	1:F:467:PHE:HB2	2.02	0.42
1:H:453:ARG:HD3	1:H:467:PHE:HB2	2.02	0.42
1:D:468:HIS:HB3	1:J:468:HIS:CD2	2.55	0.42
1:K:449:SER:HB3	1:K:472:ALA:HB2	2.02	0.42
1:A:449:SER:HB3	1:A:472:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LYS:HE2	1:B:325:ASP:OD1	2.20	0.41
1:B:449:SER:HB3	1:B:472:ALA:HB2	2.02	0.41
1:G:449:SER:HB3	1:G:472:ALA:HB2	2.02	0.41
1:H:449:SER:HB3	1:H:472:ALA:HB2	2.02	0.41
1:K:453:ARG:HD3	1:K:467:PHE:HB2	2.02	0.41
1:C:453:ARG:HD3	1:C:467:PHE:HB2	2.02	0.41
1:B:338:ILE:HG23	1:B:339:GLU:N	2.35	0.41
1:F:449:SER:HB3	1:F:472:ALA:HB2	2.02	0.41
1:I:116:ILE:HD12	1:I:116:ILE:HA	2.00	0.41
1:D:420:HIS:NE2	1:J:378:THR:OG1	2.02	0.41
1:K:116:ILE:HD12	1:K:116:ILE:HA	2.00	0.41
1:G:453:ARG:HD3	1:G:467:PHE:HB2	2.02	0.41
1:I:228:GLY:CA	1:I:254:ILE:HD11	2.51	0.41
1:I:74:ARG:CG	1:I:75:LEU:N	2.82	0.41
1:F:468:HIS:CD2	1:K:468:HIS:HB3	2.55	0.41
1:L:228:GLY:CA	1:L:254:ILE:HD11	2.51	0.41
1:A:228:GLY:CA	1:A:254:ILE:HD11	2.51	0.41
1:L:449:SER:HB3	1:L:472:ALA:HB2	2.02	0.41
1:B:453:ARG:HD3	1:B:467:PHE:HB2	2.02	0.41
1:C:228:GLY:CA	1:C:254:ILE:HD11	2.51	0.41
1:D:208:VAL:HG11	1:D:237:TRP:CE2	2.56	0.41
1:E:449:SER:HB3	1:E:472:ALA:HB2	2.02	0.41
1:G:208:VAL:HG11	1:G:237:TRP:CE2	2.56	0.41
1:G:228:GLY:CA	1:G:254:ILE:HD11	2.51	0.41
1:I:449:SER:HB3	1:I:472:ALA:HB2	2.02	0.41
1:E:208:VAL:HG11	1:E:237:TRP:CE2	2.56	0.41
1:I:208:VAL:HG11	1:I:237:TRP:CE2	2.56	0.41
1:K:228:GLY:CA	1:K:254:ILE:HD11	2.51	0.41
1:L:208:VAL:HG11	1:L:237:TRP:CE2	2.56	0.41
1:I:453:ARG:HD3	1:I:467:PHE:HB2	2.02	0.41
1:L:453:ARG:HD3	1:L:467:PHE:HB2	2.02	0.41
1:K:17:GLU:OE2	1:K:308:LEU:HD13	2.20	0.41
1:A:453:ARG:HD3	1:A:467:PHE:HB2	2.02	0.40
1:D:449:SER:HB3	1:D:472:ALA:HB2	2.02	0.40
1:E:228:GLY:CA	1:E:254:ILE:HD11	2.51	0.40
1:A:208:VAL:HG11	1:A:237:TRP:CE2	2.56	0.40
1:B:228:GLY:CA	1:B:254:ILE:HD11	2.51	0.40
1:H:208:VAL:HG11	1:H:237:TRP:CE2	2.56	0.40
1:J:208:VAL:HG11	1:J:237:TRP:CE2	2.56	0.40
1:L:201:VAL:HG13	1:L:212:PRO:HD2	2.03	0.40
1:I:201:VAL:HG13	1:I:212:PRO:HD2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:GLY:CA	1:D:254:ILE:HD11	2.51	0.40
1:E:420:HIS:NE2	1:G:378:THR:OG1	2.35	0.40
1:H:201:VAL:HG13	1:H:212:PRO:HD2	2.03	0.40
1:B:208:VAL:HG11	1:B:237:TRP:CE2	2.56	0.40
1:D:201:VAL:HG13	1:D:212:PRO:HD2	2.03	0.40
1:F:208:VAL:HG11	1:F:237:TRP:CE2	2.56	0.40
1:F:228:GLY:CA	1:F:254:ILE:HD11	2.51	0.40
1:J:228:GLY:CA	1:J:254:ILE:HD11	2.51	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	455/461 (99%)	437 (96%)	18 (4%)	0	100	100
1	B	455/461 (99%)	436 (96%)	19 (4%)	0	100	100
1	C	455/461 (99%)	437 (96%)	18 (4%)	0	100	100
1	D	455/461 (99%)	433 (95%)	22 (5%)	0	100	100
1	E	455/461 (99%)	440 (97%)	15 (3%)	0	100	100
1	F	455/461 (99%)	437 (96%)	18 (4%)	0	100	100
1	G	455/461 (99%)	435 (96%)	20 (4%)	0	100	100
1	H	455/461 (99%)	439 (96%)	16 (4%)	0	100	100
1	I	455/461 (99%)	438 (96%)	17 (4%)	0	100	100
1	J	455/461 (99%)	434 (95%)	21 (5%)	0	100	100
1	K	455/461 (99%)	439 (96%)	16 (4%)	0	100	100
1	L	455/461 (99%)	438 (96%)	17 (4%)	0	100	100
All	All	5460/5532 (99%)	5243 (96%)	217 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	391/393 (100%)	386 (99%)	5 (1%)	73	87
1	B	391/393 (100%)	384 (98%)	7 (2%)	64	84
1	C	391/393 (100%)	385 (98%)	6 (2%)	70	85
1	D	391/393 (100%)	385 (98%)	6 (2%)	70	85
1	E	391/393 (100%)	386 (99%)	5 (1%)	73	87
1	F	391/393 (100%)	385 (98%)	6 (2%)	70	85
1	G	391/393 (100%)	383 (98%)	8 (2%)	60	82
1	H	391/393 (100%)	385 (98%)	6 (2%)	70	85
1	I	391/393 (100%)	386 (99%)	5 (1%)	73	87
1	J	391/393 (100%)	386 (99%)	5 (1%)	73	87
1	K	391/393 (100%)	386 (99%)	5 (1%)	73	87
1	L	391/393 (100%)	387 (99%)	4 (1%)	80	90
All	All	4692/4716 (100%)	4624 (99%)	68 (1%)	74	86

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	45	ASN
1	A	196	LEU
1	A	306	THR
1	A	380	PHE
1	B	0	MET
1	B	45	ASN
1	B	196	LEU
1	B	305	THR
1	B	306	THR
1	B	337	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	380	PHE
1	C	0	MET
1	C	45	ASN
1	C	196	LEU
1	C	304	LEU
1	C	343	THR
1	C	380	PHE
1	D	0	MET
1	D	45	ASN
1	D	196	LEU
1	D	338	ILE
1	D	344	LYS
1	D	380	PHE
1	E	0	MET
1	E	45	ASN
1	E	196	LEU
1	E	323	LYS
1	E	380	PHE
1	F	0	MET
1	F	45	ASN
1	F	196	LEU
1	F	296	ARG
1	F	305	THR
1	F	380	PHE
1	G	0	MET
1	G	45	ASN
1	G	196	LEU
1	G	303	ILE
1	G	310	THR
1	G	317	LYS
1	G	334	THR
1	G	380	PHE
1	H	0	MET
1	H	45	ASN
1	H	196	LEU
1	H	321	ASN
1	H	343	THR
1	H	380	PHE
1	I	0	MET
1	I	45	ASN
1	I	196	LEU
1	I	317	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	380	PHE
1	J	0	MET
1	J	45	ASN
1	J	196	LEU
1	J	310	THR
1	J	380	PHE
1	K	0	MET
1	K	45	ASN
1	K	196	LEU
1	K	341	GLU
1	K	380	PHE
1	L	0	MET
1	L	45	ASN
1	L	196	LEU
1	L	380	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	76[B]	HIS
1	A	468	HIS
1	B	45	ASN
1	B	76[B]	HIS
1	B	312	ASN
1	B	416	ASN
1	B	468	HIS
1	C	45	ASN
1	C	76[B]	HIS
1	C	468	HIS
1	D	45	ASN
1	D	76[B]	HIS
1	D	468	HIS
1	E	45	ASN
1	E	76[B]	HIS
1	E	335	ASN
1	E	468	HIS
1	F	45	ASN
1	F	76[B]	HIS
1	F	468	HIS
1	G	45	ASN
1	G	76[B]	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	335	ASN
1	G	468	HIS
1	H	76[B]	HIS
1	H	321	ASN
1	H	416	ASN
1	H	468	HIS
1	I	45	ASN
1	I	76[B]	HIS
1	I	468	HIS
1	J	45	ASN
1	J	76[B]	HIS
1	J	312	ASN
1	J	468	HIS
1	K	45	ASN
1	K	76[B]	HIS
1	K	468	HIS
1	L	45	ASN
1	L	76[B]	HIS
1	L	321	ASN
1	L	468	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.